



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 PM UTC

PDB ID : 5GTY / pdb_00005gty
Title : Crystal structure of EGFR 696-1022 T790M in complex with LXX-6-26
Authors : Yan, X.E.; Yun, C.H.
Deposited on : 2016-08-23
Resolution : 3.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

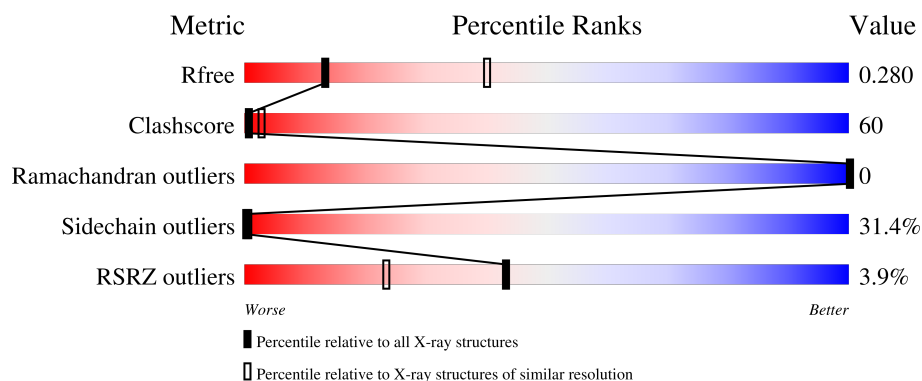
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	4% 30% 46% 15% 9%
1	B	331	3% 32% 44% 14% 10%
1	C	331	5% 25% 40% 24% 11%
1	D	331	4% 25% 48% 16% 10%
1	E	331	3% 32% 41% 15% 10%

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Mol	Chain	Length	Quality of chain
1	F	331	4% 28% 44% 18% 10%
1	G	331	2% 28% 43% 18% • 10%
1	H	331	3% 32% 40% 17% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19277 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	2	0
			2377	1529	397	432	19			
1	B	299	Total	C	N	O	S	0	0	0
			2333	1499	389	426	19			
1	D	297	Total	C	N	O	S	0	0	0
			2281	1468	377	418	18			
1	E	297	Total	C	N	O	S	0	0	0
			2297	1482	386	411	18			
1	F	297	Total	C	N	O	S	0	0	0
			2328	1499	393	417	19			
1	G	299	Total	C	N	O	S	0	1	0
			2367	1519	397	432	19			
1	H	300	Total	C	N	O	S	0	0	0
			2362	1521	392	430	19			
1	C	295	Total	C	N	O	S	0	0	0
			2325	1492	395	419	19			

There are 40 discrepancies between the modelled and reference sequences:

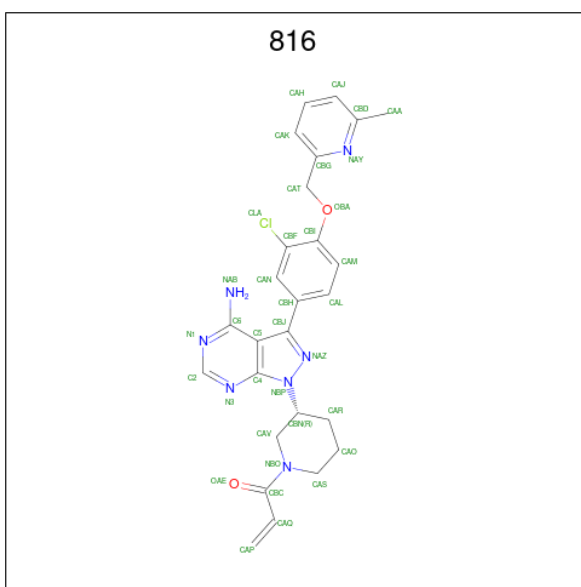
Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	expression tag	UNP P00533
A	693	ALA	-	expression tag	UNP P00533
A	694	MET	-	expression tag	UNP P00533
A	695	GLY	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	ALA	-	expression tag	UNP P00533
B	694	MET	-	expression tag	UNP P00533
B	695	GLY	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
D	692	GLY	-	expression tag	UNP P00533
D	693	ALA	-	expression tag	UNP P00533
D	694	MET	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
D	695	GLY	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
E	692	GLY	-	expression tag	UNP P00533
E	693	ALA	-	expression tag	UNP P00533
E	694	MET	-	expression tag	UNP P00533
E	695	GLY	-	expression tag	UNP P00533
E	790	MET	THR	engineered mutation	UNP P00533
F	692	GLY	-	expression tag	UNP P00533
F	693	ALA	-	expression tag	UNP P00533
F	694	MET	-	expression tag	UNP P00533
F	695	GLY	-	expression tag	UNP P00533
F	790	MET	THR	engineered mutation	UNP P00533
G	692	GLY	-	expression tag	UNP P00533
G	693	ALA	-	expression tag	UNP P00533
G	694	MET	-	expression tag	UNP P00533
G	695	GLY	-	expression tag	UNP P00533
G	790	MET	THR	engineered mutation	UNP P00533
H	692	GLY	-	expression tag	UNP P00533
H	693	ALA	-	expression tag	UNP P00533
H	694	MET	-	expression tag	UNP P00533
H	695	GLY	-	expression tag	UNP P00533
H	790	MET	THR	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	ALA	-	expression tag	UNP P00533
C	694	MET	-	expression tag	UNP P00533
C	695	GLY	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533

- Molecule 2 is 1-[(3R)-3-[4-azanyl-3-[3-chloranyl-4-[(6-methylpyridin-2-yl)methoxy]phenyl]pyrazolo[3,4-d]pyrimidin-1-yl]piperidin-1-yl]prop-2-en-1-one (CCD ID: 816) (formula: C₂₆H₂₆ClN₇O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 26	Cl 1	N 7	O 2	0	0
2	B	1	Total 36	C 26	Cl 1	N 7	O 2	0	0
2	D	1	Total 36	C 26	Cl 1	N 7	O 2	0	0
2	E	1	Total 36	C 26	Cl 1	N 7	O 2	0	0
2	F	1	Total 36	C 26	Cl 1	N 7	O 2	0	0
2	G	1	Total 36	C 26	Cl 1	N 7	O 2	0	0
2	H	1	Total 36	C 26	Cl 1	N 7	O 2	0	0
2	C	1	Total 36	C 26	Cl 1	N 7	O 2	0	0

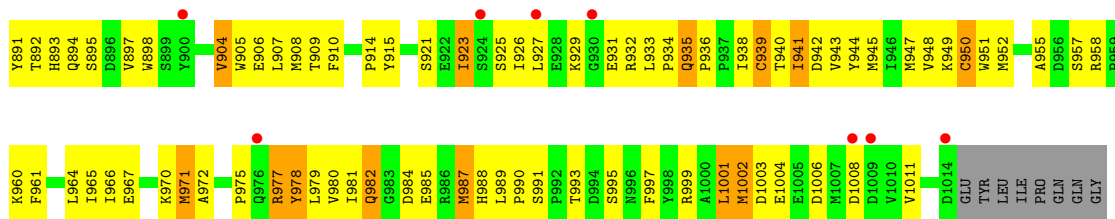
- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



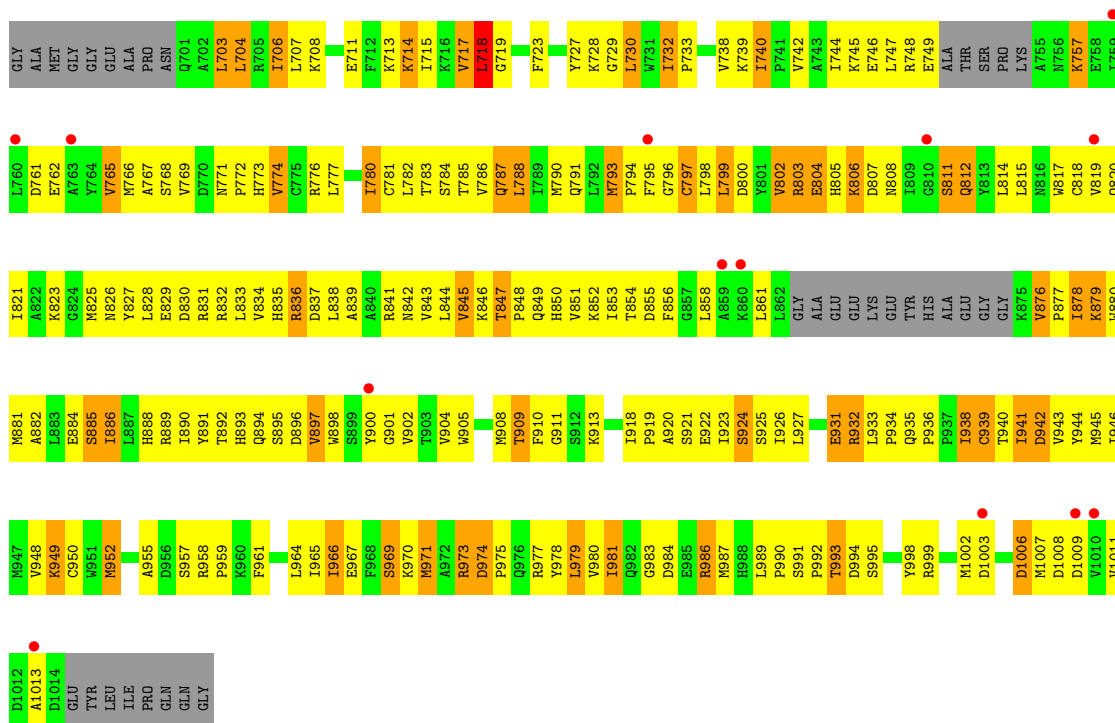
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

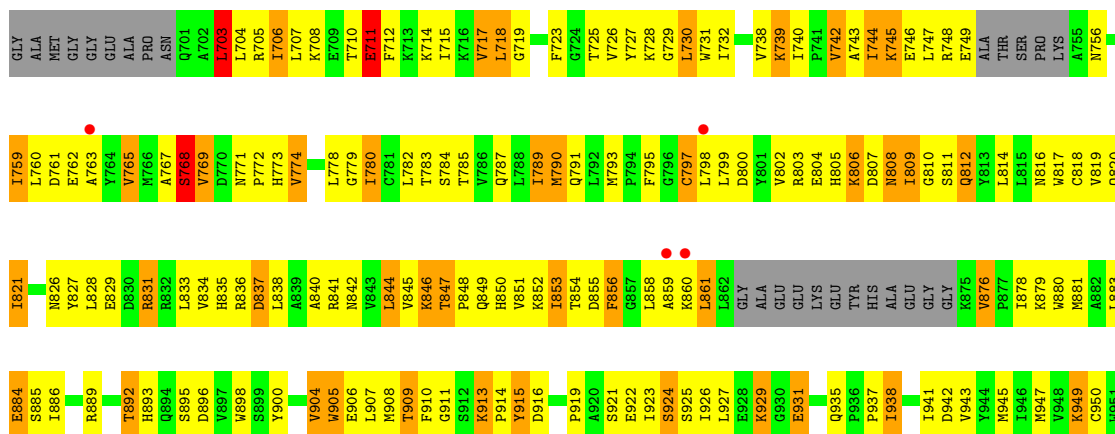
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	37	Total	O	0	0
			37	37		
4	D	19	Total	O	0	0
			19	19		
4	E	42	Total	O	0	0
			42	42		
4	F	50	Total	O	0	0
			50	50		
4	G	48	Total	O	0	0
			48	48		
4	H	27	Total	O	0	0
			27	27		
4	C	35	Total	O	0	0
			35	35		

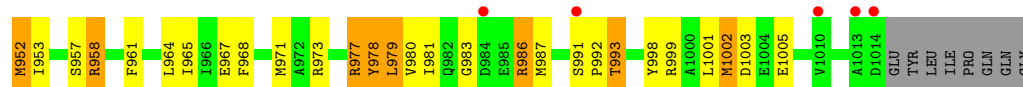


• Molecule 1: Epidermal growth factor receptor

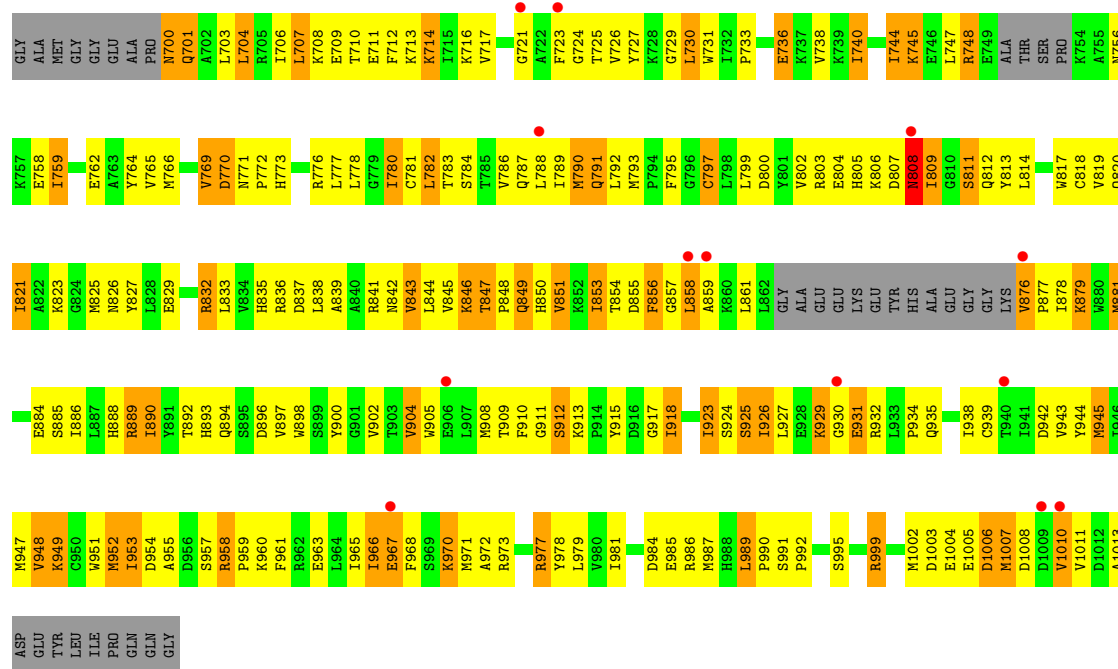


• Molecule 1: Epidermal growth factor receptor

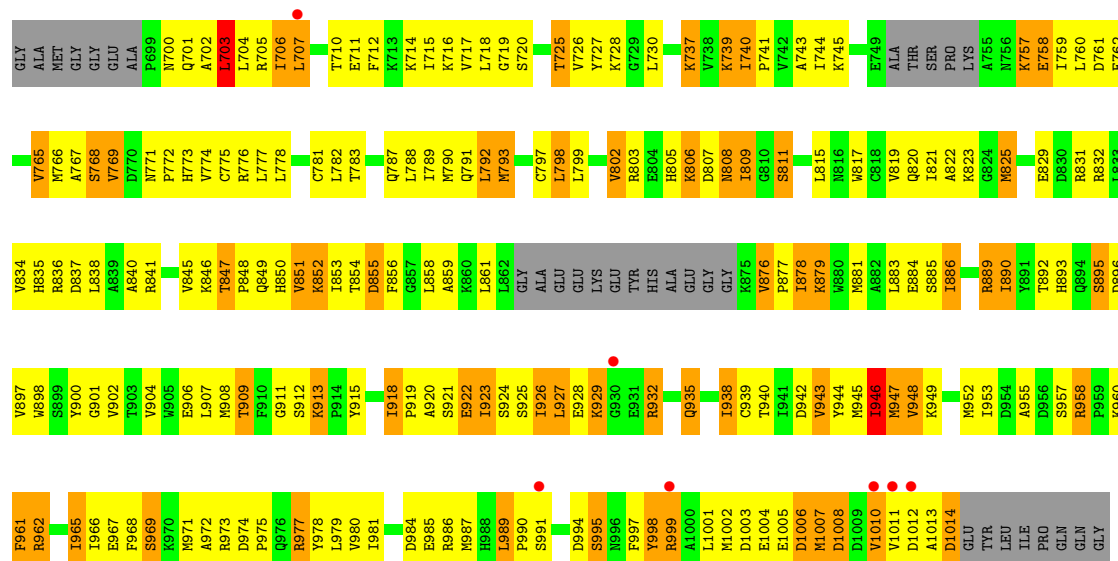




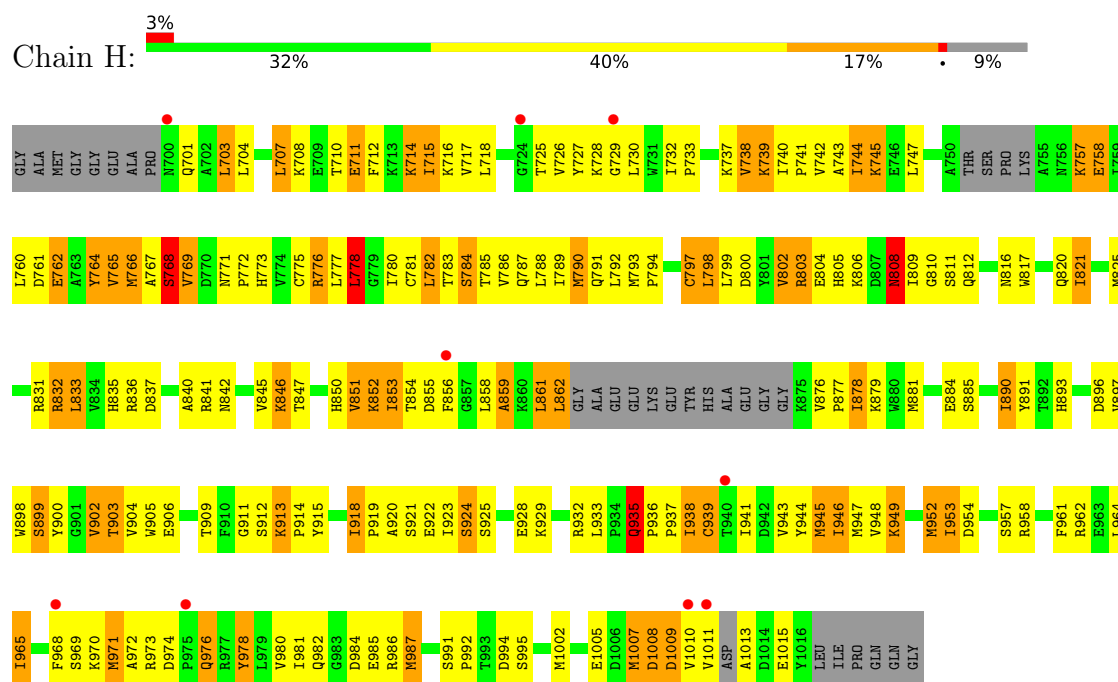
• Molecule 1: Epidermal growth factor receptor



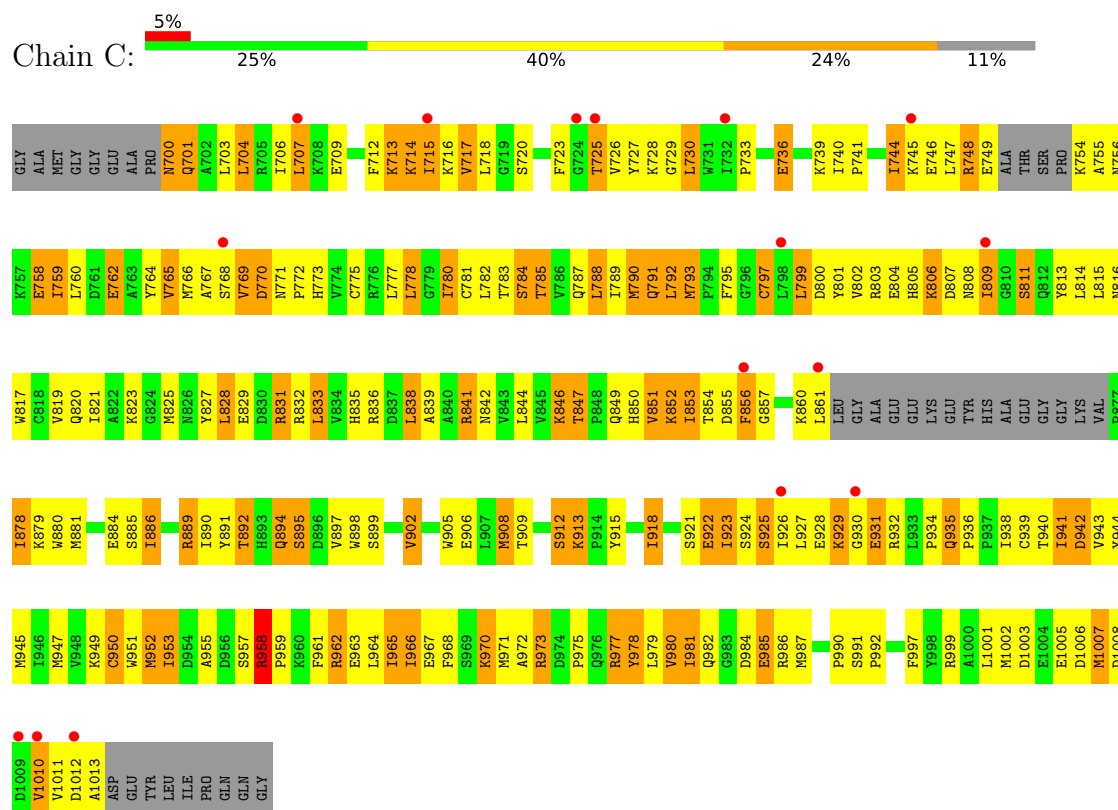
• Molecule 1: Epidermal growth factor receptor



• Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.43Å 71.80Å 152.53Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	49.81 – 3.14 49.81 – 3.14	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.81-3.14) 95.6 (49.81-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.12Å)	Xtriage
Refinement program	PHENIX (dev_2400)	Depositor
R, R_{free}	0.257 , 0.280 0.256 , 0.280	Depositor DCC
R_{free} test set	2103 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19277	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5445e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 816

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	2/2429 (0.1%)	0.96	4/3291 (0.1%)
1	B	0.65	0/2382	0.97	7/3231 (0.2%)
1	C	0.65	1/2373 (0.0%)	0.97	7/3213 (0.2%)
1	D	0.67	0/2330	0.94	3/3164 (0.1%)
1	E	0.68	1/2346 (0.0%)	0.99	10/3184 (0.3%)
1	F	0.68	1/2376 (0.0%)	0.99	7/3219 (0.2%)
1	G	0.68	2/2420 (0.1%)	0.98	6/3278 (0.2%)
1	H	0.66	0/2409	1.02	12/3260 (0.4%)
All	All	0.67	7/19065 (0.0%)	0.98	56/25840 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967[A]	GLU	CA-C	-7.53	1.43	1.52
1	A	967[B]	GLU	CA-C	-7.53	1.43	1.52
1	G	999[A]	ARG	CA-C	-7.18	1.43	1.52
1	G	999[B]	ARG	CA-C	-7.18	1.43	1.52
1	F	832	ARG	CA-C	-5.30	1.46	1.53
1	C	957	SER	C-N	5.12	1.41	1.33
1	E	905	TRP	C-N	5.07	1.40	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	715	ILE	N-CA-C	8.02	118.83	110.72
1	E	715	ILE	N-CA-C	7.57	118.36	110.72
1	F	709	GLU	N-CA-C	-7.36	103.26	111.28
1	B	978	TYR	N-CA-C	7.26	119.27	111.36
1	C	978	TYR	N-CA-C	7.03	119.03	111.36
1	A	967[A]	GLU	CA-C-O	-6.89	113.11	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	967[B]	GLU	CA-C-O	-6.89	113.11	120.42
1	F	893	HIS	N-CA-C	-6.61	104.08	111.28
1	H	808	ASN	N-CA-C	6.53	118.48	111.36
1	F	857	GLY	N-CA-C	-6.49	106.72	115.36
1	G	703	LEU	N-CA-C	6.46	117.98	111.07
1	H	846	LYS	N-CA-C	-6.19	104.54	111.28
1	A	784	SER	N-CA-C	-6.17	104.56	111.28
1	C	958	ARG	O-C-N	6.17	128.34	121.43
1	H	778	LEU	N-CA-C	6.14	118.05	111.36
1	B	817	TRP	N-CA-C	-6.06	104.68	111.28
1	E	711	GLU	N-CA-C	6.00	117.82	111.28
1	E	978	TYR	N-CA-C	5.94	119.00	111.69
1	F	784	SER	N-CA-C	-5.94	104.80	111.28
1	G	923	ILE	N-CA-C	5.89	116.63	110.62
1	H	738	VAL	N-CA-C	5.88	116.85	110.21
1	E	1002	MET	N-CA-C	5.86	117.47	111.14
1	G	946	ILE	N-CA-C	-5.86	104.64	110.62
1	F	978	TYR	N-CA-C	5.80	118.83	111.69
1	B	840	ALA	N-CA-C	-5.79	104.97	111.28
1	B	1001	LEU	N-CA-C	5.75	117.62	111.36
1	C	784	SER	N-CA-C	-5.68	105.08	111.28
1	E	846	LYS	N-CA-C	-5.67	105.10	111.28
1	E	778	LEU	N-CA-C	5.54	117.40	111.36
1	H	992	PRO	N-CA-C	-5.53	105.84	113.53
1	H	859	ALA	N-CA-C	-5.49	105.30	111.28
1	D	1007	MET	CB-CA-C	-5.46	110.26	116.54
1	G	966	ILE	N-CA-C	5.45	115.65	110.53
1	D	717	VAL	CB-CA-C	-5.41	107.17	113.22
1	E	703	LEU	N-CA-C	5.39	117.16	111.28
1	F	808	ASN	N-CA-C	5.38	119.95	113.17
1	H	784	SER	N-CA-C	-5.37	105.43	111.28
1	C	709	GLU	N-CA-C	-5.37	105.54	111.71
1	C	715	ILE	N-CA-C	5.35	116.23	111.90
1	G	846	LYS	N-CA-C	-5.31	105.49	111.28
1	G	778	LEU	N-CA-C	5.30	117.14	111.36
1	E	768	SER	N-CA-C	5.27	117.03	111.28
1	B	847	THR	N-CA-C	-5.26	103.39	108.07
1	F	1005	GLU	N-CA-C	5.26	116.88	110.41
1	C	970	LYS	N-CA-C	-5.25	105.56	111.28
1	H	978	TYR	N-CA-C	5.22	117.05	111.36
1	B	819	VAL	CB-CA-C	-5.21	105.10	112.14
1	A	723	PHE	N-CA-C	5.20	117.02	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	915	TYR	N-CA-C	-5.18	104.24	111.39
1	H	935	GLN	CA-C-N	5.18	123.44	119.66
1	H	935	GLN	C-N-CA	5.18	123.44	119.66
1	E	965	ILE	CB-CA-C	-5.13	105.22	112.14
1	H	768	SER	N-CA-C	5.08	116.81	111.28
1	B	1008	ASP	N-CA-C	5.06	116.80	111.28
1	D	718	LEU	N-CA-C	5.05	116.48	111.07
1	C	923	ILE	N-CA-C	5.05	115.77	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	0	2361	281	0
1	B	2333	0	2286	282	0
1	C	2325	0	2316	349	0
1	D	2281	0	2200	248	0
1	E	2297	0	2247	279	0
1	F	2328	0	2317	279	0
1	G	2367	0	2355	284	0
1	H	2362	0	2353	264	0
2	A	36	0	0	5	0
2	B	36	0	0	5	0
2	C	36	0	0	8	0
2	D	36	0	0	11	0
2	E	36	0	0	7	0
2	F	36	0	0	8	0
2	G	36	0	0	14	0
2	H	36	0	0	11	0
3	G	4	0	6	2	0
3	H	12	0	18	4	0
4	A	45	0	0	14	0
4	B	37	0	0	3	0
4	C	35	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	19	0	0	3	0
4	E	42	0	0	5	0
4	F	50	0	0	15	0
4	G	48	0	0	10	0
4	H	27	0	0	4	0
All	All	19277	0	18459	2238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

