



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:07 PM UTC

PDB ID : 4A0L / pdb_00004a0l
Title : Structure of DDB1-DDB2-CUL4B-RBX1 bound to a 12 bp abasic site containing DNA-duplex
Authors : Fischer, E.S.; Scrima, A.; Gut, H.; Thoma, N.H.
Deposited on : 2011-09-09
Resolution : 7.40 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:

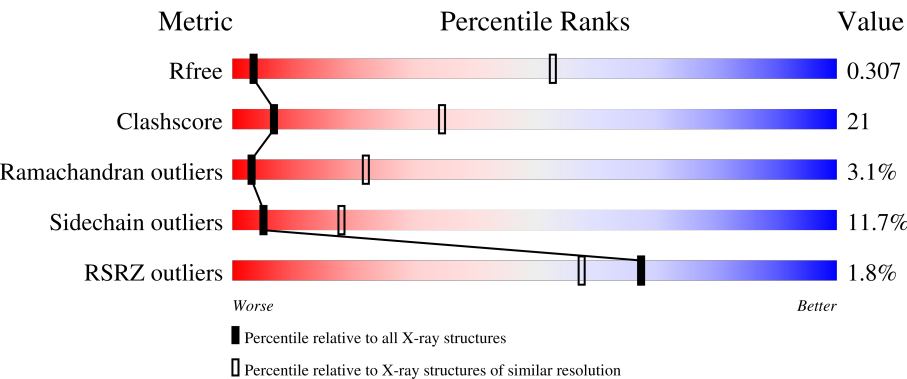
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.40 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	1144	2% 62% 25% 8%
1	C	1144	2% 63% 26% 7%
2	B	382	3% 74% 16% 7%
2	D	382	% 73% 18% 7%
3	E	726	2% 58% 32% 8%

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Mol	Chain	Length	Quality of chain
3	H	726	% 60%32%6%
4	F	98	10%6% 79%
4	I	98	13%6% 79%
5	R	12	83%17%
5	T	12	83%17%
6	S	12	58%42%
6	U	12	58%42%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35553 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 DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1105	Total	C	N	O	S	0	0	0
			8517	5403	1417	1652	45			
1	C	1105	Total	C	N	O	S	0	0	0
			8537	5409	1428	1655	45			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
C	-3	GLY	-	expression tag	UNP Q16531
C	-2	GLY	-	expression tag	UNP Q16531
C	-1	GLY	-	expression tag	UNP Q16531
C	0	ARG	-	expression tag	UNP Q16531

- Molecule 2 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	355	Total	C	N	O	S	0	0	0
			2819	1792	492	524	11			
2	D	355	Total	C	N	O	S	0	0	0
			2843	1806	499	527	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	MET	-	expression tag	UNP Q2YDS1
B	77	HIS	-	expression tag	UNP Q2YDS1
B	78	HIS	-	expression tag	UNP Q2YDS1
B	79	HIS	-	expression tag	UNP Q2YDS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	80	HIS	-	expression tag	UNP Q2YDS1
B	81	HIS	-	expression tag	UNP Q2YDS1
B	82	HIS	-	expression tag	UNP Q2YDS1
B	83	ARG	-	expression tag	UNP Q2YDS1
B	84	ARG	-	expression tag	UNP Q2YDS1
B	85	LEU	-	expression tag	UNP Q2YDS1
B	86	VAL	-	expression tag	UNP Q2YDS1
B	87	PRO	-	expression tag	UNP Q2YDS1
B	88	ARG	-	expression tag	UNP Q2YDS1
B	89	GLY	-	expression tag	UNP Q2YDS1
B	90	SER	-	expression tag	UNP Q2YDS1
B	91	GLY	-	expression tag	UNP Q2YDS1
B	92	GLY	-	expression tag	UNP Q2YDS1
B	93	ARG	-	expression tag	UNP Q2YDS1
B	180	GLN	LEU	variant	UNP Q2YDS1
B	214	ARG	TRP	variant	UNP Q2YDS1
D	76	MET	-	expression tag	UNP Q2YDS1
D	77	HIS	-	expression tag	UNP Q2YDS1
D	78	HIS	-	expression tag	UNP Q2YDS1
D	79	HIS	-	expression tag	UNP Q2YDS1
D	80	HIS	-	expression tag	UNP Q2YDS1
D	81	HIS	-	expression tag	UNP Q2YDS1
D	82	HIS	-	expression tag	UNP Q2YDS1
D	83	ARG	-	expression tag	UNP Q2YDS1
D	84	ARG	-	expression tag	UNP Q2YDS1
D	85	LEU	-	expression tag	UNP Q2YDS1
D	86	VAL	-	expression tag	UNP Q2YDS1
D	87	PRO	-	expression tag	UNP Q2YDS1
D	88	ARG	-	expression tag	UNP Q2YDS1
D	89	GLY	-	expression tag	UNP Q2YDS1
D	90	SER	-	expression tag	UNP Q2YDS1
D	91	GLY	-	expression tag	UNP Q2YDS1
D	92	GLY	-	expression tag	UNP Q2YDS1
D	93	ARG	-	expression tag	UNP Q2YDS1
D	180	GLN	LEU	variant	UNP Q2YDS1
D	214	ARG	TRP	variant	UNP Q2YDS1

- Molecule 3 is a protein called CULLIN-4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	709	Total	C	N	O	S	0	0	0
			5743	3659	979	1074	31			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	709	Total	C	N	O	S	0	0	0
			5773	3681	978	1082	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	189	GLY	-	expression tag	UNP Q13620
E	190	GLY	-	expression tag	UNP Q13620
E	191	GLY	-	expression tag	UNP Q13620
E	192	ARG	-	expression tag	UNP Q13620
H	189	GLY	-	expression tag	UNP Q13620
H	190	GLY	-	expression tag	UNP Q13620
H	191	GLY	-	expression tag	UNP Q13620
H	192	ARG	-	expression tag	UNP Q13620

- Molecule 4 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	21	Total	C	N	O	0	0	0
			175	118	31	26			
4	I	21	Total	C	N	O	0	0	0
			180	122	32	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	11	MET	-	expression tag	UNP P62878
I	11	MET	-	expression tag	UNP P62878

- Molecule 5 is a DNA chain called 12 BP THF CONTAINING DNA DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	12	Total	C	N	O	P	0	0	0
			234	111	41	70	12			
5	T	12	Total	C	N	O	P	0	0	0
			234	111	41	70	12			

- Molecule 6 is a DNA chain called 12 BP DNA DUPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S	12	Total	C	N	O	P	0	0	0
			249	118	47	72	12			

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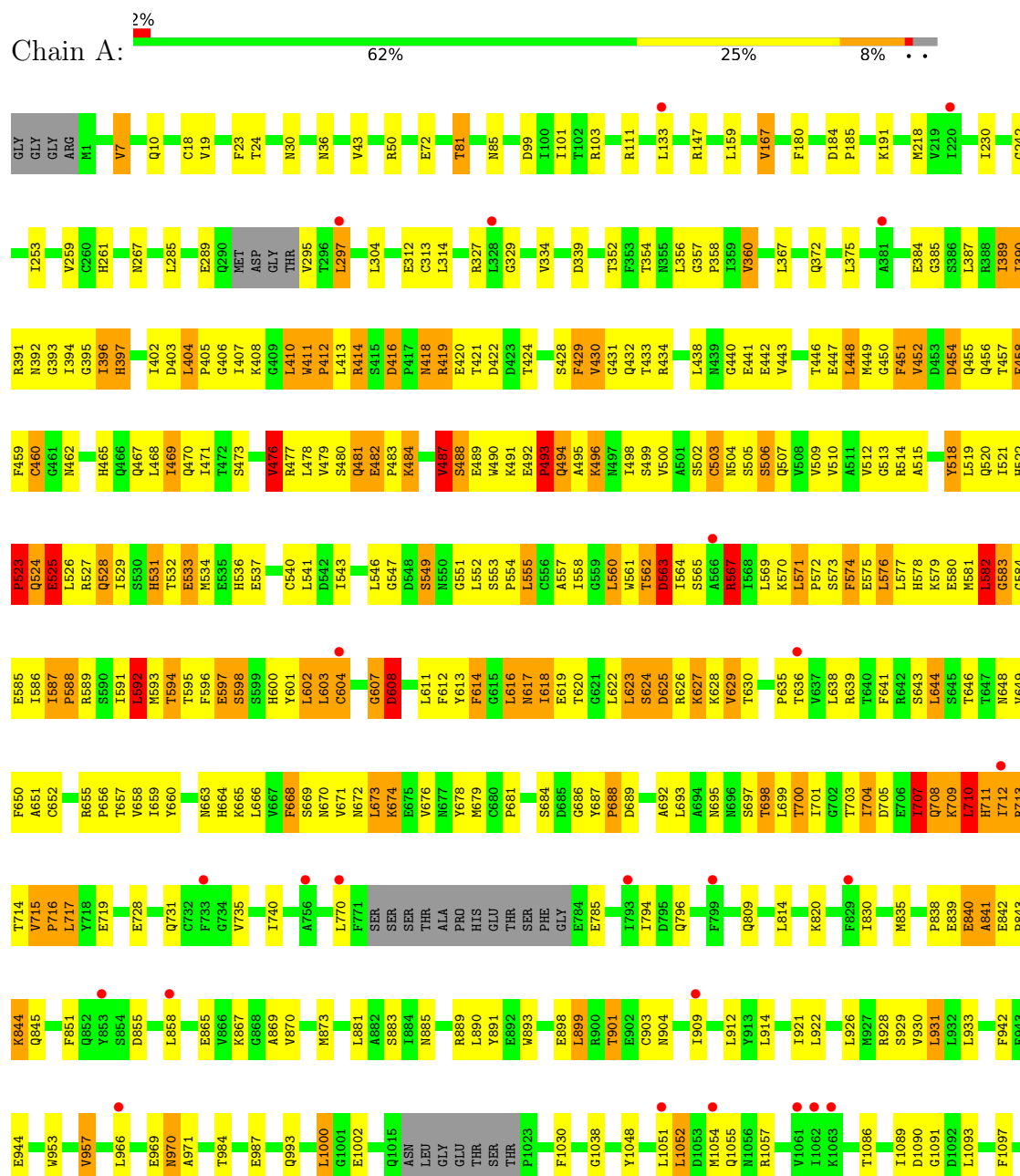
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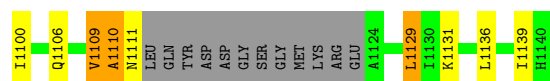
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	U	12	Total	C	N	O	P	0	0	0
			249	118	47	72	12			

3 Residue-property plots

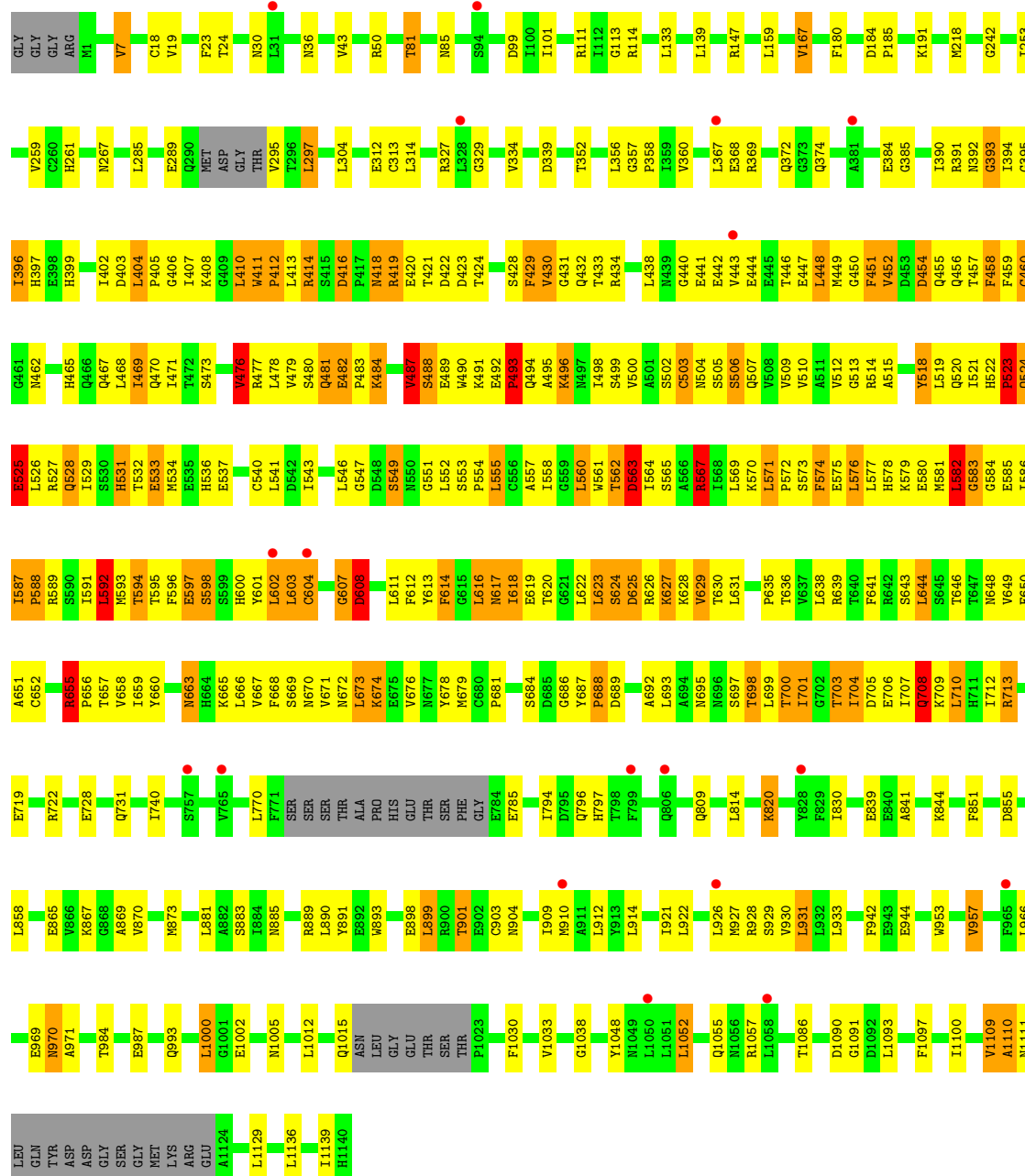
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1

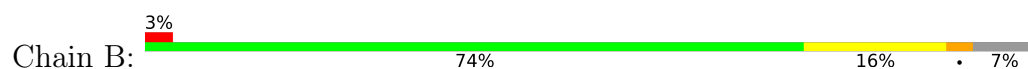


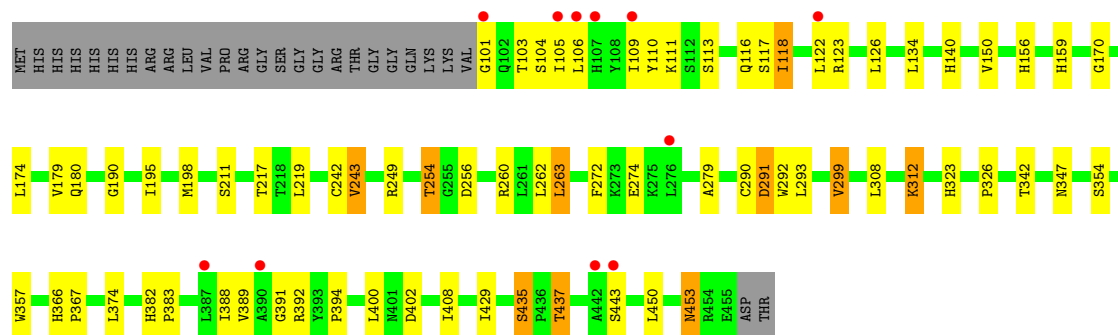


• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1

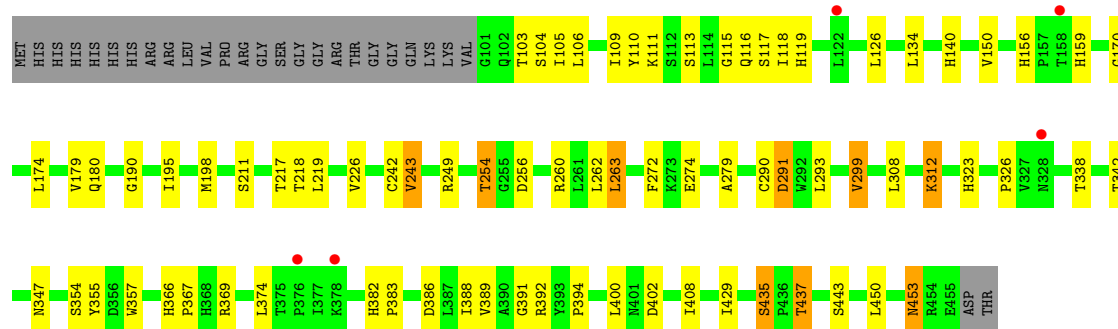
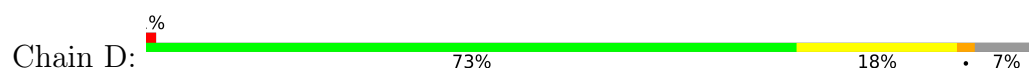


• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

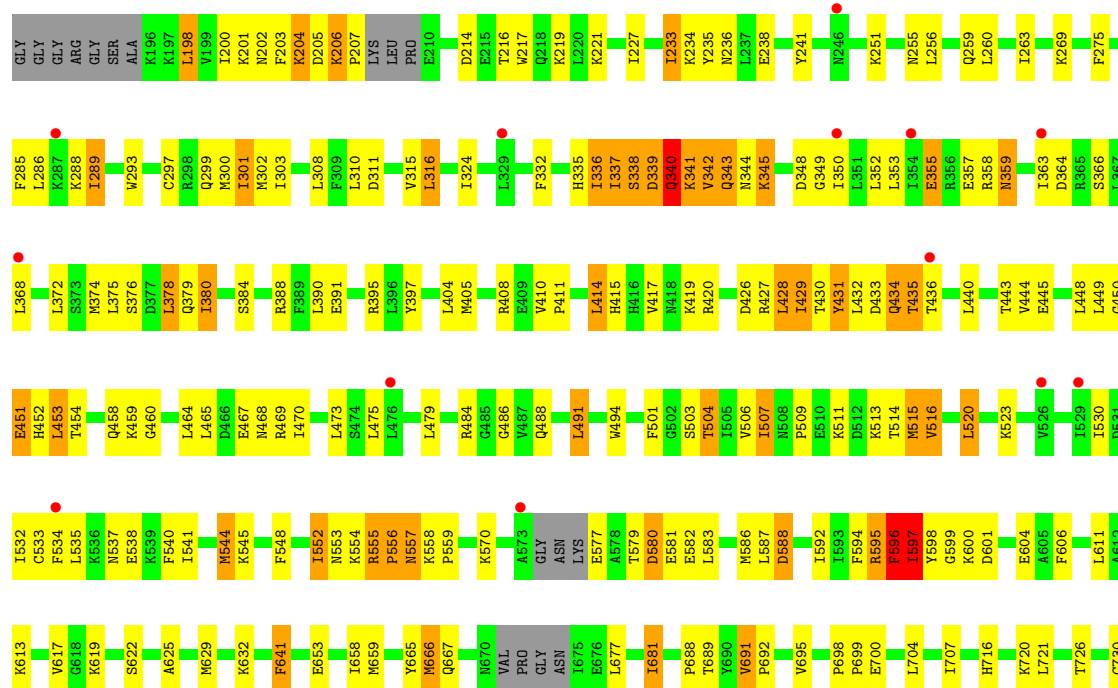


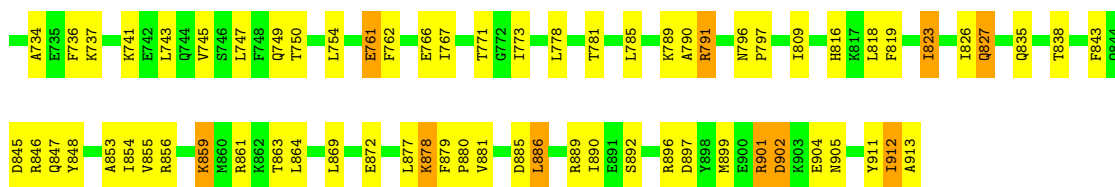


• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

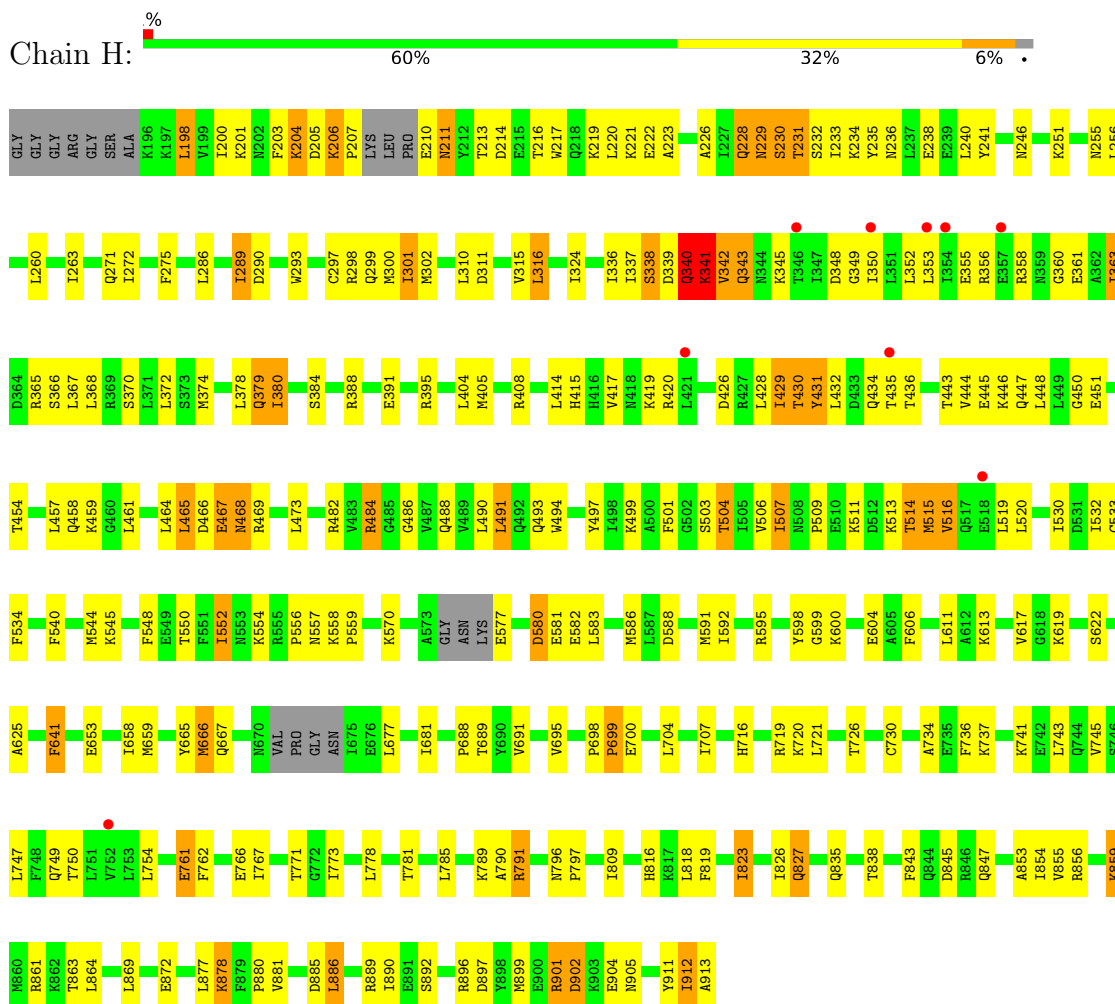


• Molecule 3: CULLIN-4B

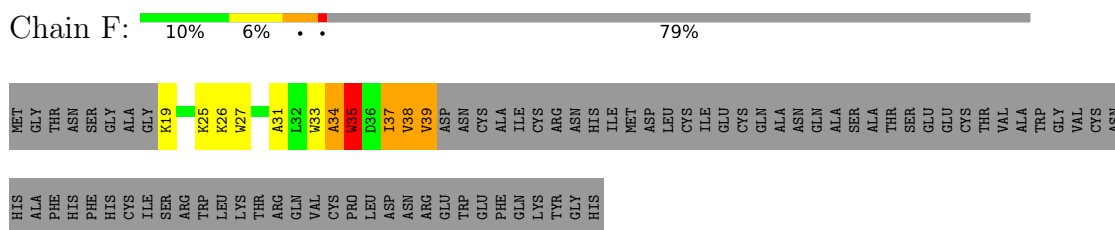




• Molecule 3: CULLIN-4B

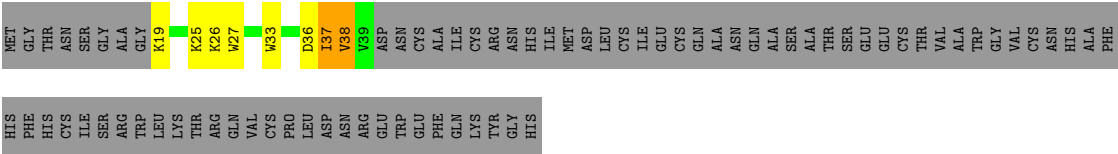


• Molecule 4: E3 UBIQUITIN-PROTEIN LIGASE RBX1

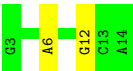
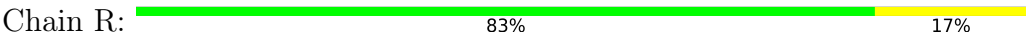


