



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:09 AM UTC

PDB ID : 3E0J / pdb_00003e0j
Title : X-ray structure of the complex of regulatory subunits of human DNA polymerase delta
Authors : Baranovskiy, A.G.; Babayeva, N.D.; Pavlov, Y.I.; Vassilyev, D.G.; Tahirov, T.H.
Deposited on : 2008-07-31
Resolution : 3.00 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:

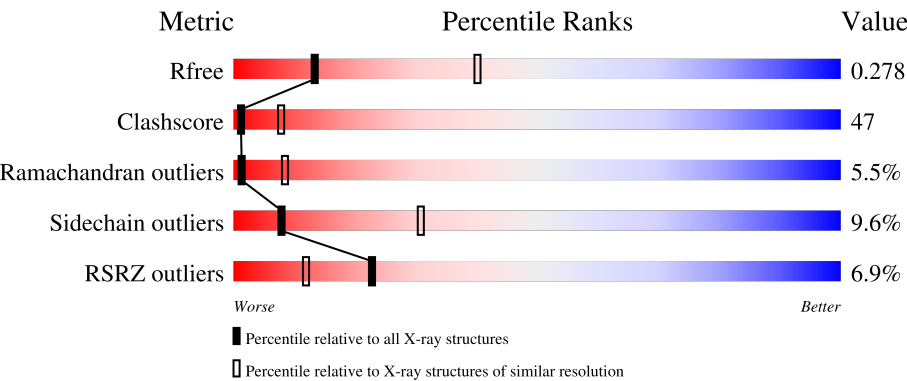
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	476	7% 27% 49% 10% • 13%
1	C	476	5% 28% 48% 9% • 14%
1	E	476	6% 26% 48% 10% • 14%
1	G	476	8% 29% 46% 9% • 14%
2	B	144	5% 40% 50% 9% •

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Mol	Chain	Length	Quality of chain
2	D	144	4% 40% 51% 9%
2	F	144	5% 39% 52% 8%
2	H	144	5% 41% 49% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17153 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 polymerase subunit delta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3185	2022	537	609	17			
1	C	409	Total	C	N	O	S	0	0	0
			3133	1991	530	595	17			
1	E	408	Total	C	N	O	S	0	0	0
			3125	1985	529	594	17			
1	G	408	Total	C	N	O	S	0	0	0
			3125	1985	529	594	17			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP P49005
A	-5	HIS	-	expression tag	UNP P49005
A	-4	HIS	-	expression tag	UNP P49005
A	-3	HIS	-	expression tag	UNP P49005
A	-2	HIS	-	expression tag	UNP P49005
A	-1	HIS	-	expression tag	UNP P49005
A	0	GLY	-	expression tag	UNP P49005
C	-6	HIS	-	expression tag	UNP P49005
C	-5	HIS	-	expression tag	UNP P49005
C	-4	HIS	-	expression tag	UNP P49005
C	-3	HIS	-	expression tag	UNP P49005
C	-2	HIS	-	expression tag	UNP P49005
C	-1	HIS	-	expression tag	UNP P49005
C	0	GLY	-	expression tag	UNP P49005
E	-6	HIS	-	expression tag	UNP P49005
E	-5	HIS	-	expression tag	UNP P49005
E	-4	HIS	-	expression tag	UNP P49005
E	-3	HIS	-	expression tag	UNP P49005
E	-2	HIS	-	expression tag	UNP P49005
E	-1	HIS	-	expression tag	UNP P49005
E	0	GLY	-	expression tag	UNP P49005

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	HIS	-	expression tag	UNP P49005
G	-5	HIS	-	expression tag	UNP P49005
G	-4	HIS	-	expression tag	UNP P49005
G	-3	HIS	-	expression tag	UNP P49005
G	-2	HIS	-	expression tag	UNP P49005
G	-1	HIS	-	expression tag	UNP P49005
G	0	GLY	-	expression tag	UNP P49005

- Molecule 2 is a protein called DNA polymerase subunit delta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			
2	D	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			
2	F	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			
2	H	143	Total	C	N	O	S	0	0	0
			1131	715	196	215	5			

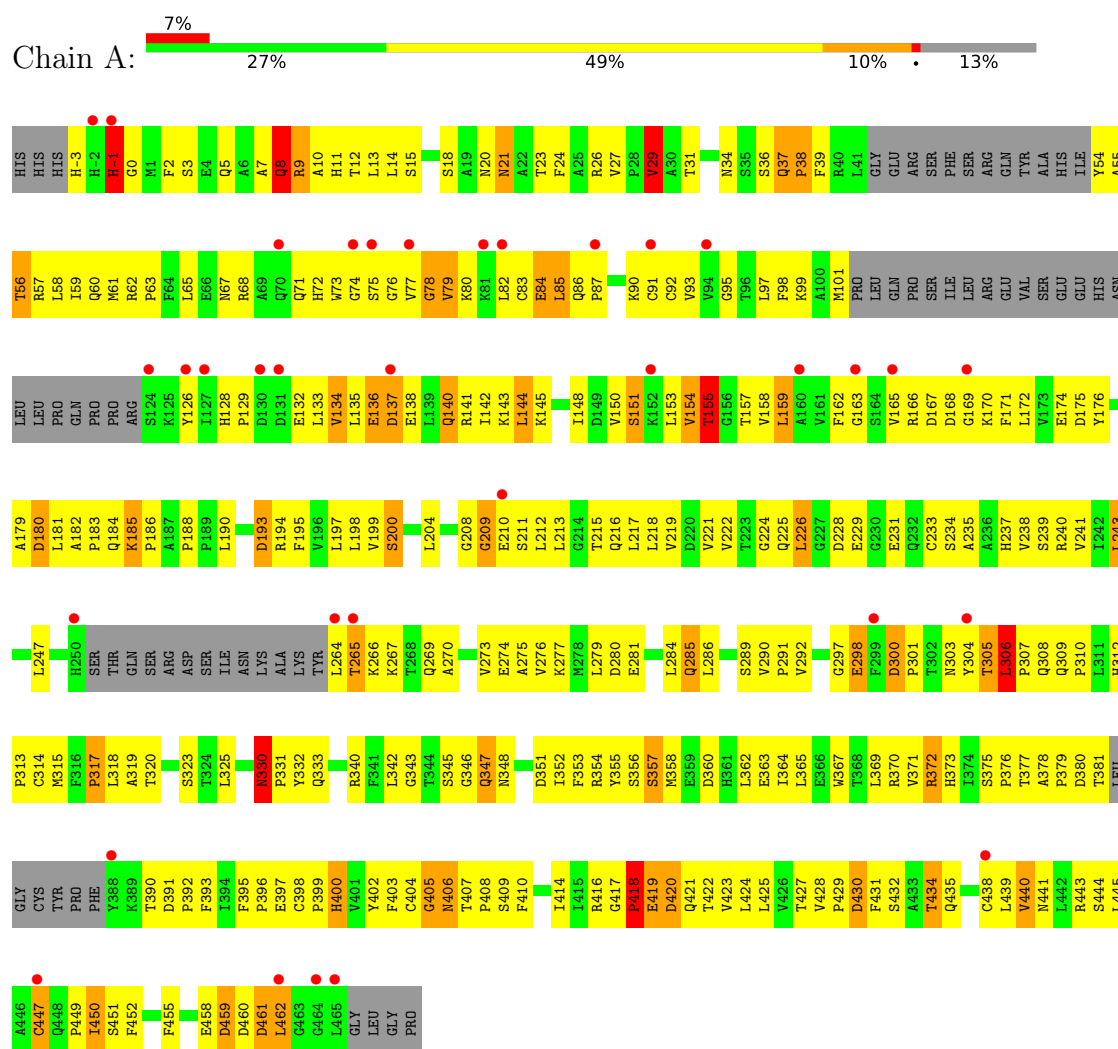
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	6	Total	O	0	0
			6	6		
3	C	12	Total	O	0	0
			12	12		
3	D	4	Total	O	0	0
			4	4		
3	E	15	Total	O	0	0
			15	15		
3	F	4	Total	O	0	0
			4	4		
3	G	8	Total	O	0	0
			8	8		
3	H	1	Total	O	0	0
			1	1		

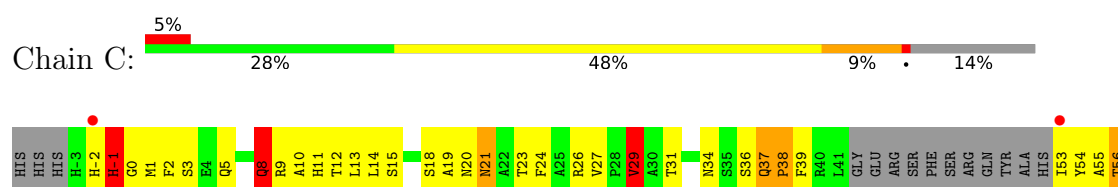
3 Residue-property plots

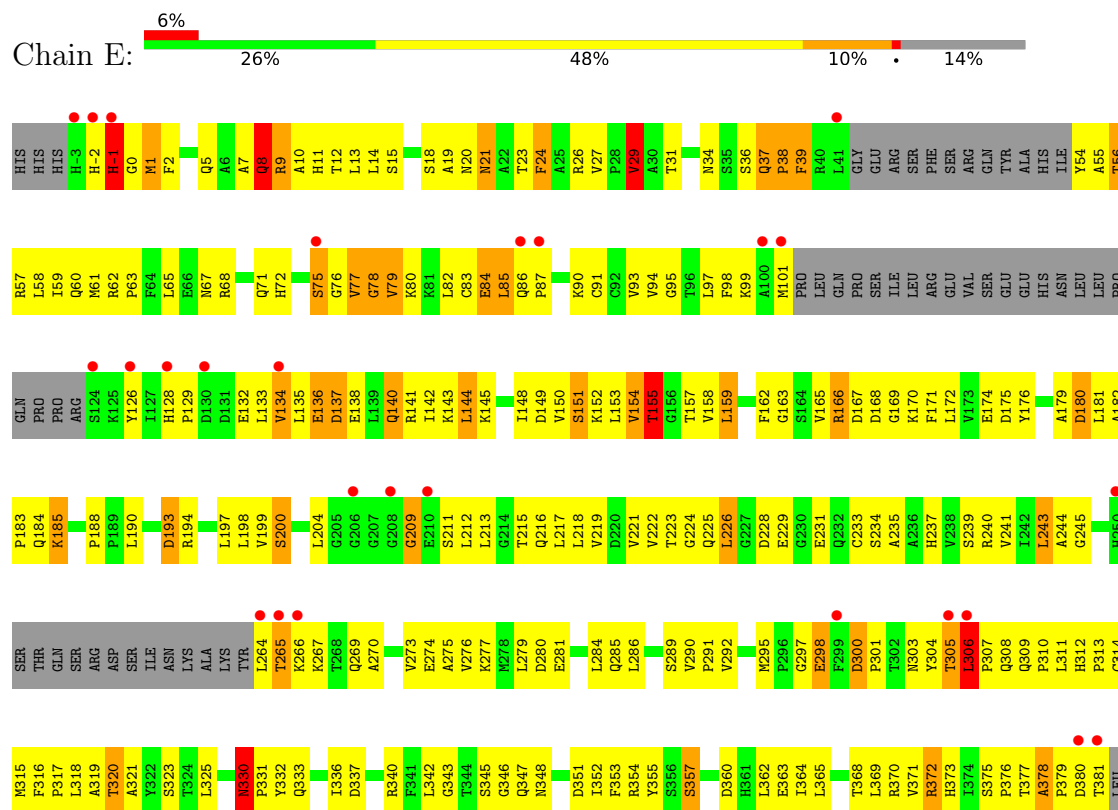
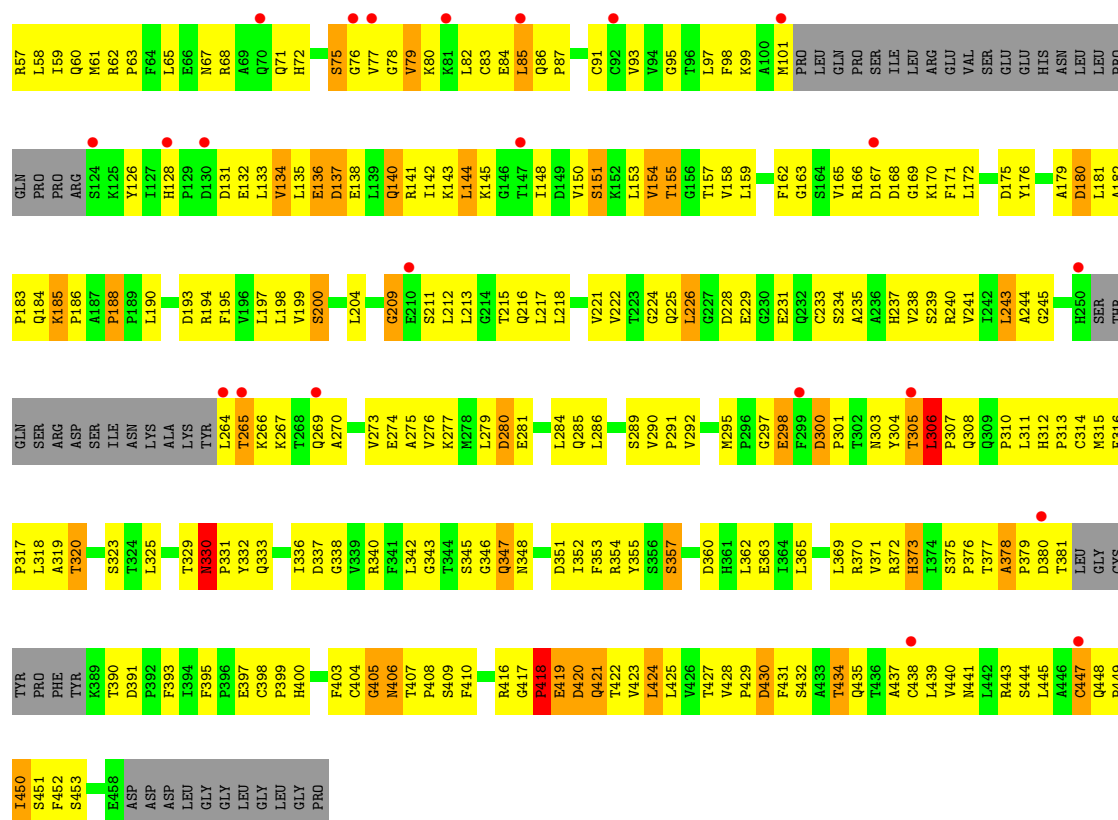
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

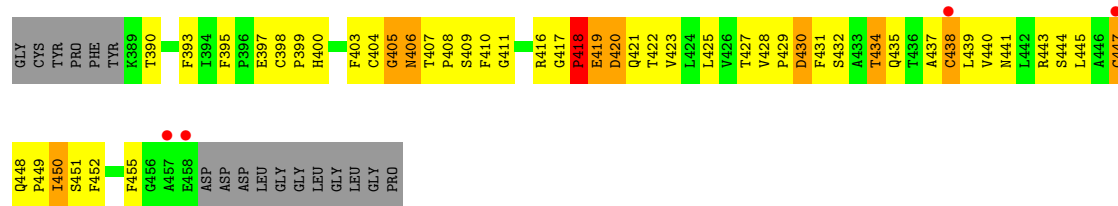
• Molecule 1: DNA polymerase subunit delta-2



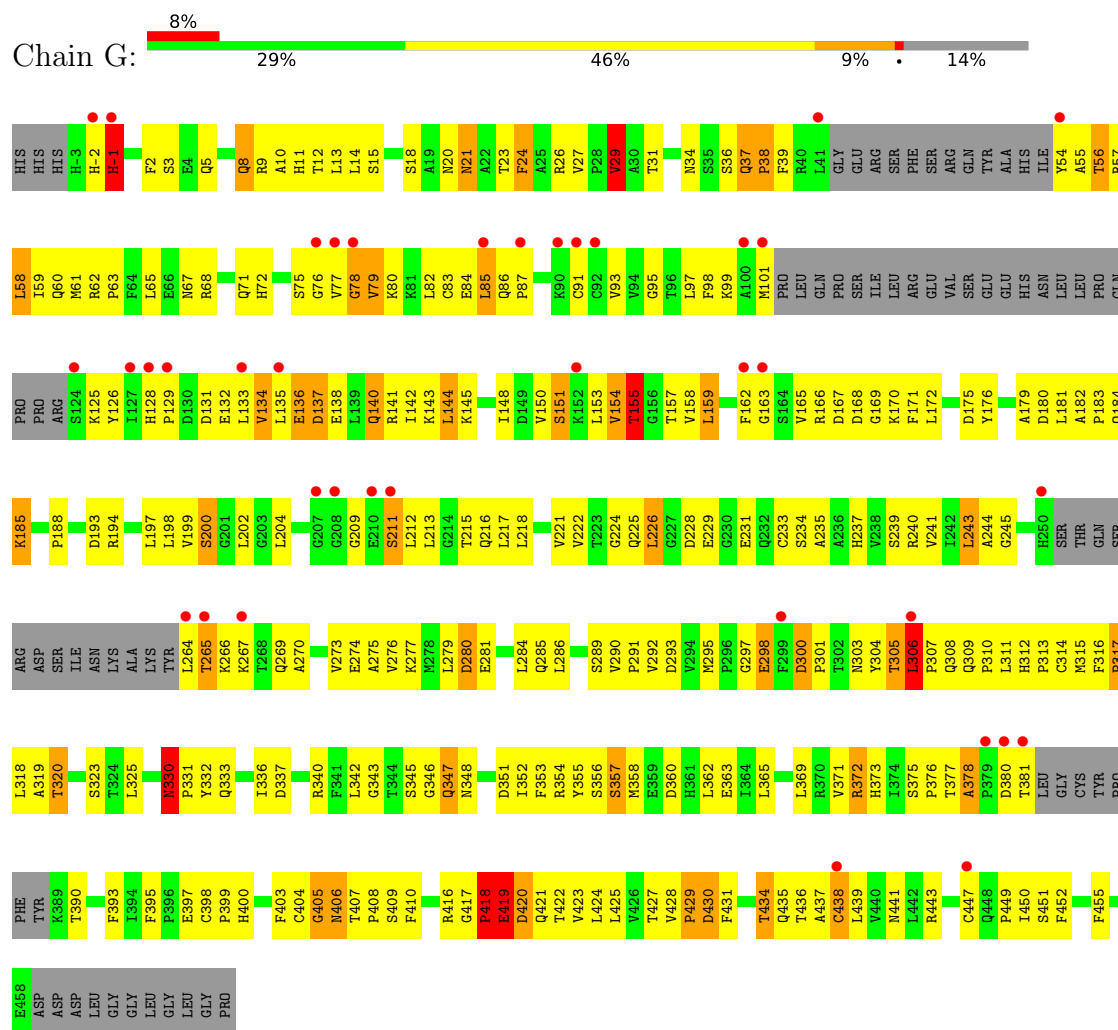
• Molecule 1: DNA polymerase subunit delta-2



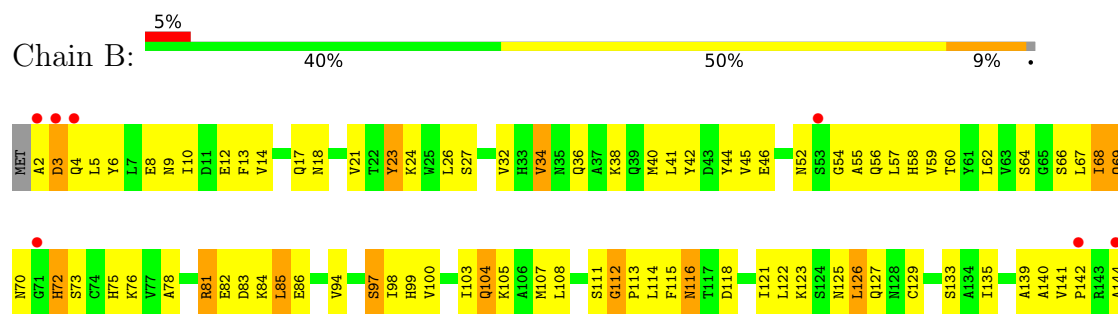




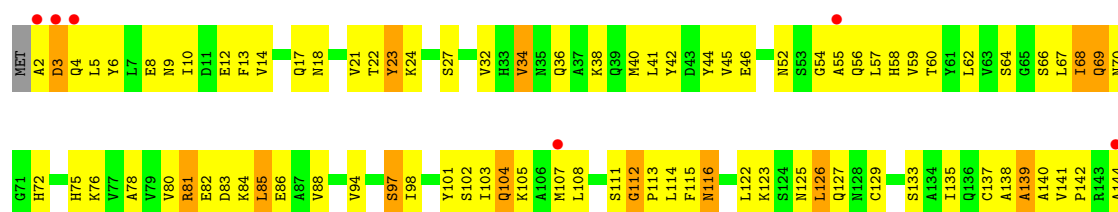
• Molecule 1: DNA polymerase subunit delta-2



• Molecule 2: DNA polymerase subunit delta-3



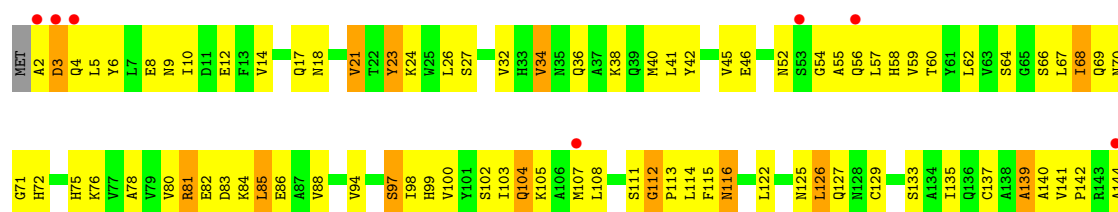
• Molecule 2: DNA polymerase subunit delta-3



• Molecule 2: DNA polymerase subunit delta-3



• Molecule 2: DNA polymerase subunit delta-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.13Å 248.53Å 103.46Å 90.00° 106.94° 90.00°	Depositor
Resolution (Å)	29.89 – 3.00 29.89 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.3 (29.89-3.00) 91.2 (29.89-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	123.02 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.281 0.256 , 0.278	Depositor DCC
R_{free} test set	4250 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17153	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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 ⓘ

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	0.70	1/3254 (0.0%)	1.18	32/4426 (0.7%)
1	C	0.70	0/3201	1.18	28/4354 (0.6%)
1	E	0.68	0/3193	1.17	31/4343 (0.7%)
1	G	0.67	0/3193	1.17	31/4343 (0.7%)
2	B	0.71	0/1150	1.01	4/1553 (0.3%)
2	D	0.69	0/1150	1.02	5/1553 (0.3%)
2	F	0.64	0/1150	1.00	6/1553 (0.4%)
2	H	0.59	0/1150	0.98	5/1553 (0.3%)
All	All	0.68	1/17441 (0.0%)	1.13	142/23678 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	VAL	CA-CB	-6.11	1.47	1.54

