



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 04:52 PM UTC

PDB ID : 6QD6 / pdb_00006qd6
Title : Molecular scaffolds expand the nanobody toolkit for cryo-EM applications:
crystal structure of Mb-cHopQ-Nb207
Authors : Uchanski, T.; Masiulis, S.; Fischer, B.; Kalichuk, V.; Wohlkonig, A.; Zogg, T.;
Remaut, H.; Vranken, W.; Aricescu, A.R.; Pardon, E.; Steyaert, J.
Deposited on : 2018-12-31
Resolution : 2.84 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

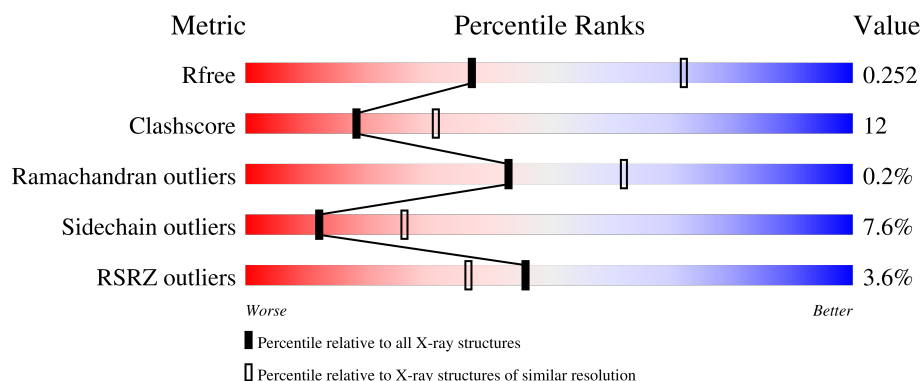
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	542	2% 67% 13% • 17%
1	B	542	5% 63% 16% • 18%
1	C	542	3% 54% 22% • 20%
1	D	542	2% 66% 14% • 18%
1	E	542	4% 61% 18% • 17%

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Mol	Chain	Length	Quality of chain
1	F	542	3% 62% 19% • 16%
1	G	542	% 62% 22% • 13%
1	H	542	4% 60% 12% • 26%
1	I	542	3% 60% 14% • 23%
1	J	542	4% 50% 17% • 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33077 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 Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3409	2107	603	686	13			
1	B	446	Total	C	N	O	S	0	0	0
			3372	2081	594	682	15			
1	C	431	Total	C	N	O	S	0	0	0
			3263	2015	573	660	15			
1	D	446	Total	C	N	O	S	0	0	0
			3384	2090	598	683	13			
1	E	451	Total	C	N	O	S	0	0	0
			3406	2103	599	689	15			
1	F	457	Total	C	N	O	S	0	0	0
			3465	2144	606	702	13			
1	G	469	Total	C	N	O	S	0	0	0
			3561	2197	626	723	15			
1	H	399	Total	C	N	O	S	0	0	0
			3015	1868	525	609	13			
1	I	419	Total	C	N	O	S	0	0	0
			3187	1976	558	640	13			
1	J	380	Total	C	N	O	S	0	0	0
			2900	1795	508	584	13			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

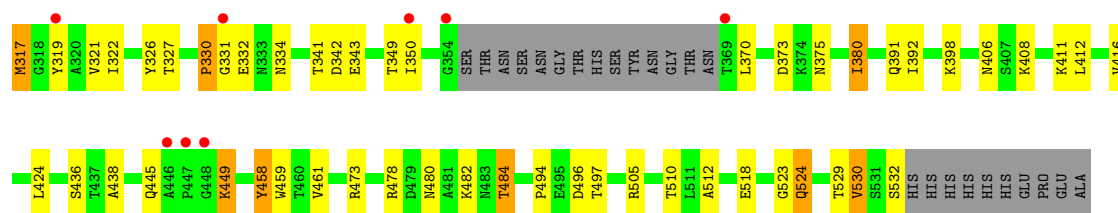
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		

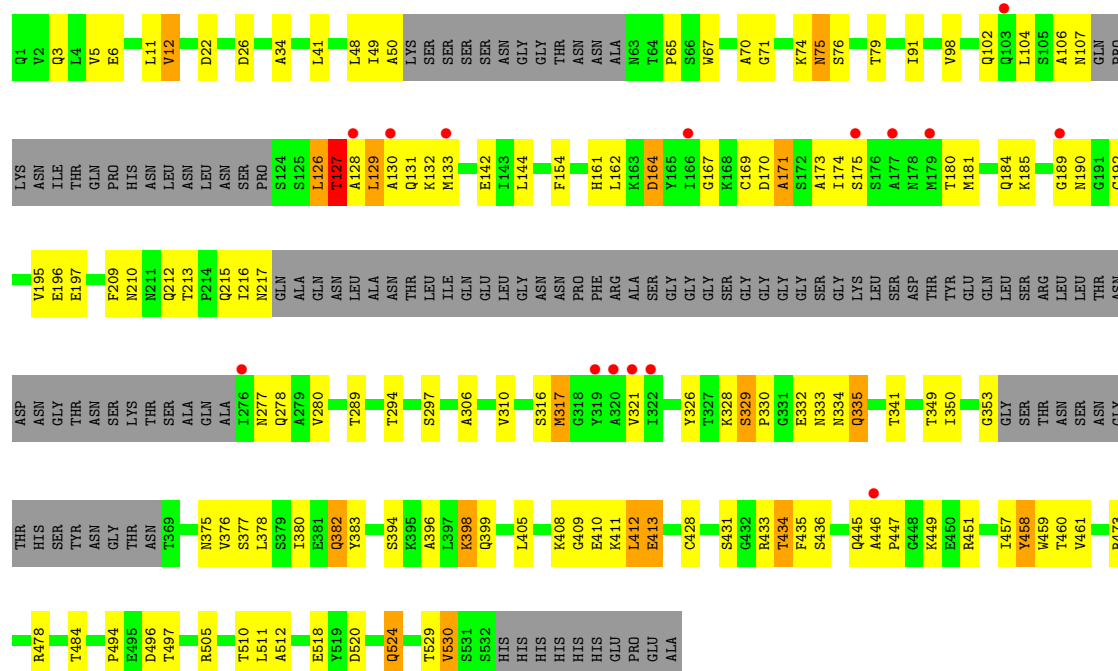
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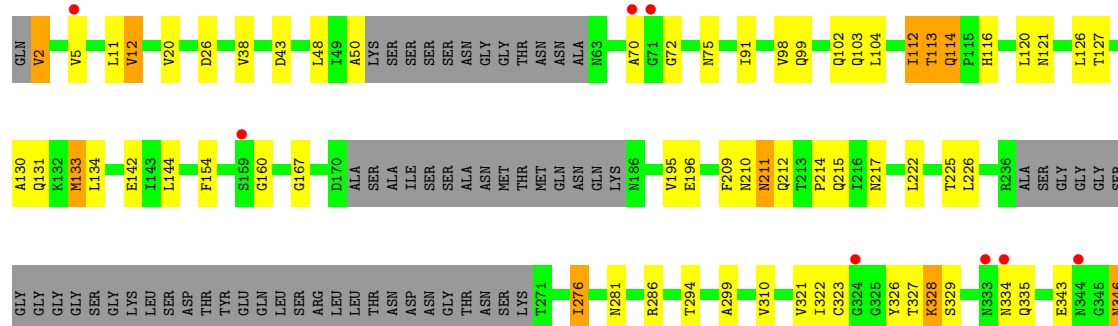
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	15	Total 15	O 15	0	0
3	C	11	Total 11	O 11	0	0
3	D	12	Total 12	O 12	0	0
3	E	8	Total 8	O 8	0	0
3	F	14	Total 14	O 14	0	0
3	G	14	Total 14	O 14	0	0
3	H	5	Total 5	O 5	0	0
3	I	12	Total 12	O 12	0	0
3	J	5	Total 5	O 5	0	0