All (2238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:707:LEU:CD1	1:H:789:ILE:HD13	1.41	1.50
1:H:707:LEU:HD13	1:H:789:ILE:CD1	1.50	1.42
1:G:989:LEU:HD22	1:G:990:PRO:CD	1.52	1.39
1:B:790:MET:HE2	2:B:1101:816:NAB	1.40	1.35
1:H:812:GLN:NE2	1:H:1013:ALA:HB2	1.43	1.29
1:C:835:HIS:CD2	1:C:856:PHE:HA	1.67	1.28
1:F:989:LEU:HD23	1:F:989:LEU:C	1.55	1.26
1:C:790:MET:HE2	2:C:1101:816:NAB	1.48	1.25
1:B:941:ILE:O	1:B:941:ILE:HD12	1.34	1.24
1:C:961:PHE:O	1:C:965:ILE:HD12	1.34	1.24
1:C:941:ILE:HD12	1:C:941:ILE:O	1.34	1.23
1:A:798:LEU:HD12	1:A:798:LEU:O	1.34	1.23
1:G:995:SER:O	1:G:999[B]:ARG:HD2	1.40	1.21
1:H:905:TRP:O	1:H:909:THR:HG23	1.40	1.20
1:C:825:MET:SD	1:C:838:LEU:CD2	2.30	1.20
1:B:835:HIS:CB	1:B:856:PHE:HB2	1.73	1.19
1:G:806:LYS:C	1:G:806:LYS:HD3	1.61	1.18
1:D:730:LEU:HD22	1:D:739:LYS:HB3	1.20	1.18
1:G:806:LYS:HD3	1:G:807:ASP:N	1.58	1.18
1:H:778:LEU:N	1:H:778:LEU:HD23	1.54	1.17
1:B:771:ASN:ND2	1:B:772:PRO:HD2	1.59	1.17
1:C:805:HIS:O	1:C:809:ILE:HG22	1.41	1.17
1:C:894:GLN:HG3	1:C:955:ALA:O	1.45	1.17
1:B:835:HIS:HB3	1:B:856:PHE:HB2	1.24	1.16
1:C:778:LEU:HD23	1:C:778:LEU:H	1.09	1.16
1:G:1007:MET:HE2	1:G:1008:ASP:O	1.43	1.16
1:F:977:ARG:HD2	1:F:977:ARG:O	1.42	1.16
1:F:842:ASN:O	1:F:854:THR:HG22	1.44	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:759:ILE:HD11	1:E:780:ILE:HD11	1.21	1.15
1:G:940:THR:HG22	1:G:943:VAL:HG23	1.24	1.15
1:B:977:ARG:HG3	1:B:977:ARG:HH21	1.02	1.14
1:E:790:MET:HE2	2:E:1101:816:NAB	1.60	1.14
1:B:982:GLN:NE2	1:B:982:GLN:H	1.46	1.14
1:D:815:LEU:CD2	1:D:979:LEU:HD11	1.77	1.13
1:F:773:HIS:O	1:F:853:ILE:HD13	1.48	1.13
1:G:1007:MET:HE1	1:G:1010:VAL:HG12	1.30	1.13
1:F:729:GLY:C	1:F:730:LEU:HD23	1.72	1.12
1:D:790:MET:HE2	2:D:1101:816:CAA	1.80	1.11
1:H:715:ILE:HD11	1:H:728:LYS:HE2	1.28	1.11
1:C:778:LEU:HD23	1:C:778:LEU:N	1.63	1.11
1:B:977:ARG:HH21	1:B:977:ARG:CG	1.65	1.10
1:D:815:LEU:HD21	1:D:979:LEU:HD11	1.19	1.10
1:E:743:ALA:C	1:E:744:ILE:HD13	1.76	1.10
1:C:835:HIS:HD2	1:C:856:PHE:HB2	1.06	1.10
1:C:856:PHE:HD1	1:C:857:GLY:N	1.49	1.10
1:H:799:LEU:O	1:H:803:ARG:HG3	1.50	1.10
1:C:760:LEU:CD1	1:C:782:LEU:HD11	1.80	1.10
1:D:815:LEU:HD21	1:D:979:LEU:CD1	1.81	1.09
1:E:945:MET:HE1	1:C:934:PRO:HG2	1.12	1.09
1:B:755:ALA:O	1:B:759:ILE:HD12	1.52	1.09
1:G:811:SER:HB3	1:G:984:ASP:OD1	1.50	1.09
1:G:989:LEU:CD2	1:G:990:PRO:CD	2.30	1.09
1:C:825:MET:SD	1:C:838:LEU:HD22	1.91	1.09
1:D:981:ILE:HB	1:D:984:ASP:HB2	1.35	1.08
1:D:771:ASN:HB3	1:D:774:VAL:HG23	1.22	1.08
1:G:849:GLN:HE21	1:G:990:PRO:HG3	1.12	1.08
1:B:831:ARG:HG2	1:B:831:ARG:HH11	1.19	1.08
1:F:771:ASN:ND2	1:F:772:PRO:HD2	1.67	1.08
1:E:937:PRO:HD2	4:E:1211:HOH:O	1.50	1.08
1:C:835:HIS:CD2	1:C:856:PHE:CA	2.36	1.08
1:G:811:SER:HB3	1:G:984:ASP:CG	1.79	1.07
1:F:876:VAL:HB	1:F:877:PRO:HD2	1.34	1.07
1:H:986:ARG:HB3	1:H:986:ARG:HH11	1.12	1.07
1:C:908:MET:HE3	1:C:979:LEU:HD21	1.08	1.07
1:E:759:ILE:CD1	1:E:780:ILE:HD11	1.83	1.06
1:F:707:LEU:H	1:F:707:LEU:HD12	1.13	1.06
1:H:832:ARG:HH11	1:H:832:ARG:HG2	1.01	1.06
1:B:809:ILE:C	1:B:987:MET:HE3	1.81	1.06
1:B:809:ILE:O	1:B:987:MET:CE	2.04	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:941:ILE:O	1:D:945:MET:HG3	1.56	1.05
1:G:989:LEU:CD2	1:G:990:PRO:HD2	1.86	1.05
1:C:760:LEU:HD13	1:C:782:LEU:CD1	1.86	1.05
1:D:730:LEU:CD2	1:D:739:LYS:HB3	1.85	1.05
1:C:913:LYS:H	1:C:913:LYS:CD	1.66	1.05
1:G:845:VAL:HG13	1:G:847:THR:O	1.57	1.04
1:C:760:LEU:HD13	1:C:782:LEU:HD11	1.05	1.04
1:C:908:MET:CG	1:C:939:CYS:SG	2.46	1.03
1:C:878:ILE:HG23	1:C:886:ILE:HD11	1.41	1.03
1:H:953:ILE:CD1	1:H:953:ILE:H	1.72	1.03
1:C:835:HIS:HD2	1:C:856:PHE:CB	1.72	1.03
1:C:909:THR:HB	1:C:912:SER:HB2	1.38	1.03
1:H:845:VAL:HG13	1:H:847:THR:O	1.57	1.02
1:E:845:VAL:HG13	1:E:847:THR:O	1.58	1.02
1:C:908:MET:HG3	1:C:939:CYS:SG	1.98	1.02
1:C:940:THR:HB	1:C:978:TYR:O	1.57	1.02
1:D:815:LEU:HD11	1:D:979:LEU:HD12	1.39	1.02
1:E:707:LEU:CD1	1:E:789:ILE:HG12	1.89	1.02
1:G:806:LYS:C	1:G:806:LYS:CD	2.30	1.02
1:H:757:LYS:HD2	1:H:757:LYS:C	1.85	1.02
1:B:988:HIS:CB	1:B:989:LEU:C	2.33	1.02
1:H:899:SER:HA	1:H:902:VAL:CG2	1.90	1.01
1:F:853:ILE:HD12	1:F:853:ILE:N	1.71	1.01
1:C:908:MET:HE3	1:C:979:LEU:CD2	1.89	1.01
1:C:908:MET:CE	1:C:979:LEU:HD21	1.90	1.01
1:A:841:ARG:HH21	1:A:841:ARG:HG2	1.20	1.01
1:E:945:MET:HE1	1:C:934:PRO:CG	1.90	1.01
1:C:700:ASN:N	1:C:703:LEU:HD12	1.76	1.01
1:A:717:VAL:O	1:A:717:VAL:HG12	1.61	1.00
1:C:717:VAL:HG23	1:C:727:TYR:CE2	1.96	1.00
1:C:894:GLN:HA	1:C:894:GLN:OE1	1.58	1.00
1:D:783:THR:HG22	1:D:784:SER:H	1.24	1.00
1:F:790:MET:HE2	2:F:1101:816:NAB	1.77	1.00
1:G:989:LEU:CD2	1:G:990:PRO:HD3	1.92	0.99
1:C:715:ILE:HD11	1:C:728:LYS:NZ	1.76	0.99
1:E:842:ASN:O	1:E:854:THR:HG22	1.61	0.99
1:E:795:PHE:HE2	1:E:1002:MET:HE1	1.26	0.99
1:D:1013:ALA:HB2	4:D:1210:HOH:O	1.61	0.99
1:H:799:LEU:HD13	1:H:840:ALA:HB3	1.41	0.99
1:A:777:LEU:HD21	1:A:788:LEU:HD23	1.44	0.99
1:F:708:LYS:N	1:F:711:GLU:HG3	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:835:HIS:CD2	1:C:856:PHE:HB2	1.97	0.99
1:G:989:LEU:HD22	1:G:990:PRO:HD2	1.01	0.98
1:F:989:LEU:C	1:F:989:LEU:CD2	2.30	0.98
1:F:990:PRO:HG3	4:F:1215:HOH:O	1.63	0.98
1:C:856:PHE:CD1	1:C:857:GLY:N	2.30	0.98
1:E:790:MET:HE3	1:E:791:GLN:O	1.62	0.98
1:F:977:ARG:HD2	1:F:977:ARG:C	1.79	0.98
1:E:795:PHE:HE2	1:E:1002:MET:CE	1.76	0.98
1:C:913:LYS:H	1:C:913:LYS:HD3	1.25	0.98
1:G:881:MET:HE3	1:G:885:SER:HB3	1.46	0.98
1:C:835:HIS:CD2	1:C:856:PHE:CB	2.46	0.98
1:G:730:LEU:HD13	1:G:739:LYS:HB3	1.46	0.97
1:E:730:LEU:HD13	1:E:739:LYS:HB3	1.46	0.97
1:E:707:LEU:HD11	1:E:789:ILE:HG12	1.45	0.97
1:B:972:ALA:HB3	1:B:1011:VAL:HG11	1.43	0.97
1:H:832:ARG:HG2	1:H:832:ARG:NH1	1.70	0.97
1:B:972:ALA:CB	1:B:1011:VAL:HG11	1.94	0.97
1:H:772:PRO:O	1:H:852:LYS:HE3	1.63	0.97
1:D:815:LEU:CD2	1:D:979:LEU:CD1	2.42	0.96
1:A:946:ILE:HD12	1:A:971:MET:HE1	1.47	0.96
1:H:762:GLU:O	1:H:765:VAL:HG23	1.63	0.96
1:H:953:ILE:HD12	1:H:953:ILE:N	1.77	0.96
1:H:812:GLN:CD	1:H:1013:ALA:HB2	1.90	0.96
1:F:707:LEU:HD12	1:F:707:LEU:N	1.81	0.95
1:G:974:ASP:OD2	3:G:1102:EDO:H21	1.67	0.95
1:D:717:VAL:HG13	1:D:727:TYR:HE2	1.29	0.95
1:C:972:ALA:O	1:C:975:PRO:HD3	1.66	0.95
1:E:847:THR:HG23	1:E:850:HIS:HB3	1.45	0.95
1:D:941:ILE:HD11	1:D:945:MET:HE3	1.47	0.95
1:F:769:VAL:O	1:F:769:VAL:HG23	1.65	0.95
1:F:853:ILE:CD1	1:F:853:ILE:H	1.80	0.95
1:B:769:VAL:HG12	1:B:827:TYR:HE2	1.29	0.95
1:E:759:ILE:CD1	1:E:780:ILE:CD1	2.45	0.94
1:G:854:THR:HG22	1:G:855:ASP:N	1.79	0.94
1:F:853:ILE:N	1:F:853:ILE:CD1	2.30	0.94
1:B:988:HIS:HA	1:B:989:LEU:CB	1.98	0.94
1:C:717:VAL:CG2	1:C:727:TYR:CE2	2.49	0.94
1:H:778:LEU:N	1:H:778:LEU:CD2	2.30	0.94
1:C:1007:MET:HG2	1:C:1008:ASP:N	1.82	0.94
1:A:946:ILE:CD1	1:A:971:MET:CE	2.46	0.94
1:D:790:MET:CE	2:D:1101:816:CAA	2.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:945:MET:CE	1:C:934:PRO:HG2	1.97	0.94
1:H:986:ARG:HH11	1:H:986:ARG:CB	1.82	0.93
1:C:707:LEU:HD11	1:C:789:ILE:HD13	1.50	0.93
1:F:989:LEU:HD23	1:F:990:PRO:N	1.81	0.93
1:H:986:ARG:CB	1:H:986:ARG:NH1	2.30	0.93
1:B:809:ILE:O	1:B:987:MET:HE2	1.68	0.93
1:E:840:ALA:HB3	1:E:906:GLU:OE2	1.67	0.93
1:B:940:THR:HB	1:B:978:TYR:O	1.67	0.93
1:D:790:MET:CE	2:D:1101:816:NAY	2.32	0.93
1:D:815:LEU:CD1	1:D:979:LEU:HD12	1.99	0.93
1:H:986:ARG:HB3	1:H:986:ARG:NH1	1.84	0.93
1:D:839:ALA:O	1:D:843:VAL:HG23	1.68	0.93
1:B:790:MET:CE	2:B:1101:816:NAB	2.30	0.93
1:E:856:PHE:CD1	1:E:856:PHE:C	2.46	0.93
1:C:717:VAL:CG2	1:C:727:TYR:HE2	1.82	0.93
1:B:809:ILE:C	1:B:987:MET:CE	2.40	0.92
1:D:717:VAL:HG13	1:D:727:TYR:CE2	2.02	0.92
1:A:977:ARG:HE	1:E:926:ILE:HD12	1.33	0.92
1:C:856:PHE:CD1	1:C:856:PHE:C	2.48	0.92
1:B:977:ARG:HG3	1:B:977:ARG:NH2	1.83	0.92
1:E:718:LEU:HB2	1:E:726:VAL:O	1.68	0.92
1:G:989:LEU:HD22	1:G:990:PRO:HD3	1.47	0.92
1:B:736:GLU:HA	1:B:736:GLU:OE2	1.70	0.91
1:B:941:ILE:HD12	1:B:941:ILE:C	1.93	0.91
1:A:798:LEU:HD12	1:A:798:LEU:C	1.92	0.91
1:C:717:VAL:HG23	1:C:727:TYR:HE2	1.32	0.91
1:H:953:ILE:CD1	1:H:953:ILE:N	2.30	0.91
1:B:894:GLN:NE2	1:B:960:LYS:HE2	1.85	0.91
1:H:778:LEU:HD23	1:H:778:LEU:H	1.32	0.91
1:H:854:THR:HG22	1:H:855:ASP:N	1.83	0.91
1:C:715:ILE:CD1	1:C:728:LYS:HZ2	1.84	0.91
1:D:815:LEU:CG	1:D:979:LEU:CD1	2.48	0.91
1:E:793:MET:HG3	1:E:844:LEU:CD1	2.02	0.90
1:F:756:ASN:ND2	1:F:782:LEU:HD13	1.86	0.90
1:E:998:TYR:O	1:E:1002:MET:HB2	1.72	0.90
1:F:778:LEU:HD23	1:F:790:MET:HA	1.52	0.90
1:E:762:GLU:O	1:E:765:VAL:HG23	1.70	0.90
1:H:899:SER:HA	1:H:902:VAL:HG23	1.53	0.90
1:G:797:CYS:SG	2:G:1101:816:OAE	2.30	0.90
1:C:704:LEU:HD12	1:C:764:TYR:HE1	1.37	0.90
1:A:946:ILE:CD1	1:A:971:MET:HE1	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:GLN:HG3	1:B:944:TYR:CD2	2.06	0.90
1:D:900:TYR:O	1:D:904:VAL:HG23	1.72	0.90
1:H:898:TRP:O	1:H:902:VAL:HG22	1.72	0.90
1:C:897:VAL:HG13	1:C:950:CYS:SG	2.11	0.90
1:H:812:GLN:NE2	1:H:1013:ALA:CB	2.33	0.89
1:G:1007:MET:HE1	1:G:1010:VAL:CG1	2.01	0.89
1:C:913:LYS:CD	1:C:913:LYS:N	2.30	0.89
1:A:777:LEU:CD2	1:A:788:LEU:HD23	2.01	0.89
1:C:715:ILE:CD1	1:C:728:LYS:NZ	2.36	0.89
1:A:830:ASP:HB3	1:C:717:VAL:HG11	1.55	0.89
1:C:941:ILE:HD12	1:C:941:ILE:C	1.96	0.89
1:E:771:ASN:HB3	1:E:774:VAL:HG23	1.52	0.89
1:H:812:GLN:HE22	1:H:1013:ALA:HB2	1.30	0.89
1:B:934:PRO:O	1:B:936:PRO:HD3	1.73	0.89
1:A:923:ILE:HA	1:A:926:ILE:HG12	1.54	0.89
1:B:737:LYS:HD3	1:B:738:VAL:CG1	2.03	0.89
1:A:705:ARG:NE	1:A:707:LEU:HD21	1.88	0.88
1:A:806:LYS:CD	1:A:806:LYS:C	2.46	0.88
1:B:982:GLN:H	1:B:982:GLN:HE21	1.17	0.88
1:H:832:ARG:HH11	1:H:832:ARG:CG	1.86	0.88
1:F:708:LYS:N	1:F:711:GLU:CG	2.36	0.88
1:F:811:SER:HB3	1:F:984:ASP:OD2	1.72	0.88
1:G:919:PRO:HD2	1:G:922:GLU:OE1	1.72	0.88
1:A:806:LYS:O	1:A:806:LYS:HD2	1.73	0.88
1:E:790:MET:CE	2:E:1101:816:NAB	2.36	0.88
1:H:899:SER:CA	1:H:902:VAL:HG23	2.04	0.88
1:B:818:CYS:SG	1:B:904:VAL:HG22	2.12	0.88
1:E:795:PHE:CE2	1:E:1002:MET:CE	2.56	0.88
1:F:955:ALA:O	1:F:958:ARG:HG3	1.73	0.88
1:A:806:LYS:C	1:A:806:LYS:HD2	1.99	0.87
1:A:834:VAL:HB	4:A:1209:HOH:O	1.74	0.87
1:G:775:CYS:SG	1:G:854:THR:OG1	2.32	0.87
1:H:817:TRP:O	1:H:821:ILE:HG13	1.74	0.87
1:D:717:VAL:HA	1:D:727:TYR:HD2	1.37	0.87
1:D:800:ASP:O	1:D:804:GLU:HG2	1.74	0.87
1:B:778:LEU:HD11	1:B:791:GLN:HG2	1.55	0.87
1:G:798:LEU:O	1:G:802:VAL:HG22	1.75	0.87
1:C:795:PHE:CE2	1:C:1002:MET:HE1	2.08	0.87
1:C:908:MET:HG2	1:C:939:CYS:SG	2.13	0.87
1:D:932:ARG:HG2	1:D:932:ARG:HH11	1.39	0.87
1:E:798:LEU:O	1:E:802:VAL:HG22	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:825:MET:HE1	1:G:853:ILE:HD13	1.57	0.87
1:C:717:VAL:O	1:C:717:VAL:HG12	1.72	0.87
1:A:878:ILE:HD12	4:A:1214:HOH:O	1.73	0.87
1:C:773:HIS:O	1:C:853:ILE:HG23	1.73	0.87
1:B:816:ASN:HA	1:B:819:VAL:HG23	1.54	0.87
1:C:897:VAL:CG1	1:C:950:CYS:SG	2.62	0.87
1:H:899:SER:C	1:H:902:VAL:HG23	1.99	0.87
1:F:876:VAL:HB	1:F:877:PRO:CD	2.04	0.86
1:A:783:THR:HB	1:A:785:THR:O	1.76	0.86
1:C:955:ALA:O	1:C:958:ARG:HG3	1.76	0.86
1:B:835:HIS:HB2	1:B:856:PHE:CA	2.05	0.86
1:E:795:PHE:CE2	1:E:1002:MET:HE1	2.10	0.86
1:H:798:LEU:O	1:H:802:VAL:HG22	1.76	0.86
1:D:717:VAL:HA	1:D:727:TYR:CD2	2.10	0.86
1:D:940:THR:HG22	1:D:943:VAL:HG23	1.58	0.86
1:G:919:PRO:HG2	1:G:922:GLU:OE1	1.76	0.86
1:A:786:VAL:HG23	4:A:1228:HOH:O	1.76	0.85
1:B:737:LYS:HD3	1:B:738:VAL:HG13	1.57	0.85
1:E:986:ARG:HG2	1:E:987:MET:N	1.89	0.85
1:C:715:ILE:HD11	1:C:728:LYS:HZ2	1.35	0.85
1:C:801:TYR:HE2	1:C:817:TRP:HH2	1.24	0.85
1:D:719:GLY:HA3	2:D:1101:816:CAS	2.07	0.85
1:H:718:LEU:HD11	1:H:792:LEU:HD11	1.56	0.85
1:A:950:CYS:O	1:A:958:ARG:HD3	1.75	0.85
1:A:977:ARG:HG2	1:E:931:GLU:OE2	1.75	0.85
1:D:815:LEU:CG	1:D:979:LEU:HD12	2.05	0.85
1:E:723:PHE:CE2	1:E:859:ALA:HA	2.09	0.85
1:H:747:LEU:HD13	1:H:862:LEU:HD21	1.59	0.85
1:B:831:ARG:HG2	1:B:831:ARG:NH1	1.83	0.85
1:D:878:ILE:HA	1:D:881:MET:HE3	1.57	0.85
1:G:854:THR:HG22	1:G:855:ASP:H	1.37	0.85
1:G:940:THR:CG2	1:G:943:VAL:HG23	2.07	0.85
1:C:940:THR:HG22	1:C:943:VAL:HG23	1.56	0.85
1:B:797:CYS:SG	1:B:800:ASP:OD2	2.35	0.85
1:B:834:VAL:HG22	1:B:893:HIS:CD2	2.12	0.85
1:C:795:PHE:HE2	1:C:1002:MET:HE1	1.41	0.85
1:E:950:CYS:O	1:E:958:ARG:HD2	1.76	0.85
1:C:714:LYS:CE	1:C:787:GLN:HE22	1.89	0.85
1:F:730:LEU:HD23	1:F:730:LEU:N	1.89	0.84
1:C:953:ILE:HD13	1:C:953:ILE:N	1.91	0.84
1:B:771:ASN:ND2	1:B:772:PRO:CD	2.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:877:PRO:O	1:D:881:MET:HG3	1.75	0.84
1:H:935:GLN:OE1	1:H:944:TYR:CD2	2.30	0.84
1:F:729:GLY:C	1:F:730:LEU:CD2	2.49	0.84
1:F:823:LYS:NZ	1:F:1008:ASP:CG	2.35	0.84
1:F:836:ARG:HB2	1:F:859:ALA:HB3	1.58	0.84
1:E:756:ASN:O	1:E:759:ILE:HG22	1.77	0.84
1:G:823:LYS:HE2	1:G:1008:ASP:OD2	1.77	0.84
1:A:856:PHE:O	1:A:856:PHE:CD1	2.30	0.84
1:E:945:MET:CE	1:C:934:PRO:CG	2.54	0.84
1:G:773:HIS:ND1	1:G:820:GLN:HB3	1.91	0.84
1:G:849:GLN:HE21	1:G:990:PRO:CG	1.89	0.84
1:B:905:TRP:O	1:B:909:THR:HG23	1.77	0.84
1:D:707:LEU:HD22	1:D:711:GLU:HB2	1.58	0.84
1:B:835:HIS:CB	1:B:856:PHE:CB	2.54	0.84
1:F:848:PRO:HB2	1:F:849:GLN:OE1	1.77	0.84
1:H:715:ILE:HD11	1:H:728:LYS:CE	2.05	0.84
1:B:817:TRP:O	1:B:821:ILE:HG13	1.78	0.83
1:E:808:ASN:O	1:E:809:ILE:HG12	1.77	0.83
1:H:762:GLU:HB3	1:H:861:LEU:HD21	1.60	0.83
1:B:945:MET:CE	1:D:909:THR:HG22	2.08	0.83
1:D:941:ILE:CD1	1:D:945:MET:HE3	2.08	0.83
1:G:878:ILE:HG23	1:G:886:ILE:HD13	1.60	0.83
1:D:878:ILE:HG13	1:D:881:MET:CE	2.09	0.83
1:E:836:ARG:HD2	1:E:860:LYS:CB	2.08	0.83
1:A:841:ARG:HG2	1:A:841:ARG:NH2	1.91	0.83
1:H:715:ILE:CD1	1:H:728:LYS:HE2	2.07	0.83
1:H:835:HIS:CE1	1:H:837:ASP:O	2.30	0.83
1:D:815:LEU:HG	1:D:979:LEU:CD1	2.08	0.83
1:D:799:LEU:O	1:D:803:ARG:HG3	1.79	0.83
1:B:798:LEU:HB2	1:B:843:VAL:HG12	1.61	0.83
1:C:905:TRP:O	1:C:909:THR:HG23	1.78	0.83
1:D:798:LEU:O	1:D:802:VAL:HG22	1.79	0.82
1:G:704:LEU:CD1	1:G:767:ALA:HB2	2.09	0.82
1:A:777:LEU:CD2	1:A:788:LEU:CD2	2.57	0.82
1:A:946:ILE:HD11	1:A:971:MET:CE	2.09	0.82
1:D:845:VAL:HG22	1:D:851:VAL:HG12	1.61	0.82
1:F:989:LEU:HD23	1:F:989:LEU:O	1.77	0.82
1:C:878:ILE:HG23	1:C:886:ILE:CD1	2.09	0.82
1:G:769:VAL:HG11	1:G:856:PHE:HZ	1.44	0.82
1:E:759:ILE:HD11	1:E:780:ILE:CD1	2.05	0.82
1:A:762:GLU:O	1:A:765:VAL:HG12	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:MET:HE2	1:C:886:ILE:HG13	1.60	0.82
1:E:744:ILE:HD13	1:E:744:ILE:N	1.84	0.82
1:F:747:LEU:HG	1:F:788:LEU:HD11	1.62	0.82
1:F:818:CYS:SG	1:F:904:VAL:HG13	2.19	0.82
1:C:1007:MET:HE2	1:C:1008:ASP:O	1.78	0.82
1:D:936:PRO:HB2	1:D:939:CYS:HB2	1.62	0.81
1:B:777:LEU:HD21	1:B:788:LEU:HD22	1.61	0.81
1:F:989:LEU:HD21	1:F:990:PRO:O	1.79	0.81
1:F:723:PHE:O	1:F:748:ARG:HG2	1.79	0.81
1:F:729:GLY:HA3	1:F:744:ILE:HD11	1.62	0.81
1:F:876:VAL:CB	1:F:877:PRO:HD2	2.10	0.81
1:H:935:GLN:HB3	1:H:944:TYR:CE2	2.15	0.81
1:H:953:ILE:H	1:H:953:ILE:HD13	1.45	0.81
1:A:705:ARG:HE	1:A:707:LEU:CD2	1.94	0.81
1:G:932:ARG:HB3	1:G:932:ARG:HH11	1.45	0.81
1:F:908:MET:HG3	1:F:939:CYS:SG	2.20	0.81
1:A:936:PRO:HB2	1:A:939:CYS:HB2	1.62	0.81
1:B:999:ARG:HH11	1:B:999:ARG:HG3	1.45	0.81
1:E:803:ARG:HG2	1:E:911:GLY:HA3	1.62	0.81
1:G:889:ARG:HH11	1:G:889:ARG:CG	1.94	0.81
1:C:879:LYS:HD3	1:C:915:TYR:HB2	1.61	0.81
1:B:997:PHE:O	1:B:997:PHE:HD1	1.63	0.80
1:E:723:PHE:HE2	1:E:859:ALA:CA	1.95	0.80
1:G:924:SER:O	1:G:928:GLU:HG3	1.81	0.80
1:H:799:LEU:HD13	1:H:840:ALA:CB	2.10	0.80
1:H:962:ARG:HA	1:H:965:ILE:HG13	1.63	0.80
1:B:977:ARG:CG	1:B:977:ARG:NH2	2.36	0.80
1:B:835:HIS:HB2	1:B:856:PHE:HA	1.62	0.80
1:H:845:VAL:CG1	1:H:847:THR:C	2.54	0.80
1:G:806:LYS:O	1:G:806:LYS:CE	2.30	0.80
1:B:769:VAL:HG12	1:B:827:TYR:CE2	2.17	0.80
1:D:707:LEU:HD22	1:D:711:GLU:CB	2.11	0.80
1:A:806:LYS:CD	1:A:806:LYS:O	2.30	0.80
1:B:935:GLN:HG3	1:B:944:TYR:CG	2.16	0.80
1:F:721:GLY:CA	1:F:724:GLY:O	2.30	0.80
1:E:743:ALA:C	1:E:744:ILE:CD1	2.54	0.80
1:F:991:SER:HB2	1:F:992:PRO:CD	2.11	0.80
1:C:816:ASN:O	1:C:820:GLN:HG3	1.80	0.80
1:C:881:MET:HE2	1:C:886:ILE:CG1	2.12	0.80
1:D:797:CYS:HB3	1:D:800:ASP:HB2	1.62	0.80
1:E:723:PHE:HE2	1:E:859:ALA:HA	1.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:ALA:O	1:B:759:ILE:CD1	2.30	0.80
1:F:944:TYR:O	1:F:948:VAL:HG22	1.81	0.80
1:G:790:MET:HG2	2:G:1101:816:CLA	2.19	0.80
1:H:743:ALA:HB2	1:H:792:LEU:HD12	1.64	0.80
1:C:913:LYS:N	1:C:913:LYS:HD2	1.96	0.80
1:A:783:THR:HG22	1:A:784:SER:H	1.47	0.79
1:D:878:ILE:HD13	1:D:920:ALA:HB1	1.63	0.79
1:F:771:ASN:ND2	1:F:772:PRO:CD	2.45	0.79
1:F:989:LEU:CD2	1:F:990:PRO:O	2.30	0.79
1:C:780:ILE:CD1	1:C:787:GLN:O	2.30	0.79
1:E:967:GLU:O	1:E:971:MET:HG3	1.82	0.79
1:E:704:LEU:HB2	1:E:767:ALA:CB	2.12	0.79
1:G:845:VAL:CG1	1:G:847:THR:O	2.30	0.79
1:E:845:VAL:CG1	1:E:847:THR:O	2.30	0.79
1:C:842:ASN:O	1:C:854:THR:HG22	1.81	0.79
1:C:894:GLN:OE1	1:C:894:GLN:CA	2.30	0.79
1:A:717:VAL:HG23	1:A:727:TYR:CE2	2.17	0.79
1:G:919:PRO:CD	1:G:922:GLU:OE1	2.30	0.79
1:A:849:GLN:OE1	1:A:995:SER:HB2	1.83	0.79
1:H:899:SER:HA	1:H:902:VAL:HG21	1.63	0.79
1:C:701:GLN:OE1	1:C:701:GLN:HA	1.81	0.79
1:H:762:GLU:O	1:H:765:VAL:CG2	2.30	0.79
1:C:894:GLN:HB3	1:C:955:ALA:HB1	1.65	0.79
1:F:769:VAL:O	1:F:769:VAL:CG2	2.30	0.79
1:F:825:MET:HE1	1:F:835:HIS:CB	2.12	0.79
1:A:900:TYR:O	1:A:904:VAL:HG23	1.83	0.78
1:B:717:VAL:O	1:B:717:VAL:HG12	1.82	0.78
1:E:844:LEU:CD2	1:E:854:THR:HG21	2.14	0.78
1:G:915:TYR:HE1	1:G:926:ILE:HD11	1.47	0.78
1:G:915:TYR:CE1	1:G:926:ILE:HD11	2.19	0.78
1:D:704:LEU:HB2	1:D:767:ALA:CB	2.12	0.78
1:C:701:GLN:OE1	1:C:701:GLN:CA	2.30	0.78
1:B:931:GLU:O	1:B:932:ARG:HD2	1.83	0.78
1:D:757:LYS:HD2	1:D:761:ASP:OD2	1.83	0.78
1:C:805:HIS:O	1:C:809:ILE:CG2	2.30	0.78
1:E:718:LEU:CB	1:E:726:VAL:O	2.32	0.78
1:E:841:ARG:HD2	4:E:1218:HOH:O	1.84	0.78
1:C:778:LEU:N	1:C:778:LEU:CD2	2.40	0.78
1:F:977:ARG:O	1:F:977:ARG:CD	2.30	0.78
1:G:919:PRO:CG	1:G:922:GLU:OE1	2.32	0.78
1:H:817:TRP:CD1	1:H:851:VAL:HG11	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:GLN:HG3	1:A:944:TYR:CG	2.19	0.78
1:H:835:HIS:CD2	1:H:856:PHE:HB3	2.19	0.78
1:C:736:GLU:HA	1:C:736:GLU:OE2	1.83	0.78
1:B:780:ILE:HD13	1:B:782:LEU:HD22	1.66	0.78
1:D:819:VAL:O	1:D:823:LYS:HG3	1.84	0.78
1:C:817:TRP:O	1:C:821:ILE:HG13	1.84	0.78
1:C:839:ALA:CB	1:C:841:ARG:HG3	2.14	0.78
1:D:790:MET:HE3	2:D:1101:816:NAY	1.99	0.78
1:G:854:THR:CG2	1:G:855:ASP:H	1.97	0.78
1:G:940:THR:HG22	1:G:943:VAL:CG2	2.10	0.77
1:B:783:THR:HG22	1:B:784:SER:N	2.00	0.77
1:H:845:VAL:CG1	1:H:847:THR:O	2.30	0.77
1:C:811:SER:HB3	1:C:984:ASP:OD1	1.85	0.77
1:D:746:GLU:HG3	1:D:787:GLN:HG2	1.65	0.77
1:F:991:SER:HB2	1:F:992:PRO:HD2	1.66	0.77
1:E:730:LEU:HD13	1:E:739:LYS:CB	2.14	0.77
1:H:800:ASP:O	1:H:804:GLU:HG3	1.84	0.77
1:H:899:SER:O	1:H:902:VAL:HG23	1.84	0.77
1:C:825:MET:SD	1:C:838:LEU:HD21	2.24	0.77
1:C:955:ALA:O	1:C:958:ARG:CG	2.32	0.77
1:A:881:MET:HE3	1:A:885:SER:CB	2.14	0.77
1:E:835:HIS:CE1	1:E:856:PHE:HA	2.18	0.77
1:F:836:ARG:HB2	1:F:859:ALA:CB	2.15	0.77
1:E:719:GLY:HA3	2:E:1101:816:CAS	2.14	0.77
1:C:707:LEU:CD1	1:C:789:ILE:HD13	2.14	0.77
1:D:941:ILE:CG1	1:D:945:MET:HE3	2.15	0.77
1:H:935:GLN:HB3	1:H:944:TYR:CD2	2.19	0.77
1:A:705:ARG:NE	1:A:707:LEU:CD2	2.48	0.76
1:G:817:TRP:CD1	1:G:851:VAL:HG11	2.20	0.76
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.20	0.76
1:D:923:ILE:O	1:D:926:ILE:HG12	1.85	0.76
1:E:898:TRP:HE3	1:E:958:ARG:NH1	1.83	0.76
1:E:706:ILE:HG22	1:E:706:ILE:O	1.86	0.76
1:F:944:TYR:O	1:F:948:VAL:CG2	2.32	0.76
1:G:854:THR:CG2	1:G:855:ASP:N	2.48	0.76
1:G:889:ARG:HH11	1:G:889:ARG:HG2	1.51	0.76
1:G:1006:ASP:CB	4:G:1220:HOH:O	2.34	0.76
1:A:700:ASN:N	1:A:703:LEU:HD12	2.00	0.76
1:H:757:LYS:C	1:H:757:LYS:CD	2.58	0.76
1:A:966:ILE:CD1	1:C:804:GLU:OE2	2.33	0.76
1:D:762:GLU:OE1	1:D:861:LEU:CB	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:717:VAL:HG22	1:G:727:TYR:CE2	2.20	0.76
1:C:801:TYR:HE2	1:C:817:TRP:CH2	2.03	0.76
1:C:973:ARG:HG2	1:C:973:ARG:NH1	2.01	0.76
1:G:703:LEU:HD23	1:G:703:LEU:N	2.01	0.76
1:H:905:TRP:O	1:H:909:THR:CG2	2.30	0.76
1:A:777:LEU:HD22	1:A:788:LEU:CD2	2.16	0.76
1:B:816:ASN:HA	1:B:819:VAL:CG2	2.14	0.76
1:D:771:ASN:HB3	1:D:774:VAL:CG2	2.10	0.76
1:A:819:VAL:HG12	1:A:823:LYS:HE3	1.66	0.76
1:C:835:HIS:NE2	1:C:856:PHE:HA	2.01	0.76
1:C:940:THR:CB	1:C:978:TYR:O	2.31	0.76
1:D:878:ILE:HA	1:D:881:MET:CE	2.16	0.76
1:A:717:VAL:O	1:A:717:VAL:CG1	2.30	0.75
1:G:704:LEU:HD13	1:G:767:ALA:HB2	1.67	0.75
1:G:825:MET:CE	1:G:853:ILE:HD13	2.16	0.75
1:G:932:ARG:HB3	1:G:932:ARG:NH1	2.00	0.75
1:D:793:MET:O	2:D:1101:816:C2	2.35	0.75
1:D:932:ARG:HG2	1:D:932:ARG:NH1	1.97	0.75
1:C:909:THR:CB	1:C:912:SER:HB2	2.14	0.75
1:A:758:GLU:OE2	1:A:758:GLU:C	2.30	0.75
1:A:815[B]:LEU:HD22	1:A:979:LEU:HD12	1.68	0.75
1:G:849:GLN:NE2	1:G:990:PRO:HG3	1.96	0.75
1:H:986:ARG:NH1	1:H:986:ARG:HB2	2.00	0.75
1:F:758:GLU:OE2	1:F:758:GLU:C	2.30	0.75
1:C:758:GLU:OE2	1:C:758:GLU:C	2.30	0.75
1:C:839:ALA:HB3	1:C:841:ARG:HG3	1.68	0.75
1:A:881:MET:CE	1:A:885:SER:HB2	2.17	0.75
1:A:946:ILE:HD11	1:A:971:MET:HE2	1.68	0.75
1:B:737:LYS:CD	1:B:738:VAL:HG13	2.16	0.75
1:G:825:MET:HG2	1:G:961:PHE:CE2	2.21	0.75
1:G:949:LYS:O	1:G:952:MET:HG2	1.87	0.75
1:G:1013:ALA:C	1:G:1014:ASP:OD1	2.30	0.75
1:E:748:ARG:HH11	1:E:748:ARG:HG3	1.52	0.75
1:A:949:LYS:O	1:A:952:MET:HG3	1.87	0.75
1:B:705:ARG:HD3	1:B:707:LEU:HD21	1.69	0.75
1:B:894:GLN:HE22	1:B:960:LYS:HE2	1.51	0.75
1:E:748:ARG:O	1:E:749:GLU:CB	2.33	0.75
1:H:879:LYS:HD2	1:H:915:TYR:HB2	1.68	0.75
1:B:717:VAL:CG2	1:B:727:TYR:CE2	2.69	0.74
1:E:833:LEU:HD13	1:E:856:PHE:CE1	2.22	0.74
1:G:743:ALA:CB	2:G:1101:816:NAB	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:923:ILE:HA	1:G:926:ILE:CG2	2.17	0.74
1:C:728:LYS:NZ	1:C:730:LEU:HD21	2.02	0.74
1:B:982:GLN:NE2	1:B:982:GLN:N	2.30	0.74
1:B:943:VAL:HG21	1:B:979:LEU:HD21	1.69	0.74
1:E:977:ARG:HG2	1:C:918:ILE:HD11	1.69	0.74
1:F:999:ARG:O	1:F:1003:ASP:C	2.30	0.74
1:G:1007:MET:CE	1:G:1008:ASP:O	2.30	0.74
1:H:758:GLU:O	1:H:758:GLU:CD	2.30	0.74
1:A:844:LEU:N	1:A:844:LEU:HD23	2.01	0.74
1:E:821:ILE:CG2	1:E:900:TYR:HE1	2.01	0.74
1:F:856:PHE:C	1:F:856:PHE:CD1	2.64	0.74
1:A:726:VAL:CG2	1:A:745:LYS:HG3	2.17	0.74
1:H:793:MET:H	2:H:1101:816:C2	2.00	0.74
1:C:1007:MET:HG2	1:C:1008:ASP:O	1.87	0.74
1:E:744:ILE:N	1:E:744:ILE:CD1	2.51	0.74
1:F:729:GLY:O	1:F:730:LEU:CD2	2.35	0.74
1:H:854:THR:CG2	1:H:855:ASP:N	2.49	0.74
1:H:781:CYS:HB3	1:H:787:GLN:HB2	1.68	0.74
1:A:881:MET:HE3	1:A:885:SER:HB3	1.69	0.74
1:C:704:LEU:HD12	1:C:764:TYR:CE1	2.22	0.74
1:C:985:GLU:H	1:C:985:GLU:CD	1.95	0.74
1:A:783:THR:HG22	1:A:784:SER:N	2.03	0.73
1:B:759:ILE:HD12	1:B:759:ILE:H	1.52	0.73
1:C:760:LEU:CD1	1:C:782:LEU:CD1	2.55	0.73
1:C:944:TYR:HA	1:C:947:MET:HE3	1.68	0.73
1:D:795:PHE:HB2	1:D:845:VAL:HG12	1.69	0.73
1:A:757:LYS:HD3	1:A:757:LYS:N	2.03	0.73
1:F:842:ASN:O	1:F:854:THR:CG2	2.32	0.73
1:H:893:HIS:O	1:H:896:ASP:HB2	1.89	0.73
1:B:982:GLN:HE21	1:B:982:GLN:N	1.86	0.73
1:G:743:ALA:HB3	2:G:1101:816:NAB	2.03	0.73
1:F:825:MET:CE	1:F:835:HIS:HB3	2.19	0.73
1:G:825:MET:CE	1:G:853:ILE:CD1	2.66	0.73
1:H:775:CYS:SG	1:H:790:MET:HE1	2.29	0.73
1:H:798:LEU:O	1:H:802:VAL:CG2	2.36	0.73
1:D:844:LEU:HD11	2:D:1101:816:CAL	2.19	0.73
1:E:806:LYS:HE2	4:E:1207:HOH:O	1.88	0.73
1:F:967:GLU:O	1:F:971:MET:HG3	1.88	0.73
1:F:972:ALA:HB3	1:F:1011:VAL:HG11	1.71	0.73
1:B:771:ASN:HD22	1:B:772:PRO:HD2	1.49	0.73
1:C:973:ARG:HG2	1:C:973:ARG:HH11	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:MET:HE2	1:A:844:LEU:HD12	1.68	0.73
1:D:878:ILE:HG23	1:D:886:ILE:HD11	1.69	0.73
1:F:717:VAL:HG22	1:F:727:TYR:CE2	2.23	0.73
1:F:823:LYS:HZ1	1:F:1008:ASP:CG	1.97	0.72
1:C:754:LYS:HG2	1:C:755:ALA:H	1.54	0.72
1:D:983:GLY:O	1:D:986:ARG:HG3	1.89	0.72
1:F:708:LYS:H	1:F:711:GLU:CD	1.96	0.72
1:A:945:MET:HE2	1:E:909:THR:HG22	1.70	0.72
1:D:900:TYR:CE2	1:D:904:VAL:HG21	2.23	0.72
1:F:1007:MET:HG2	1:F:1008:ASP:O	1.89	0.72
1:G:798:LEU:O	1:G:798:LEU:HD12	1.88	0.72
1:E:837:ASP:C	1:E:837:ASP:OD1	2.30	0.72
1:G:974:ASP:OD2	3:G:1102:EDO:C2	2.36	0.72
1:H:898:TRP:O	1:H:902:VAL:CG2	2.37	0.72
1:C:769:VAL:CG2	1:C:769:VAL:O	2.38	0.72
1:C:769:VAL:HG11	1:C:856:PHE:HE2	1.54	0.72
1:A:934:PRO:O	1:A:936:PRO:HD3	1.90	0.72
1:D:815:LEU:O	1:D:819:VAL:HG23	1.90	0.72
1:H:935:GLN:OE1	1:H:944:TYR:HD2	1.71	0.72
1:C:728:LYS:HZ3	1:C:730:LEU:HD21	1.54	0.72
1:A:704:LEU:HD12	1:A:779:GLY:HA2	1.71	0.72
1:C:744:ILE:HG23	1:C:789:ILE:HG13	1.71	0.72
1:B:748:ARG:CB	4:B:1219:HOH:O	2.37	0.72
1:B:854:THR:O	1:B:855:ASP:HB2	1.89	0.72
1:H:945:MET:HE1	3:H:1103:EDO:C2	2.19	0.72
1:A:837:ASP:HB2	4:A:1204:HOH:O	1.90	0.72
1:D:783:THR:HG22	1:D:784:SER:N	2.02	0.72
1:C:723:PHE:O	1:C:748:ARG:CG	2.37	0.72
1:C:778:LEU:H	1:C:778:LEU:CD2	1.84	0.72
1:D:940:THR:CG2	1:D:978:TYR:O	2.38	0.71
1:D:820:GLN:OE1	1:D:851:VAL:HG22	1.89	0.71
1:F:881:MET:CE	1:F:886:ILE:HG12	2.20	0.71
1:F:825:MET:SD	1:F:838:LEU:HD22	2.31	0.71
1:H:935:GLN:HB2	1:H:944:TYR:CG	2.25	0.71
1:E:881:MET:HE2	1:E:886:ILE:HG13	1.70	0.71
1:F:832:ARG:HG2	1:F:832:ARG:O	1.90	0.71
1:G:995:SER:C	1:G:999[B]:ARG:HD2	2.13	0.71
1:C:790:MET:CE	2:C:1101:816:NAB	2.42	0.71
1:B:733:PRO:HB2	1:B:736:GLU:HB2	1.72	0.71
1:E:818:CYS:SG	1:E:904:VAL:HG22	2.30	0.71
1:F:823:LYS:HG2	1:F:965:ILE:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:995:SER:O	1:G:999[B]:ARG:CD	2.31	0.71
1:H:799:LEU:O	1:H:803:ARG:CG	2.34	0.71
1:H:812:GLN:HE22	1:H:1013:ALA:CB	1.95	0.71
1:A:726:VAL:HG22	1:A:745:LYS:HG3	1.71	0.71
1:G:955:ALA:O	1:G:958:ARG:HG3	1.90	0.71
1:F:708:LYS:H	1:F:711:GLU:CG	2.02	0.71
1:G:945:MET:O	1:G:949:LYS:HG3	1.91	0.71
1:G:1006:ASP:HB3	4:G:1220:HOH:O	1.89	0.71
1:H:817:TRP:CD1	1:H:851:VAL:CG1	2.74	0.71
1:H:949:LYS:O	1:H:952:MET:HG3	1.90	0.71
1:C:913:LYS:H	1:C:913:LYS:HD2	1.53	0.71
1:G:1007:MET:HG2	1:G:1008:ASP:N	2.04	0.71
1:H:854:THR:HG22	1:H:855:ASP:H	1.56	0.71
1:B:835:HIS:HB2	1:B:856:PHE:HB2	1.70	0.71
1:F:730:LEU:N	1:F:730:LEU:CD2	2.54	0.71
1:A:967[B]:GLU:OE2	1:A:970:LYS:HD2	1.89	0.70
1:B:707:LEU:HD22	1:B:711:GLU:OE2	1.90	0.70
1:E:821:ILE:HG22	1:E:900:TYR:CE1	2.25	0.70
1:C:780:ILE:HD13	1:C:787:GLN:O	1.90	0.70
1:B:726:VAL:HG23	1:B:745:LYS:HE2	1.73	0.70
1:H:758:GLU:CD	1:H:758:GLU:C	2.59	0.70
1:A:729:GLY:HA3	1:A:744:ILE:CD1	2.21	0.70
1:A:738:VAL:HG23	4:A:1232:HOH:O	1.91	0.70
1:B:881:MET:CE	1:B:891:TYR:OH	2.39	0.70
1:E:884:GLU:HG2	1:E:885:SER:N	2.06	0.70
1:C:961:PHE:C	1:C:965:ILE:HD12	2.13	0.70
1:A:790:MET:HE1	1:A:844:LEU:HD12	1.72	0.70
1:G:989:LEU:HD23	1:G:990:PRO:HD3	1.68	0.70
1:A:977:ARG:HD2	1:A:977:ARG:O	1.92	0.70
1:C:714:LYS:HE3	1:C:787:GLN:HE22	1.56	0.70
1:E:726:VAL:CG2	1:E:745:LYS:HD2	2.22	0.70
1:E:845:VAL:CG1	1:E:847:THR:C	2.64	0.70
1:G:825:MET:HG2	1:G:961:PHE:CZ	2.26	0.70
1:C:975:PRO:HD2	1:C:1013:ALA:HB2	1.73	0.70
1:A:881:MET:CE	1:A:885:SER:CB	2.69	0.70
1:E:833:LEU:HD13	1:E:856:PHE:CZ	2.26	0.70
1:F:823:LYS:HZ2	1:F:1008:ASP:CG	1.98	0.70
1:A:757:LYS:HD3	1:A:757:LYS:H	1.56	0.70
1:B:988:HIS:CB	1:B:989:LEU:O	2.39	0.70
1:D:811:SER:HB2	1:D:981:ILE:HG13	1.72	0.70
1:E:704:LEU:HB2	1:E:767:ALA:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:756:ASN:CG	1:F:782:LEU:HD13	2.17	0.70
1:B:898:TRP:CZ2	1:B:927:LEU:HD13	2.26	0.70
1:D:704:LEU:HB2	1:D:767:ALA:HB2	1.73	0.70
1:A:898:TRP:CZ2	1:A:927:LEU:HD13	2.27	0.69
1:C:715:ILE:HG12	1:C:728:LYS:O	1.91	0.69
1:A:777:LEU:HD12	1:A:789:ILE:O	1.92	0.69
1:G:935:GLN:HB2	1:G:944:TYR:CD1	2.27	0.69
1:H:962:ARG:CA	1:H:965:ILE:HG13	2.22	0.69
1:F:799:LEU:O	1:F:803:ARG:HG3	1.92	0.69
1:H:879:LYS:HD3	1:H:923:ILE:HD11	1.75	0.69
1:C:973:ARG:HH11	1:C:973:ARG:CG	2.03	0.69
1:E:821:ILE:HG22	1:E:900:TYR:HE1	1.57	0.69
1:E:856:PHE:CD1	1:E:856:PHE:O	2.45	0.69
1:F:961:PHE:O	1:F:965:ILE:HG13	1.92	0.69
2:F:1101:816:CAP	2:F:1101:816:CAV	2.70	0.69
1:G:935:GLN:HB2	1:G:944:TYR:CG	2.27	0.69
1:B:940:THR:HG23	1:B:943:VAL:H	1.56	0.69
1:D:806:LYS:HG2	1:D:807:ASP:N	2.06	0.69
1:A:938:ILE:HD12	1:A:981:ILE:HG12	1.75	0.69
1:A:946:ILE:HD12	1:A:971:MET:CE	2.16	0.69
1:B:707:LEU:HD12	1:B:789:ILE:HD13	1.73	0.69
1:B:726:VAL:CG2	1:B:745:LYS:HE2	2.22	0.69
1:B:816:ASN:CA	1:B:819:VAL:HG23	2.23	0.69
1:D:805:HIS:CD2	4:D:1202:HOH:O	2.45	0.69
1:E:821:ILE:CG2	1:E:900:TYR:CE1	2.76	0.69
1:F:805:HIS:O	1:F:809:ILE:HG13	1.93	0.69
1:F:848:PRO:CB	1:F:849:GLN:OE1	2.40	0.69
1:A:877:PRO:O	1:A:881:MET:HG3	1.93	0.69
1:E:798:LEU:HD23	1:E:907:LEU:HD21	1.75	0.69
1:F:723:PHE:O	1:F:748:ARG:CG	2.40	0.69
1:F:853:ILE:HD13	1:F:853:ILE:H	1.56	0.69
1:F:989:LEU:CD2	1:F:989:LEU:O	2.38	0.69
1:G:898:TRP:O	1:G:902:VAL:HG23	1.92	0.69
1:C:704:LEU:O	1:C:704:LEU:HD13	1.92	0.69
1:C:790:MET:HE3	1:C:791:GLN:O	1.93	0.69
1:C:981:ILE:HG21	1:C:987:MET:HE3	1.75	0.69
1:H:757:LYS:HD2	1:H:757:LYS:O	1.93	0.69
1:A:856:PHE:CD1	1:A:856:PHE:C	2.71	0.68
1:D:730:LEU:HD22	1:D:739:LYS:CB	2.13	0.68
1:H:800:ASP:O	1:H:804:GLU:CG	2.42	0.68
1:H:878:ILE:HD13	1:H:920:ALA:HB1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:VAL:HG22	1:C:968:PHE:HB3	1.75	0.68
1:B:818:CYS:SG	1:B:904:VAL:CG2	2.80	0.68
1:E:856:PHE:O	1:E:856:PHE:CG	2.46	0.68
1:G:893:HIS:O	1:G:896:ASP:HB2	1.93	0.68
1:H:943:VAL:O	1:H:946:ILE:HG22	1.93	0.68
1:C:813:TYR:OH	1:C:990:PRO:HD3	1.93	0.68
1:F:708:LYS:O	1:F:711:GLU:CG	2.41	0.68
1:F:898:TRP:HE3	1:F:958:ARG:NH2	1.92	0.68
2:A:1101:816:CAP	2:A:1101:816:CAV	2.71	0.68
1:D:938:ILE:HD11	1:D:979:LEU:HD22	1.75	0.68
1:E:759:ILE:HD13	1:E:780:ILE:HD12	1.76	0.68
1:E:835:HIS:O	1:E:836:ARG:HB2	1.91	0.68
1:E:879:LYS:HE2	1:E:923:ILE:HD11	1.75	0.68
1:F:977:ARG:C	1:F:977:ARG:CD	2.53	0.68
1:F:999:ARG:HA	1:F:1003:ASP:CB	2.24	0.68
1:H:762:GLU:HB3	1:H:861:LEU:CD2	2.24	0.68
1:A:705:ARG:CD	1:A:707:LEU:HD21	2.23	0.68
1:E:879:LYS:CE	1:E:923:ILE:HD11	2.23	0.68
1:G:923:ILE:O	1:G:927:LEU:HG	1.93	0.68
1:F:724:GLY:HA2	1:F:748:ARG:HD2	1.76	0.68
1:B:835:HIS:HB2	1:B:856:PHE:CB	2.23	0.68
1:E:762:GLU:O	1:E:765:VAL:CG2	2.41	0.68
1:F:773:HIS:CE1	1:F:820:GLN:HG2	2.29	0.68
1:F:825:MET:HE1	1:F:835:HIS:CG	2.29	0.68
1:A:815[B]:LEU:HD22	1:A:979:LEU:CD1	2.22	0.67
1:D:765:VAL:HG12	1:D:766:MET:N	2.09	0.67
1:D:919:PRO:HB2	1:D:922:GLU:HG3	1.76	0.67
1:E:790:MET:HG2	2:E:1101:816:CLA	2.30	0.67
1:H:938:ILE:HG13	1:H:939:CYS:N	2.04	0.67
1:D:832:ARG:CG	4:G:1202:HOH:O	2.42	0.67
1:F:990:PRO:CG	4:F:1215:HOH:O	2.32	0.67
1:A:705:ARG:HE	1:A:707:LEU:HD23	1.58	0.67
1:D:894:GLN:O	1:D:897:VAL:HG23	1.94	0.67
1:A:748:ARG:O	1:A:749:GLU:CB	2.41	0.67
1:B:972:ALA:HB1	1:B:1011:VAL:HG11	1.76	0.67
1:G:815:LEU:O	1:G:819:VAL:HG23	1.95	0.67
1:G:803:ARG:HG2	1:G:911:GLY:HA3	1.76	0.67
1:G:806:LYS:HD3	1:G:807:ASP:CA	2.25	0.67
1:C:770:ASP:C	1:C:770:ASP:OD1	2.38	0.67
1:A:854:THR:O	1:A:855:ASP:HB2	1.94	0.67
1:A:945:MET:CE	1:E:909:THR:HG22	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:MET:HE1	1:B:891:TYR:OH	1.95	0.67
1:E:706:ILE:O	1:E:706:ILE:CG2	2.43	0.67
1:F:708:LYS:O	1:F:711:GLU:HG3	1.93	0.67
1:G:766:MET:HE2	1:G:777:LEU:HD22	1.77	0.67
1:A:777:LEU:HD21	1:A:788:LEU:CD2	2.17	0.67
1:F:721:GLY:HA3	1:F:724:GLY:O	1.95	0.67
1:F:707:LEU:HB2	1:F:711:GLU:CG	2.25	0.67
1:F:817:TRP:O	1:F:821:ILE:HG13	1.95	0.67
1:A:817:TRP:O	1:A:821:ILE:HG13	1.95	0.67
1:B:708:LYS:O	1:B:711:GLU:HG3	1.95	0.67
1:F:856:PHE:CD1	1:F:856:PHE:O	2.48	0.67
1:E:783:THR:HG22	1:E:784:SER:N	2.08	0.66
1:F:825:MET:CE	1:F:835:HIS:CB	2.72	0.66
1:D:878:ILE:HG23	1:D:886:ILE:CD1	2.24	0.66
1:E:844:LEU:HD23	1:E:854:THR:HG21	1.76	0.66
1:C:717:VAL:HG23	1:C:727:TYR:CD2	2.30	0.66
1:B:756:ASN:HA	1:B:759:ILE:HD13	1.77	0.66
1:D:837:ASP:CG	1:D:837:ASP:O	2.38	0.66
1:D:950:CYS:O	1:D:958:ARG:CD	2.43	0.66
1:F:701:GLN:CA	1:F:701:GLN:OE1	2.44	0.66
1:F:797:CYS:HB3	1:F:800:ASP:HB2	1.76	0.66
1:G:845:VAL:CG1	1:G:847:THR:C	2.68	0.66
1:E:938:ILE:HD11	1:E:979:LEU:HD13	1.77	0.66
1:E:950:CYS:O	1:E:958:ARG:CD	2.43	0.66
1:F:825:MET:HE1	1:F:835:HIS:HB3	1.77	0.66
1:B:798:LEU:O	1:B:802:VAL:HG22	1.96	0.66
1:D:790:MET:CE	2:D:1101:816:CBD	2.72	0.66
1:D:854:THR:O	1:D:855:ASP:HB2	1.95	0.66
1:E:881:MET:HE2	1:E:886:ILE:CG1	2.25	0.66
1:A:790:MET:HE2	2:A:1101:816:NAB	2.11	0.66
1:B:997:PHE:O	1:B:997:PHE:CD1	2.46	0.66
1:D:790:MET:HE1	2:D:1101:816:NAY	2.11	0.66
1:D:940:THR:CG2	1:D:943:VAL:HG23	2.24	0.66
1:A:945:MET:CE	1:E:909:THR:CG2	2.73	0.66
1:B:737:LYS:HD3	1:B:738:VAL:HG12	1.78	0.66
1:G:817:TRP:CD1	1:G:851:VAL:CG1	2.79	0.66
1:H:987:MET:CE	4:H:1214:HOH:O	2.42	0.66
1:A:940:THR:HB	1:A:978:TYR:O	1.94	0.66
1:B:910:PHE:CE2	1:B:938:ILE:HD11	2.31	0.66
1:F:990:PRO:HD3	4:F:1215:HOH:O	1.95	0.66
1:G:823:LYS:HA	1:G:965:ILE:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:CYS:CB	1:A:800:ASP:OD2	2.44	0.66
1:G:825:MET:HE2	1:G:853:ILE:CD1	2.26	0.66
1:G:881:MET:CE	1:G:885:SER:HB3	2.25	0.66
1:E:793:MET:HG3	1:E:844:LEU:HD12	1.76	0.65
1:C:926:ILE:HB	1:C:931:GLU:HG3	1.76	0.65
1:B:802:VAL:HG11	1:B:907:LEU:HD22	1.78	0.65
1:A:711:GLU:O	1:A:732:ILE:HG22	1.96	0.65
1:B:831:ARG:HH11	1:B:831:ARG:CG	2.00	0.65
1:B:808:ASN:N	1:B:808:ASN:OD1	2.30	0.65
1:C:835:HIS:O	1:C:836:ARG:HB2	1.96	0.65
1:F:707:LEU:H	1:F:707:LEU:CD1	2.01	0.65
1:G:1014:ASP:OD1	1:G:1014:ASP:N	2.30	0.65
1:C:801:TYR:CE2	1:C:817:TRP:CH2	2.84	0.65
1:A:982:GLN:OE1	1:A:982:GLN:N	2.30	0.65
1:B:811:SER:OG	1:B:975:PRO:HB2	1.96	0.65
1:H:835:HIS:O	1:H:836:ARG:HB2	1.95	0.65
1:C:817:TRP:CD1	1:C:851:VAL:CG1	2.80	0.65
1:C:704:LEU:HD13	1:C:704:LEU:C	2.22	0.65
1:C:835:HIS:NE2	1:C:856:PHE:CA	2.57	0.65
1:E:835:HIS:ND1	1:E:837:ASP:O	2.30	0.65
1:F:849:GLN:OE1	1:F:849:GLN:N	2.30	0.65
1:F:878:ILE:HD13	1:F:881:MET:CE	2.27	0.65
1:G:704:LEU:HD12	1:G:767:ALA:HB2	1.79	0.65