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ASP	N-CA-C	-9.82	98.89	112.25
1	E	306	LEU	CA-C-N	-9.74	107.67	119.84
1	E	306	LEU	C-N-CA	-9.74	107.67	119.84
1	G	306	LEU	CA-C-N	-9.55	107.91	119.84
1	G	306	LEU	C-N-CA	-9.55	107.91	119.84
1	C	306	LEU	CA-C-N	-9.20	108.34	119.84
1	C	306	LEU	C-N-CA	-9.20	108.34	119.84
1	A	18	SER	N-CA-C	-8.71	96.64	110.14
1	C	185	LYS	CA-C-N	8.59	128.61	119.76
1	C	185	LYS	C-N-CA	8.59	128.61	119.76
1	C	18	SER	N-CA-C	-8.22	97.41	110.14
1	A	306	LEU	CA-C-N	-7.99	109.86	119.84
1	A	306	LEU	C-N-CA	-7.99	109.86	119.84
1	G	18	SER	N-CA-C	-7.99	97.76	110.14
1	A	185	LYS	CA-C-N	7.70	127.69	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LYS	C-N-CA	7.70	127.69	119.76
1	G	185	LYS	CA-C-N	7.65	127.64	119.76
1	G	185	LYS	C-N-CA	7.65	127.64	119.76
1	E	18	SER	N-CA-C	-7.50	97.99	109.85
1	C	169	GLY	N-CA-C	-6.99	106.37	114.69
1	A	235	ALA	N-CA-C	-6.97	103.69	111.28
1	C	235	ALA	N-CA-C	-6.94	103.72	111.28
1	E	235	ALA	N-CA-C	-6.89	103.77	111.28
1	G	169	GLY	N-CA-C	-6.89	106.49	114.69
1	E	330	ASN	CA-C-N	-6.76	111.39	119.84
1	E	330	ASN	C-N-CA	-6.76	111.39	119.84
1	E	357	SER	N-CA-C	-6.71	105.25	113.50
1	E	306	LEU	N-CA-C	6.71	121.29	112.17
1	E	169	GLY	N-CA-C	-6.69	106.73	114.69
1	E	185	LYS	CA-C-N	6.68	126.64	119.76
1	E	185	LYS	C-N-CA	6.68	126.64	119.76
1	A	306	LEU	N-CA-C	6.62	121.18	112.17
1	A	461	ASP	N-CA-C	-6.58	103.35	112.30
1	C	306	LEU	N-CA-C	6.57	121.10	112.17
1	G	330	ASN	CA-C-N	-6.57	111.63	119.84
1	G	330	ASN	C-N-CA	-6.57	111.63	119.84
1	G	188	PRO	CA-C-N	6.55	126.31	119.76
1	G	188	PRO	C-N-CA	6.55	126.31	119.76
1	G	235	ALA	N-CA-C	-6.54	104.15	111.28
1	A	169	GLY	N-CA-C	-6.54	106.91	114.69
1	C	330	ASN	CA-C-N	-6.53	111.68	119.84
1	C	330	ASN	C-N-CA	-6.53	111.68	119.84
1	A	330	ASN	CA-C-N	-6.37	111.87	119.84
1	A	330	ASN	C-N-CA	-6.37	111.87	119.84
2	D	21	VAL	N-CA-C	6.33	116.50	106.88
1	E	309	GLN	CA-C-N	6.27	127.68	119.84
1	E	309	GLN	C-N-CA	6.27	127.68	119.84
1	A	247	LEU	N-CA-C	-6.08	106.02	113.50
1	G	166	ARG	N-CA-C	6.08	119.07	110.14
1	A	357	SER	N-CA-C	-6.05	106.06	113.50
1	G	137	ASP	N-CA-C	-6.05	101.24	110.14
1	A	137	ASP	N-CA-C	-6.04	101.27	110.14
1	G	357	SER	N-CA-C	-6.04	106.08	113.50
1	C	166	ARG	N-CA-C	6.02	118.99	110.14
1	E	137	ASP	N-CA-C	-5.97	101.37	110.14
1	C	34	ASN	N-CA-C	-5.95	101.47	110.28
1	G	400	HIS	N-CA-C	-5.91	105.73	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	306	LEU	N-CA-C	5.90	120.19	112.17
2	B	21	VAL	N-CA-C	5.89	115.83	106.88
1	C	188	PRO	CA-C-N	5.89	125.65	119.76
1	C	188	PRO	C-N-CA	5.89	125.65	119.76
1	C	137	ASP	N-CA-C	-5.88	101.50	110.14
2	F	73	SER	N-CA-C	5.88	118.03	108.63
1	A	188	PRO	CA-C-N	5.86	125.62	119.76
1	A	188	PRO	C-N-CA	5.86	125.62	119.76
1	E	166	ARG	N-CA-C	5.85	118.74	110.14
1	G	154	VAL	N-CA-C	5.84	116.77	108.42
1	E	450	ILE	N-CA-C	-5.82	99.73	108.12
1	E	300	ASP	N-CA-C	-5.81	102.09	110.40
2	D	139	ALA	N-CA-C	5.80	117.69	111.36
1	G	159	LEU	N-CA-C	5.78	118.28	109.95
1	E	34	ASN	N-CA-C	-5.75	101.77	110.28
1	A	450	ILE	N-CA-C	-5.75	99.85	108.12
2	H	21	VAL	N-CA-C	5.73	115.58	106.88
1	A	166	ARG	N-CA-C	5.68	118.50	110.14
1	E	400	HIS	N-CA-C	-5.66	106.05	113.12
1	A	400	HIS	N-CA-C	-5.65	106.05	113.12
1	E	159	LEU	N-CA-C	5.65	118.09	109.95
1	G	300	ASP	N-CA-C	-5.64	102.33	110.40
1	E	154	VAL	N-CA-C	5.64	116.48	108.42
1	G	24	PHE	N-CA-C	5.64	119.43	109.96
2	H	97	SER	N-CA-C	5.62	118.63	109.24
1	C	357	SER	N-CA-C	-5.61	106.59	113.50
1	G	9	ARG	N-CA-C	5.58	117.75	108.99
1	G	309	GLN	CA-C-N	5.56	126.79	119.84
1	G	309	GLN	C-N-CA	5.56	126.79	119.84
2	D	78	ALA	N-CA-C	5.55	117.83	109.23
1	A	309	GLN	CA-C-N	5.54	126.76	119.84
1	A	309	GLN	C-N-CA	5.54	126.76	119.84
1	A	144	LEU	N-CA-C	5.51	118.45	109.24
2	H	139	ALA	N-CA-C	5.51	117.37	111.36
2	F	139	ALA	N-CA-C	5.51	117.36	111.36
1	A	34	ASN	N-CA-C	-5.50	102.13	110.28
1	E	144	LEU	N-CA-C	5.50	118.42	109.24
1	E	1	MET	N-CA-C	-5.49	103.24	110.43
1	C	300	ASP	N-CA-C	-5.43	102.63	110.40
1	C	280	ASP	N-CA-C	-5.43	105.01	111.03
1	A	210	GLU	N-CA-C	-5.42	105.46	111.36
1	A	9	ARG	N-CA-C	5.38	117.44	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	VAL	N-CA-C	5.36	116.08	108.42
2	D	97	SER	N-CA-C	5.34	118.17	109.24
1	C	421	GLN	N-CA-C	-5.34	101.41	109.85
1	A	159	LEU	N-CA-C	5.34	117.64	109.95
1	G	378	ALA	CA-C-N	5.34	125.31	120.03
1	G	378	ALA	C-N-CA	5.34	125.31	120.03
1	E	24	PHE	N-CA-C	5.33	118.91	109.96
1	C	9	ARG	N-CA-C	5.33	117.35	108.99
1	A	455	PHE	N-CA-C	5.30	117.14	110.24
1	C	144	LEU	N-CA-C	5.29	118.08	109.24
2	B	73	SER	N-CA-C	5.29	116.92	108.41
1	C	378	ALA	CA-C-N	5.27	125.24	120.03
1	C	378	ALA	C-N-CA	5.27	125.24	120.03
1	A	300	ASP	N-CA-C	-5.23	102.56	110.50
2	B	78	ALA	N-CA-C	5.23	117.94	109.06
1	G	34	ASN	N-CA-C	-5.22	102.55	110.28
2	F	21	VAL	N-CA-C	5.22	115.28	107.51
1	E	78	GLY	N-CA-C	-5.22	107.44	115.73
2	H	137	CYS	N-CA-C	5.21	117.22	107.99
1	C	154	VAL	N-CA-C	5.20	115.86	108.42
1	E	378	ALA	CA-C-N	5.19	125.17	120.03
1	E	378	ALA	C-N-CA	5.19	125.17	120.03
1	A	440	VAL	CB-CA-C	-5.17	103.89	110.98
2	F	137	CYS	N-CA-C	5.17	117.13	107.99
2	D	101	TYR	N-CA-C	-5.16	106.12	112.72
2	F	78	ALA	N-CA-C	5.14	117.81	109.06
2	F	101	TYR	N-CA-C	-5.13	106.16	112.72
1	G	144	LEU	N-CA-C	5.13	117.81	109.24
1	G	280	ASP	N-CA-C	-5.13	105.60	111.14
1	E	9	ARG	N-CA-C	5.12	117.03	108.99
1	C	450	ILE	N-CA-C	-5.10	100.78	108.12
1	A	78	GLY	N-CA-C	-5.10	107.63	115.73
2	B	97	SER	N-CA-C	5.10	117.75	109.24
1	C	391	ASP	CA-C-N	5.08	124.58	119.19
1	C	391	ASP	C-N-CA	5.08	124.58	119.19
1	E	188	PRO	CA-C-N	5.08	124.83	119.76
1	E	188	PRO	C-N-CA	5.08	124.83	119.76
1	C	373	HIS	N-CA-C	5.07	115.82	107.20
2	H	78	ALA	N-CA-C	5.07	117.68	109.06
1	E	39	PHE	N-CA-C	-5.07	108.12	114.56
1	G	419	GLU	N-CA-C	-5.05	98.83	108.17
1	G	78	GLY	N-CA-C	-5.02	107.75	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	211	SER	N-CA-C	-5.00	105.96	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3185	0	3150	338	0
1	C	3133	0	3112	346	0
1	E	3125	0	3101	334	0
1	G	3125	0	3101	332	0
2	B	1131	0	1138	98	0
2	D	1131	0	1138	96	0
2	F	1131	0	1138	85	0
2	H	1131	0	1138	91	0
3	A	11	0	0	1	0
3	B	6	0	0	0	0
3	C	12	0	0	3	0
3	D	4	0	0	0	0
3	E	15	0	0	2	0
3	F	4	0	0	0	0
3	G	8	0	0	2	0
3	H	1	0	0	0	0
All	All	17153	0	17016	1619	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 47.