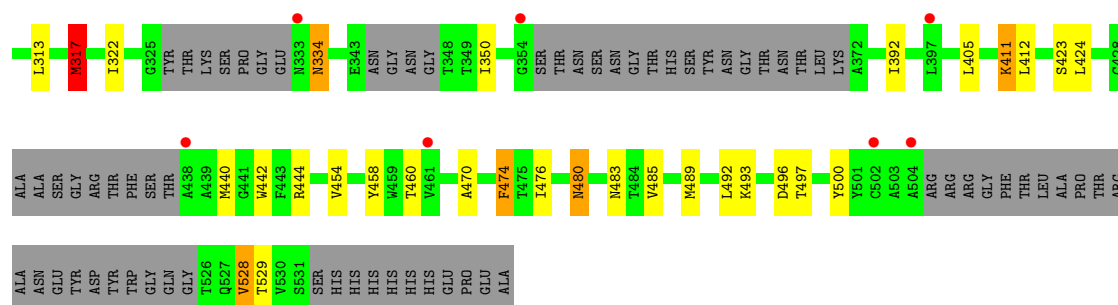


● Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207

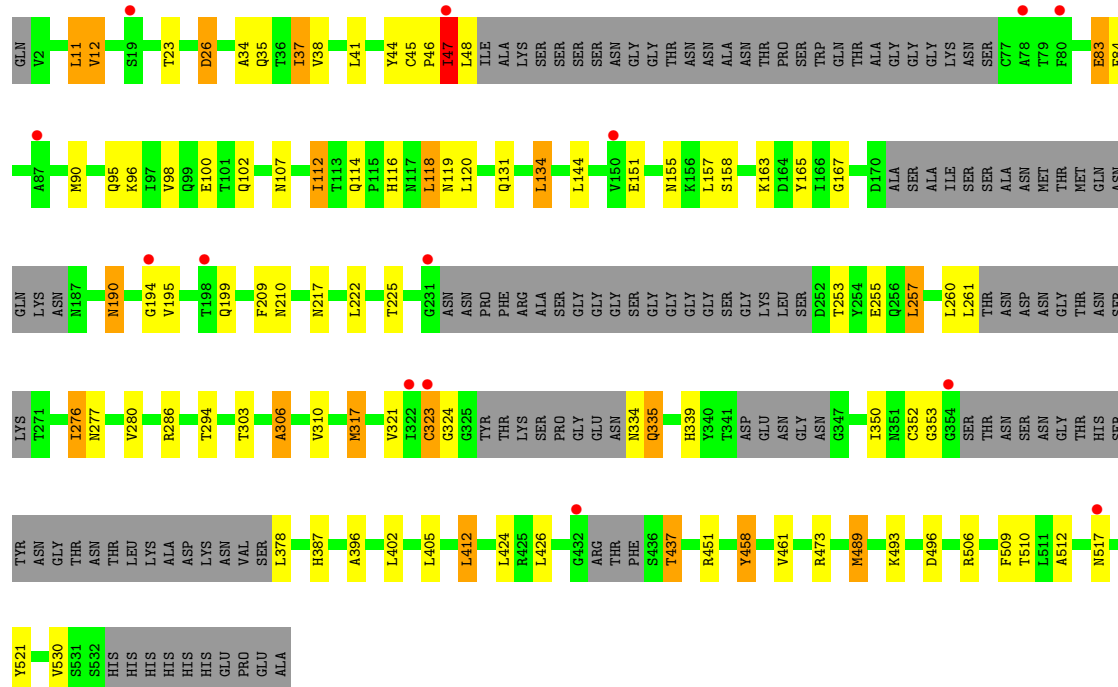


● Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207

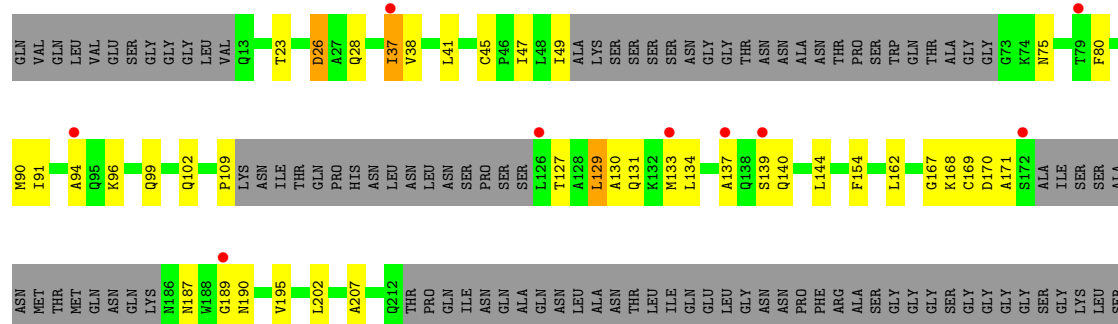


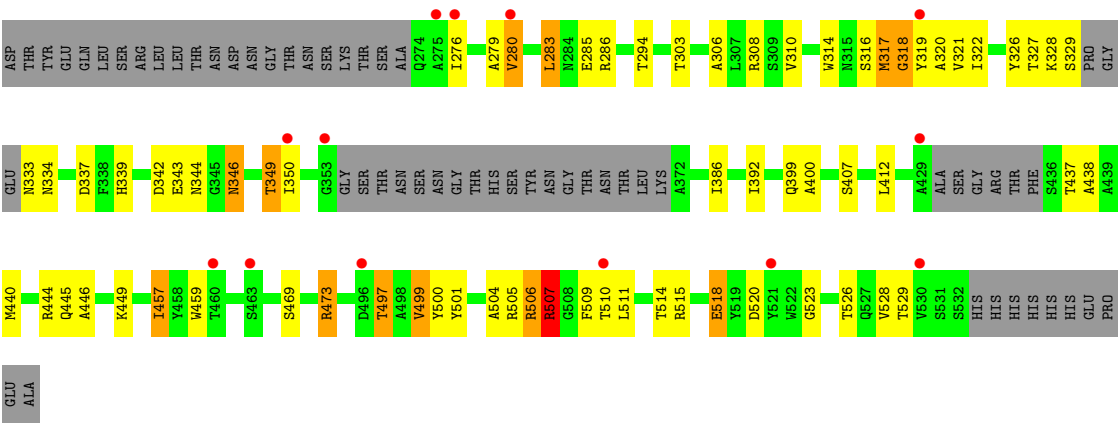


- Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207



- Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.17Å 92.92Å 244.22Å 92.05° 96.93° 112.15°	Depositor
Resolution (Å)	41.45 – 2.84 41.45 – 2.84	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.45-2.84) 95.6 (41.45-2.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.204 , 0.239 0.226 , 0.252	Depositor DCC
R_{free} test set	6538 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 98.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33077	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.84	1/3461 (0.0%)	1.39	19/4690 (0.4%)
1	B	0.88	1/3419 (0.0%)	1.40	24/4625 (0.5%)
1	C	0.89	0/3310	1.44	30/4479 (0.7%)
1	D	0.86	1/3432 (0.0%)	1.39	23/4647 (0.5%)
1	E	0.86	0/3453	1.37	24/4676 (0.5%)
1	F	0.89	4/3514 (0.1%)	1.41	27/4760 (0.6%)
1	G	0.83	0/3610	1.39	15/4887 (0.3%)
1	H	0.82	0/3051	1.39	13/4124 (0.3%)
1	I	0.83	2/3229 (0.1%)	1.40	35/4369 (0.8%)
1	J	0.89	1/2939 (0.0%)	1.40	27/3971 (0.7%)
All	All	0.86	10/33418 (0.0%)	1.40	237/45228 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	489	MET	SD-CE	-6.99	1.62	1.79
1	F	317	MET	CA-C	6.75	1.61	1.52
1	F	317	MET	N-CA	-5.98	1.36	1.45
1	J	170	ASP	CA-C	5.88	1.59	1.52
1	F	489	MET	SD-CE	-5.63	1.65	1.79
1	A	121	ASN	CA-C	-5.32	1.47	1.53
1	I	45	CYS	CA-C	5.25	1.57	1.53
1	F	461	VAL	N-CA	-5.20	1.40	1.46
1	B	160	GLY	N-CA	5.16	1.50	1.45
1	D	328	LYS	CA-C	5.03	1.59	1.52