1:G:835:HIS:ND1	1:G:837:ASP:O	2.30	0.65
1:F:701:GLN:OE1	1:F:701:GLN:N	2.30	0.65
1:H:935:GLN:CB	1:H:944:TYR:CD2	2.79	0.65
1:G:703:LEU:N	1:G:703:LEU:CD2	2.59	0.65
1:G:889:ARG:CG	1:G:889:ARG:NH1	2.58	0.65
1:A:922:GLU:OE2	1:A:926:ILE:CG2	2.46	0.64
1:A:949:LYS:O	1:A:952:MET:CG	2.45	0.64
1:B:783:THR:CG2	1:B:784:SER:N	2.61	0.64
1:B:940:THR:CB	1:B:978:TYR:O	2.43	0.64
1:F:900:TYR:O	1:F:904:VAL:HG23	1.97	0.64
1:G:878:ILE:HG23	1:G:886:ILE:CD1	2.28	0.64
1:H:757:LYS:CD	1:H:757:LYS:O	2.44	0.64
1:C:716:LYS:HG3	1:C:717:VAL:N	2.11	0.64
1:C:801:TYR:CE2	1:C:817:TRP:HH2	2.13	0.64
1:A:835:HIS:O	1:A:836:ARG:HB2	1.96	0.64
1:E:991:SER:OG	1:E:992:PRO:HD2	1.97	0.64
1:H:808:ASN:N	1:H:808:ASN:OD1	2.30	0.64
1:H:825:MET:HE2	1:H:961:PHE:HZ	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:ILE:HD11	1:C:814:LEU:HG	1.79	0.64
1:G:923:ILE:HA	1:G:926:ILE:HG23	1.79	0.64
1:H:777:LEU:HB2	2:H:1101:816:CAA	2.27	0.64
1:C:762:GLU:O	1:C:766:MET:HG3	1.97	0.64
1:F:945:MET:C	1:F:948:VAL:HG23	2.22	0.64
1:B:771:ASN:HB3	1:B:774:VAL:HG23	1.78	0.64
1:G:808:ASN:OD1	1:G:808:ASN:N	2.30	0.64
1:G:879:LYS:HG2	1:G:915:TYR:HB2	1.79	0.64
1:G:923:ILE:O	1:G:926:ILE:HG23	1.97	0.64
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.31	0.64
1:C:894:GLN:HG3	1:C:955:ALA:C	2.21	0.64
1:F:745:LYS:NZ	4:F:1201:HOH:O	2.30	0.64
1:H:904:VAL:HG12	1:H:947:MET:HE2	1.78	0.64
1:B:831:ARG:O	1:B:832:ARG:HB2	1.96	0.64
1:E:880:TRP:NE1	1:E:906:GLU:OE1	2.31	0.64
1:F:905:TRP:O	1:F:909:THR:HG23	1.98	0.64
1:G:960:LYS:CD	4:G:1203:HOH:O	2.44	0.64
1:C:952:MET:O	1:C:958:ARG:NH1	2.30	0.64
1:A:717:VAL:HG23	1:A:727:TYR:CD2	2.33	0.64
1:F:808:ASN:OD1	1:F:808:ASN:N	2.30	0.64
1:F:898:TRP:CE3	1:F:958:ARG:NH2	2.64	0.64
1:G:985:GLU:HG2	1:G:986:ARG:N	2.12	0.64
1:F:729:GLY:O	1:F:730:LEU:HD22	1.98	0.64
1:F:758:GLU:OE2	1:F:759:ILE:N	2.30	0.64
1:B:910:PHE:HE2	1:B:938:ILE:HD11	1.62	0.64
1:B:988:HIS:CA	1:B:989:LEU:CB	2.75	0.64
1:G:740:ILE:HG22	1:G:741:PRO:HD2	1.79	0.64
1:G:1008:ASP:N	1:G:1008:ASP:OD1	2.31	0.64
1:B:704:LEU:HB2	1:B:767:ALA:CB	2.29	0.63
1:B:771:ASN:HD22	1:B:772:PRO:CD	2.06	0.63
1:E:793:MET:HE1	1:E:846:LYS:HB2	1.80	0.63
1:G:944:TYR:O	1:G:947:MET:HB2	1.98	0.63
1:H:925:SER:OG	1:H:929:LYS:NZ	2.30	0.63
1:C:827:TYR:CZ	1:C:831:ARG:CD	2.81	0.63
1:G:737:LYS:CG	1:G:737:LYS:O	2.46	0.63
1:H:790:MET:HG2	2:H:1101:816:NAB	2.13	0.63
1:B:941:ILE:C	1:B:941:ILE:CD1	2.66	0.63
1:D:707:LEU:CD2	1:D:711:GLU:CB	2.76	0.63
1:H:825:MET:HB3	1:H:961:PHE:CZ	2.33	0.63
1:C:717:VAL:O	1:C:717:VAL:CG1	2.43	0.63
1:C:758:GLU:OE2	1:C:759:ILE:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:LEU:O	1:C:819:VAL:HG23	1.99	0.63
1:A:806:LYS:NZ	4:A:1201:HOH:O	2.30	0.63
1:D:718:LEU:HD13	1:D:728:LYS:HB2	1.80	0.63
1:D:835:HIS:O	1:D:836:ARG:HB2	1.98	0.63
1:E:759:ILE:HD13	1:E:780:ILE:CD1	2.29	0.63
1:E:812:GLN:O	1:E:816:ASN:ND2	2.30	0.63
1:H:703:LEU:HD13	1:H:768:SER:HA	1.79	0.63
1:A:808:ASN:OD1	1:A:808:ASN:N	2.30	0.63
1:D:949:LYS:O	1:D:952:MET:HG3	1.99	0.63
1:F:721:GLY:N	1:F:724:GLY:O	2.32	0.63
1:G:835:HIS:NE2	1:G:856:PHE:HB3	2.13	0.63
1:D:745:LYS:NZ	1:D:855:ASP:OD1	2.31	0.63
1:D:941:ILE:HD11	1:D:945:MET:CE	2.25	0.63
1:E:844:LEU:HD21	1:E:854:THR:HG21	1.80	0.63
1:F:736:GLU:HA	1:F:736:GLU:OE2	1.98	0.63
1:G:775:CYS:HB2	1:G:854:THR:OG1	1.98	0.63
1:A:799:LEU:O	1:A:802:VAL:HG23	1.98	0.63
1:A:815[A]:LEU:HG	1:A:979:LEU:HD11	1.79	0.63
1:A:972:ALA:O	1:A:975:PRO:HD3	1.98	0.63
1:G:825:MET:SD	1:G:838:LEU:HD22	2.39	0.63
1:H:837:ASP:O	1:H:842:ASN:ND2	2.30	0.63
1:H:854:THR:CG2	1:H:855:ASP:H	2.08	0.63
1:C:728:LYS:HG3	1:C:792:LEU:HD11	1.81	0.63
1:C:894:GLN:CB	1:C:955:ALA:HB1	2.29	0.63
1:A:762:GLU:OE1	1:A:861:LEU:CD2	2.47	0.63
1:A:813:TYR:OH	1:A:990:PRO:HD3	1.99	0.63
1:C:723:PHE:O	1:C:748:ARG:HG2	1.99	0.63
1:B:999:ARG:HH11	1:B:999:ARG:CG	2.12	0.62
1:D:846:LYS:O	1:D:847:THR:HG22	1.98	0.62
1:C:961:PHE:HA	1:C:964:LEU:HD12	1.81	0.62
1:B:945:MET:HE1	1:D:909:THR:HG22	1.80	0.62
1:E:904:VAL:CG1	1:E:947:MET:HE2	2.28	0.62
1:F:858:LEU:HD13	2:F:1101:816:CAK	2.28	0.62
1:H:961:PHE:O	1:H:965:ILE:HG12	1.99	0.62
1:C:799:LEU:O	1:C:802:VAL:HG22	1.99	0.62
1:D:774:VAL:HG21	1:D:827:TYR:CD2	2.34	0.62
1:F:945:MET:O	1:F:948:VAL:HG23	1.99	0.62
1:G:773:HIS:HE1	1:G:820:GLN:HG2	1.64	0.62
1:G:835:HIS:CE1	1:G:837:ASP:O	2.52	0.62
1:H:757:LYS:NZ	1:H:761:ASP:OD2	2.30	0.62
1:A:977:ARG:NE	1:E:926:ILE:HD12	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:LEU:O	1:B:819:VAL:HG23	1.99	0.62
1:F:780:ILE:HD13	1:F:787:GLN:O	2.00	0.62
1:H:845:VAL:HG13	1:H:847:THR:C	2.23	0.62
1:C:1007:MET:CG	1:C:1008:ASP:O	2.47	0.62
1:F:781:CYS:SG	1:F:783:THR:CG2	2.87	0.62
1:G:767:ALA:O	1:G:776:ARG:NH1	2.30	0.62
1:B:843:VAL:HG12	1:B:843:VAL:O	1.98	0.62
1:D:991:SER:OG	1:D:992:PRO:HD2	2.00	0.62
1:C:769:VAL:O	1:C:769:VAL:HG23	2.00	0.62
1:C:797:CYS:SG	1:C:800:ASP:OD2	2.58	0.62
1:C:849:GLN:OE1	1:C:849:GLN:N	2.30	0.62
1:E:949:LYS:O	1:E:958:ARG:HG3	1.98	0.62
1:H:985:GLU:HG2	1:H:986:ARG:N	2.12	0.62
1:B:717:VAL:HG22	1:B:727:TYR:CD2	2.35	0.62
1:A:799:LEU:O	1:A:799:LEU:HD12	1.99	0.62
1:E:748:ARG:HG3	1:E:748:ARG:NH1	2.14	0.62
1:G:877:PRO:O	1:G:881:MET:HG3	1.99	0.62
1:H:924:SER:O	1:H:928:GLU:HG3	2.00	0.62
1:C:717:VAL:CG2	1:C:727:TYR:CD2	2.83	0.62
1:C:918:ILE:HG22	1:C:918:ILE:O	1.99	0.62
1:A:769:VAL:HG12	1:A:827:TYR:HE2	1.64	0.62
1:D:739:LYS:C	1:D:740:ILE:HD13	2.24	0.62
1:F:832:ARG:HG2	4:F:1211:HOH:O	2.00	0.62
1:G:883:LEU:HD22	1:G:953:ILE:CD1	2.29	0.62
1:B:837:ASP:OD2	1:B:841:ARG:NH1	2.33	0.61
1:B:940:THR:CG2	1:B:943:VAL:H	2.13	0.61
1:E:836:ARG:HD2	1:E:860:LYS:CA	2.29	0.61
1:E:941:ILE:HG13	1:E:945:MET:HE2	1.81	0.61
1:F:733:PRO:HB2	1:F:736:GLU:HB2	1.81	0.61
1:E:840:ALA:CB	1:E:906:GLU:OE2	2.45	0.61
1:F:700:ASN:CB	1:F:703:LEU:HD12	2.28	0.61
1:G:705:ARG:NH2	1:G:711:GLU:OE1	2.31	0.61
1:G:772:PRO:O	1:G:852:LYS:HD2	1.99	0.61
1:G:805:HIS:O	1:G:809:ILE:HG13	2.00	0.61
1:C:1007:MET:CE	1:C:1008:ASP:O	2.48	0.61
1:A:983:GLY:O	1:A:987:MET:HG2	2.00	0.61
1:B:950:CYS:O	1:B:958:ARG:NE	2.33	0.61
1:D:967:GLU:O	1:D:971:MET:HG3	2.00	0.61
1:E:886:ILE:HG21	1:E:924:SER:HB2	1.82	0.61
1:F:925:SER:O	1:F:929:LYS:N	2.30	0.61
1:F:947:MET:HB3	1:F:951:TRP:CH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:757:LYS:C	1:G:757:LYS:CD	2.72	0.61
1:C:880:TRP:NE1	1:C:906:GLU:OE2	2.32	0.61
1:D:795:PHE:CB	1:D:845:VAL:HG12	2.30	0.61
1:D:799:LEU:O	1:D:802:VAL:HG23	2.00	0.61
1:G:766:MET:O	1:G:769:VAL:HG13	2.00	0.61
1:C:980:VAL:CG2	1:C:980:VAL:O	2.49	0.61
1:A:705:ARG:HD3	1:A:707:LEU:HD21	1.83	0.61
1:B:799:LEU:O	1:B:803:ARG:HG3	2.00	0.61
1:E:983:GLY:O	1:E:986:ARG:HD3	2.01	0.61
1:G:999[B]:ARG:HB3	1:G:1003:ASP:O	2.00	0.61
1:A:922:GLU:O	1:A:926:ILE:HG23	2.00	0.61
1:A:952:MET:O	1:A:958:ARG:NH2	2.30	0.61
1:F:707:LEU:HB2	1:F:711:GLU:HG3	1.83	0.61
2:F:1101:816:NAB	2:F:1101:816:CAN	2.63	0.61
1:G:940:THR:HB	1:G:978:TYR:O	2.00	0.61
1:G:969:SER:O	1:G:972:ALA:HB3	2.00	0.61
1:A:926:ILE:HG13	1:A:927:LEU:N	2.15	0.61
1:D:842:ASN:O	1:D:854:THR:HG22	2.00	0.61
1:G:700:ASN:C	1:G:700:ASN:OD1	2.42	0.61
1:G:835:HIS:CD2	1:G:856:PHE:HB3	2.36	0.61
1:H:771:ASN:OD1	1:H:773:HIS:N	2.30	0.61
1:C:942:ASP:OD1	1:C:977:ARG:NH2	2.34	0.61
1:B:766:MET:HE1	1:B:858:LEU:HD12	1.83	0.61
1:G:790:MET:HE2	2:G:1101:816:NAB	2.14	0.61
1:H:743:ALA:HB3	2:H:1101:816:NAB	2.16	0.61
1:H:962:ARG:O	1:H:965:ILE:HG13	2.00	0.61
1:A:800:ASP:HB3	4:A:1218:HOH:O	2.01	0.61
1:E:797:CYS:HB2	1:E:800:ASP:H	1.65	0.61
1:G:799:LEU:O	1:G:803:ARG:HG3	2.00	0.61
1:H:777:LEU:C	1:H:778:LEU:HD23	2.24	0.61
1:C:898:TRP:HE3	1:C:958:ARG:NH1	1.98	0.61
1:C:953:ILE:N	1:C:953:ILE:CD1	2.62	0.61
1:D:703:LEU:HD12	1:D:768:SER:HA	1.82	0.60
1:E:769:VAL:HG12	1:E:827:TYR:HE2	1.66	0.60
1:E:783:THR:CG2	1:E:784:SER:N	2.64	0.60
1:B:790:MET:HE3	1:B:791:GLN:O	2.01	0.60
1:D:739:LYS:O	1:D:740:ILE:HD13	2.02	0.60
1:E:898:TRP:CE3	1:E:958:ARG:NH1	2.66	0.60
1:H:835:HIS:HE1	1:H:837:ASP:O	1.81	0.60
1:H:1008:ASP:OD2	1:H:1008:ASP:N	2.30	0.60
1:C:701:GLN:OE1	1:C:701:GLN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:TRP:CZ2	1:C:927:LEU:HD13	2.36	0.60
1:F:805:HIS:HB3	1:F:809:ILE:HG12	1.83	0.60
1:A:876:VAL:HG23	1:A:878:ILE:HG13	1.84	0.60
1:A:881:MET:HE2	1:A:885:SER:HB2	1.83	0.60
1:E:793:MET:HE2	1:E:844:LEU:HD12	1.83	0.60
1:G:743:ALA:CB	2:G:1101:816:C6	2.79	0.60
1:C:854:THR:O	1:C:855:ASP:HB2	2.00	0.60
1:C:905:TRP:CD2	1:C:909:THR:HG21	2.36	0.60
1:H:776:ARG:CG	1:H:776:ARG:HH11	2.13	0.60
1:A:774:VAL:HG23	1:A:824:GLY:CA	2.32	0.60
1:B:877:PRO:O	1:B:881:MET:HG3	2.02	0.60
1:F:856:PHE:O	1:F:856:PHE:CG	2.54	0.60
1:H:797:CYS:SG	2:H:1101:816:OAE	2.60	0.60
1:C:935:GLN:HB2	1:C:944:TYR:CG	2.37	0.60
1:C:940:THR:HG23	1:C:943:VAL:H	1.66	0.60
1:F:966:ILE:HG23	1:F:970:LYS:HE3	1.84	0.60
1:G:775:CYS:CB	1:G:854:THR:OG1	2.50	0.60
1:H:881:MET:CE	1:H:891:TYR:OH	2.50	0.60
1:A:708:LYS:O	1:A:711:GLU:HG3	2.01	0.60
1:B:737:LYS:H	1:B:737:LYS:HD2	1.67	0.60
1:E:719:GLY:HA3	2:E:1101:816:CAO	2.32	0.60
1:G:962:ARG:NH2	4:G:1201:HOH:O	2.34	0.60
1:A:774:VAL:HG23	1:A:824:GLY:HA2	1.83	0.60
1:A:881:MET:HE3	1:A:885:SER:HB2	1.80	0.60
1:A:999:ARG:O	1:A:1003:ASP:C	2.44	0.60
1:D:780:ILE:HG12	1:D:781:CYS:N	2.17	0.60
1:G:737:LYS:O	1:G:737:LYS:HG2	2.01	0.60
1:G:769:VAL:O	1:G:769:VAL:CG2	2.47	0.60
1:C:973:ARG:O	1:C:1013:ALA:HA	2.01	0.60
1:A:798:LEU:O	1:A:802:VAL:HG22	2.01	0.60
1:C:879:LYS:NZ	1:C:915:TYR:O	2.34	0.60
1:B:881:MET:HE2	1:B:891:TYR:CE1	2.36	0.59
1:E:783:THR:O	1:E:784:SER:C	2.44	0.59
1:F:770:ASP:C	1:F:770:ASP:OD1	2.44	0.59
1:H:797:CYS:HB3	1:H:841:ARG:O	2.02	0.59
1:H:825:MET:HG2	1:H:853:ILE:CD1	2.31	0.59
1:C:926:ILE:O	1:C:930:GLY:N	2.36	0.59
1:C:941:ILE:C	1:C:941:ILE:CD1	2.69	0.59
1:A:966:ILE:HD11	1:C:804:GLU:OE2	2.01	0.59
1:G:999[A]:ARG:NH1	1:G:1005:GLU:O	2.35	0.59
1:H:987:MET:HE3	4:H:1214:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1009:ASP:N	1:H:1009:ASP:OD1	2.35	0.59
1:D:811:SER:CB	1:D:981:ILE:HG13	2.31	0.59
1:G:811:SER:CB	1:G:984:ASP:OD1	2.38	0.59
1:F:858:LEU:CD1	2:F:1101:816:CAK	2.79	0.59
1:C:800:ASP:O	1:C:804:GLU:HG3	2.02	0.59
1:C:972:ALA:O	1:C:975:PRO:CD	2.48	0.59
1:A:935:GLN:HG3	1:A:944:TYR:CD2	2.37	0.59
1:B:893:HIS:O	1:B:897:VAL:HG23	2.02	0.59
1:F:884:GLU:HG2	1:F:885:SER:N	2.16	0.59
1:C:985:GLU:OE1	1:C:985:GLU:N	2.30	0.59
1:D:908:MET:SD	1:D:979:LEU:HD21	2.42	0.59
1:C:748:ARG:O	1:C:749:GLU:CB	2.51	0.59
1:A:704:LEU:HB2	1:A:767:ALA:CB	2.33	0.59
1:B:791:GLN:HG3	4:B:1211:HOH:O	2.02	0.59
1:F:881:MET:HE3	1:F:886:ILE:HG12	1.84	0.59
1:H:776:ARG:O	1:H:778:LEU:CD2	2.50	0.59
1:D:820:GLN:NE2	1:D:849:GLN:O	2.30	0.59
1:F:826:ASN:ND2	4:F:1202:HOH:O	2.36	0.59
1:G:700:ASN:OD1	1:G:701:GLN:N	2.36	0.59
1:H:899:SER:CA	1:H:902:VAL:CG2	2.67	0.59
1:A:778:LEU:HD11	1:A:791:GLN:HG2	1.85	0.59
1:B:972:ALA:HB1	1:B:1011:VAL:CG1	2.32	0.59
1:D:815:LEU:CD2	1:D:979:LEU:HD12	2.30	0.59
1:D:846:LYS:C	1:D:847:THR:CG2	2.75	0.59
1:E:771:ASN:HB3	1:E:774:VAL:CG2	2.29	0.59
1:F:876:VAL:CB	1:F:877:PRO:CD	2.74	0.59
1:G:769:VAL:HG11	1:G:856:PHE:CZ	2.33	0.59
1:H:877:PRO:O	1:H:881:MET:HG3	2.02	0.59
1:A:900:TYR:CE2	1:A:964:LEU:HD13	2.38	0.59
1:B:719:GLY:HA3	2:B:1101:816:CAO	2.33	0.59
1:F:707:LEU:N	1:F:707:LEU:CD1	2.56	0.59
1:F:817:TRP:CD1	1:F:851:VAL:HG22	2.38	0.59
1:H:730:LEU:HD13	1:H:739:LYS:HB2	1.85	0.59
1:B:809:ILE:N	1:B:987:MET:HE3	2.17	0.58
1:B:851:VAL:O	1:B:851:VAL:HG23	2.01	0.58
1:D:714:LYS:O	1:D:714:LYS:HG2	2.01	0.58
1:E:898:TRP:CD1	1:E:898:TRP:C	2.81	0.58
1:F:707:LEU:C	1:F:711:GLU:HG3	2.27	0.58
2:A:1101:816:NAB	2:A:1101:816:CAN	2.66	0.58
1:E:941:ILE:CG1	1:E:945:MET:HE2	2.33	0.58
2:H:1101:816:NAB	2:H:1101:816:CAN	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:MET:HE1	1:D:852:LYS:HD3	1.85	0.58
1:D:955:ALA:O	1:D:958:ARG:HB2	2.03	0.58
1:E:842:ASN:O	1:E:854:THR:CG2	2.45	0.58
1:F:835:HIS:CD2	1:F:856:PHE:HB2	2.38	0.58
1:D:940:THR:HG22	1:D:978:TYR:O	2.01	0.58
1:E:833:LEU:CD1	1:E:856:PHE:CZ	2.86	0.58
1:F:942:ASP:OD1	1:F:977:ARG:NH1	2.32	0.58
1:H:949:LYS:O	1:H:952:MET:CG	2.51	0.58
1:C:715:ILE:CD1	1:C:728:LYS:HZ1	2.16	0.58
1:C:715:ILE:HD11	1:C:728:LYS:CE	2.34	0.58
1:C:977:ARG:CD	1:C:977:ARG:C	2.76	0.58
1:D:769:VAL:HG23	1:D:769:VAL:O	2.02	0.58
1:D:940:THR:HB	1:D:978:TYR:O	2.02	0.58
1:E:814:LEU:HD23	1:E:817:TRP:CE3	2.39	0.58
1:H:790:MET:HG3	1:H:791:GLN:N	2.17	0.58
1:C:797:CYS:CB	1:C:800:ASP:OD2	2.52	0.58
1:C:849:GLN:HB3	1:C:1010:VAL:HG11	1.85	0.58
1:B:717:VAL:CG2	1:B:727:TYR:CD2	2.86	0.58
2:G:1101:816:NAB	2:G:1101:816:CAN	2.67	0.58
1:H:776:ARG:NH1	1:H:776:ARG:HG2	2.17	0.58
1:C:745:LYS:HB3	1:C:788:LEU:HD13	1.86	0.58
1:A:815[B]:LEU:HD13	1:A:979:LEU:HD11	1.85	0.58
1:D:767:ALA:O	1:D:776:ARG:HG3	2.04	0.58
1:C:745:LYS:HB3	1:C:788:LEU:CD1	2.33	0.58
1:F:878:ILE:HD13	1:F:881:MET:HE1	1.86	0.58
1:G:700:ASN:OD1	1:G:702:ALA:N	2.30	0.58
1:G:997:PHE:CE2	1:G:1001:LEU:HD11	2.39	0.58
1:C:712:PHE:HZ	1:C:787:GLN:OE1	1.87	0.58
1:C:881:MET:HE2	1:C:886:ILE:HG12	1.85	0.58
1:E:820:GLN:NE2	1:E:849:GLN:O	2.33	0.58
1:G:806:LYS:O	1:G:806:LYS:HE3	2.04	0.58
1:G:851:VAL:C	1:G:852:LYS:HG2	2.27	0.58
1:H:825:MET:CE	1:H:961:PHE:CZ	2.87	0.58
1:A:950:CYS:O	1:A:958:ARG:CD	2.50	0.57
1:B:736:GLU:OE2	1:B:736:GLU:CA	2.48	0.57
1:G:878:ILE:HD13	1:G:920:ALA:HB1	1.85	0.57
1:C:980:VAL:O	1:C:980:VAL:HG23	2.03	0.57
1:E:809:ILE:HG22	1:E:810:GLY:N	2.18	0.57
1:C:715:ILE:HD13	1:C:728:LYS:NZ	2.19	0.57
1:C:782:LEU:C	1:C:783:THR:HG23	2.29	0.57
1:H:961:PHE:HA	1:H:964:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:962:ARG:C	1:H:965:ILE:HG13	2.28	0.57
1:C:827:TYR:CZ	1:C:831:ARG:HD3	2.39	0.57
1:C:836:ARG:HG2	1:C:891:TYR:CD1	2.39	0.57
1:A:819:VAL:O	1:A:823:LYS:HG3	2.04	0.57
1:E:759:ILE:HG23	1:E:760:LEU:N	2.18	0.57
1:B:809:ILE:CA	1:B:987:MET:HE3	2.35	0.57
1:B:876:VAL:HG21	1:B:889:ARG:NH1	2.19	0.57
1:B:905:TRP:O	1:B:909:THR:CG2	2.50	0.57
1:F:923:ILE:HD12	1:F:926:ILE:HD11	1.86	0.57
1:G:825:MET:HE2	1:G:853:ILE:HD12	1.86	0.57
1:G:999[A]:ARG:HH12	1:G:1006:ASP:HA	1.68	0.57
1:C:716:LYS:O	1:C:728:LYS:N	2.34	0.57
1:C:828:LEU:HD11	1:C:856:PHE:HB2	1.86	0.57
1:C:839:ALA:HB1	1:C:841:ARG:CG	2.34	0.57
1:C:898:TRP:CD1	1:C:898:TRP:C	2.81	0.57
1:A:805:HIS:O	1:A:809:ILE:HG13	2.05	0.57
1:A:898:TRP:CH2	1:A:927:LEU:HD13	2.39	0.57
1:A:1006:ASP:OD1	1:A:1006:ASP:N	2.30	0.57
1:E:846:LYS:CE	1:E:1005:GLU:OE1	2.53	0.57
1:E:952:MET:O	1:E:958:ARG:NH1	2.35	0.57
1:H:769:VAL:HG11	1:H:856:PHE:HZ	1.70	0.57
1:H:986:ARG:HB2	1:H:986:ARG:CZ	2.34	0.57
1:D:900:TYR:CE2	1:D:904:VAL:CG2	2.87	0.57
1:E:885:SER:O	1:E:889:ARG:HA	2.04	0.57
1:G:836:ARG:HG3	4:G:1210:HOH:O	2.05	0.57
1:C:833:LEU:HD13	1:C:856:PHE:CZ	2.39	0.57
1:D:812:GLN:HG2	1:D:975:PRO:CG	2.34	0.57
1:D:894:GLN:C	1:D:897:VAL:HG23	2.30	0.57
1:F:832:ARG:CG	4:F:1211:HOH:O	2.51	0.57
1:G:823:LYS:HG2	1:G:965:ILE:CD1	2.35	0.57
1:G:856:PHE:CD1	1:G:856:PHE:O	2.57	0.57
1:H:718:LEU:HD11	1:H:792:LEU:CD1	2.31	0.57
1:H:961:PHE:O	1:H:965:ILE:CG1	2.53	0.57
1:C:815:LEU:CD1	1:C:975:PRO:HA	2.34	0.57
1:A:707:LEU:HD22	1:A:711:GLU:CD	2.30	0.57
1:A:793:MET:HE3	1:A:844:LEU:CB	2.35	0.57
1:B:997:PHE:CD1	1:B:997:PHE:C	2.78	0.57
1:D:786:VAL:HG13	1:D:786:VAL:O	2.05	0.57
1:E:847:THR:HG23	1:E:850:HIS:CB	2.28	0.57
1:F:845:VAL:HG12	1:F:847:THR:O	2.04	0.57
1:F:897:VAL:HG21	4:F:1228:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:989:LEU:HD23	1:F:990:PRO:O	2.04	0.57
1:G:835:HIS:O	1:G:836:ARG:HB2	2.04	0.57
1:G:897:VAL:O	1:G:901:GLY:N	2.33	0.57
1:A:798:LEU:C	1:A:798:LEU:CD1	2.65	0.57
1:D:884:GLU:HG2	1:D:885:SER:N	2.18	0.57
1:E:745:LYS:HZ1	1:E:858:LEU:HD21	1.69	0.57
1:C:940:THR:CG2	1:C:978:TYR:O	2.53	0.57
1:A:830:ASP:HB3	1:C:717:VAL:CG1	2.32	0.56
1:B:704:LEU:HB2	1:B:767:ALA:HB2	1.86	0.56
1:F:819:VAL:HG23	1:F:968:PHE:HB3	1.86	0.56
1:F:1007:MET:HG2	1:F:1008:ASP:N	2.15	0.56
1:G:823:LYS:HG2	1:G:965:ILE:HD13	1.86	0.56
1:G:997:PHE:CE2	1:G:1001:LEU:CD1	2.88	0.56
1:B:835:HIS:CG	1:B:856:PHE:HB2	2.37	0.56
1:F:825:MET:HG2	1:F:961:PHE:CZ	2.40	0.56
1:C:726:VAL:HG22	1:C:745:LYS:HG3	1.86	0.56
1:B:988:HIS:CB	1:B:990:PRO:N	2.67	0.56
1:D:732:ILE:O	1:D:732:ILE:HG13	2.03	0.56
1:D:991:SER:OG	1:D:992:PRO:CD	2.54	0.56
1:E:803:ARG:O	1:E:806:LYS:HD2	2.06	0.56
1:F:793:MET:HE2	1:F:844:LEU:HB2	1.87	0.56
1:F:835:HIS:CE1	1:F:837:ASP:O	2.58	0.56
1:F:995:SER:O	1:F:999:ARG:HG3	2.05	0.56
1:G:769:VAL:O	1:G:769:VAL:HG22	2.04	0.56
1:H:715:ILE:HG12	1:H:728:LYS:O	2.06	0.56
1:C:940:THR:CG2	1:C:943:VAL:HG23	2.30	0.56
1:A:775:CYS:HB2	1:A:853:ILE:O	2.06	0.56
1:B:982:GLN:H	1:B:982:GLN:CD	2.13	0.56
1:D:845:VAL:HG12	1:D:845:VAL:O	2.05	0.56
1:F:835:HIS:HE1	1:F:837:ASP:O	1.87	0.56
1:F:889:ARG:HD2	4:F:1209:HOH:O	2.04	0.56
1:D:961:PHE:HA	1:D:964:LEU:HB2	1.88	0.56
1:E:876:VAL:HG11	1:E:889:ARG:HH12	1.70	0.56
1:E:879:LYS:HD3	1:E:915:TYR:HB2	1.87	0.56
1:E:913:LYS:CD	1:E:913:LYS:N	2.68	0.56
1:G:881:MET:HE3	1:G:885:SER:CB	2.28	0.56
1:H:835:HIS:CD2	1:H:856:PHE:CB	2.89	0.56
1:H:971:MET:O	1:H:974:ASP:C	2.48	0.56
1:C:723:PHE:O	1:C:748:ARG:HG3	2.06	0.56
1:C:878:ILE:HG22	1:C:923:ILE:HG21	1.87	0.56
1:B:905:TRP:CE2	1:B:909:THR:HG21	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:LYS:HB2	1:E:910:PHE:HB3	1.86	0.56
1:F:700:ASN:HB2	1:F:703:LEU:HD12	1.86	0.56
1:A:931:GLU:O	1:A:932:ARG:HD3	2.06	0.56
1:B:708:LYS:HB2	1:B:711:GLU:CG	2.35	0.56
1:B:716:LYS:HB3	1:B:728:LYS:HB3	1.86	0.56
1:D:821:ILE:HG23	1:D:853:ILE:HD11	1.87	0.56
1:B:780:ILE:HD13	1:B:782:LEU:CD2	2.34	0.56
1:D:815:LEU:HD21	1:D:979:LEU:HD12	1.81	0.56
1:D:938:ILE:HD11	1:D:979:LEU:CD2	2.35	0.56
1:F:790:MET:HG2	2:F:1101:816:CLA	2.42	0.56
1:A:841:ARG:NH2	1:A:841:ARG:CG	2.62	0.56
1:H:925:SER:O	1:H:929:LYS:HG3	2.06	0.56
1:H:935:GLN:CB	1:H:944:TYR:CG	2.88	0.56
1:H:946:ILE:CG2	1:H:947:MET:N	2.69	0.56
1:E:879:LYS:HG2	1:E:923:ILE:CD1	2.36	0.55
1:G:705:ARG:HG3	1:G:706:ILE:N	2.21	0.55
1:C:793:MET:HE2	1:C:844:LEU:HB2	1.87	0.55
1:C:1007:MET:SD	1:C:1008:ASP:O	2.64	0.55
1:A:846:LYS:HE3	1:A:1005:GLU:OE1	2.07	0.55
1:F:850:HIS:O	1:F:850:HIS:CD2	2.60	0.55
1:C:926:ILE:HA	1:C:929:LYS:HB2	1.87	0.55
1:A:815[A]:LEU:HG	1:A:979:LEU:CD1	2.36	0.55
1:A:878:ILE:CD1	4:A:1214:HOH:O	2.41	0.55
1:B:878:ILE:HG23	1:B:886:ILE:HD13	1.87	0.55
1:B:947:MET:O	1:B:950:CYS:HB2	2.07	0.55
1:D:773:HIS:CE1	1:D:850:HIS:CE1	2.94	0.55
1:E:765:VAL:O	1:E:768:SER:CB	2.54	0.55
1:G:949:LYS:O	1:G:952:MET:CG	2.53	0.55
1:B:831:ARG:HB3	1:B:833:LEU:CD1	2.36	0.55
1:B:1003:ASP:C	1:B:1003:ASP:OD1	2.48	0.55
1:D:805:HIS:HD2	4:D:1202:HOH:O	1.83	0.55
1:H:817:TRP:O	1:H:821:ILE:CG1	2.49	0.55
1:H:825:MET:HE2	1:H:961:PHE:CZ	2.41	0.55
2:H:1101:816:N3	2:H:1101:816:CAR	2.70	0.55
1:A:705:ARG:HD3	1:A:707:LEU:CD2	2.36	0.55
1:A:811:SER:HB3	1:A:984:ASP:OD1	2.06	0.55
1:D:803:ARG:HG2	1:D:911:GLY:HA3	1.88	0.55
1:H:729:GLY:HA3	1:H:744:ILE:HD11	1.89	0.55
1:B:717:VAL:CG2	1:B:727:TYR:HE2	2.18	0.55
1:D:765:VAL:CG1	1:D:766:MET:N	2.66	0.55
1:E:803:ARG:CG	1:E:911:GLY:HA3	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1003:ASP:OD1	1:E:1005:GLU:HG2	2.06	0.55
1:A:830:ASP:CB	1:C:717:VAL:HG11	2.32	0.55
1:E:816:ASN:O	1:E:820:GLN:HG3	2.06	0.55
1:F:850:HIS:CD2	1:F:850:HIS:C	2.84	0.55
1:F:923:ILE:HA	1:F:926:ILE:HD11	1.88	0.55
1:F:977:ARG:NH2	1:G:926:ILE:HD12	2.22	0.55
1:G:971:MET:HA	1:G:978:TYR:CE2	2.42	0.55
1:H:943:VAL:HG12	1:H:947:MET:HE3	1.88	0.55
1:H:974:ASP:O	1:H:978:TYR:HD2	1.89	0.55
1:C:825:MET:CG	1:C:838:LEU:HD21	2.36	0.55
1:A:813:TYR:OH	1:A:990:PRO:HG3	2.07	0.55
1:A:974:ASP:OD2	1:E:929:LYS:HE3	2.06	0.55
1:F:845:VAL:CG1	1:F:847:THR:O	2.55	0.55
1:F:999:ARG:O	1:F:1003:ASP:N	2.39	0.55
1:B:943:VAL:HG21	1:B:979:LEU:CD2	2.37	0.55
1:D:772:PRO:O	1:D:852:LYS:HG2	2.07	0.55
1:E:799:LEU:O	1:E:803:ARG:HG3	2.07	0.55
1:E:809:ILE:CG2	1:E:810:GLY:N	2.70	0.55
1:F:803:ARG:HG2	1:F:911:GLY:HA3	1.89	0.55
1:F:811:SER:HA	1:F:981:ILE:CD1	2.37	0.55
1:G:890:ILE:HG22	1:G:890:ILE:O	2.06	0.55
1:G:940:THR:CG2	1:G:978:TYR:O	2.54	0.55
1:A:974:ASP:OD2	1:E:929:LYS:CE	2.55	0.55
1:D:974:ASP:HB3	1:D:977:ARG:HB3	1.89	0.55
1:E:793:MET:HG3	1:E:844:LEU:HD13	1.88	0.55
1:G:745:LYS:NZ	1:G:855:ASP:OD1	2.40	0.55
1:G:774:VAL:CG1	1:G:856:PHE:CE2	2.90	0.55
1:C:839:ALA:CB	1:C:841:ARG:CG	2.85	0.55
1:A:797:CYS:HB2	1:A:800:ASP:OD2	2.07	0.54
1:D:938:ILE:CG1	1:D:979:LEU:HD23	2.37	0.54
1:F:898:TRP:CD1	1:F:898:TRP:C	2.85	0.54
1:H:825:MET:HE3	1:H:961:PHE:CE2	2.42	0.54
1:E:854:THR:O	1:E:855:ASP:HB2	2.07	0.54
1:F:811:SER:HB2	1:F:981:ILE:HD12	1.87	0.54
1:F:977:ARG:HG2	1:F:977:ARG:HH21	1.73	0.54
1:G:822:ALA:CB	1:G:965:ILE:HG12	2.37	0.54
1:H:986:ARG:CB	1:H:986:ARG:CZ	2.84	0.54
1:B:809:ILE:HG21	1:B:814:LEU:HD11	1.89	0.54
1:F:966:ILE:CG2	1:F:970:LYS:HE3	2.37	0.54
1:G:847:THR:OG1	1:G:848:PRO:CD	2.55	0.54
1:H:879:LYS:HD3	1:H:923:ILE:CD1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:946:ILE:HG22	1:H:947:MET:N	2.21	0.54
1:C:839:ALA:HB1	1:C:841:ARG:HG3	1.85	0.54
1:B:898:TRP:CH2	1:B:927:LEU:HD13	2.43	0.54
1:B:997:PHE:HD1	1:B:997:PHE:C	2.15	0.54
1:D:817:TRP:HA	1:D:820:GLN:HB2	1.90	0.54
1:E:847:THR:CG2	1:E:850:HIS:HB3	2.29	0.54
1:F:849:GLN:N	1:F:849:GLN:CD	2.65	0.54
1:H:939:CYS:SG	1:H:947:MET:HE1	2.47	0.54
1:C:842:ASN:O	1:C:854:THR:CG2	2.54	0.54
1:D:811:SER:HB2	1:D:981:ILE:CG1	2.37	0.54
1:E:817:TRP:O	1:E:821:ILE:HD12	2.08	0.54
1:G:806:LYS:CD	1:G:806:LYS:O	2.53	0.54
1:H:778:LEU:HG	1:H:790:MET:HA	1.88	0.54
1:B:813:TYR:OH	1:B:990:PRO:HG3	2.08	0.54
1:B:972:ALA:CB	1:B:1011:VAL:CG1	2.78	0.54
1:E:814:LEU:HD23	1:E:817:TRP:CZ3	2.42	0.54
1:F:778:LEU:HD23	1:F:790:MET:CA	2.33	0.54
1:F:917:GLY:C	1:F:918:ILE:HD13	2.33	0.54
1:E:904:VAL:HG13	1:E:947:MET:HE2	1.89	0.54
1:H:743:ALA:CB	2:H:1101:816:C6	2.86	0.54
1:H:897:VAL:HA	1:H:900:TYR:HB3	1.90	0.54
1:C:756:ASN:CG	1:C:782:LEU:HD22	2.33	0.54
1:C:897:VAL:HG12	1:C:950:CYS:SG	2.47	0.54
1:A:717:VAL:CG2	1:A:727:TYR:CE2	2.89	0.54
1:B:941:ILE:HG23	1:B:942:ASP:OD1	2.08	0.54
1:D:703:LEU:O	1:D:776:ARG:NH1	2.37	0.54
1:E:783:THR:CG2	1:E:784:SER:H	2.21	0.54
1:C:714:LYS:HD3	1:C:727:TYR:CD1	2.43	0.54
1:B:783:THR:CG2	1:B:784:SER:H	2.20	0.54
1:G:932:ARG:HH11	1:G:932:ARG:CB	2.19	0.54
1:H:726:VAL:HG22	1:H:745:LYS:HB2	1.88	0.54
1:C:825:MET:SD	1:C:838:LEU:HD23	2.40	0.54
1:B:881:MET:HE2	1:B:891:TYR:HE1	1.73	0.54
1:E:883:LEU:HD22	1:E:953:ILE:CD1	2.38	0.54
1:G:823:LYS:CE	1:G:1008:ASP:OD2	2.53	0.54
1:C:782:LEU:C	1:C:783:THR:CG2	2.81	0.54
1:C:962:ARG:NH1	4:C:1205:HOH:O	2.41	0.54
1:E:836:ARG:HD2	1:E:860:LYS:HA	1.90	0.53
1:E:945:MET:HE3	1:C:934:PRO:CG	2.38	0.53
1:F:832:ARG:O	1:F:832:ARG:CG	2.56	0.53
1:H:805:HIS:HB3	1:H:809:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:955:ALA:O	1:C:958:ARG:HG2	2.07	0.53
1:C:981:ILE:HG21	1:C:987:MET:CE	2.37	0.53
1:A:700:ASN:CB	1:A:703:LEU:CD1	2.86	0.53
1:A:738:VAL:CG2	4:A:1232:HOH:O	2.54	0.53
1:B:811:SER:HB3	1:B:984:ASP:OD2	2.07	0.53
1:E:717:VAL:HG13	1:E:727:TYR:HE2	1.73	0.53
1:H:707:LEU:CD1	1:H:789:ILE:CD1	2.38	0.53
1:H:925:SER:O	1:H:929:LYS:CG	2.56	0.53
1:C:765:VAL:HG12	1:C:766:MET:N	2.22	0.53
1:C:790:MET:HG2	2:C:1101:816:CLA	2.45	0.53
1:A:705:ARG:CD	1:A:707:LEU:CD2	2.85	0.53
1:B:718:LEU:HD11	1:B:728:LYS:HB2	1.90	0.53
1:D:830:ASP:HA	1:G:720:SER:HB2	1.89	0.53
1:D:999:ARG:HA	1:D:1003:ASP:HB3	1.91	0.53
1:F:845:VAL:HG12	1:F:847:THR:C	2.34	0.53
1:G:799:LEU:O	1:G:802:VAL:HG23	2.07	0.53
1:C:846:LYS:C	1:C:847:THR:CG2	2.81	0.53
1:D:790:MET:HG2	1:D:791:GLN:N	2.24	0.53
1:E:913:LYS:N	1:E:913:LYS:HD2	2.22	0.53
1:F:708:LYS:N	1:F:711:GLU:OE2	2.30	0.53
1:A:938:ILE:HG13	1:A:938:ILE:O	2.08	0.53
1:B:894:GLN:CB	1:B:955:ALA:HB1	2.39	0.53
1:G:847:THR:OG1	1:G:848:PRO:HD2	2.08	0.53
1:H:831:ARG:HB3	1:H:833:LEU:CD1	2.38	0.53
1:C:714:LYS:NZ	4:C:1204:HOH:O	2.41	0.53
1:A:813:TYR:CZ	1:A:990:PRO:HD3	2.44	0.53
1:F:704:LEU:HD23	1:F:764:TYR:CE1	2.43	0.53
1:F:909:THR:O	1:F:910:PHE:HB2	2.07	0.53
1:C:922:GLU:O	1:C:926:ILE:HG23	2.09	0.53
1:A:762:GLU:OE1	1:A:861:LEU:HD23	2.09	0.53
1:H:803:ARG:HG2	1:H:911:GLY:HA3	1.90	0.53
1:C:765:VAL:O	1:C:768:SER:HB2	2.08	0.53
1:A:767:ALA:O	1:A:776:ARG:NH1	2.37	0.53
1:A:777:LEU:CD1	1:A:789:ILE:O	2.57	0.53
1:A:815[B]:LEU:CD2	1:A:979:LEU:HD12	2.38	0.53
1:D:1006:ASP:OD1	1:D:1006:ASP:N	2.37	0.53
2:E:1101:816:NAB	2:E:1101:816:CAN	2.72	0.53
1:F:701:GLN:OE1	1:F:701:GLN:HA	2.08	0.53
1:G:757:LYS:HD2	1:G:758:GLU:N	2.23	0.53
1:C:971:MET:HA	1:C:978:TYR:CE2	2.44	0.53
1:A:923:ILE:CA	1:A:926:ILE:HG12	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:THR:HG23	1:A:941:ILE:N	2.24	0.53
1:B:705:ARG:HG2	1:B:707:LEU:HD23	1.89	0.53
1:B:737:LYS:CD	1:B:737:LYS:C	2.81	0.53
1:E:743:ALA:O	1:E:744:ILE:CD1	2.57	0.53
1:E:941:ILE:HG23	1:E:945:MET:HE3	1.90	0.53
1:G:821:ILE:HG22	1:G:900:TYR:CE1	2.43	0.53
1:H:776:ARG:O	1:H:778:LEU:HD21	2.08	0.53
1:A:880:TRP:CZ2	1:A:906:GLU:OE2	2.62	0.53
1:F:781:CYS:SG	1:F:783:THR:HG23	2.49	0.53
1:F:879:LYS:NZ	1:F:918:ILE:O	2.36	0.53
1:G:773:HIS:CE1	1:G:820:GLN:HG2	2.43	0.53
1:G:998:TYR:HE2	4:G:1227:HOH:O	1.92	0.53
1:C:714:LYS:HA	1:C:729:GLY:HA2	1.90	0.53
1:F:707:LEU:CB	1:F:711:GLU:CD	2.82	0.52
1:D:842:ASN:O	1:D:854:THR:CG2	2.57	0.52
1:E:726:VAL:HG23	1:E:745:LYS:HD2	1.92	0.52
1:B:894:GLN:HB3	1:B:955:ALA:HB1	1.91	0.52
1:E:821:ILE:HA	1:E:853:ILE:HD11	1.92	0.52
1:F:747:LEU:HG	1:F:788:LEU:CD1	2.37	0.52
1:F:778:LEU:HD22	1:F:778:LEU:N	2.24	0.52
1:F:878:ILE:HD13	1:F:881:MET:HE2	1.91	0.52
1:C:999:ARG:O	1:C:1003:ASP:C	2.52	0.52
1:D:790:MET:HE3	2:D:1101:816:CAA	2.38	0.52
1:D:846:LYS:HD2	1:D:850:HIS:HD2	1.74	0.52
1:D:876:VAL:HG12	1:D:877:PRO:HD2	1.91	0.52
1:H:858:LEU:O	1:H:861:LEU:HB2	2.08	0.52
1:A:762:GLU:CD	1:A:861:LEU:HD21	2.34	0.52
1:D:981:ILE:HB	1:D:984:ASP:CB	2.24	0.52
1:E:745:LYS:O	1:E:787:GLN:HA	2.10	0.52
1:H:954:ASP:HB3	1:H:957:SER:OG	2.10	0.52
1:C:825:MET:CG	1:C:838:LEU:CD2	2.88	0.52
1:B:945:MET:HE1	1:D:909:THR:CG2	2.39	0.52
1:E:771:ASN:OD1	1:E:772:PRO:N	2.42	0.52
1:C:714:LYS:CE	1:C:787:GLN:NE2	2.67	0.52
1:C:817:TRP:CD1	1:C:851:VAL:HG11	2.45	0.52
1:B:798:LEU:HB2	1:B:843:VAL:CG1	2.36	0.52
1:D:942:ASP:O	1:D:946:ILE:HG13	2.09	0.52
1:G:728:LYS:HG3	1:G:792:LEU:HD13	1.90	0.52
1:H:769:VAL:HG11	1:H:856:PHE:CZ	2.45	0.52
1:A:793:MET:HE3	1:A:844:LEU:HB2	1.90	0.52
1:A:799:LEU:HB2	1:A:840:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:773:HIS:O	1:E:853:ILE:HG13	2.09	0.52
1:E:835:HIS:CE1	1:E:837:ASP:O	2.63	0.52
1:F:800:ASP:O	1:F:804:GLU:HG3	2.09	0.52
1:G:766:MET:CE	1:G:777:LEU:HD22	2.39	0.52
1:G:1007:MET:HG2	1:G:1008:ASP:O	2.09	0.52
1:H:718:LEU:HD21	1:H:728:LYS:HB2	1.92	0.52
1:A:705:ARG:HG2	1:A:706:ILE:O	2.10	0.52
1:A:757:LYS:N	1:A:757:LYS:CD	2.73	0.52
1:D:846:LYS:C	1:D:847:THR:HG22	2.35	0.52
1:G:819:VAL:HG22	1:G:968:PHE:HB3	1.92	0.52
1:H:1007:MET:SD	1:H:1008:ASP:O	2.68	0.52
1:C:712:PHE:CZ	1:C:787:GLN:OE1	2.63	0.52
1:C:780:ILE:HD12	1:C:787:GLN:O	2.07	0.52
1:C:929:LYS:HD2	1:C:931:GLU:OE2	2.10	0.52
1:B:762:GLU:O	1:B:766:MET:HG3	2.10	0.51
1:F:945:MET:CA	1:F:948:VAL:HG23	2.40	0.51
1:G:790:MET:HG2	2:G:1101:816:CBF	2.39	0.51
1:C:849:GLN:HB3	1:C:1010:VAL:CG1	2.41	0.51
1:C:894:GLN:NE2	1:C:958:ARG:O	2.42	0.51
1:A:898:TRP:CD1	1:A:898:TRP:C	2.88	0.51
1:D:878:ILE:HG13	1:D:881:MET:HE2	1.92	0.51
1:D:941:ILE:HG12	1:D:945:MET:HE3	1.90	0.51
1:E:780:ILE:O	1:E:780:ILE:HG22	2.10	0.51
1:E:950:CYS:O	1:E:958:ARG:CG	2.58	0.51
1:G:771:ASN:HB3	1:G:774:VAL:HG23	1.92	0.51
1:H:708:LYS:CG	1:H:711:GLU:OE2	2.58	0.51
1:H:716:LYS:CG	1:H:717:VAL:N	2.73	0.51
1:C:808:ASN:HB3	4:C:1222:HOH:O	2.10	0.51
1:C:827:TYR:CZ	1:C:831:ARG:HD2	2.44	0.51
1:B:915:TYR:OH	1:B:927:LEU:HD21	2.10	0.51
1:E:759:ILE:CD1	1:E:780:ILE:HD12	2.28	0.51
1:E:799:LEU:HD22	1:E:841:ARG:HB3	1.93	0.51
1:F:900:TYR:HH	1:F:968:PHE:HE2	1.58	0.51
1:F:945:MET:HA	1:F:948:VAL:CG2	2.40	0.51
2:F:1101:816:CAR	4:F:1231:HOH:O	2.57	0.51
1:H:708:LYS:HG3	1:H:711:GLU:HB2	1.93	0.51
1:D:748:ARG:O	1:D:749:GLU:C	2.53	0.51
1:F:726:VAL:CG2	1:F:745:LYS:HE2	2.41	0.51
1:A:888:HIS:HA	1:D:888:HIS:O	2.11	0.51
1:G:806:LYS:C	1:G:806:LYS:CE	2.80	0.51
1:G:924:SER:O	1:G:928:GLU:CG	2.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:TRP:CZ2	1:B:927:LEU:CD1	2.92	0.51
1:D:806:LYS:HB2	1:D:910:PHE:HB3	1.92	0.51
1:F:991:SER:CB	1:F:992:PRO:CD	2.83	0.51
1:C:713:LYS:O	1:C:713:LYS:HG3	2.11	0.51
1:A:932:ARG:HB3	1:A:951:TRP:CE3	2.45	0.51
1:B:988:HIS:CA	1:B:989:LEU:C	2.84	0.51
1:D:703:LEU:C	1:D:776:ARG:HH12	2.18	0.51
1:D:825:MET:HG3	1:D:838:LEU:HD22	1.92	0.51
1:E:922:GLU:O	1:E:926:ILE:HG23	2.10	0.51
1:F:949:LYS:O	1:F:952:MET:HB2	2.10	0.51
1:G:806:LYS:O	1:G:806:LYS:HE2	2.09	0.51
1:A:721:GLY:HA3	4:A:1207:HOH:O	2.10	0.51
1:C:846:LYS:O	1:C:847:THR:HG22	2.10	0.51
1:A:806:LYS:O	1:A:806:LYS:HD3	2.09	0.51
1:B:851:VAL:O	1:B:851:VAL:CG2	2.59	0.51
1:E:806:LYS:HG2	1:E:807:ASP:N	2.25	0.51
2:G:1101:816:N3	2:G:1101:816:CAR	2.74	0.51
1:A:700:ASN:N	1:A:703:LEU:CD1	2.73	0.51
1:B:788:LEU:O	2:B:1101:816:CLA	2.66	0.51
1:B:977:ARG:HE	1:D:931:GLU:HB2	1.75	0.51
1:E:992:PRO:HD2	1:E:993:THR:H	1.76	0.51
1:F:955:ALA:O	1:F:958:ARG:CG	2.53	0.51
1:G:925:SER:O	1:G:929:LYS:HG2	2.11	0.51
1:G:940:THR:HG23	1:G:943:VAL:H	1.75	0.51
1:H:707:LEU:HD13	1:H:789:ILE:CG1	2.35	0.51
1:C:713:LYS:NZ	4:C:1206:HOH:O	2.43	0.51
1:C:899:SER:O	1:C:902:VAL:HG23	2.11	0.51
1:A:783:THR:CG2	1:A:784:SER:H	2.21	0.50
1:D:940:THR:HG22	1:D:943:VAL:CG2	2.34	0.50
1:E:707:LEU:HD11	1:E:789:ILE:CG1	2.31	0.50
1:F:1008:ASP:O	1:F:1008:ASP:OD2	2.30	0.50
1:G:743:ALA:HB2	2:G:1101:816:N1	2.27	0.50
1:H:945:MET:HE1	3:H:1103:EDO:H22	1.92	0.50
1:A:949:LYS:O	1:A:958:ARG:HG3	2.11	0.50
1:D:932:ARG:HH11	1:D:932:ARG:CG	2.14	0.50
1:E:950:CYS:HA	1:E:958:ARG:HG2	1.93	0.50
1:F:835:HIS:O	1:F:896:ASP:CG	2.54	0.50
1:G:774:VAL:HG12	1:G:856:PHE:HE2	1.76	0.50
1:H:767:ALA:O	1:H:776:ARG:NH1	2.44	0.50
1:B:809:ILE:O	1:B:809:ILE:HG22	2.10	0.50
1:D:939:CYS:SG	1:D:943:VAL:CG1	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:940:THR:CB	1:D:978:TYR:O	2.58	0.50
1:F:932:ARG:HH22	1:F:953:ILE:HD13	1.76	0.50
1:E:819:VAL:HG23	1:E:968:PHE:HB3	1.91	0.50
1:F:894:GLN:O	1:F:897:VAL:HB	2.11	0.50
1:F:945:MET:HA	1:F:948:VAL:HG23	1.94	0.50
1:G:881:MET:CE	1:G:885:SER:CB	2.89	0.50
1:A:850:HIS:ND1	1:A:1003:ASP:OD2	2.45	0.50
1:B:1003:ASP:OD1	1:B:1003:ASP:O	2.30	0.50
1:E:919:PRO:HB2	1:E:922:GLU:HG3	1.93	0.50
1:F:776:ARG:NH1	4:F:1203:HOH:O	2.38	0.50
1:F:902:VAL:O	1:F:905:TRP:HB3	2.11	0.50
1:G:943:VAL:HG21	1:G:979:LEU:HD23	1.92	0.50
1:G:1012:ASP:O	1:G:1014:ASP:OD1	2.30	0.50
1:H:987:MET:HE1	4:H:1214:HOH:O	2.08	0.50
1:C:817:TRP:CD1	1:C:851:VAL:HG13	2.46	0.50
1:B:999:ARG:O	1:B:1003:ASP:C	2.55	0.50
1:D:837:ASP:O	1:D:837:ASP:OD1	2.30	0.50
1:E:999:ARG:O	1:E:1003:ASP:O	2.30	0.50
1:F:707:LEU:HB2	1:F:711:GLU:CD	2.36	0.50
1:C:770:ASP:OD1	1:C:770:ASP:O	2.30	0.50
1:C:947:MET:HB3	1:C:951:TRP:CH2	2.47	0.50
1:A:945:MET:O	1:A:949:LYS:HG3	2.10	0.50
1:A:1013:ALA:O	1:A:1014:ASP:O	2.30	0.50
1:F:985:GLU:HG2	1:F:986:ARG:N	2.27	0.50
1:G:719:GLY:HA3	2:G:1101:816:CAS	2.42	0.50
1:C:881:MET:CE	1:C:886:ILE:HG13	2.38	0.50
1:A:932:ARG:HH22	1:A:953:ILE:HD11	1.76	0.50
1:B:783:THR:O	1:B:784:SER:C	2.54	0.50
1:B:846:LYS:O	1:B:847:THR:HG22	2.11	0.50
1:D:707:LEU:HD23	1:D:711:GLU:CG	2.41	0.50
1:E:848:PRO:HD2	1:E:998:TYR:CE1	2.47	0.50
1:G:773:HIS:ND1	1:G:820:GLN:CB	2.71	0.50
1:A:743:ALA:O	2:A:1101:816:CLA	2.67	0.50
1:A:846:LYS:HD3	1:A:852:LYS:HD2	1.94	0.50
1:B:737:LYS:HD2	1:B:737:LYS:N	2.26	0.50
1:B:821:ILE:CG2	1:B:853:ILE:HD11	2.42	0.50
1:F:731:TRP:CE3	1:F:740:ILE:HG13	2.47	0.50
1:G:718:LEU:HD21	1:G:728:LYS:HB2	1.93	0.50
1:G:975:PRO:HG3	1:G:1013:ALA:HB2	1.94	0.50
1:C:935:GLN:HB2	1:C:944:TYR:CD1	2.47	0.50
1:A:985:GLU:HG2	1:A:986:ARG:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:818:CYS:SG	1:D:904:VAL:HG13	2.51	0.49
1:F:717:VAL:HG22	1:F:727:TYR:HE2	1.71	0.49
1:C:756:ASN:ND2	1:C:782:LEU:HD22	2.27	0.49
1:C:860:LYS:O	1:C:861:LEU:O	2.30	0.49
1:C:940:THR:CG2	1:C:943:VAL:H	2.25	0.49
1:A:888:HIS:O	1:D:888:HIS:HB3	2.11	0.49
1:B:932:ARG:HG3	1:B:951:TRP:CE3	2.48	0.49
1:D:814:LEU:HD23	1:D:817:TRP:CZ3	2.47	0.49
1:D:856:PHE:O	1:D:856:PHE:CG	2.63	0.49
1:E:726:VAL:HG22	1:E:745:LYS:HD2	1.93	0.49
1:E:914:PRO:O	1:E:915:TYR:C	2.55	0.49
1:F:790:MET:HE3	1:F:791:GLN:O	2.12	0.49
1:F:999:ARG:O	1:F:1003:ASP:O	2.30	0.49
1:G:912:SER:HA	1:G:913:LYS:HE3	1.94	0.49
1:C:781:CYS:HB3	1:C:787:GLN:HB2	1.94	0.49
1:C:999:ARG:HG2	1:C:1003:ASP:HB3	1.94	0.49
1:A:780:ILE:HG12	1:A:781:CYS:N	2.27	0.49
1:B:704:LEU:HD23	1:B:764:TYR:CE1	2.47	0.49
1:B:999:ARG:CG	1:B:999:ARG:NH1	2.73	0.49
1:D:839:ALA:HB3	1:D:842:ASN:HD22	1.77	0.49
1:E:803:ARG:NE	1:E:911:GLY:O	2.45	0.49
1:F:811:SER:CB	1:F:984:ASP:OD2	2.55	0.49
1:G:967:GLU:O	1:G:971:MET:HG3	2.12	0.49
1:H:879:LYS:HB3	1:H:915:TYR:HD2	1.77	0.49
1:B:882:ALA:HA	1:B:898:TRP:CD2	2.46	0.49
1:E:821:ILE:HG21	1:E:900:TYR:CE1	2.47	0.49
1:F:945:MET:HE1	1:G:909:THR:HG22	1.94	0.49
1:G:892:THR:H	1:G:895:SER:HB3	1.77	0.49
1:H:758:GLU:O	1:H:758:GLU:OE2	2.30	0.49
1:C:977:ARG:HG3	1:C:978:TYR:N	2.27	0.49
1:A:732:ILE:HG23	1:A:732:ILE:O	2.12	0.49
1:B:831:ARG:NH2	4:B:1204:HOH:O	2.45	0.49
1:D:771:ASN:ND2	1:D:772:PRO:HD2	2.27	0.49
1:E:943:VAL:HG12	1:E:947:MET:HE3	1.95	0.49
1:F:949:LYS:HB3	1:F:959:PRO:HD3	1.94	0.49
1:H:902:VAL:O	1:H:906:GLU:HG3	2.13	0.49
1:C:938:ILE:HG13	1:C:939:CYS:N	2.27	0.49
1:B:898:TRP:HZ2	1:B:927:LEU:CD1	2.26	0.49
1:D:757:LYS:HD2	1:D:761:ASP:CG	2.37	0.49
1:E:941:ILE:HG23	1:C:934:PRO:HG3	1.93	0.49