• Molecule 4: E3 UBIQUITIN-PROTEIN LIGASE RBX1

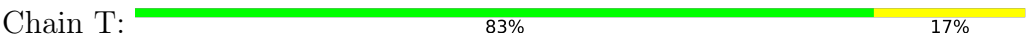




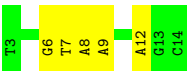
● Molecule 5: 12 BP THF CONTAINING DNA DUPLEX



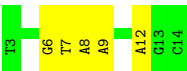
● Molecule 5: 12 BP THF CONTAINING DNA DUPLEX



● Molecule 6: 12 BP DNA DUPLEX



● Molecule 6: 12 BP DNA DUPLEX



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.80Å 155.84Å 255.39Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	29.86 – 7.40 29.86 – 7.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.86-7.40) 97.5 (29.86-7.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 7.23Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.318 , 0.320 0.312 , 0.307	Depositor DCC
R_{free} test set	1355 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	444.7	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 296.2	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	0.76	EDS
Total number of atoms	35553	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 3DR

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	0.53	1/8668 (0.0%)	0.92	45/11756 (0.4%)
1	C	0.54	2/8688 (0.0%)	0.94	47/11783 (0.4%)
2	B	0.48	0/2891	0.78	1/3928 (0.0%)
2	D	0.49	0/2917	0.78	0/3962
3	E	0.52	3/5831 (0.1%)	0.86	7/7832 (0.1%)
3	H	0.48	1/5865 (0.0%)	0.84	2/7878 (0.0%)
4	F	0.44	0/179	0.57	0/241
4	I	0.53	0/186	0.63	0/251
5	R	0.37	0/248	0.72	0/377
5	T	0.37	0/248	0.72	0/377
6	S	0.39	0/279	0.83	0/429
6	U	0.39	0/279	0.82	0/429
All	All	0.51	7/36279 (0.0%)	0.88	102/49243 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	579	THR	C-N	-10.08	1.20	1.33
3	E	376	SER	C-N	8.98	1.47	1.33
3	E	537	ASN	C-N	-8.89	1.22	1.34
1	C	582	LEU	C-N	8.10	1.45	1.33
1	A	582	LEU	C-N	8.05	1.45	1.33
3	H	447	GLN	C-N	6.09	1.42	1.33
1	C	710	LEU	CA-C	5.13	1.59	1.52

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	710	LEU	N-CA-C	10.54	125.71	108.96
1	A	524	GLN	OE1-CD-NE2	-9.65	112.94	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	524	GLN	OE1-CD-NE2	-9.41	113.19	122.60
1	A	624	SER	N-CA-C	9.02	130.01	110.80
1	C	624	SER	N-CA-C	8.99	129.95	110.80
1	C	411	TRP	CA-C-N	8.61	130.60	119.84
1	C	411	TRP	C-N-CA	8.61	130.60	119.84
1	A	411	TRP	CA-C-N	8.60	130.59	119.84
1	A	411	TRP	C-N-CA	8.60	130.59	119.84
3	E	537	ASN	CA-C-N	8.57	132.62	120.28
3	E	537	ASN	C-N-CA	8.57	132.62	120.28
1	A	689	ASP	N-CA-C	-8.21	93.32	110.80
1	A	688	PRO	N-CA-C	8.19	129.34	112.47
1	C	688	PRO	N-CA-C	8.10	129.16	112.47
1	C	689	ASP	N-CA-C	-8.08	93.59	110.80
3	E	376	SER	O-C-N	7.81	131.05	122.15
1	A	451	PHE	N-CA-C	7.41	120.09	110.53
1	C	451	PHE	N-CA-C	7.22	119.84	110.53
1	A	655	ARG	CA-C-N	7.04	128.65	119.84
1	A	655	ARG	C-N-CA	7.04	128.65	119.84
1	C	655	ARG	CA-C-N	6.99	128.57	119.84
1	C	655	ARG	C-N-CA	6.99	128.57	119.84
1	A	524	GLN	CG-CD-NE2	6.93	126.79	116.40
3	E	579	THR	CA-C-N	6.86	133.75	120.99
3	E	579	THR	C-N-CA	6.86	133.75	120.99
1	C	524	GLN	CG-CD-NE2	6.74	126.51	116.40
1	C	698	THR	N-CA-C	6.71	119.52	108.99
1	A	698	THR	N-CA-C	6.63	119.41	108.99
1	C	393	GLY	N-CA-C	6.44	120.50	111.10
1	C	458	PHE	N-CA-C	-6.44	106.01	114.31
1	A	458	PHE	N-CA-C	-6.32	106.15	114.31
1	A	574	PHE	N-CA-C	-6.23	105.63	113.23
1	C	688	PRO	CA-N-CD	-6.23	103.28	112.00
1	A	429	PHE	N-CA-C	-6.21	100.36	109.18
1	A	688	PRO	CA-N-CD	-6.21	103.31	112.00
1	C	429	PHE	N-CA-C	-6.21	100.37	109.18
1	A	571	LEU	N-CA-C	6.17	123.45	109.81
1	C	423	ASP	N-CA-C	-6.05	105.20	114.16
1	C	571	LEU	N-CA-C	5.94	122.94	109.81
1	C	525	GLU	N-CA-C	5.94	118.32	108.99
1	C	555	LEU	N-CA-C	5.88	119.25	110.14
1	A	651	ALA	N-CA-C	5.83	118.67	108.52
1	C	574	PHE	N-CA-C	-5.81	106.14	113.23
1	A	525	GLU	N-CA-C	5.77	118.05	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	555	LEU	N-CA-C	5.77	119.08	110.14
1	C	624	SER	CB-CA-C	-5.74	99.00	110.42
1	C	528	GLN	N-CA-C	5.73	118.22	109.62
1	A	624	SER	CB-CA-C	-5.70	99.07	110.42
1	C	651	ALA	N-CA-C	5.70	118.44	108.52
1	A	487	VAL	N-CA-C	5.65	117.63	112.43
1	C	523	PRO	CA-N-CD	-5.63	104.11	112.00
1	A	528	GLN	N-CA-C	5.61	118.04	109.62
1	A	524	GLN	N-CA-C	-5.59	103.85	111.56
1	A	523	PRO	CA-N-CD	-5.55	104.23	112.00
1	A	416	ASP	CA-C-N	5.55	125.22	119.56
1	A	416	ASP	C-N-CA	5.55	125.22	119.56
1	A	484	LYS	N-CA-C	5.53	117.38	110.91
1	A	523	PRO	N-CA-C	5.49	123.78	112.47
3	H	666	MET	N-CA-C	5.48	119.23	112.54
1	A	607	GLY	N-CA-C	-5.47	107.13	115.66
1	C	625	ASP	N-CA-C	-5.47	99.16	110.80
1	C	506	SER	N-CA-C	5.46	119.94	113.12
1	C	588	PRO	N-CA-C	-5.43	102.92	111.34
1	A	582	LEU	O-C-N	5.43	129.81	122.59
1	A	625	ASP	N-CA-C	-5.42	99.25	110.80
1	C	524	GLN	N-CA-C	-5.42	104.08	111.56
1	C	523	PRO	N-CA-C	5.40	123.60	112.47
1	C	487	VAL	N-CA-C	5.40	117.40	112.43
1	C	607	GLY	N-CA-C	-5.40	107.24	115.66
3	E	666	MET	N-CA-C	5.39	119.12	112.54
1	A	506	SER	N-CA-C	5.36	119.83	113.12
1	C	582	LEU	O-C-N	5.34	129.70	122.59
1	A	608	ASP	N-CA-C	-5.29	105.41	111.07
1	C	929	SER	N-CA-C	5.29	116.34	108.31
1	A	929	SER	N-CA-C	5.28	116.33	108.31
1	C	416	ASP	CA-C-N	5.26	124.92	119.56
1	C	416	ASP	C-N-CA	5.26	124.92	119.56
1	C	687	TYR	CA-C-N	5.25	126.40	119.84
1	C	687	TYR	C-N-CA	5.25	126.40	119.84
3	E	342	VAL	N-CA-C	5.24	115.45	110.53
1	C	397	HIS	N-CA-C	-5.24	102.11	109.96
1	A	604	CYS	N-CA-C	-5.21	103.04	110.59
1	A	567	ARG	N-CA-C	5.21	117.79	110.14
1	A	496	LYS	N-CA-C	-5.20	103.67	110.53
1	A	397	HIS	N-CA-C	-5.19	102.18	109.96
1	C	554	PRO	N-CA-C	-5.19	106.97	114.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	PRO	N-CA-C	-5.18	103.30	111.34
1	A	554	PRO	N-CA-C	-5.18	106.99	114.18
1	C	484	LYS	N-CA-C	5.16	117.46	111.02
1	A	523	PRO	N-CA-CB	-5.15	97.84	103.25
1	C	567	ARG	N-CA-C	5.14	117.70	110.14
1	A	687	TYR	CA-C-N	5.12	126.24	119.84
1	A	687	TYR	C-N-CA	5.12	126.24	119.84
1	C	604	CYS	N-CA-C	-5.12	103.17	110.59
1	C	608	ASP	N-CA-C	-5.10	105.61	111.07
1	A	476	VAL	N-CA-C	-5.10	101.06	109.12
1	C	496	LYS	N-CA-C	-5.08	103.83	110.53
1	C	523	PRO	N-CA-CB	-5.07	97.92	103.25
1	C	476	VAL	N-CA-C	-5.07	101.11	109.12
2	B	118	ILE	N-CA-C	5.06	119.86	109.34
3	H	447	GLN	O-C-N	5.02	128.27	122.25
1	A	494	GLN	N-CA-C	5.01	118.88	112.26

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	8517	0	8394	497	0
1	C	8537	0	8432	412	0
2	B	2819	0	2745	91	0
2	D	2843	0	2788	76	0
3	E	5743	0	5774	306	0
3	H	5773	0	5798	253	0
4	F	175	0	184	22	0
4	I	180	0	178	6	0
5	R	234	0	132	3	0
5	T	234	0	132	3	0
6	S	249	0	136	7	0
6	U	249	0	136	7	0
All	All	35553	0	34829	1496	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 21.