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	191	GLY	N-CA-C	10.55	124.74	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	ALA	N-CA-C	10.40	122.20	111.07
1	G	431	SER	N-CA-C	10.28	122.57	111.36
1	C	127	THR	N-CA-C	-9.94	100.43	111.07
1	E	333	ASN	N-CA-C	9.13	121.59	110.91
1	C	329	SER	CA-C-N	9.12	129.18	119.78
1	C	329	SER	C-N-CA	9.12	129.18	119.78
1	F	76	SER	N-CA-C	9.09	121.19	111.28
1	A	78	ALA	N-CA-C	-8.95	102.15	113.43
1	J	506	ARG	N-CA-C	-8.64	97.70	110.23
1	A	459	TRP	N-CA-C	8.45	120.49	111.28
1	C	398	LYS	N-CA-C	8.44	120.56	111.36
1	B	332	GLU	N-CA-C	7.93	121.74	110.23
1	D	471	LYS	N-CA-C	7.92	119.54	111.07
1	B	281	ASN	CA-C-N	7.90	130.71	120.44
1	B	281	ASN	C-N-CA	7.90	130.71	120.44
1	C	70	ALA	N-CA-C	7.80	119.86	111.36
1	E	26	ASP	CA-CB-CG	7.78	120.38	112.60
1	J	523	GLY	CA-C-N	7.75	131.00	120.54
1	J	523	GLY	C-N-CA	7.75	131.00	120.54
1	I	253	THR	N-CA-C	-7.65	104.09	113.50
1	F	211	ASN	CA-C-N	7.56	133.02	120.70
1	F	211	ASN	C-N-CA	7.56	133.02	120.70
1	D	327	THR	CB-CA-C	7.54	123.02	109.29
1	H	483	ASN	CA-CB-CG	7.43	120.03	112.60
1	F	253	THR	N-CA-C	-7.32	103.45	112.38
1	J	334	ASN	N-CA-C	7.29	121.58	111.74
1	J	318	GLY	CA-C-N	7.23	130.69	120.28
1	J	318	GLY	C-N-CA	7.23	130.69	120.28
1	I	120	LEU	N-CA-C	-7.13	104.71	113.41
1	E	175	SER	N-CA-C	7.04	119.45	108.96
1	F	479	ASP	CA-C-N	7.02	129.99	120.38
1	F	479	ASP	C-N-CA	7.02	129.99	120.38
1	E	100	GLU	N-CA-C	-6.99	105.28	113.88
1	J	129	LEU	N-CA-C	-6.94	103.72	111.71
1	J	499	VAL	N-CA-CB	6.93	118.27	110.72
1	F	399	GLN	N-CA-C	6.88	118.86	111.36
1	C	510	THR	N-CA-C	-6.79	105.00	113.55
1	A	398	LYS	N-CA-C	6.65	118.61	111.36
1	G	316	SER	N-CA-C	6.46	118.12	111.14
1	A	45	CYS	N-CA-C	6.44	124.05	109.81
1	E	461	VAL	N-CA-C	-6.44	106.68	111.90
1	J	169	CYS	CA-C-N	6.43	131.66	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	169	CYS	C-N-CA	6.43	131.66	121.44
1	F	72	GLY	N-CA-C	6.42	120.43	112.73
1	G	335	GLN	N-CA-C	6.41	119.66	110.24
1	I	44	TYR	CB-CA-C	6.41	119.41	109.03
1	C	435	PHE	N-CA-C	-6.31	104.74	112.88
1	J	507	ARG	N-CA-C	6.29	118.91	110.35
1	F	252	ASP	N-CA-C	-6.28	105.37	113.16
1	I	253	THR	CA-C-N	6.27	128.60	120.44
1	I	253	THR	C-N-CA	6.27	128.60	120.44
1	C	184	GLN	N-CA-C	6.27	117.99	111.03
1	A	76	SER	CA-C-N	-6.19	115.50	126.45
1	A	76	SER	C-N-CA	-6.19	115.50	126.45
1	C	131	GLN	CA-C-N	6.18	131.04	120.72
1	C	131	GLN	C-N-CA	6.18	131.04	120.72
1	I	306	ALA	CA-C-N	6.18	128.47	120.44
1	I	306	ALA	C-N-CA	6.18	128.47	120.44
1	I	437	THR	CA-C-N	6.11	129.08	120.28
1	I	437	THR	C-N-CA	6.11	129.08	120.28
1	E	3	GLN	N-CA-C	6.09	118.96	109.52
1	H	528	VAL	N-CA-CB	6.08	119.79	111.41
1	F	294	THR	CA-C-N	6.06	128.69	120.38
1	F	294	THR	C-N-CA	6.06	128.69	120.38
1	G	164	ASP	CA-CB-CG	6.06	118.66	112.60
1	B	331	GLY	N-CA-C	6.04	121.72	113.99
1	J	327	THR	N-CA-C	-6.01	106.07	113.41
1	I	165	TYR	N-CA-C	6.01	118.99	111.24
1	H	196	GLU	CA-C-N	6.00	128.25	120.44
1	H	196	GLU	C-N-CA	6.00	128.25	120.44
1	E	165	TYR	N-CA-C	5.95	120.59	112.68
1	D	160	GLY	CA-C-N	5.90	129.00	120.38
1	D	160	GLY	C-N-CA	5.90	129.00	120.38
1	I	190	ASN	CA-CB-CG	5.88	118.48	112.60
1	F	75	ASN	CA-C-N	5.87	128.15	120.28
1	F	75	ASN	C-N-CA	5.87	128.15	120.28
1	H	158	SER	N-CA-C	5.87	117.76	111.36
1	I	45	CYS	CA-C-N	-5.87	113.54	120.11
1	I	45	CYS	C-N-CA	-5.87	113.54	120.11
1	C	409	GLY	N-CA-C	-5.84	105.74	112.29
1	B	178	ASN	CA-CB-CG	5.84	118.44	112.60
1	E	186	ASN	N-CA-C	5.80	117.42	109.18
1	G	224	ASN	CA-CB-CG	5.80	118.40	112.60
1	F	510	THR	N-CA-C	-5.80	105.21	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	44	TYR	CA-C-N	5.80	128.66	123.10
1	I	44	TYR	C-N-CA	5.80	128.66	123.10
1	I	84	PHE	CA-CB-CG	5.79	119.58	113.80
1	I	34	ALA	CA-C-N	5.78	127.95	120.44
1	I	34	ALA	C-N-CA	5.78	127.95	120.44
1	A	322	ILE	N-CA-CB	5.76	117.41	110.95
1	E	76	SER	N-CA-C	5.76	117.56	111.28
1	I	112	ILE	N-CA-CB	5.75	118.06	111.39
1	E	376	VAL	N-CA-C	5.75	121.29	109.34
1	D	211	ASN	CA-CB-CG	5.75	118.34	112.60
1	D	281	ASN	CA-CB-CG	5.75	118.34	112.60
1	D	103	GLN	CA-C-N	5.73	127.89	120.44
1	D	103	GLN	C-N-CA	5.73	127.89	120.44
1	D	142	GLU	CB-CG-CD	5.72	122.33	112.60
1	E	78	ALA	N-CA-C	-5.70	104.45	111.75
1	B	282	ASN	CA-CB-CG	5.70	118.30	112.60
1	C	171	ALA	CA-C-N	5.68	128.21	120.54
1	C	171	ALA	C-N-CA	5.68	128.21	120.54
1	E	103	GLN	CA-C-N	5.68	127.89	120.28
1	E	103	GLN	C-N-CA	5.68	127.89	120.28
1	F	254	TYR	CA-C-N	5.68	129.34	120.82
1	F	254	TYR	C-N-CA	5.68	129.34	120.82
1	I	107	ASN	CA-CB-CG	5.66	118.26	112.60
1	B	342	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	510	THR	N-CA-C	-5.64	106.44	113.55
1	E	63	ASN	CA-C-N	5.64	129.24	120.60
1	E	63	ASN	C-N-CA	5.64	129.24	120.60
1	A	400	ALA	N-CA-C	-5.63	106.95	113.88
1	B	294	THR	CA-C-N	5.63	128.10	120.38
1	B	294	THR	C-N-CA	5.63	128.10	120.38
1	D	374	LYS	N-CA-C	5.62	118.16	110.24
1	C	341	THR	CA-C-N	5.60	132.24	121.54
1	C	341	THR	C-N-CA	5.60	132.24	121.54
1	C	12	VAL	CA-C-N	5.60	128.66	120.71
1	C	12	VAL	C-N-CA	5.60	128.66	120.71
1	J	207	ALA	CA-C-N	5.60	127.78	120.28
1	J	207	ALA	C-N-CA	5.60	127.78	120.28
1	I	225	THR	CA-C-N	5.59	128.23	120.29
1	I	225	THR	C-N-CA	5.59	128.23	120.29
1	F	458	TYR	N-CA-C	5.58	118.50	109.40