1:F:770:ASP:OD1	1:F:770:ASP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:802:VAL:HG12	1:G:809:ILE:CD1	2.42	0.49
1:H:708:LYS:HG3	1:H:711:GLU:OE2	2.12	0.49
1:H:758:GLU:OE1	1:H:762:GLU:OE1	2.30	0.49
1:C:884:GLU:HG2	1:C:885:SER:H	1.77	0.49
1:B:790:MET:HE1	1:B:844:LEU:CD1	2.42	0.49
1:B:981:ILE:O	1:B:984:ASP:HB2	2.13	0.49
1:F:820:GLN:NE2	1:F:1010:VAL:HG12	2.28	0.49
1:G:774:VAL:HG12	1:G:856:PHE:CE2	2.48	0.49
1:H:802:VAL:HG12	1:H:809:ILE:HD12	1.94	0.49
1:H:847:THR:O	1:H:850:HIS:O	2.30	0.49
1:C:898:TRP:CH2	1:C:927:LEU:HD13	2.47	0.49
2:C:1101:816:NAB	2:C:1101:816:CAN	2.76	0.49
1:B:995:SER:O	1:B:999:ARG:HG2	2.12	0.49
1:E:718:LEU:HG	1:E:728:LYS:N	2.28	0.49
1:G:952:MET:HE2	1:G:957:SER:HB3	1.94	0.49
1:H:809:ILE:CG2	1:H:810:GLY:N	2.75	0.49
1:C:707:LEU:CD1	1:C:789:ILE:CD1	2.89	0.49
1:A:726:VAL:HG23	1:A:745:LYS:HG3	1.92	0.49
1:B:949:LYS:O	1:B:952:MET:CG	2.61	0.49
1:D:769:VAL:O	1:D:769:VAL:CG2	2.61	0.49
1:E:992:PRO:CD	1:E:993:THR:H	2.26	0.49
1:G:822:ALA:HB1	1:G:965:ILE:HG12	1.93	0.49
1:H:766:MET:HE2	1:H:777:LEU:HD22	1.94	0.49
1:H:903:THR:HA	1:H:906:GLU:HG3	1.93	0.49
1:C:905:TRP:O	1:C:909:THR:CG2	2.56	0.49
1:A:774:VAL:CG2	1:A:824:GLY:O	2.61	0.49
1:A:880:TRP:NE1	1:A:906:GLU:OE2	2.44	0.49
1:E:876:VAL:HG11	1:E:889:ARG:NH1	2.28	0.49
1:C:745:LYS:O	1:C:787:GLN:HA	2.13	0.49
1:A:745:LYS:NZ	4:A:1207:HOH:O	2.46	0.48
1:A:999:ARG:NH2	1:A:1006:ASP:HA	2.28	0.48
1:D:767:ALA:O	1:D:776:ARG:CG	2.60	0.48
1:C:759:ILE:HA	1:C:762:GLU:HG3	1.94	0.48
1:C:783:THR:OG1	1:C:785:THR:O	2.30	0.48
1:C:898:TRP:CE3	1:C:958:ARG:NH1	2.80	0.48
1:C:961:PHE:O	1:C:965:ILE:CD1	2.30	0.48
1:A:793:MET:CE	1:A:844:LEU:HB2	2.43	0.48
1:A:898:TRP:CZ2	1:A:927:LEU:CD1	2.96	0.48
1:D:848:PRO:HD2	1:D:998:TYR:CE1	2.48	0.48
1:F:909:THR:HB	1:F:912:SER:HB2	1.94	0.48
1:G:717:VAL:HG22	1:G:727:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:940:THR:HG22	1:G:978:TYR:O	2.14	0.48
1:C:823:LYS:HG2	1:C:965:ILE:HG12	1.94	0.48
1:A:708:LYS:N	1:A:711:GLU:OE2	2.42	0.48
1:A:819:VAL:CG1	1:A:823:LYS:HE3	2.42	0.48
1:B:729:GLY:HA3	1:B:744:ILE:HD11	1.95	0.48
1:D:783:THR:CG2	1:D:784:SER:H	2.08	0.48
1:D:803:ARG:NH2	1:D:911:GLY:O	2.40	0.48
1:E:723:PHE:CE2	1:E:859:ALA:CA	2.78	0.48
1:E:768:SER:OG	1:E:831:ARG:NH1	2.45	0.48
1:F:713:LYS:HA	4:F:1223:HOH:O	2.13	0.48
1:B:949:LYS:O	1:B:952:MET:HG2	2.13	0.48
1:D:795:PHE:CZ	1:D:848:PRO:HD3	2.48	0.48
1:E:771:ASN:OD1	1:E:773:HIS:N	2.30	0.48
1:E:783:THR:O	1:E:785:THR:N	2.46	0.48
1:F:736:GLU:N	4:F:1206:HOH:O	2.46	0.48
1:H:741:PRO:C	1:H:742:VAL:HG13	2.37	0.48
1:C:713:LYS:HD2	4:C:1206:HOH:O	2.14	0.48
1:A:811:SER:OG	1:A:975:PRO:HB2	2.13	0.48
1:A:837:ASP:O	1:A:842:ASN:ND2	2.43	0.48
1:B:816:ASN:O	1:B:820:GLN:HG3	2.14	0.48
1:D:723:PHE:O	1:D:747:LEU:HD23	2.13	0.48
1:D:808:ASN:OD1	1:D:808:ASN:O	2.30	0.48
1:F:989:LEU:HD23	1:F:990:PRO:CA	2.42	0.48
1:G:798:LEU:HD12	1:G:798:LEU:C	2.39	0.48
1:G:821:ILE:HG22	1:G:900:TYR:HE1	1.79	0.48
1:C:908:MET:HB3	1:C:936:PRO:HG2	1.95	0.48
1:A:758:GLU:OE2	1:A:758:GLU:O	2.30	0.48
1:A:811:SER:HB3	1:A:984:ASP:CG	2.38	0.48
1:A:815[A]:LEU:O	1:A:818:CYS:HB2	2.14	0.48
1:A:843:VAL:C	1:A:844:LEU:HD23	2.38	0.48
1:B:809:ILE:N	1:B:987:MET:CE	2.77	0.48
1:B:932:ARG:HG3	1:B:951:TRP:HE3	1.79	0.48
1:D:815:LEU:HG	1:D:979:LEU:HD13	1.94	0.48
1:E:783:THR:C	1:E:785:THR:N	2.69	0.48
1:F:799:LEU:O	1:F:802:VAL:CG2	2.61	0.48
1:G:944:TYR:O	1:G:947:MET:CB	2.61	0.48
1:H:884:GLU:HG2	1:H:885:SER:N	2.28	0.48
1:H:969:SER:O	1:H:972:ALA:HB3	2.13	0.48
1:C:726:VAL:CG2	1:C:745:LYS:HE2	2.42	0.48
1:C:955:ALA:HA	1:C:958:ARG:NE	2.29	0.48
1:A:831:ARG:O	1:A:832:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:793:MET:H	2:G:1101:816:C2	2.26	0.48
1:H:835:HIS:NE2	1:H:854:THR:O	2.40	0.48
1:H:991:SER:OG	1:H:994:ASP:OD2	2.30	0.48
1:A:815[B]:LEU:O	1:A:818:CYS:HB2	2.14	0.48
1:A:904:VAL:O	1:A:908:MET:HG2	2.13	0.48
1:D:999:ARG:O	1:D:1003:ASP:C	2.57	0.48
1:E:806:LYS:CE	4:E:1207:HOH:O	2.56	0.48
1:H:714:LYS:NZ	1:H:787:GLN:HE22	2.12	0.48
1:A:765:VAL:CG1	1:A:766:MET:N	2.76	0.48
1:B:846:LYS:HD3	1:B:852:LYS:HD2	1.96	0.48
1:E:706:ILE:HG13	1:E:780:ILE:HG22	1.96	0.48
1:E:708:LYS:O	1:E:711:GLU:N	2.43	0.48
1:E:898:TRP:CZ2	1:E:927:LEU:HD22	2.49	0.48
1:C:803:ARG:O	1:C:806:LYS:HG2	2.14	0.48
1:A:894:GLN:HB3	1:A:955:ALA:HB1	1.96	0.48
1:A:1013:ALA:O	1:A:1014:ASP:C	2.56	0.48
1:B:726:VAL:CG2	1:B:745:LYS:CE	2.91	0.48
1:B:815:LEU:O	1:B:818:CYS:HB2	2.14	0.48
1:F:960:LYS:HA	4:F:1228:HOH:O	2.13	0.48
1:H:762:GLU:CB	1:H:861:LEU:CD2	2.90	0.48
1:A:938:ILE:HB	1:A:980:VAL:O	2.14	0.47
1:B:831:ARG:HD3	1:B:833:LEU:HD11	1.95	0.47
1:B:834:VAL:CG2	1:B:893:HIS:CD2	2.91	0.47
1:B:940:THR:HG23	1:B:942:ASP:N	2.29	0.47
1:E:855:ASP:OD2	1:E:858:LEU:HD23	2.13	0.47
1:F:717:VAL:HG22	1:F:727:TYR:CD2	2.49	0.47
1:H:782:LEU:C	1:H:783:THR:HG23	2.39	0.47
1:B:809:ILE:CG2	1:B:814:LEU:HD11	2.44	0.47
1:B:831:ARG:O	1:B:832:ARG:CB	2.61	0.47
1:E:759:ILE:O	1:E:763:ALA:N	2.35	0.47
1:F:879:LYS:HD3	1:F:915:TYR:HB2	1.96	0.47
1:F:898:TRP:CZ2	1:F:927:LEU:HD13	2.49	0.47
1:G:703:LEU:HD23	1:G:703:LEU:H	1.76	0.47
1:H:714:LYS:HZ1	1:H:787:GLN:HE22	1.60	0.47
1:H:825:MET:HE3	1:H:961:PHE:CZ	2.49	0.47
1:H:878:ILE:CG2	1:H:923:ILE:HG13	2.44	0.47
1:H:970:LYS:HA	1:H:973:ARG:HD2	1.96	0.47
1:B:835:HIS:CG	1:B:856:PHE:CB	2.95	0.47
1:B:846:LYS:C	1:B:847:THR:CG2	2.87	0.47
1:B:931:GLU:O	1:B:932:ARG:CD	2.58	0.47
1:F:731:TRP:CZ3	1:F:740:ILE:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:798:LEU:HG	1:G:907:LEU:HD21	1.95	0.47
1:G:884:GLU:HG2	1:G:885:SER:N	2.29	0.47
1:G:940:THR:CB	1:G:978:TYR:O	2.62	0.47
1:H:708:LYS:HG3	1:H:711:GLU:CG	2.43	0.47
1:H:717:VAL:HG22	1:H:727:TYR:CE2	2.49	0.47
1:C:704:LEU:HB2	1:C:767:ALA:HB2	1.94	0.47
1:C:765:VAL:CG1	1:C:766:MET:N	2.76	0.47
1:C:846:LYS:HG3	1:C:847:THR:CG2	2.44	0.47
1:C:975:PRO:HD2	1:C:1013:ALA:CB	2.43	0.47
1:C:975:PRO:CD	1:C:1013:ALA:HB2	2.42	0.47
1:B:843:VAL:HG22	1:B:853:ILE:HG12	1.97	0.47
1:D:796:GLY:O	1:D:845:VAL:N	2.34	0.47
1:E:805:HIS:O	1:E:808:ASN:O	2.33	0.47
1:H:729:GLY:C	1:H:730:LEU:HD23	2.40	0.47
1:C:714:LYS:HA	1:C:729:GLY:CA	2.45	0.47
1:C:811:SER:CB	1:C:984:ASP:OD1	2.58	0.47
1:B:966:ILE:HG22	1:B:970:LYS:HE3	1.96	0.47
1:D:767:ALA:O	1:D:776:ARG:HD2	2.13	0.47
1:G:855:ASP:OD1	1:G:858:LEU:CD2	2.62	0.47
1:H:776:ARG:O	1:H:778:LEU:HD23	2.14	0.47
1:C:771:ASN:ND2	1:C:772:PRO:HD2	2.29	0.47
1:C:856:PHE:HD1	1:C:857:GLY:H	1.51	0.47
1:A:799:LEU:HB2	1:A:840:ALA:CB	2.44	0.47
1:A:900:TYR:O	1:A:904:VAL:CG2	2.59	0.47
1:A:927:LEU:HD11	4:A:1213:HOH:O	2.14	0.47
1:B:835:HIS:ND1	1:B:856:PHE:HA	2.30	0.47
1:F:1008:ASP:OD2	1:F:1008:ASP:C	2.58	0.47
1:A:856:PHE:O	1:A:856:PHE:CG	2.68	0.47
1:B:882:ALA:HA	1:B:898:TRP:CE2	2.50	0.47
1:B:935:GLN:CG	1:B:944:TYR:CG	2.93	0.47
1:D:894:GLN:HA	1:D:897:VAL:CG2	2.45	0.47
1:E:765:VAL:O	1:E:768:SER:OG	2.30	0.47
1:E:905:TRP:O	1:E:909:THR:OG1	2.30	0.47
1:E:973:ARG:HG2	1:E:973:ARG:HH11	1.80	0.47
1:F:795:PHE:HB2	1:F:845:VAL:O	2.15	0.47
1:F:817:TRP:CD1	1:F:851:VAL:CG2	2.97	0.47
1:F:935:GLN:HB3	1:F:944:TYR:CD2	2.50	0.47
1:G:758:GLU:O	1:G:761:ASP:HB2	2.15	0.47
1:H:962:ARG:HA	1:H:965:ILE:CG1	2.40	0.47
1:C:855:ASP:HA	2:C:1101:816:CAK	2.44	0.47
1:B:729:GLY:HA3	1:B:744:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:926:ILE:O	1:F:930:GLY:N	2.46	0.47
1:F:999:ARG:HA	1:F:1003:ASP:HB2	1.95	0.47
1:A:771:ASN:OD1	1:A:772:PRO:HD2	2.15	0.47
1:B:717:VAL:HG23	1:B:727:TYR:CE2	2.49	0.47
1:B:880:TRP:NE1	1:B:906:GLU:OE2	2.36	0.47
1:E:943:VAL:HG21	1:E:979:LEU:CD2	2.45	0.47
1:F:729:GLY:HA3	1:F:744:ILE:CD1	2.37	0.47
1:H:729:GLY:HA3	1:H:744:ILE:CD1	2.45	0.47
1:H:831:ARG:CB	1:H:833:LEU:HD12	2.45	0.47
1:H:935:GLN:CD	1:H:944:TYR:CD2	2.91	0.47
1:C:816:ASN:O	1:C:820:GLN:CG	2.59	0.47
1:C:849:GLN:N	1:C:849:GLN:CD	2.72	0.47
1:C:1007:MET:HG2	1:C:1008:ASP:C	2.40	0.47
1:A:992:PRO:O	1:A:996:ASN:HB2	2.14	0.47
1:B:813:TYR:OH	1:B:990:PRO:HB3	2.15	0.47
1:B:835:HIS:HE2	1:B:838:LEU:HB2	1.80	0.47
1:E:707:LEU:HD13	1:E:789:ILE:HG12	1.92	0.47
1:D:812:GLN:NE2	1:D:1011:VAL:O	2.43	0.46
1:D:942:ASP:CG	1:F:934:PRO:HG3	2.40	0.46
1:E:795:PHE:HB2	1:E:845:VAL:HB	1.96	0.46
1:E:795:PHE:N	1:E:795:PHE:CD2	2.84	0.46
1:F:844:LEU:O	1:F:851:VAL:HG12	2.15	0.46
1:H:974:ASP:O	1:H:978:TYR:CD2	2.67	0.46
1:A:900:TYR:C	1:A:900:TYR:CD2	2.93	0.46
1:A:999:ARG:O	1:A:1003:ASP:O	2.34	0.46
1:B:771:ASN:HD21	1:B:772:PRO:HD2	1.70	0.46
1:B:778:LEU:HD11	1:B:791:GLN:CG	2.38	0.46
1:B:783:THR:HG22	1:B:784:SER:H	1.75	0.46
1:F:811:SER:HB3	1:F:984:ASP:CG	2.39	0.46
1:F:926:ILE:HB	1:F:931:GLU:HG3	1.97	0.46
1:G:707:LEU:HD13	1:G:789:ILE:HD13	1.97	0.46
1:H:991:SER:HG	1:H:994:ASP:CG	2.22	0.46
1:A:940:THR:CG2	1:A:942:ASP:H	2.28	0.46
1:B:712:PHE:CE2	1:B:789:ILE:HD11	2.50	0.46
1:D:706:ILE:N	1:D:706:ILE:CD1	2.78	0.46
1:D:795:PHE:CB	1:D:845:VAL:CG1	2.93	0.46
1:F:772:PRO:HB3	1:F:1007:MET:HA	1.97	0.46
1:F:839:ALA:O	1:F:843:VAL:HG23	2.15	0.46
1:F:989:LEU:HD23	1:F:990:PRO:C	2.40	0.46
1:F:995:SER:O	1:F:999:ARG:CG	2.62	0.46
1:C:777:LEU:HB2	2:C:1101:816:CAA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:942:ASP:OD2	1:C:942:ASP:N	2.43	0.46
1:A:966:ILE:HG22	1:A:970:LYS:HE3	1.96	0.46
1:B:905:TRP:CD2	1:B:933:LEU:HD13	2.50	0.46
1:E:892:THR:O	1:E:895:SER:HB2	2.15	0.46
1:F:855:ASP:HA	1:F:858:LEU:HD13	1.97	0.46
1:F:888:HIS:HB2	1:F:890:ILE:HG13	1.97	0.46
1:G:943:VAL:O	1:G:946:ILE:HB	2.15	0.46
1:H:825:MET:HG2	1:H:853:ILE:HD12	1.97	0.46
1:A:769:VAL:HG21	1:A:856:PHE:CZ	2.51	0.46
1:A:774:VAL:HG21	1:A:824:GLY:O	2.16	0.46
1:A:894:GLN:CB	1:A:955:ALA:HB1	2.46	0.46
1:E:829:GLU:HA	1:E:893:HIS:CE1	2.50	0.46
1:H:707:LEU:HD13	1:H:789:ILE:HD13	0.57	0.46
1:H:741:PRO:C	1:H:742:VAL:CG1	2.88	0.46
1:A:812:GLN:HE21	1:A:812:GLN:HB2	1.49	0.46
1:B:704:LEU:HD23	1:B:764:TYR:CD1	2.50	0.46
1:D:826:ASN:HB2	1:D:961:PHE:HB3	1.97	0.46
1:D:844:LEU:HG	1:D:854:THR:HG21	1.98	0.46
1:D:970:LYS:HA	1:D:973:ARG:HG3	1.97	0.46
1:C:905:TRP:CE3	1:C:909:THR:HG21	2.50	0.46
1:A:716:LYS:HB3	1:A:728:LYS:HB3	1.97	0.46
1:A:834:VAL:CB	4:A:1209:HOH:O	2.49	0.46
1:D:926:ILE:HB	1:D:931:GLU:HG3	1.98	0.46
1:E:793:MET:HE3	1:E:846:LYS:CA	2.46	0.46
1:E:793:MET:HE3	1:E:846:LYS:N	2.31	0.46
1:E:846:LYS:CE	1:E:1003:ASP:OD2	2.64	0.46
1:G:900:TYR:O	1:G:904:VAL:HG23	2.16	0.46
1:H:715:ILE:HD11	1:H:728:LYS:CD	2.45	0.46
1:H:845:VAL:HG12	1:H:847:THR:C	2.36	0.46
1:D:717:VAL:CG1	1:D:727:TYR:HE2	2.15	0.46
1:D:897:VAL:HG11	1:D:959:PRO:O	2.15	0.46
1:E:892:THR:H	1:E:895:SER:HB2	1.81	0.46
1:C:777:LEU:HD12	1:C:789:ILE:O	2.15	0.46
1:C:780:ILE:O	1:C:780:ILE:CG2	2.62	0.46
1:C:836:ARG:HG2	1:C:891:TYR:CG	2.51	0.46
1:A:811:SER:CB	1:A:984:ASP:OD2	2.64	0.46
1:A:835:HIS:C	1:A:835:HIS:ND1	2.74	0.46
1:B:939:CYS:SG	1:B:943:VAL:HG11	2.56	0.46
1:E:950:CYS:HA	1:E:958:ARG:CG	2.46	0.46
1:E:977:ARG:CG	1:C:918:ILE:HD11	2.42	0.46
1:F:885:SER:OG	1:F:890:ILE:O	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:946:ILE:HD12	1:G:971:MET:CE	2.46	0.46
1:C:968:PHE:O	1:C:971:MET:HB2	2.16	0.46
1:A:811:SER:HB3	1:A:984:ASP:OD2	2.16	0.45
1:B:821:ILE:HG23	1:B:853:ILE:HD11	1.97	0.45
1:B:961:PHE:HA	1:B:964:LEU:HB2	1.98	0.45
1:E:793:MET:O	2:E:1101:816:C2	2.64	0.45
1:E:798:LEU:CD2	1:E:907:LEU:HD21	2.45	0.45
1:G:940:THR:HG23	1:G:942:ASP:N	2.31	0.45
1:C:769:VAL:O	1:C:769:VAL:HG22	2.17	0.45
1:C:825:MET:HB3	1:C:961:PHE:CE1	2.52	0.45
1:C:856:PHE:CD1	1:C:857:GLY:CA	2.98	0.45
1:A:880:TRP:HA	1:A:902:VAL:HG21	1.98	0.45
1:A:881:MET:CE	1:A:885:SER:HB3	2.40	0.45
1:B:780:ILE:CD1	1:B:782:LEU:HD22	2.42	0.45
1:B:910:PHE:CE2	1:B:938:ILE:CD1	2.99	0.45
1:B:977:ARG:O	1:D:918:ILE:HD11	2.16	0.45
1:D:833:LEU:HD13	1:D:856:PHE:CE1	2.52	0.45
1:D:961:PHE:O	1:D:965:ILE:HG13	2.15	0.45
1:E:708:LYS:O	1:E:711:GLU:HB2	2.16	0.45
1:E:759:ILE:CG2	1:E:760:LEU:N	2.79	0.45
1:E:836:ARG:CD	1:E:860:LYS:HA	2.45	0.45
1:F:929:LYS:HA	1:F:929:LYS:HD2	1.71	0.45
1:H:708:LYS:O	1:H:712:PHE:CE1	2.69	0.45
1:H:743:ALA:CB	2:H:1101:816:NAB	2.78	0.45
1:H:762:GLU:HG2	1:H:861:LEU:HD23	1.99	0.45
1:C:972:ALA:C	1:C:975:PRO:HD3	2.37	0.45
1:A:700:ASN:CB	1:A:703:LEU:HD11	2.46	0.45
1:A:767:ALA:CB	1:A:777:LEU:O	2.64	0.45
1:B:798:LEU:HD12	1:B:801:TYR:HB3	1.97	0.45
1:G:718:LEU:HD11	1:G:792:LEU:HD12	1.97	0.45
1:G:908:MET:HE1	1:G:979:LEU:HD11	1.98	0.45
1:H:945:MET:HE3	3:H:1104:EDO:H22	1.98	0.45
1:B:895:SER:O	1:B:898:TRP:HB3	2.16	0.45
1:F:999:ARG:HA	1:F:1003:ASP:HB3	1.96	0.45
1:G:861:LEU:HD23	1:G:861:LEU:N	2.31	0.45
1:G:897:VAL:HA	1:G:900:TYR:HB3	1.98	0.45
1:H:778:LEU:CD2	1:H:778:LEU:H	2.06	0.45
1:D:950:CYS:HA	1:D:958:ARG:HG2	1.98	0.45
1:E:818:CYS:O	1:E:900:TYR:OH	2.31	0.45
1:F:813:TYR:CE1	1:F:989:LEU:HB2	2.52	0.45
1:F:923:ILE:O	1:F:927:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:915:TYR:CE1	1:G:926:ILE:CD1	2.93	0.45
1:H:775:CYS:HG	1:H:854:THR:HG1	1.58	0.45
1:H:859:ALA:O	1:H:862:LEU:C	2.59	0.45
1:A:708:LYS:O	1:A:711:GLU:CG	2.64	0.45
1:A:972:ALA:O	1:A:975:PRO:HG3	2.17	0.45
1:D:707:LEU:HD23	1:D:711:GLU:CD	2.42	0.45
1:E:991:SER:OG	1:E:992:PRO:CD	2.64	0.45
1:G:777:LEU:HD11	1:G:788:LEU:HB3	1.97	0.45
1:G:944:TYR:O	1:G:948:VAL:N	2.45	0.45
1:C:780:ILE:O	1:C:780:ILE:HG22	2.15	0.45
1:D:719:GLY:HA3	2:D:1101:816:CAO	2.46	0.45
1:E:961:PHE:HA	1:E:964:LEU:HB2	1.98	0.45
1:G:971:MET:O	1:G:974:ASP:C	2.59	0.45
1:G:990:PRO:HB2	1:G:994:ASP:HB2	1.99	0.45
1:C:720:SER:OG	1:C:725:THR:HG22	2.17	0.45
1:C:940:THR:HG23	1:C:942:ASP:N	2.31	0.45
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.50	0.45
1:A:915:TYR:OH	1:A:927:LEU:HD21	2.17	0.45
1:A:938:ILE:O	1:A:938:ILE:CG1	2.63	0.45
1:B:835:HIS:O	1:B:835:HIS:CD2	2.70	0.45
1:D:886:ILE:HG21	1:D:924:SER:HB2	1.99	0.45
1:E:850:HIS:ND1	1:E:1003:ASP:OD2	2.32	0.45
1:E:973:ARG:HH11	1:E:973:ARG:CG	2.30	0.45
1:F:733:PRO:HB2	1:F:736:GLU:CB	2.44	0.45
1:G:855:ASP:OD1	1:G:858:LEU:HD22	2.17	0.45
1:G:858:LEU:HD12	1:G:861:LEU:HG	1.99	0.45
1:H:739:LYS:HB3	1:H:739:LYS:HE3	1.57	0.45
1:C:932:ARG:HH22	1:C:953:ILE:HD11	1.81	0.45
1:A:793:MET:HE3	1:A:844:LEU:HB3	1.98	0.45
1:B:717:VAL:HG23	1:B:727:TYR:CD2	2.52	0.45
1:D:729:GLY:HA3	1:D:744:ILE:CD1	2.47	0.45
1:E:826:ASN:O	1:E:829:GLU:HB3	2.17	0.45
1:G:782:LEU:C	1:G:783:THR:HG23	2.42	0.45
1:C:825:MET:CB	1:C:961:PHE:CE1	2.99	0.45
1:C:878:ILE:CG2	1:C:886:ILE:HD11	2.28	0.45
1:A:831:ARG:O	1:A:832:ARG:CB	2.63	0.45
1:A:966:ILE:O	1:A:970:LYS:HG3	2.16	0.45
1:B:999:ARG:HB3	1:B:999:ARG:CZ	2.47	0.45
1:D:939:CYS:SG	1:D:943:VAL:HG11	2.57	0.45
1:D:977:ARG:HG2	1:D:978:TYR:CE2	2.52	0.45
1:E:837:ASP:OD1	1:E:838:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:971:MET:HA	1:E:978:TYR:CE2	2.51	0.45
1:G:943:VAL:HG21	1:G:979:LEU:CD2	2.46	0.45
1:H:816:ASN:O	1:H:820:GLN:HG3	2.17	0.45
1:H:913:LYS:NZ	4:H:1204:HOH:O	2.49	0.45
1:C:715:ILE:HD11	1:C:728:LYS:HD3	1.99	0.45
1:C:780:ILE:HD13	1:C:780:ILE:HA	1.62	0.45
1:A:885:SER:HB3	1:A:891:TYR:CE1	2.52	0.44
1:B:723:PHE:HB3	1:B:858:LEU:HD23	1.99	0.44
1:B:898:TRP:CE3	1:B:951:TRP:HA	2.52	0.44
1:H:708:LYS:HG3	1:H:711:GLU:CD	2.42	0.44
1:H:971:MET:HA	1:H:978:TYR:CE2	2.52	0.44
1:A:793:MET:CE	1:A:844:LEU:CB	2.96	0.44
1:B:777:LEU:HD12	1:B:789:ILE:O	2.17	0.44
1:B:835:HIS:CE1	1:B:837:ASP:O	2.70	0.44
1:E:879:LYS:HG2	1:E:923:ILE:HD13	1.99	0.44
1:F:836:ARG:CB	1:F:859:ALA:HB3	2.38	0.44
1:G:765:VAL:O	1:G:768:SER:HB3	2.16	0.44
1:H:764:TYR:HD1	1:H:764:TYR:HA	1.71	0.44
1:H:935:GLN:HB2	1:H:944:TYR:CD1	2.52	0.44
1:A:719:GLY:HA3	2:A:1101:816:CAS	2.48	0.44
1:B:961:PHE:O	1:B:965:ILE:HG13	2.17	0.44
1:E:771:ASN:CG	1:E:772:PRO:HD2	2.42	0.44
1:F:944:TYR:O	1:F:948:VAL:HG23	2.16	0.44
1:F:977:ARG:O	1:G:918:ILE:HD11	2.18	0.44
1:G:757:LYS:C	1:G:757:LYS:HD2	2.41	0.44
1:G:825:MET:CE	1:G:838:LEU:HD22	2.47	0.44
1:H:965:ILE:O	1:H:969:SER:OG	2.30	0.44
1:C:835:HIS:NE2	1:C:856:PHE:N	2.65	0.44
1:A:762:GLU:OE1	1:A:861:LEU:HD21	2.17	0.44
1:D:898:TRP:CD1	1:D:898:TRP:C	2.95	0.44
1:E:718:LEU:HB2	1:E:726:VAL:C	2.39	0.44
1:E:941:ILE:HG13	1:E:945:MET:CE	2.48	0.44
1:G:821:ILE:CG2	1:G:900:TYR:HE1	2.30	0.44
1:G:850:HIS:HD2	1:G:851:VAL:N	2.14	0.44
1:G:879:LYS:CG	1:G:915:TYR:HB2	2.47	0.44
1:G:925:SER:O	1:G:929:LYS:CG	2.65	0.44
1:H:766:MET:CE	1:H:777:LEU:HD22	2.47	0.44
1:C:889:ARG:HD3	1:C:889:ARG:HA	1.36	0.44
1:A:771:ASN:CG	1:A:772:PRO:HD2	2.43	0.44
1:B:923:ILE:HA	1:B:926:ILE:HG12	1.98	0.44
1:D:831:ARG:HE	1:D:831:ARG:HB3	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:949:LYS:HB2	1:D:949:LYS:HE3	1.60	0.44
1:E:745:LYS:HZ1	1:E:858:LEU:CD2	2.31	0.44
1:E:949:LYS:HB2	1:E:949:LYS:HE3	1.48	0.44
1:E:961:PHE:O	1:E:964:LEU:N	2.50	0.44
1:F:881:MET:HE3	1:F:886:ILE:CG1	2.46	0.44
1:G:855:ASP:HA	2:G:1101:816:CAK	2.47	0.44
1:H:936:PRO:HA	1:H:937:PRO:HD3	1.90	0.44
1:H:952:MET:HB2	1:H:958:ARG:HG2	1.99	0.44
1:C:717:VAL:HG22	1:C:727:TYR:CD2	2.52	0.44
1:A:849:GLN:OE1	1:A:995:SER:CB	2.61	0.44
1:A:849:GLN:HE21	1:A:849:GLN:H	1.64	0.44
1:E:861:LEU:HD22	1:E:861:LEU:HA	1.76	0.44
1:F:708:LYS:CA	1:F:711:GLU:CG	2.96	0.44
1:G:790:MET:HE2	1:G:791:GLN:O	2.18	0.44
1:G:883:LEU:HD22	1:G:953:ILE:HD12	1.99	0.44
1:G:902:VAL:O	1:G:906:GLU:HG3	2.18	0.44
1:C:730:LEU:HD12	1:C:739:LYS:HB3	2.00	0.44
1:C:747:LEU:HD21	1:C:788:LEU:HD11	1.99	0.44
1:A:715:ILE:HG12	1:A:728:LYS:O	2.17	0.44
1:A:736:GLU:OE2	1:A:736:GLU:HA	2.18	0.44
1:D:965:ILE:O	1:D:969:SER:OG	2.31	0.44
1:E:743:ALA:O	1:E:744:ILE:HD12	2.18	0.44
1:F:714:LYS:HE2	1:F:787:GLN:OE1	2.18	0.44
1:F:954:ASP:O	1:F:957:SER:OG	2.34	0.44
1:G:898:TRP:HZ3	1:G:952:MET:O	2.01	0.44
1:H:913:LYS:HA	1:H:914:PRO:HD3	1.84	0.44
1:C:769:VAL:HG11	1:C:856:PHE:CE2	2.44	0.44
1:C:772:PRO:O	1:C:852:LYS:HG2	2.16	0.44
1:C:935:GLN:HA	1:C:936:PRO:HD3	1.76	0.44
1:B:777:LEU:CD2	1:B:788:LEU:HD22	2.38	0.44
1:B:881:MET:CE	1:B:891:TYR:CE1	2.99	0.44
1:D:707:LEU:CD2	1:D:711:GLU:CG	2.96	0.44
1:D:933:LEU:HB3	1:D:934:PRO:HD2	2.00	0.44
1:E:703:LEU:N	1:E:703:LEU:HD23	2.33	0.44
1:F:747:LEU:CG	1:F:788:LEU:HD11	2.43	0.44
1:A:835:HIS:CE1	1:A:837:ASP:O	2.70	0.44
1:E:774:VAL:HG11	1:E:828:LEU:HD21	2.00	0.44
1:E:780:ILE:O	1:E:780:ILE:CG2	2.63	0.44
1:G:889:ARG:NH1	1:G:889:ARG:HG3	2.31	0.44
1:G:904:VAL:HG12	1:G:947:MET:HE2	1.99	0.44
1:C:715:ILE:HD11	1:C:728:LYS:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:LEU:O	1:C:802:VAL:CG2	2.66	0.44
1:C:806:LYS:HB2	1:C:806:LYS:HE2	1.38	0.44
1:B:967:GLU:O	1:B:971:MET:HG3	2.18	0.43
1:D:729:GLY:HA3	1:D:744:ILE:HD12	2.00	0.43
1:D:799:LEU:O	1:D:802:VAL:CG2	2.65	0.43
1:D:879:LYS:H	1:D:879:LYS:HG2	1.56	0.43
1:D:893:HIS:O	1:D:896:ASP:HB2	2.19	0.43
1:F:708:LYS:CA	1:F:711:GLU:HG3	2.47	0.43
1:B:760:LEU:HD12	1:B:760:LEU:HA	1.84	0.43
1:B:802:VAL:HG11	1:B:907:LEU:CD2	2.46	0.43
1:B:813:TYR:HE1	1:B:988:HIS:O	2.01	0.43
1:E:908:MET:O	1:E:938:ILE:CG2	2.66	0.43
1:G:944:TYR:O	1:G:947:MET:N	2.51	0.43
1:H:938:ILE:HA	1:H:980:VAL:O	2.18	0.43
1:A:735:GLY:N	4:A:1203:HOH:O	2.52	0.43
1:A:783:THR:CG2	1:A:784:SER:N	2.73	0.43
1:B:904:VAL:O	1:B:908:MET:HG2	2.18	0.43
1:B:926:ILE:O	1:B:929:LYS:HB2	2.18	0.43
1:D:830:ASP:O	1:G:725:THR:HG23	2.18	0.43
1:D:966:ILE:O	1:D:970:LYS:HG3	2.19	0.43
1:F:707:LEU:HD22	1:F:712:PHE:HD1	1.83	0.43
1:F:878:ILE:CG2	1:F:923:ILE:HG21	2.48	0.43
1:A:958:ARG:HA	1:A:959:PRO:HD3	1.86	0.43
1:B:708:LYS:HB2	1:B:711:GLU:HG2	1.99	0.43
1:B:977:ARG:NE	1:D:931:GLU:HB2	2.33	0.43
1:D:774:VAL:HG11	1:D:828:LEU:HD21	1.99	0.43
1:D:898:TRP:CZ2	1:D:927:LEU:HD13	2.54	0.43
1:E:844:LEU:HD23	1:E:854:THR:CG2	2.47	0.43
1:E:893:HIS:O	1:E:896:ASP:HB2	2.19	0.43
1:F:799:LEU:O	1:F:802:VAL:HG22	2.17	0.43
1:F:813:TYR:OH	1:F:849:GLN:NE2	2.51	0.43
1:G:790:MET:CE	1:G:791:GLN:O	2.67	0.43
1:G:823:LYS:CA	1:G:965:ILE:HD11	2.45	0.43
1:B:705:ARG:HG2	1:B:707:LEU:CD2	2.48	0.43
1:B:783:THR:C	1:B:785:THR:N	2.73	0.43
1:B:940:THR:CG2	1:B:978:TYR:O	2.66	0.43
1:D:992:PRO:HD2	1:D:993:THR:H	1.84	0.43
1:F:897:VAL:CG2	4:F:1228:HOH:O	2.62	0.43
1:G:985:GLU:CG	1:G:986:ARG:N	2.81	0.43
1:H:976:GLN:HG2	1:H:984:ASP:OD2	2.19	0.43
1:C:925:SER:O	1:C:929:LYS:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:TRP:CE3	1:A:740:ILE:HD13	2.54	0.43
1:B:730:LEU:HB3	1:B:739:LYS:HB3	2.00	0.43
1:E:913:LYS:NZ	4:E:1203:HOH:O	2.52	0.43
1:F:898:TRP:HZ2	1:F:927:LEU:HD13	1.83	0.43
1:F:973:ARG:O	1:F:1013:ALA:HA	2.19	0.43
1:G:923:ILE:C	1:G:926:ILE:HG23	2.44	0.43
1:C:745:LYS:O	1:C:788:LEU:HD12	2.17	0.43
1:C:897:VAL:HG21	1:C:959:PRO:O	2.18	0.43
1:A:893:HIS:HA	1:A:896:ASP:HB2	2.01	0.43
1:B:760:LEU:HD13	1:B:782:LEU:CD2	2.48	0.43
1:B:790:MET:HE1	1:B:844:LEU:HD12	2.01	0.43
1:B:941:ILE:HG23	1:B:942:ASP:N	2.33	0.43
1:D:941:ILE:O	1:D:941:ILE:HG13	2.14	0.43
1:E:950:CYS:O	1:E:958:ARG:HG2	2.18	0.43
1:F:884:GLU:H	1:F:884:GLU:CD	2.26	0.43
1:F:926:ILE:HA	1:F:929:LYS:HB2	2.01	0.43
1:F:977:ARG:HH21	1:F:977:ARG:CG	2.31	0.43
1:H:1007:MET:HE1	1:H:1010:VAL:CG1	2.48	0.43
1:C:881:MET:CE	1:C:886:ILE:CG1	2.91	0.43
1:A:805:HIS:HB3	1:A:809:ILE:CG1	2.48	0.43
1:B:813:TYR:CE1	1:B:988:HIS:O	2.72	0.43
1:B:939:CYS:SG	1:B:943:VAL:CG1	3.07	0.43
1:E:771:ASN:OD1	1:E:772:PRO:HD2	2.19	0.43
1:G:850:HIS:CD2	1:G:850:HIS:C	2.97	0.43
1:G:977:ARG:NH2	1:G:978:TYR:CE1	2.86	0.43
1:G:991:SER:HB2	1:G:994:ASP:OD2	2.18	0.43
1:H:745:LYS:HB2	1:H:745:LYS:HE3	1.49	0.43
1:B:831:ARG:HB3	1:B:833:LEU:HD12	1.99	0.43
1:F:972:ALA:CB	1:F:1011:VAL:HG11	2.43	0.43
1:F:1007:MET:CG	1:F:1008:ASP:O	2.64	0.43
1:A:885:SER:HA	1:A:890:ILE:H	1.84	0.43
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.54	0.43
1:F:884:GLU:O	1:F:888:HIS:N	2.32	0.43
1:G:821:ILE:CG2	1:G:900:TYR:CE1	3.02	0.43
1:H:768:SER:OG	1:H:831:ARG:NH2	2.52	0.43
1:C:712:PHE:CD2	1:C:712:PHE:C	2.97	0.43
1:C:846:LYS:HG3	1:C:847:THR:HG23	2.01	0.43
1:C:940:THR:HG22	1:C:943:VAL:CG2	2.38	0.43
1:A:846:LYS:HD3	1:A:852:LYS:CD	2.49	0.42
1:D:885:SER:O	1:D:889:ARG:HA	2.18	0.42
1:D:902:VAL:O	1:D:905:TRP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:771:ASN:HD21	1:F:772:PRO:HD2	1.73	0.42
1:G:776:ARG:NH1	1:G:776:ARG:HG2	2.35	0.42
1:G:939:CYS:SG	1:G:947:MET:HE1	2.59	0.42
1:G:971:MET:O	1:G:974:ASP:N	2.51	0.42
1:H:935:GLN:HA	1:H:936:PRO:HD3	1.74	0.42
1:B:856:PHE:O	1:B:856:PHE:CG	2.72	0.42
1:D:777:LEU:HD11	1:D:788:LEU:CB	2.50	0.42
1:E:772:PRO:O	1:E:852:LYS:HG2	2.18	0.42
1:E:884:GLU:OE2	1:E:895:SER:OG	2.33	0.42
1:E:913:LYS:O	1:E:916:ASP:HB2	2.18	0.42
1:E:941:ILE:HG23	1:E:945:MET:CE	2.49	0.42
1:F:721:GLY:C	1:F:724:GLY:O	2.62	0.42
1:F:1006:ASP:OD2	1:F:1006:ASP:N	2.52	0.42
1:H:743:ALA:CB	2:H:1101:816:N1	2.83	0.42
1:H:878:ILE:HG22	1:H:923:ILE:HG13	2.01	0.42
1:C:984:ASP:OD2	1:C:984:ASP:O	2.37	0.42
1:C:991:SER:HB2	1:C:992:PRO:CD	2.50	0.42
1:A:974:ASP:OD2	1:E:929:LYS:HE2	2.19	0.42
1:B:889:ARG:HD2	1:B:889:ARG:HA	1.83	0.42
1:D:821:ILE:HG22	1:D:900:TYR:HE1	1.84	0.42
1:D:950:CYS:O	1:D:958:ARG:CG	2.67	0.42
1:D:1008:ASP:OD1	1:D:1009:ASP:N	2.51	0.42
1:E:793:MET:HE1	1:E:852:LYS:HD3	2.02	0.42
1:E:814:LEU:HD11	1:E:910:PHE:HE1	1.84	0.42
1:E:818:CYS:SG	1:E:904:VAL:CG2	3.05	0.42
1:F:846:LYS:C	1:F:847:THR:CG2	2.92	0.42
1:G:772:PRO:HB2	1:G:773:HIS:CD2	2.54	0.42
1:G:952:MET:HE3	1:G:952:MET:HB3	1.69	0.42
1:H:757:LYS:O	1:H:757:LYS:HD3	2.20	0.42
1:H:846:LYS:C	1:H:847:THR:CG2	2.92	0.42
1:H:903:THR:O	1:H:906:GLU:HB2	2.19	0.42
1:H:904:VAL:CG1	1:H:947:MET:HE2	2.49	0.42
1:C:1007:MET:CG	1:C:1008:ASP:N	2.68	0.42
1:A:707:LEU:HB3	1:A:712:PHE:HE1	1.85	0.42
1:A:878:ILE:CD1	1:A:920:ALA:HB1	2.49	0.42
1:B:850:HIS:C	1:B:850:HIS:CD2	2.96	0.42
1:D:732:ILE:HA	1:D:733:PRO:HD2	1.92	0.42
1:D:845:VAL:HG13	1:D:847:THR:O	2.19	0.42
1:E:712:PHE:CE2	1:E:744:ILE:HG13	2.54	0.42
1:F:813:TYR:HE1	1:F:989:LEU:HA	1.83	0.42
1:G:726:VAL:HG22	1:G:745:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:889:ARG:HA	1:G:889:ARG:HD2	1.53	0.42
1:C:728:LYS:HZ3	1:C:730:LEU:CD2	2.27	0.42
1:C:855:ASP:H	2:C:1101:816:CAH	2.33	0.42
1:D:714:LYS:HB3	1:D:744:ILE:HD13	2.00	0.42
1:D:901:GLY:O	1:D:905:TRP:N	2.47	0.42
1:D:941:ILE:HG13	1:D:945:MET:HG3	2.01	0.42
1:E:730:LEU:HD23	1:E:730:LEU:HA	1.61	0.42
1:E:795:PHE:H	1:E:795:PHE:HD2	1.66	0.42
1:F:805:HIS:O	1:F:809:ILE:CG1	2.67	0.42
1:F:977:ARG:HH21	1:G:926:ILE:HD12	1.85	0.42
1:F:999:ARG:HB3	1:F:1003:ASP:HB3	2.01	0.42
1:G:938:ILE:HB	1:G:980:VAL:O	2.20	0.42
1:H:704:LEU:HB3	1:H:764:TYR:CE1	2.54	0.42
1:C:973:ARG:C	1:C:975:PRO:HD3	2.43	0.42
1:A:738:VAL:HG22	1:A:739:LYS:N	2.35	0.42
1:A:922:GLU:OE2	1:A:926:ILE:HG22	2.18	0.42
1:A:933:LEU:HA	1:A:934:PRO:HD3	1.79	0.42
1:B:884:GLU:OE1	1:B:958:ARG:NH1	2.41	0.42
1:B:890:ILE:O	1:B:890:ILE:HG22	2.19	0.42
1:D:757:LYS:HD3	1:D:761:ASP:OD1	2.18	0.42
1:D:877:PRO:HB2	1:D:880:TRP:HB2	2.02	0.42
1:E:806:LYS:O	1:E:910:PHE:CE2	2.73	0.42
1:C:707:LEU:HD11	1:C:789:ILE:CD1	2.35	0.42
1:B:733:PRO:HB2	1:B:736:GLU:CB	2.46	0.42
1:E:819:VAL:CG2	1:E:968:PHE:HB3	2.50	0.42
1:F:778:LEU:HD22	1:F:778:LEU:H	1.84	0.42
1:G:773:HIS:CE1	1:G:820:GLN:CG	3.03	0.42
1:C:758:GLU:OE2	1:C:759:ILE:HA	2.19	0.42
1:C:884:GLU:HG2	1:C:885:SER:N	2.34	0.42
1:A:821:ILE:O	1:A:825:MET:HG2	2.19	0.42
1:A:881:MET:HE2	1:A:881:MET:HB3	1.84	0.42
1:B:898:TRP:CZ3	1:B:951:TRP:O	2.73	0.42
1:B:966:ILE:CG2	1:B:970:LYS:HE3	2.49	0.42
1:D:894:GLN:HA	1:D:897:VAL:HG23	2.02	0.42
1:D:950:CYS:O	1:D:958:ARG:HG2	2.20	0.42
1:E:806:LYS:CG	1:E:807:ASP:N	2.83	0.42
1:E:835:HIS:NE2	1:E:856:PHE:HA	2.35	0.42
1:G:712:PHE:CZ	1:G:781:CYS:SG	3.13	0.42
1:H:729:GLY:O	1:H:730:LEU:HD23	2.18	0.42
1:H:856:PHE:CD1	1:H:856:PHE:C	2.98	0.42
1:C:973:ARG:O	1:C:1013:ALA:CA	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:LEU:O	1:A:783:THR:OG1	2.35	0.42
1:B:829:GLU:HG3	1:B:893:HIS:CG	2.55	0.42
1:B:1002:MET:HB2	1:B:1002:MET:HE2	1.77	0.42
1:E:845:VAL:HG12	1:E:847:THR:C	2.42	0.42
1:F:769:VAL:HB	1:F:827:TYR:HE2	1.85	0.42
1:F:776:ARG:O	2:F:1101:816:CAA	2.68	0.42
1:G:831:ARG:NH2	4:G:1206:HOH:O	2.52	0.42
1:G:876:VAL:HG11	1:G:889:ARG:HH21	1.85	0.42
1:H:732:ILE:HA	1:H:733:PRO:HD3	1.84	0.42
1:B:813:TYR:CE1	1:B:990:PRO:HD3	2.55	0.42
1:D:989:LEU:CB	1:D:990:PRO:HD2	2.50	0.42
1:G:858:LEU:O	1:G:859:ALA:C	2.59	0.42
1:H:798:LEU:HD12	1:H:798:LEU:HA	1.75	0.42
1:H:856:PHE:CD1	1:H:856:PHE:O	2.73	0.42
1:C:733:PRO:HB2	1:C:736:GLU:HB2	2.01	0.42
2:C:1101:816:CAP	2:C:1101:816:CAV	2.98	0.42
1:A:922:GLU:OE2	1:A:926:ILE:HG21	2.20	0.41
1:B:790:MET:HG2	2:B:1101:816:CLA	2.57	0.41
1:B:923:ILE:O	1:B:926:ILE:HG12	2.19	0.41
1:E:881:MET:HE2	1:E:886:ILE:HG12	2.00	0.41
1:E:904:VAL:HG12	1:E:905:TRP:N	2.33	0.41
1:E:913:LYS:HZ2	1:E:913:LYS:HG2	1.66	0.41
1:F:748:ARG:HG2	1:F:748:ARG:H	1.44	0.41
1:G:760:LEU:HD12	1:G:760:LEU:HA	1.73	0.41
1:G:1012:ASP:OD1	1:G:1013:ALA:N	2.53	0.41
1:H:793:MET:HA	1:H:794:PRO:HD3	1.89	0.41
1:H:918:ILE:HA	1:H:919:PRO:HD3	1.94	0.41
1:C:740:ILE:HA	1:C:741:PRO:HD3	1.86	0.41
1:A:769:VAL:HG21	1:A:856:PHE:HZ	1.85	0.41
1:A:858:LEU:HD13	1:A:858:LEU:HA	1.85	0.41
1:B:759:ILE:HD12	1:B:759:ILE:N	2.29	0.41
1:B:811:SER:OG	1:B:975:PRO:CB	2.66	0.41
1:D:812:GLN:HG2	1:D:975:PRO:HG3	2.00	0.41
1:D:923:ILE:O	1:D:926:ILE:CG1	2.63	0.41
1:E:723:PHE:CE2	1:E:859:ALA:CB	3.03	0.41
1:E:723:PHE:O	1:E:747:LEU:HD23	2.20	0.41
1:E:846:LYS:CE	1:E:1003:ASP:CG	2.93	0.41
1:F:806:LYS:HB3	1:F:910:PHE:HB3	2.00	0.41
1:F:841:ARG:HH12	1:F:877:PRO:HB3	1.84	0.41
1:G:938:ILE:HG13	1:G:939:CYS:N	2.31	0.41
1:H:708:LYS:HG2	1:H:711:GLU:OE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:LEU:HD12	1:C:839:ALA:N	2.34	0.41
1:A:815[B]:LEU:CD2	1:A:979:LEU:CD1	2.97	0.41
1:E:731:TRP:HB3	1:E:740:ILE:HB	2.01	0.41
1:G:822:ALA:HB3	1:G:965:ILE:HG12	2.02	0.41
1:H:841:ARG:CG	1:H:842:ASN:N	2.83	0.41
1:H:861:LEU:C	1:H:862:LEU:HG	2.43	0.41
1:A:878:ILE:HD13	1:A:920:ALA:HB1	2.01	0.41
1:D:771:ASN:CB	1:D:774:VAL:HG23	2.16	0.41
1:D:931:GLU:H	1:D:931:GLU:HG2	1.45	0.41
1:D:944:TYR:O	1:D:948:VAL:HG23	2.20	0.41
1:H:809:ILE:O	1:H:987:MET:SD	2.79	0.41
1:H:831:ARG:HB3	1:H:833:LEU:HD12	2.00	0.41
1:C:850:HIS:HD2	1:C:851:VAL:N	2.18	0.41
1:A:898:TRP:HZ2	1:A:927:LEU:HD13	1.79	0.41
1:A:945:MET:HE1	1:E:909:THR:CG2	2.49	0.41
1:B:815:LEU:O	1:B:819:VAL:CG2	2.66	0.41
1:F:839:ALA:HB3	1:F:841:ARG:HG2	2.02	0.41
1:F:923:ILE:O	1:F:926:ILE:HG12	2.20	0.41
1:C:856:PHE:HD1	1:C:857:GLY:CA	2.27	0.41
1:A:818:CYS:SG	1:A:904:VAL:HG13	2.61	0.41
1:B:955:ALA:HA	1:B:958:ARG:NH1	2.36	0.41
1:E:942:ASP:CG	1:E:977:ARG:NH1	2.79	0.41
1:G:852:LYS:HE3	1:G:852:LYS:HB3	1.84	0.41
1:G:883:LEU:CD2	1:G:953:ILE:HD12	2.50	0.41
1:H:900:TYR:O	1:H:904:VAL:HG23	2.20	0.41
1:C:775:CYS:N	1:C:853:ILE:O	2.51	0.41
1:C:809:ILE:C	1:C:987:MET:SD	3.04	0.41
1:C:997:PHE:O	1:C:1001:LEU:HD12	2.20	0.41
1:A:700:ASN:CA	1:A:703:LEU:HD12	2.48	0.41
1:A:888:HIS:O	1:D:888:HIS:CB	2.68	0.41
1:A:1002:MET:HE2	1:A:1002:MET:HB2	1.78	0.41
1:B:705:ARG:HD3	1:B:707:LEU:CD2	2.44	0.41
1:B:793:MET:HE3	1:B:844:LEU:CB	2.50	0.41
1:E:712:PHE:HE2	1:E:744:ILE:HG13	1.85	0.41
1:E:718:LEU:HB2	1:E:727:TYR:HA	2.02	0.41
1:E:793:MET:CE	1:E:846:LYS:HB2	2.49	0.41
1:F:835:HIS:CD2	1:F:856:PHE:CB	3.02	0.41
1:H:945:MET:HE1	3:H:1103:EDO:O2	2.20	0.41
1:C:892:THR:H	1:C:895:SER:HB3	1.85	0.41
1:C:966:ILE:HG22	1:C:967:GLU:N	2.34	0.41
1:A:982:GLN:OE1	1:A:982:GLN:CA	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:ALA:O	1:B:776:ARG:CG	2.69	0.41
1:B:775:CYS:HB2	1:B:853:ILE:O	2.21	0.41
1:B:777:LEU:HD21	1:B:788:LEU:CD2	2.41	0.41
1:E:705:ARG:O	1:E:779:GLY:HA2	2.20	0.41
1:E:723:PHE:HE2	1:E:859:ALA:CB	2.33	0.41
1:H:771:ASN:HA	1:H:772:PRO:HD3	1.95	0.41
1:C:880:TRP:CZ2	1:C:906:GLU:OE2	2.74	0.41
1:A:806:LYS:C	1:A:806:LYS:HD3	2.43	0.41
1:B:801:TYR:CE1	1:B:805:HIS:CE1	3.09	0.41
1:B:835:HIS:CB	1:B:856:PHE:HA	2.42	0.41
1:B:961:PHE:O	1:B:965:ILE:N	2.45	0.41
1:D:782:LEU:O	1:D:783:THR:OG1	2.35	0.41
1:D:793:MET:HA	1:D:794:PRO:HD2	1.97	0.41
1:D:827:TYR:O	1:D:830:ASP:HB2	2.21	0.41
1:E:723:PHE:N	1:E:723:PHE:CD1	2.89	0.41
1:F:762:GLU:H	1:F:762:GLU:HG2	1.59	0.41
1:F:1007:MET:HE2	1:F:1008:ASP:O	2.21	0.41
1:G:802:VAL:HG12	1:G:809:ILE:HD12	2.03	0.41
1:G:904:VAL:CG1	1:G:947:MET:HE2	2.51	0.41
1:G:908:MET:HG3	1:G:939:CYS:SG	2.61	0.41
1:H:762:GLU:HG2	1:H:861:LEU:CD2	2.51	0.41
1:C:716:LYS:HG3	1:C:717:VAL:H	1.80	0.41
1:C:835:HIS:HE2	1:C:856:PHE:N	2.18	0.41
1:A:778:LEU:HG	1:A:790:MET:HA	2.03	0.41
1:A:813:TYR:OH	1:A:990:PRO:CD	2.68	0.41
1:A:976:GLN:H	1:A:976:GLN:HG2	1.34	0.41
1:E:717:VAL:HG13	1:E:727:TYR:CE2	2.55	0.41
1:E:945:MET:HE3	1:C:934:PRO:HG3	2.02	0.41
1:F:884:GLU:HG2	1:F:885:SER:H	1.82	0.41
1:F:935:GLN:HB3	1:F:944:TYR:CE2	2.56	0.41
1:G:960:LYS:HA	4:G:1203:HOH:O	2.19	0.41
1:H:905:TRP:CZ2	1:H:933:LEU:HD22	2.56	0.41
1:D:961:PHE:O	1:D:964:LEU:N	2.54	0.40
1:E:898:TRP:CH2	1:E:927:LEU:HD22	2.56	0.40
1:H:744:ILE:HA	1:H:788:LEU:O	2.20	0.40
1:C:736:GLU:OE2	1:C:736:GLU:CA	2.54	0.40
1:A:811:SER:OG	1:A:975:PRO:CB	2.68	0.40
1:A:977:ARG:CD	1:A:977:ARG:C	2.95	0.40
1:B:782:LEU:HA	1:B:782:LEU:HD13	1.75	0.40
1:B:820:GLN:NE2	1:B:849:GLN:O	2.50	0.40
1:G:898:TRP:CZ3	1:G:952:MET:O	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:783:THR:OG1	1:H:785:THR:O	2.37	0.40
1:H:791:GLN:HG3	1:H:792:LEU:N	2.36	0.40
1:C:703:LEU:HD13	1:C:768:SER:HA	2.03	0.40
1:C:827:TYR:OH	1:C:831:ARG:HD2	2.22	0.40
1:C:879:LYS:NZ	1:C:918:ILE:O	2.43	0.40
1:A:898:TRP:HZ2	1:A:927:LEU:CD1	2.34	0.40
1:B:938:ILE:HG22	1:B:979:LEU:HB3	2.03	0.40
1:B:952:MET:O	1:B:958:ARG:CZ	2.70	0.40
1:D:812:GLN:CG	1:D:975:PRO:HG2	2.51	0.40
1:D:814:LEU:HD11	1:D:910:PHE:HE1	1.87	0.40
1:D:836:ARG:HG2	1:D:891:TYR:CD1	2.56	0.40
1:D:938:ILE:HG12	1:D:939:CYS:N	2.32	0.40
1:E:729:GLY:N	1:E:742:VAL:O	2.52	0.40
1:F:744:ILE:HG23	1:F:789:ILE:HG13	2.04	0.40
1:H:811:SER:N	1:H:981:ILE:HD12	2.37	0.40
1:H:890:ILE:O	1:H:890:ILE:HG22	2.17	0.40
1:H:1007:MET:HE1	1:H:1010:VAL:HG12	2.03	0.40
1:A:790:MET:HG3	1:A:791:GLN:O	2.21	0.40
1:A:815[B]:LEU:CD1	1:A:979:LEU:HD11	2.51	0.40
1:B:905:TRP:CZ3	1:B:914:PRO:HA	2.57	0.40
1:G:799:LEU:HD13	1:G:840:ALA:HB3	2.03	0.40
1:G:953:ILE:HB	4:G:1207:HOH:O	2.21	0.40
1:H:758:GLU:O	1:H:758:GLU:OE1	2.38	0.40
1:C:758:GLU:OE2	1:C:759:ILE:CA	2.69	0.40
1:A:709:GLU:H	1:A:709:GLU:HG2	1.39	0.40
1:A:841:ARG:HH21	1:A:841:ARG:CG	2.02	0.40
1:A:977:ARG:HD2	1:A:977:ARG:C	2.44	0.40
1:B:891:TYR:C	1:B:892:THR:HG23	2.46	0.40
1:D:942:ASP:OD1	1:D:942:ASP:N	2.40	0.40
1:E:885:SER:O	1:E:889:ARG:CA	2.69	0.40
1:F:979:LEU:HD23	1:F:979:LEU:HA	1.89	0.40
1:G:730:LEU:HD13	1:G:739:LYS:CB	2.32	0.40
1:G:773:HIS:O	1:G:852:LYS:HA	2.22	0.40
1:G:792:LEU:HA	2:G:1101:816:N1	2.37	0.40
1:H:777:LEU:N	2:H:1101:816:CAA	2.85	0.40
1:H:968:PHE:HA	1:H:971:MET:HG3	2.04	0.40
1:C:977:ARG:CD	1:C:977:ARG:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/331 (89%)	290 (98%)	6 (2%)	0	100	100
1	B	293/331 (88%)	286 (98%)	7 (2%)	0	100	100
1	C	289/331 (87%)	285 (99%)	4 (1%)	0	100	100
1	D	291/331 (88%)	282 (97%)	9 (3%)	0	100	100
1	E	291/331 (88%)	286 (98%)	5 (2%)	0	100	100
1	F	291/331 (88%)	287 (99%)	4 (1%)	0	100	100
1	G	294/331 (89%)	291 (99%)	3 (1%)	0	100	100
1	H	292/331 (88%)	286 (98%)	6 (2%)	0	100	100
All	All	2337/2648 (88%)	2293 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/288 (88%)	183 (72%)	71 (28%)	0	1
1	B	246/288 (85%)	179 (73%)	67 (27%)	0	1
1	C	248/288 (86%)	153 (62%)	95 (38%)	0	0
1	D	234/288 (81%)	159 (68%)	75 (32%)	0	0
1	E	236/288 (82%)	168 (71%)	68 (29%)	0	1
1	F	245/288 (85%)	161 (66%)	84 (34%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	256/288 (89%)	177 (69%)	79 (31%)	0	0
1	H	252/288 (88%)	173 (69%)	79 (31%)	0	0
All	All	1971/2304 (86%)	1353 (69%)	618 (31%)	0	0