All (1496) 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)
3:E:555:ARG:CG	3:E:559:PRO:HD3	1.32	1.56
1:A:354:THR:CG2	1:A:712:ILE:HG21	1.37	1.53
3:E:552:ILE:CG2	3:E:597:ILE:HG12	1.42	1.48
3:H:365:ARG:CB	3:H:430:THR:HG22	1.44	1.45
3:E:555:ARG:HB3	3:E:559:PRO:CG	1.52	1.37
1:A:926:LEU:HD11	2:B:122:LEU:CD2	1.54	1.36
3:E:285:PHE:CE2	3:E:345:LYS:HD2	1.63	1.32
3:E:552:ILE:HG21	3:E:597:ILE:CG1	1.60	1.32
1:A:926:LEU:CD1	2:B:122:LEU:HD21	1.60	1.31
1:C:499:SER:HB3	3:H:238:GLU:CB	1.59	1.30
3:H:220:LEU:CD2	3:H:240:LEU:HD22	1.59	1.30
3:E:449:LEU:CD1	3:E:479:LEU:HD22	1.66	1.26
3:H:220:LEU:HD23	3:H:240:LEU:CD2	1.65	1.25
1:A:709:LYS:O	1:A:710:LEU:HD23	1.39	1.22
3:E:555:ARG:CB	3:E:559:PRO:HG3	1.69	1.21
1:C:841:ALA:O	2:D:104:SER:HA	1.36	1.20
1:A:354:THR:HG21	1:A:712:ILE:CG2	1.70	1.20
3:E:428:LEU:CD2	3:E:432:LEU:HD23	1.73	1.19
1:A:704:ILE:N	1:A:704:ILE:HD12	1.54	1.18
3:E:555:ARG:CG	3:E:559:PRO:CD	2.22	1.17
3:H:226:ALA:HB1	3:H:233:ILE:N	1.58	1.15
1:A:111:ARG:HG3	2:B:292:TRP:CZ2	1.80	1.15
1:A:394:ILE:HG23	1:A:705:ASP:HB3	1.25	1.14
1:A:354:THR:CG2	1:A:712:ILE:CG2	2.24	1.14
1:A:354:THR:HG21	1:A:712:ILE:HG21	1.16	1.13
3:E:449:LEU:HD11	3:E:479:LEU:HD22	1.22	1.13
3:E:285:PHE:CZ	3:E:345:LYS:HD2	1.83	1.13
3:E:555:ARG:HB3	3:E:559:PRO:CD	1.78	1.13
1:C:910:MET:HE1	2:D:105:ILE:HG21	1.25	1.13
1:A:111:ARG:NE	2:B:292:TRP:HE1	1.43	1.12
1:A:354:THR:HG23	1:A:712:ILE:HG21	1.32	1.10
3:E:494:TRP:CE3	3:E:540:PHE:HD2	1.70	1.10
1:A:562:THR:O	1:A:564:ILE:HG13	1.53	1.09
1:C:562:THR:O	1:C:564:ILE:HG13	1.52	1.09
3:E:340:GLN:HG2	3:E:341:LYS:N	1.65	1.09
3:H:365:ARG:CB	3:H:430:THR:CG2	2.30	1.08
1:A:714:THR:HG22	1:A:716:PRO:HD3	1.15	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HD21	1:A:712:ILE:HG23	1.28	1.08
1:A:912:LEU:HD21	2:B:109:ILE:HG12	1.08	1.08
3:E:552:ILE:HD12	3:E:597:ILE:HD11	1.10	1.08
1:A:354:THR:HG21	1:A:712:ILE:CB	1.84	1.08
3:E:429:ILE:HG12	3:E:429:ILE:O	1.47	1.08
1:A:840:GLU:H	2:B:103:THR:CB	1.66	1.07
3:E:587:LEU:HD22	3:E:629:MET:SD	1.95	1.07
1:A:912:LEU:HD22	2:B:109:ILE:CG2	1.85	1.07
3:E:553:ASN:CB	3:E:598:TYR:HB2	1.84	1.07
1:A:664:HIS:HB2	1:A:1131:LYS:HE3	1.37	1.06
1:A:704:ILE:H	1:A:704:ILE:CD1	1.66	1.06
1:C:910:MET:CE	2:D:105:ILE:HG21	1.84	1.06
3:H:363:ILE:HD13	3:H:363:ILE:C	1.79	1.06
3:E:555:ARG:HB3	3:E:559:PRO:HG3	1.05	1.05
3:E:555:ARG:HG2	3:E:559:PRO:HD3	1.38	1.05
1:A:843:PRO:CB	2:B:104:SER:CB	2.36	1.04
3:E:374:MET:HG2	3:E:378:LEU:HD23	1.37	1.04
3:E:428:LEU:HD22	3:E:432:LEU:HD23	1.40	1.04
1:A:912:LEU:HD21	2:B:109:ILE:CG1	1.87	1.03
3:H:286:LEU:HD21	3:H:349:GLY:HA3	1.40	1.03
3:E:555:ARG:HG3	3:E:559:PRO:CD	1.85	1.03
1:A:111:ARG:CG	2:B:292:TRP:HZ2	1.71	1.02
1:A:704:ILE:HD12	1:A:704:ILE:H	0.87	1.02
3:E:555:ARG:CB	3:E:559:PRO:CD	2.36	1.02
3:H:272:ILE:HD11	3:H:340:GLN:HE22	1.17	1.02
1:A:356:LEU:CD2	1:A:712:ILE:HG23	1.90	1.02
3:E:552:ILE:HD12	3:E:597:ILE:CD1	1.90	1.01
1:C:111:ARG:HH22	2:D:290:CYS:HA	1.21	1.01
1:A:354:THR:CG2	1:A:712:ILE:HD12	1.90	1.01
1:A:354:THR:HG21	1:A:712:ILE:CD1	1.91	1.00
3:E:555:ARG:HG3	3:E:559:PRO:HD3	1.04	1.00
1:C:585:GLU:HG3	3:H:301:ILE:CG2	1.91	1.00
3:H:363:ILE:HD13	3:H:363:ILE:O	1.61	0.99
1:A:714:THR:CG2	1:A:716:PRO:HD3	1.90	0.99
3:E:397:TYR:CD2	3:E:444:VAL:HG13	1.96	0.99
1:C:708:GLN:HA	1:C:708:GLN:NE2	1.75	0.98
1:A:354:THR:CG2	1:A:712:ILE:CD1	2.41	0.98
1:A:912:LEU:CD2	2:B:109:ILE:HG12	1.92	0.98
3:H:220:LEU:HD23	3:H:240:LEU:HD22	0.99	0.98
3:E:555:ARG:CB	3:E:559:PRO:CG	2.33	0.97
3:E:720:LYS:HG3	4:F:34:ALA:HB2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:465:LEU:HB3	3:H:497:TYR:CZ	2.01	0.96
1:A:111:ARG:HG3	2:B:292:TRP:HZ2	1.18	0.96
3:E:555:ARG:CB	3:E:559:PRO:HD3	1.95	0.96
1:A:708:GLN:O	1:A:709:LYS:HD3	1.67	0.95
3:H:353:LEU:HD22	3:H:363:ILE:CB	1.96	0.95
1:A:987:GLU:OE2	2:B:156:HIS:HE1	1.49	0.94
3:H:272:ILE:HD11	3:H:340:GLN:NE2	1.83	0.94
1:C:465:HIS:ND1	1:C:523:PRO:HD3	1.82	0.93
3:E:340:GLN:CG	3:E:341:LYS:H	1.80	0.93
3:H:428:LEU:HA	3:H:432:LEU:CB	1.98	0.93
1:A:465:HIS:ND1	1:A:523:PRO:HD3	1.82	0.93
3:H:457:LEU:HB2	3:H:493:GLN:HE21	1.32	0.93
4:F:37:ILE:HG13	4:F:38:VAL:N	1.83	0.93
3:E:340:GLN:CG	3:E:341:LYS:N	2.30	0.92
3:H:226:ALA:HB1	3:H:233:ILE:H	1.25	0.92
1:A:912:LEU:HD22	2:B:109:ILE:HG23	1.48	0.92
3:H:340:GLN:HG2	3:H:341:LYS:HG2	1.50	0.92
3:E:720:LYS:CG	4:F:34:ALA:HB2	2.00	0.92
3:H:353:LEU:HD22	3:H:363:ILE:CG1	2.00	0.92
3:H:417:VAL:HG22	3:H:448:LEU:HD13	1.49	0.92
1:A:715:VAL:HG12	1:A:715:VAL:O	1.71	0.91
1:C:507:GLN:NE2	1:C:552:LEU:HA	1.85	0.91
3:E:494:TRP:CE3	3:E:540:PHE:CD2	2.57	0.91
3:E:597:ILE:HG22	3:E:600:LYS:HG2	1.49	0.91
1:A:507:GLN:NE2	1:A:552:LEU:HA	1.85	0.91
3:E:588:ASP:HA	3:E:632:LYS:HZ1	1.32	0.91
3:E:286:LEU:HD21	3:E:349:GLY:HA3	1.52	0.91
3:H:223:ALA:CB	3:H:240:LEU:HD11	2.01	0.91
1:C:392:ASN:HB2	1:C:1012:LEU:O	1.70	0.90
1:C:111:ARG:NH2	2:D:290:CYS:HA	1.84	0.90
3:H:339:ASP:O	3:H:340:GLN:HB3	1.72	0.90
1:A:465:HIS:CE1	1:A:523:PRO:HD3	2.07	0.90
3:E:588:ASP:HA	3:E:632:LYS:NZ	1.86	0.90
1:C:18:CYS:HB2	1:C:313:CYS:SG	2.12	0.90
1:C:329:GLY:HA3	1:C:384:GLU:HG2	1.54	0.89
3:E:588:ASP:CA	3:E:632:LYS:HZ1	1.86	0.89
1:A:111:ARG:HE	2:B:292:TRP:HE1	1.20	0.89
3:E:338:SER:O	3:E:343:GLN:HB2	1.72	0.89
1:C:465:HIS:CE1	1:C:523:PRO:HD3	2.07	0.89
3:H:426:ASP:O	3:H:429:ILE:HG23	1.73	0.89
1:A:18:CYS:HB2	1:A:313:CYS:SG	2.12	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.54	0.88
1:A:714:THR:HG22	1:A:716:PRO:CD	2.03	0.88
2:D:323:HIS:NE2	2:D:342:THR:HG21	1.89	0.88
4:F:38:VAL:C	4:F:39:VAL:HG23	1.99	0.88
1:C:987:GLU:OE2	2:D:156:HIS:CE1	2.26	0.88
2:B:323:HIS:NE2	2:B:342:THR:HG21	1.88	0.88
1:C:578:HIS:CD2	1:C:623:LEU:HD12	2.09	0.87
1:A:23:PHE:H	1:A:30:ASN:HD22	1.21	0.87
1:A:578:HIS:CD2	1:A:623:LEU:HD12	2.09	0.87
3:E:552:ILE:CG2	3:E:597:ILE:CG1	2.35	0.87
3:E:552:ILE:CD1	3:E:597:ILE:HD11	2.00	0.87
3:H:226:ALA:CB	3:H:233:ILE:N	2.37	0.87
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.56	0.87
1:C:910:MET:SD	2:D:105:ILE:HD13	2.15	0.87
3:H:340:GLN:HG2	3:H:341:LYS:N	1.87	0.86
1:C:649:VAL:HG12	1:C:650:PHE:H	1.39	0.86
1:A:482:GLU:CD	1:A:483:PRO:HD3	2.00	0.86
1:C:218:MET:HE3	1:C:261:HIS:HD2	1.40	0.86
3:H:226:ALA:CB	3:H:233:ILE:H	1.86	0.86
1:A:375:LEU:O	1:A:389:ILE:CA	2.23	0.85
3:H:290:ASP:CG	3:H:367:LEU:HD13	2.02	0.85
3:E:340:GLN:CG	3:E:341:LYS:HG2	2.06	0.85
1:C:482:GLU:CD	1:C:483:PRO:HD3	2.00	0.85
1:A:499:SER:HB3	3:E:238:GLU:CB	2.06	0.85
1:C:23:PHE:H	1:C:30:ASN:HD22	1.21	0.85
1:C:111:ARG:CZ	2:D:290:CYS:SG	2.64	0.85
1:C:507:GLN:HE22	1:C:553:SER:H	1.24	0.85
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.41	0.85
1:A:218:MET:HE3	1:A:261:HIS:HD2	1.41	0.85
1:A:520:GLN:HG3	1:A:529:ILE:HG13	1.59	0.85
4:F:38:VAL:O	4:F:39:VAL:HG23	1.77	0.84
1:A:649:VAL:HG12	1:A:650:PHE:H	1.38	0.84
3:H:353:LEU:HD22	3:H:363:ILE:HB	1.57	0.84
3:E:595:ARG:C	3:E:596:PHE:CG	2.55	0.84
3:H:378:LEU:O	3:H:379:GLN:HB2	1.77	0.84
1:A:375:LEU:O	1:A:389:ILE:HA	1.78	0.84
3:E:428:LEU:HD23	3:E:432:LEU:HD23	1.58	0.84
3:E:595:ARG:O	3:E:596:PHE:CG	2.30	0.84
1:C:520:GLN:HG3	1:C:529:ILE:HG13	1.60	0.84
4:F:38:VAL:O	4:F:38:VAL:HG22	1.74	0.84
3:H:220:LEU:HD22	3:H:240:LEU:HD22	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:GLU:HG3	1:A:840:GLU:O	1.76	0.83
1:C:81:THR:HG21	1:C:85:ASN:HD22	1.41	0.83
1:C:841:ALA:O	2:D:104:SER:CA	2.25	0.83
1:A:926:LEU:HD11	2:B:122:LEU:HD21	0.85	0.83
1:C:430:VAL:HG13	3:H:246:ASN:HB3	1.58	0.83
1:A:714:THR:O	1:A:715:VAL:HB	1.77	0.83
1:A:111:ARG:CB	2:B:292:TRP:HZ2	1.91	0.83
1:A:446:THR:HG22	1:A:447:GLU:H	1.43	0.82
1:A:507:GLN:HE22	1:A:553:SER:H	1.25	0.82
1:A:394:ILE:HG23	1:A:705:ASP:CB	2.07	0.82
3:E:339:ASP:CG	3:E:340:GLN:N	2.37	0.82
1:A:394:ILE:CG2	1:A:705:ASP:HB3	2.08	0.82
1:C:534:MET:HE1	1:C:569:LEU:HD21	1.62	0.82
3:H:465:LEU:HB3	3:H:497:TYR:CE2	2.14	0.82
1:A:111:ARG:NE	2:B:292:TRP:NE1	2.26	0.82
1:A:404:LEU:HD21	3:E:200:ILE:HD11	1.61	0.82
1:A:585:GLU:OE2	3:E:301:ILE:HG23	1.79	0.82
3:E:332:PHE:CE1	3:E:336:ILE:HG21	2.14	0.82
3:H:461:LEU:HD22	3:H:493:GLN:HB3	1.61	0.82
1:A:509:VAL:HG23	1:A:543:ILE:HD13	1.62	0.81
1:A:987:GLU:OE2	2:B:156:HIS:CE1	2.33	0.81
1:C:585:GLU:OE2	3:H:301:ILE:HG23	1.79	0.81
1:A:602:LEU:C	1:A:603:LEU:HD23	2.05	0.81
1:C:446:THR:HG22	1:C:447:GLU:H	1.43	0.81
1:C:602:LEU:C	1:C:603:LEU:HD23	2.04	0.81
3:E:617:VAL:HG11	3:E:827:GLN:HB3	1.62	0.81
3:H:457:LEU:HB3	3:H:493:GLN:HG2	1.60	0.81
1:A:534:MET:HE1	1:A:569:LEU:HD21	1.62	0.81
1:C:926:LEU:CD2	2:D:105:ILE:HD11	2.10	0.81
3:H:340:GLN:HG2	3:H:341:LYS:H	1.46	0.81
3:H:617:VAL:HG11	3:H:827:GLN:HB3	1.62	0.81
1:A:912:LEU:HD22	2:B:109:ILE:HG21	1.62	0.81
1:A:111:ARG:CB	2:B:292:TRP:CZ2	2.65	0.80
1:A:413:LEU:HB2	1:A:424:THR:HB	1.63	0.80
1:A:537:GLU:OE1	3:E:236:ASN:HB2	1.81	0.80
3:E:449:LEU:HD13	3:E:479:LEU:HD22	1.64	0.80
1:A:664:HIS:C	1:A:1131:LYS:HE2	2.07	0.80
1:C:509:VAL:HG23	1:C:543:ILE:HD13	1.62	0.80
1:C:987:GLU:OE2	2:D:156:HIS:HE1	1.62	0.80
1:A:356:LEU:HD21	1:A:712:ILE:CG2	2.10	0.80
1:C:413:LEU:HB2	1:C:424:THR:HB	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ARG:HG3	1:A:714:THR:H	1.47	0.79
1:C:430:VAL:HG22	3:H:246:ASN:HB3	1.63	0.79
1:C:412:PRO:HB2	1:C:422:ASP:OD2	1.83	0.79
1:C:705:ASP:OD1	1:C:707:ILE:HG13	1.83	0.79
1:A:111:ARG:HB3	2:B:290:CYS:SG	2.22	0.78
3:H:220:LEU:CD2	3:H:240:LEU:CD2	2.42	0.78
3:H:340:GLN:CG	3:H:341:LYS:HG2	2.12	0.78
1:A:708:GLN:O	1:A:709:LYS:CD	2.31	0.78
1:A:987:GLU:CD	2:B:156:HIS:CE1	2.61	0.78
3:E:285:PHE:CE2	3:E:345:LYS:CD	2.58	0.78
1:A:578:HIS:NE2	1:A:623:LEU:HD12	1.99	0.78
1:C:814:LEU:HD11	2:D:106:LEU:HD13	1.66	0.78
1:A:111:ARG:CG	2:B:292:TRP:CZ2	2.53	0.78
3:E:491:LEU:HG	3:E:540:PHE:CZ	2.18	0.78
3:H:901:ARG:O	3:H:902:ASP:HB2	1.84	0.78
3:E:350:ILE:HA	3:E:368:LEU:HD21	1.65	0.78
1:A:354:THR:HG21	1:A:712:ILE:HD12	1.59	0.77
1:A:532:THR:HG1	1:A:574:PHE:HD2	1.29	0.77
1:A:708:GLN:O	1:A:709:LYS:CE	2.31	0.77
1:C:578:HIS:NE2	1:C:623:LEU:HD12	1.99	0.77
1:A:412:PRO:HB2	1:A:422:ASP:OD2	1.83	0.77
1:A:23:PHE:H	1:A:30:ASN:ND2	1.82	0.77
1:C:507:GLN:HE22	1:C:552:LEU:HA	1.48	0.77
1:A:507:GLN:HE22	1:A:552:LEU:HA	1.48	0.77
3:E:901:ARG:O	3:E:902:ASP:HB2	1.84	0.76
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.15	0.76
1:C:649:VAL:HG12	1:C:650:PHE:N	2.00	0.76
1:C:708:GLN:HA	1:C:708:GLN:HE21	1.50	0.76
1:A:707:ILE:O	1:A:708:GLN:CB	2.33	0.76
1:A:709:LYS:O	1:A:710:LEU:CD2	2.30	0.76
1:C:23:PHE:H	1:C:30:ASN:ND2	1.82	0.76
3:E:520:LEU:CD2	3:E:586:MET:HE1	2.15	0.76
1:A:649:VAL:HG12	1:A:650:PHE:N	2.00	0.76
3:E:417:VAL:HG21	3:E:449:LEU:HD21	1.66	0.76
1:A:450:GLY:HA3	1:A:479:VAL:CG2	2.17	0.75
3:H:229:ASN:C	3:H:231:THR:H	1.94	0.75
1:A:448:LEU:HB3	1:A:451:PHE:HD2	1.52	0.75
1:A:452:VAL:HG12	1:A:454:ASP:OD1	1.86	0.75
1:C:329:GLY:HA3	1:C:384:GLU:CG	2.16	0.75
3:E:587:LEU:HB3	3:E:632:LYS:HD3	1.67	0.75
3:H:340:GLN:NE2	3:H:342:VAL:HG22	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:PRO:HA	2:B:101:GLY:HA2	1.68	0.75
1:A:987:GLU:OE1	2:B:159:HIS:HB2	1.86	0.74
1:C:452:VAL:HG12	1:C:454:ASP:OD1	1.86	0.74
3:E:595:ARG:O	3:E:596:PHE:CD2	2.40	0.74
4:F:35:TRP:HA	4:F:35:TRP:CE3	2.20	0.74
3:H:299:GLN:HA	3:H:302:MET:HE2	1.68	0.74
1:A:10:GLN:OE1	1:A:710:LEU:HD11	1.87	0.74
1:C:450:GLY:HA3	1:C:479:VAL:CG2	2.17	0.74
1:A:375:LEU:O	1:A:389:ILE:CB	2.36	0.74
3:E:299:GLN:HA	3:E:302:MET:HE2	1.68	0.74
1:C:585:GLU:CG	3:H:301:ILE:CG2	2.66	0.74
1:A:354:THR:HG22	1:A:712:ILE:CD1	2.17	0.74
1:A:664:HIS:CB	1:A:1131:LYS:HE3	2.18	0.74
3:E:556:PRO:O	3:E:557:ASN:CG	2.30	0.74
1:A:589:ARG:NH1	3:E:241:TYR:HE2	1.85	0.74
1:C:928:ARG:HD2	2:D:437:THR:HG23	1.68	0.74
3:E:374:MET:HG2	3:E:378:LEU:CD2	2.15	0.74
3:H:457:LEU:HB2	3:H:493:GLN:NE2	2.03	0.74
1:A:451:PHE:CD1	1:A:470:GLN:HB2	2.23	0.73
1:C:469:ILE:HD11	1:C:476:VAL:HG23	1.69	0.73
1:C:585:GLU:HG3	3:H:301:ILE:HG21	1.68	0.73
3:H:293:TRP:CH2	3:H:370:SER:HB2	2.22	0.73
1:A:835:MET:HG2	1:A:845:GLN:O	1.88	0.73
1:A:469:ILE:HD11	1:A:476:VAL:HG23	1.69	0.73
1:A:657:THR:HG22	1:A:658:VAL:H	1.53	0.73
1:C:910:MET:CE	2:D:105:ILE:HD13	2.19	0.73
1:A:844:LYS:O	1:A:845:GLN:HG3	1.88	0.73
1:A:111:ARG:HB2	2:B:292:TRP:CZ2	2.24	0.73
1:C:448:LEU:HB3	1:C:451:PHE:HD2	1.52	0.73
1:C:563:ASP:OD2	1:C:565:SER:HB3	1.87	0.73
1:A:926:LEU:HD21	2:B:122:LEU:CG	2.18	0.73
1:C:451:PHE:CD1	1:C:470:GLN:HB2	2.23	0.73
1:A:563:ASP:OD2	1:A:565:SER:HB3	1.87	0.72
1:A:354:THR:HG21	1:A:712:ILE:CG1	2.18	0.72
1:A:578:HIS:CD2	1:A:623:LEU:H	2.06	0.72
3:H:465:LEU:HD21	3:H:494:TRP:HD1	1.53	0.72
1:C:578:HIS:CD2	1:C:623:LEU:H	2.06	0.72
1:C:404:LEU:HD21	3:H:200:ILE:HD11	1.70	0.72
1:C:657:THR:HG22	1:C:658:VAL:H	1.52	0.72
1:C:841:ALA:HA	2:D:103:THR:O	1.90	0.72
3:E:353:LEU:CB	3:E:368:LEU:HD11	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:597:ILE:O	3:E:600:LYS:HE2	1.89	0.72
1:C:926:LEU:HD21	2:D:105:ILE:HD11	1.71	0.72
3:H:847:GLN:HB3	3:H:889:ARG:HD2	1.72	0.72
1:A:111:ARG:HG3	2:B:292:TRP:CE2	2.25	0.72
1:C:585:GLU:OE2	3:H:301:ILE:CG2	2.38	0.72
3:H:461:LEU:CD2	3:H:493:GLN:HB3	2.18	0.72
1:A:912:LEU:CD2	2:B:109:ILE:CG1	2.62	0.72
3:E:450:GLY:C	3:E:452:HIS:H	1.97	0.72
3:E:594:PHE:C	3:E:596:PHE:H	1.96	0.72
3:E:597:ILE:O	3:E:600:LYS:HG2	1.88	0.72
1:C:1055:GLN:HE22	1:C:1090:ASP:H	1.36	0.72
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.72	0.72
1:A:664:HIS:HB2	1:A:1131:LYS:CE	2.18	0.72
1:A:840:GLU:N	2:B:103:THR:CB	2.48	0.72
1:A:842:GLU:O	1:A:844:LYS:HD3	1.90	0.72
1:C:537:GLU:OE1	3:H:236:ASN:HB2	1.89	0.72
1:A:218:MET:HE3	1:A:261:HIS:CD2	2.25	0.71
1:A:465:HIS:HB2	1:A:467:GLN:HE21	1.54	0.71
1:C:589:ARG:NH1	3:H:241:TYR:CE2	2.58	0.71
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.37	0.71
1:C:469:ILE:HD13	1:C:470:GLN:N	2.06	0.71
1:C:465:HIS:O	1:C:467:GLN:HG3	1.89	0.71
1:A:394:ILE:HG22	1:A:395:GLY:N	2.05	0.71
3:E:847:GLN:HB3	3:E:889:ARG:HD2	1.72	0.71
1:C:465:HIS:HB2	1:C:467:GLN:HE21	1.54	0.71
1:C:579:LYS:HG2	1:C:581:MET:HE3	1.72	0.71
3:E:555:ARG:HB2	3:E:559:PRO:HG3	1.68	0.71
1:A:450:GLY:HA3	1:A:479:VAL:HG21	1.73	0.71
1:A:465:HIS:O	1:A:467:GLN:HG3	1.89	0.71
1:A:889:ARG:HD3	1:A:901:THR:HB	1.73	0.71
3:H:290:ASP:CG	3:H:367:LEU:CD1	2.64	0.71
1:A:710:LEU:O	1:A:711:HIS:C	2.34	0.71
1:C:451:PHE:CE1	1:C:470:GLN:HB2	2.26	0.71
1:C:889:ARG:HD3	1:C:901:THR:HB	1.73	0.71
3:E:449:LEU:HD11	3:E:479:LEU:CD2	2.13	0.71
3:H:272:ILE:CD1	3:H:340:GLN:HE22	1.99	0.71
1:A:451:PHE:CE1	1:A:470:GLN:HB2	2.25	0.70
1:A:532:THR:HG22	1:A:533:GLU:N	2.06	0.70
1:A:652:CYS:HB3	1:A:676:VAL:O	1.91	0.70
1:C:399:HIS:NE2	1:C:703:THR:HG22	2.05	0.70
1:C:532:THR:HG22	1:C:533:GLU:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:GLU:CG	3:H:301:ILE:HG23	2.21	0.70
3:H:428:LEU:CA	3:H:432:LEU:CB	2.69	0.70
3:H:434:GLN:C	3:H:436:THR:H	1.99	0.70
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.73	0.70
1:C:707:ILE:HG22	1:C:707:ILE:O	1.90	0.70
1:A:480:SER:O	1:A:484:LYS:HA	1.92	0.70
3:H:457:LEU:CB	3:H:493:GLN:HE21	2.04	0.70
2:D:263:LEU:HB2	2:D:272:PHE:HB3	1.72	0.70
3:E:530:ILE:HA	3:E:534:PHE:HB2	1.73	0.70
1:A:715:VAL:O	1:A:715:VAL:CG1	2.40	0.70
3:E:595:ARG:C	3:E:596:PHE:CD1	2.70	0.70
1:C:218:MET:HE3	1:C:261:HIS:CD2	2.25	0.70
1:C:561:TRP:O	1:C:587:ILE:CG2	2.40	0.70
3:E:429:ILE:O	3:E:429:ILE:CG1	2.35	0.69
3:H:223:ALA:HB2	3:H:240:LEU:HD11	1.72	0.69
1:C:450:GLY:HA3	1:C:479:VAL:HG21	1.73	0.69
3:E:203:PHE:O	3:E:204:LYS:C	2.35	0.69
1:A:469:ILE:HD13	1:A:470:GLN:N	2.06	0.69
3:E:597:ILE:O	3:E:600:LYS:CG	2.40	0.69
3:H:530:ILE:HA	3:H:534:PHE:HB2	1.73	0.69
1:C:652:CYS:HB3	1:C:676:VAL:O	1.91	0.69
4:F:37:ILE:HG13	4:F:38:VAL:H	1.57	0.69
3:H:363:ILE:C	3:H:363:ILE:CD1	2.53	0.69
1:C:430:VAL:HG13	3:H:246:ASN:CB	2.21	0.69
1:A:452:VAL:HG23	1:A:470:GLN:OE1	1.93	0.69
1:A:561:TRP:O	1:A:587:ILE:CG2	2.40	0.69
1:C:596:PHE:HE1	1:C:648:ASN:HA	1.58	0.69
3:E:428:LEU:HD22	3:E:432:LEU:CD2	2.20	0.69
3:H:336:ILE:O	3:H:342:VAL:HG11	1.91	0.69
1:C:480:SER:O	1:C:484:LYS:HA	1.92	0.69
1:C:592:LEU:HD23	1:C:593:MET:O	1.92	0.69
3:E:350:ILE:HG12	3:E:368:LEU:CD2	2.23	0.69
3:H:203:PHE:O	3:H:204:LYS:C	2.35	0.69
3:H:230:SER:C	3:H:232:SER:H	2.00	0.69
1:A:389:ILE:O	1:A:390:ILE:CB	2.40	0.69
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.75	0.69
3:E:339:ASP:O	3:E:340:GLN:HB3	1.93	0.69
1:A:596:PHE:HE1	1:A:648:ASN:HA	1.57	0.68
3:H:337:ILE:HG13	3:H:374:MET:CE	2.22	0.68
1:C:618:ILE:HG13	1:C:619:GLU:N	2.08	0.68
3:H:450:GLY:O	3:H:451:GLU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:ILE:HD12	1:C:704:ILE:H	1.57	0.68
3:E:555:ARG:O	3:E:556:PRO:C	2.36	0.68
1:A:579:LYS:HG2	1:A:581:MET:HE3	1.73	0.68
3:H:762:PHE:HB3	3:H:766:GLU:HG3	1.76	0.68
1:A:592:LEU:HD23	1:A:593:MET:O	1.92	0.68
3:E:598:TYR:CD2	3:E:878:LYS:O	2.46	0.68
3:E:340:GLN:HG2	3:E:341:LYS:HG2	1.76	0.68
1:A:926:LEU:HD11	2:B:122:LEU:HD23	1.70	0.68
3:E:339:ASP:CG	3:E:340:GLN:H	1.99	0.68
1:A:618:ILE:HG13	1:A:619:GLU:N	2.07	0.68
1:C:402:ILE:CD1	3:H:198:LEU:HB3	2.23	0.68
3:E:417:VAL:HG21	3:E:449:LEU:CD2	2.24	0.68
3:E:762:PHE:HB3	3:E:766:GLU:HG3	1.76	0.68
1:A:111:ARG:NH1	2:B:290:CYS:SG	2.67	0.67
1:A:356:LEU:CD2	1:A:712:ILE:CG2	2.70	0.67
1:C:452:VAL:HG23	1:C:470:GLN:OE1	1.93	0.67
3:E:507:ILE:HD11	3:E:554:LYS:NZ	2.09	0.67
3:E:588:ASP:CA	3:E:632:LYS:NZ	2.53	0.67
1:C:430:VAL:CG1	3:H:246:ASN:HB3	2.24	0.67
1:C:499:SER:CB	3:H:238:GLU:CB	2.55	0.67
1:A:397:HIS:HB2	1:A:703:THR:CG2	2.25	0.67
3:E:520:LEU:HD22	3:E:586:MET:HE1	1.76	0.67
1:A:354:THR:HG22	1:A:712:ILE:HD13	1.76	0.67
3:E:552:ILE:HG21	3:E:597:ILE:HG12	0.71	0.67
1:C:585:GLU:CD	3:H:301:ILE:HG23	2.19	0.67
3:E:552:ILE:HG23	3:E:597:ILE:HG12	1.65	0.67
1:A:440:GLY:O	1:A:686:GLY:HA3	1.94	0.67
1:A:840:GLU:O	1:A:840:GLU:CG	2.43	0.67
1:A:912:LEU:CD2	2:B:109:ILE:CG2	2.69	0.67
1:C:440:GLY:O	1:C:686:GLY:HA3	1.94	0.67
3:H:226:ALA:HB1	3:H:232:SER:C	2.18	0.67
1:C:926:LEU:HD21	2:D:126:LEU:HD11	1.76	0.66
3:E:374:MET:CG	3:E:378:LEU:HD23	2.20	0.66
1:A:111:ARG:HB2	2:B:292:TRP:HZ2	1.60	0.66
1:A:714:THR:O	1:A:715:VAL:CB	2.44	0.66
2:D:443:SER:HB2	2:D:450:LEU:HB2	1.76	0.66
4:F:35:TRP:HA	4:F:35:TRP:HE3	1.58	0.66
3:E:340:GLN:HG3	3:E:341:LYS:H	1.59	0.66
1:A:460:CYS:HA	1:A:469:ILE:O	1.96	0.66
1:C:630:THR:CB	1:C:797:HIS:CE1	2.78	0.66
3:E:720:LYS:HG2	4:F:34:ALA:CB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:CG2	1:A:712:ILE:HD13	2.24	0.66
1:C:630:THR:HB	1:C:797:HIS:CE1	2.30	0.66
1:A:536:HIS:CD2	1:A:563:ASP:HB3	2.31	0.66
3:H:340:GLN:CD	3:H:341:LYS:HG2	2.20	0.66
1:C:926:LEU:HD22	2:D:105:ILE:CD1	2.26	0.66
3:E:332:PHE:CZ	3:E:336:ILE:HG21	2.31	0.66
3:E:599:GLY:HA2	3:E:879:PHE:HB3	1.78	0.66
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.76	0.65
1:C:460:CYS:HA	1:C:469:ILE:O	1.95	0.65
1:C:564:ILE:HG22	1:C:564:ILE:O	1.96	0.65
1:A:926:LEU:HD21	2:B:122:LEU:HD11	1.78	0.65
3:H:911:TYR:O	3:H:912:ILE:HG13	1.96	0.65
1:C:582:LEU:O	1:C:583:GLY:O	2.14	0.65
3:E:555:ARG:CD	3:E:556:PRO:HD2	2.27	0.65
3:H:464:LEU:HB3	3:H:473:LEU:HD21	1.78	0.65
1:A:354:THR:HG23	1:A:712:ILE:CG2	2.12	0.65
1:C:987:GLU:OE1	2:D:159:HIS:HB2	1.97	0.65
1:A:582:LEU:O	1:A:583:GLY:O	2.14	0.65
3:H:223:ALA:CB	3:H:240:LEU:CD1	2.75	0.65
3:H:340:GLN:HG2	3:H:341:LYS:CG	2.26	0.65
3:E:285:PHE:CZ	3:E:345:LYS:CD	2.71	0.65
3:E:494:TRP:HE3	3:E:540:PHE:HD2	1.41	0.65
1:C:394:ILE:HD12	1:C:706:GLU:HA	1.78	0.65
1:C:536:HIS:CD2	1:C:563:ASP:HB3	2.31	0.65
3:E:417:VAL:HG11	3:E:449:LEU:HD11	1.79	0.65
1:A:711:HIS:O	1:A:713:ARG:N	2.30	0.65
1:C:910:MET:HE1	2:D:105:ILE:CG2	2.16	0.65
1:A:562:THR:O	1:A:564:ILE:N	2.30	0.64
1:C:446:THR:CG2	1:C:447:GLU:H	2.05	0.64
3:E:720:LYS:CG	4:F:34:ALA:CB	2.74	0.64
1:A:564:ILE:HG22	1:A:564:ILE:O	1.96	0.64
1:C:507:GLN:HE22	1:C:553:SER:N	1.94	0.64
1:C:518:TYR:HD1	1:C:519:LEU:N	1.95	0.64
3:E:911:TYR:O	3:E:912:ILE:HG13	1.96	0.64
1:C:667:VAL:HG22	1:C:1015:GLN:O	1.98	0.64
3:E:434:GLN:O	3:E:436:THR:N	2.30	0.64
3:E:594:PHE:O	3:E:596:PHE:N	2.30	0.64
3:H:434:GLN:O	3:H:436:THR:N	2.30	0.64
1:C:392:ASN:HD22	1:C:1012:LEU:C	2.06	0.64
1:C:520:GLN:HG3	1:C:529:ILE:CG1	2.27	0.64
3:E:494:TRP:CZ3	3:E:540:PHE:HD2	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:434:GLN:C	3:E:436:THR:H	2.03	0.64
1:A:589:ARG:NH1	3:E:241:TYR:CE2	2.65	0.64
3:E:415:HIS:O	3:E:419:LYS:HG2	1.97	0.64
1:A:507:GLN:NE2	1:A:553:SER:H	1.95	0.64
1:A:601:TYR:CE2	1:A:666:LEU:HD21	2.33	0.64
1:A:708:GLN:O	1:A:709:LYS:NZ	2.31	0.64
1:C:562:THR:O	1:C:564:ILE:N	2.30	0.64
3:E:450:GLY:O	3:E:452:HIS:N	2.30	0.64
3:E:555:ARG:O	3:E:557:ASN:N	2.30	0.64
1:A:715:VAL:N	1:A:716:PRO:CD	2.60	0.64
1:C:402:ILE:HD13	3:H:198:LEU:CB	2.28	0.64
3:H:467:GLU:HG2	3:H:469:ARG:HE	1.63	0.64
1:A:692:ALA:C	1:A:693:LEU:HD23	2.23	0.63
1:A:710:LEU:O	1:A:712:ILE:N	2.32	0.63
1:C:926:LEU:CD2	2:D:105:ILE:CD1	2.76	0.63
3:H:230:SER:O	3:H:232:SER:N	2.30	0.63
3:E:411:PRO:HG3	3:E:464:LEU:HD21	1.81	0.63
1:A:507:GLN:HE22	1:A:553:SER:N	1.95	0.63
1:C:430:VAL:CG2	3:H:246:ASN:HB3	2.27	0.63
1:C:601:TYR:CE2	1:C:666:LEU:HD21	2.33	0.63
3:H:229:ASN:O	3:H:231:THR:N	2.30	0.63
3:H:336:ILE:O	3:H:342:VAL:CB	2.45	0.63
3:H:337:ILE:O	3:H:338:SER:C	2.41	0.63
3:H:599:GLY:H	3:H:878:LYS:HG2	1.63	0.63
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.81	0.63
3:E:431:TYR:O	3:E:432:LEU:HB2	1.98	0.63
3:E:595:ARG:HB2	3:E:596:PHE:CZ	2.33	0.63
4:F:38:VAL:C	4:F:39:VAL:CG2	2.71	0.63
1:A:518:TYR:HD1	1:A:519:LEU:N	1.96	0.63
3:E:359:ASN:N	3:E:359:ASN:OD1	2.32	0.63
1:A:414:ARG:CB	1:A:462:ASN:HD21	2.12	0.63
3:E:555:ARG:HD2	3:E:556:PRO:HD2	1.81	0.63
3:H:229:ASN:N	3:H:229:ASN:OD1	2.30	0.63
3:H:340:GLN:O	3:H:341:LYS:C	2.41	0.63
1:A:705:ASP:O	1:A:707:ILE:HG13	1.98	0.63
1:C:692:ALA:C	1:C:693:LEU:HD23	2.23	0.63
1:C:414:ARG:CB	1:C:462:ASN:HD21	2.12	0.62
2:D:249:ARG:HE	2:D:291:ASP:HB3	1.64	0.62
1:A:520:GLN:HG3	1:A:529:ILE:CG1	2.27	0.62
1:C:476:VAL:HG13	1:C:490:TRP:HB3	1.81	0.62
1:C:482:GLU:OE1	1:C:483:PRO:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:ASN:HD21	1:C:619:GLU:HB2	1.64	0.62
1:C:507:GLN:NE2	1:C:553:SER:H	1.94	0.62
1:C:562:THR:HG22	1:C:563:ASP:N	2.14	0.62
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	1.81	0.62
1:C:839:GLU:H	2:D:103:THR:HG21	1.63	0.62
1:C:928:ARG:NH1	2:D:437:THR:CG2	2.62	0.62
1:C:7:VAL:HG13	1:C:1091:GLY:HA3	1.82	0.62
1:A:709:LYS:C	1:A:710:LEU:HD23	2.21	0.62
1:C:928:ARG:NH1	2:D:437:THR:HG23	2.14	0.62