1	B	160	GLY	CA-C-N	5.58	128.02	120.38
1	B	160	GLY	C-N-CA	5.58	128.02	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	SER	N-CA-C	5.57	115.30	108.11
1	G	399	GLN	N-CA-C	5.56	120.33	112.93
1	C	458	TYR	N-CA-C	5.56	118.61	109.72
1	B	196	GLU	CA-C-N	5.54	127.98	120.44
1	B	196	GLU	C-N-CA	5.54	127.98	120.44
1	C	434	THR	N-CA-C	5.53	117.87	110.35
1	B	12	VAL	CA-C-N	5.52	128.55	120.71
1	B	12	VAL	C-N-CA	5.52	128.55	120.71
1	B	480	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	528	VAL	N-CA-CB	5.50	118.79	111.64
1	F	211	ASN	CA-CB-CG	5.50	118.10	112.60
1	E	528	VAL	N-CA-CB	5.49	118.78	111.64
1	H	458	TYR	N-CA-C	5.47	118.14	109.50
1	J	407	SER	CA-C-N	5.45	128.13	120.28
1	J	407	SER	C-N-CA	5.45	128.13	120.28
1	F	252	ASP	CA-C-N	5.44	129.31	120.60
1	F	252	ASP	C-N-CA	5.44	129.31	120.60
1	C	294	THR	CA-C-N	5.44	127.83	120.38
1	C	294	THR	C-N-CA	5.44	127.83	120.38
1	I	353	GLY	N-CA-C	5.43	122.85	115.30
1	A	142	GLU	CB-CG-CD	5.43	121.83	112.60
1	F	212	GLN	CA-C-N	5.43	126.87	120.09
1	F	212	GLN	C-N-CA	5.43	126.87	120.09
1	G	294	THR	CA-C-N	5.42	127.80	120.38
1	G	294	THR	C-N-CA	5.42	127.80	120.38
1	A	77	CYS	CB-CA-C	-5.40	102.28	110.06
1	D	407	SER	CA-C-N	5.40	127.52	120.28
1	D	407	SER	C-N-CA	5.40	127.52	120.28
1	D	299	ALA	N-CA-C	-5.40	105.04	111.03
1	B	373	ASP	CA-CB-CG	5.39	117.99	112.60
1	I	510	THR	N-CA-C	-5.39	105.51	112.68
1	F	202	LEU	N-CA-C	-5.38	104.29	112.04
1	I	119	ASN	N-CA-C	5.36	117.13	111.28
1	J	328	LYS	N-CA-C	-5.36	107.39	114.04
1	J	497	THR	CB-CA-C	-5.36	102.52	110.67
1	B	341	THR	CB-CA-C	5.36	119.03	109.65
1	F	461	VAL	N-CA-C	-5.36	105.16	111.00
1	H	317	MET	N-CA-C	5.36	121.00	113.02
1	E	174	ILE	N-CA-C	-5.35	100.68	108.17
1	J	139	SER	CA-C-N	5.33	127.43	120.28
1	J	139	SER	C-N-CA	5.33	127.43	120.28
1	C	380	ILE	N-CA-CB	5.30	117.75	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	294	THR	CA-C-N	5.30	127.64	120.38
1	I	294	THR	C-N-CA	5.30	127.64	120.38
1	D	133	MET	CA-C-N	5.29	127.63	120.65
1	D	133	MET	C-N-CA	5.29	127.63	120.65
1	E	380	ILE	N-CA-CB	5.29	117.73	110.54
1	E	294	THR	CA-C-N	5.28	127.62	120.38
1	E	294	THR	C-N-CA	5.28	127.62	120.38
1	G	217	ASN	N-CA-C	-5.28	105.57	112.23
1	D	450	GLU	N-CA-C	5.27	117.94	110.50
1	A	211	ASN	CA-CB-CG	5.27	117.87	112.60
1	G	458	TYR	N-CA-C	5.25	117.66	109.52
1	I	517	ASN	CA-CB-CG	5.25	117.85	112.60
1	B	316	SER	N-CA-C	5.24	117.07	111.36
1	A	196	GLU	CA-C-N	5.24	127.25	120.44
1	A	196	GLU	C-N-CA	5.24	127.25	120.44
1	J	294	THR	CA-C-N	5.18	127.47	120.38
1	J	294	THR	C-N-CA	5.18	127.47	120.38
1	J	509	PHE	N-CA-C	5.17	116.39	108.42
1	C	142	GLU	CB-CG-CD	5.17	121.38	112.60
1	D	506	ARG	CA-C-N	5.16	128.54	120.75
1	D	506	ARG	C-N-CA	5.16	128.54	120.75
1	G	255	GLU	CA-C-N	5.16	127.45	120.65
1	G	255	GLU	C-N-CA	5.16	127.45	120.65
1	I	194	GLY	CA-C-N	5.15	127.79	120.53
1	I	194	GLY	C-N-CA	5.15	127.79	120.53
1	A	294	THR	CA-C-N	5.12	127.40	120.38
1	A	294	THR	C-N-CA	5.12	127.40	120.38
1	H	214	PRO	CA-C-N	5.12	127.14	120.28
1	H	214	PRO	C-N-CA	5.12	127.14	120.28
1	B	221	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	231	GLY	CA-C-N	5.09	127.93	120.71
1	A	231	GLY	C-N-CA	5.09	127.93	120.71
1	C	65	PRO	CA-C-N	5.09	127.05	120.44
1	C	65	PRO	C-N-CA	5.09	127.05	120.44
1	H	221	ASN	CA-C-N	5.08	127.50	120.29
1	H	221	ASN	C-N-CA	5.08	127.50	120.29
1	C	341	THR	CB-CA-C	5.08	117.66	110.24
1	I	165	TYR	CB-CA-C	-5.08	102.48	110.86
1	C	102	GLN	CA-C-N	5.07	127.08	120.28
1	C	102	GLN	C-N-CA	5.07	127.08	120.28
1	D	528	VAL	N-CA-CB	5.07	118.23	111.64
1	F	347	GLY	CA-C-N	5.06	132.09	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	347	GLY	C-N-CA	5.06	132.09	123.03
1	I	26	ASP	CA-CB-CG	5.05	117.65	112.60
1	I	199	GLN	CA-C-N	5.04	127.04	120.28
1	I	199	GLN	C-N-CA	5.04	127.04	120.28
1	E	102	GLN	CA-C-N	5.04	127.30	120.44
1	E	102	GLN	C-N-CA	5.04	127.30	120.44
1	H	474	PHE	CA-CB-CG	5.04	118.84	113.80
1	D	294	THR	CA-C-N	5.04	127.28	120.38
1	D	294	THR	C-N-CA	5.04	127.28	120.38
1	J	501	TYR	CA-C-N	5.04	128.62	121.42
1	J	501	TYR	C-N-CA	5.04	128.62	121.42
1	I	458	TYR	N-CA-C	5.03	117.60	109.40
1	B	44	TYR	N-CA-C	5.03	120.41	113.97
1	J	134	LEU	CA-C-N	5.03	127.33	120.54
1	J	134	LEU	C-N-CA	5.03	127.33	120.54
1	E	65	PRO	CA-C-N	5.02	126.97	120.44
1	E	65	PRO	C-N-CA	5.02	126.97	120.44
1	B	221	ASN	CA-C-N	5.02	127.51	120.28
1	B	221	ASN	C-N-CA	5.02	127.51	120.28
1	D	510	THR	N-CA-C	-5.02	106.00	112.68
1	G	196	GLU	CA-C-N	5.01	126.95	120.44
1	G	196	GLU	C-N-CA	5.01	126.95	120.44
1	C	383	TYR	CA-C-N	5.01	126.99	120.28
1	C	383	TYR	C-N-CA	5.01	126.99	120.28
1	F	380	ILE	N-CA-CB	5.01	117.35	110.54
1	H	322	ILE	N-CA-CB	5.00	116.17	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3409	0	3318	66	0
1	B	3372	0	3291	67	0
1	C	3263	0	3181	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3384	0	3298	48	0
1	E	3406	0	3329	100	0
1	F	3465	0	3388	87	0
1	G	3561	0	3477	127	0
1	H	3015	0	2948	58	0
1	I	3187	0	3118	60	0
1	J	2900	0	2817	105	0
2	A	1	0	0	0	0
3	A	18	0	0	0	0
3	B	15	0	0	0	0
3	C	11	0	0	0	0
3	D	12	0	0	1	0
3	E	8	0	0	3	0
3	F	14	0	0	0	0
3	G	14	0	0	0	0
3	H	5	0	0	0	0
3	I	12	0	0	2	0
3	J	5	0	0	0	0
All	All	33077	0	32165	788	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 12.