All (1619) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HG11	1:C:291:PRO:HG2	1.19	1.18
1:C:58:LEU:HD21	1:C:95:GLY:HA2	1.25	1.13
1:E:58:LEU:HD21	1:E:95:GLY:HA2	1.25	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD21	1:A:95:GLY:HA2	1.26	1.09
1:G:29:VAL:HG11	1:G:291:PRO:HG2	1.24	1.09
1:G:58:LEU:HD21	1:G:95:GLY:HA2	1.29	1.09
1:A:29:VAL:HG11	1:A:291:PRO:HG2	1.12	1.07
1:E:29:VAL:HG11	1:E:291:PRO:HG2	1.21	1.07
1:G:193:ASP:HB3	1:G:443:ARG:NH1	1.74	1.00
1:C:193:ASP:HB3	1:C:443:ARG:NH1	1.80	0.97
1:A:193:ASP:HB3	1:A:443:ARG:NH1	1.81	0.94
1:G:330:ASN:HB3	1:G:331:PRO:HD3	1.50	0.94
1:C:330:ASN:HB3	1:C:331:PRO:HD3	1.48	0.94
1:G:98:PHE:HB2	1:G:134:VAL:HG13	1.51	0.92
1:C:193:ASP:HB3	1:C:443:ARG:HH11	1.33	0.91
1:E:330:ASN:HB3	1:E:331:PRO:HD3	1.49	0.91
2:B:116:ASN:H	2:B:116:ASN:HD22	1.17	0.90
2:F:116:ASN:HD22	2:F:116:ASN:H	1.20	0.90
1:E:193:ASP:HB3	1:E:443:ARG:NH1	1.86	0.89
1:A:330:ASN:HB3	1:A:331:PRO:HD3	1.55	0.89
1:E:99:LYS:H	1:E:155:THR:HG23	1.38	0.89
1:A:340:ARG:HH12	1:A:397:GLU:HB3	1.38	0.89
1:G:99:LYS:H	1:G:155:THR:HG23	1.39	0.88
1:A:193:ASP:HB3	1:A:443:ARG:HH11	1.34	0.88
1:A:98:PHE:HB2	1:A:134:VAL:HG13	1.53	0.88
1:A:407:THR:HG22	1:A:409:SER:H	1.37	0.87
1:C:99:LYS:H	1:C:155:THR:HG23	1.40	0.87
1:C:340:ARG:HH12	1:C:397:GLU:HB3	1.39	0.87
1:C:98:PHE:HB2	1:C:134:VAL:HG13	1.56	0.87
2:H:116:ASN:HD22	2:H:116:ASN:H	1.22	0.87
1:G:193:ASP:HB3	1:G:443:ARG:HH11	1.31	0.86
1:C:407:THR:HG22	1:C:409:SER:H	1.39	0.86
1:E:98:PHE:HB2	1:E:134:VAL:HG13	1.57	0.86
1:E:182:ALA:HB1	1:E:183:PRO:HD2	1.58	0.86
1:A:290:VAL:HG22	1:A:291:PRO:HD2	1.57	0.86
1:A:99:LYS:H	1:A:155:THR:HG23	1.39	0.86
1:A:29:VAL:CG1	1:A:291:PRO:HG2	2.03	0.85
1:G:340:ARG:HH12	1:G:397:GLU:HB3	1.39	0.85
1:A:182:ALA:HB1	1:A:183:PRO:HD2	1.58	0.85
1:C:193:ASP:CB	1:C:441:ASN:HD21	1.90	0.85
1:G:407:THR:HG22	1:G:409:SER:H	1.42	0.84
1:C:182:ALA:HB1	1:C:183:PRO:HD2	1.56	0.84
2:D:116:ASN:H	2:D:116:ASN:HD22	1.20	0.84
1:G:39:PHE:CE2	1:G:331:PRO:HB2	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ARG:HH12	1:E:397:GLU:HB3	1.40	0.83
1:C:323:SER:HA	2:D:144:ALA:HB3	1.61	0.83
1:G:182:ALA:HB1	1:G:183:PRO:HD2	1.58	0.83
2:B:116:ASN:HD22	2:B:116:ASN:N	1.72	0.83
1:E:82:LEU:HD11	1:E:142:ILE:CG2	2.09	0.83
1:E:406:ASN:N	1:E:406:ASN:HD22	1.76	0.83
2:F:116:ASN:HD22	2:F:116:ASN:N	1.75	0.82
1:A:323:SER:HA	2:B:144:ALA:HB3	1.59	0.82
1:E:407:THR:HG22	1:E:409:SER:H	1.44	0.82
1:C:61:MET:HE3	1:C:158:VAL:HB	1.59	0.82
1:G:145:LYS:HE3	1:G:170:LYS:HB2	1.61	0.82
1:E:39:PHE:CE2	1:E:331:PRO:HB2	2.15	0.82
1:A:226:LEU:HD12	1:A:226:LEU:C	2.04	0.81
1:E:61:MET:HE3	1:E:158:VAL:HB	1.60	0.81
1:E:193:ASP:CB	1:E:441:ASN:HD21	1.93	0.81
2:D:116:ASN:HD22	2:D:116:ASN:N	1.74	0.81
1:E:145:LYS:HE3	1:E:170:LYS:HB2	1.63	0.81
1:G:82:LEU:HD21	1:G:142:ILE:H	1.47	0.80
1:G:82:LEU:HD11	1:G:142:ILE:CG2	2.11	0.80
1:A:56:THR:HA	1:A:59:ILE:HD12	1.64	0.80
1:C:82:LEU:HD11	1:C:142:ILE:CG2	2.11	0.80
1:C:406:ASN:N	1:C:406:ASN:HD22	1.80	0.80
1:G:323:SER:HA	2:H:144:ALA:HB3	1.62	0.80
1:G:406:ASN:N	1:G:406:ASN:HD22	1.79	0.80
1:G:308:GLN:HB2	1:G:330:ASN:HB2	1.64	0.79
1:A:82:LEU:HD11	1:A:142:ILE:CG2	2.11	0.79
1:G:62:ARG:HB3	1:G:63:PRO:HD3	1.64	0.79
1:E:193:ASP:HB3	1:E:443:ARG:HH11	1.41	0.79
1:A:148:ILE:HG13	1:A:176:TYR:CE2	2.17	0.79
1:A:193:ASP:CB	1:A:441:ASN:HD21	1.95	0.79
1:A:308:GLN:HB2	1:A:330:ASN:HB2	1.62	0.79
1:E:193:ASP:O	1:E:194:ARG:HD3	1.81	0.79
1:A:62:ARG:HB3	1:A:63:PRO:HD3	1.64	0.79
1:C:308:GLN:HB2	1:C:330:ASN:HB2	1.63	0.79
1:E:151:SER:HB2	1:E:357:SER:HB2	1.65	0.79
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.65	0.79
1:A:419:GLU:O	1:A:421:GLN:HG3	1.83	0.79
1:G:56:THR:HA	1:G:59:ILE:HD12	1.64	0.79
2:B:116:ASN:H	2:B:116:ASN:ND2	1.82	0.78
1:C:145:LYS:HE3	1:C:170:LYS:HB2	1.64	0.78
1:C:330:ASN:HB3	1:C:331:PRO:CD	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:LEU:CD1	1:E:450:ILE:HD11	2.14	0.78
1:G:37:GLN:HE21	1:G:38:PRO:HD2	1.48	0.78
1:A:193:ASP:O	1:A:194:ARG:HD3	1.84	0.78
1:C:193:ASP:HB3	1:C:441:ASN:HD21	1.47	0.78
1:C:439:LEU:CD1	1:C:450:ILE:HD11	2.13	0.78
1:A:193:ASP:HB3	1:A:441:ASN:HD21	1.48	0.78
1:G:193:ASP:CB	1:G:441:ASN:HD21	1.95	0.78
2:H:116:ASN:HD22	2:H:116:ASN:N	1.78	0.78
1:A:54:TYR:HA	1:A:380:ASP:OD1	1.83	0.78
1:A:226:LEU:HD22	2:B:62:LEU:HD11	1.64	0.78
1:E:29:VAL:CG1	1:E:291:PRO:HG2	2.11	0.78
1:E:323:SER:HA	2:F:144:ALA:HB3	1.64	0.78
1:C:56:THR:HA	1:C:59:ILE:HD12	1.66	0.78
1:A:39:PHE:CE2	1:A:331:PRO:HB2	2.18	0.77
1:A:330:ASN:O	1:A:331:PRO:C	2.26	0.77
1:E:306:LEU:HB3	1:E:307:PRO:HD3	1.66	0.77
1:G:330:ASN:HB3	1:G:331:PRO:CD	2.14	0.77
1:G:54:TYR:HA	1:G:380:ASP:OD1	1.85	0.77
1:E:159:LEU:HD23	1:E:159:LEU:H	1.49	0.77
1:A:61:MET:HE3	1:A:158:VAL:HB	1.66	0.77
1:A:406:ASN:N	1:A:406:ASN:HD22	1.82	0.77
1:C:62:ARG:HB3	1:C:63:PRO:HD3	1.65	0.77
1:C:217:LEU:O	1:C:221:VAL:HG23	1.84	0.77
1:G:226:LEU:C	1:G:226:LEU:HD12	2.10	0.77
1:A:145:LYS:HE3	1:A:170:LYS:HB2	1.67	0.77
1:E:193:ASP:HB3	1:E:441:ASN:HD21	1.48	0.77
1:C:82:LEU:HD21	1:C:142:ILE:H	1.47	0.76
1:C:148:ILE:HG13	1:C:176:TYR:CE2	2.20	0.76
1:G:439:LEU:CD1	1:G:450:ILE:HD11	2.15	0.76
1:A:303:ASN:HD22	1:A:305:THR:CG2	1.97	0.76
1:C:29:VAL:CG1	1:C:291:PRO:HG2	2.09	0.76
1:E:82:LEU:HD21	1:E:142:ILE:H	1.51	0.76
1:E:308:GLN:HB2	1:E:330:ASN:HB2	1.67	0.76
1:G:148:ILE:HG13	1:G:176:TYR:CE2	2.19	0.76
1:E:226:LEU:HD22	2:F:62:LEU:HD11	1.66	0.76
1:E:330:ASN:HB3	1:E:331:PRO:CD	2.14	0.76
1:G:290:VAL:HG22	1:G:291:PRO:HD2	1.67	0.76
1:C:290:VAL:HG22	1:C:291:PRO:HD2	1.67	0.76
1:G:306:LEU:HB3	1:G:307:PRO:HD3	1.68	0.76
1:C:419:GLU:O	1:C:421:GLN:HG3	1.85	0.75
2:F:116:ASN:H	2:F:116:ASN:ND2	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:GLN:HG2	2:F:40:MET:HE3	1.67	0.75
1:G:419:GLU:O	1:G:421:GLN:HG3	1.86	0.75
1:E:148:ILE:HG13	1:E:176:TYR:CE2	2.22	0.75
1:C:39:PHE:CE2	1:C:331:PRO:HB2	2.20	0.75
2:D:116:ASN:H	2:D:116:ASN:ND2	1.85	0.75
1:E:56:THR:HA	1:E:59:ILE:HD12	1.67	0.75
1:G:95:GLY:HA3	1:G:135:LEU:HD11	1.68	0.75
1:A:37:GLN:HE21	1:A:38:PRO:HD2	1.52	0.75
1:C:193:ASP:O	1:C:194:ARG:HD3	1.87	0.75
2:D:36:GLN:HG2	2:D:40:MET:HE3	1.67	0.75
1:A:82:LEU:HD21	1:A:142:ILE:H	1.50	0.75
1:E:37:GLN:HE21	1:E:38:PRO:HD2	1.52	0.75
1:G:217:LEU:O	1:G:221:VAL:HG23	1.87	0.75
1:E:226:LEU:C	1:E:226:LEU:HD12	2.12	0.74
1:E:419:GLU:O	1:E:421:GLN:HG3	1.85	0.74
1:G:303:ASN:HD22	1:G:305:THR:CG2	1.99	0.74
1:E:290:VAL:HG22	1:E:291:PRO:HD2	1.66	0.74
1:A:151:SER:HB2	1:A:357:SER:HB2	1.69	0.74
1:C:303:ASN:HD22	1:C:305:THR:CG2	2.00	0.74
2:B:66:SER:HB3	2:B:94:VAL:HG12	1.70	0.74
1:A:82:LEU:HD11	1:A:142:ILE:HG21	1.70	0.74
1:A:330:ASN:HB3	1:A:331:PRO:CD	2.18	0.74
1:C:226:LEU:HD22	2:D:62:LEU:HD11	1.70	0.74
1:G:61:MET:HE3	1:G:158:VAL:HB	1.68	0.74
1:G:193:ASP:O	1:G:194:ARG:HD3	1.86	0.74
1:E:82:LEU:HD11	1:E:142:ILE:HG21	1.68	0.73
1:G:330:ASN:O	1:G:331:PRO:C	2.28	0.73
1:C:37:GLN:HE21	1:C:38:PRO:HD2	1.52	0.73
1:C:82:LEU:HD11	1:C:142:ILE:HG21	1.70	0.73
1:C:226:LEU:HD12	1:C:226:LEU:C	2.14	0.73
1:C:333:GLN:HG2	1:C:342:LEU:HD13	1.71	0.73
1:A:29:VAL:HG11	1:A:291:PRO:CG	2.07	0.73
1:E:95:GLY:HA3	1:E:135:LEU:HD11	1.71	0.73
2:F:85:LEU:HD12	2:F:85:LEU:O	1.88	0.73
1:G:333:GLN:HG2	1:G:342:LEU:HD13	1.70	0.73
1:A:95:GLY:HA3	1:A:135:LEU:HD11	1.69	0.72
1:E:62:ARG:HB3	1:E:63:PRO:HD3	1.70	0.72
1:A:142:ILE:HD13	1:A:171:PHE:HB2	1.69	0.72
1:G:151:SER:HB2	1:G:357:SER:HB2	1.71	0.72
1:G:184:GLN:HB2	1:G:398:CYS:HB3	1.69	0.72
1:A:77:VAL:HG13	1:A:79:VAL:HG23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:SER:HB2	1:C:357:SER:HB2	1.71	0.72
1:G:365:LEU:HD13	1:G:404:CYS:HB2	1.71	0.72
1:G:82:LEU:HD11	1:G:142:ILE:HG21	1.70	0.72
1:G:221:VAL:HG22	1:G:226:LEU:HD11	1.72	0.72
1:A:439:LEU:CD1	1:A:450:ILE:HD11	2.20	0.72
1:C:54:TYR:HA	1:C:380:ASP:OD1	1.90	0.72
1:C:159:LEU:H	1:C:159:LEU:HD23	1.54	0.71
1:A:418:PRO:HB2	1:A:419:GLU:OE1	1.88	0.71
1:G:142:ILE:HD13	1:G:171:PHE:HB2	1.70	0.71
2:H:116:ASN:H	2:H:116:ASN:ND2	1.87	0.71
1:A:407:THR:HG23	1:A:408:PRO:HD2	1.71	0.71
1:E:330:ASN:O	1:E:331:PRO:C	2.28	0.71
1:G:193:ASP:HB3	1:G:441:ASN:HD21	1.54	0.71
1:A:333:GLN:HG2	1:A:342:LEU:HD13	1.72	0.71
1:E:221:VAL:HG22	1:E:226:LEU:HD11	1.72	0.71
1:E:303:ASN:HD22	1:E:305:THR:CG2	2.03	0.71
1:C:95:GLY:HA3	1:C:135:LEU:HD11	1.70	0.71
1:C:142:ILE:HD13	1:C:171:PHE:HB2	1.71	0.71
1:C:330:ASN:O	1:C:331:PRO:C	2.30	0.71
1:C:365:LEU:HD13	1:C:404:CYS:HB2	1.73	0.71
1:A:315:MET:O	1:A:317:PRO:HD3	1.92	0.70
1:A:217:LEU:O	1:A:221:VAL:HG23	1.91	0.70
2:B:85:LEU:HD12	2:B:85:LEU:O	1.90	0.70
2:D:70:ASN:H	2:D:72:HIS:CD2	2.08	0.70
1:G:75:SER:O	1:G:77:VAL:N	2.23	0.70
1:G:226:LEU:HD22	2:H:62:LEU:HD11	1.71	0.70
1:C:75:SER:O	1:C:77:VAL:N	2.24	0.70
1:A:159:LEU:H	1:A:159:LEU:HD23	1.57	0.70
1:C:315:MET:O	1:C:317:PRO:HD3	1.92	0.70
1:A:86:GLN:HE21	1:A:86:GLN:HA	1.57	0.69
3:C:471:HOH:O	1:E:21:ASN:HB2	1.92	0.69
1:G:29:VAL:CG1	1:G:291:PRO:HG2	2.14	0.69
1:E:54:TYR:HA	1:E:380:ASP:OD1	1.91	0.69
1:E:418:PRO:HB2	1:E:419:GLU:OE1	1.92	0.69
1:A:303:ASN:HA	1:C:303:ASN:HA	1.74	0.69
1:C:329:THR:HG23	3:C:476:HOH:O	1.91	0.69
1:A:80:LYS:HD2	1:A:84:GLU:HB2	1.74	0.69
1:A:82:LEU:O	1:A:85:LEU:HD22	1.92	0.69
2:B:36:GLN:HG2	2:B:40:MET:HE3	1.73	0.69
1:G:333:GLN:CG	1:G:342:LEU:HD13	2.22	0.69
1:G:406:ASN:HD22	1:G:406:ASN:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:GLU:O	1:C:285:GLN:HG3	1.91	0.69
1:E:75:SER:O	1:E:77:VAL:N	2.26	0.69
1:E:142:ILE:HD13	1:E:171:PHE:HB2	1.73	0.69
1:G:82:LEU:O	1:G:85:LEU:HD22	1.91	0.69
1:A:75:SER:O	1:A:77:VAL:N	2.25	0.69
1:E:27:VAL:CG1	1:E:237:HIS:HA	2.22	0.69
2:H:36:GLN:HG2	2:H:40:MET:HE3	1.73	0.69
1:G:39:PHE:CD2	1:G:331:PRO:HB2	2.27	0.69
1:G:340:ARG:NH1	1:G:397:GLU:HB3	2.08	0.69
1:A:58:LEU:HD21	1:A:95:GLY:CA	2.17	0.68
2:F:139:ALA:O	2:F:141:VAL:N	2.24	0.68
1:G:277:LYS:HE2	1:G:281:GLU:OE2	1.94	0.68
2:D:85:LEU:HD12	2:D:85:LEU:O	1.93	0.68
1:A:303:ASN:HD22	1:A:305:THR:HG23	1.59	0.68
1:A:65:LEU:HD21	1:A:158:VAL:O	1.94	0.68
1:E:37:GLN:HE21	1:E:38:PRO:CD	2.06	0.68
1:A:365:LEU:HD13	1:A:404:CYS:HB2	1.75	0.68
1:G:159:LEU:HD23	1:G:159:LEU:H	1.58	0.68
2:H:85:LEU:O	2:H:85:LEU:HD12	1.93	0.68
1:E:151:SER:HB2	1:E:357:SER:CB	2.24	0.68
1:C:306:LEU:HB3	1:C:307:PRO:HD3	1.76	0.68
1:E:82:LEU:O	1:E:85:LEU:HD22	1.93	0.68
1:A:77:VAL:HG13	1:A:79:VAL:CG2	2.24	0.67
1:A:340:ARG:NH1	1:A:397:GLU:HB3	2.09	0.67
1:C:133:LEU:O	1:C:144:LEU:HD12	1.94	0.67
1:C:340:ARG:NH1	1:C:397:GLU:HB3	2.07	0.67
1:A:37:GLN:HE21	1:A:38:PRO:CD	2.07	0.67
1:G:82:LEU:HD21	1:G:142:ILE:N	2.09	0.67
1:E:184:GLN:HB2	1:E:398:CYS:HB3	1.75	0.67
1:E:419:GLU:CD	1:E:419:GLU:H	2.01	0.67
1:C:453:SER:HA	3:C:473:HOH:O	1.93	0.67
1:G:315:MET:O	1:G:317:PRO:HD3	1.93	0.67
1:A:80:LYS:CD	1:A:84:GLU:HB2	2.24	0.67
2:B:57:LEU:HD11	2:B:103:ILE:HG23	1.77	0.67
1:E:148:ILE:HA	1:E:176:TYR:HE2	1.59	0.67
1:C:82:LEU:O	1:C:85:LEU:HD22	1.95	0.67
1:C:181:LEU:HD12	1:C:417:GLY:HA3	1.76	0.67
1:E:77:VAL:HG13	1:E:79:VAL:HG23	1.76	0.67
1:G:97:LEU:HG	1:G:159:LEU:HD21	1.77	0.67
2:B:68:ILE:HD12	2:B:68:ILE:N	2.10	0.67
2:F:68:ILE:N	2:F:68:ILE:HD12	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:PRO:HB2	1:C:419:GLU:OE1	1.94	0.66
1:G:80:LYS:HD2	1:G:84:GLU:HB2	1.78	0.66
1:G:86:GLN:HE21	1:G:86:GLN:HA	1.59	0.66
1:A:419:GLU:CD	1:A:419:GLU:H	2.03	0.66
1:C:86:GLN:HA	1:C:86:GLN:HE21	1.60	0.66
1:E:277:LYS:HE2	1:E:281:GLU:OE2	1.93	0.66
1:E:406:ASN:HD22	1:E:406:ASN:H	1.42	0.66
1:G:37:GLN:HE21	1:G:38:PRO:CD	2.09	0.66
1:G:77:VAL:HG13	1:G:79:VAL:HG23	1.76	0.66
1:C:303:ASN:HD22	1:C:305:THR:HG23	1.60	0.66
1:E:365:LEU:HD13	1:E:404:CYS:HB2	1.76	0.66
1:A:27:VAL:CG1	1:A:237:HIS:HA	2.25	0.66
1:E:39:PHE:CD2	1:E:331:PRO:HB2	2.30	0.66
1:G:330:ASN:O	1:G:332:TYR:N	2.29	0.66
1:G:418:PRO:HB2	1:G:419:GLU:OE1	1.95	0.66
1:G:430:ASP:O	1:G:434:THR:HG23	1.95	0.66
1:A:221:VAL:HG22	1:A:226:LEU:HD11	1.77	0.66
2:D:139:ALA:O	2:D:141:VAL:N	2.25	0.66
1:G:417:GLY:HA3	1:G:421:GLN:OE1	1.96	0.66
1:A:82:LEU:HD21	1:A:142:ILE:N	2.10	0.66
1:C:82:LEU:HD21	1:C:142:ILE:N	2.10	0.66
1:E:226:LEU:HD22	2:F:62:LEU:CD1	2.26	0.66
1:A:97:LEU:HG	1:A:159:LEU:HD21	1.77	0.66
1:E:410:PHE:HE1	1:E:438:CYS:HB2	1.61	0.66
2:F:57:LEU:HD11	2:F:103:ILE:HG23	1.76	0.66
1:G:319:ALA:HB1	1:G:325:LEU:HD22	1.77	0.66
1:A:410:PHE:HE1	1:A:438:CYS:HB2	1.61	0.65
1:C:184:GLN:HB2	1:C:398:CYS:HB3	1.77	0.65
1:E:417:GLY:HA3	1:E:421:GLN:OE1	1.96	0.65
1:E:430:ASP:O	1:E:434:THR:HG23	1.96	0.65
1:A:330:ASN:O	1:A:332:TYR:N	2.30	0.65
1:G:65:LEU:HD21	1:G:158:VAL:O	1.96	0.65
1:G:303:ASN:HD22	1:G:305:THR:HG23	1.60	0.65
1:A:417:GLY:HA3	1:A:421:GLN:OE1	1.97	0.65
1:C:37:GLN:HE21	1:C:38:PRO:CD	2.08	0.65
2:D:69:GLN:HB2	2:D:72:HIS:CD2	2.31	0.65
1:A:27:VAL:HG13	1:A:237:HIS:HA	1.78	0.65
1:C:142:ILE:CD1	1:C:171:PHE:HB2	2.26	0.65
1:C:151:SER:HB2	1:C:357:SER:CB	2.27	0.65
1:G:37:GLN:O	1:G:39:PHE:N	2.28	0.65
1:G:133:LEU:O	1:G:144:LEU:HD12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:THR:HG23	1:G:408:PRO:HD2	1.77	0.65
2:H:125:ASN:O	2:H:127:GLN:N	2.29	0.65
1:C:37:GLN:H	1:C:37:GLN:NE2	1.95	0.65
1:C:80:LYS:HD2	1:C:84:GLU:HB2	1.79	0.65
1:C:126:TYR:HD2	1:C:355:TYR:HE1	1.44	0.65
1:G:37:GLN:C	1:G:39:PHE:H	2.05	0.65
1:A:142:ILE:CD1	1:A:171:PHE:HB2	2.27	0.65
1:A:151:SER:HB2	1:A:357:SER:CB	2.27	0.65
2:D:70:ASN:C	2:D:72:HIS:H	2.05	0.64
1:E:306:LEU:O	1:E:308:GLN:N	2.30	0.64
1:G:181:LEU:HD12	1:G:417:GLY:HA3	1.79	0.64
1:G:439:LEU:HG	1:G:450:ILE:HD11	1.79	0.64
2:F:70:ASN:C	2:F:72:HIS:H	2.04	0.64
2:B:67:LEU:HD23	2:B:76:LYS:HE3	1.80	0.64
1:G:145:LYS:CE	1:G:170:LYS:HB2	2.28	0.64
1:G:209:GLY:O	1:G:212:LEU:HB2	1.97	0.64
2:H:57:LEU:HD11	2:H:103:ILE:HG23	1.77	0.64
1:A:439:LEU:HG	1:A:450:ILE:HD11	1.79	0.64
1:C:65:LEU:HD21	1:C:158:VAL:O	1.98	0.64
1:C:410:PHE:HE1	1:C:438:CYS:HB2	1.63	0.64
1:E:54:TYR:N	3:E:477:HOH:O	2.31	0.64
1:E:330:ASN:O	1:E:332:TYR:N	2.29	0.64
2:H:66:SER:HB3	2:H:94:VAL:HG12	1.78	0.64
2:H:68:ILE:N	2:H:68:ILE:HD12	2.13	0.64
1:C:97:LEU:HG	1:C:159:LEU:HD21	1.79	0.64
1:C:277:LYS:HE2	1:C:281:GLU:OE2	1.98	0.64
1:C:406:ASN:HD22	1:C:406:ASN:H	1.45	0.64
1:E:154:VAL:HG11	1:E:355:TYR:HB2	1.80	0.64
1:G:410:PHE:HE1	1:G:438:CYS:HB2	1.61	0.64
1:G:419:GLU:CD	1:G:419:GLU:H	2.06	0.64
1:A:184:GLN:HB2	1:A:398:CYS:HB3	1.78	0.64
1:A:406:ASN:HD22	1:A:406:ASN:H	1.45	0.64
1:E:37:GLN:O	1:E:39:PHE:N	2.31	0.64
1:G:37:GLN:NE2	1:G:37:GLN:H	1.95	0.64
1:A:277:LYS:HE2	1:A:281:GLU:OE2	1.98	0.64
1:C:77:VAL:HG13	1:C:79:VAL:HG23	1.80	0.64
1:C:80:LYS:CD	1:C:84:GLU:HB2	2.28	0.64
1:G:77:VAL:HG13	1:G:79:VAL:CG2	2.28	0.64
1:G:269:GLN:O	1:G:273:VAL:HG23	1.98	0.64
1:A:37:GLN:C	1:A:39:PHE:H	2.06	0.64
1:E:77:VAL:HG13	1:E:79:VAL:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:LYS:HD2	1:E:84:GLU:HB2	1.80	0.64
1:E:86:GLN:HE21	1:E:86:GLN:HA	1.62	0.64
1:C:333:GLN:CG	1:C:342:LEU:HD13	2.27	0.63
2:D:57:LEU:HD11	2:D:103:ILE:HG23	1.80	0.63
1:G:27:VAL:HG13	1:G:237:HIS:HA	1.81	0.63
1:G:151:SER:HB2	1:G:357:SER:CB	2.28	0.63
1:E:55:ALA:O	1:E:59:ILE:HG13	1.98	0.63
1:A:37:GLN:O	1:A:39:PHE:N	2.30	0.63
2:B:12:GLU:O	2:B:17:GLN:HG3	1.98	0.63
1:C:193:ASP:HB2	1:C:441:ASN:HD21	1.63	0.63
1:G:27:VAL:CG1	1:G:237:HIS:HA	2.28	0.63
1:G:142:ILE:CD1	1:G:171:PHE:HB2	2.28	0.63
1:A:226:LEU:C	1:A:226:LEU:CD1	2.70	0.63
1:A:269:GLN:O	1:A:273:VAL:HG23	1.98	0.63
1:E:82:LEU:HD21	1:E:142:ILE:N	2.12	0.63
1:A:407:THR:CG2	1:A:408:PRO:HD2	2.28	0.63
1:C:439:LEU:HG	1:C:450:ILE:HD11	1.80	0.63
2:D:69:GLN:HB2	2:D:72:HIS:NE2	2.13	0.63
1:E:303:ASN:HD22	1:E:305:THR:HG23	1.61	0.63
1:C:209:GLY:O	1:C:212:LEU:HB2	1.99	0.63
1:C:231:GLU:HG3	2:D:97:SER:OG	1.98	0.63
1:A:319:ALA:HB1	1:A:325:LEU:HD22	1.80	0.63
1:C:27:VAL:CG1	1:C:237:HIS:HA	2.28	0.63
2:B:70:ASN:H	2:B:72:HIS:CD2	2.16	0.63
1:C:430:ASP:O	1:C:434:THR:HG23	1.99	0.63
1:E:333:GLN:HG2	1:E:342:LEU:HD13	1.81	0.63
2:H:139:ALA:O	2:H:141:VAL:N	2.30	0.63
1:A:181:LEU:HD12	1:A:417:GLY:HA3	1.80	0.62
1:A:290:VAL:HG22	1:A:291:PRO:CD	2.27	0.62
1:A:333:GLN:CG	1:A:342:LEU:HD13	2.28	0.62
1:A:343:GLY:HA3	1:A:403:PHE:CE1	2.34	0.62
1:C:19:ALA:HB1	1:E:193:ASP:H	1.61	0.62
1:C:419:GLU:CD	1:C:419:GLU:H	2.07	0.62
1:E:319:ALA:HB1	1:E:325:LEU:HD22	1.80	0.62
2:B:139:ALA:O	2:B:141:VAL:N	2.27	0.62
1:C:226:LEU:HD22	2:D:62:LEU:CD1	2.28	0.62
1:C:330:ASN:O	1:C:332:TYR:N	2.31	0.62
1:G:80:LYS:CD	1:G:84:GLU:HB2	2.29	0.62
1:G:148:ILE:HA	1:G:176:TYR:HE2	1.63	0.62
1:G:281:GLU:O	1:G:285:GLN:HG3	1.99	0.62
1:C:193:ASP:HB2	1:C:441:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ILE:HD12	2:D:68:ILE:N	2.14	0.62
1:E:75:SER:O	1:E:77:VAL:HG23	2.00	0.62
1:E:27:VAL:HG13	1:E:237:HIS:HA	1.82	0.62
1:E:209:GLY:O	1:E:212:LEU:HB2	2.00	0.62
1:E:407:THR:HG23	1:E:408:PRO:HD2	1.80	0.62
1:G:126:TYR:HD2	1:G:355:TYR:HE1	1.47	0.62
1:E:37:GLN:NE2	1:E:38:PRO:HD2	2.15	0.62
1:C:407:THR:OG1	1:C:427:THR:HB	1.99	0.62
1:C:26:ARG:HG3	1:C:27:VAL:N	2.15	0.62
1:E:333:GLN:CG	1:E:342:LEU:HD13	2.30	0.62
2:F:66:SER:HB3	2:F:94:VAL:HG12	1.81	0.62
1:C:148:ILE:HA	1:C:176:TYR:HE2	1.65	0.62
1:G:243:LEU:N	1:G:243:LEU:HD23	2.14	0.62
1:E:37:GLN:C	1:E:39:PHE:H	2.09	0.61
2:H:70:ASN:C	2:H:72:HIS:H	2.09	0.61
1:A:55:ALA:O	1:A:59:ILE:HG13	2.00	0.61
1:C:65:LEU:CD2	1:C:158:VAL:HG12	2.30	0.61
1:E:281:GLU:O	1:E:285:GLN:HG3	2.00	0.61
1:G:13:LEU:HD13	2:H:38:LYS:HD2	1.82	0.61
1:A:281:GLU:O	1:A:285:GLN:HG3	2.00	0.61
1:C:417:GLY:HA3	1:C:421:GLN:OE1	1.99	0.61
1:A:37:GLN:H	1:A:37:GLN:NE2	1.99	0.61
1:C:27:VAL:HG13	1:C:237:HIS:HA	1.81	0.61
1:C:132:GLU:OE2	1:C:143:LYS:HE2	2.00	0.61
1:E:65:LEU:HD21	1:E:158:VAL:O	2.00	0.61
1:E:133:LEU:O	1:E:144:LEU:HD12	2.00	0.61
1:E:340:ARG:NH1	1:E:397:GLU:HB3	2.11	0.61
1:G:65:LEU:CD2	1:G:158:VAL:HG12	2.31	0.61
1:G:226:LEU:HB2	2:H:62:LEU:CD1	2.30	0.61
1:G:343:GLY:HA3	1:G:403:PHE:CE1	2.36	0.61
1:C:55:ALA:O	1:C:59:ILE:HG13	2.01	0.61
1:G:65:LEU:HD23	1:G:159:LEU:O	1.99	0.61
1:A:226:LEU:HD22	2:B:62:LEU:CD1	2.29	0.61
1:C:193:ASP:H	1:E:19:ALA:HB1	1.65	0.61
1:C:319:ALA:HB1	1:C:325:LEU:HD22	1.83	0.61
1:G:439:LEU:CG	1:G:450:ILE:HD11	2.31	0.61
1:C:439:LEU:CG	1:C:450:ILE:HD11	2.30	0.61
1:G:37:GLN:NE2	1:G:38:PRO:HD2	2.16	0.61
1:G:55:ALA:O	1:G:59:ILE:HG13	2.01	0.61
2:D:125:ASN:O	2:D:127:GLN:N	2.33	0.61
1:G:133:LEU:HD21	1:G:150:VAL:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:SER:O	2:B:114:LEU:HB2	2.00	0.61
1:G:290:VAL:HG22	1:G:291:PRO:CD	2.31	0.61
1:C:37:GLN:C	1:C:39:PHE:H	2.09	0.60
1:C:39:PHE:CD2	1:C:331:PRO:HB2	2.36	0.60
1:C:97:LEU:HD22	1:C:133:LEU:HB3	1.83	0.60
1:C:221:VAL:HG22	1:C:226:LEU:HD11	1.83	0.60
1:G:154:VAL:HG11	1:G:355:TYR:HB2	1.83	0.60
1:A:209:GLY:O	1:A:212:LEU:HB2	2.00	0.60
1:E:145:LYS:CE	1:E:170:LYS:HB2	2.31	0.60
1:G:406:ASN:N	1:G:406:ASN:ND2	2.50	0.60
2:H:67:LEU:HD23	2:H:76:LYS:HE3	1.82	0.60
1:A:290:VAL:CG2	1:A:291:PRO:HD2	2.31	0.60
1:A:39:PHE:CD2	1:A:331:PRO:HB2	2.37	0.60
1:E:97:LEU:HG	1:E:159:LEU:HD21	1.83	0.60
1:G:193:ASP:HB2	1:G:441:ASN:ND2	2.17	0.60
1:C:58:LEU:HD21	1:C:95:GLY:CA	2.17	0.60
1:E:315:MET:O	1:E:317:PRO:HD3	2.02	0.60
1:E:343:GLY:HA3	1:E:403:PHE:CE1	2.36	0.60
1:E:142:ILE:CD1	1:E:171:PHE:HB2	2.32	0.60
1:E:419:GLU:CD	1:E:419:GLU:N	2.59	0.60
1:A:126:TYR:HD2	1:A:355:TYR:HE1	1.49	0.60
1:A:148:ILE:HA	1:A:176:TYR:HE2	1.66	0.60
1:E:68:ARG:HG3	1:E:179:ALA:HA	1.84	0.60
1:G:193:ASP:HB2	1:G:441:ASN:HD21	1.66	0.60
1:A:193:ASP:C	1:A:194:ARG:HD3	2.26	0.60
2:D:66:SER:HB3	2:D:94:VAL:HG12	1.83	0.60
1:A:-1:HIS:ND1	1:A:0:GLY:N	2.50	0.60
1:E:58:LEU:HD21	1:E:95:GLY:CA	2.17	0.60
1:G:226:LEU:HD22	2:H:62:LEU:CD1	2.32	0.60
1:G:306:LEU:O	1:G:308:GLN:N	2.35	0.60
1:C:286:LEU:HB3	1:C:292:VAL:HG21	1.84	0.60
1:E:65:LEU:HD23	1:E:159:LEU:O	2.02	0.60
1:A:5:GLN:O	1:A:8:GLN:HB2	2.02	0.59
1:G:226:LEU:C	1:G:226:LEU:CD1	2.76	0.59
1:G:439:LEU:HG	1:G:450:ILE:CD1	2.32	0.59
1:C:133:LEU:HD21	1:C:150:VAL:HG13	1.84	0.59
1:A:314:CYS:SG	1:C:315:MET:HG2	2.42	0.59
1:E:193:ASP:OD2	1:E:193:ASP:N	2.34	0.59
1:E:193:ASP:HB2	1:E:441:ASN:ND2	2.17	0.59
1:E:231:GLU:HG3	2:F:97:SER:OG	2.03	0.59
1:G:380:ASP:O	1:G:381:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:O	1:A:144:LEU:HD12	2.02	0.59
1:A:154:VAL:HG11	1:A:355:TYR:HB2	1.84	0.59
1:C:13:LEU:HD13	2:D:38:LYS:HD2	1.84	0.59
1:E:37:GLN:NE2	1:E:37:GLN:H	2.00	0.59
1:G:68:ARG:HG3	1:G:179:ALA:HA	1.85	0.59
2:B:66:SER:HB3	2:B:94:VAL:CG1	2.32	0.59
1:C:101:MET:HB2	1:C:128:HIS:CG	2.38	0.59
1:E:80:LYS:CD	1:E:84:GLU:HB2	2.32	0.59
1:A:65:LEU:HD21	1:A:158:VAL:C	2.27	0.58
1:A:430:ASP:O	1:A:434:THR:HG23	2.03	0.58
1:A:439:LEU:HG	1:A:450:ILE:CD1	2.33	0.58
2:B:125:ASN:O	2:B:127:GLN:N	2.36	0.58
1:E:82:LEU:HD11	1:E:142:ILE:HG22	1.83	0.58
1:A:348:ASN:CB	1:A:375:SER:HB2	2.32	0.58
1:A:439:LEU:CG	1:A:450:ILE:HD11	2.33	0.58
1:C:193:ASP:OD2	1:C:193:ASP:N	2.36	0.58
1:C:77:VAL:HG13	1:C:79:VAL:CG2	2.33	0.58
1:C:407:THR:O	1:C:429:PRO:HA	2.03	0.58
1:E:193:ASP:C	1:E:194:ARG:HD3	2.27	0.58
1:E:217:LEU:O	1:E:221:VAL:HG23	2.03	0.58
2:F:64:SER:OG	2:F:97:SER:HB2	2.03	0.58
1:G:407:THR:CG2	1:G:408:PRO:HD2	2.33	0.58
1:A:407:THR:OG1	1:A:427:THR:HB	2.03	0.58
1:C:406:ASN:N	1:C:406:ASN:ND2	2.51	0.58
1:E:133:LEU:HD21	1:E:150:VAL:HG13	1.85	0.58
1:A:185:LYS:HE3	1:A:397:GLU:OE2	2.04	0.58
1:G:274:GLU:O	1:G:277:LYS:HB3	2.03	0.58
1:C:269:GLN:O	1:C:273:VAL:HG23	2.04	0.58
1:E:97:LEU:HD22	1:E:133:LEU:HB3	1.85	0.58
1:E:193:ASP:HB2	1:E:441:ASN:HD21	1.68	0.58
1:E:286:LEU:HB3	1:E:292:VAL:HG21	1.86	0.58
1:A:97:LEU:HD22	1:A:133:LEU:HB3	1.84	0.58
1:A:459:ASP:C	1:A:461:ASP:H	2.11	0.58
1:G:26:ARG:HG3	1:G:27:VAL:N	2.18	0.58
1:G:65:LEU:HD21	1:G:158:VAL:C	2.29	0.58
1:G:82:LEU:HD11	1:G:142:ILE:HG22	1.85	0.58
1:A:419:GLU:CD	1:A:419:GLU:N	2.61	0.58
2:F:125:ASN:O	2:F:127:GLN:N	2.37	0.58
1:A:101:MET:HB2	1:A:128:HIS:CG	2.39	0.58
1:A:226:LEU:HB2	2:B:62:LEU:CD1	2.34	0.58
1:E:274:GLU:O	1:E:277:LYS:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:GLY:HA3	1:E:403:PHE:CD1	2.39	0.58
1:A:193:ASP:HB2	1:A:441:ASN:ND2	2.19	0.58
1:C:306:LEU:HD12	1:C:306:LEU:O	2.03	0.58
1:E:226:LEU:HB2	2:F:62:LEU:CD1	2.34	0.58
1:A:132:GLU:OE2	1:A:143:LYS:HE2	2.04	0.57
1:C:145:LYS:CE	1:C:170:LYS:HB2	2.34	0.57
1:C:154:VAL:HG11	1:C:355:TYR:HB2	1.85	0.57
1:G:297:GLY:N	1:G:300:ASP:OD2	2.37	0.57
1:G:371:VAL:HG12	1:G:371:VAL:O	2.04	0.57
1:A:37:GLN:NE2	1:A:38:PRO:HD2	2.17	0.57
1:A:83:CYS:HA	1:A:140:GLN:HE22	1.70	0.57
1:E:290:VAL:HG22	1:E:291:PRO:CD	2.34	0.57
1:G:286:LEU:HB3	1:G:292:VAL:HG21	1.85	0.57
2:H:125:ASN:C	2:H:127:GLN:N	2.62	0.57
1:C:330:ASN:CB	1:C:331:PRO:HD3	2.29	0.57
1:E:181:LEU:HD12	1:E:417:GLY:HA3	1.86	0.57
1:E:407:THR:O	1:E:429:PRO:HA	2.05	0.57
1:C:290:VAL:HG22	1:C:291:PRO:CD	2.34	0.57
1:E:226:LEU:C	1:E:226:LEU:CD1	2.76	0.57
1:C:65:LEU:HD21	1:C:158:VAL:HG12	1.87	0.57
1:G:101:MET:HB2	1:G:128:HIS:CG	2.40	0.57
1:G:200:SER:HB3	1:G:428:VAL:HG12	1.86	0.57
1:A:193:ASP:HB2	1:A:441:ASN:HD21	1.69	0.57
1:A:193:ASP:OD2	1:A:193:ASP:N	2.38	0.57
1:G:154:VAL:HG12	1:G:155:THR:N	2.19	0.57
1:G:343:GLY:HA3	1:G:403:PHE:CD1	2.39	0.57
1:C:297:GLY:N	1:C:300:ASP:OD2	2.37	0.57
1:C:419:GLU:CD	1:C:419:GLU:N	2.63	0.57
1:C:439:LEU:HG	1:C:450:ILE:CD1	2.34	0.57
1:A:24:PHE:CZ	1:A:233:CYS:HB2	2.40	0.57
1:A:36:SER:HB3	1:A:333:GLN:H	1.69	0.57
1:A:226:LEU:HD12	1:A:226:LEU:O	2.03	0.57
1:C:343:GLY:HA3	1:C:403:PHE:CE1	2.40	0.57
1:E:65:LEU:CD2	1:E:158:VAL:HG12	2.34	0.57
1:E:126:TYR:HD2	1:E:355:TYR:HE1	1.51	0.57
1:E:224:GLY:HA3	2:F:135:ILE:HG13	1.86	0.57
1:A:343:GLY:HA3	1:A:403:PHE:CD1	2.40	0.56
1:A:212:LEU:O	1:A:213:LEU:C	2.46	0.56
2:B:70:ASN:HB2	2:B:72:HIS:CE1	2.40	0.56
1:C:37:GLN:N	1:C:38:PRO:HD2	2.20	0.56