3:E:340:GLN:HG3	3:E:341:LYS:HG2	1.82	0.62
3:E:397:TYR:CD2	3:E:444:VAL:CG1	2.78	0.62
1:A:669:SER:O	1:A:670:ASN:C	2.43	0.62
2:B:249:ARG:HE	2:B:291:ASP:HB3	1.63	0.62
1:A:591:ILE:O	1:A:592:LEU:HB2	2.00	0.62
1:A:926:LEU:HD21	2:B:122:LEU:CD1	2.30	0.62
1:C:926:LEU:HD22	2:D:105:ILE:HD11	1.82	0.62
3:E:720:LYS:HG2	4:F:34:ALA:HB2	1.82	0.62
3:E:405:MET:HE3	3:E:405:MET:HA	1.82	0.61
1:A:354:THR:HG21	1:A:712:ILE:HB	1.78	0.61
1:A:582:LEU:HD13	1:A:583:GLY:H	1.64	0.61
3:E:598:TYR:HD2	3:E:878:LYS:O	1.83	0.61
1:A:562:THR:HG22	1:A:563:ASP:N	2.14	0.61
1:A:617:ASN:HD21	1:A:619:GLU:HB2	1.64	0.61
1:A:926:LEU:HD21	2:B:122:LEU:HG	1.80	0.61
1:C:912:LEU:CD2	2:D:109:ILE:HD13	2.30	0.61
1:C:928:ARG:CZ	2:D:437:THR:CG2	2.78	0.61
4:F:38:VAL:O	4:F:39:VAL:CG2	2.47	0.61
1:A:492:GLU:HG3	1:A:496:LYS:HB2	1.83	0.61
1:C:889:ARG:HG3	1:C:904:ASN:ND2	2.16	0.61
1:C:111:ARG:NH2	2:D:290:CYS:SG	2.73	0.61
1:A:657:THR:HG21	1:A:668:PHE:HB3	1.82	0.61
1:C:591:ILE:O	1:C:592:LEU:HB2	2.00	0.61
3:E:501:PHE:O	3:E:504:THR:HG22	2.01	0.61
5:R:12:DG:N2	6:S:6:DG:C2	2.69	0.61
1:A:889:ARG:HG3	1:A:904:ASN:ND2	2.16	0.61
5:T:12:DG:N2	6:U:6:DG:C2	2.69	0.61
1:A:482:GLU:OE1	1:A:483:PRO:HD3	1.99	0.61
1:C:396:ILE:HD13	1:C:396:ILE:H	1.66	0.60
1:C:669:SER:O	1:C:670:ASN:C	2.43	0.60
3:H:415:HIS:O	3:H:419:LYS:HG2	2.00	0.60
1:A:394:ILE:CG2	1:A:395:GLY:N	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:405:MET:HE3	3:H:405:MET:HA	1.83	0.60
3:H:465:LEU:HD21	3:H:494:TRP:CD1	2.35	0.60
3:H:501:PHE:O	3:H:504:THR:HG22	2.01	0.60
1:A:518:TYR:CD1	1:A:518:TYR:C	2.80	0.60
1:C:582:LEU:HD13	1:C:583:GLY:H	1.65	0.60
3:E:414:LEU:HB3	3:E:475:LEU:CD2	2.32	0.60
3:H:206:LYS:CB	3:H:207:PRO:CD	2.79	0.60
1:A:446:THR:CG2	1:A:447:GLU:H	2.05	0.60
1:C:492:GLU:HG3	1:C:496:LYS:HB2	1.83	0.60
1:A:387:LEU:CD1	1:A:735:VAL:HG21	2.31	0.60
3:H:290:ASP:OD1	3:H:367:LEU:CD1	2.50	0.60
3:E:286:LEU:HD21	3:E:349:GLY:CA	2.30	0.60
3:E:587:LEU:CB	3:E:632:LYS:HD3	2.31	0.60
1:A:912:LEU:HD21	2:B:109:ILE:CD1	2.31	0.60
1:A:589:ARG:HD3	3:E:241:TYR:OH	2.02	0.60
1:A:397:HIS:HB2	1:A:703:THR:HG23	1.84	0.59
1:A:889:ARG:HG3	1:A:904:ASN:HD21	1.67	0.59
3:E:596:PHE:CD1	3:E:596:PHE:N	2.69	0.59
1:A:573:SER:OG	1:A:575:GLU:HB2	2.02	0.59
1:A:673:LEU:HD23	1:A:674:LYS:H	1.67	0.59
1:C:851:PHE:HB3	1:C:858:LEU:HD22	1.85	0.59
3:H:446:LYS:HG3	3:H:484:ARG:HH22	1.67	0.59
1:C:402:ILE:HD12	3:H:198:LEU:HB3	1.85	0.59
3:E:337:ILE:O	3:E:342:VAL:CB	2.50	0.59
1:C:441:GLU:HG2	1:C:441:GLU:O	2.02	0.59
3:E:350:ILE:HA	3:E:368:LEU:CD2	2.32	0.59
3:E:375:LEU:HD22	3:E:380:ILE:HB	1.83	0.59
1:A:851:PHE:HB3	1:A:858:LEU:HD22	1.85	0.59
1:C:912:LEU:HD22	2:D:109:ILE:HD13	1.85	0.59
1:A:454:ASP:OD1	1:A:454:ASP:N	2.28	0.59
1:A:498:ILE:HD12	1:A:498:ILE:N	2.18	0.59
1:A:588:PRO:HB3	1:A:604:CYS:SG	2.43	0.59
1:C:890:LEU:HB3	1:C:903:CYS:HB2	1.84	0.59
3:E:374:MET:O	3:E:378:LEU:N	2.36	0.59
3:E:730:CYS:HB2	4:F:26:LYS:O	2.03	0.59
1:A:396:ILE:HD13	1:A:396:ILE:H	1.68	0.58
1:A:407:ILE:HG21	1:A:410:LEU:HD23	1.85	0.58
1:C:518:TYR:C	1:C:518:TYR:CD1	2.79	0.58
1:C:912:LEU:HD21	2:D:109:ILE:CD1	2.33	0.58
3:E:506:VAL:O	3:E:555:ARG:HD3	2.03	0.58
3:H:444:VAL:HG12	3:H:448:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.84	0.58
1:A:432:GLN:NE2	3:E:207:PRO:HG3	2.18	0.58
1:A:922:LEU:HD23	1:A:957:VAL:HG13	1.84	0.58
1:C:498:ILE:HD12	1:C:498:ILE:N	2.18	0.58
1:C:889:ARG:HG3	1:C:904:ASN:HD21	1.67	0.58
3:E:375:LEU:HD23	3:E:380:ILE:HD12	1.85	0.58
1:A:841:ALA:N	2:B:103:THR:CB	2.65	0.58
3:H:519:LEU:HD21	3:H:552:ILE:HD11	1.85	0.58
1:A:441:GLU:O	1:A:441:GLU:HG2	2.02	0.58
1:C:446:THR:HG22	1:C:447:GLU:N	2.16	0.58
1:C:910:MET:HE1	2:D:105:ILE:HD13	1.86	0.58
3:H:231:THR:O	3:H:232:SER:C	2.45	0.58
3:H:604:GLU:HB2	3:H:641:PHE:CE2	2.39	0.58
1:A:926:LEU:CD2	2:B:122:LEU:HD11	2.33	0.58
1:C:414:ARG:HB3	1:C:462:ASN:HD21	1.68	0.58
1:C:573:SER:OG	1:C:575:GLU:HB2	2.02	0.58
1:C:477:ARG:HG2	1:C:489:GLU:HG3	1.86	0.58
1:A:433:THR:HG22	1:A:434:ARG:H	1.69	0.58
1:C:588:PRO:HB3	1:C:604:CYS:SG	2.43	0.58
1:C:600:HIS:HB2	1:C:616:LEU:O	2.04	0.58
1:A:432:GLN:HA	1:A:455:GLN:O	2.04	0.58
1:A:841:ALA:C	2:B:103:THR:O	2.46	0.58
1:C:673:LEU:HD23	1:C:674:LYS:H	1.68	0.58
3:E:604:GLU:HB2	3:E:641:PHE:CE2	2.38	0.58
3:H:336:ILE:O	3:H:342:VAL:CG1	2.51	0.58
1:C:695:ASN:OD1	1:C:697:SER:N	2.30	0.58
3:E:491:LEU:HG	3:E:540:PHE:CE1	2.39	0.58
1:A:354:THR:CB	1:A:712:ILE:HD12	2.33	0.58
1:A:493:PRO:HB2	1:A:494:GLN:HE22	1.69	0.58
1:C:502:SER:O	1:C:503:CYS:HB2	2.04	0.58
1:C:814:LEU:HD11	2:D:106:LEU:CD1	2.32	0.58
1:C:903:CYS:HB3	1:C:942:PHE:CE2	2.38	0.58
1:C:953:TRP:CG	2:D:119:HIS:HE1	2.21	0.58
3:E:596:PHE:O	3:E:597:ILE:HG13	2.04	0.58
3:H:339:ASP:O	3:H:340:GLN:CB	2.48	0.58
3:H:464:LEU:HB3	3:H:473:LEU:CD2	2.32	0.58
1:A:502:SER:O	1:A:503:CYS:HB2	2.04	0.57
1:A:890:LEU:HB3	1:A:903:CYS:HB2	1.85	0.57
3:H:734:ALA:HB3	3:H:741:LYS:O	2.04	0.57
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.69	0.57
1:C:553:SER:O	1:C:571:LEU:HD12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:LEU:HD12	1:C:622:LEU:C	2.29	0.57
3:H:730:CYS:HB2	4:I:26:LYS:O	2.03	0.57
6:U:7:DT:H73	6:U:8:DA:C6	2.39	0.57
1:C:402:ILE:HD13	3:H:198:LEU:HB3	1.86	0.57
1:C:414:ARG:HH11	1:C:414:ARG:HG2	1.69	0.57
1:A:622:LEU:C	1:A:622:LEU:HD12	2.29	0.57
1:A:903:CYS:HB3	1:A:942:PHE:CE2	2.39	0.57
1:C:167:VAL:HG13	1:C:180:PHE:HB3	1.84	0.57
1:C:407:ILE:HG21	1:C:410:LEU:HD23	1.85	0.57
1:C:430:VAL:HG12	1:C:431:GLY:N	2.19	0.57
3:E:734:ALA:HB3	3:E:741:LYS:O	2.04	0.57
3:H:228:GLN:HB3	3:H:229:ASN:OD1	2.04	0.57
6:S:7:DT:H73	6:S:8:DA:C6	2.39	0.57
1:A:534:MET:HE2	1:A:558:ILE:HD13	1.87	0.57
1:A:553:SER:O	1:A:571:LEU:HD12	2.03	0.57
2:B:242:CYS:O	2:B:254:THR:HG23	2.05	0.57
3:H:353:LEU:CD2	3:H:363:ILE:HB	2.33	0.57
1:C:841:ALA:C	2:D:104:SER:HA	2.25	0.57
1:C:922:LEU:HD23	1:C:957:VAL:HG13	1.85	0.57
3:E:588:ASP:N	3:E:632:LYS:NZ	2.53	0.57
1:A:414:ARG:HB3	1:A:462:ASN:HD21	1.68	0.57
1:C:432:GLN:HA	1:C:455:GLN:O	2.04	0.57
1:C:910:MET:SD	2:D:105:ILE:HG21	2.44	0.57
3:E:417:VAL:HG11	3:E:449:LEU:CG	2.35	0.57
3:E:771:THR:HG23	3:E:773:ILE:HG12	1.86	0.57
4:F:38:VAL:O	4:F:38:VAL:CG2	2.48	0.57
3:H:337:ILE:HG13	3:H:374:MET:HE1	1.87	0.57
1:A:600:HIS:HB2	1:A:616:LEU:O	2.04	0.57
1:C:433:THR:HG22	1:C:434:ARG:H	1.69	0.57
1:C:493:PRO:HB2	1:C:494:GLN:HE22	1.70	0.57
1:C:578:HIS:CE1	1:C:623:LEU:HD12	2.39	0.57
1:C:589:ARG:NH1	3:H:241:TYR:HE2	2.02	0.57
1:A:111:ARG:CZ	2:B:292:TRP:HE1	2.14	0.56
3:E:506:VAL:HA	3:E:515:MET:HE2	1.87	0.56
3:H:771:THR:HG23	3:H:773:ILE:HG12	1.86	0.56
1:A:503:CYS:SG	1:A:504:ASN:N	2.78	0.56
1:C:534:MET:HE2	1:C:558:ILE:HD13	1.87	0.56
3:E:417:VAL:HG11	3:E:449:LEU:HD21	1.87	0.56
3:H:204:LYS:O	3:H:205:ASP:HB3	2.04	0.56
1:A:928:ARG:NH1	2:B:437:THR:HG23	2.21	0.56
1:C:429:PHE:O	1:C:430:VAL:O	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:CYS:SG	1:C:504:ASN:N	2.78	0.56
1:C:927:MET:SD	2:D:126:LEU:HD13	2.45	0.56
3:H:658:ILE:HG21	3:H:716:HIS:HE1	1.71	0.56
2:D:242:CYS:O	2:D:254:THR:HG23	2.04	0.56
3:H:353:LEU:HB3	3:H:363:ILE:HG13	1.87	0.56
1:A:430:VAL:HG12	1:A:431:GLY:N	2.19	0.56
1:A:578:HIS:CE1	1:A:623:LEU:HD12	2.40	0.56
3:H:506:VAL:HA	3:H:515:MET:HE2	1.87	0.56
1:C:1000:LEU:HD13	1:C:1002:GLU:HB2	1.88	0.56
3:E:410:VAL:HB	3:E:411:PRO:HD3	1.86	0.56
3:E:730:CYS:HB3	4:F:27:TRP:HA	1.88	0.56
1:A:477:ARG:HG2	1:A:489:GLU:HG3	1.86	0.56
1:C:928:ARG:CZ	2:D:437:THR:HG21	2.35	0.56
3:E:467:GLU:HG2	3:E:469:ARG:HE	1.70	0.56
1:A:111:ARG:CZ	2:B:290:CYS:SG	2.94	0.56
1:A:354:THR:HG22	1:A:712:ILE:HG21	1.70	0.56
1:A:659:ILE:HG22	1:A:660:TYR:N	2.21	0.56
1:A:695:ASN:OD1	1:A:697:SER:N	2.30	0.56
1:C:518:TYR:CD1	1:C:519:LEU:N	2.74	0.56
1:A:664:HIS:CB	1:A:1131:LYS:CE	2.80	0.56
1:A:715:VAL:H	1:A:716:PRO:CD	2.18	0.56
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.88	0.56
3:E:339:ASP:HA	3:E:343:GLN:HB2	1.88	0.56
1:A:429:PHE:O	1:A:430:VAL:O	2.22	0.56
1:A:493:PRO:HB2	1:A:494:GLN:NE2	2.21	0.56
1:A:587:ILE:HD11	3:E:308:LEU:CD2	2.36	0.55
1:A:703:THR:OG1	1:A:704:ILE:N	2.39	0.55
1:C:706:GLU:O	1:C:706:GLU:HG2	2.05	0.55
1:A:513:GLY:HA2	3:E:236:ASN:ND2	2.21	0.55
1:A:582:LEU:CD1	1:A:583:GLY:H	2.19	0.55
1:C:493:PRO:HB2	1:C:494:GLN:NE2	2.21	0.55
3:E:658:ILE:HG21	3:E:716:HIS:HE1	1.71	0.55
1:A:403:ASP:HA	1:A:698:THR:HG22	1.88	0.55
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.88	0.55
1:A:532:THR:CG2	1:A:533:GLU:N	2.69	0.55
1:A:987:GLU:CD	2:B:156:HIS:HE1	2.04	0.55
1:C:490:TRP:CG	1:C:491:LYS:H	2.24	0.55
1:C:582:LEU:CD1	1:C:583:GLY:H	2.20	0.55
1:A:663:ASN:O	1:A:1131:LYS:HE2	2.06	0.55
1:C:479:VAL:HG12	1:C:480:SER:N	2.22	0.55
1:C:557:ALA:HB2	1:C:593:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:THR:HG22	1:A:447:GLU:N	2.15	0.55
3:H:444:VAL:CG1	3:H:448:LEU:HD12	2.35	0.55
1:A:490:TRP:CG	1:A:491:LYS:H	2.23	0.55
1:A:518:TYR:CD1	1:A:519:LEU:N	2.75	0.55
1:C:522:HIS:HB3	1:C:523:PRO:HD2	1.89	0.55
1:A:432:GLN:HE22	3:E:207:PRO:CG	2.19	0.55
1:A:448:LEU:HD23	1:A:451:PHE:CE2	2.42	0.55
1:A:479:VAL:HG12	1:A:480:SER:N	2.22	0.55
1:A:663:ASN:O	1:A:1131:LYS:CE	2.55	0.55
1:C:403:ASP:HA	1:C:698:THR:HG22	1.88	0.55
1:C:433:THR:HG22	1:C:434:ARG:N	2.22	0.55
1:C:502:SER:OG	1:C:543:ILE:HG12	2.07	0.55
1:C:525:GLU:OE2	1:C:527:ARG:NH2	2.39	0.55
3:E:597:ILE:O	3:E:600:LYS:CE	2.53	0.55
3:E:734:ALA:HB1	3:E:736:PHE:CE2	2.42	0.55
3:H:730:CYS:HB3	4:I:27:TRP:HA	1.88	0.55
3:H:734:ALA:HB1	3:H:736:PHE:CE2	2.42	0.55
1:A:502:SER:OG	1:A:543:ILE:HG12	2.07	0.55
1:A:571:LEU:O	1:A:572:PRO:C	2.50	0.55
1:A:713:ARG:HG3	1:A:714:THR:N	2.21	0.55
1:C:562:THR:C	1:C:564:ILE:N	2.64	0.55
3:H:226:ALA:O	3:H:232:SER:N	2.40	0.55
3:H:428:LEU:O	3:H:432:LEU:CB	2.55	0.55
3:H:457:LEU:CD1	3:H:490:LEU:HA	2.37	0.55
1:A:532:THR:OG1	1:A:574:PHE:HD2	1.90	0.54
1:A:557:ALA:HB2	1:A:593:MET:HE2	1.88	0.54
1:A:404:LEU:HD21	3:E:200:ILE:CD1	2.36	0.54
1:A:649:VAL:CG1	1:A:650:PHE:H	2.16	0.54
1:C:532:THR:OG1	1:C:574:PHE:HD2	1.90	0.54
3:E:357:GLU:O	3:E:427:ARG:NH2	2.41	0.54
3:E:659:MET:HE2	3:E:659:MET:HA	1.90	0.54
1:A:562:THR:C	1:A:564:ILE:N	2.64	0.54
1:A:926:LEU:CG	2:B:122:LEU:HD21	2.35	0.54
2:B:140:HIS:HB2	2:B:453:ASN:HB2	1.88	0.54
1:C:614:PHE:N	1:C:614:PHE:CD1	2.75	0.54
1:A:841:ALA:HA	2:B:103:THR:O	2.07	0.54
1:C:289:GLU:HA	1:C:295:VAL:HA	1.89	0.54
3:E:507:ILE:HD11	3:E:554:LYS:HZ3	1.73	0.54
3:H:220:LEU:HD23	3:H:240:LEU:HD23	1.81	0.54
1:A:525:GLU:OE2	1:A:527:ARG:NE	2.41	0.54
1:C:431:GLY:O	1:C:432:GLN:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:LEU:HD23	1:C:451:PHE:CE2	2.42	0.54
1:C:1033:VAL:HG11	2:D:115:GLY:HA3	1.89	0.54
2:D:140:HIS:HB2	2:D:453:ASN:HB2	1.89	0.54
3:E:430:THR:O	3:E:431:TYR:CB	2.54	0.54
1:A:289:GLU:HA	1:A:295:VAL:HA	1.88	0.54
1:A:431:GLY:O	1:A:432:GLN:HB3	2.07	0.54
1:A:614:PHE:CD1	1:A:614:PHE:N	2.75	0.54
3:E:374:MET:CG	3:E:378:LEU:CD2	2.83	0.54
2:B:299:VAL:HA	2:B:326:PRO:HB3	1.89	0.54
3:E:553:ASN:CB	3:E:598:TYR:CB	2.73	0.54
1:A:602:LEU:C	1:A:602:LEU:HD13	2.33	0.54
1:C:285:LEU:HB3	1:C:297:LEU:HD11	1.89	0.54
1:C:602:LEU:C	1:C:602:LEU:HD13	2.33	0.54
2:D:299:VAL:HA	2:D:326:PRO:HB3	1.89	0.54
1:C:18:CYS:HB2	1:C:313:CYS:HG	1.70	0.54
1:C:571:LEU:O	1:C:572:PRO:C	2.50	0.54
3:E:595:ARG:HB2	3:E:596:PHE:CE1	2.43	0.54
3:E:789:LYS:HB2	3:E:791:ARG:HH12	1.73	0.54
1:A:708:GLN:C	1:A:709:LYS:HD3	2.30	0.54
1:C:931:LEU:HD21	1:C:944:GLU:HG3	1.90	0.54
3:E:665:TYR:HD2	3:E:666:MET:SD	2.31	0.54
1:A:111:ARG:CZ	2:B:292:TRP:NE1	2.71	0.53
1:A:525:GLU:OE2	1:A:527:ARG:NH2	2.39	0.53
3:E:449:LEU:HD13	3:E:479:LEU:HB3	1.90	0.53
3:H:223:ALA:HB1	3:H:240:LEU:HD11	1.85	0.53
3:H:230:SER:C	3:H:232:SER:N	2.67	0.53
3:H:789:LYS:HB2	3:H:791:ARG:HH12	1.74	0.53
1:A:578:HIS:HD2	1:A:623:LEU:H	1.56	0.53
3:E:677:LEU:HD13	4:F:27:TRP:CE3	2.43	0.53
1:A:596:PHE:CZ	1:A:649:VAL:HG23	2.43	0.53
1:A:602:LEU:O	1:A:603:LEU:HD23	2.07	0.53
3:E:767:ILE:O	3:E:771:THR:HG22	2.09	0.53
3:H:336:ILE:O	3:H:342:VAL:HG21	2.09	0.53
1:A:450:GLY:HA3	1:A:479:VAL:HG22	1.91	0.53
1:A:536:HIS:HB2	1:A:560:LEU:HD13	1.90	0.53
1:C:659:ILE:HG22	1:C:660:TYR:N	2.22	0.53
1:A:285:LEU:HB3	1:A:297:LEU:HD11	1.90	0.53
1:A:587:ILE:HD11	3:E:308:LEU:HD22	1.91	0.53
3:E:414:LEU:HB3	3:E:475:LEU:HD23	1.90	0.53
3:H:222:GLU:O	3:H:233:ILE:CB	2.57	0.53
3:H:338:SER:O	3:H:343:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:7:DT:H73	6:U:8:DA:N6	2.24	0.53
1:A:433:THR:HG22	1:A:434:ARG:N	2.23	0.53
1:C:596:PHE:CZ	1:C:649:VAL:HG23	2.43	0.53
1:C:602:LEU:O	1:C:603:LEU:HD23	2.08	0.53
1:A:679:MET:SD	1:A:679:MET:C	2.92	0.53
1:C:113:GLY:H	2:D:338:THR:HG22	1.74	0.53
1:C:649:VAL:CG1	1:C:650:PHE:N	2.71	0.53
3:H:226:ALA:HB2	3:H:233:ILE:CB	2.39	0.53
3:H:271:GLN:HB3	3:H:336:ILE:HD11	1.91	0.53
1:C:536:HIS:HB2	1:C:560:LEU:HD13	1.89	0.53
1:C:578:HIS:HD2	1:C:623:LEU:H	1.55	0.53
3:E:350:ILE:HG21	3:E:372:LEU:HD21	1.90	0.53
3:H:659:MET:HE2	3:H:659:MET:HA	1.90	0.53
3:H:665:TYR:HD2	3:H:666:MET:SD	2.31	0.53
1:A:487:VAL:O	1:A:488:SER:HB2	2.09	0.52
1:C:532:THR:CG2	1:C:533:GLU:N	2.69	0.52
3:H:336:ILE:O	3:H:342:VAL:HB	2.07	0.52
3:H:365:ARG:O	3:H:431:TYR:CB	2.57	0.52
3:H:767:ILE:O	3:H:771:THR:HG22	2.09	0.52
1:A:111:ARG:HE	2:B:292:TRP:NE1	1.97	0.52
1:A:869:ALA:HB2	2:B:106:LEU:CB	2.39	0.52
1:C:525:GLU:OE2	1:C:527:ARG:NE	2.41	0.52
3:E:704:LEU:HA	3:E:707:ILE:HG22	1.91	0.52
1:A:594:THR:CG2	1:A:595:THR:N	2.73	0.52
1:C:679:MET:SD	1:C:679:MET:C	2.92	0.52
3:E:206:LYS:N	3:E:207:PRO:HD2	2.23	0.52
3:H:677:LEU:HD13	4:I:27:TRP:CE3	2.44	0.52
3:H:854:ILE:HG21	3:H:899:MET:HE1	1.91	0.52
6:S:7:DT:H73	6:S:8:DA:N6	2.24	0.52
1:C:659:ILE:H	1:C:659:ILE:HD12	1.75	0.52
3:E:520:LEU:HD21	3:E:586:MET:HE1	1.90	0.52
2:B:217:THR:OG1	2:B:254:THR:HG21	2.09	0.52
1:C:912:LEU:HD21	2:D:109:ILE:HD11	1.92	0.52
1:A:658:VAL:HG12	1:A:658:VAL:O	2.09	0.52
3:E:556:PRO:C	3:E:557:ASN:CG	2.77	0.52
1:A:664:HIS:O	1:A:1131:LYS:HE2	2.08	0.52
1:A:931:LEU:HD21	1:A:944:GLU:HG3	1.91	0.52
1:C:487:VAL:O	1:C:488:SER:HB2	2.09	0.52
1:C:631:LEU:O	1:C:655:ARG:HB2	2.10	0.52
1:C:649:VAL:CG1	1:C:650:PHE:H	2.17	0.52
3:H:206:LYS:H	3:H:207:PRO:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:353:LEU:HD22	3:H:363:ILE:HG12	1.88	0.52
1:C:594:THR:CG2	1:C:595:THR:N	2.73	0.52
2:D:217:THR:OG1	2:D:254:THR:HG21	2.10	0.52
3:E:417:VAL:HG11	3:E:449:LEU:CD1	2.40	0.52
1:A:448:LEU:HD23	1:A:451:PHE:HE2	1.75	0.52
1:C:402:ILE:O	1:C:698:THR:HB	2.10	0.52
1:A:408:LYS:HA	1:A:678:TYR:CE1	2.45	0.51
1:A:912:LEU:CD2	2:B:109:ILE:CD1	2.88	0.51
1:C:402:ILE:CD1	3:H:198:LEU:CB	2.87	0.51
1:C:561:TRP:HA	1:C:587:ILE:HG21	1.92	0.51
3:E:854:ILE:HG21	3:E:899:MET:HE1	1.91	0.51
4:F:38:VAL:O	4:F:39:VAL:CB	2.57	0.51
1:A:402:ILE:O	1:A:698:THR:HB	2.10	0.51
1:A:659:ILE:HD12	1:A:659:ILE:H	1.75	0.51
1:C:393:GLY:O	1:C:709:LYS:N	2.38	0.51
1:C:578:HIS:CE1	1:C:623:LEU:CD1	2.93	0.51
1:A:578:HIS:CE1	1:A:623:LEU:CD1	2.93	0.51
3:E:311:ASP:O	3:E:316:LEU:HB2	2.10	0.51
3:E:557:ASN:ND2	3:E:843:PHE:HZ	2.09	0.51
3:H:457:LEU:HD11	3:H:490:LEU:HA	1.93	0.51
1:A:838:PRO:CA	2:B:101:GLY:HA2	2.38	0.51
1:A:840:GLU:O	1:A:841:ALA:C	2.54	0.51
1:C:658:VAL:O	1:C:658:VAL:HG12	2.09	0.51
3:E:390:LEU:HD22	3:E:440:LEU:HD13	1.91	0.51
3:E:491:LEU:HA	3:E:540:PHE:CE2	2.46	0.51
3:E:494:TRP:HE3	3:E:540:PHE:CD2	2.21	0.51
1:A:573:SER:O	1:A:574:PHE:HB2	2.10	0.51
1:C:374:GLN:HG2	1:C:391:ARG:CB	2.39	0.51
3:E:600:LYS:HG3	3:E:878:LYS:HG3	1.91	0.51
3:H:205:ASP:CG	3:H:205:ASP:O	2.53	0.51
3:H:704:LEU:HA	3:H:707:ILE:HG22	1.91	0.51
1:A:459:PHE:CD2	1:A:460:CYS:N	2.79	0.51
1:A:471:ILE:HA	1:A:476:VAL:HA	1.92	0.51
1:A:570:LYS:O	1:A:574:PHE:N	2.42	0.51
1:C:459:PHE:CD2	1:C:460:CYS:N	2.79	0.51
1:C:573:SER:O	1:C:574:PHE:HB2	2.10	0.51
3:E:340:GLN:O	3:E:344:ASN:OD1	2.28	0.51
1:C:451:PHE:HD1	1:C:470:GLN:HB2	1.74	0.51
3:H:206:LYS:N	3:H:207:PRO:HD2	2.26	0.51
3:H:598:TYR:HD1	3:H:878:LYS:O	1.94	0.51
3:H:600:LYS:HG3	3:H:878:LYS:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:523:LYS:CE	3:E:544:MET:HE2	2.41	0.51
3:H:338:SER:O	3:H:343:GLN:HG3	2.10	0.51
1:A:613:TYR:CE1	1:A:627:LYS:HB2	2.46	0.51
1:A:709:LYS:C	1:A:710:LEU:CG	2.84	0.51
1:C:369:ARG:CB	1:C:668:PHE:CB	2.89	0.51
1:C:408:LYS:HA	1:C:678:TYR:CE1	2.46	0.51
1:C:454:ASP:OD1	1:C:454:ASP:N	2.28	0.51
3:H:337:ILE:HG21	3:H:374:MET:HE3	1.92	0.51
1:A:711:HIS:O	1:A:711:HIS:CD2	2.64	0.51
1:C:970:ASN:OD1	2:D:119:HIS:ND1	2.42	0.51
3:E:340:GLN:HG2	3:E:341:LYS:H	1.42	0.51
3:E:428:LEU:HD22	3:E:432:LEU:HB3	1.91	0.51
3:E:594:PHE:C	3:E:596:PHE:N	2.63	0.51
3:H:864:LEU:HD23	3:H:869:LEU:HD12	1.92	0.51
1:C:490:TRP:CG	1:C:491:LYS:N	2.79	0.50
1:C:671:VAL:O	1:C:673:LEU:N	2.38	0.50
1:A:416:ASP:OD1	1:A:418:ASN:HB2	2.11	0.50
1:A:814:LEU:HD21	2:B:110:TYR:HB2	1.93	0.50
1:C:430:VAL:HG22	3:H:246:ASN:HD22	1.76	0.50
1:C:613:TYR:CE1	1:C:627:LYS:HB2	2.46	0.50
3:H:311:ASP:O	3:H:316:LEU:HB2	2.10	0.50
1:A:394:ILE:CG2	1:A:395:GLY:H	2.24	0.50
1:A:612:PHE:CE2	1:A:628:LYS:HD2	2.47	0.50
1:A:671:VAL:O	1:A:673:LEU:N	2.38	0.50
1:C:471:ILE:HA	1:C:476:VAL:HA	1.92	0.50
1:A:715:VAL:O	1:A:716:PRO:C	2.55	0.50
1:C:430:VAL:HG22	3:H:246:ASN:CB	2.36	0.50
3:E:494:TRP:CH2	3:E:530:ILE:HG21	2.46	0.50
3:H:216:THR:HA	3:H:219:LYS:HB2	1.93	0.50
1:A:512:VAL:HB	1:A:515:ALA:HB3	1.93	0.50
3:E:761:GLU:HB3	3:E:809:ILE:HG22	1.94	0.50
3:H:434:GLN:C	3:H:436:THR:N	2.59	0.50
3:H:457:LEU:HB3	3:H:493:GLN:CG	2.39	0.50
1:A:391:ARG:O	1:A:393:GLY:N	2.44	0.50
1:C:587:ILE:HD12	1:C:587:ILE:H	1.77	0.50
3:E:886:LEU:O	3:E:890:ILE:HG12	2.12	0.50
1:A:492:GLU:CG	1:A:496:LYS:HB2	2.42	0.50
1:C:512:VAL:HB	1:C:515:ALA:HB3	1.94	0.50
1:A:1054:MET:SD	1:A:1129:LEU:HD11	2.52	0.50
3:H:345:LYS:HA	3:H:348:ASP:HB2	1.93	0.50
3:H:380:ILE:HG22	3:H:384:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:494:TRP:CH2	3:H:530:ILE:HG21	2.46	0.50
1:A:561:TRP:HA	1:A:587:ILE:HG21	1.93	0.49
1:A:893:TRP:HE3	1:A:899:LEU:HD13	1.77	0.49
1:A:912:LEU:CD2	2:B:109:ILE:HG23	2.33	0.49
1:C:399:HIS:CE1	1:C:703:THR:HG22	2.47	0.49
1:C:416:ASP:OD1	1:C:418:ASN:HB2	2.11	0.49
1:C:612:PHE:CE2	1:C:628:LYS:HD2	2.46	0.49
1:A:490:TRP:CG	1:A:491:LYS:N	2.79	0.49
1:A:668:PHE:N	1:A:668:PHE:CD1	2.80	0.49
2:B:256:ASP:OD2	2:B:260:ARG:HB2	2.12	0.49
1:C:448:LEU:HD23	1:C:451:PHE:HE2	1.75	0.49
3:E:587:LEU:CB	3:E:632:LYS:CD	2.90	0.49
1:C:490:TRP:CD2	1:C:491:LYS:N	2.81	0.49
1:C:695:ASN:OD1	1:C:698:THR:N	2.42	0.49
2:D:211:SER:HB3	2:D:243:VAL:HG13	1.95	0.49
3:E:216:THR:HA	3:E:219:LYS:HB2	1.93	0.49
3:E:350:ILE:HG12	3:E:368:LEU:HD22	1.91	0.49
1:C:707:ILE:O	1:C:708:GLN:O	2.30	0.49
1:C:928:ARG:NH1	2:D:437:THR:HG21	2.27	0.49
3:E:796:ASN:HB2	3:E:797:PRO:HD3	1.94	0.49
3:H:557:ASN:ND2	3:H:843:PHE:HZ	2.10	0.49
1:C:492:GLU:CG	1:C:496:LYS:HB2	2.42	0.49
1:C:570:LYS:O	1:C:574:PHE:N	2.41	0.49
3:E:864:LEU:HD23	3:E:869:LEU:HD12	1.92	0.49
1:A:354:THR:HB	1:A:712:ILE:HD12	1.93	0.49
1:A:1055:GLN:NE2	1:A:1090:ASP:H	2.09	0.49
1:C:893:TRP:HE3	1:C:899:LEU:HD13	1.77	0.49
1:A:664:HIS:O	1:A:1131:LYS:NZ	2.46	0.49
1:C:450:GLY:HA3	1:C:479:VAL:HG22	1.91	0.49
3:E:380:ILE:HG22	3:E:384:SER:HB2	1.95	0.49
3:E:555:ARG:NE	3:E:556:PRO:HD2	2.27	0.49
3:H:365:ARG:CB	3:H:430:THR:O	2.60	0.49
2:D:256:ASP:OD2	2:D:260:ARG:HB2	2.13	0.49
3:E:414:LEU:HG	3:E:479:LEU:HD12	1.94	0.49
1:A:587:ILE:N	1:A:587:ILE:HD12	2.28	0.49
1:A:596:PHE:CE2	1:A:659:ILE:HG22	2.48	0.49
1:C:394:ILE:HG22	1:C:395:GLY:N	2.27	0.49
3:H:591:MET:HE2	3:H:591:MET:HA	1.95	0.49
3:H:622:SER:HB3	3:H:625:ALA:HB2	1.95	0.49
1:A:641:PHE:CE2	1:A:650:PHE:HB2	2.48	0.49
1:A:912:LEU:CD2	2:B:109:ILE:HG21	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:ILE:O	1:C:707:ILE:CG2	2.60	0.49
1:C:1055:GLN:NE2	1:C:1090:ASP:H	2.09	0.49
3:E:397:TYR:CE2	3:E:444:VAL:CG1	2.96	0.49
3:H:886:LEU:O	3:H:890:ILE:HG12	2.12	0.49
1:A:459:PHE:O	1:A:460:CYS:HB3	2.13	0.48
1:A:840:GLU:O	1:A:841:ALA:O	2.30	0.48
3:E:345:LYS:HA	3:E:348:ASP:HB2	1.94	0.48
3:H:781:THR:HG22	3:H:826:ILE:HD13	1.95	0.48
1:A:490:TRP:CD2	1:A:491:LYS:N	2.81	0.48
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.77	0.48
2:B:211:SER:HB3	2:B:243:VAL:HG13	1.94	0.48
1:C:587:ILE:HD12	1:C:587:ILE:N	2.27	0.48
1:A:443:VAL:HG12	1:A:443:VAL:O	2.13	0.48
1:A:562:THR:O	1:A:563:ASP:C	2.56	0.48
1:C:655:ARG:NH1	1:C:713:ARG:NE	2.60	0.48
3:E:339:ASP:HA	3:E:343:GLN:CB	2.43	0.48
3:E:426:ASP:O	3:E:429:ILE:HG23	2.12	0.48
3:E:622:SER:HB3	3:E:625:ALA:HB2	1.95	0.48
1:A:587:ILE:HD12	1:A:587:ILE:H	1.78	0.48
1:A:596:PHE:HZ	1:A:649:VAL:HG23	1.78	0.48
1:A:659:ILE:O	1:A:660:TYR:HB3	2.13	0.48
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.78	0.48
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.13	0.48
2:B:394:PRO:HB3	2:B:402:ASP:HB3	1.96	0.48
3:E:340:GLN:HG3	3:E:341:LYS:CD	2.43	0.48
3:H:761:GLU:HB3	3:H:809:ILE:HG22	1.94	0.48
1:A:385:GLY:HA3	1:A:719:GLU:O	2.14	0.48
1:A:432:GLN:HE22	3:E:207:PRO:HG3	1.79	0.48
1:A:450:GLY:O	1:A:477:ARG:NH2	2.45	0.48
1:A:695:ASN:OD1	1:A:698:THR:N	2.42	0.48
1:C:393:GLY:O	1:C:708:GLN:HA	2.14	0.48
1:C:459:PHE:O	1:C:460:CYS:HB3	2.13	0.48
1:C:596:PHE:HZ	1:C:649:VAL:HG23	1.78	0.48
1:C:722:ARG:NH2	2:D:110:TYR:CD2	2.82	0.48
3:E:781:THR:HG22	3:E:826:ILE:HD13	1.94	0.48
3:H:796:ASN:HB2	3:H:797:PRO:HD3	1.94	0.48
1:A:433:THR:O	1:A:434:ARG:HG3	2.14	0.48
1:C:641:PHE:HB2	1:C:681:PRO:HG3	1.95	0.48
2:D:394:PRO:HB3	2:D:402:ASP:HB3	1.96	0.48
3:E:233:ILE:HD13	3:E:233:ILE:H	1.78	0.48
3:E:434:GLN:C	3:E:436:THR:N	2.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:587:LEU:HB2	3:E:632:LYS:HE3	1.95	0.48
4:I:37:ILE:O	4:I:38:VAL:C	2.56	0.48
1:A:638:LEU:O	1:A:639:ARG:HG2	2.14	0.48
1:C:392:ASN:CB	1:C:1012:LEU:O	2.54	0.48
1:C:596:PHE:CE2	1:C:659:ILE:HG22	2.47	0.48
1:C:641:PHE:CE2	1:C:650:PHE:HB2	2.48	0.48
1:A:594:THR:HG23	1:A:595:THR:N	2.28	0.48
1:A:611:LEU:C	1:A:611:LEU:HD23	2.39	0.48
1:C:657:THR:HG22	1:C:658:VAL:N	2.24	0.48
1:C:659:ILE:O	1:C:660:TYR:HB3	2.13	0.48
3:E:300:MET:C	3:E:302:MET:H	2.22	0.48
3:H:681:ILE:HD11	3:H:721:LEU:HD22	1.95	0.48
1:A:396:ILE:HD13	1:A:396:ILE:N	2.29	0.48
1:A:459:PHE:CG	1:A:460:CYS:N	2.82	0.48
1:A:708:GLN:C	1:A:709:LYS:HE2	2.39	0.48
1:A:711:HIS:O	1:A:711:HIS:CG	2.66	0.48
3:E:588:ASP:N	3:E:632:LYS:HZ1	2.09	0.48
3:H:582:GLU:O	3:H:586:MET:HG2	2.14	0.48
1:A:479:VAL:CG1	1:A:480:SER:N	2.77	0.48
1:C:514:ARG:HG3	1:C:514:ARG:HH11	1.78	0.48
1:C:731:GLN:HA	1:C:796:GLN:HE21	1.78	0.48
1:C:770:LEU:HD13	1:C:865:GLU:HB2	1.95	0.48