All (618) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	704	LEU
1	A	709	GLU
1	A	711	GLU
1	A	714	LYS
1	A	717	VAL
1	A	725	THR
1	A	728	LYS
1	A	732	ILE
1	A	739	LYS
1	A	745	LYS
1	A	746	GLU
1	A	757	LYS
1	A	758	GLU
1	A	762	GLU
1	A	765	VAL
1	A	769	VAL
1	A	775	CYS
1	A	780	ILE
1	A	788	LEU
1	A	789	ILE
1	A	790	MET
1	A	792	LEU
1	A	793	MET
1	A	797	CYS
1	A	798	LEU
1	A	802	VAL
1	A	806	LYS
1	A	807	ASP
1	A	808	ASN
1	A	809	ILE
1	A	811	SER
1	A	812	GLN
1	A	832	ARG
1	A	841	ARG

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Mol	Chain	Res	Type
1	A	844	LEU
1	A	846	LYS
1	A	849	GLN
1	A	851	VAL
1	A	854	THR
1	A	858	LEU
1	A	889	ARG
1	A	896	ASP
1	A	904	VAL
1	A	913	LYS
1	A	921	SER
1	A	922	GLU
1	A	923	ILE
1	A	925	SER
1	A	928	GLU
1	A	935	GLN
1	A	938	ILE
1	A	939	CYS
1	A	940	THR
1	A	948	VAL
1	A	952	MET
1	A	957	SER
1	A	967[A]	GLU
1	A	967[B]	GLU
1	A	973	ARG
1	A	976	GLN
1	A	980	VAL
1	A	982	GLN
1	A	991	SER
1	A	994	ASP
1	A	1001	LEU
1	A	1002	MET
1	A	1006	ASP
1	A	1009	ASP
1	A	1010	VAL
1	A	1011	VAL
1	A	1012	ASP
1	B	701	GLN
1	B	707	LEU
1	B	709	GLU
1	B	711	GLU
1	B	713	LYS