All (788) 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:J:326:TYR:CD1	1:J:329:SER:HB3	1.50	1.46
1:F:45:CYS:SG	1:F:77:CYS:CB	2.23	1.27
1:J:326:TYR:CG	1:J:329:SER:HB3	1.70	1.26
1:A:45:CYS:SG	1:A:77:CYS:SG	1.45	1.24
1:F:45:CYS:CB	1:F:77:CYS:SG	2.25	1.23
1:J:437:THR:HG22	1:J:507:ARG:NH2	1.54	1.22
1:G:63:ASN:O	1:G:174:ILE:HG22	1.39	1.21
1:G:326:TYR:CD2	1:G:330:PRO:HB3	1.76	1.19
1:G:169:CYS:SG	1:G:192:CYS:SG	1.37	1.16
1:G:326:TYR:CE2	1:G:330:PRO:HB3	1.80	1.15
1:G:181:MET:HE3	1:G:186:ASN:OD1	1.44	1.13
1:J:326:TYR:CG	1:J:329:SER:CB	2.30	1.13
1:E:173:ALA:CB	1:E:185:LYS:HD2	1.79	1.11
1:A:76:SER:O	1:A:77:CYS:HB2	1.33	1.10
1:I:323:CYS:SG	1:I:352:CYS:SG	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:THR:HG22	1:E:530:VAL:H	1.15	1.08
1:F:169:CYS:SG	1:F:192:CYS:CB	2.48	1.02
1:F:169:CYS:SG	1:F:192:CYS:SG	1.20	1.02
1:I:323:CYS:CB	1:I:352:CYS:SG	2.47	1.02
1:G:169:CYS:CB	1:G:192:CYS:SG	2.48	1.01
1:J:326:TYR:CD1	1:J:329:SER:CB	2.41	1.01
1:E:172:SER:HB2	1:E:174:ILE:HG23	1.44	1.00
1:E:173:ALA:HB2	1:E:185:LYS:CD	1.91	0.99
1:G:170:ASP:H	1:G:190:ASN:ND2	1.59	0.99
1:E:173:ALA:HB2	1:E:185:LYS:HD2	0.97	0.97
1:F:497:THR:HG22	1:F:530:VAL:H	1.30	0.97
1:J:326:TYR:CD2	1:J:329:SER:HB2	1.99	0.97
1:I:47:ILE:HD12	1:I:47:ILE:H	1.29	0.96
1:G:497:THR:HG22	1:G:530:VAL:H	1.29	0.96
1:A:45:CYS:CB	1:A:77:CYS:SG	2.54	0.95
1:E:303:THR:HG21	1:E:405:LEU:HD21	1.46	0.95
1:E:172:SER:HB2	1:E:174:ILE:CG2	1.95	0.95
1:I:303:THR:HG21	1:I:405:LEU:HD21	1.49	0.94
1:E:3:GLN:HG2	1:E:4:LEU:H	1.26	0.94
1:E:3:GLN:HG2	1:E:4:LEU:N	1.81	0.94
1:G:433:ARG:NH1	1:G:506:ARG:HG3	1.83	0.94
1:G:173:ALA:HB2	1:G:185:LYS:HD3	1.52	0.92
1:C:127:THR:CG2	1:C:128:ALA:N	2.33	0.91
1:J:437:THR:HG22	1:J:507:ARG:HH21	1.17	0.91
1:C:497:THR:HG22	1:C:530:VAL:H	1.34	0.91
1:F:118:LEU:HD22	1:F:253:THR:HG22	1.53	0.89
1:G:317:MET:HE2	1:G:317:MET:C	1.97	0.88
1:G:143:ILE:HG21	1:G:290:LEU:HD11	1.55	0.88
1:C:127:THR:HG22	1:C:128:ALA:N	1.87	0.87
1:H:130:ALA:HB2	1:H:226:LEU:HD22	1.57	0.87
1:G:317:MET:HE2	1:G:317:MET:O	1.74	0.87
1:A:370:LEU:HD11	1:A:377:SER:HB2	1.56	0.87
1:C:175:SER:HB3	1:C:181:MET:HE1	1.55	0.87
1:G:175:SER:OG	1:G:181:MET:SD	2.33	0.87
1:A:76:SER:O	1:A:77:CYS:CB	2.19	0.86
1:H:454:VAL:HG13	1:H:470:ALA:HB2	1.56	0.86
1:C:180:THR:HB	1:C:349:THR:CG2	2.06	0.86
1:G:63:ASN:O	1:G:174:ILE:CG2	2.23	0.86
1:C:127:THR:HG22	1:C:128:ALA:H	1.40	0.86
1:J:133:MET:HE1	1:J:279:ALA:O	1.76	0.85
1:H:84:PHE:CE1	1:H:317:MET:CE	2.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:PHE:HE1	1:H:317:MET:CE	1.90	0.84
1:G:211:ASN:O	1:G:214:PRO:HD2	1.76	0.84
1:E:517:ASN:HD22	1:E:517:ASN:H	1.26	0.84
1:B:449:LYS:HA	1:B:449:LYS:CE	2.07	0.83
1:E:48:LEU:HD11	1:E:76:SER:HA	1.59	0.83
1:C:34:ALA:HB1	1:C:310:VAL:HG21	1.61	0.83
1:E:34:ALA:HB1	1:E:310:VAL:HG21	1.60	0.83
1:J:133:MET:CE	1:J:279:ALA:O	2.26	0.83
1:J:342:ASP:HB3	1:J:346:ASN:OD1	1.79	0.82
1:E:175:SER:OG	1:E:181:MET:HE1	1.79	0.82
1:C:175:SER:CB	1:C:181:MET:HE1	2.09	0.81
1:G:326:TYR:CD2	1:G:330:PRO:CB	2.60	0.81
1:H:84:PHE:HE1	1:H:317:MET:HE3	1.45	0.81
1:E:3:GLN:CG	1:E:4:LEU:H	1.94	0.81
1:G:175:SER:OG	1:G:181:MET:HE1	1.79	0.81
1:C:180:THR:HB	1:C:349:THR:HG23	1.62	0.81
1:G:433:ARG:HH12	1:G:506:ARG:HG3	1.44	0.80
1:A:144:LEU:HD21	1:A:209:PHE:HB3	1.64	0.80
1:F:34:ALA:HB1	1:F:310:VAL:HG21	1.64	0.79
1:C:144:LEU:HD21	1:C:209:PHE:HB3	1.64	0.79
1:D:113:THR:C	1:D:114:GLN:HG2	2.05	0.79
1:D:91:ILE:HD11	1:D:310:VAL:HG21	1.63	0.79
1:G:326:TYR:CG	1:G:330:PRO:HB3	2.17	0.79
1:D:144:LEU:HD21	1:D:209:PHE:HB3	1.65	0.79
1:E:183:ASN:HB2	3:E:606:HOH:O	1.83	0.78
1:I:23:THR:HG23	1:I:412:LEU:HD11	1.65	0.78
1:J:47:ILE:HG13	1:J:322:ILE:HD12	1.66	0.78