3:E:892:SER:O	3:E:896:ARG:HD3	2.14	0.48
2:B:272:PHE:HE2	2:B:312:LYS:HA	1.79	0.47
1:C:385:GLY:HA3	1:C:719:GLU:O	2.13	0.47
3:E:582:GLU:O	3:E:586:MET:HG2	2.14	0.47
3:H:300:MET:C	3:H:302:MET:H	2.22	0.47
3:H:358:ARG:O	3:H:420:ARG:NH1	2.47	0.47
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.44	0.47
1:A:457:THR:HG22	1:A:458:PHE:N	2.29	0.47
1:C:218:MET:CE	1:C:261:HIS:HD2	2.21	0.47
3:H:892:SER:O	3:H:896:ARG:HD3	2.14	0.47
1:A:414:ARG:HB3	1:A:462:ASN:ND2	2.29	0.47
1:A:707:ILE:HG13	1:A:707:ILE:H	1.35	0.47
1:C:414:ARG:HB3	1:C:462:ASN:ND2	2.29	0.47
1:C:450:GLY:O	1:C:477:ARG:NH2	2.46	0.47
1:C:1136:LEU:O	1:C:1139:ILE:HG12	2.13	0.47
3:E:555:ARG:HD2	3:E:555:ARG:HA	1.61	0.47
3:E:681:ILE:HD11	3:E:721:LEU:HD22	1.95	0.47
1:A:562:THR:C	1:A:564:ILE:H	2.23	0.47
1:A:641:PHE:HB2	1:A:681:PRO:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ILE:HG22	1:C:403:ASP:H	1.80	0.47
1:C:403:ASP:O	1:C:405:PRO:HD3	2.15	0.47
1:C:611:LEU:C	1:C:611:LEU:HD23	2.40	0.47
3:E:509:PRO:C	3:E:511:LYS:H	2.23	0.47
1:A:402:ILE:HD13	3:E:198:LEU:HB3	1.97	0.47
1:C:459:PHE:CG	1:C:460:CYS:N	2.82	0.47
1:C:562:THR:C	1:C:564:ILE:H	2.23	0.47
1:C:638:LEU:O	1:C:639:ARG:HG2	2.15	0.47
2:D:272:PHE:HE2	2:D:312:LYS:HA	1.79	0.47
3:E:355:GLU:O	3:E:359:ASN:OD1	2.32	0.47
1:A:403:ASP:O	1:A:405:PRO:HD3	2.15	0.47
1:A:715:VAL:H	1:A:716:PRO:HD3	1.80	0.47
1:C:479:VAL:CG1	1:C:480:SER:N	2.77	0.47
1:C:641:PHE:CD1	1:C:641:PHE:C	2.93	0.47
3:E:206:LYS:CB	3:E:207:PRO:CD	2.92	0.47
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.96	0.47
1:A:490:TRP:O	1:A:491:LYS:HB2	2.14	0.47
1:A:531:HIS:ND1	1:A:532:THR:N	2.63	0.47
1:A:656:PRO:HG2	1:A:676:VAL:HG23	1.97	0.47
1:A:843:PRO:N	2:B:104:SER:CB	2.78	0.47
1:A:926:LEU:CD2	2:B:122:LEU:HD21	2.44	0.47
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.15	0.47
1:C:23:PHE:N	1:C:30:ASN:ND2	2.59	0.47
1:C:184:ASP:HB2	1:C:185:PRO:CD	2.44	0.47
1:C:407:ILE:CD1	1:C:699:LEU:HB2	2.45	0.47
1:C:443:VAL:HG12	1:C:443:VAL:O	2.13	0.47
1:C:532:THR:HG22	1:C:533:GLU:H	1.80	0.47
1:C:594:THR:HG23	1:C:595:THR:N	2.28	0.47
1:C:708:GLN:HE21	1:C:708:GLN:CA	2.20	0.47
3:E:847:GLN:HE22	3:E:885:ASP:HB3	1.80	0.47
1:A:407:ILE:CD1	1:A:699:LEU:HB2	2.45	0.47
1:C:585:GLU:OE2	3:H:301:ILE:HG12	2.15	0.47
1:A:396:ILE:HD13	1:A:396:ILE:O	2.15	0.47
1:C:396:ILE:HD13	1:C:396:ILE:O	2.15	0.47
1:C:433:THR:O	1:C:434:ARG:HG3	2.14	0.47
3:E:203:PHE:O	3:E:205:ASP:N	2.47	0.47
3:E:341:LYS:H	3:E:341:LYS:HD2	1.79	0.47
1:A:714:THR:HG22	1:A:715:VAL:N	2.30	0.47
1:A:770:LEU:HD13	1:A:865:GLU:HB2	1.95	0.47
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.50	0.47
1:C:113:GLY:N	2:D:338:THR:HG22	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:THR:HG22	1:C:458:PHE:N	2.29	0.47
3:E:417:VAL:CG2	3:E:449:LEU:HD21	2.43	0.47
3:E:587:LEU:HB2	3:E:632:LYS:CD	2.44	0.47
3:E:597:ILE:N	3:E:600:LYS:HE2	2.29	0.47
1:A:451:PHE:HD1	1:A:470:GLN:HB2	1.73	0.46
1:A:512:VAL:O	1:A:515:ALA:HB3	2.15	0.46
1:A:579:LYS:HE3	1:A:581:MET:CE	2.45	0.46
1:A:709:LYS:C	1:A:710:LEU:HG	2.40	0.46
1:C:531:HIS:ND1	1:C:532:THR:N	2.63	0.46
1:C:562:THR:O	1:C:563:ASP:C	2.56	0.46
1:C:643:SER:OG	1:C:644:LEU:N	2.46	0.46
1:C:889:ARG:HD2	1:C:891:TYR:CZ	2.50	0.46
3:E:468:ASN:C	3:E:468:ASN:HD22	2.22	0.46
3:E:859:LYS:HB3	3:E:859:LYS:HE3	1.80	0.46
3:H:468:ASN:C	3:H:468:ASN:HD22	2.23	0.46
1:A:402:ILE:HG22	1:A:403:ASP:H	1.80	0.46
1:A:432:GLN:HE22	3:E:207:PRO:HG2	1.80	0.46
1:C:114:ARG:NH2	2:D:386:ASP:OD2	2.47	0.46
1:C:356:LEU:HD21	1:C:712:ILE:HD13	1.96	0.46
1:C:438:LEU:CD1	1:C:684:SER:HB2	2.46	0.46
1:C:576:LEU:C	1:C:577:LEU:HD23	2.41	0.46
1:C:704:ILE:H	1:C:704:ILE:CD1	2.21	0.46
3:E:350:ILE:HG12	3:E:368:LEU:HD23	1.94	0.46
3:E:414:LEU:HG	3:E:479:LEU:CD1	2.45	0.46
3:H:430:THR:O	3:H:431:TYR:CB	2.61	0.46
3:H:466:ASP:O	3:H:467:GLU:C	2.55	0.46
3:H:509:PRO:C	3:H:511:LYS:H	2.22	0.46
3:H:911:TYR:CE2	3:H:913:ALA:HB2	2.50	0.46
1:A:360:VAL:HG22	2:B:113:SER:O	2.15	0.46
1:A:451:PHE:HE1	1:A:470:GLN:HB2	1.79	0.46
1:C:579:LYS:HE3	1:C:581:MET:CE	2.45	0.46
1:C:596:PHE:CZ	1:C:659:ILE:HG22	2.50	0.46
1:C:1048:TYR:O	1:C:1052:LEU:HB2	2.15	0.46
1:A:560:LEU:HG	1:A:565:SER:OG	2.16	0.46
1:C:396:ILE:N	1:C:396:ILE:CD1	2.78	0.46
3:E:555:ARG:HE	3:E:556:PRO:HD2	1.80	0.46
3:E:599:GLY:H	3:E:878:LYS:HG2	1.80	0.46
1:A:442:GLU:HG3	1:A:443:VAL:H	1.81	0.46
1:A:641:PHE:CD1	1:A:641:PHE:C	2.93	0.46
1:A:664:HIS:O	1:A:1131:LYS:CE	2.64	0.46
1:A:708:GLN:C	1:A:709:LYS:CD	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:ALA:CB	2:B:106:LEU:CB	2.93	0.46
1:C:512:VAL:O	1:C:515:ALA:HB3	2.15	0.46
1:C:560:LEU:HG	1:C:565:SER:OG	2.16	0.46
1:A:596:PHE:CZ	1:A:659:ILE:HG22	2.50	0.46
1:A:641:PHE:HB3	1:A:679:MET:HE1	1.97	0.46
3:E:338:SER:C	3:E:343:GLN:HB2	2.40	0.46
3:E:341:LYS:O	3:E:345:LYS:HG2	2.15	0.46
3:H:223:ALA:HB1	3:H:240:LEU:CD1	2.43	0.46
1:A:657:THR:HG22	1:A:658:VAL:N	2.24	0.46
1:C:43:VAL:HG21	1:C:50:ARG:CZ	2.46	0.46
3:E:363:ILE:O	3:E:364:ASP:C	2.58	0.46
3:E:597:ILE:HG22	3:E:597:ILE:O	2.15	0.46
4:F:33:TRP:O	4:F:34:ALA:O	2.34	0.46
1:A:396:ILE:N	1:A:396:ILE:CD1	2.78	0.46
1:A:438:LEU:CD1	1:A:684:SER:HB2	2.45	0.46
1:A:708:GLN:C	1:A:709:LYS:CE	2.88	0.46
1:C:987:GLU:CD	2:D:156:HIS:CE1	2.94	0.46
3:H:226:ALA:CB	3:H:233:ILE:CB	2.94	0.46
3:H:698:PRO:O	3:H:700:GLU:N	2.48	0.46
3:H:847:GLN:HE22	3:H:885:ASP:HB3	1.80	0.46
1:A:576:LEU:C	1:A:577:LEU:HD23	2.41	0.46
1:C:490:TRP:O	1:C:491:LYS:HB2	2.15	0.46
3:E:350:ILE:HD13	3:E:372:LEU:CD2	2.45	0.46
3:E:698:PRO:O	3:E:700:GLU:N	2.48	0.46
3:E:720:LYS:HG3	4:F:34:ALA:CB	2.34	0.46
1:A:218:MET:CE	1:A:261:HIS:HD2	2.21	0.46
1:A:407:ILE:HD11	1:A:699:LEU:HB2	1.98	0.46
1:A:587:ILE:H	1:A:587:ILE:CD1	2.29	0.46
1:A:643:SER:O	1:A:644:LEU:C	2.59	0.46
1:A:830:ILE:HG22	1:A:873:MET:HE1	1.99	0.46
1:C:184:ASP:HB2	1:C:185:PRO:HD2	1.97	0.46
1:C:656:PRO:HG2	1:C:676:VAL:HG23	1.97	0.46
1:C:1005:ASN:ND2	2:D:113:SER:O	2.46	0.46
1:C:442:GLU:HG3	1:C:443:VAL:H	1.81	0.45
1:C:643:SER:O	1:C:644:LEU:C	2.59	0.45
1:C:830:ILE:HG22	1:C:873:MET:HE1	1.98	0.45
1:C:869:ALA:H	1:C:885:ASN:ND2	2.14	0.45
1:C:953:TRP:HB2	1:C:970:ASN:HB2	1.98	0.45
1:A:953:TRP:HZ2	2:B:123:ARG:NH1	2.15	0.45
1:C:513:GLY:HA2	3:H:236:ASN:ND2	2.32	0.45
1:C:546:LEU:O	1:C:549:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:GLU:O	1:C:598:SER:HB3	2.16	0.45
3:E:911:TYR:CE2	3:E:913:ALA:HB2	2.50	0.45
1:A:476:VAL:HG22	1:A:526:LEU:CD1	2.47	0.45
3:E:332:PHE:CZ	3:E:336:ILE:HD12	2.51	0.45
3:E:417:VAL:HG11	3:E:449:LEU:CD2	2.47	0.45
3:E:558:LYS:N	3:E:559:PRO:HD2	2.32	0.45
3:H:272:ILE:HD11	3:H:340:GLN:CD	2.41	0.45
1:C:926:LEU:CD2	2:D:126:LEU:HD11	2.45	0.45
3:H:340:GLN:NE2	3:H:342:VAL:CG2	2.76	0.45
1:A:411:TRP:HB2	1:A:460:CYS:SG	2.56	0.45
1:C:407:ILE:HD11	1:C:699:LEU:HB2	1.99	0.45
1:C:564:ILE:HG22	1:C:582:LEU:CD1	2.47	0.45
2:D:388:ILE:O	2:D:408:ILE:HA	2.17	0.45
3:E:341:LYS:H	3:E:341:LYS:CD	2.29	0.45
3:E:691:VAL:HA	3:E:692:PRO:HD3	1.85	0.45
3:H:491:LEU:HG	3:H:540:PHE:CZ	2.51	0.45
1:A:835:MET:CG	1:A:845:GLN:O	2.61	0.45
3:E:269:LYS:HD2	3:E:335:HIS:CE1	2.52	0.45
1:A:354:THR:HG22	1:A:712:ILE:HD12	1.84	0.45
1:A:589:ARG:CZ	3:E:241:TYR:CE2	3.00	0.45
1:A:657:THR:CG2	1:A:668:PHE:HB3	2.47	0.45
1:A:705:ASP:C	1:A:705:ASP:OD1	2.59	0.45
1:A:707:ILE:HB	1:A:708:GLN:H	1.45	0.45
1:A:889:ARG:CD	1:A:901:THR:HB	2.45	0.45
1:A:1109:VAL:O	1:A:1111:ASN:N	2.42	0.45
1:C:390:ILE:HG22	1:C:391:ARG:N	2.32	0.45
1:C:655:ARG:NH1	1:C:713:ARG:HE	2.15	0.45
3:H:350:ILE:HG21	3:H:372:LEU:HD21	1.98	0.45
6:S:7:DT:C7	6:S:8:DA:C6	2.99	0.45
1:A:629:VAL:HG23	1:A:630:THR:N	2.31	0.45
1:A:664:HIS:C	1:A:1131:LYS:CE	2.84	0.45
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.97	0.45
1:C:411:TRP:HB2	1:C:460:CYS:SG	2.57	0.45
1:C:641:PHE:HB3	1:C:679:MET:HE1	1.98	0.45
3:E:580:ASP:HA	3:E:583:LEU:HB3	1.99	0.45
3:H:436:THR:HG22	3:H:436:THR:O	2.16	0.45
3:H:580:ASP:HA	3:H:583:LEU:HB3	1.98	0.45
3:H:720:LYS:HB3	4:I:36:ASP:HB2	1.98	0.45
1:A:564:ILE:HG22	1:A:582:LEU:CD1	2.47	0.45
1:C:528:GLN:O	1:C:528:GLN:HG2	2.17	0.45
1:A:43:VAL:HG21	1:A:50:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:HG3	1:A:327:ARG:HD2	1.98	0.45
1:A:597:GLU:O	1:A:598:SER:HB3	2.17	0.45
1:A:643:SER:OG	1:A:644:LEU:N	2.47	0.45
1:A:841:ALA:CA	2:B:103:THR:O	2.65	0.45
1:C:444:GLU:HB3	3:H:201:LYS:HB2	1.98	0.45
3:H:861:ARG:NH1	3:H:872:GLU:OE2	2.50	0.45
6:U:7:DT:C7	6:U:8:DA:C6	3.00	0.45
1:A:312:GLU:HG3	1:A:327:ARG:CD	2.47	0.44
1:A:397:HIS:HB2	1:A:703:THR:HG22	1.99	0.44
1:A:528:GLN:O	1:A:528:GLN:HG2	2.17	0.44
1:A:532:THR:CG2	1:A:533:GLU:H	2.30	0.44
1:A:546:LEU:O	1:A:549:SER:HB3	2.17	0.44
1:A:740:ILE:HG23	1:A:785:GLU:HG3	1.99	0.44
1:C:557:ALA:N	1:C:593:MET:HE2	2.32	0.44
1:C:580:GLU:OE2	1:C:626:ARG:HD2	2.17	0.44
1:C:629:VAL:HG23	1:C:630:THR:N	2.31	0.44
3:E:545:LYS:HE2	3:E:545:LYS:HB3	1.82	0.44
1:A:564:ILE:O	1:A:582:LEU:HD12	2.17	0.44
1:C:312:GLU:HG3	1:C:327:ARG:HD2	1.98	0.44
1:C:396:ILE:HD13	1:C:396:ILE:N	2.29	0.44
1:C:476:VAL:HG22	1:C:526:LEU:CD1	2.47	0.44
1:C:607:GLY:HA2	1:C:635:PRO:HB3	1.99	0.44
1:A:580:GLU:OE2	1:A:626:ARG:HD2	2.17	0.44
1:A:659:ILE:CG2	1:A:660:TYR:N	2.79	0.44
1:C:534:MET:CE	1:C:569:LEU:HD11	2.47	0.44
3:E:494:TRP:CZ3	3:E:540:PHE:HB3	2.52	0.44
3:H:340:GLN:HB3	3:H:340:GLN:HE21	1.52	0.44
3:H:391:GLU:HG2	3:H:395:ARG:HH22	1.81	0.44
3:H:719:ARG:HD3	4:I:33:TRP:CE3	2.53	0.44
3:H:853:ALA:HA	3:H:856:ARG:HG2	2.00	0.44
1:A:478:LEU:HB3	1:A:488:SER:HB3	1.99	0.44
1:A:692:ALA:O	1:A:693:LEU:HD23	2.17	0.44
1:A:869:ALA:H	1:A:885:ASN:ND2	2.15	0.44
1:C:692:ALA:O	1:C:693:LEU:HD23	2.17	0.44
1:C:889:ARG:CD	1:C:901:THR:HB	2.45	0.44
1:C:1057:ARG:HH12	1:C:1110:ALA:HB3	1.83	0.44
3:E:275:PHE:CE2	3:E:289:ILE:HD13	2.53	0.44
3:E:391:GLU:HG2	3:E:395:ARG:HH22	1.81	0.44
3:H:336:ILE:O	3:H:342:VAL:CG2	2.65	0.44
1:A:953:TRP:CZ2	2:B:123:ARG:NH1	2.86	0.44
1:C:659:ILE:CG2	1:C:660:TYR:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:558:LYS:N	3:H:559:PRO:HD2	2.32	0.44
3:H:749:GLN:HG2	3:H:785:LEU:HD11	2.00	0.44
1:C:534:MET:HE2	1:C:569:LEU:HD11	2.00	0.44
3:E:293:TRP:O	3:E:297:CYS:HB2	2.18	0.44
3:E:514:THR:O	3:E:515:MET:C	2.60	0.44
3:E:743:LEU:HD22	3:E:823:ILE:HD11	2.00	0.44
3:E:853:ALA:HA	3:E:856:ARG:HG2	2.00	0.44
3:H:275:PHE:CE2	3:H:289:ILE:HD13	2.53	0.44
3:H:736:PHE:HB2	3:H:737:LYS:H	1.62	0.44
1:A:419:ARG:HD3	1:A:421:THR:O	2.18	0.44
1:A:429:PHE:O	1:A:456:GLN:HG3	2.18	0.44
1:A:534:MET:CE	1:A:569:LEU:HD11	2.47	0.44
1:C:740:ILE:HG23	1:C:785:GLU:HG3	2.00	0.44
1:C:921:ILE:HB	1:C:933:LEU:HB2	1.99	0.44
3:E:375:LEU:CD2	3:E:380:ILE:HD12	2.48	0.44
3:H:514:THR:O	3:H:515:MET:C	2.60	0.44
3:H:743:LEU:HD22	3:H:823:ILE:HD11	2.00	0.44
1:A:921:ILE:HB	1:A:933:LEU:HB2	1.99	0.44
1:A:926:LEU:HD21	2:B:122:LEU:CD2	2.48	0.44
1:A:1057:ARG:HH12	1:A:1110:ALA:HB3	1.82	0.44
3:E:336:ILE:HG22	3:E:337:ILE:HD13	2.00	0.44
3:H:293:TRP:O	3:H:297:CYS:HB2	2.18	0.44
1:A:557:ALA:N	1:A:593:MET:HE2	2.33	0.43
1:A:709:LYS:C	1:A:710:LEU:CD2	2.88	0.43
3:E:622:SER:HB3	3:E:625:ALA:CB	2.48	0.43
5:T:12:DG:C2	6:U:6:DG:C2	3.06	0.43
1:A:534:MET:HE2	1:A:569:LEU:HD11	2.01	0.43
1:A:582:LEU:CD1	1:A:583:GLY:N	2.81	0.43
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.99	0.43
1:A:969:GLU:CD	1:A:971:ALA:H	2.26	0.43
1:C:139:LEU:HG	2:D:355:TYR:HB2	1.99	0.43
1:C:312:GLU:HG3	1:C:327:ARG:CD	2.47	0.43
1:C:430:VAL:O	1:C:456:GLN:HB2	2.19	0.43
1:C:447:GLU:O	1:C:448:LEU:HD12	2.18	0.43
3:E:749:GLN:HG2	3:E:785:LEU:HD11	2.00	0.43
3:H:353:LEU:HD12	3:H:368:LEU:HD21	1.99	0.43
3:H:854:ILE:HD13	3:H:890:ILE:HD13	2.00	0.43
2:B:323:HIS:CD2	2:B:342:THR:HG21	2.53	0.43
2:B:388:ILE:O	2:B:408:ILE:HA	2.17	0.43
1:C:428:SER:OG	1:C:456:GLN:HG2	2.19	0.43
1:C:602:LEU:HD22	1:C:603:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:507:ILE:HD11	3:E:554:LYS:HZ2	1.81	0.43
3:E:861:ARG:NH1	3:E:872:GLU:OE2	2.51	0.43
3:H:741:LYS:HG2	3:H:818:LEU:O	2.19	0.43
1:A:697:SER:C	1:A:698:THR:HG23	2.43	0.43
1:A:926:LEU:HD21	2:B:122:LEU:HD21	2.01	0.43
2:B:382:HIS:CG	2:B:383:PRO:HD2	2.54	0.43
1:C:697:SER:C	1:C:698:THR:HG23	2.44	0.43
1:C:969:GLU:CD	1:C:971:ALA:H	2.26	0.43
2:D:383:PRO:HG3	2:D:435:SER:O	2.18	0.43
3:E:555:ARG:HD2	3:E:556:PRO:CD	2.47	0.43
3:E:741:LYS:HG2	3:E:818:LEU:O	2.19	0.43
5:R:12:DG:C2	6:S:6:DG:C2	3.06	0.43
1:C:429:PHE:O	1:C:456:GLN:HG3	2.18	0.43
1:C:564:ILE:O	1:C:582:LEU:HD12	2.18	0.43
3:H:229:ASN:O	3:H:231:THR:HG23	2.18	0.43
3:H:750:THR:O	3:H:754:LEU:HB2	2.19	0.43
1:A:602:LEU:HD22	1:A:603:LEU:N	2.34	0.43
1:A:912:LEU:CD2	2:B:109:ILE:HD13	2.48	0.43
2:B:105:ILE:HD12	2:B:126:LEU:HD21	2.01	0.43
2:B:367:PRO:HG2	2:B:392:ARG:HG3	2.01	0.43
3:E:340:GLN:HG3	3:E:341:LYS:CG	2.46	0.43
1:A:448:LEU:HD12	1:A:448:LEU:HA	1.80	0.43
1:A:1109:VAL:C	1:A:1111:ASN:H	2.26	0.43
1:C:673:LEU:HD23	1:C:674:LYS:N	2.33	0.43
3:H:466:ASP:O	3:H:468:ASN:N	2.51	0.43
1:A:428:SER:OG	1:A:456:GLN:HG2	2.19	0.43
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.18	0.43
1:C:655:ARG:CG	1:C:655:ARG:HH11	2.31	0.43
1:C:655:ARG:NH2	1:C:713:ARG:HD3	2.34	0.43
3:H:337:ILE:HG21	3:H:374:MET:CE	2.48	0.43
3:H:341:LYS:HB3	3:H:341:LYS:HE3	1.79	0.43
1:A:586:ILE:HG21	1:A:608:ASP:N	2.34	0.43
1:C:419:ARG:HD3	1:C:421:THR:O	2.18	0.43
1:C:478:LEU:HB3	1:C:488:SER:HB3	1.99	0.43
3:E:227:ILE:HD11	3:E:303:ILE:HG13	2.01	0.43
3:H:356:ARG:HD2	3:H:361:GLU:CD	2.44	0.43
3:H:457:LEU:CD1	3:H:493:GLN:HB2	2.49	0.43
3:H:507:ILE:HD11	3:H:554:LYS:HB3	2.00	0.43
5:R:6:DA:C2	6:S:12:DA:C2	3.07	0.43
1:A:843:PRO:C	1:A:844:LYS:HD2	2.43	0.43
1:C:567:ARG:HB3	1:C:579:LYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:PHE:O	1:C:1100:ILE:HG12	2.19	0.43
3:E:450:GLY:HA2	3:E:453:LEU:HD21	2.01	0.43
3:H:229:ASN:C	3:H:231:THR:N	2.61	0.43
1:A:494:GLN:O	1:A:495:ALA:HB3	2.19	0.42
2:B:391:GLY:HA3	2:B:429:ILE:O	2.19	0.42
1:C:492:GLU:CD	1:C:496:LYS:HB2	2.44	0.42
1:C:603:LEU:HD23	1:C:603:LEU:N	2.34	0.42
1:C:893:TRP:CE3	1:C:899:LEU:HD13	2.54	0.42
3:E:854:ILE:HD13	3:E:890:ILE:HD13	1.99	0.42
3:H:467:GLU:O	3:H:468:ASN:CB	2.66	0.42
3:H:622:SER:HB3	3:H:625:ALA:CB	2.48	0.42
1:A:357:GLY:HA2	1:A:358:PRO:C	2.44	0.42
1:C:579:LYS:CG	1:C:581:MET:HE3	2.47	0.42
2:D:382:HIS:CG	2:D:383:PRO:HD2	2.54	0.42
3:E:201:LYS:O	3:E:202:ASN:HB2	2.18	0.42
3:E:311:ASP:HA	3:E:315:VAL:HG23	2.00	0.42
5:T:6:DA:C2	6:U:12:DA:C2	3.07	0.42
1:A:230:ILE:HD11	1:A:285:LEU:HD21	2.02	0.42
1:A:505:SER:OG	1:A:506:SER:N	2.52	0.42
1:C:357:GLY:HA2	1:C:358:PRO:C	2.43	0.42
1:C:582:LEU:CD1	1:C:583:GLY:N	2.81	0.42
2:D:367:PRO:HG2	2:D:392:ARG:HG3	2.01	0.42
3:H:311:ASP:HA	3:H:315:VAL:HG23	2.01	0.42
1:A:23:PHE:N	1:A:30:ASN:ND2	2.59	0.42
1:A:414:ARG:HH11	1:A:414:ARG:CG	2.32	0.42
1:A:430:VAL:O	1:A:456:GLN:HB2	2.18	0.42
1:A:586:ILE:HG22	1:A:607:GLY:H	1.83	0.42
1:A:842:GLU:O	1:A:844:LYS:CD	2.65	0.42
1:C:586:ILE:HG22	1:C:607:GLY:H	1.82	0.42
1:C:1109:VAL:C	1:C:1111:ASN:H	2.26	0.42
3:E:556:PRO:C	3:E:557:ASN:ND2	2.77	0.42
3:E:599:GLY:N	3:E:878:LYS:HG2	2.34	0.42
1:A:567:ARG:HB3	1:A:579:LYS:HA	2.01	0.42
2:B:383:PRO:HG3	2:B:435:SER:O	2.18	0.42
2:D:391:GLY:HA3	2:D:429:ILE:O	2.20	0.42
3:E:397:TYR:CD1	3:E:448:LEU:HD11	2.55	0.42
3:E:750:THR:O	3:E:754:LEU:HB2	2.19	0.42
3:H:467:GLU:O	3:H:468:ASN:HB3	2.20	0.42
1:A:111:ARG:HH21	2:B:292:TRP:CD1	2.38	0.42
1:A:492:GLU:CD	1:A:496:LYS:HB2	2.43	0.42
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:LEU:HB3	1:C:414:ARG:H	1.69	0.42
1:A:447:GLU:O	1:A:448:LEU:HD12	2.18	0.42
1:C:448:LEU:HD12	1:C:448:LEU:HA	1.80	0.42
1:C:500:VAL:HG12	1:C:541:LEU:HD12	2.01	0.42
1:C:557:ALA:H	1:C:593:MET:HE2	1.84	0.42
1:C:699:LEU:HD13	1:C:700:THR:N	2.35	0.42
3:E:523:LYS:CE	3:E:544:MET:CE	2.98	0.42
3:E:599:GLY:C	3:E:601:ASP:N	2.77	0.42
1:C:1030:PHE:CZ	1:C:1038:GLY:HA3	2.54	0.42
2:D:170:GLY:C	2:D:195:ILE:HD11	2.45	0.42
3:E:338:SER:O	3:E:343:GLN:CB	2.57	0.42
3:E:390:LEU:CD2	3:E:440:LEU:HD13	2.50	0.42
3:E:533:CYS:HB2	3:E:534:PHE:HD1	1.85	0.42
1:A:23:PHE:N	1:A:30:ASN:HD22	2.02	0.42
1:A:500:VAL:HG12	1:A:541:LEU:HD12	2.01	0.42
1:A:578:HIS:CG	1:A:623:LEU:HD12	2.54	0.42
1:C:451:PHE:HE1	1:C:470:GLN:HB2	1.79	0.42
1:C:494:GLN:O	1:C:495:ALA:HB3	2.19	0.42
1:C:505:SER:OG	1:C:506:SER:N	2.52	0.42
2:D:279:ALA:HB1	2:D:299:VAL:HG22	2.02	0.42
3:E:552:ILE:CG2	3:E:597:ILE:CD1	2.97	0.42
3:E:736:PHE:HB2	3:E:737:LYS:H	1.62	0.42
3:H:445:GLU:OE2	3:H:482:ARG:NE	2.53	0.42
2:B:347:ASN:HA	2:B:366:HIS:O	2.20	0.42
2:D:105:ILE:HD12	2:D:126:LEU:HD21	2.01	0.42
3:H:340:GLN:O	3:H:343:GLN:N	2.52	0.42
3:H:855:VAL:O	3:H:859:LYS:HB2	2.20	0.42
1:A:375:LEU:O	1:A:389:ILE:C	2.63	0.41
1:A:407:ILE:HD13	1:A:699:LEU:HD23	2.01	0.41
1:A:502:SER:O	1:A:503:CYS:CB	2.68	0.41
1:A:1055:GLN:HE22	1:A:1090:ASP:N	2.11	0.41
1:C:368:GLU:O	1:C:629:VAL:HB	2.20	0.41
3:E:855:VAL:O	3:E:859:LYS:HB2	2.20	0.41
2:B:170:GLY:C	2:B:195:ILE:HD11	2.45	0.41
1:C:523:PRO:HB3	1:C:524:GLN:NE2	2.35	0.41
1:C:532:THR:CG2	1:C:533:GLU:H	2.30	0.41
1:C:586:ILE:HG21	1:C:608:ASP:N	2.34	0.41
3:E:606:PHE:CZ	3:E:838:THR:HG23	2.55	0.41
1:A:24:THR:H	1:A:30:ASN:ND2	2.18	0.41
1:A:580:GLU:C	1:A:581:MET:HE2	2.45	0.41
2:B:354:SER:HA	2:B:357:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:THR:H	1:C:30:ASN:ND2	2.18	0.41
1:C:111:ARG:NE	2:D:290:CYS:SG	2.93	0.41
3:E:340:GLN:HB3	3:E:340:GLN:HE21	1.66	0.41
3:H:515:MET:O	3:H:516:VAL:C	2.63	0.41
2:B:279:ALA:HB1	2:B:299:VAL:HG22	2.02	0.41
1:C:407:ILE:HD13	1:C:699:LEU:HD23	2.01	0.41
1:C:565:SER:CB	1:C:567:ARG:HH11	2.34	0.41
3:E:397:TYR:CG	3:E:444:VAL:HG13	2.50	0.41
3:E:494:TRP:CZ3	3:E:540:PHE:CD2	3.00	0.41
3:H:606:PHE:CZ	3:H:838:THR:HG23	2.55	0.41
3:H:698:PRO:HA	3:H:699:PRO:HD3	1.98	0.41
1:A:111:ARG:NH2	2:B:292:TRP:CD1	2.89	0.41
1:A:712:ILE:O	1:A:713:ARG:O	2.38	0.41
2:D:354:SER:HA	2:D:357:TRP:CE2	2.56	0.41
3:H:465:LEU:HG	3:H:497:TYR:CD2	2.55	0.41
1:C:592:LEU:HD23	1:C:592:LEU:C	2.45	0.41
1:C:641:PHE:CD2	1:C:679:MET:HE1	2.56	0.41
2:D:347:ASN:HA	2:D:366:HIS:O	2.20	0.41
3:E:410:VAL:HG21	3:E:460:GLY:HA3	2.02	0.41
3:H:341:LYS:H	3:H:341:LYS:HD2	1.85	0.41
3:H:533:CYS:HB2	3:H:534:PHE:HD1	1.85	0.41
1:A:663:ASN:C	1:A:665:LYS:N	2.77	0.41
1:C:416:ASP:OD1	1:C:416:ASP:C	2.63	0.41
1:C:565:SER:OG	1:C:567:ARG:NH1	2.54	0.41
1:C:580:GLU:C	1:C:581:MET:HE2	2.45	0.41
3:E:288:LYS:HD3	3:E:288:LYS:HA	1.88	0.41
3:E:358:ARG:HG3	3:E:427:ARG:HH12	1.86	0.41
3:E:464:LEU:HB3	3:E:473:LEU:CD2	2.51	0.41
3:E:899:MET:HA	3:E:911:TYR:O	2.21	0.41
1:A:394:ILE:HG22	1:A:395:GLY:H	1.82	0.41
1:A:416:ASP:OD1	1:A:416:ASP:C	2.63	0.41
1:A:641:PHE:CD2	1:A:679:MET:HE1	2.56	0.41
1:A:699:LEU:HD13	1:A:699:LEU:C	2.46	0.41
1:C:585:GLU:CD	3:H:301:ILE:CG2	2.89	0.41
3:H:206:LYS:CB	3:H:207:PRO:HD3	2.50	0.41
3:H:211:ASN:C	3:H:213:THR:H	2.28	0.41
3:H:298:ARG:HB3	3:H:298:ARG:CZ	2.50	0.41
3:H:415:HIS:C	3:H:419:LYS:HZ3	2.29	0.41
3:H:545:LYS:HB3	3:H:545:LYS:HE2	1.82	0.41
1:A:448:LEU:HB3	1:A:451:PHE:CD2	2.43	0.41
1:A:523:PRO:HB3	1:A:524:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ALA:H	1:A:593:MET:HE2	1.85	0.41
1:A:565:SER:CB	1:A:567:ARG:HH11	2.34	0.41
1:A:592:LEU:HD23	1:A:592:LEU:C	2.46	0.41
1:A:699:LEU:HD13	1:A:700:THR:N	2.35	0.41
1:A:703:THR:OG1	1:A:704:ILE:HD12	2.20	0.41
1:C:404:LEU:HD12	1:C:429:PHE:CZ	2.55	0.41
1:C:926:LEU:HD21	2:D:105:ILE:CD1	2.43	0.41
2:D:323:HIS:CD2	2:D:342:THR:HG21	2.53	0.41
3:E:404:LEU:HD22	3:E:408:ARG:HH21	1.86	0.41
3:E:515:MET:O	3:E:516:VAL:C	2.63	0.41
3:E:538:GLU:HA	3:E:541:ILE:HG22	2.03	0.41
3:H:206:LYS:O	3:H:207:PRO:C	2.64	0.41
3:H:741:LYS:HA	3:H:819:PHE:CE1	2.56	0.41
1:A:561:TRP:O	1:A:587:ILE:HG21	2.19	0.41
1:C:457:THR:CG2	1:C:459:PHE:O	2.69	0.41
1:C:699:LEU:HD13	1:C:699:LEU:C	2.46	0.41
3:E:436:THR:O	3:E:436:THR:HG22	2.20	0.41
3:E:468:ASN:HD21	3:E:470:ILE:HG23	1.86	0.41
3:H:494:TRP:CE3	3:H:540:PHE:HD2	2.38	0.41
3:H:499:LYS:HE2	3:H:550:THR:HG21	2.02	0.41
6:S:8:DA:C2	6:S:9:DA:N6	2.88	0.41
1:C:414:ARG:HH11	1:C:414:ARG:CG	2.32	0.40
1:C:701:ILE:H	1:C:701:ILE:HD12	1.86	0.40
1:C:820:LYS:H	1:C:820:LYS:HG2	1.79	0.40
1:C:1055:GLN:HE22	1:C:1090:ASP:N	2.11	0.40
2:D:218:THR:CG2	2:D:226:VAL:HG13	2.51	0.40
3:E:534:PHE:O	3:E:535:LEU:C	2.65	0.40
3:E:741:LYS:HA	3:E:819:PHE:CE1	2.56	0.40
3:E:835:GLN:HA	3:E:838:THR:HG22	2.03	0.40
3:E:846:ARG:C	3:E:848:TYR:H	2.29	0.40
3:H:404:LEU:HD22	3:H:408:ARG:HH21	1.86	0.40
3:H:457:LEU:CB	3:H:493:GLN:HG2	2.43	0.40
3:H:466:ASP:C	3:H:468:ASN:N	2.79	0.40
6:U:8:DA:C2	6:U:9:DA:N6	2.88	0.40
1:A:72:GLU:CD	1:A:103:ARG:HH22	2.29	0.40
1:A:404:LEU:HD12	1:A:429:PHE:CZ	2.56	0.40
1:A:870:VAL:HA	1:A:883:SER:O	2.21	0.40
1:C:487:VAL:O	1:C:487:VAL:HG23	2.21	0.40
3:H:226:ALA:HB1	3:H:232:SER:CA	2.51	0.40
3:H:293:TRP:CZ3	3:H:370:SER:HB2	2.53	0.40
1:A:329:GLY:HA3	1:A:384:GLU:HG3	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD13	1:A:468:LEU:HD23	2.03	0.40
1:A:469:ILE:HD13	1:A:469:ILE:C	2.46	0.40
1:A:523:PRO:C	1:A:524:GLN:NE2	2.80	0.40
1:A:565:SER:OG	1:A:567:ARG:NH1	2.54	0.40
1:C:469:ILE:HD13	1:C:469:ILE:C	2.46	0.40
1:C:870:VAL:HA	1:C:883:SER:O	2.21	0.40
3:E:449:LEU:O	3:E:453:LEU:HD13	2.21	0.40
3:E:596:PHE:O	3:E:597:ILE:CG1	2.68	0.40
1:A:457:THR:CG2	1:A:459:PHE:O	2.69	0.40
1:C:429:PHE:O	1:C:430:VAL:C	2.64	0.40
1:C:663:ASN:C	1:C:665:LYS:N	2.77	0.40
1:C:1057:ARG:NH1	1:C:1109:VAL:O	2.55	0.40
3:E:681:ILE:HD12	4:F:31:ALA:HB3	2.03	0.40
3:H:198:LEU:HD22	3:H:198:LEU:HA	1.92	0.40
3:H:211:ASN:C	3:H:213:THR:N	2.76	0.40
3:H:859:LYS:HB3	3:H:859:LYS:HE3	1.80	0.40
3:H:899:MET:HA	3:H:911:TYR:O	2.21	0.40
1:A:893:TRP:CE3	1:A:899:LEU:HD13	2.54	0.40
1:C:413:LEU:HD13	1:C:468:LEU:HD23	2.03	0.40
1:C:452:VAL:HG22	1:C:477:ARG:NH1	2.37	0.40
1:C:928:ARG:HH11	2:D:437:THR:HG23	1.82	0.40
3:E:358:ARG:O	3:E:420:ARG:NH2	2.55	0.40
3:E:445:GLU:O	3:E:449:LEU:HB2	2.21	0.40
3:H:835:GLN:HA	3:H:838:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1095/1144 (96%)	948 (87%)	105 (10%)	42 (4%)	2 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1095/1144 (96%)	967 (88%)	97 (9%)	31 (3%)	4	24
2	B	353/382 (92%)	333 (94%)	16 (4%)	4 (1%)	11	46
2	D	353/382 (92%)	333 (94%)	16 (4%)	4 (1%)	11	46
3	E	701/726 (97%)	603 (86%)	73 (10%)	25 (4%)	2	20
3	H	701/726 (97%)	604 (86%)	72 (10%)	25 (4%)	2	20
4	F	19/98 (19%)	14 (74%)	2 (10%)	3 (16%)	0	2
4	I	19/98 (19%)	16 (84%)	2 (10%)	1 (5%)	1	15
All	All	4336/4700 (92%)	3818 (88%)	383 (9%)	135 (3%)	3	22