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Mol	Chain	Res	Type
1	B	716	LYS
1	B	717	VAL
1	B	734	GLU
1	B	736	GLU
1	B	737	LYS
1	B	745	LYS
1	B	758	GLU
1	B	760	LEU
1	B	762	GLU
1	B	768	SER
1	B	769	VAL
1	B	774	VAL
1	B	780	ILE
1	B	782	LEU
1	B	789	ILE
1	B	790	MET
1	B	792	LEU
1	B	793	MET
1	B	807	ASP
1	B	808	ASN
1	B	809	ILE
1	B	811	SER
1	B	819	VAL
1	B	821	ILE
1	B	831	ARG
1	B	832	ARG
1	B	833	LEU
1	B	835	HIS
1	B	836	ARG
1	B	841	ARG
1	B	843	VAL
1	B	846	LYS
1	B	847	THR
1	B	853	ILE
1	B	858	LEU
1	B	861	LEU
1	B	878	ILE
1	B	884	GLU
1	B	889	ARG
1	B	890	ILE
1	B	904	VAL
1	B	921	SER

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Mol	Chain	Res	Type
1	B	923	ILE
1	B	925	SER
1	B	935	GLN
1	B	939	CYS
1	B	941	ILE
1	B	948	VAL
1	B	950	CYS
1	B	957	SER
1	B	971	MET
1	B	977	ARG
1	B	980	VAL
1	B	982	GLN
1	B	985	GLU
1	B	987	MET
1	B	991	SER
1	B	993	THR
1	B	1001	LEU
1	B	1002	MET
1	B	1004	GLU
1	B	1006	ASP
1	D	703	LEU
1	D	704	LEU
1	D	706	ILE
1	D	708	LYS
1	D	713	LYS
1	D	714	LYS
1	D	715	ILE
1	D	718	LEU
1	D	730	LEU
1	D	732	ILE
1	D	738	VAL
1	D	740	ILE
1	D	742	VAL
1	D	757	LYS
1	D	765	VAL
1	D	774	VAL
1	D	780	ILE
1	D	785	THR
1	D	787	GLN
1	D	788	LEU
1	D	793	MET
1	D	797	CYS

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Mol	Chain	Res	Type
1	D	799	LEU
1	D	802	VAL
1	D	803	ARG
1	D	804	GLU
1	D	806	LYS
1	D	811	SER
1	D	812	GLN
1	D	829	GLU
1	D	834	VAL
1	D	836	ARG
1	D	841	ARG
1	D	845	VAL
1	D	847	THR
1	D	858	LEU
1	D	876	VAL
1	D	878	ILE
1	D	879	LYS
1	D	885	SER
1	D	886	ILE
1	D	890	ILE
1	D	892	THR
1	D	895	SER
1	D	897	VAL
1	D	909	THR
1	D	913	LYS
1	D	921	SER
1	D	924	SER
1	D	925	SER
1	D	931	GLU
1	D	932	ARG
1	D	935	GLN
1	D	938	ILE
1	D	939	CYS
1	D	941	ILE
1	D	942	ASP
1	D	949	LYS
1	D	952	MET
1	D	957	SER
1	D	966	ILE
1	D	969	SER
1	D	971	MET
1	D	973	ARG