1:C:82:LEU:HD11	1:C:142:ILE:HG22	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:C	1:C:194:ARG:HD3	2.30	0.56
1:A:65:LEU:CD2	1:A:158:VAL:HG12	2.35	0.56
1:A:231:GLU:HG3	2:B:97:SER:OG	2.04	0.56
1:A:303:ASN:HD22	1:A:305:THR:HG22	1.70	0.56
1:A:407:THR:O	1:A:429:PRO:HA	2.05	0.56
1:E:269:GLN:O	1:E:273:VAL:HG23	2.04	0.56
1:G:97:LEU:HD22	1:G:133:LEU:HB3	1.87	0.56
1:C:145:LYS:HE2	1:C:168:ASP:OD1	2.05	0.56
1:E:351:ASP:O	1:E:352:ILE:C	2.49	0.56
1:E:360:ASP:OD2	1:E:362:LEU:HB3	2.05	0.56
2:F:111:SER:O	2:F:114:LEU:HB2	2.04	0.56
1:A:65:LEU:HD23	1:A:159:LEU:O	2.04	0.56
1:C:348:ASN:HB2	1:C:375:SER:HB2	1.86	0.56
1:E:26:ARG:HG3	1:E:27:VAL:N	2.20	0.56
1:E:36:SER:HB3	1:E:333:GLN:H	1.71	0.56
2:H:62:LEU:C	2:H:62:LEU:HD23	2.30	0.56
2:B:6:TYR:HA	2:B:9:ASN:HD22	1.71	0.56
1:C:37:GLN:O	1:C:39:PHE:N	2.38	0.56
1:C:65:LEU:HD21	1:C:158:VAL:C	2.31	0.56
1:E:243:LEU:HD23	1:E:243:LEU:N	2.20	0.56
1:E:313:PRO:HB2	1:G:273:VAL:HG22	1.88	0.56
1:G:348:ASN:CB	1:G:375:SER:HB2	2.35	0.56
2:H:12:GLU:O	2:H:17:GLN:HG3	2.06	0.56
2:D:111:SER:O	2:D:114:LEU:HB2	2.06	0.56
1:G:193:ASP:OD2	1:G:193:ASP:N	2.39	0.56
1:C:14:LEU:HD11	2:D:98:ILE:CG2	2.36	0.56
2:D:64:SER:OG	2:D:97:SER:HB2	2.06	0.56
2:F:67:LEU:HD23	2:F:76:LYS:HE3	1.86	0.56
1:A:75:SER:O	1:A:77:VAL:HG23	2.06	0.56
1:A:348:ASN:HB2	1:A:375:SER:HB2	1.87	0.56
1:C:393:PHE:N	1:C:393:PHE:CD2	2.72	0.56
2:D:45:VAL:HG23	2:D:46:GLU:N	2.21	0.56
2:F:66:SER:HB3	2:F:94:VAL:CG1	2.36	0.56
1:G:99:LYS:N	1:G:155:THR:HG23	2.16	0.56
1:G:345:SER:C	1:G:405:GLY:HA3	2.31	0.56
1:G:407:THR:O	1:G:429:PRO:HA	2.06	0.56
1:A:77:VAL:CG1	1:A:79:VAL:HB	2.36	0.55
1:A:82:LEU:HD11	1:A:142:ILE:HG22	1.85	0.55
1:C:407:THR:HG23	1:C:408:PRO:HD2	1.87	0.55
1:A:145:LYS:CE	1:A:170:LYS:HB2	2.35	0.55
1:E:410:PHE:CE1	1:E:438:CYS:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:GLU:OE2	1:G:143:LYS:HE2	2.06	0.55
1:A:306:LEU:HD12	1:A:306:LEU:O	2.06	0.55
2:B:6:TYR:CD1	2:B:40:MET:HG2	2.40	0.55
1:C:199:VAL:HG12	1:C:200:SER:N	2.22	0.55
1:C:348:ASN:CB	1:C:375:SER:HB2	2.36	0.55
1:E:65:LEU:HD21	1:E:158:VAL:C	2.32	0.55
1:A:26:ARG:HG3	1:A:27:VAL:N	2.21	0.55
1:C:26:ARG:HG3	1:C:27:VAL:H	1.71	0.55
2:F:58:HIS:CE1	2:F:107:MET:HB2	2.41	0.55
1:G:65:LEU:HD21	1:G:158:VAL:HG12	1.86	0.55
1:G:410:PHE:CE1	1:G:438:CYS:HB2	2.41	0.55
2:H:58:HIS:CE1	2:H:107:MET:HB2	2.41	0.55
1:A:306:LEU:O	1:A:308:GLN:N	2.38	0.55
1:C:37:GLN:NE2	1:C:38:PRO:HD2	2.18	0.55
1:C:99:LYS:N	1:C:155:THR:HG23	2.18	0.55
2:D:2:ALA:O	2:D:5:LEU:HB3	2.06	0.55
1:E:37:GLN:N	1:E:38:PRO:HD2	2.21	0.55
1:G:185:LYS:HE3	1:G:397:GLU:OE2	2.07	0.55
1:G:330:ASN:CB	1:G:331:PRO:HD3	2.32	0.55
1:A:68:ARG:HG3	1:A:179:ALA:HA	1.89	0.55
1:C:5:GLN:O	1:C:8:GLN:HB2	2.07	0.55
1:C:19:ALA:HB2	1:E:443:ARG:CZ	2.37	0.55
1:C:284:LEU:HD22	1:C:318:LEU:HB3	1.89	0.55
1:C:330:ASN:CB	1:C:331:PRO:CD	2.84	0.55
2:F:24:LYS:O	2:F:27:SER:HB3	2.06	0.55
1:C:14:LEU:HD11	2:D:98:ILE:HG22	1.89	0.55
1:A:37:GLN:N	1:A:38:PRO:HD2	2.21	0.55
1:A:274:GLU:O	1:A:277:LYS:HB3	2.07	0.55
1:C:99:LYS:HE2	1:C:150:VAL:HG12	1.89	0.55
1:C:154:VAL:HG12	1:C:155:THR:N	2.20	0.55
1:C:226:LEU:HB2	2:D:62:LEU:CD1	2.37	0.55
2:D:67:LEU:HD23	2:D:76:LYS:HE3	1.89	0.55
2:D:70:ASN:HB2	2:D:72:HIS:CE1	2.42	0.55
1:E:279:LEU:HD12	1:E:279:LEU:O	2.07	0.55
1:E:393:PHE:N	1:E:393:PHE:CD2	2.73	0.55
1:G:77:VAL:CG1	1:G:79:VAL:HB	2.36	0.55
1:G:451:SER:HB2	2:H:76:LYS:HD3	1.89	0.55
1:C:315:MET:C	1:C:317:PRO:HD3	2.33	0.55
1:G:199:VAL:HG12	1:G:200:SER:N	2.22	0.55
1:G:351:ASP:O	1:G:352:ILE:C	2.50	0.55
1:E:5:GLN:O	1:E:8:GLN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:HD13	2:F:38:LYS:HD2	1.89	0.54
1:C:21:ASN:H	1:E:237:HIS:CE1	2.24	0.54
1:C:343:GLY:HA3	1:C:403:PHE:CD1	2.42	0.54
1:C:360:ASP:OD2	1:C:362:LEU:HB3	2.07	0.54
2:D:6:TYR:HA	2:D:9:ASN:HD22	1.72	0.54
2:D:125:ASN:C	2:D:127:GLN:N	2.64	0.54
1:E:77:VAL:CG1	1:E:79:VAL:HB	2.37	0.54
1:E:204:LEU:HD12	1:E:279:LEU:HB2	1.89	0.54
1:E:373:HIS:HA	1:E:393:PHE:O	2.07	0.54
1:G:290:VAL:CG2	1:G:291:PRO:HD2	2.34	0.54
1:G:419:GLU:CD	1:G:419:GLU:N	2.64	0.54
1:A:133:LEU:HD21	1:A:150:VAL:HG13	1.88	0.54
1:C:226:LEU:HD13	2:D:62:LEU:HD11	1.89	0.54
1:C:279:LEU:HD12	1:C:279:LEU:O	2.06	0.54
1:E:212:LEU:O	1:E:213:LEU:C	2.48	0.54
1:C:36:SER:HB3	1:C:333:GLN:H	1.72	0.54
1:E:68:ARG:O	1:E:72:HIS:HB2	2.07	0.54
1:E:228:ASP:OD1	1:E:229:GLU:N	2.39	0.54
1:E:303:ASN:HB2	1:E:305:THR:HG22	1.90	0.54
1:E:380:ASP:O	1:E:381:THR:HG23	2.08	0.54
1:G:68:ARG:O	1:G:72:HIS:HB2	2.07	0.54
1:A:68:ARG:O	1:A:72:HIS:HB2	2.07	0.54
1:A:145:LYS:HE2	1:A:168:ASP:OD1	2.07	0.54
2:B:58:HIS:CE1	2:B:107:MET:HB2	2.42	0.54
1:E:410:PHE:HA	1:E:429:PRO:HD3	1.90	0.54
1:G:279:LEU:HD12	1:G:279:LEU:O	2.08	0.54
1:G:303:ASN:HD22	1:G:305:THR:HG22	1.73	0.54
1:A:286:LEU:HB3	1:A:292:VAL:HG21	1.90	0.54
1:A:297:GLY:N	1:A:300:ASP:OD2	2.41	0.54
1:A:380:ASP:O	1:A:381:THR:HG23	2.07	0.54
1:E:275:ALA:O	1:E:276:VAL:C	2.51	0.54
1:E:290:VAL:CG2	1:E:291:PRO:HD2	2.37	0.54
1:E:371:VAL:HG12	1:E:371:VAL:O	2.07	0.54
1:A:154:VAL:HG12	1:A:155:THR:N	2.23	0.54
1:A:243:LEU:HD23	1:A:243:LEU:N	2.23	0.54
1:C:226:LEU:C	1:C:226:LEU:CD1	2.81	0.54
1:C:380:ASP:O	1:C:381:THR:HG23	2.06	0.54
1:E:407:THR:CG2	1:E:408:PRO:HD2	2.38	0.54
1:A:360:ASP:OD2	1:A:362:LEU:HB3	2.08	0.54
1:A:373:HIS:HA	1:A:393:PHE:O	2.07	0.54
1:C:303:ASN:HB2	1:C:305:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:HIS:CE1	2:D:107:MET:HB2	2.43	0.54
1:E:399:PRO:O	1:E:423:VAL:HG22	2.06	0.54
1:G:82:LEU:HD13	1:G:93:VAL:HG11	1.89	0.54
2:H:6:TYR:CD1	2:H:40:MET:HG2	2.43	0.54
2:B:62:LEU:HD23	2:B:62:LEU:C	2.33	0.54
1:C:224:GLY:HA3	2:D:135:ILE:HG13	1.90	0.54
2:D:62:LEU:C	2:D:62:LEU:HD23	2.33	0.54
1:E:345:SER:C	1:E:405:GLY:HA3	2.33	0.54
1:G:-2:HIS:O	1:G:-1:HIS:HB2	2.08	0.54
1:C:306:LEU:O	1:C:308:GLN:N	2.39	0.54
1:C:351:ASP:O	1:C:352:ILE:C	2.50	0.54
1:E:98:PHE:HA	1:E:155:THR:HG22	1.88	0.54
1:E:163:GLY:HA3	1:E:172:LEU:O	2.08	0.54
1:E:303:ASN:HA	1:G:303:ASN:HA	1.90	0.54
1:G:224:GLY:HA3	2:H:135:ILE:HG13	1.90	0.54
1:A:406:ASN:N	1:A:406:ASN:ND2	2.53	0.53
1:C:26:ARG:NH1	1:C:289:SER:O	2.40	0.53
1:C:57:ARG:NH2	1:C:378:ALA:O	2.41	0.53
1:C:68:ARG:HG3	1:C:179:ALA:HA	1.90	0.53
1:E:101:MET:HB2	1:E:128:HIS:CG	2.42	0.53
2:F:12:GLU:O	2:F:17:GLN:HG3	2.07	0.53
1:G:360:ASP:OD2	1:G:362:LEU:HB3	2.08	0.53
1:C:243:LEU:HD23	1:C:243:LEU:N	2.24	0.53
1:G:393:PHE:N	1:G:393:PHE:CD2	2.73	0.53
2:H:111:SER:O	2:H:114:LEU:HB2	2.08	0.53
1:A:82:LEU:HD13	1:A:93:VAL:HG11	1.89	0.53
1:C:346:GLY:CA	1:C:405:GLY:HA3	2.39	0.53
1:E:407:THR:OG1	1:E:427:THR:HB	2.07	0.53
1:G:307:PRO:HG3	1:G:393:PHE:CZ	2.43	0.53
1:A:303:ASN:ND2	1:A:308:GLN:HA	2.22	0.53
1:C:26:ARG:CG	1:C:27:VAL:N	2.72	0.53
1:C:98:PHE:HA	1:C:155:THR:HG22	1.91	0.53
1:E:83:CYS:HA	1:E:140:GLN:HE22	1.72	0.53
1:G:29:VAL:HG11	1:G:291:PRO:CG	2.18	0.53
1:G:275:ALA:O	1:G:276:VAL:C	2.51	0.53
1:G:315:MET:C	1:G:317:PRO:HD3	2.33	0.53
2:H:45:VAL:HG23	2:H:46:GLU:N	2.22	0.53
1:C:77:VAL:CG1	1:C:79:VAL:HB	2.38	0.53
1:C:163:GLY:HA3	1:C:172:LEU:O	2.08	0.53
1:C:266:LYS:HG3	1:C:267:LYS:HG3	1.91	0.53
2:F:6:TYR:HA	2:F:9:ASN:HD22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:O	1:A:352:ILE:C	2.51	0.53
1:G:83:CYS:HA	1:G:140:GLN:HE22	1.73	0.53
1:G:99:LYS:HE2	1:G:150:VAL:HG12	1.90	0.53
2:H:52:ASN:CB	2:H:55:ALA:HB2	2.38	0.53
1:A:57:ARG:NH2	1:A:378:ALA:O	2.42	0.53
1:C:83:CYS:HA	1:C:140:GLN:HE22	1.73	0.53
1:C:290:VAL:CG2	1:C:291:PRO:HD2	2.38	0.53
1:C:371:VAL:HG12	1:C:371:VAL:O	2.08	0.53
2:F:23:TYR:CD1	2:F:38:LYS:HE2	2.44	0.53
1:A:212:LEU:O	1:A:215:THR:N	2.42	0.53
1:E:37:GLN:H	1:E:37:GLN:CD	2.17	0.53
1:E:65:LEU:HD21	1:E:158:VAL:HG12	1.90	0.53
2:F:2:ALA:O	2:F:5:LEU:HB3	2.09	0.53
1:A:438:CYS:SG	1:A:439:LEU:N	2.82	0.53
1:C:439:LEU:HD12	1:C:450:ILE:HD11	1.91	0.53
1:G:330:ASN:CB	1:G:331:PRO:CD	2.87	0.53
1:A:37:GLN:H	1:A:37:GLN:CD	2.17	0.53
1:A:351:ASP:HA	1:A:354:ARG:HD2	1.90	0.53
2:B:52:ASN:CB	2:B:55:ALA:HB2	2.39	0.53
1:C:75:SER:O	1:C:77:VAL:HG23	2.09	0.53
1:E:193:ASP:CB	1:E:441:ASN:ND2	2.67	0.53
1:E:419:GLU:O	1:E:420:ASP:C	2.52	0.53
1:A:199:VAL:HG12	1:A:200:SER:N	2.23	0.52
1:A:266:LYS:HG3	1:A:267:LYS:HG3	1.91	0.52
1:A:279:LEU:HD12	1:A:279:LEU:O	2.08	0.52
1:E:197:LEU:HD21	1:E:218:LEU:HD11	1.90	0.52
1:E:212:LEU:O	1:E:215:THR:N	2.42	0.52
1:E:269:GLN:NE2	1:G:320:THR:HB	2.24	0.52
1:G:419:GLU:O	1:G:420:ASP:C	2.52	0.52
2:H:66:SER:HB3	2:H:94:VAL:CG1	2.40	0.52
1:A:99:LYS:N	1:A:155:THR:HG23	2.17	0.52
1:A:303:ASN:HB2	1:A:305:THR:HG22	1.91	0.52
2:B:23:TYR:CD2	2:B:24:LYS:N	2.77	0.52
1:A:193:ASP:CB	1:A:441:ASN:ND2	2.69	0.52
1:C:200:SER:HB3	1:C:428:VAL:HG12	1.92	0.52
1:E:98:PHE:HA	1:E:155:THR:CG2	2.39	0.52
1:E:297:GLY:N	1:E:300:ASP:OD2	2.43	0.52
1:E:439:LEU:HD12	1:E:450:ILE:HD11	1.89	0.52
2:F:62:LEU:C	2:F:62:LEU:HD23	2.33	0.52
1:C:86:GLN:O	1:C:87:PRO:C	2.53	0.52
2:D:12:GLU:O	2:D:17:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:GLN:H	1:G:37:GLN:CD	2.18	0.52
1:G:37:GLN:N	1:G:38:PRO:HD2	2.24	0.52
1:E:65:LEU:HD23	1:E:159:LEU:C	2.34	0.52
1:E:303:ASN:ND2	1:E:308:GLN:HA	2.24	0.52
1:E:315:MET:HG2	1:G:314:CYS:SG	2.49	0.52
2:F:10:ILE:O	2:F:14:VAL:HG23	2.10	0.52
1:G:58:LEU:HD21	1:G:95:GLY:CA	2.19	0.52
1:G:303:ASN:HB2	1:G:305:THR:HG22	1.90	0.52
1:G:407:THR:OG1	1:G:427:THR:HB	2.09	0.52
2:B:122:LEU:O	2:B:125:ASN:N	2.38	0.52
1:C:37:GLN:H	1:C:37:GLN:CD	2.17	0.52
1:C:82:LEU:HD13	1:C:93:VAL:HG11	1.91	0.52
1:C:274:GLU:O	1:C:277:LYS:HB3	2.09	0.52
1:E:148:ILE:HA	1:E:176:TYR:CE2	2.42	0.52
1:E:395:PHE:H	1:E:395:PHE:HD1	1.58	0.52
1:G:395:PHE:H	1:G:395:PHE:HD1	1.58	0.52
1:A:371:VAL:HG12	1:A:371:VAL:O	2.09	0.52
1:C:68:ARG:O	1:C:72:HIS:HB2	2.09	0.52
1:E:348:ASN:CB	1:E:375:SER:HB2	2.40	0.52
2:F:41:LEU:HD22	2:F:103:ILE:HD12	1.90	0.52
1:G:21:ASN:OD1	2:H:36:GLN:HB2	2.10	0.52
1:A:14:LEU:HD11	2:B:98:ILE:HG22	1.92	0.52
1:A:200:SER:HB3	1:A:428:VAL:HG12	1.91	0.52
1:C:225:GLN:HE21	2:D:133:SER:HB2	1.74	0.52
1:E:99:LYS:N	1:E:155:THR:HG23	2.17	0.52
1:A:26:ARG:HD3	1:A:290:VAL:HG23	1.91	0.52
2:B:125:ASN:C	2:B:127:GLN:N	2.66	0.52
1:C:82:LEU:HB2	1:C:137:ASP:HB2	1.92	0.52
1:C:264:LEU:HD23	1:C:265:THR:N	2.25	0.52
1:C:303:ASN:ND2	1:C:308:GLN:HA	2.24	0.52
1:C:393:PHE:N	1:C:393:PHE:HD2	2.08	0.52
1:E:330:ASN:CB	1:E:331:PRO:HD3	2.33	0.52
1:E:393:PHE:N	1:E:393:PHE:HD2	2.08	0.52
1:G:98:PHE:HA	1:G:155:THR:HG22	1.91	0.52
1:G:197:LEU:HD21	1:G:218:LEU:HD11	1.92	0.52
1:A:393:PHE:N	1:A:393:PHE:CD2	2.75	0.51
2:B:68:ILE:N	2:B:68:ILE:CD1	2.72	0.51
1:C:145:LYS:HZ1	1:C:168:ASP:HB2	1.75	0.51
2:D:10:ILE:O	2:D:14:VAL:HG23	2.10	0.51
1:E:330:ASN:CB	1:E:331:PRO:CD	2.87	0.51
2:F:68:ILE:N	2:F:68:ILE:CD1	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:TYR:HA	2:H:9:ASN:HD22	1.75	0.51
1:E:197:LEU:HB3	1:E:241:VAL:HG22	1.91	0.51
1:A:315:MET:C	1:A:317:PRO:HD3	2.35	0.51
1:G:193:ASP:C	1:G:194:ARG:HD3	2.35	0.51
1:G:348:ASN:HB3	1:G:375:SER:HB2	1.92	0.51
1:A:14:LEU:HD11	2:B:98:ILE:CG2	2.41	0.51
2:B:41:LEU:HD22	2:B:103:ILE:HD12	1.92	0.51
1:C:419:GLU:O	1:C:420:ASP:C	2.53	0.51
1:E:315:MET:C	1:E:317:PRO:HD3	2.35	0.51
2:F:122:LEU:O	2:F:125:ASN:N	2.42	0.51
2:H:10:ILE:O	2:H:14:VAL:HG23	2.10	0.51
1:A:65:LEU:HD23	1:A:159:LEU:C	2.36	0.51
1:C:5:GLN:HG3	1:C:193:ASP:OD1	2.11	0.51
1:E:154:VAL:HG12	1:E:155:THR:N	2.26	0.51
2:F:125:ASN:C	2:F:127:GLN:N	2.67	0.51
1:A:65:LEU:HD21	1:A:158:VAL:HG12	1.93	0.51
1:E:199:VAL:HG12	1:E:200:SER:N	2.24	0.51
1:G:57:ARG:NH2	1:G:378:ALA:O	2.44	0.51
1:G:226:LEU:HD12	1:G:226:LEU:O	2.10	0.51
1:A:5:GLN:HG3	1:A:193:ASP:OD1	2.10	0.51
1:C:65:LEU:HD23	1:C:159:LEU:O	2.10	0.51
1:C:145:LYS:HZ1	1:C:168:ASP:CB	2.24	0.51
1:C:239:SER:O	1:C:240:ARG:HG2	2.10	0.51
1:C:303:ASN:HD22	1:C:305:THR:HG22	1.74	0.51
2:D:6:TYR:CD1	2:D:40:MET:HG2	2.46	0.51
1:G:204:LEU:HD12	1:G:279:LEU:HB2	1.93	0.51
1:G:212:LEU:O	1:G:215:THR:N	2.44	0.51
1:G:351:ASP:HA	1:G:354:ARG:HD2	1.93	0.51
1:A:225:GLN:NE2	2:B:133:SER:HB2	2.26	0.51
1:A:264:LEU:HD23	1:A:265:THR:N	2.25	0.51
2:B:64:SER:OG	2:B:97:SER:HB2	2.11	0.51
2:B:81:ARG:NH1	2:B:108:LEU:O	2.44	0.51
1:C:53:ILE:HG22	1:C:55:ALA:H	1.76	0.51
1:C:216:GLN:HE21	2:D:115:PHE:HD1	1.57	0.51
1:A:224:GLY:HA3	2:B:135:ILE:HG13	1.93	0.51
1:E:82:LEU:HD13	1:E:93:VAL:HG11	1.91	0.51
1:E:264:LEU:HD23	1:E:265:THR:N	2.26	0.51
1:G:86:GLN:O	1:G:87:PRO:C	2.54	0.51
1:G:231:GLU:HG3	2:H:97:SER:OG	2.11	0.51
1:C:410:PHE:HA	1:C:429:PRO:HD3	1.93	0.51
1:E:99:LYS:HE2	1:E:150:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:LEU:CG	1:E:450:ILE:HD11	2.41	0.51
2:F:42:TYR:O	2:F:45:VAL:HG22	2.11	0.51
1:G:5:GLN:O	1:G:8:GLN:HB2	2.10	0.51
1:G:36:SER:HB3	1:G:333:GLN:H	1.76	0.51
1:G:239:SER:O	1:G:240:ARG:HG2	2.10	0.51
1:G:284:LEU:HD22	1:G:318:LEU:HB3	1.92	0.51
1:C:19:ALA:HB1	1:E:193:ASP:OD2	2.11	0.50
2:D:115:PHE:O	2:D:116:ASN:C	2.55	0.50
1:E:307:PRO:HG3	1:E:393:PHE:CZ	2.46	0.50
1:E:351:ASP:HA	1:E:354:ARG:HD2	1.93	0.50
1:G:277:LYS:HE2	1:G:281:GLU:CD	2.36	0.50
2:H:85:LEU:HD12	2:H:85:LEU:C	2.36	0.50
1:A:225:GLN:HE21	2:B:133:SER:HB2	1.75	0.50
2:B:23:TYR:CD1	2:B:38:LYS:HE2	2.46	0.50
1:A:13:LEU:HD13	2:B:38:LYS:HD2	1.92	0.50
1:C:410:PHE:CE1	1:C:438:CYS:HB2	2.45	0.50
2:D:41:LEU:HD22	2:D:103:ILE:HD12	1.92	0.50
2:D:86:GLU:OE2	2:D:86:GLU:HA	2.10	0.50
1:E:200:SER:HB3	1:E:428:VAL:HG12	1.92	0.50
1:G:5:GLN:HG3	1:G:193:ASP:OD1	2.11	0.50
2:H:2:ALA:O	2:H:5:LEU:HB3	2.12	0.50
1:A:211:SER:HA	1:A:435:GLN:NE2	2.27	0.50
1:E:225:GLN:NE2	2:F:133:SER:HB2	2.26	0.50
1:G:65:LEU:HD23	1:G:159:LEU:C	2.36	0.50
2:H:23:TYR:CD2	2:H:24:LYS:N	2.79	0.50
2:H:24:LYS:O	2:H:27:SER:HB3	2.10	0.50
1:C:423:VAL:HG12	1:C:425:LEU:HD23	1.93	0.50
1:E:154:VAL:HG11	1:E:355:TYR:CB	2.41	0.50
1:G:393:PHE:N	1:G:393:PHE:HD2	2.10	0.50
2:B:2:ALA:O	2:B:5:LEU:HB3	2.12	0.50
1:C:231:GLU:CG	2:D:97:SER:OG	2.60	0.50
1:C:373:HIS:HA	1:C:393:PHE:O	2.11	0.50
2:F:58:HIS:NE2	2:F:107:MET:HE3	2.26	0.50
1:C:29:VAL:HG11	1:C:291:PRO:CG	2.13	0.50
1:E:132:GLU:OE2	1:E:143:LYS:HE2	2.12	0.50
2:F:52:ASN:CB	2:F:55:ALA:HB2	2.42	0.50
1:A:26:ARG:CD	1:A:290:VAL:HG23	2.42	0.50
2:B:72:HIS:HD2	2:B:72:HIS:O	1.94	0.50
2:B:112:GLY:O	2:B:113:PRO:C	2.55	0.50
1:C:65:LEU:HD12	1:C:179:ALA:HB2	1.94	0.50
1:G:266:LYS:HG3	1:G:267:LYS:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:LEU:O	1:G:306:LEU:HD12	2.11	0.50
1:A:37:GLN:C	1:A:39:PHE:N	2.70	0.50
1:A:86:GLN:O	1:A:87:PRO:C	2.53	0.50
1:A:330:ASN:CB	1:A:331:PRO:CD	2.89	0.50
2:D:85:LEU:HD12	2:D:85:LEU:C	2.36	0.50
1:E:266:LYS:HG3	1:E:267:LYS:HG3	1.94	0.50
1:E:439:LEU:HG	1:E:450:ILE:HD11	1.94	0.50
1:A:277:LYS:HE2	1:A:281:GLU:CD	2.37	0.49
1:A:459:ASP:O	1:A:462:LEU:HG	2.13	0.49
2:B:99:HIS:ND1	2:B:100:VAL:O	2.40	0.49
1:C:65:LEU:HD23	1:C:159:LEU:C	2.37	0.49
1:E:26:ARG:HD3	1:E:290:VAL:HG23	1.94	0.49
1:G:172:LEU:HD22	3:G:474:HOH:O	2.11	0.49
2:B:86:GLU:OE2	2:B:86:GLU:HA	2.11	0.49
1:C:151:SER:O	1:C:357:SER:N	2.45	0.49
1:C:225:GLN:NE2	2:D:133:SER:HB2	2.27	0.49
1:E:221:VAL:HG21	1:E:452:PHE:HE2	1.77	0.49
1:G:154:VAL:HG11	1:G:355:TYR:CB	2.41	0.49
1:G:212:LEU:O	1:G:213:LEU:C	2.53	0.49
1:A:98:PHE:HA	1:A:155:THR:HG22	1.93	0.49
1:A:190:LEU:HB2	1:A:443:ARG:HB2	1.94	0.49
1:A:303:ASN:HD21	1:A:308:GLN:HA	1.77	0.49
1:A:307:PRO:HG3	1:A:393:PHE:CZ	2.47	0.49
1:A:410:PHE:HA	1:A:429:PRO:HD3	1.94	0.49
2:B:52:ASN:HB3	2:B:55:ALA:HB2	1.95	0.49
1:C:399:PRO:O	1:C:423:VAL:HG22	2.12	0.49
1:E:303:ASN:HB3	1:G:304:TYR:CD1	2.47	0.49
1:G:67:ASN:O	1:G:71:GLN:HG2	2.12	0.49
1:A:410:PHE:CE1	1:A:438:CYS:HB2	2.44	0.49
2:F:45:VAL:HG23	2:F:46:GLU:N	2.27	0.49
1:G:218:LEU:HD22	1:G:431:PHE:CE2	2.48	0.49
2:B:3:ASP:CG	2:B:4:GLN:N	2.69	0.49
2:D:66:SER:HB3	2:D:94:VAL:CG1	2.42	0.49
2:D:81:ARG:NH1	2:D:108:LEU:O	2.45	0.49
1:E:11:HIS:CD2	1:E:11:HIS:N	2.81	0.49
1:E:14:LEU:HD11	2:F:98:ILE:CG2	2.42	0.49
1:A:419:GLU:O	1:A:420:ASP:C	2.55	0.49
2:B:103:ILE:N	2:B:104:GLN:HE21	2.10	0.49
1:C:67:ASN:O	1:C:71:GLN:HG2	2.12	0.49
1:C:157:THR:HG23	1:C:371:VAL:HG11	1.93	0.49
1:E:159:LEU:HD23	1:E:159:LEU:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:LYS:HE3	1:C:397:GLU:OE2	2.12	0.49
1:E:5:GLN:HG3	1:E:193:ASP:OD1	2.12	0.49
1:G:439:LEU:HD12	1:G:450:ILE:HD11	1.94	0.49
1:A:348:ASN:HB3	1:A:375:SER:HB2	1.95	0.49
1:A:395:PHE:H	1:A:395:PHE:HD1	1.58	0.49
1:C:407:THR:CG2	1:C:408:PRO:HD2	2.41	0.49
1:E:60:GLN:O	1:E:63:PRO:HD2	2.13	0.49
2:F:81:ARG:NH1	2:F:108:LEU:O	2.46	0.49
1:G:82:LEU:HB2	1:G:137:ASP:HB2	1.95	0.49
1:G:98:PHE:HA	1:G:155:THR:CG2	2.43	0.49
1:G:264:LEU:HD23	1:G:265:THR:N	2.27	0.49
2:H:58:HIS:NE2	2:H:107:MET:HE3	2.27	0.49
1:A:26:ARG:NH1	1:A:289:SER:O	2.45	0.49
1:C:345:SER:C	1:C:405:GLY:HA3	2.37	0.49
1:C:360:ASP:O	1:C:363:GLU:HB3	2.13	0.49
1:E:151:SER:O	1:E:357:SER:N	2.46	0.49
1:G:75:SER:O	1:G:77:VAL:HG23	2.13	0.49
1:A:26:ARG:HG3	1:A:27:VAL:H	1.77	0.49
1:A:204:LEU:HD12	1:A:279:LEU:HB2	1.94	0.49
1:A:444:SER:O	1:A:445:LEU:HB2	2.12	0.49
2:B:85:LEU:HD12	2:B:85:LEU:C	2.37	0.49
1:C:218:LEU:HD22	1:C:431:PHE:CE2	2.47	0.49
1:C:237:HIS:CE1	1:E:21:ASN:H	2.31	0.49
1:C:351:ASP:HA	1:C:354:ARG:HD2	1.94	0.49
1:C:354:ARG:C	1:C:355:TYR:HD1	2.21	0.49
1:E:185:LYS:HE3	1:E:397:GLU:OE2	2.12	0.49
1:A:346:GLY:CA	1:A:405:GLY:HA3	2.43	0.48
2:B:10:ILE:O	2:B:14:VAL:HG23	2.13	0.48
2:D:45:VAL:CG2	2:D:46:GLU:N	2.76	0.48
2:F:85:LEU:HD12	2:F:85:LEU:C	2.37	0.48
2:H:125:ASN:C	2:H:127:GLN:H	2.20	0.48
1:A:3:SER:OG	2:B:75:HIS:ND1	2.34	0.48
1:A:221:VAL:HG21	1:A:452:PHE:HE2	1.78	0.48
2:D:3:ASP:CG	2:D:4:GLN:N	2.71	0.48
1:E:406:ASN:N	1:E:406:ASN:ND2	2.47	0.48
1:G:95:GLY:CA	1:G:135:LEU:HD11	2.42	0.48
1:G:423:VAL:HG12	1:G:425:LEU:HD23	1.96	0.48
2:H:64:SER:OG	2:H:97:SER:HB2	2.12	0.48
1:A:2:PHE:CG	1:A:439:LEU:HD12	2.48	0.48
1:A:7:ALA:O	1:A:9:ARG:N	2.47	0.48
2:B:70:ASN:C	2:B:72:HIS:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ARG:NH2	1:E:378:ALA:O	2.47	0.48
1:G:148:ILE:HA	1:G:176:TYR:CE2	2.46	0.48
1:G:410:PHE:HA	1:G:429:PRO:HD3	1.94	0.48
1:A:11:HIS:N	1:A:11:HIS:CD2	2.81	0.48
1:A:280:ASP:CG	1:A:318:LEU:HB2	2.38	0.48
1:C:98:PHE:HA	1:C:155:THR:CG2	2.43	0.48
1:C:182:ALA:HB1	1:C:183:PRO:CD	2.37	0.48
1:C:373:HIS:O	1:C:376:PRO:HD3	2.13	0.48
2:D:24:LYS:O	2:D:27:SER:HB3	2.13	0.48
1:E:452:PHE:CD1	1:E:452:PHE:N	2.81	0.48
2:H:41:LEU:HD22	2:H:103:ILE:HD12	1.94	0.48
1:A:-1:HIS:ND1	1:A:-1:HIS:C	2.72	0.48
2:B:45:VAL:HG23	2:B:46:GLU:N	2.27	0.48
1:E:430:ASP:OD1	1:E:432:SER:HB3	2.13	0.48
1:G:24:PHE:CZ	1:G:233:CYS:HB2	2.49	0.48
1:G:319:ALA:CB	1:G:325:LEU:HD22	2.42	0.48
1:A:67:ASN:O	1:A:71:GLN:HG2	2.14	0.48
1:A:269:GLN:NE2	1:C:320:THR:HB	2.29	0.48
1:C:443:ARG:CZ	1:E:19:ALA:HB2	2.43	0.48
1:E:94:VAL:HB	3:E:484:HOH:O	2.12	0.48
1:E:319:ALA:O	1:E:321:ALA:N	2.47	0.48
2:F:3:ASP:C	2:F:5:LEU:N	2.70	0.48
1:G:60:GLN:O	1:G:63:PRO:HD2	2.14	0.48
1:G:354:ARG:C	1:G:355:TYR:HD1	2.21	0.48
2:B:24:LYS:O	2:B:27:SER:HB3	2.12	0.48
1:C:269:GLN:O	1:C:270:ALA:C	2.57	0.48
2:F:3:ASP:CG	2:F:4:GLN:N	2.72	0.48
1:G:14:LEU:HD11	2:H:98:ILE:CG2	2.44	0.48
1:G:348:ASN:HB2	1:G:375:SER:HB2	1.95	0.48
2:H:42:TYR:O	2:H:45:VAL:HG22	2.13	0.48
2:H:68:ILE:N	2:H:68:ILE:CD1	2.77	0.48
2:B:23:TYR:CG	2:B:24:LYS:N	2.82	0.48
2:B:42:TYR:O	2:B:45:VAL:HG22	2.14	0.48
1:G:11:HIS:N	1:G:11:HIS:CD2	2.80	0.48
1:G:151:SER:O	1:G:357:SER:N	2.45	0.48
1:G:162:PHE:HB3	1:G:175:ASP:O	2.14	0.48
1:C:21:ASN:OD1	2:D:36:GLN:HB2	2.14	0.48
1:E:218:LEU:HD22	1:E:431:PHE:CE2	2.49	0.48
1:E:225:GLN:HE21	2:F:133:SER:HB2	1.78	0.48
1:E:244:ALA:HA	1:E:295:MET:HB2	1.96	0.48
1:G:311:LEU:HD23	1:G:311:LEU:HA	1.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:103:ILE:C	2:H:104:GLN:HE21	2.22	0.48
1:A:163:GLY:HA3	1:A:172:LEU:O	2.13	0.48
1:A:284:LEU:HD22	1:A:318:LEU:HB3	1.96	0.48
2:B:58:HIS:NE2	2:B:107:MET:HE3	2.29	0.48
2:D:52:ASN:HB3	2:D:55:ALA:HB2	1.96	0.48
1:E:82:LEU:HB2	1:E:137:ASP:HB2	1.96	0.48
1:E:157:THR:HG23	1:E:371:VAL:HG11	1.95	0.48
1:A:97:LEU:CD2	1:A:133:LEU:HB3	2.44	0.47
1:A:378:ALA:HA	1:A:379:PRO:HD3	1.75	0.47
1:E:29:VAL:HG11	1:E:291:PRO:CG	2.16	0.47
1:E:136:GLU:HG2	1:E:141:ARG:HB3	1.96	0.47
1:E:319:ALA:CB	1:E:325:LEU:HD22	2.44	0.47
1:G:163:GLY:HA3	1:G:172:LEU:O	2.14	0.47
1:G:193:ASP:CB	1:G:443:ARG:NH1	2.64	0.47
2:H:103:ILE:N	2:H:104:GLN:HE21	2.12	0.47
1:A:151:SER:O	1:A:357:SER:N	2.47	0.47
1:C:204:LEU:HD12	1:C:279:LEU:HB2	1.96	0.47
1:C:307:PRO:HG3	1:C:393:PHE:CZ	2.48	0.47
2:D:52:ASN:CB	2:D:55:ALA:HB2	2.43	0.47
1:E:198:LEU:HB3	1:E:428:VAL:HG21	1.96	0.47
1:E:216:GLN:HE21	2:F:115:PHE:HD1	1.61	0.47
1:E:355:TYR:N	1:E:355:TYR:CD1	2.82	0.47
1:G:373:HIS:HA	1:G:393:PHE:O	2.14	0.47
1:A:83:CYS:HA	1:A:140:GLN:NE2	2.28	0.47
2:B:72:HIS:CD2	2:B:72:HIS:O	2.68	0.47
1:C:195:PHE:HB2	1:C:238:VAL:HG22	1.96	0.47
1:C:228:ASP:OD1	1:C:229:GLU:N	2.45	0.47
1:E:90:LYS:NZ	1:E:174:GLU:OE2	2.45	0.47
1:E:97:LEU:CD2	1:E:133:LEU:HB3	2.43	0.47
1:G:65:LEU:HD12	1:G:179:ALA:HB2	1.95	0.47
1:A:416:ARG:HA	1:A:421:GLN:O	2.14	0.47
2:B:125:ASN:C	2:B:127:GLN:H	2.22	0.47
1:C:19:ALA:CB	1:E:193:ASP:OD2	2.63	0.47
1:C:275:ALA:O	1:C:276:VAL:C	2.55	0.47
1:G:145:LYS:HE2	1:G:168:ASP:OD1	2.15	0.47
1:G:157:THR:HG23	1:G:371:VAL:HG11	1.96	0.47
2:H:3:ASP:CG	2:H:4:GLN:N	2.72	0.47
2:D:23:TYR:CD1	2:D:38:LYS:HE2	2.50	0.47
2:D:72:HIS:HD2	2:D:72:HIS:O	1.97	0.47
1:E:99:LYS:HE2	1:E:150:VAL:CG1	2.44	0.47
1:E:153:LEU:HD12	1:E:153:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:ILE:O	1:E:337:ASP:C	2.58	0.47
1:E:398:CYS:SG	1:E:423:VAL:HG21	2.54	0.47
1:G:136:GLU:HG2	1:G:141:ARG:HB3	1.96	0.47
1:G:239:SER:O	1:G:240:ARG:CG	2.62	0.47
2:B:3:ASP:C	2:B:5:LEU:N	2.72	0.47
1:C:-2:HIS:O	1:C:-1:HIS:HB2	2.15	0.47
1:C:395:PHE:HD1	1:C:395:PHE:H	1.57	0.47
2:D:122:LEU:O	2:D:125:ASN:N	2.46	0.47
1:E:280:ASP:CG	1:E:318:LEU:HB2	2.39	0.47
1:E:423:VAL:HG12	1:E:425:LEU:HD23	1.97	0.47
1:E:439:LEU:HG	1:E:450:ILE:CD1	2.44	0.47
1:G:221:VAL:HG21	1:G:452:PHE:HE2	1.80	0.47
1:G:228:ASP:OD1	1:G:229:GLU:N	2.43	0.47
1:A:226:LEU:HB3	2:B:23:TYR:OH	2.15	0.47
2:B:59:VAL:HG12	2:B:60:THR:N	2.29	0.47
1:C:65:LEU:HD22	1:C:158:VAL:HG12	1.96	0.47
1:C:212:LEU:O	1:C:215:THR:N	2.48	0.47
2:D:68:ILE:N	2:D:68:ILE:CD1	2.77	0.47
1:E:37:GLN:HB2	1:E:38:PRO:CD	2.45	0.47
1:E:86:GLN:O	1:E:87:PRO:C	2.56	0.47
1:E:306:LEU:O	1:E:306:LEU:HD12	2.14	0.47
1:E:354:ARG:C	1:E:355:TYR:HD1	2.22	0.47
1:A:303:ASN:HB3	1:C:304:TYR:CD1	2.50	0.47
1:A:354:ARG:C	1:A:355:TYR:HD1	2.23	0.47
2:D:3:ASP:C	2:D:5:LEU:N	2.69	0.47
2:D:23:TYR:CD2	2:D:24:LYS:N	2.81	0.47
2:D:70:ASN:O	2:D:72:HIS:N	2.46	0.47
1:E:303:ASN:HD21	1:E:308:GLN:HA	1.80	0.47
1:E:416:ARG:HA	1:E:421:GLN:O	2.15	0.47
1:G:346:GLY:CA	1:G:405:GLY:HA3	2.45	0.47
1:A:65:LEU:HD12	1:A:179:ALA:HB2	1.97	0.47
1:A:82:LEU:HB2	1:A:137:ASP:HB2	1.96	0.47
1:A:393:PHE:N	1:A:393:PHE:HD2	2.13	0.47
2:B:103:ILE:C	2:B:104:GLN:HE21	2.23	0.47
1:C:83:CYS:HA	1:C:140:GLN:NE2	2.30	0.47
1:E:395:PHE:CD1	1:E:395:PHE:N	2.82	0.47
1:A:26:ARG:CG	1:A:27:VAL:N	2.77	0.47
1:A:418:PRO:CB	1:A:419:GLU:OE1	2.62	0.47
1:A:423:VAL:HG12	1:A:425:LEU:HD23	1.97	0.47
1:C:11:HIS:N	1:C:11:HIS:CD2	2.82	0.47
2:D:58:HIS:NE2	2:D:107:MET:HE3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:LYS:HE2	1:E:168:ASP:OD1	2.15	0.47
1:E:348:ASN:HB2	1:E:375:SER:HB2	1.97	0.47
2:F:38:LYS:HD3	2:F:99:HIS:CE1	2.50	0.47
1:G:86:GLN:HA	1:G:86:GLN:NE2	2.29	0.47
1:G:145:LYS:HZ1	1:G:168:ASP:CB	2.28	0.47
1:G:198:LEU:HB3	1:G:428:VAL:HG21	1.97	0.47
1:A:78:GLY:O	1:A:91:CYS:HB2	2.15	0.46
1:A:275:ALA:O	1:A:276:VAL:C	2.57	0.46
2:B:115:PHE:O	2:B:116:ASN:C	2.58	0.46
1:C:211:SER:HA	1:C:435:GLN:NE2	2.30	0.46
1:C:438:CYS:SG	1:C:439:LEU:N	2.88	0.46
2:D:103:ILE:C	2:D:104:GLN:HE21	2.23	0.46
1:G:226:LEU:HD13	2:H:62:LEU:HD11	1.96	0.46