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	LEU
1	A	390	ILE
1	A	430	VAL
1	A	583	GLY
1	A	598	SER
1	A	672	ASN
1	A	707	ILE
1	A	708	GLN
1	A	711	HIS
1	A	712	ILE
1	A	713	ARG
1	A	715	VAL
1	A	841	ALA
1	C	367	LEU
1	C	430	VAL
1	C	583	GLY
1	C	598	SER
1	C	672	ASN
1	C	674	LYS
1	C	708	GLN
3	E	204	LYS
3	E	431	TYR
3	E	515	MET
3	E	556	PRO
3	E	595	ARG
3	E	597	ILE
3	E	902	ASP
4	F	34	ALA

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Mol	Chain	Res	Type
4	F	38	VAL
3	H	204	LYS
3	H	431	TYR
3	H	515	MET
3	H	902	ASP
4	I	38	VAL
1	A	389	ILE
1	A	392	ASN
1	A	549	SER
1	A	562	THR
1	A	563	ASP
1	A	584	GLY
1	A	674	LYS
1	A	855	ASP
1	A	1110	ALA
2	B	117	SER
1	C	547	GLY
1	C	549	SER
1	C	562	THR
1	C	563	ASP
1	C	584	GLY
1	C	855	ASP
1	C	1110	ALA
2	D	117	SER
3	E	337	ILE
3	E	435	THR
3	E	596	PHE
3	E	761	GLU
3	E	880	PRO
3	E	912	ILE
3	H	206	LYS
3	H	230	SER
3	H	231	THR
3	H	338	SER
3	H	435	THR
3	H	761	GLU
3	H	880	PRO
3	H	912	ILE
1	A	372	GLN
1	A	418	ASN
1	A	449	MET
1	A	481	GLN