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Mol	Chain	Res	Type
1	D	974	ASP
1	D	979	LEU
1	D	980	VAL
1	D	981	ILE
1	D	986	ARG
1	D	987	MET
1	D	993	THR
1	D	994	ASP
1	D	995	SER
1	D	1002	MET
1	D	1006	ASP
1	E	703	LEU
1	E	706	ILE
1	E	710	THR
1	E	711	GLU
1	E	714	LYS
1	E	717	VAL
1	E	718	LEU
1	E	725	THR
1	E	730	LEU
1	E	732	ILE
1	E	738	VAL
1	E	739	LYS
1	E	742	VAL
1	E	744	ILE
1	E	745	LYS
1	E	746	GLU
1	E	759	ILE
1	E	761	ASP
1	E	765	VAL
1	E	768	SER
1	E	769	VAL
1	E	774	VAL
1	E	780	ILE
1	E	782	LEU
1	E	789	ILE
1	E	790	MET
1	E	797	CYS
1	E	804	GLU
1	E	806	LYS
1	E	808	ASN
1	E	809	ILE

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Mol	Chain	Res	Type
1	E	811	SER
1	E	812	GLN
1	E	821	ILE
1	E	831	ARG
1	E	834	VAL
1	E	837	ASP
1	E	844	LEU
1	E	847	THR
1	E	851	VAL
1	E	853	ILE
1	E	856	PHE
1	E	861	LEU
1	E	876	VAL
1	E	878	ILE
1	E	884	GLU
1	E	892	THR
1	E	904	VAL
1	E	909	THR
1	E	913	LYS
1	E	921	SER
1	E	924	SER
1	E	925	SER
1	E	929	LYS
1	E	931	GLU
1	E	935	GLN
1	E	938	ILE
1	E	949	LYS
1	E	952	MET
1	E	957	SER
1	E	958	ARG
1	E	977	ARG
1	E	979	LEU
1	E	980	VAL
1	E	981	ILE
1	E	986	ARG
1	E	993	THR
1	E	1001	LEU
1	F	700	ASN
1	F	701	GLN
1	F	704	LEU
1	F	706	ILE
1	F	707	LEU

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Mol	Chain	Res	Type
1	F	710	THR
1	F	714	LYS
1	F	716	LYS
1	F	725	THR
1	F	730	LEU
1	F	736	GLU
1	F	738	VAL
1	F	740	ILE
1	F	744	ILE
1	F	745	LYS
1	F	748	ARG
1	F	759	ILE
1	F	765	VAL
1	F	766	MET
1	F	769	VAL
1	F	770	ASP
1	F	777	LEU
1	F	780	ILE
1	F	782	LEU
1	F	786	VAL
1	F	790	MET
1	F	791	GLN
1	F	792	LEU
1	F	797	CYS
1	F	807	ASP
1	F	808	ASN
1	F	809	ILE
1	F	811	SER
1	F	812	GLN
1	F	814	LEU
1	F	821	ILE
1	F	829	GLU
1	F	833	LEU
1	F	843	VAL
1	F	846	LYS
1	F	847	THR
1	F	849	GLN
1	F	851	VAL
1	F	853	ILE
1	F	856	PHE
1	F	858	LEU
1	F	861	LEU

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Mol	Chain	Res	Type
1	F	876	VAL
1	F	879	LYS
1	F	881	MET
1	F	889	ARG
1	F	890	ILE
1	F	892	THR
1	F	904	VAL
1	F	912	SER
1	F	913	LYS
1	F	918	ILE
1	F	923	ILE
1	F	924	SER
1	F	925	SER
1	F	926	ILE
1	F	929	LYS
1	F	931	GLU
1	F	938	ILE
1	F	943	VAL
1	F	945	MET
1	F	948	VAL
1	F	949	LYS
1	F	952	MET
1	F	953	ILE
1	F	958	ARG
1	F	963	GLU
1	F	966	ILE
1	F	967	GLU
1	F	970	LYS
1	F	977	ARG
1	F	987	MET
1	F	989	LEU
1	F	999	ARG
1	F	1002	MET
1	F	1004	GLU
1	F	1006	ASP
1	F	1007	MET
1	F	1010	VAL
1	G	703	LEU
1	G	706	ILE
1	G	707	LEU
1	G	710	THR
1	G	714	LYS

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Mol	Chain	Res	Type
1	G	715	ILE
1	G	716	LYS
1	G	725	THR
1	G	737	LYS
1	G	739	LYS
1	G	740	ILE
1	G	744	ILE
1	G	757	LYS
1	G	758	GLU
1	G	759	ILE
1	G	762	GLU
1	G	765	VAL
1	G	768	SER
1	G	769	VAL
1	G	787	GLN
1	G	792	LEU
1	G	793	MET
1	G	798	LEU
1	G	802	VAL
1	G	806	LYS
1	G	808	ASN
1	G	809	ILE
1	G	811	SER
1	G	825	MET
1	G	829	GLU
1	G	832	ARG
1	G	834	VAL
1	G	841	ARG
1	G	847	THR
1	G	851	VAL
1	G	852	LYS
1	G	855	ASP
1	G	876	VAL
1	G	878	ILE
1	G	879	LYS
1	G	886	ILE
1	G	889	ARG
1	G	890	ILE
1	G	895	SER
1	G	909	THR
1	G	913	LYS
1	G	918	ILE

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Mol	Chain	Res	Type
1	G	921	SER
1	G	922	GLU
1	G	926	ILE
1	G	927	LEU
1	G	929	LYS
1	G	932	ARG
1	G	935	GLN
1	G	938	ILE
1	G	943	VAL
1	G	946	ILE
1	G	947	MET
1	G	948	VAL
1	G	958	ARG
1	G	961	PHE
1	G	962	ARG
1	G	965	ILE
1	G	969	SER
1	G	973	ARG
1	G	977	ARG
1	G	981	ILE
1	G	987	MET
1	G	989	LEU
1	G	995	SER
1	G	998	TYR
1	G	1002	MET
1	G	1004	GLU
1	G	1006	ASP
1	G	1007	MET
1	G	1008	ASP
1	G	1010	VAL
1	G	1011	VAL
1	G	1014	ASP
1	H	701	GLN
1	H	703	LEU
1	H	707	LEU
1	H	710	THR
1	H	711	GLU
1	H	714	LYS
1	H	725	THR
1	H	737	LYS
1	H	738	VAL
1	H	739	LYS

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Mol	Chain	Res	Type
1	H	740	ILE
1	H	744	ILE
1	H	745	LYS
1	H	757	LYS
1	H	758	GLU
1	H	760	LEU
1	H	762	GLU
1	H	764	TYR
1	H	765	VAL
1	H	766	MET
1	H	768	SER
1	H	769	VAL
1	H	776	ARG
1	H	778	LEU
1	H	780	ILE
1	H	782	LEU
1	H	784	SER
1	H	786	VAL
1	H	790	MET
1	H	797	CYS
1	H	798	LEU
1	H	802	VAL
1	H	803	ARG
1	H	806	LYS
1	H	808	ASN
1	H	821	ILE
1	H	832	ARG
1	H	833	LEU
1	H	851	VAL
1	H	852	LYS
1	H	853	ILE
1	H	861	LEU
1	H	862	LEU
1	H	876	VAL
1	H	878	ILE
1	H	890	ILE
1	H	899	SER
1	H	902	VAL
1	H	903	THR
1	H	912	SER
1	H	913	LYS
1	H	918	ILE

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Mol	Chain	Res	Type
1	H	921	SER
1	H	922	GLU
1	H	924	SER
1	H	932	ARG
1	H	935	GLN
1	H	938	ILE
1	H	939	CYS
1	H	941	ILE
1	H	945	MET
1	H	946	ILE
1	H	948	VAL
1	H	949	LYS
1	H	952	MET
1	H	953	ILE
1	H	965	ILE
1	H	971	MET
1	H	976	GLN
1	H	982	GLN
1	H	987	MET
1	H	995	SER
1	H	1002	MET
1	H	1005	GLU
1	H	1007	MET
1	H	1008	ASP
1	H	1009	ASP
1	H	1011	VAL
1	H	1015	GLU
1	C	700	ASN
1	C	701	GLN
1	C	704	LEU
1	C	706	ILE
1	C	707	LEU
1	C	713	LYS
1	C	714	LYS
1	C	717	VAL
1	C	718	LEU
1	C	725	THR
1	C	730	LEU
1	C	736	GLU
1	C	744	ILE
1	C	746	GLU
1	C	748	ARG

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Mol	Chain	Res	Type
1	C	758	GLU
1	C	759	ILE
1	C	762	GLU
1	C	765	VAL
1	C	769	VAL
1	C	770	ASP
1	C	778	LEU
1	C	780	ILE
1	C	784	SER
1	C	785	THR
1	C	788	LEU
1	C	790	MET
1	C	791	GLN
1	C	792	LEU
1	C	793	MET
1	C	797	CYS
1	C	799	LEU
1	C	806	LYS
1	C	807	ASP
1	C	809	ILE
1	C	811	SER
1	C	828	LEU
1	C	829	GLU
1	C	831	ARG
1	C	832	ARG
1	C	833	LEU
1	C	838	LEU
1	C	841	ARG
1	C	846	LYS
1	C	847	THR
1	C	851	VAL
1	C	852	LYS
1	C	853	ILE
1	C	856	PHE
1	C	878	ILE
1	C	886	ILE
1	C	889	ARG
1	C	890	ILE
1	C	892	THR
1	C	894	GLN
1	C	895	SER
1	C	902	VAL

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Mol	Chain	Res	Type
1	C	908	MET
1	C	912	SER
1	C	913	LYS
1	C	918	ILE
1	C	921	SER
1	C	922	GLU
1	C	924	SER
1	C	925	SER
1	C	928	GLU
1	C	929	LYS
1	C	931	GLU
1	C	935	GLN
1	C	941	ILE
1	C	942	ASP
1	C	945	MET
1	C	949	LYS
1	C	950	CYS
1	C	952	MET
1	C	953	ILE
1	C	958	ARG
1	C	962	ARG
1	C	963	GLU
1	C	965	ILE
1	C	966	ILE
1	C	970	LYS
1	C	973	ARG
1	C	977	ARG
1	C	980	VAL
1	C	981	ILE
1	C	982	GLN
1	C	985	GLU
1	C	986	ARG
1	C	1005	GLU
1	C	1006	ASP
1	C	1007	MET
1	C	1010	VAL
1	C	1011	VAL
1	C	1012	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	849	GLN
1	B	894	GLN
1	B	982	GLN
1	D	771	ASN
1	D	773	HIS
1	D	805	HIS
1	D	808	ASN
1	D	816	ASN
1	D	826	ASN
1	D	850	HIS
1	E	808	ASN
1	E	826	ASN
1	E	935	GLN
1	F	771	ASN
1	F	835	HIS
1	G	849	GLN
1	H	701	GLN
1	H	787	GLN
1	H	816	ASN
1	H	976	GLN
1	C	700	ASN
1	C	787	GLN
1	C	808	ASN
1	C	835	HIS
1	C	888	HIS
1	C	982	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	EDO	H	1102	-	3,3,3	0.30	0	2,2,2	0.54	0
2	816	F	1101	1	40,40,40	3.57	12 (30%)	57,57,57	2.73	22 (38%)
3	EDO	H	1103	-	3,3,3	0.36	0	2,2,2	0.51	0
2	816	E	1101	1	40,40,40	3.67	12 (30%)	57,57,57	2.77	19 (33%)
2	816	B	1101	1	40,40,40	3.86	12 (30%)	57,57,57	2.76	20 (35%)
2	816	C	1101	1	40,40,40	3.76	12 (30%)	57,57,57	2.61	20 (35%)
2	816	G	1101	1	40,40,40	4.03	13 (32%)	57,57,57	2.75	23 (40%)
3	EDO	G	1102	-	3,3,3	0.44	0	2,2,2	0.31	0
2	816	D	1101	1	40,40,40	3.99	12 (30%)	57,57,57	2.75	16 (28%)
2	816	H	1101	1	40,40,40	3.97	12 (30%)	57,57,57	2.92	22 (38%)
3	EDO	H	1104	-	3,3,3	0.51	0	2,2,2	0.27	0
2	816	A	1101	1	40,40,40	3.85	12 (30%)	57,57,57	2.65	20 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	H	1102	-	-	1/1/1/1	-
2	816	F	1101	1	-	5/19/29/29	0/5/5/5
3	EDO	H	1103	-	-	1/1/1/1	-
2	816	E	1101	1	-	3/19/29/29	0/5/5/5
2	816	B	1101	1	-	3/19/29/29	0/5/5/5
2	816	C	1101	1	-	5/19/29/29	0/5/5/5
2	816	G	1101	1	-	5/19/29/29	0/5/5/5
3	EDO	G	1102	-	-	0/1/1/1	-
2	816	D	1101	1	-	5/19/29/29	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	816	H	1101	1	-	3/19/29/29	0/5/5/5
3	EDO	H	1104	-	-	1/1/1/1	-
2	816	A	1101	1	-	5/19/29/29	0/5/5/5

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	816	NBP-NAZ	-14.67	1.11	1.38
2	D	1101	816	NBP-NAZ	-14.62	1.11	1.38
2	G	1101	816	NBP-NAZ	-14.10	1.12	1.38
2	H	1101	816	NBP-NAZ	-13.75	1.12	1.38
2	A	1101	816	NBP-NAZ	-13.58	1.13	1.38
2	C	1101	816	NBP-NAZ	-13.33	1.13	1.38
2	E	1101	816	NBP-NAZ	-12.69	1.14	1.38
2	H	1101	816	CBH-CBJ	-12.04	1.32	1.49
2	D	1101	816	CBH-CBJ	-11.93	1.32	1.49
2	G	1101	816	CBH-CBJ	-11.68	1.32	1.49
2	C	1101	816	CBH-CBJ	-11.26	1.33	1.49
2	A	1101	816	CBH-CBJ	-11.12	1.33	1.49
2	B	1101	816	CBH-CBJ	-11.12	1.33	1.49
2	F	1101	816	CBH-CBJ	-10.80	1.33	1.49
2	E	1101	816	CBH-CBJ	-10.58	1.34	1.49
2	F	1101	816	NBP-NAZ	-10.38	1.19	1.38
2	F	1101	816	C5-C6	-9.10	1.32	1.42
2	D	1101	816	C5-C6	-9.01	1.32	1.42
2	H	1101	816	C5-C6	-8.88	1.32	1.42
2	E	1101	816	C5-C6	-8.81	1.32	1.42
2	G	1101	816	C5-C6	-8.64	1.32	1.42
2	A	1101	816	C5-C6	-8.55	1.32	1.42
2	B	1101	816	C5-C6	-8.41	1.33	1.42
2	C	1101	816	C5-C6	-7.97	1.33	1.42
2	H	1101	816	C5-C4	-7.36	1.31	1.40
2	G	1101	816	C5-C4	-6.94	1.31	1.40
2	A	1101	816	C5-C4	-6.91	1.31	1.40
2	B	1101	816	C5-C4	-6.74	1.32	1.40
2	F	1101	816	C5-C4	-6.74	1.32	1.40
2	C	1101	816	C5-C4	-6.60	1.32	1.40
2	D	1101	816	C5-C4	-6.56	1.32	1.40
2	G	1101	816	CBF-CLA	-6.31	1.58	1.73
2	E	1101	816	C5-C4	-6.19	1.32	1.40
2	A	1101	816	CBF-CLA	-6.14	1.59	1.73
2	G	1101	816	CAA-CBD	-5.54	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	816	CAA-CBD	-5.54	1.37	1.50
2	C	1101	816	CAA-CBD	-5.44	1.38	1.50
2	B	1101	816	CAA-CBD	-5.37	1.38	1.50
2	D	1101	816	CAA-CBD	-5.34	1.38	1.50
2	E	1101	816	CAA-CBD	-5.30	1.38	1.50
2	A	1101	816	CAA-CBD	-5.25	1.38	1.50
2	H	1101	816	CAA-CBD	-5.24	1.38	1.50
2	A	1101	816	CAT-CBG	-5.20	1.38	1.50
2	G	1101	816	CAT-CBG	-5.20	1.38	1.50
2	H	1101	816	C5-CBJ	-5.14	1.31	1.44
2	E	1101	816	CAT-CBG	-5.12	1.38	1.50
2	D	1101	816	C5-CBJ	-5.04	1.31	1.44
2	D	1101	816	CAT-CBG	-5.03	1.38	1.50
2	C	1101	816	CBF-CLA	-4.91	1.62	1.73
2	F	1101	816	C5-CBJ	-4.89	1.32	1.44
2	F	1101	816	CAP-CAQ	4.79	1.53	1.30
2	H	1101	816	CAT-CBG	-4.79	1.39	1.50
2	G	1101	816	C5-CBJ	-4.79	1.32	1.44
2	F	1101	816	CAT-CBG	-4.79	1.39	1.50
2	C	1101	816	C5-CBJ	-4.74	1.32	1.44
2	C	1101	816	CAP-CAQ	4.68	1.52	1.30
2	C	1101	816	CAT-CBG	-4.67	1.39	1.50
2	B	1101	816	CAP-CAQ	4.65	1.52	1.30
2	H	1101	816	CAP-CAQ	4.64	1.52	1.30
2	D	1101	816	CAP-CAQ	4.63	1.52	1.30
2	A	1101	816	C5-CBJ	-4.63	1.32	1.44
2	E	1101	816	C5-CBJ	-4.63	1.32	1.44
2	B	1101	816	C5-CBJ	-4.62	1.32	1.44
2	B	1101	816	CAT-CBG	-4.60	1.39	1.50
2	E	1101	816	CAP-CAQ	4.59	1.52	1.30
2	H	1101	816	CBF-CLA	-4.58	1.62	1.73
2	A	1101	816	CAP-CAQ	4.57	1.52	1.30
2	G	1101	816	CAP-CAQ	4.48	1.51	1.30
2	E	1101	816	CBF-CLA	-4.17	1.63	1.73
2	F	1101	816	CBF-CLA	-4.06	1.64	1.73
2	D	1101	816	CBF-CLA	-3.97	1.64	1.73
2	H	1101	816	C4-NBP	-3.76	1.32	1.36
2	G	1101	816	C4-NBP	-3.50	1.32	1.36
2	B	1101	816	C4-NBP	-3.43	1.32	1.36
2	H	1101	816	C2-N1	3.20	1.39	1.33
2	F	1101	816	C4-NBP	-3.19	1.32	1.36
2	G	1101	816	C2-N1	3.12	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	816	CBF-CLA	-3.11	1.66	1.73
2	D	1101	816	C2-N3	3.08	1.39	1.33
2	D	1101	816	C2-N1	3.07	1.39	1.33
2	E	1101	816	C2-N1	2.97	1.39	1.33
2	C	1101	816	C2-N3	2.96	1.39	1.33
2	C	1101	816	C4-NBP	-2.95	1.33	1.36
2	C	1101	816	C2-N1	2.89	1.39	1.33
2	G	1101	816	C2-N3	2.89	1.39	1.33
2	A	1101	816	C4-NBP	-2.89	1.33	1.36
2	E	1101	816	C2-N3	2.88	1.39	1.33
2	H	1101	816	C2-N3	2.78	1.38	1.33
2	F	1101	816	C2-N3	2.78	1.38	1.33
2	B	1101	816	C2-N3	2.75	1.38	1.33
2	A	1101	816	C2-N3	2.74	1.38	1.33
2	F	1101	816	C2-N1	2.67	1.38	1.33
2	B	1101	816	C2-N1	2.64	1.38	1.33
2	D	1101	816	C4-NBP	-2.61	1.33	1.36
2	E	1101	816	C4-NBP	-2.44	1.33	1.36
2	A	1101	816	C2-N1	2.27	1.38	1.33
2	G	1101	816	CBN-NBP	-2.13	1.43	1.46

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1101	816	CAP-CAQ-CBC	-8.78	103.45	121.27
2	H	1101	816	CAP-CAQ-CBC	-8.00	105.02	121.27
2	B	1101	816	N3-C2-N1	-7.45	117.30	128.58
2	E	1101	816	CAR-CBN-NBP	-7.43	104.85	111.88
2	H	1101	816	C6-C5-C4	7.42	121.30	115.74
2	D	1101	816	C6-C5-C4	7.41	121.29	115.74
2	A	1101	816	N3-C2-N1	-7.38	117.41	128.58
2	F	1101	816	N3-C2-N1	-7.30	117.53	128.58
2	D	1101	816	CBJ-NAZ-NBP	7.27	110.80	106.97
2	G	1101	816	N3-C2-N1	-7.21	117.66	128.58
2	D	1101	816	N3-C2-N1	-7.11	117.81	128.58
2	E	1101	816	C6-C5-C4	7.05	121.02	115.74
2	C	1101	816	N3-C2-N1	-7.01	117.97	128.58
2	H	1101	816	N3-C2-N1	-6.95	118.06	128.58
2	B	1101	816	CBJ-NAZ-NBP	6.77	110.54	106.97
2	E	1101	816	N3-C2-N1	-6.74	118.38	128.58
2	B	1101	816	CAP-CAQ-CBC	-6.67	107.73	121.27
2	D	1101	816	CAP-CAQ-CBC	-6.66	107.75	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	816	C6-C5-C4	6.64	120.71	115.74
2	C	1101	816	CAP-CAQ-CBC	-6.43	108.21	121.27
2	A	1101	816	CAP-CAQ-CBC	-6.43	108.21	121.27
2	A	1101	816	C6-C5-C4	6.33	120.48	115.74
2	G	1101	816	C6-C5-C4	6.32	120.47	115.74
2	E	1101	816	CAP-CAQ-CBC	-6.23	108.61	121.27
2	F	1101	816	C6-C5-C4	6.21	120.39	115.74
2	A	1101	816	C5-C4-N3	-6.03	120.57	126.97
2	B	1101	816	C6-C5-C4	5.82	120.10	115.74
2	E	1101	816	C5-C4-N3	-5.82	120.80	126.97
2	C	1101	816	CBJ-NAZ-NBP	5.81	110.03	106.97
2	D	1101	816	C5-C4-N3	-5.80	120.82	126.97
2	C	1101	816	C5-C4-N3	-5.79	120.83	126.97
2	D	1101	816	CAR-CBN-NBP	-5.65	106.53	111.88
2	B	1101	816	CAR-CBN-NBP	-5.64	106.54	111.88
2	E	1101	816	CBJ-NAZ-NBP	5.56	109.90	106.97
2	F	1101	816	C5-C4-N3	-5.55	121.08	126.97
2	H	1101	816	C4-NBP-CBN	-5.41	115.55	128.97
2	B	1101	816	C5-C4-N3	-5.34	121.31	126.97
2	A	1101	816	CBJ-NAZ-NBP	5.29	109.75	106.97
2	H	1101	816	CAT-OBA-CBI	-5.28	107.30	117.76
2	F	1101	816	CBN-NBP-NAZ	5.21	132.12	119.89
2	H	1101	816	CBN-NBP-NAZ	5.20	132.09	119.89
2	H	1101	816	C5-C4-N3	-5.15	121.51	126.97
2	F	1101	816	C5-C6-NAB	-5.07	116.71	123.40
2	D	1101	816	C5-C6-NAB	-5.07	116.71	123.40
2	A	1101	816	C5-C6-NAB	-5.03	116.76	123.40
2	G	1101	816	C5-C4-N3	-4.98	121.69	126.97
2	E	1101	816	C5-C6-NAB	-4.90	116.93	123.40
2	G	1101	816	C5-C6-NAB	-4.84	117.00	123.40
2	H	1101	816	C5-C6-NAB	-4.79	117.08	123.40
2	B	1101	816	C5-C6-NAB	-4.77	117.10	123.40
2	D	1101	816	N3-C4-NBP	4.77	132.26	126.05
2	F	1101	816	CAP-CAQ-CBC	-4.76	111.61	121.27
2	F	1101	816	CBJ-NAZ-NBP	4.74	109.47	106.97
2	A	1101	816	N3-C4-NBP	4.72	132.20	126.05
2	F	1101	816	C4-NBP-CBN	-4.48	117.85	128.97
2	E	1101	816	N3-C4-NBP	4.48	131.89	126.05
2	C	1101	816	C5-C6-NAB	-4.47	117.50	123.40
2	F	1101	816	CBH-CBJ-NAZ	4.32	124.53	118.91
2	C	1101	816	N3-C4-NBP	4.28	131.63	126.05
2	B	1101	816	N3-C4-NBP	4.23	131.57	126.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1101	816	CBH-CBJ-NAZ	4.21	124.39	118.91
2	B	1101	816	CAT-OBA-CBI	-4.13	109.57	117.76
2	G	1101	816	N3-C4-NBP	4.13	131.42	126.05
2	H	1101	816	CAR-CBN-NBP	-4.09	108.01	111.88
2	H	1101	816	N3-C4-NBP	4.02	131.29	126.05
2	H	1101	816	C5-CBJ-CBH	-4.01	126.52	131.28
2	F	1101	816	C6-C5-CBJ	-4.00	135.02	139.07
2	G	1101	816	CBJ-NAZ-NBP	3.93	109.04	106.97
2	C	1101	816	CAT-OBA-CBI	-3.91	110.02	117.76
2	F	1101	816	N3-C4-NBP	3.83	131.04	126.05
2	G	1101	816	CAR-CBN-NBP	-3.83	108.25	111.88
2	G	1101	816	CAT-OBA-CBI	-3.81	110.20	117.76
2	G	1101	816	C4-NBP-CBN	-3.76	119.65	128.97
2	B	1101	816	C5-CBJ-NAZ	-3.74	107.62	110.19
2	F	1101	816	C5-C6-N1	3.70	121.97	118.64
2	A	1101	816	CAT-OBA-CBI	-3.68	110.47	117.76
2	H	1101	816	CBN-CAV-NBO	-3.67	104.56	109.46
2	A	1101	816	C5-C6-N1	3.57	121.84	118.64
2	A	1101	816	C2-N3-C4	3.53	120.45	111.83
2	E	1101	816	C6-C5-CBJ	-3.48	135.54	139.07
2	C	1101	816	CAS-NBO-CAV	3.48	119.78	113.07
2	B	1101	816	C5-C6-N1	3.44	121.73	118.64
2	C	1101	816	C5-C6-N1	3.42	121.71	118.64
2	D	1101	816	CBN-CAV-NBO	3.41	114.00	109.46
2	F	1101	816	CAT-OBA-CBI	-3.40	111.02	117.76
2	B	1101	816	C2-N3-C4	3.39	120.11	111.83
2	E	1101	816	C5-C6-N1	3.35	121.65	118.64
2	G	1101	816	CBN-NBP-NAZ	3.35	127.75	119.89
2	A	1101	816	CBH-CBJ-NAZ	3.34	123.26	118.91
2	C	1101	816	C2-N3-C4	3.32	119.93	111.83
2	F	1101	816	C2-N3-C4	3.31	119.92	111.83
2	B	1101	816	CAO-CAS-NBO	-3.28	104.02	110.67
2	G	1101	816	C5-C6-N1	3.27	121.58	118.64
2	F	1101	816	CAV-CBN-NBP	3.26	113.51	109.47
2	F	1101	816	C5-CBJ-CBH	-3.25	127.42	131.28
2	E	1101	816	CBI-CBF-CLA	-3.22	115.76	119.44
2	C	1101	816	CBH-CBJ-NAZ	3.19	123.05	118.91
2	D	1101	816	C2-N3-C4	3.18	119.60	111.83
2	H	1101	816	C6-C5-CBJ	-3.16	135.87	139.07
2	A	1101	816	CAQ-CBC-NBO	-3.14	114.20	117.66
2	D	1101	816	C6-C5-CBJ	-3.14	135.89	139.07
2	G	1101	816	C2-N3-C4	3.13	119.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1101	816	C5-CBJ-NAZ	-3.12	108.05	110.19
2	G	1101	816	CBH-CBJ-NAZ	3.11	122.96	118.91
2	G	1101	816	CAS-NBO-CAV	3.09	119.03	113.07
2	E	1101	816	C2-N3-C4	3.09	119.38	111.83
2	D	1101	816	C5-C6-N1	3.03	121.36	118.64
2	A	1101	816	C5-CBJ-NAZ	-3.01	108.12	110.19
2	H	1101	816	C2-N3-C4	2.98	119.12	111.83
2	H	1101	816	CBJ-NAZ-NBP	2.97	108.53	106.97
2	E	1101	816	C5-CBJ-NAZ	-2.89	108.21	110.19
2	D	1101	816	CAS-NBO-CAV	2.87	118.61	113.07
2	A	1101	816	CAS-NBO-CAV	2.87	118.59	113.07
2	D	1101	816	CAR-CAO-CAS	-2.83	107.03	110.75
2	E	1101	816	CBH-CBJ-NAZ	2.83	122.59	118.91
2	H	1101	816	CAS-NBO-CAV	2.82	118.51	113.07
2	D	1101	816	C5-CBJ-NAZ	-2.82	108.25	110.19
2	G	1101	816	C4-C5-CBJ	-2.80	102.79	104.74
2	D	1101	816	C4-C5-CBJ	-2.76	102.81	104.74
2	H	1101	816	C4-C5-CBJ	-2.74	102.83	104.74
2	E	1101	816	CAN-CBF-CLA	2.74	122.94	118.45
2	A	1101	816	C6-C5-CBJ	-2.73	136.31	139.07
2	B	1101	816	C4-C5-CBJ	-2.68	102.87	104.74
2	H	1101	816	C5-C6-N1	2.67	121.04	118.64
2	C	1101	816	C6-C5-CBJ	-2.66	136.38	139.07
2	G	1101	816	C4-NBP-NAZ	2.64	112.60	110.90
2	B	1101	816	CAK-CBG-NAY	-2.64	119.06	122.40
2	C	1101	816	C4-C5-CBJ	-2.62	102.91	104.74
2	C	1101	816	C5-CBJ-NAZ	-2.61	108.39	110.19
2	B	1101	816	CAT-CBG-NAY	2.60	120.93	115.69
2	B	1101	816	CBH-CBJ-NAZ	2.52	122.18	118.91
2	C	1101	816	CAQ-CBC-NBO	-2.49	114.92	117.66
2	H	1101	816	CAV-CBN-NBP	2.47	112.53	109.47
2	G	1101	816	C5-CBJ-CBH	-2.47	128.35	131.28
2	G	1101	816	CBI-CBF-CLA	-2.47	116.62	119.44
2	A	1101	816	C4-NBP-CBN	-2.45	122.89	128.97
2	F	1101	816	CAS-NBO-CAV	2.44	117.77	113.07
2	E	1101	816	CAS-NBO-CAV	2.43	117.76	113.07
2	A	1101	816	OAE-CBC-NBO	2.43	124.62	121.18
2	F	1101	816	CAN-CBF-CLA	2.43	122.43	118.45
2	E	1101	816	CAO-CAS-NBO	-2.42	105.75	110.67
2	B	1101	816	CAS-NBO-CAV	2.42	117.74	113.07
2	F	1101	816	CAO-CAR-CBN	2.39	115.36	110.81
2	E	1101	816	CAR-CAO-CAS	-2.36	107.65	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	816	CBN-NBP-NAZ	2.36	125.43	119.89
2	G	1101	816	CAN-CBF-CLA	2.33	122.27	118.45
2	C	1101	816	CAT-CBG-NAY	2.32	120.37	115.69
2	H	1101	816	CAT-CBG-NAY	2.30	120.33	115.69
2	G	1101	816	C6-C5-CBJ	-2.30	136.74	139.07
2	C	1101	816	C5-CBJ-CBH	-2.30	128.55	131.28
2	H	1101	816	C4-NBP-NAZ	2.26	112.36	110.90
2	A	1101	816	C5-CBJ-CBH	-2.26	128.60	131.28
2	F	1101	816	CAR-CBN-CAV	2.22	113.51	110.83
2	E	1101	816	CAT-OBA-CBI	-2.21	113.38	117.76
2	A	1101	816	C4-C5-CBJ	-2.19	103.21	104.74
2	G	1101	816	C5-CBJ-NAZ	-2.19	108.69	110.19
2	F	1101	816	CBI-CBF-CLA	-2.19	116.94	119.44
2	B	1101	816	CAO-CAR-CBN	2.13	114.85	110.81
2	C	1101	816	OAE-CBC-NBO	2.08	124.12	121.18
2	C	1101	816	CAN-CBF-CLA	2.06	121.83	118.45
2	G	1101	816	CBN-CAV-NBO	-2.02	106.76	109.46
2	B	1101	816	C6-C5-CBJ	-2.02	137.03	139.07

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1101	816	CAP-CAQ-CBC-OAE
2	H	1101	816	CBG-CAT-OBA-CBI
2	F	1101	816	CBG-CAT-OBA-CBI
2	G	1101	816	CBG-CAT-OBA-CBI
2	A	1101	816	CAP-CAQ-CBC-OAE
2	C	1101	816	CAP-CAQ-CBC-OAE
2	E	1101	816	CAP-CAQ-CBC-NBO
2	C	1101	816	CAP-CAQ-CBC-NBO
2	D	1101	816	CBG-CAT-OBA-CBI
2	C	1101	816	CBG-CAT-OBA-CBI
2	B	1101	816	CBG-CAT-OBA-CBI
2	E	1101	816	CBG-CAT-OBA-CBI
2	D	1101	816	CAP-CAQ-CBC-OAE
2	F	1101	816	CAP-CAQ-CBC-OAE
2	G	1101	816	CAP-CAQ-CBC-OAE
2	A	1101	816	CAP-CAQ-CBC-NBO
2	F	1101	816	CAP-CAQ-CBC-NBO
2	C	1101	816	OBA-CAT-CBG-NAY
2	C	1101	816	OBA-CAT-CBG-CAK

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Mol	Chain	Res	Type	Atoms
2	G	1101	816	OBA-CAT-CBG-NAY
3	H	1103	EDO	O1-C1-C2-O2
2	D	1101	816	CAP-CAQ-CBC-NBO
2	G	1101	816	CAP-CAQ-CBC-NBO
3	H	1102	EDO	O1-C1-C2-O2
3	H	1104	EDO	O1-C1-C2-O2
2	G	1101	816	OBA-CAT-CBG-CAK
2	B	1101	816	OBA-CAT-CBG-NAY
2	A	1101	816	OBA-CAT-CBG-CAK
2	A	1101	816	CAV-CBN-NBP-NAZ
2	A	1101	816	OBA-CAT-CBG-NAY
2	F	1101	816	OBA-CAT-CBG-NAY
2	H	1101	816	OBA-CAT-CBG-NAY
2	D	1101	816	OBA-CAT-CBG-NAY
2	B	1101	816	OBA-CAT-CBG-CAK
2	H	1101	816	OBA-CAT-CBG-CAK
2	F	1101	816	OBA-CAT-CBG-CAK
2	D	1101	816	OBA-CAT-CBG-CAK

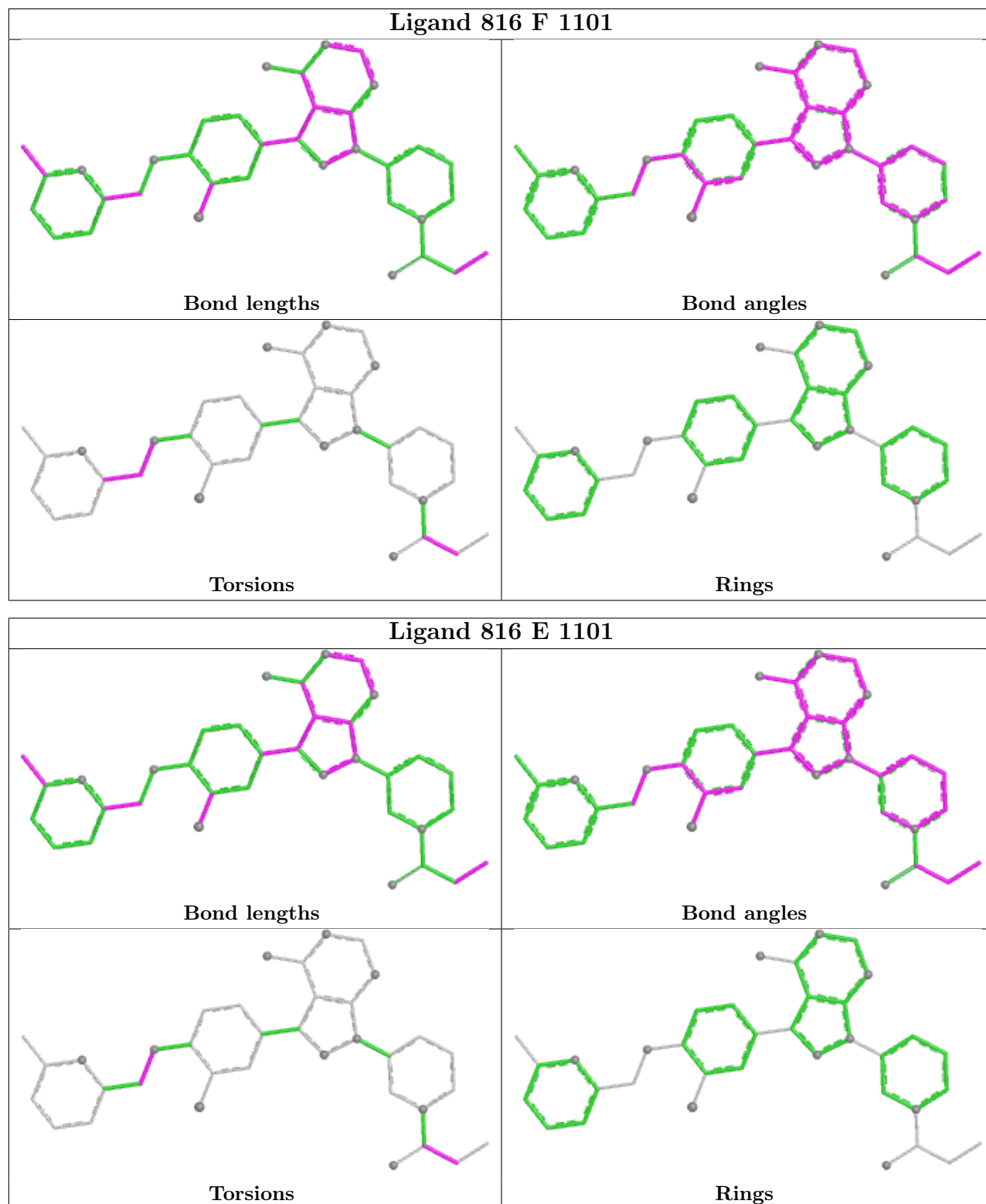
There are no ring outliers.