1:G:346:GLY:O	1:G:347:GLN:C	2.58	0.46
2:H:52:ASN:HB3	2:H:55:ALA:HB2	1.95	0.46
1:A:153:LEU:N	1:A:153:LEU:HD12	2.30	0.46
1:A:345:SER:C	1:A:405:GLY:HA3	2.41	0.46
2:F:23:TYR:CD2	2:F:24:LYS:N	2.81	0.46
1:A:73:TRP:HZ3	1:A:92:CYS:SG	2.38	0.46
1:A:395:PHE:CD1	1:A:395:PHE:N	2.83	0.46
1:C:95:GLY:CA	1:C:135:LEU:HD11	2.41	0.46
1:C:277:LYS:HE2	1:C:281:GLU:CD	2.40	0.46
1:C:428:VAL:HA	1:C:429:PRO:HD2	1.72	0.46
1:E:226:LEU:HD12	1:E:226:LEU:O	2.14	0.46
2:F:58:HIS:CE1	2:F:107:MET:HE3	2.51	0.46
1:G:65:LEU:HD22	1:G:158:VAL:HG12	1.98	0.46
1:A:98:PHE:HA	1:A:155:THR:CG2	2.45	0.46
1:A:208:GLY:N	3:A:474:HOH:O	2.48	0.46
1:A:216:GLN:HE21	2:B:115:PHE:HD1	1.62	0.46
1:A:430:ASP:OD1	1:A:432:SER:HB3	2.15	0.46
1:C:145:LYS:NZ	1:C:168:ASP:HB2	2.30	0.46
2:D:23:TYR:CG	2:D:24:LYS:N	2.84	0.46
2:F:59:VAL:HG12	2:F:60:THR:N	2.30	0.46
1:A:182:ALA:HB1	1:A:183:PRO:CD	2.39	0.46
2:B:116:ASN:N	2:B:116:ASN:ND2	2.44	0.46
2:B:122:LEU:O	2:B:123:LYS:C	2.59	0.46
1:C:197:LEU:HD21	1:C:218:LEU:HD11	1.97	0.46
1:C:378:ALA:HA	1:C:379:PRO:HD3	1.75	0.46
1:C:410:PHE:CD2	1:C:449:PRO:HG3	2.51	0.46
2:D:58:HIS:CE1	2:D:107:MET:HE3	2.49	0.46
1:E:67:ASN:O	1:E:71:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:GLY:O	1:E:91:CYS:HB2	2.16	0.46
2:F:23:TYR:CE1	2:F:38:LYS:HE2	2.50	0.46
2:H:58:HIS:CE1	2:H:107:MET:HE3	2.51	0.46
1:A:369:LEU:CD2	1:A:423:VAL:HG11	2.46	0.46
1:E:83:CYS:HA	1:E:140:GLN:NE2	2.31	0.46
1:E:360:ASP:O	1:E:363:GLU:HB3	2.16	0.46
2:F:70:ASN:C	2:F:72:HIS:N	2.69	0.46
2:F:103:ILE:N	2:F:104:GLN:HE21	2.14	0.46
1:G:97:LEU:HG	1:G:159:LEU:CD2	2.45	0.46
1:G:145:LYS:NZ	1:G:168:ASP:HB2	2.30	0.46
1:G:333:GLN:HG3	1:G:342:LEU:HD13	1.95	0.46
1:G:399:PRO:O	1:G:423:VAL:HG22	2.15	0.46
1:A:351:ASP:C	1:A:353:PHE:N	2.74	0.46
1:C:-1:HIS:ND1	1:C:0:GLY:N	2.63	0.46
1:E:306:LEU:HD23	1:E:393:PHE:HE1	1.79	0.46
2:F:52:ASN:HB3	2:F:55:ALA:HB2	1.97	0.46
1:G:26:ARG:HD3	1:G:290:VAL:HG23	1.97	0.46
1:G:99:LYS:HE2	1:G:150:VAL:CG1	2.45	0.46
2:H:3:ASP:C	2:H:5:LEU:N	2.72	0.46
2:H:23:TYR:CD1	2:H:38:LYS:HE2	2.50	0.46
2:H:115:PHE:O	2:H:116:ASN:C	2.58	0.46
1:A:228:ASP:OD1	1:A:229:GLU:N	2.47	0.46
2:D:59:VAL:O	2:D:82:GLU:HB2	2.15	0.46
1:G:452:PHE:CD1	1:G:452:PHE:N	2.84	0.46
2:H:23:TYR:CG	2:H:24:LYS:N	2.83	0.46
1:A:373:HIS:O	1:A:376:PRO:HD3	2.16	0.46
1:C:60:GLN:O	1:C:63:PRO:HD2	2.16	0.46
1:C:97:LEU:CD2	1:C:133:LEU:HB3	2.43	0.46
1:C:351:ASP:C	1:C:353:PHE:N	2.73	0.46
1:C:440:VAL:HG22	1:C:447:CYS:SG	2.56	0.46
2:D:125:ASN:C	2:D:127:GLN:H	2.24	0.46
1:E:333:GLN:HG3	1:E:342:LEU:HD13	1.98	0.46
2:F:23:TYR:CD1	2:F:34:VAL:HG22	2.51	0.46
2:F:86:GLU:OE2	2:F:86:GLU:HA	2.15	0.46
2:F:99:HIS:ND1	2:F:100:VAL:O	2.45	0.46
2:H:23:TYR:CD1	2:H:34:VAL:HG22	2.50	0.46
1:A:372:ARG:NH1	1:A:395:PHE:O	2.49	0.46
1:C:60:GLN:OE1	1:C:390:THR:HG23	2.16	0.46
2:D:112:GLY:O	2:D:113:PRO:C	2.56	0.46
1:E:194:ARG:NH1	1:E:194:ARG:HG3	2.31	0.46
1:G:216:GLN:HE21	2:H:115:PHE:HD1	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:VAL:CG2	2:H:46:GLU:N	2.79	0.46
1:A:80:LYS:HD3	1:A:84:GLU:HB2	1.98	0.45
1:A:198:LEU:HB3	1:A:428:VAL:HG21	1.97	0.45
1:C:37:GLN:C	1:C:39:PHE:N	2.73	0.45
1:C:212:LEU:O	1:C:213:LEU:C	2.56	0.45
1:C:239:SER:O	1:C:240:ARG:CG	2.64	0.45
1:C:280:ASP:CG	1:C:318:LEU:HB2	2.40	0.45
1:E:180:ASP:HA	1:E:370:ARG:O	2.17	0.45
1:A:60:GLN:O	1:A:63:PRO:HD2	2.16	0.45
1:A:157:THR:HG23	1:A:371:VAL:HG11	1.97	0.45
1:A:225:GLN:O	2:B:23:TYR:HE1	2.00	0.45
1:C:148:ILE:HG13	1:C:176:TYR:CZ	2.51	0.45
1:C:162:PHE:HB3	1:C:175:ASP:O	2.15	0.45
1:E:95:GLY:CA	1:E:135:LEU:HD11	2.44	0.45
1:E:353:PHE:CD1	1:E:353:PHE:C	2.94	0.45
1:G:145:LYS:HZ1	1:G:168:ASP:HB2	1.81	0.45
1:A:269:GLN:O	1:A:270:ALA:C	2.60	0.45
1:A:355:TYR:CD1	1:A:355:TYR:N	2.83	0.45
1:C:78:GLY:O	1:C:91:CYS:HB2	2.16	0.45
1:C:154:VAL:HG11	1:C:355:TYR:CB	2.46	0.45
1:C:226:LEU:HB3	2:D:23:TYR:OH	2.17	0.45
1:C:424:LEU:C	1:C:424:LEU:HD12	2.41	0.45
1:E:60:GLN:OE1	1:E:390:THR:HG23	2.16	0.45
1:E:162:PHE:HB3	1:E:175:ASP:O	2.15	0.45
1:G:153:LEU:HD12	1:G:153:LEU:N	2.31	0.45
1:A:21:ASN:OD1	2:B:36:GLN:HB2	2.16	0.45
1:C:395:PHE:CD1	1:C:395:PHE:N	2.83	0.45
2:D:72:HIS:CD2	2:D:72:HIS:O	2.70	0.45
2:D:125:ASN:O	2:D:126:LEU:C	2.58	0.45
1:G:290:VAL:CG2	1:G:291:PRO:CD	2.94	0.45
2:H:26:LEU:HD22	2:H:41:LEU:HD21	1.98	0.45
1:A:86:GLN:HA	1:A:86:GLN:NE2	2.29	0.45
1:E:61:MET:O	1:E:62:ARG:C	2.60	0.45
1:E:277:LYS:HE2	1:E:281:GLU:CD	2.40	0.45
1:G:436:THR:HA	1:G:450:ILE:O	2.17	0.45
1:A:304:TYR:CD1	1:C:303:ASN:HB3	2.52	0.45
2:B:10:ILE:O	2:B:13:PHE:HB2	2.17	0.45
2:D:3:ASP:C	2:D:5:LEU:H	2.25	0.45
1:E:231:GLU:CG	2:F:97:SER:OG	2.64	0.45
1:E:438:CYS:SG	1:E:439:LEU:N	2.89	0.45
1:G:303:ASN:ND2	1:G:308:GLN:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:351:ASP:HB2	1:G:377:THR:HG21	1.99	0.45
1:G:353:PHE:CD1	1:G:353:PHE:C	2.95	0.45
1:G:428:VAL:HA	1:G:429:PRO:HD2	1.77	0.45
2:H:86:GLU:HA	2:H:86:GLU:OE2	2.16	0.45
2:H:125:ASN:O	2:H:126:LEU:C	2.59	0.45
1:A:24:PHE:O	2:B:135:ILE:HA	2.16	0.45
1:A:86:GLN:HE21	1:A:86:GLN:CA	2.23	0.45
1:A:356:SER:OG	1:A:357:SER:N	2.50	0.45
1:C:3:SER:OG	2:D:75:HIS:ND1	2.35	0.45
1:C:99:LYS:HE2	1:C:150:VAL:CG1	2.46	0.45
1:C:274:GLU:O	1:C:275:ALA:C	2.59	0.45
1:E:274:GLU:O	1:E:275:ALA:C	2.60	0.45
1:G:60:GLN:OE1	1:G:390:THR:HG23	2.16	0.45
1:G:355:TYR:N	1:G:355:TYR:CD1	2.84	0.45
2:H:112:GLY:O	2:H:113:PRO:C	2.60	0.45
1:A:60:GLN:OE1	1:A:390:THR:HG23	2.16	0.45
1:A:65:LEU:HD22	1:A:158:VAL:HG12	1.99	0.45
1:A:148:ILE:HA	1:A:176:TYR:CE2	2.50	0.45
1:A:451:SER:HB2	2:B:76:LYS:HD3	1.99	0.45
1:C:11:HIS:C	1:C:12:THR:CG2	2.89	0.45
2:D:70:ASN:C	2:D:72:HIS:N	2.72	0.45
1:E:198:LEU:O	1:E:437:ALA:HB1	2.16	0.45
2:F:23:TYR:CG	2:F:24:LYS:N	2.84	0.45
2:H:59:VAL:HG12	2:H:60:THR:N	2.31	0.45
1:A:360:ASP:O	1:A:363:GLU:HB3	2.16	0.45
1:C:221:VAL:HG21	1:C:452:PHE:HE2	1.81	0.45
1:E:351:ASP:C	1:E:353:PHE:N	2.71	0.45
2:H:59:VAL:O	2:H:82:GLU:HB2	2.17	0.45
1:A:319:ALA:CB	1:A:325:LEU:HD22	2.46	0.45
2:B:23:TYR:CE1	2:B:38:LYS:HE2	2.52	0.45
1:C:13:LEU:HD13	2:D:38:LYS:CD	2.46	0.45
1:C:316:PHE:O	1:C:320:THR:HG23	2.16	0.45
1:E:451:SER:HB2	2:F:76:LYS:HD3	1.99	0.45
2:F:125:ASN:C	2:F:127:GLN:H	2.24	0.45
1:G:280:ASP:OD1	1:G:317:PRO:HD2	2.17	0.45
1:A:136:GLU:HG2	1:A:141:ARG:HB3	1.98	0.44
1:A:218:LEU:HD22	1:A:431:PHE:CE2	2.52	0.44
1:G:373:HIS:O	1:G:376:PRO:HD3	2.17	0.44
2:B:18:ASN:OD1	2:B:105:LYS:HE2	2.17	0.44
1:C:86:GLN:HA	1:C:86:GLN:NE2	2.31	0.44
1:C:244:ALA:HA	1:C:295:MET:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASP:OD1	1:C:317:PRO:HD2	2.16	0.44
1:C:303:ASN:HD21	1:C:308:GLN:HA	1.82	0.44
1:C:351:ASP:HB2	1:C:377:THR:HG21	1.98	0.44
1:E:37:GLN:C	1:E:39:PHE:N	2.72	0.44
1:G:360:ASP:O	1:G:363:GLU:HB3	2.17	0.44
1:A:95:GLY:CA	1:A:135:LEU:HD11	2.43	0.44
1:A:440:VAL:HG22	1:A:447:CYS:SG	2.57	0.44
1:C:198:LEU:HB3	1:C:428:VAL:HG21	1.99	0.44
2:D:103:ILE:N	2:D:104:GLN:HE21	2.14	0.44
1:E:24:PHE:CZ	1:E:233:CYS:HB2	2.52	0.44
2:F:59:VAL:O	2:F:82:GLU:HB2	2.17	0.44
1:G:26:ARG:HG3	1:G:27:VAL:H	1.81	0.44
1:G:26:ARG:NH1	1:G:289:SER:O	2.48	0.44
1:A:351:ASP:HB2	1:A:377:THR:HG21	1.99	0.44
1:C:444:SER:O	1:C:445:LEU:HB2	2.17	0.44
1:E:311:LEU:HD23	1:E:311:LEU:HA	1.75	0.44
1:E:418:PRO:CB	1:E:419:GLU:OE1	2.64	0.44
2:F:6:TYR:CD1	2:F:40:MET:HG2	2.52	0.44
1:G:2:PHE:CG	1:G:439:LEU:HD12	2.52	0.44
1:G:83:CYS:HA	1:G:140:GLN:NE2	2.32	0.44
1:A:99:LYS:HE2	1:A:150:VAL:HG12	1.98	0.44
1:C:37:GLN:NE2	1:C:37:GLN:N	2.64	0.44
1:C:132:GLU:CD	1:C:143:LYS:HE2	2.43	0.44
1:E:269:GLN:O	1:E:270:ALA:C	2.60	0.44
1:E:351:ASP:HB2	1:E:377:THR:HG21	1.98	0.44
1:G:78:GLY:O	1:G:91:CYS:HB2	2.17	0.44
1:G:97:LEU:CD2	1:G:133:LEU:HB3	2.47	0.44
1:G:138:GLU:H	1:G:138:GLU:CD	2.26	0.44
1:G:398:CYS:SG	1:G:423:VAL:HG21	2.57	0.44
1:A:132:GLU:CD	1:A:143:LYS:HE2	2.42	0.44
1:A:197:LEU:HB3	1:A:241:VAL:HG22	1.99	0.44
1:A:226:LEU:HB2	2:B:62:LEU:HD13	1.99	0.44
2:B:8:GLU:O	2:B:9:ASN:C	2.61	0.44
1:C:61:MET:O	1:C:62:ARG:C	2.58	0.44
1:C:138:GLU:CD	1:C:138:GLU:H	2.26	0.44
1:C:151:SER:CB	1:C:357:SER:HB2	2.45	0.44
1:E:211:SER:HA	1:E:435:GLN:NE2	2.32	0.44
2:F:137:CYS:O	2:F:138:ALA:C	2.59	0.44
1:G:11:HIS:C	1:G:12:THR:CG2	2.91	0.44
1:G:438:CYS:SG	1:G:439:LEU:N	2.91	0.44
1:G:455:PHE:CD1	1:G:455:PHE:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:CYS:SG	1:A:423:VAL:HG21	2.58	0.44
1:C:128:HIS:ND1	1:C:131:ASP:OD1	2.51	0.44
1:C:194:ARG:NH1	1:C:194:ARG:HG3	2.32	0.44
1:E:239:SER:O	1:E:240:ARG:HG2	2.18	0.44
1:E:303:ASN:HD22	1:E:305:THR:HG22	1.79	0.44
1:C:2:PHE:CG	1:C:439:LEU:HD12	2.53	0.44
1:C:193:ASP:CB	1:C:443:ARG:NH1	2.68	0.44
2:F:122:LEU:O	2:F:126:LEU:N	2.51	0.44
1:A:197:LEU:HD21	1:A:218:LEU:HD11	2.00	0.44
1:A:266:LYS:HD2	1:A:266:LYS:C	2.43	0.44
1:C:403:PHE:CD1	1:C:403:PHE:C	2.96	0.44
2:D:137:CYS:O	2:D:138:ALA:C	2.61	0.44
1:E:65:LEU:HD22	1:E:158:VAL:HG12	2.00	0.44
1:E:151:SER:CB	1:E:357:SER:HB2	2.42	0.44
1:G:26:ARG:CG	1:G:27:VAL:N	2.81	0.44
1:A:148:ILE:HG13	1:A:176:TYR:CZ	2.51	0.43
1:A:185:LYS:HA	1:A:186:PRO:HD3	1.79	0.43
1:A:353:PHE:CD1	1:A:353:PHE:C	2.95	0.43
1:A:452:PHE:N	1:A:452:PHE:CD1	2.85	0.43
1:C:24:PHE:O	2:D:135:ILE:HA	2.18	0.43
1:C:26:ARG:HD3	1:C:290:VAL:HG23	1.98	0.43
1:E:26:ARG:CD	1:E:290:VAL:HG23	2.48	0.43
1:E:269:GLN:HE22	1:G:320:THR:HB	1.83	0.43
1:E:348:ASN:HB3	1:E:375:SER:HB2	1.99	0.43
1:E:440:VAL:HG22	1:E:447:CYS:SG	2.58	0.43
1:G:244:ALA:HA	1:G:295:MET:HB2	1.99	0.43
2:H:81:ARG:NH1	2:H:108:LEU:O	2.51	0.43
1:A:145:LYS:NZ	1:A:168:ASP:HB2	2.33	0.43
1:A:284:LEU:HD23	2:B:126:LEU:HD11	2.00	0.43
1:A:330:ASN:CB	1:A:331:PRO:HD3	2.35	0.43
1:C:308:GLN:OE1	1:C:330:ASN:ND2	2.39	0.43
1:C:342:LEU:HD12	1:C:343:GLY:H	1.83	0.43
1:C:418:PRO:CB	1:C:419:GLU:OE1	2.65	0.43
1:E:14:LEU:HD11	2:F:98:ILE:HG22	1.99	0.43
1:E:372:ARG:NH1	1:E:395:PHE:O	2.51	0.43
1:G:-2:HIS:O	1:G:-1:HIS:CB	2.66	0.43
1:G:37:GLN:HB2	1:G:38:PRO:CD	2.48	0.43
1:G:197:LEU:HB3	1:G:241:VAL:HG22	2.00	0.43
1:G:243:LEU:N	1:G:243:LEU:CD2	2.81	0.43
1:G:395:PHE:CD1	1:G:395:PHE:N	2.83	0.43
2:H:103:ILE:CA	2:H:104:GLN:HE21	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:HB3	1:A:175:ASP:O	2.17	0.43
1:A:298:GLU:OE1	1:A:298:GLU:HA	2.18	0.43
1:A:315:MET:HG2	1:C:314:CYS:SG	2.58	0.43
2:B:32:VAL:CG1	2:B:36:GLN:OE1	2.65	0.43
2:B:59:VAL:CG1	2:B:60:THR:N	2.81	0.43
1:G:148:ILE:HG13	1:G:176:TYR:CZ	2.52	0.43
1:G:269:GLN:O	1:G:270:ALA:C	2.61	0.43
1:G:416:ARG:HA	1:G:421:GLN:O	2.18	0.43
1:G:443:ARG:HH11	1:G:443:ARG:HG2	1.83	0.43
1:A:11:HIS:C	1:A:12:THR:CG2	2.90	0.43
1:A:85:LEU:CG	1:A:165:VAL:HG21	2.48	0.43
1:C:148:ILE:HA	1:C:176:TYR:CE2	2.49	0.43
2:D:23:TYR:CD1	2:D:34:VAL:HG22	2.53	0.43
1:E:82:LEU:HD21	1:E:142:ILE:HG22	2.00	0.43
1:E:172:LEU:C	1:E:172:LEU:HD23	2.44	0.43
2:F:44:TYR:CD2	2:F:44:TYR:C	2.96	0.43
1:G:24:PHE:O	2:H:135:ILE:HA	2.18	0.43
1:G:274:GLU:O	1:G:275:ALA:C	2.59	0.43
2:H:18:ASN:OD1	2:H:105:LYS:HE2	2.18	0.43
2:H:55:ALA:O	2:H:57:LEU:N	2.52	0.43
1:A:36:SER:O	1:A:37:GLN:C	2.61	0.43
1:A:62:ARG:CB	1:A:63:PRO:HD3	2.44	0.43
1:C:185:LYS:H	1:C:185:LYS:HG2	1.69	0.43
2:D:32:VAL:CG1	2:D:36:GLN:OE1	2.65	0.43
1:E:373:HIS:O	1:E:376:PRO:HD3	2.17	0.43
2:F:24:LYS:HB3	2:F:118:ASP:OD1	2.19	0.43
2:F:26:LEU:HD22	2:F:41:LEU:HD21	2.00	0.43
1:G:82:LEU:HD21	1:G:142:ILE:HG22	2.01	0.43
1:G:231:GLU:CG	2:H:97:SER:OG	2.66	0.43
1:G:346:GLY:N	1:G:405:GLY:HA3	2.34	0.43
1:A:154:VAL:HG11	1:A:355:TYR:CB	2.46	0.43
2:B:23:TYR:CD1	2:B:34:VAL:HG22	2.53	0.43
2:D:3:ASP:O	2:D:5:LEU:N	2.52	0.43
2:H:34:VAL:O	2:H:38:LYS:HG3	2.18	0.43
2:B:59:VAL:O	2:B:82:GLU:HB2	2.18	0.43
1:C:194:ARG:HG3	1:C:194:ARG:HH11	1.84	0.43
1:C:239:SER:C	1:C:240:ARG:CG	2.92	0.43
2:D:22:THR:O	2:D:23:TYR:C	2.61	0.43
1:G:298:GLU:OE1	1:G:298:GLU:HA	2.18	0.43
1:A:239:SER:O	1:A:240:ARG:HG2	2.19	0.43
2:B:17:GLN:O	2:B:18:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ALA:O	2:B:57:LEU:N	2.52	0.43
2:B:103:ILE:CA	2:B:104:GLN:HE21	2.32	0.43
1:C:80:LYS:HD3	1:C:84:GLU:HB2	2.01	0.43
1:C:266:LYS:C	1:C:266:LYS:HD2	2.44	0.43
1:C:346:GLY:N	1:C:405:GLY:HA3	2.34	0.43
1:C:365:LEU:CD1	1:C:404:CYS:HB2	2.47	0.43
2:D:4:GLN:O	2:D:8:GLU:HG3	2.19	0.43
1:E:280:ASP:OD1	1:E:317:PRO:HD2	2.19	0.43
1:G:61:MET:O	1:G:62:ARG:C	2.61	0.43
1:G:239:SER:C	1:G:240:ARG:CG	2.92	0.43
1:A:399:PRO:O	1:A:423:VAL:HG22	2.19	0.43
1:C:136:GLU:HG2	1:C:141:ARG:HB3	2.01	0.43
2:F:20:ILE:HG23	2:F:104:GLN:HG3	2.01	0.43
1:G:306:LEU:HD23	1:G:393:PHE:HE1	1.82	0.43
1:A:369:LEU:HD21	1:A:423:VAL:HG11	2.01	0.43
2:D:44:TYR:CD2	2:D:44:TYR:C	2.96	0.43
1:E:194:ARG:HG3	1:E:194:ARG:HH11	1.83	0.43
1:E:346:GLY:CA	1:E:405:GLY:HA3	2.48	0.43
1:G:226:LEU:HB3	2:H:23:TYR:OH	2.19	0.43
1:A:-3:HIS:H1	1:A:-3:HIS:CD2	2.37	0.42
1:A:231:GLU:CG	2:B:97:SER:OG	2.66	0.42
1:C:101:MET:HB2	1:C:128:HIS:CD2	2.54	0.42
1:C:451:SER:HB2	2:D:76:LYS:HD3	2.01	0.42
2:D:10:ILE:O	2:D:13:PHE:HB2	2.19	0.42
2:D:60:THR:OG1	2:D:102:SER:OG	2.27	0.42
1:G:128:HIS:ND1	1:G:131:ASP:OD1	2.52	0.42
1:G:145:LYS:CE	1:G:168:ASP:HB3	2.49	0.42
1:G:151:SER:CB	1:G:357:SER:HB2	2.45	0.42
1:G:182:ALA:HB1	1:G:183:PRO:CD	2.39	0.42
1:A:151:SER:CB	1:A:357:SER:HB2	2.45	0.42
1:C:355:TYR:N	1:C:355:TYR:CD1	2.86	0.42
2:D:34:VAL:O	2:D:38:LYS:HG3	2.19	0.42
1:E:11:HIS:C	1:E:12:THR:CG2	2.92	0.42
1:E:138:GLU:CD	1:E:138:GLU:H	2.27	0.42
1:A:274:GLU:O	1:A:275:ALA:C	2.62	0.42
1:C:188:PRO:HD2	1:C:338:GLY:O	2.19	0.42
1:C:197:LEU:HB3	1:C:241:VAL:HG22	2.01	0.42
1:E:26:ARG:NH1	1:E:289:SER:O	2.51	0.42
2:F:18:ASN:OD1	2:F:105:LYS:HE2	2.20	0.42
1:G:36:SER:O	1:G:37:GLN:C	2.60	0.42
1:G:125:LYS:NZ	1:G:356:SER:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:VAL:CG1	2:H:60:THR:N	2.82	0.42
1:A:37:GLN:HB2	1:A:38:PRO:CD	2.50	0.42
1:A:395:PHE:HA	1:A:396:PRO:HD3	1.87	0.42
1:C:-1:HIS:ND1	1:C:-1:HIS:C	2.76	0.42
2:D:42:TYR:O	2:D:45:VAL:HG22	2.20	0.42
1:E:312:HIS:ND1	1:E:313:PRO:HD2	2.33	0.42
1:E:439:LEU:HD11	1:E:450:ILE:HD11	2.00	0.42
2:F:112:GLY:O	2:F:113:PRO:C	2.61	0.42
2:F:115:PHE:O	2:F:116:ASN:C	2.63	0.42
1:C:14:LEU:HD23	1:C:14:LEU:HA	1.90	0.42
1:C:190:LEU:HB2	1:C:443:ARG:HB2	2.01	0.42
1:C:312:HIS:ND1	1:C:313:PRO:HD2	2.34	0.42
1:C:342:LEU:HD12	1:C:343:GLY:N	2.34	0.42
1:E:-1:HIS:ND1	1:E:0:GLY:N	2.67	0.42
1:E:182:ALA:HB1	1:E:183:PRO:CD	2.38	0.42
1:E:209:GLY:HA2	1:E:212:LEU:HD12	2.01	0.42
1:E:277:LYS:O	1:E:280:ASP:HB3	2.20	0.42
1:E:346:GLY:O	1:E:347:GLN:C	2.62	0.42
1:E:411:GLY:HA3	1:E:427:THR:OG1	2.19	0.42
1:E:443:ARG:HH11	1:E:443:ARG:HG2	1.84	0.42
1:G:211:SER:HA	1:G:435:GLN:NE2	2.34	0.42
1:G:307:PRO:HG3	1:G:393:PHE:HZ	1.83	0.42
1:G:376:PRO:C	1:G:378:ALA:H	2.27	0.42
1:A:304:TYR:C	1:A:305:THR:O	2.63	0.42
1:C:145:LYS:NZ	1:C:168:ASP:CB	2.82	0.42
1:C:148:ILE:O	1:C:148:ILE:HG23	2.19	0.42
1:E:65:LEU:HD12	1:E:179:ALA:HB2	2.01	0.42
1:E:284:LEU:HD22	1:E:318:LEU:HB3	2.01	0.42
1:G:86:GLN:HE21	1:G:86:GLN:CA	2.24	0.42
1:G:145:LYS:NZ	1:G:168:ASP:CB	2.82	0.42
2:B:69:GLN:HE21	2:B:69:GLN:HB2	1.60	0.42
1:C:346:GLY:O	1:C:347:GLN:C	2.62	0.42
1:C:353:PHE:CD1	1:C:353:PHE:C	2.97	0.42
1:E:185:LYS:H	1:E:185:LYS:HG2	1.70	0.42
1:E:314:CYS:SG	1:G:315:MET:HG2	2.59	0.42
1:G:37:GLN:NE2	1:G:37:GLN:N	2.63	0.42
1:G:369:LEU:CD2	1:G:423:VAL:HG11	2.50	0.42
2:H:6:TYR:O	2:H:10:ILE:HG13	2.20	0.42
1:A:90:LYS:NZ	1:A:174:GLU:OE2	2.47	0.42
1:A:346:GLY:O	1:A:347:GLN:C	2.62	0.42
1:C:37:GLN:HB2	1:C:38:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ASP:HA	1:C:370:ARG:O	2.20	0.42
1:E:-2:HIS:O	1:E:-1:HIS:HB2	2.19	0.42
1:E:55:ALA:O	1:E:56:THR:C	2.63	0.42
1:E:128:HIS:O	1:E:129:PRO:C	2.62	0.42
1:E:403:PHE:CD1	1:E:403:PHE:C	2.97	0.42
1:G:225:GLN:HE21	2:H:133:SER:HB2	1.85	0.42
1:G:365:LEU:CD1	1:G:404:CYS:HB2	2.46	0.42
2:H:21:VAL:O	2:H:102:SER:HA	2.20	0.42
1:A:101:MET:HB2	1:A:128:HIS:CD2	2.54	0.42
1:A:280:ASP:OD1	1:A:317:PRO:HD2	2.19	0.42
1:C:1:MET:SD	1:C:448:GLN:HB2	2.59	0.42
1:C:85:LEU:CG	1:C:165:VAL:HG21	2.50	0.42
1:C:430:ASP:O	1:C:430:ASP:CG	2.62	0.42
2:D:80:VAL:HG11	2:D:88:VAL:HG21	2.01	0.42
1:E:24:PHE:O	2:F:135:ILE:HA	2.19	0.42
1:E:455:PHE:CD1	1:E:455:PHE:C	2.97	0.42
1:G:198:LEU:O	1:G:437:ALA:HB1	2.20	0.42
2:H:99:HIS:ND1	2:H:100:VAL:O	2.45	0.42
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.87	0.42
1:C:298:GLU:HA	1:C:298:GLU:OE1	2.20	0.42
1:C:416:ARG:HA	1:C:421:GLN:O	2.19	0.42
2:D:59:VAL:HG12	2:D:60:THR:N	2.33	0.42
1:E:149:ASP:OD2	1:E:152:LYS:HB2	2.20	0.42
2:F:59:VAL:CG1	2:F:60:THR:N	2.81	0.42
2:F:69:GLN:HE21	2:F:69:GLN:HB2	1.59	0.42
1:G:101:MET:HB2	1:G:128:HIS:CD2	2.55	0.42
1:G:225:GLN:OE1	2:H:24:LYS:HE3	2.20	0.42
1:G:336:ILE:O	1:G:337:ASP:C	2.63	0.42
1:A:85:LEU:HD12	1:A:165:VAL:CG2	2.50	0.41
1:A:97:LEU:HG	1:A:159:LEU:CD2	2.47	0.41
2:B:3:ASP:C	2:B:5:LEU:H	2.27	0.41
2:B:24:LYS:HB3	2:B:118:ASP:OD1	2.20	0.41
1:C:340:ARG:HB2	1:C:400:HIS:ND1	2.35	0.41
1:C:424:LEU:HD12	1:C:425:LEU:N	2.35	0.41
2:F:3:ASP:C	2:F:5:LEU:H	2.27	0.41
2:F:32:VAL:CG1	2:F:36:GLN:OE1	2.68	0.41
1:G:85:LEU:CG	1:G:165:VAL:HG21	2.50	0.41
1:G:372:ARG:NH1	1:G:395:PHE:O	2.51	0.41
2:H:64:SER:HA	2:H:76:LYS:O	2.20	0.41
1:C:153:LEU:N	1:C:153:LEU:HD12	2.35	0.41
1:C:213:LEU:O	1:C:217:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:SER:HA	2:D:76:LYS:O	2.20	0.41
1:E:36:SER:O	1:E:37:GLN:C	2.63	0.41
2:F:17:GLN:O	2:F:18:ASN:HB2	2.20	0.41
1:G:239:SER:C	1:G:240:ARG:HG3	2.46	0.41
1:G:351:ASP:C	1:G:353:PHE:N	2.74	0.41
2:B:122:LEU:O	2:B:126:LEU:N	2.53	0.41
1:C:239:SER:C	1:C:240:ARG:HG3	2.46	0.41
2:D:59:VAL:CG1	2:D:60:THR:N	2.82	0.41
1:E:197:LEU:HA	1:E:439:LEU:HD23	2.03	0.41
1:E:266:LYS:C	1:E:266:LYS:HD2	2.46	0.41
1:E:298:GLU:HA	1:E:298:GLU:OE1	2.20	0.41
1:E:369:LEU:CD2	1:E:423:VAL:HG11	2.50	0.41
1:E:410:PHE:CD2	1:E:449:PRO:HG3	2.55	0.41
1:G:14:LEU:HD11	2:H:98:ILE:HG22	2.01	0.41
1:A:77:VAL:HG13	1:A:79:VAL:CB	2.50	0.41
1:A:138:GLU:CD	1:A:138:GLU:H	2.29	0.41
1:A:376:PRO:C	1:A:378:ALA:H	2.29	0.41
1:A:403:PHE:CD1	1:A:403:PHE:C	2.98	0.41
1:A:410:PHE:CD2	1:A:449:PRO:HG3	2.55	0.41
2:B:26:LEU:HD22	2:B:41:LEU:HD21	2.01	0.41
1:E:1:MET:SD	1:E:448:GLN:HB2	2.60	0.41
1:E:26:ARG:CG	1:E:27:VAL:N	2.84	0.41
2:F:45:VAL:CG2	2:F:46:GLU:N	2.82	0.41
1:G:37:GLN:C	1:G:39:PHE:N	2.69	0.41
1:G:185:LYS:H	1:G:185:LYS:HG2	1.73	0.41
2:H:3:ASP:O	2:H:5:LEU:N	2.54	0.41
2:H:38:LYS:HD3	2:H:99:HIS:CE1	2.56	0.41
1:A:-3:HIS:H3	1:A:414:ILE:HD12	1.86	0.41
1:A:180:ASP:HA	1:A:370:ARG:O	2.20	0.41
1:A:290:VAL:CG2	1:A:291:PRO:CD	2.94	0.41
1:A:405:GLY:O	1:A:428:VAL:O	2.38	0.41
2:B:62:LEU:O	2:B:98:ILE:HA	2.20	0.41
2:F:3:ASP:O	2:F:5:LEU:N	2.54	0.41
2:H:3:ASP:C	2:H:5:LEU:H	2.28	0.41
2:H:80:VAL:HG11	2:H:88:VAL:HG21	2.03	0.41
2:H:122:LEU:O	2:H:126:LEU:N	2.54	0.41
1:A:99:LYS:HE2	1:A:150:VAL:CG1	2.50	0.41
2:D:18:ASN:OD1	2:D:105:LYS:HE2	2.20	0.41
1:E:37:GLN:NE2	1:E:37:GLN:N	2.67	0.41
1:E:342:LEU:HD12	1:E:343:GLY:N	2.35	0.41
1:G:3:SER:OG	2:H:75:HIS:ND1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:HIS:C	1:G:12:THR:HG23	2.45	0.41
1:G:132:GLU:CD	1:G:143:LYS:HE2	2.45	0.41
1:G:172:LEU:CD2	3:G:474:HOH:O	2.66	0.41
1:G:357:SER:O	1:G:358:MET:C	2.63	0.41
1:G:410:PHE:CD2	1:G:449:PRO:HG3	2.55	0.41
2:H:23:TYR:CE1	2:H:38:LYS:HE2	2.55	0.41
2:H:32:VAL:CG1	2:H:36:GLN:OE1	2.69	0.41
1:A:55:ALA:O	1:A:56:THR:C	2.64	0.41
1:A:277:LYS:O	1:A:280:ASP:HB3	2.20	0.41
1:A:391:ASP:HA	1:A:392:PRO:HD3	1.80	0.41
1:A:430:ASP:O	1:A:430:ASP:CG	2.63	0.41
1:C:83:CYS:HB3	1:C:140:GLN:OE1	2.20	0.41
1:E:330:ASN:ND2	1:E:345:SER:OG	2.53	0.41
1:E:364:ILE:O	1:E:368:THR:HG23	2.20	0.41
1:G:55:ALA:O	1:G:56:THR:C	2.63	0.41
1:G:316:PHE:O	1:G:320:THR:HG23	2.21	0.41
2:B:58:HIS:CE1	2:B:107:MET:HE3	2.56	0.41
1:E:2:PHE:CG	1:E:439:LEU:HD12	2.56	0.41
1:E:132:GLU:CD	1:E:143:LYS:HE2	2.46	0.41
1:E:304:TYR:C	1:E:305:THR:O	2.62	0.41
2:F:20:ILE:HG23	2:F:104:GLN:CG	2.51	0.41
1:G:293:ASP:OD1	1:G:332:TYR:OH	2.33	0.41
1:A:74:GLY:O	1:A:75:SER:C	2.64	0.41
1:A:82:LEU:HD21	1:A:142:ILE:HG22	2.02	0.41
1:A:84:GLU:H	1:A:84:GLU:HG3	1.63	0.41
1:A:342:LEU:HD12	1:A:343:GLY:N	2.36	0.41
1:A:346:GLY:N	1:A:405:GLY:HA3	2.36	0.41
1:A:364:ILE:O	1:A:367:TRP:HB3	2.20	0.41
2:B:3:ASP:O	2:B:5:LEU:N	2.53	0.41
1:C:24:PHE:CZ	1:C:233:CYS:HB2	2.56	0.41
1:C:135:LEU:HB2	1:C:144:LEU:HD11	2.03	0.41
1:C:171:PHE:CD2	1:C:171:PHE:C	2.99	0.41
1:C:229:GLU:OE2	1:E:9:ARG:NH1	2.52	0.41
1:C:333:GLN:HG3	1:C:342:LEU:HD13	2.02	0.41
1:E:226:LEU:HB3	2:F:23:TYR:OH	2.21	0.41
1:E:376:PRO:C	1:E:378:ALA:H	2.29	0.41
1:E:378:ALA:HA	1:E:379:PRO:HD3	1.77	0.41
2:F:80:VAL:HG11	2:F:88:VAL:HG21	2.03	0.41
1:G:77:VAL:HG13	1:G:79:VAL:CB	2.51	0.41
1:G:225:GLN:NE2	2:H:133:SER:HB2	2.35	0.41
1:G:266:LYS:C	1:G:266:LYS:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:CE	1:C:168:ASP:HB3	2.51	0.41
1:C:336:ILE:O	1:C:337:ASP:C	2.64	0.41
1:C:348:ASN:HB3	1:C:375:SER:HB2	2.03	0.41
1:C:354:ARG:C	1:C:355:TYR:CD1	2.99	0.41
2:D:23:TYR:O	2:D:24:LYS:C	2.64	0.41
2:D:122:LEU:O	2:D:123:LYS:C	2.64	0.41
1:G:14:LEU:HD23	1:G:14:LEU:HA	1.88	0.41
1:A:197:LEU:HD13	1:A:439:LEU:HD23	2.03	0.40
2:B:4:GLN:O	2:B:8:GLU:HG3	2.21	0.40
2:B:45:VAL:CG2	2:B:46:GLU:N	2.84	0.40
1:C:82:LEU:HD21	1:C:142:ILE:HG22	2.03	0.40
1:C:185:LYS:HA	1:C:186:PRO:HD3	1.80	0.40
1:C:276:VAL:O	1:C:277:LYS:C	2.63	0.40
1:C:311:LEU:HD23	1:C:311:LEU:HA	1.73	0.40
1:C:430:ASP:OD1	1:C:432:SER:HB3	2.21	0.40
1:E:159:LEU:H	1:E:159:LEU:CD2	2.27	0.40
1:G:277:LYS:O	1:G:281:GLU:HG3	2.21	0.40
2:H:70:ASN:O	2:H:72:HIS:N	2.54	0.40
1:A:61:MET:O	1:A:62:ARG:C	2.63	0.40
1:A:195:PHE:HB2	1:A:238:VAL:HG22	2.03	0.40
1:A:458:GLU:HG2	1:A:459:ASP:N	2.36	0.40
1:C:55:ALA:O	1:C:56:THR:C	2.64	0.40
1:C:80:LYS:HD2	1:C:84:GLU:O	2.21	0.40
1:C:198:LEU:O	1:C:437:ALA:HB1	2.21	0.40
1:C:369:LEU:CD2	1:C:423:VAL:HG11	2.51	0.40
1:E:21:ASN:OD1	2:F:36:GLN:HB2	2.21	0.40
1:E:219:VAL:O	1:E:223:THR:OG1	2.32	0.40
1:G:-1:HIS:C	1:G:-1:HIS:ND1	2.79	0.40
1:G:126:TYR:HD2	1:G:355:TYR:CE1	2.34	0.40
1:A:312:HIS:ND1	1:A:313:PRO:HD2	2.36	0.40
1:A:340:ARG:HB2	1:A:400:HIS:ND1	2.36	0.40
1:A:342:LEU:O	1:A:402:TYR:HA	2.21	0.40
1:A:357:SER:O	1:A:358:MET:C	2.62	0.40
1:C:197:LEU:HA	1:C:439:LEU:HD23	2.03	0.40
1:E:85:LEU:CG	1:E:165:VAL:HG21	2.52	0.40
1:G:82:LEU:HD12	1:G:82:LEU:HA	1.83	0.40
1:G:148:ILE:HG23	1:G:148:ILE:O	2.20	0.40
1:G:202:LEU:HD23	1:G:202:LEU:HA	1.89	0.40
1:G:312:HIS:ND1	1:G:313:PRO:HD2	2.36	0.40
1:A:197:LEU:HD13	1:A:439:LEU:CD2	2.51	0.40
1:A:410:PHE:CG	1:A:449:PRO:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:TYR:CD2	2:B:44:TYR:C	2.99	0.40
2:B:121:ILE:HD12	2:B:121:ILE:HA	1.92	0.40
2:H:4:GLN:O	2:H:8:GLU:HG3	2.21	0.40
2:H:8:GLU:O	2:H:9:ASN:C	2.65	0.40
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.95	0.40
1:A:128:HIS:O	1:A:129:PRO:C	2.64	0.40
1:A:172:LEU:HD23	1:A:172:LEU:C	2.47	0.40
2:B:5:LEU:O	2:B:9:ASN:ND2	2.54	0.40
1:C:226:LEU:HB2	2:D:62:LEU:HD13	2.03	0.40
1:E:7:ALA:O	1:E:9:ARG:N	2.55	0.40
1:E:190:LEU:HB2	1:E:443:ARG:HB2	2.02	0.40
1:E:316:PHE:O	1:E:320:THR:HG23	2.22	0.40
1:E:444:SER:O	1:E:445:LEU:HB2	2.22	0.40
1:G:128:HIS:O	1:G:129:PRO:C	2.65	0.40
1:G:280:ASP:CG	1:G:318:LEU:HB2	2.46	0.40
1:G:306:LEU:HB3	1:G:307:PRO:CD	2.47	0.40
2:H:41:LEU:HD13	2:H:103:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	406/476 (85%)	321 (79%)	63 (16%)	22 (5%)	1	9
1	C	399/476 (84%)	317 (79%)	60 (15%)	22 (6%)	1	8
1	E	398/476 (84%)	325 (82%)	50 (13%)	23 (6%)	1	8
1	G	398/476 (84%)	319 (80%)	56 (14%)	23 (6%)	1	8
2	B	141/144 (98%)	110 (78%)	24 (17%)	7 (5%)	1	10
2	D	141/144 (98%)	115 (82%)	19 (14%)	7 (5%)	1	10
2	F	141/144 (98%)	113 (80%)	21 (15%)	7 (5%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	141/144 (98%)	114 (81%)	19 (14%)	8 (6%)	1	8
All	All	2165/2480 (87%)	1734 (80%)	312 (14%)	119 (6%)	1	8