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Mol	Chain	Res	Type
1	A	547	GLY
1	A	624	SER
1	A	644	LEU
1	A	710	LEU
1	A	1109	VAL
1	C	418	ASN
1	C	449	MET
1	C	481	GLN
1	C	624	SER
1	C	644	LEU
1	C	1109	VAL
3	E	557	ASN
3	H	340	GLN
3	H	341	LYS
3	H	468	ASN
1	A	36	ASN
1	A	488	SER
2	B	190	GLY
1	C	36	ASN
1	C	372	GLN
1	C	488	SER
1	C	503	CYS
2	D	190	GLY
3	E	338	SER
3	E	340	GLN
3	E	451	GLU
3	E	699	PRO
3	H	699	PRO
1	A	503	CYS
1	A	592	LEU
1	C	242	GLY
1	C	592	LEU
2	D	291	ASP
3	E	790	ALA
3	H	360	GLY
3	H	467	GLU
3	H	556	PRO
3	H	790	ALA
1	A	242	GLY
1	A	460	CYS
2	B	291	ASP
1	C	460	CYS

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Mol	Chain	Res	Type
4	F	35	TRP
1	A	493	PRO
1	A	551	GLY
2	B	118	ILE
1	C	493	PRO
1	C	551	GLY
2	D	118	ILE
3	E	301	ILE
3	E	688	PRO
3	E	881	VAL
3	H	301	ILE
3	H	688	PRO
3	H	881	VAL
1	A	406	GLY
1	C	406	GLY
3	E	516	VAL
3	H	516	VAL
1	A	523	PRO
1	A	716	PRO
1	C	523	PRO
3	E	206	LYS
3	E	486	GLY
3	H	486	GLY