1:I:144:LEU:HD21	1:I:209:PHE:HB3	1.65	0.78
1:J:326:TYR:CD2	1:J:329:SER:CB	2.64	0.78
1:E:184:GLN:O	1:E:185:LYS:HD3	1.82	0.78
1:G:170:ASP:H	1:G:190:ASN:HD21	1.27	0.78
1:I:11:LEU:HD21	3:I:601:HOH:O	1.84	0.77
1:E:288:LYS:HA	1:E:288:LYS:HE2	1.66	0.77
1:G:497:THR:CG2	1:G:530:VAL:H	1.96	0.77
1:B:84:PHE:HE1	1:B:317:MET:CE	1.97	0.77
1:B:41:LEU:HD13	1:B:317:MET:HE1	1.67	0.77
1:I:83:GLU:HB3	1:I:157:LEU:CD1	2.14	0.77
1:J:507:ARG:H	1:J:507:ARG:NE	1.82	0.77
1:I:98:VAL:O	1:I:102:GLN:HG2	1.84	0.77
1:G:281:ASN:O	1:G:285:GLU:HG3	1.84	0.76
1:G:326:TYR:CE2	1:G:371:LYS:N	2.54	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:MET:CE	1:G:186:ASN:OD1	2.28	0.76
1:F:197:GLU:O	1:F:201:LEU:CD1	2.33	0.76
1:G:212:GLN:O	1:G:215:GLN:HG2	1.85	0.76
1:F:497:THR:CG2	1:F:530:VAL:H	1.99	0.75
1:C:329:SER:OG	1:C:330:PRO:HD2	1.87	0.75
1:G:326:TYR:CE2	1:G:330:PRO:CB	2.68	0.75
1:J:133:MET:HE3	1:J:283:LEU:HD22	1.68	0.75
1:E:75:ASN:OD1	1:E:78:ALA:HB2	1.87	0.75
1:F:169:CYS:CB	1:F:192:CYS:SG	2.72	0.75
1:J:342:ASP:CB	1:J:346:ASN:OD1	2.34	0.75
1:F:226:LEU:O	1:F:229:GLU:HB2	1.86	0.74
1:I:83:GLU:HB3	1:I:157:LEU:HD12	1.68	0.74
1:G:213:THR:OG1	1:G:214:PRO:HD3	1.87	0.74
1:F:144:LEU:HD21	1:F:209:PHE:HB3	1.70	0.74
1:I:335:GLN:C	1:I:335:GLN:HE21	1.96	0.74
1:B:144:LEU:HD21	1:B:209:PHE:HB3	1.68	0.74
1:B:449:LYS:HA	1:B:449:LYS:HE2	1.67	0.73
1:G:175:SER:OG	1:G:181:MET:CE	2.36	0.73
1:H:214:PRO:O	1:H:218:GLN:HG3	1.87	0.73
1:F:47:ILE:HA	1:F:75:ASN:HA	1.70	0.73
1:C:326:TYR:CZ	1:C:330:PRO:HG3	2.24	0.73
1:G:326:TYR:CZ	1:G:330:PRO:HB3	2.22	0.73
1:I:35:GLN:HE22	1:I:95:GLN:HE22	1.37	0.72
1:F:154:PHE:CE1	1:F:195:VAL:CG1	2.72	0.72
1:A:500:TYR:CD1	1:A:528:VAL:HG13	2.25	0.72
1:B:178:ASN:OD1	1:B:350:ILE:HG23	1.90	0.72
1:D:500:TYR:CD1	1:D:528:VAL:HG13	2.25	0.72
1:C:459:TRP:O	1:C:478:ARG:NH2	2.22	0.72
1:D:346:ASN:OD1	1:D:346:ASN:N	2.21	0.72
1:E:3:GLN:CG	1:E:4:LEU:N	2.53	0.72
1:A:154:PHE:CE1	1:A:195:VAL:CG1	2.72	0.72
1:C:130:ALA:HB1	1:C:133:MET:HE2	1.71	0.72
1:E:500:TYR:CD1	1:E:528:VAL:HG13	2.24	0.72
1:G:506:ARG:O	1:G:507:ARG:HB3	1.88	0.72
1:F:228:GLN:O	1:F:228:GLN:HG2	1.89	0.72
1:C:497:THR:CG2	1:C:530:VAL:H	2.03	0.71
1:J:399:GLN:CG	1:J:400:ALA:N	2.52	0.71
1:B:334:ASN:O	1:B:380:ILE:HD13	1.91	0.71
1:B:45:CYS:HG	1:B:77:CYS:CB	2.03	0.71
1:J:326:TYR:CG	1:J:329:SER:HB2	2.12	0.71
1:F:341:THR:HA	1:F:347:GLY:HA2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:ALA:CB	1:H:226:LEU:HD22	2.21	0.70
1:H:334:ASN:H	1:H:334:ASN:ND2	1.88	0.70
1:A:154:PHE:CZ	1:A:195:VAL:HG12	2.26	0.70
1:I:222:LEU:HD21	1:I:276:ILE:HG22	1.73	0.70
1:F:154:PHE:CZ	1:F:195:VAL:HG12	2.26	0.70
1:G:71:GLY:HA2	1:G:74:LYS:HE2	1.74	0.70
1:D:326:TYR:HD2	1:D:329:SER:H	1.40	0.70
1:E:172:SER:CB	1:E:174:ILE:HG23	2.18	0.70
1:E:497:THR:CG2	1:E:530:VAL:H	2.01	0.70
1:G:326:TYR:CE1	1:G:371:LYS:HD2	2.27	0.70
1:I:48:LEU:O	1:I:48:LEU:HG	1.90	0.70
1:G:352:CYS:HB3	1:G:380:ILE:CD1	2.22	0.69
1:A:133:MET:HE1	1:A:222:LEU:HD22	1.74	0.69
1:C:378:LEU:HD22	1:C:382:GLN:HG3	1.73	0.69
1:F:105:SER:O	1:F:108:GLN:NE2	2.26	0.69
1:I:257:LEU:HD13	1:I:257:LEU:O	1.93	0.69
1:F:119:ASN:ND2	1:G:471:LYS:HE2	2.07	0.69
1:J:342:ASP:CG	1:J:346:ASN:OD1	2.35	0.69
1:H:440:MET:SD	1:H:485:VAL:CG2	2.80	0.69
1:A:133:MET:HE2	1:A:223:ALA:HB2	1.75	0.69
1:J:440:MET:HG3	1:J:459:TRP:CE3	2.27	0.69
1:G:144:LEU:HD21	1:G:209:PHE:HB3	1.75	0.69
1:G:369:THR:HG23	1:G:370:LEU:CD2	2.22	0.69
1:I:23:THR:CG2	1:I:412:LEU:HD11	2.23	0.69
1:B:49:ILE:HD13	1:B:49:ILE:N	2.07	0.69
1:H:480:ASN:OD1	1:H:480:ASN:N	2.22	0.68
1:J:127:THR:O	1:J:130:ALA:HB3	1.93	0.68
1:F:326:TYR:CE2	1:F:371:LYS:N	2.61	0.68