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ALA
1	A	76	GLY
1	A	79	VAL
1	A	330	ASN
1	A	405	GLY
2	B	140	ALA
1	C	-1	HIS
1	C	10	ALA
1	C	76	GLY
1	C	79	VAL
1	C	330	ASN
1	C	405	GLY
2	D	140	ALA
1	E	-1	HIS
1	E	76	GLY
1	E	79	VAL
1	E	330	ASN
1	E	405	GLY
2	F	140	ALA
1	G	-1	HIS
1	G	76	GLY
1	G	79	VAL
1	G	330	ASN
1	G	405	GLY
2	H	126	LEU
2	H	140	ALA
1	A	-1	HIS
1	A	8	GLN
1	A	310	PRO
1	A	420	ASP
2	B	56	GLN
2	B	84	LYS
2	B	126	LEU
1	C	8	GLN
1	C	310	PRO
1	C	420	ASP

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Mol	Chain	Res	Type
2	D	84	LYS
2	D	126	LEU
1	E	8	GLN
1	E	10	ALA
1	E	320	THR
1	E	420	ASP
2	F	84	LYS
2	F	126	LEU
1	G	8	GLN
1	G	10	ALA
1	G	310	PRO
1	G	420	ASP
2	H	56	GLN
2	H	84	LYS
1	A	38	PRO
1	A	180	ASP
1	A	265	THR
1	A	298	GLU
1	A	305	THR
1	A	320	THR
1	C	298	GLU
1	C	305	THR
1	C	320	THR
2	D	56	GLN
1	E	38	PRO
1	E	75	SER
1	E	298	GLU
1	E	305	THR
1	E	310	PRO
2	F	56	GLN
1	G	38	PRO
1	G	298	GLU
1	G	305	THR
1	G	320	THR
1	A	209	GLY
1	A	347	GLN
1	C	38	PRO
1	C	265	THR
1	C	301	PRO
1	C	347	GLN
1	E	180	ASP
1	E	301	PRO