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	938/1000 (94%)	832 (89%)	106 (11%)	5	19
1	C	944/1000 (94%)	840 (89%)	104 (11%)	6	20
2	B	306/335 (91%)	282 (92%)	24 (8%)	11	32
2	D	313/335 (93%)	288 (92%)	25 (8%)	11	31
3	E	625/660 (95%)	532 (85%)	93 (15%)	3	12
3	H	631/660 (96%)	546 (86%)	85 (14%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	17/83 (20%)	12 (71%)	5 (29%)	0	2
4	I	16/83 (19%)	13 (81%)	3 (19%)	1	8
All	All	3790/4156 (91%)	3345 (88%)	445 (12%)	5	18

All (445) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	19	VAL
1	A	81	THR
1	A	99	ASP
1	A	101	ILE
1	A	133	LEU
1	A	147	ARG
1	A	159	LEU
1	A	167	VAL
1	A	191	LYS
1	A	253	ILE
1	A	259	VAL
1	A	267	ASN
1	A	297	LEU
1	A	304	LEU
1	A	314	LEU
1	A	334	VAL
1	A	339	ASP
1	A	352	THR
1	A	360	VAL
1	A	396	ILE
1	A	404	LEU
1	A	410	LEU
1	A	412	PRO
1	A	414	ARG
1	A	419	ARG
1	A	420	GLU
1	A	448	LEU
1	A	452	VAL
1	A	454	ASP
1	A	469	ILE
1	A	473	SER
1	A	476	VAL
1	A	481	GLN

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Mol	Chain	Res	Type
1	A	482	GLU
1	A	487	VAL
1	A	493	PRO
1	A	510	VAL
1	A	518	TYR
1	A	521	ILE
1	A	523	PRO
1	A	525	GLU
1	A	531	HIS
1	A	533	GLU
1	A	540	CYS
1	A	555	LEU
1	A	560	LEU
1	A	563	ASP
1	A	567	ARG
1	A	576	LEU
1	A	582	LEU
1	A	587	ILE
1	A	592	LEU
1	A	594	THR
1	A	597	GLU
1	A	602	LEU
1	A	603	LEU
1	A	608	ASP
1	A	614	PHE
1	A	616	LEU
1	A	617	ASN
1	A	618	ILE
1	A	620	THR
1	A	623	LEU
1	A	625	ASP
1	A	627	LYS
1	A	629	VAL
1	A	636	THR
1	A	646	THR
1	A	668	PHE
1	A	673	LEU
1	A	688	PRO
1	A	700	THR
1	A	701	ILE
1	A	704	ILE
1	A	707	ILE

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Mol	Chain	Res	Type
1	A	709	LYS
1	A	710	LEU
1	A	717	LEU
1	A	728	GLU
1	A	794	ILE
1	A	809	GLN
1	A	820	LYS
1	A	839	GLU
1	A	840	GLU
1	A	844	LYS
1	A	867	LYS
1	A	881	LEU
1	A	898	GLU
1	A	899	LEU
1	A	901	THR
1	A	909	ILE
1	A	914	LEU
1	A	930	VAL
1	A	931	LEU
1	A	957	VAL
1	A	966	LEU
1	A	970	ASN
1	A	984	THR
1	A	993	GLN
1	A	1000	LEU
1	A	1052	LEU
1	A	1086	THR
1	A	1093	LEU
1	A	1106	GLN
1	A	1129	LEU
2	B	111	LYS
2	B	116	GLN
2	B	134	LEU
2	B	150	VAL
2	B	174	LEU
2	B	179	VAL
2	B	180	GLN
2	B	198	MET
2	B	219	LEU
2	B	243	VAL
2	B	254	THR
2	B	262	LEU

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Mol	Chain	Res	Type
2	B	263	LEU
2	B	274	GLU
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	312	LYS
2	B	374	LEU
2	B	389	VAL
2	B	400	LEU
2	B	435	SER
2	B	437	THR
2	B	453	ASN
1	C	7	VAL
1	C	19	VAL
1	C	81	THR
1	C	99	ASP
1	C	101	ILE
1	C	133	LEU
1	C	147	ARG
1	C	159	LEU
1	C	167	VAL
1	C	191	LYS
1	C	253	ILE
1	C	259	VAL
1	C	267	ASN
1	C	297	LEU
1	C	304	LEU
1	C	314	LEU
1	C	334	VAL
1	C	339	ASP
1	C	352	THR
1	C	360	VAL
1	C	396	ILE
1	C	404	LEU
1	C	410	LEU
1	C	412	PRO
1	C	414	ARG
1	C	419	ARG
1	C	420	GLU
1	C	448	LEU
1	C	452	VAL
1	C	454	ASP

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Mol	Chain	Res	Type
1	C	469	ILE
1	C	473	SER
1	C	476	VAL
1	C	481	GLN
1	C	482	GLU
1	C	487	VAL
1	C	493	PRO
1	C	510	VAL
1	C	518	TYR
1	C	521	ILE
1	C	523	PRO
1	C	525	GLU
1	C	531	HIS
1	C	533	GLU
1	C	540	CYS
1	C	555	LEU
1	C	560	LEU
1	C	563	ASP
1	C	567	ARG
1	C	576	LEU
1	C	582	LEU
1	C	587	ILE
1	C	592	LEU
1	C	594	THR
1	C	597	GLU
1	C	602	LEU
1	C	603	LEU
1	C	608	ASP
1	C	614	PHE
1	C	616	LEU
1	C	617	ASN
1	C	618	ILE
1	C	620	THR
1	C	623	LEU
1	C	625	ASP
1	C	627	LYS
1	C	629	VAL
1	C	636	THR
1	C	646	THR
1	C	655	ARG
1	C	663	ASN
1	C	673	LEU

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Mol	Chain	Res	Type
1	C	688	PRO
1	C	700	THR
1	C	701	ILE
1	C	703	THR
1	C	704	ILE
1	C	708	GLN
1	C	710	LEU
1	C	713	ARG
1	C	728	GLU
1	C	794	ILE
1	C	809	GLN
1	C	820	LYS
1	C	844	LYS
1	C	867	LYS
1	C	881	LEU
1	C	898	GLU
1	C	899	LEU
1	C	901	THR
1	C	909	ILE
1	C	914	LEU
1	C	930	VAL
1	C	931	LEU
1	C	957	VAL
1	C	966	LEU
1	C	970	ASN
1	C	984	THR
1	C	993	GLN
1	C	1000	LEU
1	C	1052	LEU
1	C	1086	THR
1	C	1093	LEU
1	C	1129	LEU
2	D	111	LYS
2	D	116	GLN
2	D	134	LEU
2	D	150	VAL
2	D	174	LEU
2	D	179	VAL
2	D	180	GLN
2	D	198	MET
2	D	219	LEU
2	D	243	VAL

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Mol	Chain	Res	Type
2	D	254	THR
2	D	262	LEU
2	D	263	LEU
2	D	274	GLU
2	D	293	LEU
2	D	299	VAL
2	D	308	LEU
2	D	312	LYS
2	D	369	ARG
2	D	374	LEU
2	D	389	VAL
2	D	400	LEU
2	D	435	SER
2	D	437	THR
2	D	453	ASN
3	E	198	LEU
3	E	214	ASP
3	E	217	TRP
3	E	221	LYS
3	E	233	ILE
3	E	234	LYS
3	E	235	TYR
3	E	251	LYS
3	E	255	ASN
3	E	256	LEU
3	E	259	GLN
3	E	260	LEU
3	E	263	ILE
3	E	289	ILE
3	E	310	LEU
3	E	316	LEU
3	E	324	ILE
3	E	336	ILE
3	E	339	ASP
3	E	340	GLN
3	E	341	LYS
3	E	343	GLN
3	E	345	LYS
3	E	352	LEU
3	E	355	GLU
3	E	359	ASN
3	E	366	SER

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Mol	Chain	Res	Type
3	E	378	LEU
3	E	379	GLN
3	E	380	ILE
3	E	388	ARG
3	E	414	LEU
3	E	428	LEU
3	E	429	ILE
3	E	433	ASP
3	E	434	GLN
3	E	435	THR
3	E	443	THR
3	E	451	GLU
3	E	453	LEU
3	E	454	THR
3	E	458	GLN
3	E	459	LYS
3	E	465	LEU
3	E	484	ARG
3	E	488	GLN
3	E	491	LEU
3	E	503	SER
3	E	504	THR
3	E	507	ILE
3	E	513	LYS
3	E	520	LEU
3	E	532	ILE
3	E	544	MET
3	E	548	PHE
3	E	552	ILE
3	E	555	ARG
3	E	570	LYS
3	E	577	GLU
3	E	580	ASP
3	E	581	GLU
3	E	588	ASP
3	E	592	ILE
3	E	596	PHE
3	E	597	ILE
3	E	611	LEU
3	E	613	LYS
3	E	619	LYS
3	E	641	PHE

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Mol	Chain	Res	Type
3	E	653	GLU
3	E	667	GLN
3	E	681	ILE
3	E	689	THR
3	E	691	VAL
3	E	695	VAL
3	E	726	THR
3	E	745	VAL
3	E	747	LEU
3	E	778	LEU
3	E	791	ARG
3	E	816	HIS
3	E	823	ILE
3	E	827	GLN
3	E	845	ASP
3	E	859	LYS
3	E	863	THR
3	E	877	LEU
3	E	878	LYS
3	E	886	LEU
3	E	897	ASP
3	E	901	ARG
3	E	904	GLU
3	E	905	ASN
4	F	19	LYS
4	F	25	LYS
4	F	35	TRP
4	F	37	ILE
4	F	39	VAL
3	H	198	LEU
3	H	210	GLU
3	H	211	ASN
3	H	214	ASP
3	H	217	TRP
3	H	221	LYS
3	H	228	GLN
3	H	229	ASN
3	H	234	LYS
3	H	235	TYR
3	H	251	LYS
3	H	255	ASN
3	H	256	LEU

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Mol	Chain	Res	Type
3	H	260	LEU
3	H	263	ILE
3	H	289	ILE
3	H	310	LEU
3	H	316	LEU
3	H	324	ILE
3	H	340	GLN
3	H	341	LYS
3	H	342	VAL
3	H	343	GLN
3	H	352	LEU
3	H	355	GLU
3	H	363	ILE
3	H	366	SER
3	H	379	GLN
3	H	380	ILE
3	H	388	ARG
3	H	414	LEU
3	H	429	ILE
3	H	430	THR
3	H	443	THR
3	H	454	THR
3	H	458	GLN
3	H	459	LYS
3	H	465	LEU
3	H	484	ARG
3	H	488	GLN
3	H	491	LEU
3	H	503	SER
3	H	504	THR
3	H	507	ILE
3	H	513	LYS
3	H	514	THR
3	H	520	LEU
3	H	532	ILE
3	H	544	MET
3	H	548	PHE
3	H	552	ILE
3	H	570	LYS
3	H	577	GLU
3	H	580	ASP
3	H	581	GLU

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Mol	Chain	Res	Type
3	H	588	ASP
3	H	592	ILE
3	H	595	ARG
3	H	611	LEU
3	H	613	LYS
3	H	619	LYS
3	H	641	PHE
3	H	653	GLU
3	H	667	GLN
3	H	689	THR
3	H	691	VAL
3	H	695	VAL
3	H	726	THR
3	H	745	VAL
3	H	747	LEU
3	H	778	LEU
3	H	791	ARG
3	H	816	HIS
3	H	823	ILE
3	H	827	GLN
3	H	845	ASP
3	H	859	LYS
3	H	863	THR
3	H	877	LEU
3	H	878	LYS
3	H	886	LEU
3	H	897	ASP
3	H	901	ARG
3	H	904	GLU
3	H	905	ASN
4	I	19	LYS
4	I	25	LYS
4	I	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	30	ASN
1	A	85	ASN
1	A	156	ASN
1	A	241	ASN

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Mol	Chain	Res	Type
1	A	261	HIS
1	A	319	ASN
1	A	374	GLN
1	A	455	GLN
1	A	462	ASN
1	A	467	GLN
1	A	481	GLN
1	A	494	GLN
1	A	507	GLN
1	A	524	GLN
1	A	536	HIS
1	A	550	ASN
1	A	578	HIS
1	A	634	GLN
1	A	648	ASN
1	A	677	ASN
1	A	711	HIS
1	A	731	GLN
1	A	796	GLN
1	A	877	ASN
1	A	885	ASN
1	A	904	ASN
1	A	907	ASN
1	A	950	ASN
1	A	993	GLN
1	A	1034	ASN
1	A	1055	GLN
2	B	121	GLN
2	B	156	HIS
2	B	269	HIS
2	B	370	GLN
2	B	397	GLN
2	B	419	GLN
2	B	453	ASN
1	C	4	ASN
1	C	30	ASN
1	C	85	ASN
1	C	156	ASN
1	C	241	ASN
1	C	261	HIS
1	C	319	ASN
1	C	374	GLN

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Mol	Chain	Res	Type
1	C	392	ASN
1	C	456	GLN
1	C	462	ASN
1	C	467	GLN
1	C	481	GLN
1	C	494	GLN
1	C	507	GLN
1	C	524	GLN
1	C	536	HIS
1	C	550	ASN
1	C	578	HIS
1	C	634	GLN
1	C	648	ASN
1	C	663	ASN
1	C	677	ASN
1	C	708	GLN
1	C	731	GLN
1	C	796	GLN
1	C	797	HIS
1	C	852	GLN
1	C	877	ASN
1	C	885	ASN
1	C	904	ASN
1	C	907	ASN
1	C	993	GLN
1	C	1034	ASN
1	C	1055	GLN
2	D	121	GLN
2	D	269	HIS
2	D	370	GLN
2	D	397	GLN
2	D	419	GLN
2	D	424	ASN
2	D	453	ASN
3	E	211	ASN
3	E	255	ASN
3	E	296	HIS
3	E	318	ASN
3	E	340	GLN
3	E	379	GLN
3	E	402	GLN
3	E	434	GLN

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Mol	Chain	Res	Type
3	E	468	ASN
3	E	542	ASN
3	E	557	ASN
3	E	716	HIS
3	E	724	GLN
3	E	744	GLN
3	E	827	GLN
3	E	847	GLN
3	E	905	ASN
3	E	907	ASN
3	E	910	ASN
3	H	246	ASN
3	H	255	ASN
3	H	296	HIS
3	H	318	ASN
3	H	340	GLN
3	H	379	GLN
3	H	394	ASN
3	H	402	GLN
3	H	418	ASN
3	H	434	GLN
3	H	447	GLN
3	H	452	HIS
3	H	468	ASN
3	H	493	GLN
3	H	542	ASN
3	H	557	ASN
3	H	716	HIS
3	H	724	GLN
3	H	744	GLN
3	H	827	GLN
3	H	847	GLN
3	H	905	ASN
3	H	907	ASN
3	H	910	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
5	3DR	R	9	5	8,11,12	0.36	0	7,14,17	1.20	0
5	3DR	T	9	5	8,11,12	0.37	0	7,14,17	1.19	0

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
5	3DR	R	9	5	-	1/3/15/16	0/1/1/1
5	3DR	T	9	5	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	9	3DR	C3'-C4'-C5'-O5'
5	T	9	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	1105/1144 (96%)	-0.04	24 (2%) 62 53	98, 183, 251, 326	0
1	C	1105/1144 (96%)	-0.11	18 (1%) 70 59	130, 197, 349, 378	0
2	B	355/382 (92%)	-0.06	11 (3%) 51 46	275, 328, 394, 423	0
2	D	355/382 (92%)	-0.21	5 (1%) 73 62	193, 275, 343, 370	0
3	E	709/726 (97%)	-0.02	13 (1%) 67 58	131, 321, 394, 414	0
3	H	709/726 (97%)	-0.09	9 (1%) 75 64	226, 289, 381, 399	0
4	F	21/98 (21%)	-0.13	0 100 100	368, 383, 396, 398	0
4	I	21/98 (21%)	-0.25	0 100 100	340, 358, 380, 389	0
5	R	11/12 (91%)	0.24	0 100 100	301, 317, 376, 403	0
5	T	11/12 (91%)	-0.06	0 100 100	257, 344, 355, 356	0
6	S	12/12 (100%)	-0.12	0 100 100	317, 326, 386, 386	0
6	U	12/12 (100%)	0.04	0 100 100	286, 320, 350, 363	0
All	All	4426/4748 (93%)	-0.08	80 (1%) 67 58	98, 240, 379, 423	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	109	ILE	8.0
2	B	106	LEU	7.0
1	C	328	LEU	6.2
3	H	350	ILE	5.7
3	E	350	ILE	5.3
2	D	328	ASN	4.2
2	B	105	ILE	3.9
3	E	529	ILE	3.8
1	A	966	LEU	3.8
1	C	381	ALA	3.7
3	H	353	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	376	PRO	3.6
3	E	526	VAL	3.5
1	A	712	ILE	3.5
3	E	246	ASN	3.5
2	B	122	LEU	3.5
3	E	573	ALA	3.4
1	A	1063	LYS	3.4
1	A	858	LEU	3.2
3	E	354	ILE	3.2
3	H	354	ILE	3.1
1	C	367	LEU	3.0
3	H	357	GLU	3.0
3	E	363	ILE	2.9
1	C	965	PHE	2.9
1	A	853	TYR	2.9
1	A	381	ALA	2.9
1	A	297	LEU	2.8
3	E	534	PHE	2.8
1	A	328	LEU	2.7
1	A	1062	ILE	2.7
1	C	910	MET	2.7
3	E	329	LEU	2.7
1	C	806	GLN	2.7
3	H	752	VAL	2.7
2	D	378	LYS	2.7
1	C	1050	LEU	2.7
2	D	122	LEU	2.7
2	B	107	HIS	2.6
1	C	799	PHE	2.6
1	A	1061	VAL	2.6
1	C	443	VAL	2.5
3	H	346	THR	2.5
3	H	421	LEU	2.5
1	C	1058	LEU	2.5
1	A	756	ALA	2.4
1	A	133	LEU	2.4
2	D	158	THR	2.4
1	C	31	LEU	2.4
2	B	443	SER	2.3
1	A	566	ALA	2.3
3	E	436	THR	2.3
1	A	604	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	793	ILE	2.2
1	A	770	LEU	2.2
3	E	368	LEU	2.2
1	A	829	PHE	2.2
2	B	276	LEU	2.2
1	A	733	PHE	2.2
1	C	757	SER	2.2
1	C	926	LEU	2.2
1	A	909	ILE	2.2
3	H	518	GLU	2.2
2	B	390	ALA	2.2
1	A	1051	LEU	2.2
1	C	828	TYR	2.2
2	B	101	GLY	2.1
3	H	435	THR	2.1
1	C	94	SER	2.1
2	B	442	ALA	2.1
2	B	387	LEU	2.1
3	E	476	LEU	2.1
1	A	799	PHE	2.1
1	A	1054	MET	2.1
1	C	602	LEU	2.1
3	E	287	LYS	2.1
1	A	636	THR	2.1
1	A	220	ILE	2.0
1	C	604	CYS	2.0
1	C	765	VAL	2.0

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

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(Å ²)	Q<0.9
5	3DR	R	9	11/12	0.77	0.05	318,324,336,339	0
5	3DR	T	9	11/12	0.85	0.10	347,358,362,362	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.