1:I:112:ILE:HG12	1:I:276:ILE:HD11	1.74	0.68
1:J:342:ASP:HB2	1:J:346:ASN:O	1.94	0.68
1:A:478:ARG:HD2	1:A:478:ARG:O	1.93	0.68
1:C:446:ALA:HB1	1:C:447:PRO:CD	2.24	0.68
1:J:171:ALA:HB2	1:J:344:ASN:HD21	1.58	0.68
1:F:197:GLU:O	1:F:201:LEU:HD12	1.93	0.68
1:H:169:CYS:SG	1:H:190:ASN:HB3	2.34	0.68
1:E:222:LEU:HD21	1:E:276:ILE:HG22	1.76	0.67
1:B:84:PHE:CE1	1:B:317:MET:CE	2.77	0.67
1:F:227:ILE:C	1:F:229:GLU:H	2.03	0.67
1:H:84:PHE:CZ	1:H:317:MET:HE1	2.29	0.67
1:E:184:GLN:O	1:E:185:LYS:CD	2.42	0.67
1:G:176:SER:OG	1:G:179:MET:HB3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:GLN:HA	1:G:352:CYS:O	1.94	0.67
1:A:411:LYS:HG2	1:A:412:LEU:N	2.09	0.67
1:I:426:LEU:HG	1:I:489:MET:HE2	1.75	0.67
1:E:335:GLN:NE2	1:E:491:SER:OG	2.28	0.66
1:F:200:SER:OG	1:F:201:LEU:HD12	1.95	0.66
1:G:509:PHE:CE2	1:G:512:ALA:HA	2.30	0.66
1:C:329:SER:OG	1:C:330:PRO:CD	2.43	0.66
1:E:524:GLN:HG2	1:E:525:GLY:N	2.10	0.66
1:A:162:LEU:O	1:A:166:ILE:HG22	1.94	0.66
1:C:34:ALA:CB	1:C:310:VAL:HG21	2.25	0.66
1:J:505:ARG:HG3	1:J:506:ARG:O	1.94	0.66
1:A:370:LEU:HD12	1:A:370:LEU:C	2.21	0.66
1:E:497:THR:HG22	1:E:530:VAL:N	2.00	0.66
1:J:440:MET:HG3	1:J:459:TRP:CZ3	2.31	0.66
1:C:164:ASP:OD1	1:C:164:ASP:N	2.28	0.66
1:B:120:LEU:HG	1:B:121:ASN:H	1.61	0.65
1:G:150:VAL:HG21	1:G:302:ALA:HB1	1.78	0.65
1:C:328:LYS:HG3	1:C:329:SER:H	1.61	0.65
1:E:34:ALA:CB	1:E:310:VAL:HG21	2.25	0.65
1:F:34:ALA:CB	1:F:310:VAL:HG21	2.26	0.65
1:F:337:ASP:HB3	1:F:349:THR:CG2	2.27	0.65
1:F:119:ASN:HD22	1:G:471:LYS:HE2	1.61	0.65
1:C:326:TYR:CE2	1:C:330:PRO:HG3	2.32	0.65
1:E:288:LYS:HA	1:E:288:LYS:CE	2.26	0.65
1:F:296:ASN:OD1	1:F:296:ASN:N	2.29	0.65
1:E:75:ASN:OD1	1:E:78:ALA:CB	2.45	0.64
1:A:396:ALA:HB2	1:A:412:LEU:HD11	1.79	0.64
1:D:326:TYR:HD1	1:D:334:ASN:HD22	1.45	0.64
1:A:208:ASP:OD2	1:A:286:ARG:NH1	2.31	0.64
1:C:212:GLN:O	1:C:215:GLN:HG2	1.98	0.64
1:G:335:GLN:CG	1:G:351:ASN:HD21	2.11	0.64
1:A:370:LEU:HD11	1:A:377:SER:CB	2.28	0.64
1:I:118:LEU:HD12	1:I:257:LEU:HD23	1.79	0.64
1:H:154:PHE:CE1	1:H:195:VAL:CG1	2.80	0.64
1:J:317:MET:HE2	1:J:317:MET:O	1.98	0.63
1:G:175:SER:HG	1:G:181:MET:CE	2.09	0.63
1:G:155:ASN:O	1:G:159:SER:HB3	1.98	0.63
1:I:412:LEU:C	1:I:412:LEU:HD12	2.24	0.63
1:B:449:LYS:HA	1:B:449:LYS:HE3	1.81	0.63
1:C:277:ASN:HA	1:C:280:VAL:HG22	1.81	0.63
1:E:183:ASN:ND2	1:E:347:GLY:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:GLN:HG3	1:G:351:ASN:HD21	1.64	0.63
1:J:154:PHE:CE1	1:J:195:VAL:CG2	2.82	0.63
1:G:497:THR:HG22	1:G:530:VAL:N	2.08	0.63
1:I:458:TYR:HB3	1:I:509:PHE:HZ	1.63	0.63
1:E:473:ARG:HB3	1:E:491:SER:HB2	1.81	0.63
1:G:170:ASP:N	1:G:190:ASN:HD21	1.97	0.62
1:F:497:THR:HG22	1:F:530:VAL:N	2.10	0.62
1:J:133:MET:HE2	1:J:279:ALA:O	1.99	0.62
1:G:326:TYR:CD2	1:G:370:LEU:C	2.76	0.62
1:H:442:TRP:HD1	1:H:476:ILE:HD12	1.64	0.62
1:B:343:GLU:OE2	1:B:398:LYS:HD3	1.98	0.62
1:F:326:TYR:CZ	1:F:371:LYS:HB2	2.35	0.62
1:H:440:MET:SD	1:H:485:VAL:HG23	2.40	0.62
1:I:46:PRO:HG2	1:I:378:LEU:HD13	1.81	0.62
1:B:459:TRP:O	1:B:478:ARG:NH2	2.31	0.62
1:D:38:VAL:HG21	1:D:91:ILE:HD12	1.80	0.62
1:A:47:ILE:HA	1:A:75:ASN:HA	1.82	0.62
1:C:154:PHE:CE1	1:C:195:VAL:CG2	2.83	0.62
1:F:225:THR:O	1:F:229:GLU:HG2	1.99	0.62
1:C:174:ILE:HD11	1:C:189:GLY:HA3	1.82	0.62
1:A:277:ASN:HA	1:A:280:VAL:HG12	1.81	0.61
1:E:173:ALA:CB	1:E:185:LYS:CD	2.65	0.61
1:E:337:ASP:HB3	1:E:349:THR:CG2	2.30	0.61
1:F:150:VAL:HG21	1:F:302:ALA:HB1	1.82	0.61
1:G:173:ALA:HB2	1:G:185:LYS:CD	2.29	0.61
1:J:326:TYR:CE1	1:J:329:SER:HB3	2.28	0.61
1:J:342:ASP:CB	1:J:346:ASN:O	2.48	0.61
1:E:398:LYS:HG3	1:E:399:GLN:HG3	1.83	0.61
1:C:170:ASP:H	1:C:190:ASN:HD22	1.48	0.61
1:I:277:ASN:HA	1:I:280:VAL:HG22	1.83	0.61