11 monomers are involved in 75 short contacts:

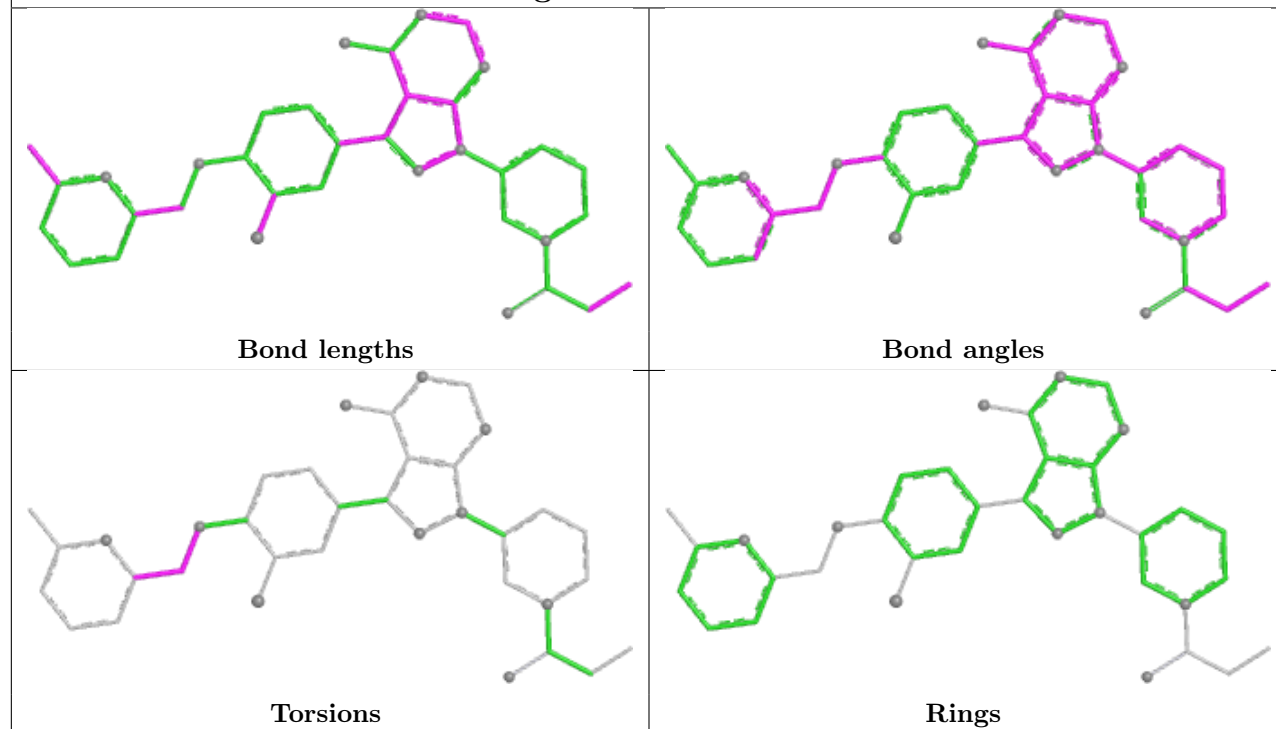
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1101	816	8	0
3	H	1103	EDO	3	0
2	E	1101	816	7	0
2	B	1101	816	5	0
2	C	1101	816	8	0
2	G	1101	816	14	0
3	G	1102	EDO	2	0
2	D	1101	816	11	0
2	H	1101	816	11	0
3	H	1104	EDO	1	0
2	A	1101	816	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

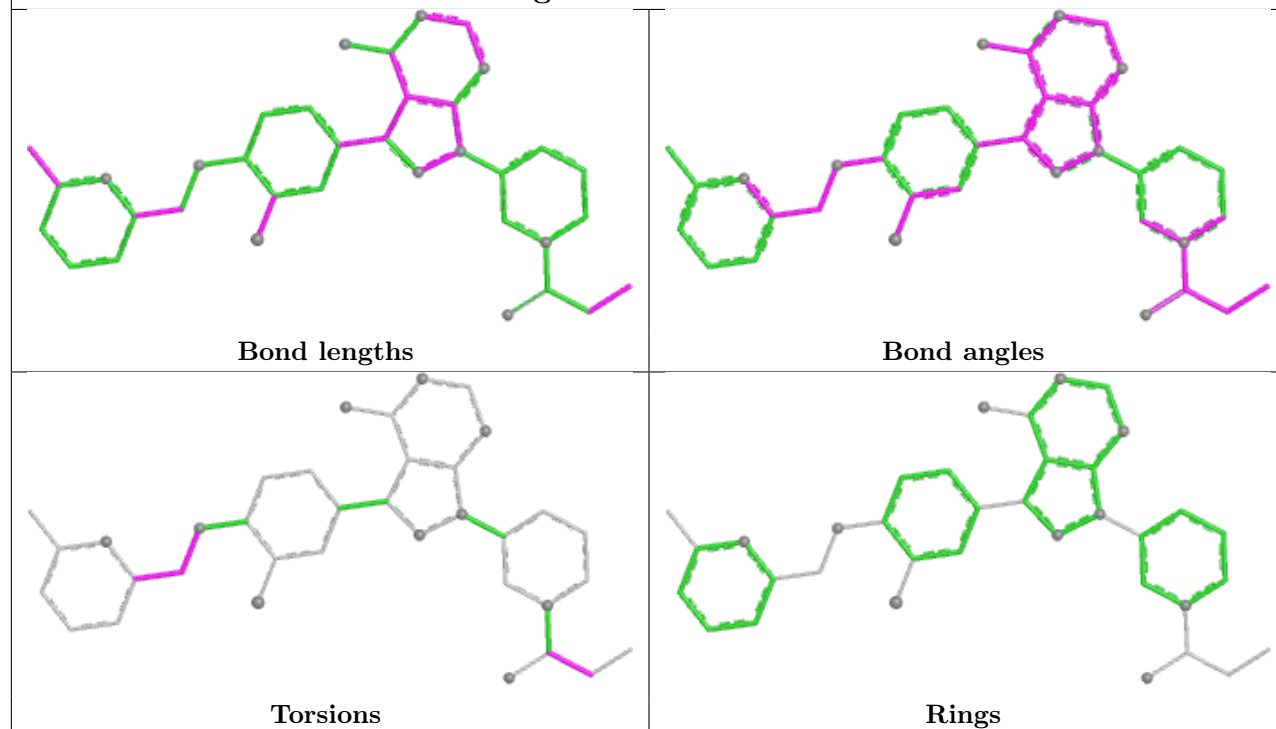
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



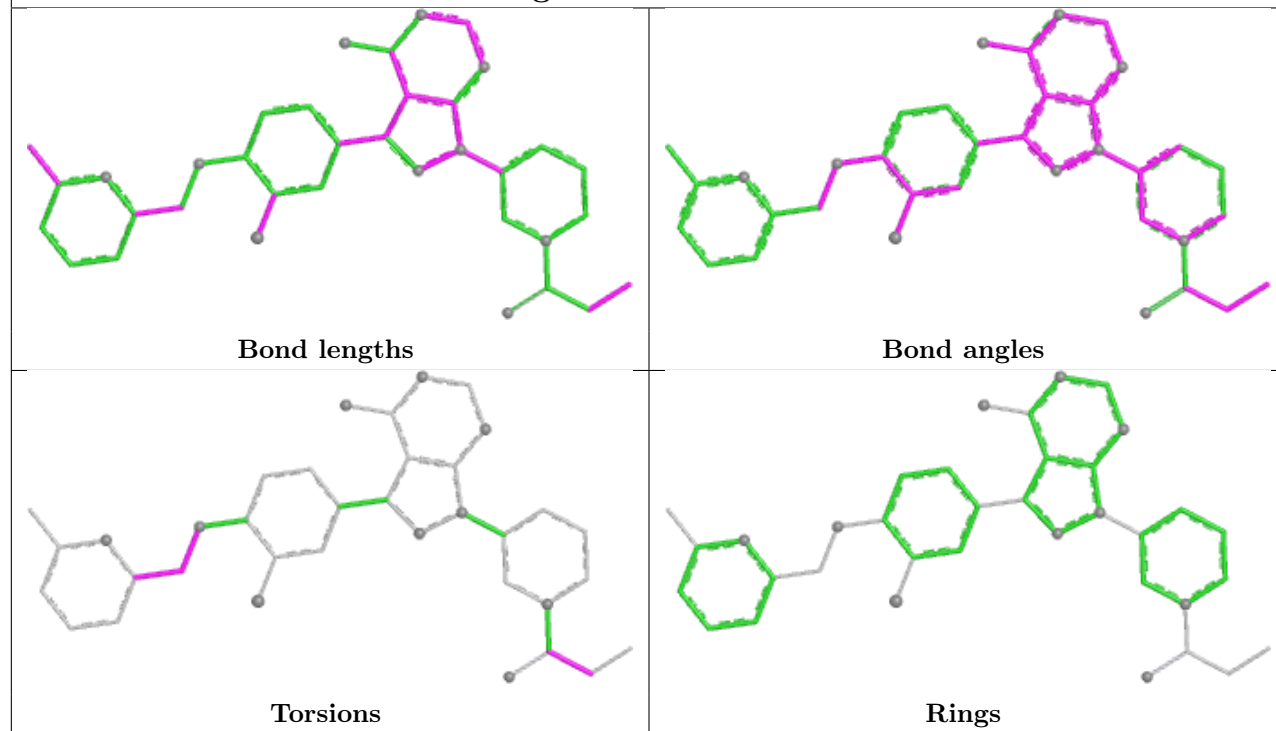
Ligand 816 B 1101



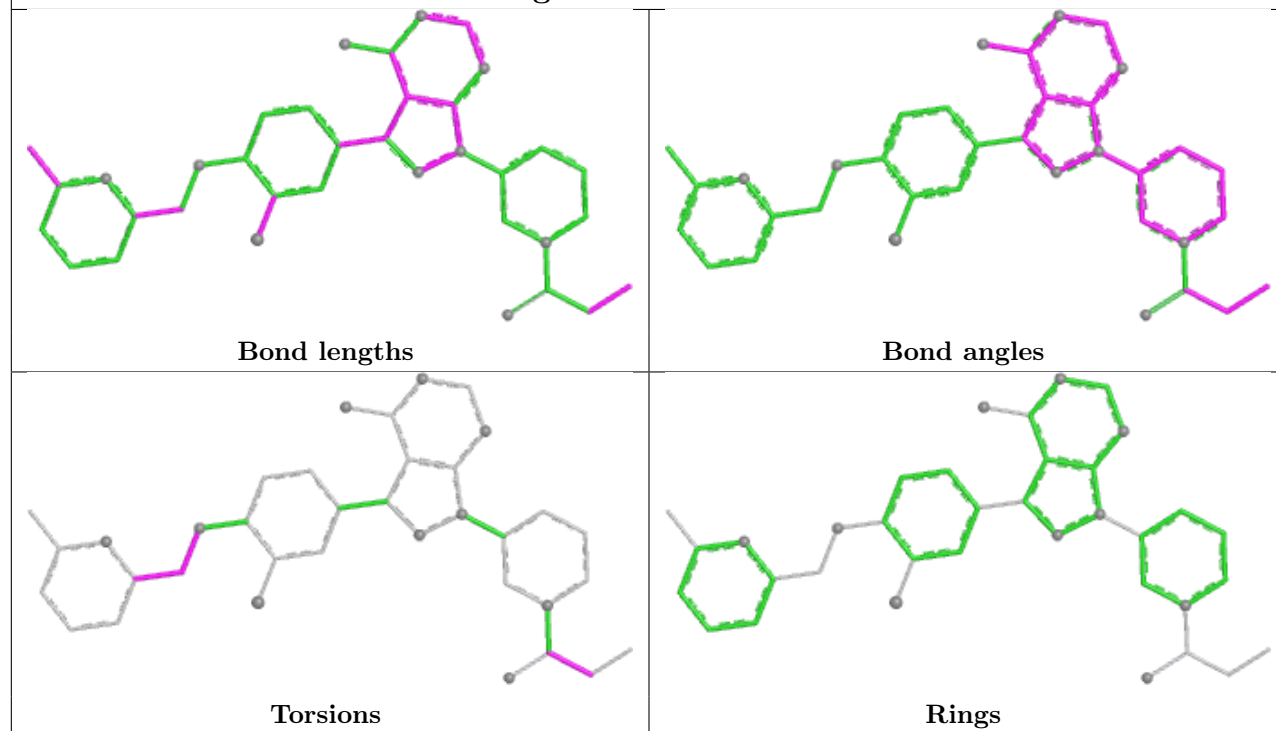
Ligand 816 C 1101

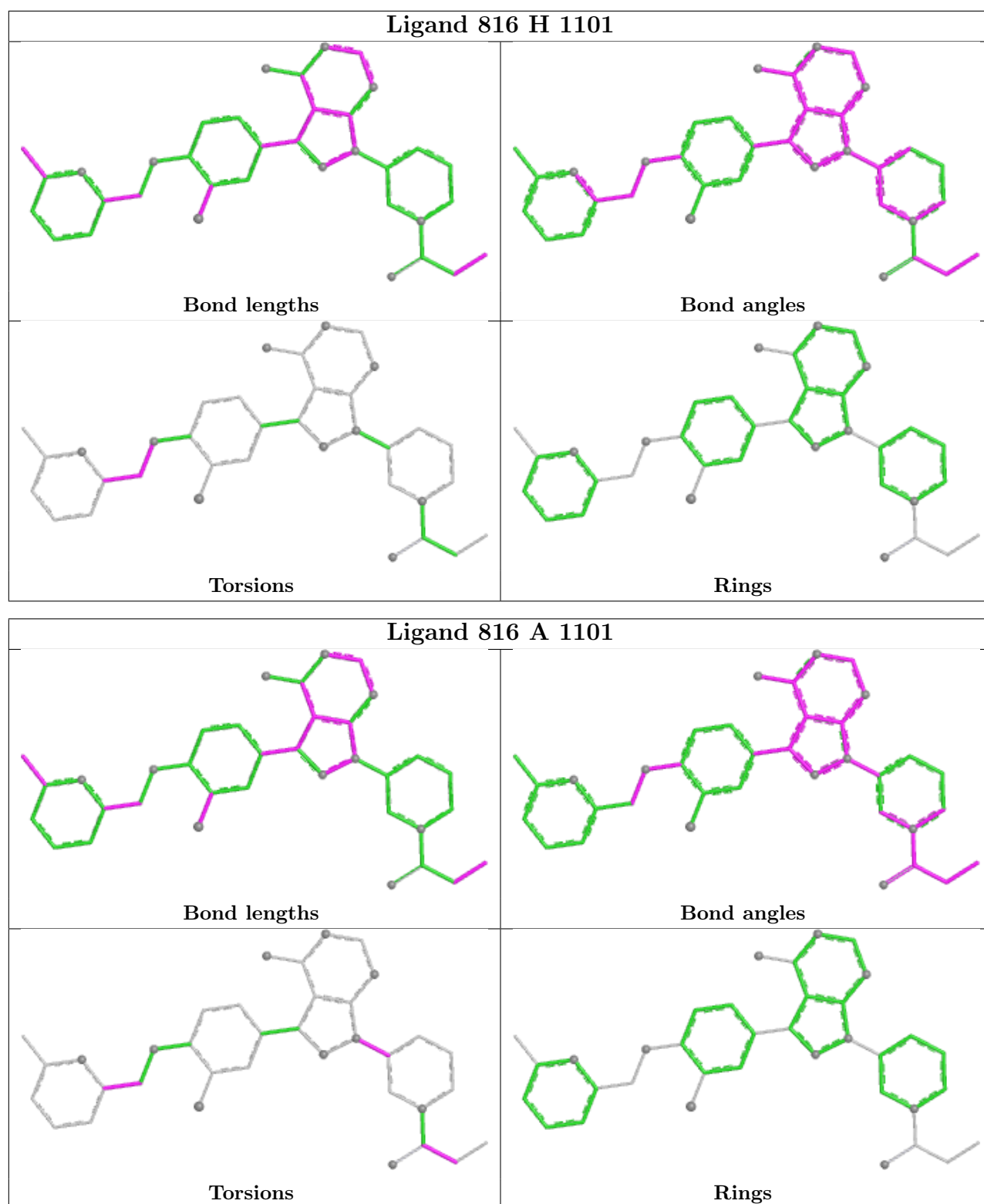


Ligand 816 G 1101



Ligand 816 D 1101





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	300/331 (90%)	0.54	14 (4%)	36	19	19, 48, 89, 111	3 (1%)
1	B	299/331 (90%)	0.44	11 (3%)	45	25	29, 48, 85, 112	0
1	C	295/331 (89%)	0.59	16 (5%)	31	16	31, 52, 89, 125	0
1	D	297/331 (89%)	0.57	13 (4%)	39	20	29, 48, 97, 121	1 (0%)
1	E	297/331 (89%)	0.41	9 (3%)	52	31	26, 49, 94, 112	0
1	F	297/331 (89%)	0.50	13 (4%)	39	20	31, 48, 82, 93	0
1	G	299/331 (90%)	0.49	7 (2%)	61	39	31, 50, 88, 99	1 (0%)
1	H	300/331 (90%)	0.45	9 (3%)	52	31	31, 48, 92, 107	0
All	All	2384/2648 (90%)	0.50	92 (3%)	43	23	19, 49, 89, 125	5 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	763	ALA	6.2
1	E	860	LYS	5.0
1	F	859	ALA	5.0
1	F	1009	ASP	4.7
1	C	724	GLY	4.6
1	B	761	ASP	4.3
1	C	856	PHE	4.2
1	C	930	GLY	3.8
1	C	1009	ASP	3.8
1	C	768	SER	3.8
1	F	930	GLY	3.6
1	H	940	THR	3.6
1	D	760	LEU	3.5
1	A	915	TYR	3.3
1	C	1010	VAL	3.3
1	F	940	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	729	GLY	3.2
1	F	788	LEU	3.1
1	E	763	ALA	3.0
1	H	724	GLY	3.0
1	D	859	ALA	3.0
1	B	927	LEU	2.9
1	G	1011	VAL	2.9
1	C	732	ILE	2.9
1	B	837	ASP	2.9
1	C	715	ILE	2.8
1	E	859	ALA	2.8
1	G	999[A]	ARG	2.8
1	D	759	ILE	2.7
1	A	1009	ASP	2.7
1	D	860	LYS	2.7
1	A	912	SER	2.7
1	B	900	TYR	2.7
1	G	1010	VAL	2.7
1	E	1010	VAL	2.6
1	A	732	ILE	2.6
1	C	1012	ASP	2.6
1	A	877	PRO	2.5
1	G	1012	ASP	2.5
1	G	991	SER	2.5
1	C	725	THR	2.5
1	E	798	LEU	2.5
1	E	991	SER	2.4
1	B	1009	ASP	2.4
1	D	1003	ASP	2.4
1	E	1013	ALA	2.4
1	D	1013	ALA	2.4
1	B	1014	ASP	2.4
1	C	707	LEU	2.4
1	A	734	GLU	2.4
1	D	1010	VAL	2.3
1	B	924	SER	2.3
1	H	856	PHE	2.3
1	B	807	ASP	2.3
1	A	931	GLU	2.2
1	C	926	ILE	2.2
1	C	809	ILE	2.2
1	A	930	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	900	TYR	2.2
1	A	916	ASP	2.2
1	E	984	ASP	2.2
1	D	795	PHE	2.2
1	A	895	SER	2.1
1	D	810	GLY	2.1
1	H	700	ASN	2.1
1	B	1008	ASP	2.1
1	D	1009	ASP	2.1
1	A	1010	VAL	2.1
1	H	1010	VAL	2.1
1	C	861	LEU	2.1
1	F	858	LEU	2.1
1	F	721	GLY	2.1
1	G	930	GLY	2.1
1	F	808	ASN	2.1
1	F	876	VAL	2.1
1	B	976	GLN	2.1
1	F	906	GLU	2.1
1	A	1011	VAL	2.1
1	C	745	LYS	2.1
1	F	967	GLU	2.1
1	H	1011	VAL	2.0
1	G	707	LEU	2.0
1	A	835	HIS	2.0
1	E	1014	ASP	2.0
1	B	930	GLY	2.0
1	F	723	PHE	2.0
1	H	975	PRO	2.0
1	F	1010	VAL	2.0
1	C	798	LEU	2.0
1	H	968	PHE	2.0
1	A	802	VAL	2.0
1	D	819	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

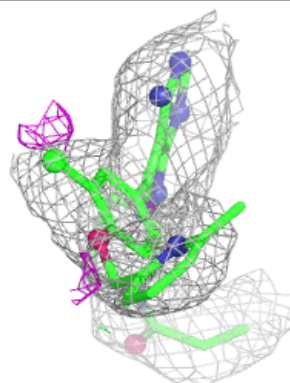
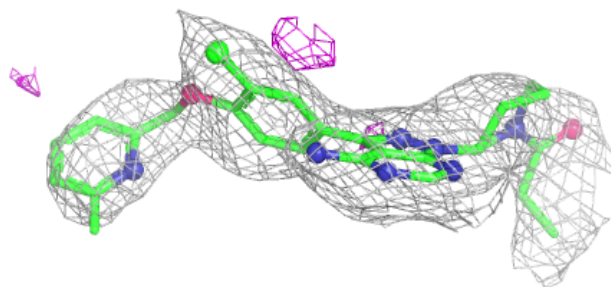
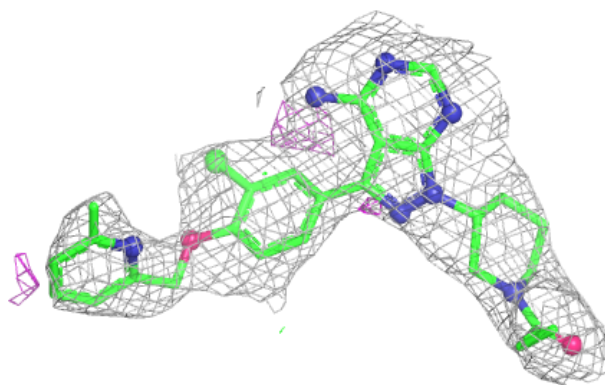
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	H	1103	4/4	0.49	0.21	70,70,70,70	0
3	EDO	H	1104	4/4	0.54	0.29	71,71,71,71	0
3	EDO	H	1102	4/4	0.63	0.15	65,65,65,65	0
3	EDO	G	1102	4/4	0.74	0.15	55,55,55,55	0
2	816	E	1101	36/36	0.83	0.16	42,56,66,70	0
2	816	H	1101	36/36	0.83	0.15	44,50,60,61	0
2	816	A	1101	36/36	0.86	0.13	31,39,51,61	0
2	816	C	1101	36/36	0.86	0.11	43,51,62,77	0
2	816	G	1101	36/36	0.86	0.15	40,51,62,67	0
2	816	F	1101	36/36	0.88	0.14	33,45,50,62	0
2	816	D	1101	36/36	0.88	0.12	41,53,66,68	0
2	816	B	1101	36/36	0.92	0.10	36,42,49,51	0

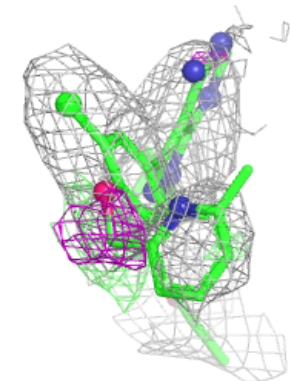
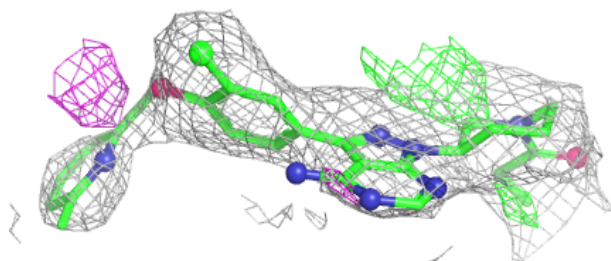
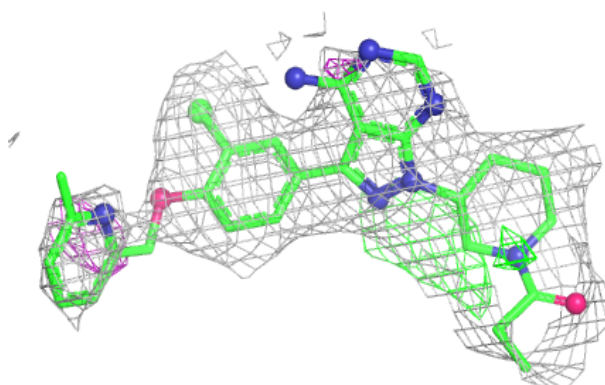
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 816 E 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

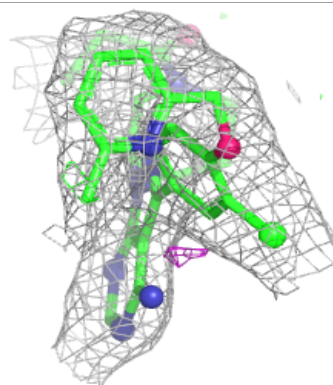
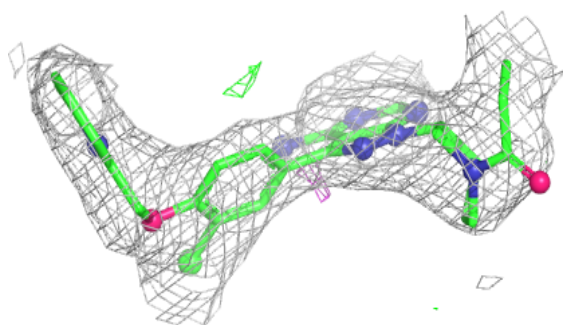
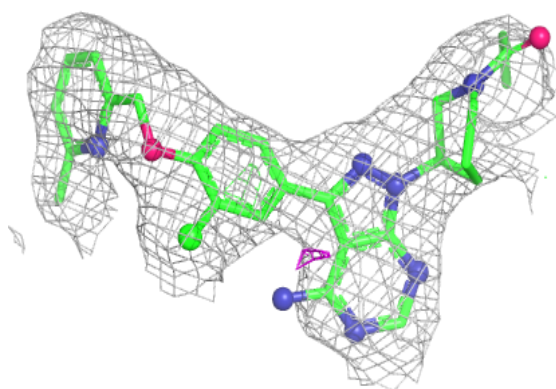
**Electron density around 816 H 1101:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

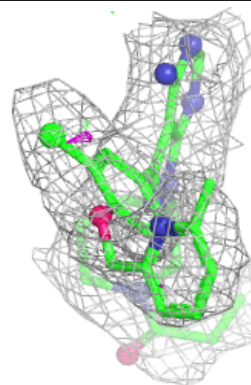
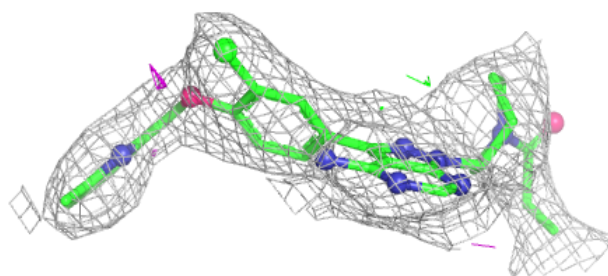
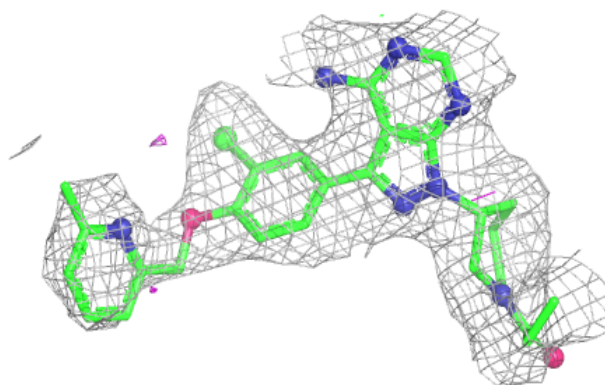


Electron density around 816 A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

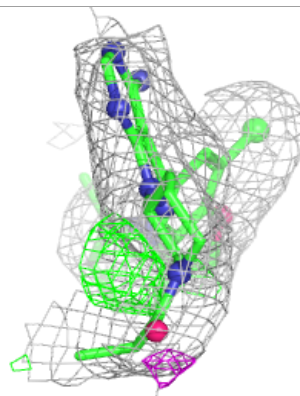
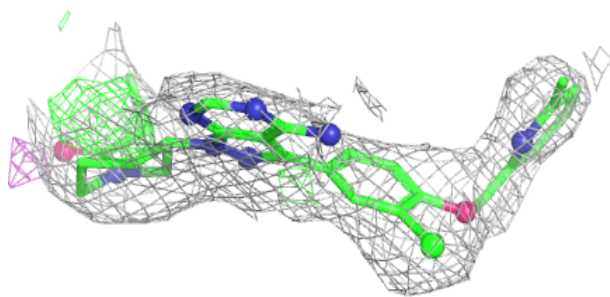
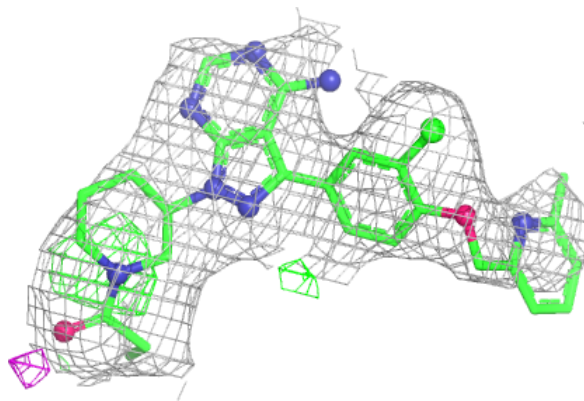
**Electron density around 816 C 1101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

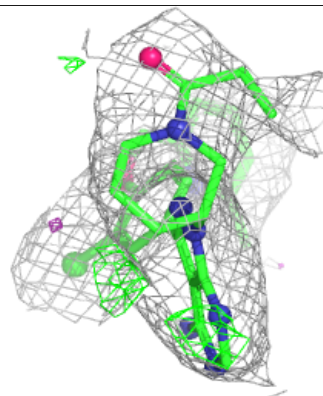
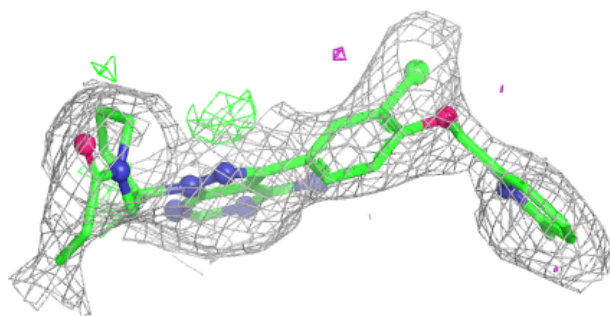
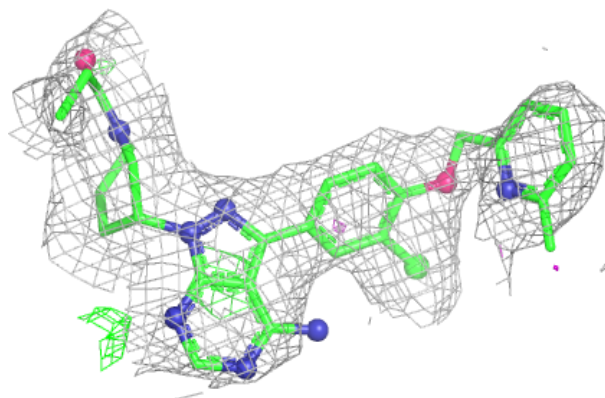


Electron density around 816 G 1101:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

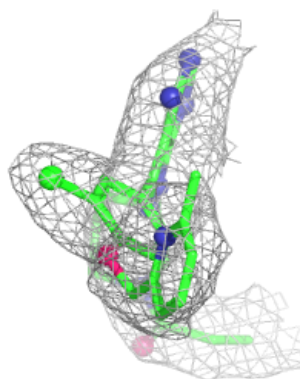
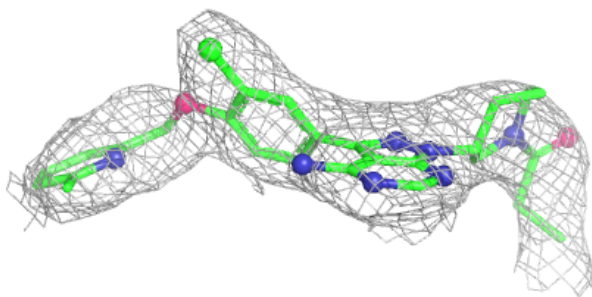
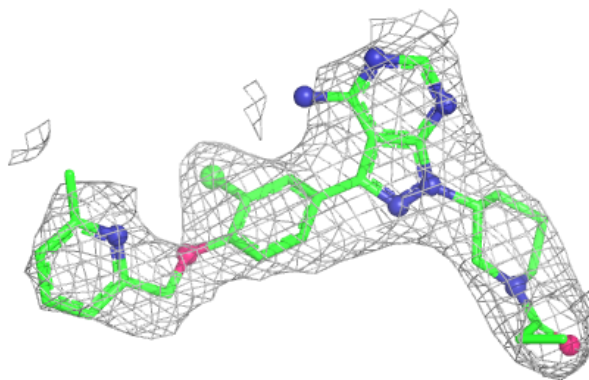
**Electron density around 816 F 1101:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

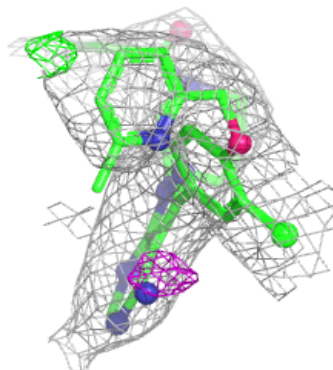
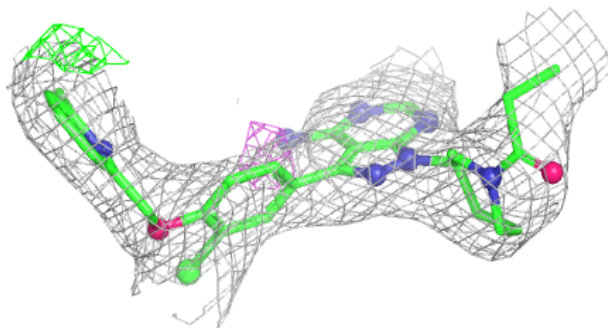
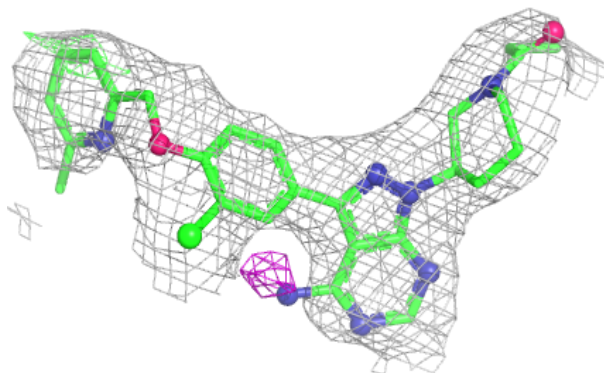


Electron density around 816 D 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 816 B 1101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.