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Mol	Chain	Res	Type
1	G	155	THR
1	G	180	ASP
1	G	265	THR
1	G	301	PRO
1	A	155	THR
1	A	301	PRO
2	B	142	PRO
1	C	180	ASP
1	C	209	GLY
1	E	155	THR
1	E	209	GLY
1	E	265	THR
1	E	418	PRO
2	F	142	PRO
1	G	347	GLN
1	A	29	VAL
1	A	418	PRO
2	B	112	GLY
1	C	75	SER
1	C	418	PRO
2	D	142	PRO
1	E	245	GLY
1	G	29	VAL
1	G	418	PRO
2	H	142	PRO
2	B	54	GLY
1	C	29	VAL
2	F	54	GLY
1	G	245	GLY
2	H	54	GLY
2	D	54	GLY
2	D	112	GLY
1	E	29	VAL
1	C	245	GLY
1	E	77	VAL
2	F	112	GLY
2	H	71	GLY
1	A	317	PRO
1	G	317	PRO
1	G	429	PRO
2	H	112	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	355/409 (87%)	318 (90%)	37 (10%)	7	28
1	C	350/409 (86%)	318 (91%)	32 (9%)	9	33
1	E	349/409 (85%)	314 (90%)	35 (10%)	7	29
1	G	349/409 (85%)	316 (90%)	33 (10%)	8	31
2	B	125/126 (99%)	113 (90%)	12 (10%)	8	31
2	D	125/126 (99%)	114 (91%)	11 (9%)	9	35
2	F	125/126 (99%)	114 (91%)	11 (9%)	9	35
2	H	125/126 (99%)	114 (91%)	11 (9%)	9	35
All	All	1903/2140 (89%)	1721 (90%)	182 (10%)	8	31

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	8	GLN
1	A	15	SER
1	A	20	ASN
1	A	21	ASN
1	A	23	THR
1	A	29	VAL
1	A	31	THR
1	A	37	GLN
1	A	56	THR
1	A	84	GLU
1	A	85	LEU
1	A	134	VAL
1	A	136	GLU
1	A	140	GLN
1	A	151	SER
1	A	155	THR
1	A	167	ASP
1	A	193	ASP

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Mol	Chain	Res	Type
1	A	200	SER
1	A	222	VAL
1	A	226	LEU
1	A	234	SER
1	A	243	LEU
1	A	285	GLN
1	A	306	LEU
1	A	372	ARG
1	A	406	ASN
1	A	418	PRO
1	A	419	GLU
1	A	422	THR
1	A	424	LEU
1	A	430	ASP
1	A	434	THR
1	A	447	CYS
1	A	459	ASP
1	A	462	LEU
2	B	3	ASP
2	B	23	TYR
2	B	34	VAL
2	B	68	ILE
2	B	69	GLN
2	B	72	HIS
2	B	81	ARG
2	B	83	ASP
2	B	85	LEU
2	B	104	GLN
2	B	116	ASN
2	B	129	CYS
1	C	-1	HIS
1	C	8	GLN
1	C	15	SER
1	C	20	ASN
1	C	21	ASN
1	C	23	THR
1	C	29	VAL
1	C	31	THR
1	C	37	GLN
1	C	56	THR
1	C	85	LEU
1	C	134	VAL

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Mol	Chain	Res	Type
1	C	136	GLU
1	C	140	GLN
1	C	151	SER
1	C	155	THR
1	C	167	ASP
1	C	200	SER
1	C	222	VAL
1	C	226	LEU
1	C	234	SER
1	C	243	LEU
1	C	306	LEU
1	C	372	ARG
1	C	406	ASN
1	C	418	PRO
1	C	419	GLU
1	C	422	THR
1	C	424	LEU
1	C	430	ASP
1	C	434	THR
1	C	447	CYS
2	D	3	ASP
2	D	23	TYR
2	D	34	VAL
2	D	68	ILE
2	D	69	GLN
2	D	81	ARG
2	D	83	ASP
2	D	85	LEU
2	D	104	GLN
2	D	116	ASN
2	D	129	CYS
1	E	-1	HIS
1	E	8	GLN
1	E	15	SER
1	E	20	ASN
1	E	21	ASN
1	E	23	THR
1	E	29	VAL
1	E	31	THR
1	E	37	GLN
1	E	56	THR
1	E	84	GLU

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Mol	Chain	Res	Type
1	E	85	LEU
1	E	134	VAL
1	E	136	GLU
1	E	140	GLN
1	E	151	SER
1	E	155	THR
1	E	166	ARG
1	E	167	ASP
1	E	193	ASP
1	E	200	SER
1	E	222	VAL
1	E	226	LEU
1	E	234	SER
1	E	243	LEU
1	E	306	LEU
1	E	372	ARG
1	E	406	ASN
1	E	418	PRO
1	E	419	GLU
1	E	422	THR
1	E	430	ASP
1	E	434	THR
1	E	438	CYS
1	E	447	CYS
2	F	3	ASP
2	F	34	VAL
2	F	63	VAL
2	F	68	ILE
2	F	69	GLN
2	F	81	ARG
2	F	83	ASP
2	F	85	LEU
2	F	104	GLN
2	F	116	ASN
2	F	129	CYS
1	G	-1	HIS
1	G	15	SER
1	G	20	ASN
1	G	21	ASN
1	G	23	THR
1	G	29	VAL
1	G	31	THR

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Mol	Chain	Res	Type
1	G	37	GLN
1	G	56	THR
1	G	58	LEU
1	G	85	LEU
1	G	134	VAL
1	G	136	GLU
1	G	140	GLN
1	G	151	SER
1	G	155	THR
1	G	167	ASP
1	G	200	SER
1	G	222	VAL
1	G	226	LEU
1	G	234	SER
1	G	243	LEU
1	G	306	LEU
1	G	372	ARG
1	G	406	ASN
1	G	418	PRO
1	G	419	GLU
1	G	422	THR
1	G	424	LEU
1	G	430	ASP
1	G	434	THR
1	G	438	CYS
1	G	447	CYS
2	H	3	ASP
2	H	23	TYR
2	H	34	VAL
2	H	68	ILE
2	H	69	GLN
2	H	81	ARG
2	H	83	ASP
2	H	85	LEU
2	H	104	GLN
2	H	116	ASN
2	H	129	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS

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Mol	Chain	Res	Type
1	A	5	GLN
1	A	20	ASN
1	A	37	GLN
1	A	70	GLN
1	A	86	GLN
1	A	216	GLN
1	A	246	ASN
1	A	269	GLN
1	A	285	GLN
1	A	326	GLN
1	A	333	GLN
1	A	361	HIS
2	B	9	ASN
2	B	69	GLN
2	B	70	ASN
2	B	72	HIS
2	B	104	GLN
2	B	116	ASN
2	B	127	GLN
2	B	128	ASN
1	C	-3	HIS
1	C	5	GLN
1	C	37	GLN
1	C	67	ASN
1	C	70	GLN
1	C	86	GLN
1	C	216	GLN
1	C	269	GLN
1	C	285	GLN
1	C	333	GLN
1	C	361	HIS
1	C	406	ASN
2	D	9	ASN
2	D	56	GLN
2	D	69	GLN
2	D	70	ASN
2	D	72	HIS
2	D	116	ASN
2	D	127	GLN
2	D	128	ASN
1	E	-3	HIS
1	E	5	GLN

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Mol	Chain	Res	Type
1	E	11	HIS
1	E	37	GLN
1	E	70	GLN
1	E	86	GLN
1	E	216	GLN
1	E	269	GLN
1	E	285	GLN
1	E	326	GLN
1	E	333	GLN
1	E	406	ASN
2	F	9	ASN
2	F	56	GLN
2	F	69	GLN
2	F	104	GLN
2	F	116	ASN
2	F	127	GLN
2	F	128	ASN
2	F	136	GLN
1	G	-2	HIS
1	G	11	HIS
1	G	37	GLN
1	G	70	GLN
1	G	86	GLN
1	G	216	GLN
1	G	326	GLN
1	G	333	GLN
1	G	361	HIS
1	G	406	ASN
2	H	9	ASN
2	H	69	GLN
2	H	70	ASN
2	H	104	GLN
2	H	116	ASN
2	H	127	GLN
2	H	128	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	416/476 (87%)	0.46	34 (8%) 17 9	21, 54, 104, 113	0
1	C	409/476 (85%)	0.33	24 (5%) 28 14	20, 50, 98, 108	0
1	E	408/476 (85%)	0.36	30 (7%) 20 10	24, 53, 94, 107	0
1	G	408/476 (85%)	0.51	38 (9%) 14 7	27, 58, 103, 114	0
2	B	143/144 (99%)	0.29	7 (4%) 35 18	29, 52, 90, 113	0
2	D	143/144 (99%)	0.16	6 (4%) 40 22	32, 49, 83, 102	0
2	F	143/144 (99%)	0.45	7 (4%) 35 18	38, 64, 88, 116	0
2	H	143/144 (99%)	0.43	7 (4%) 35 18	34, 68, 93, 111	0
All	All	2213/2480 (89%)	0.39	153 (6%) 23 12	20, 56, 100, 116	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	210	GLU	5.4
1	A	465	LEU	5.4
1	E	264	LEU	5.2
2	D	3	ASP	5.2
2	H	144	ALA	5.2
1	E	250	HIS	4.6
1	C	264	LEU	4.5
1	C	438	CYS	4.5
2	D	2	ALA	4.4
2	H	4	GLN	4.3
1	G	264	LEU	4.0
1	A	264	LEU	4.0
1	E	438	CYS	4.0
1	A	464	GLY	4.0
1	C	-2	HIS	4.0
2	B	2	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	144	ALA	3.9
1	C	124	SER	3.9
1	E	130	ASP	3.9
1	A	265	THR	3.9
1	C	53	ILE	3.9
1	G	250	HIS	3.9
1	G	265	THR	3.9
1	G	128	HIS	3.8
1	C	447	CYS	3.7
1	G	438	CYS	3.7
2	F	144	ALA	3.6
1	C	265	THR	3.6
1	G	87	PRO	3.6
1	E	210	GLU	3.5
1	E	-1	HIS	3.5
2	F	142	PRO	3.4
2	B	3	ASP	3.4
1	G	41	LEU	3.4
1	G	-2	HIS	3.4
2	B	142	PRO	3.4
1	A	299	PHE	3.3
1	E	128	HIS	3.3
1	A	388	TYR	3.3
2	H	3	ASP	3.3
1	A	87	PRO	3.3
1	C	250	HIS	3.3
1	C	380	ASP	3.3
1	A	447	CYS	3.3
1	G	92	CYS	3.2
1	E	41	LEU	3.1
1	A	165	VAL	3.1
1	G	127	ILE	3.1
1	C	147	THR	3.1
1	E	447	CYS	3.1
1	A	250	HIS	3.1
1	G	91	CYS	3.1
1	G	447	CYS	3.1
1	G	76	GLY	3.0
1	C	210	GLU	3.0
1	A	131	ASP	3.0
1	A	91	CYS	3.0
1	C	305	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	438	CYS	3.0
1	E	265	THR	3.0
1	E	457	ALA	2.9
2	F	2	ALA	2.9
1	G	101	MET	2.9
1	A	75	SER	2.9
1	C	130	ASP	2.9
2	D	144	ALA	2.8
1	G	124	SER	2.8
1	A	210	GLU	2.8
1	A	-1	HIS	2.8
1	G	381	THR	2.8
1	A	462	LEU	2.8
1	C	128	HIS	2.8
1	C	92	CYS	2.8
1	G	129	PRO	2.8
1	A	130	ASP	2.7
1	C	77	VAL	2.7
1	E	87	PRO	2.7
1	C	299	PHE	2.7
1	E	299	PHE	2.7
2	H	2	ALA	2.7
1	A	126	TYR	2.7
2	B	53	SER	2.6
2	F	4	GLN	2.6
1	G	207	GLY	2.6
1	C	81	LYS	2.6
1	E	134	VAL	2.6
1	E	124	SER	2.6
1	E	-2	HIS	2.5
1	E	458	GLU	2.5
1	A	137	ASP	2.5
1	A	160	ALA	2.5
1	G	380	ASP	2.5
2	F	143	ARG	2.5
2	H	107	MET	2.5
2	F	3	ASP	2.5
1	A	-2	HIS	2.5
1	A	70	GLN	2.4
1	E	101	MET	2.4
1	E	266	LYS	2.4
1	G	152	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	85	LEU	2.4
1	G	299	PHE	2.4
1	A	163	GLY	2.4
1	C	76	GLY	2.4
1	E	380	ASP	2.4
1	G	90	LYS	2.4
2	F	86	GLU	2.4
1	G	211	SER	2.4
2	D	4	GLN	2.3
1	E	305	THR	2.3
1	G	78	GLY	2.3
1	A	152	LYS	2.3
1	G	100	ALA	2.3
2	D	107	MET	2.3
1	C	85	LEU	2.3
2	H	53	SER	2.3
1	C	269	GLN	2.3
1	G	163	GLY	2.2
1	G	379	PRO	2.2
1	C	101	MET	2.2
1	G	306	LEU	2.2
1	A	77	VAL	2.2
1	A	94	VAL	2.2
1	G	133	LEU	2.2
1	E	-3	HIS	2.2
1	A	124	SER	2.2
1	E	86	GLN	2.2
2	B	4	GLN	2.2
2	D	55	ALA	2.2
1	G	162	PHE	2.2
1	E	126	TYR	2.2
1	E	75	SER	2.2
1	E	306	LEU	2.2
1	C	167	ASP	2.2
1	E	381	THR	2.1
2	B	71	GLY	2.1
1	A	127	ILE	2.1
1	A	82	LEU	2.1
1	E	100	ALA	2.1
1	A	74	GLY	2.1
1	G	77	VAL	2.1
1	A	304	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	70	GLN	2.1
1	G	267	LYS	2.1
1	G	135	LEU	2.1
1	E	206	GLY	2.1
1	G	208	GLY	2.1
1	A	81	LYS	2.0
1	G	-1	HIS	2.0
1	A	169	GLY	2.0
1	G	54	TYR	2.0
1	E	208	GLY	2.0
2	H	56	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.