1:J:469:SER:O	1:J:473:ARG:CZ	2.49	0.61
1:J:109:PRO:HG2	1:J:133:MET:SD	2.40	0.61
1:E:111:ASN:OD1	1:E:277:ASN:ND2	2.34	0.60
1:I:11:LEU:CD2	3:I:601:HOH:O	2.44	0.60
1:A:370:LEU:HD13	1:A:376:VAL:CG2	2.32	0.60
1:C:497:THR:HG22	1:C:530:VAL:N	2.14	0.60
1:H:12:VAL:HG22	1:H:424:LEU:HD13	1.84	0.60
1:A:343:GLU:O	1:A:344:ASN:CB	2.46	0.60
1:F:229:GLU:OE1	1:F:229:GLU:HA	2.01	0.60
1:C:41:LEU:HD13	1:C:317:MET:HE1	1.83	0.60
1:E:471:LYS:HD2	1:E:472:GLY:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:154:PHE:CE1	1:J:195:VAL:HG22	2.36	0.60
1:G:27:ALA:O	1:G:31:LEU:HG	2.01	0.60
1:E:65:PRO:HG3	1:E:174:ILE:HD12	1.83	0.60
1:B:84:PHE:CE1	1:B:317:MET:HE2	2.37	0.60
1:G:509:PHE:HD2	1:G:511:LEU:O	1.84	0.60
1:F:201:LEU:HD12	1:F:201:LEU:N	2.16	0.60
1:J:154:PHE:CZ	1:J:195:VAL:HG22	2.37	0.60
1:C:446:ALA:HB1	1:C:447:PRO:HD2	1.83	0.59
1:I:96:LYS:O	1:I:100:GLU:HG2	2.02	0.59
1:E:160:GLY:O	1:E:163:LYS:HG2	2.03	0.59
1:B:494:PRO:HA	1:B:530:VAL:HB	1.84	0.59
1:F:201:LEU:HD12	1:F:201:LEU:H	1.66	0.59
1:I:458:TYR:HB3	1:I:509:PHE:CZ	2.37	0.59
1:J:507:ARG:H	1:J:507:ARG:CD	2.11	0.59
1:F:65:PRO:HD2	1:F:68:GLN:HE21	1.67	0.59
1:H:154:PHE:CZ	1:H:195:VAL:HG12	2.37	0.59
1:E:90:MET:HE1	1:E:157:LEU:HD22	1.83	0.59
1:D:91:ILE:HD11	1:D:310:VAL:CG2	2.32	0.59
1:E:47:ILE:HG22	1:E:48:LEU:N	2.17	0.59
1:G:480:ASN:OD1	1:G:480:ASN:N	2.35	0.59
1:J:399:GLN:HG2	1:J:400:ALA:N	2.16	0.59
1:I:37:ILE:HG13	1:I:38:VAL:N	2.18	0.59
1:E:326:TYR:HB2	1:E:329:SER:O	2.02	0.59
1:H:84:PHE:CE1	1:H:317:MET:HE1	2.35	0.59
1:C:154:PHE:CE1	1:C:195:VAL:HG22	2.37	0.59
1:D:334:ASN:O	1:D:380:ILE:CD1	2.50	0.59
1:H:454:VAL:CG1	1:H:470:ALA:HB2	2.31	0.58
1:A:459:TRP:HZ2	1:A:483:ASN:OD1	1.86	0.58
1:D:113:THR:C	1:D:114:GLN:CG	2.76	0.58
1:I:47:ILE:HD12	1:I:47:ILE:N	2.07	0.58
1:C:154:PHE:CZ	1:C:195:VAL:HG22	2.39	0.58
1:C:494:PRO:HA	1:C:530:VAL:O	2.04	0.58
1:J:437:THR:CG2	1:J:507:ARG:NH2	2.49	0.58
1:J:507:ARG:H	1:J:507:ARG:HE	1.48	0.58
1:F:200:SER:HG	1:F:201:LEU:HD12	1.67	0.58
1:G:324:GLY:HA2	1:G:380:ILE:HD11	1.86	0.58
1:J:343:GLU:OE2	1:J:343:GLU:HA	2.03	0.58
1:C:6:GLU:OE1	1:C:524:GLN:HG3	2.03	0.58
1:D:154:PHE:CE1	1:D:195:VAL:CG2	2.86	0.58
1:A:71:GLY:HA3	1:A:79:THR:HG21	1.86	0.58
1:E:176:SER:OG	1:E:319:TYR:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:440:MET:HB2	1:H:485:VAL:HG21	1.85	0.58
1:A:343:GLU:O	1:A:344:ASN:HB2	2.04	0.58
1:F:118:LEU:CD2	1:F:253:THR:HG22	2.32	0.58
1:G:326:TYR:CZ	1:G:371:LYS:HB2	2.39	0.58
1:C:167:GLY:HA2	1:C:195:VAL:HG12	1.86	0.57
1:C:458:TYR:CZ	1:C:512:ALA:HB1	2.39	0.57
1:G:326:TYR:CE2	1:G:370:LEU:C	2.81	0.57
1:J:133:MET:HE1	1:J:283:LEU:HB2	1.86	0.57
1:H:84:PHE:CZ	1:H:317:MET:CE	2.85	0.57
1:J:187:ASN:OD1	1:J:342:ASP:OD1	2.23	0.57
1:J:506:ARG:HB3	1:J:520:ASP:CG	2.29	0.57
1:E:165:TYR:N	1:E:165:TYR:CD1	2.73	0.57
1:F:326:TYR:CE2	1:F:370:LEU:C	2.82	0.57
1:H:193:ALA:HB3	1:H:195:VAL:HG23	1.85	0.57
1:J:457:ILE:HG23	1:J:457:ILE:O	2.04	0.57
1:D:154:PHE:CZ	1:D:195:VAL:HG22	2.39	0.57
1:G:112:ILE:HB	1:G:277:ASN:HD21	1.70	0.56
1:A:370:LEU:HD13	1:A:376:VAL:HG22	1.86	0.56
1:E:194:GLY:HA3	1:E:308:ARG:NH1	2.20	0.56
1:E:506:ARG:HD3	1:E:521:TYR:CE2	2.41	0.56
1:C:175:SER:HB2	1:C:181:MET:HE1	1.87	0.56
1:E:458:TYR:HB3	1:E:461:VAL:HB	1.86	0.56
1:G:387:HIS:O	1:G:391:GLN:HG2	2.05	0.56
1:J:505:ARG:HD3	1:J:518:GLU:O	2.05	0.56
1:A:465:TYR:N	1:A:465:TYR:CD1	2.72	0.56
1:G:489:MET:HE2	1:G:492:LEU:HD21	1.87	0.56
1:C:48:LEU:CD1	1:C:76:SER:HA	2.35	0.56
1:B:334:ASN:HB2	1:B:380:ILE:HD12	1.88	0.56
1:H:442:TRP:CD1	1:H:476:ILE:HD12	2.41	0.56
1:J:316:SER:O	1:J:319:TYR:HE1	1.88	0.56
1:D:500:TYR:HD1	1:D:528:VAL:HG13	1.67	0.56
1:B:84:PHE:HE1	1:B:317:MET:HE2	1.71	0.56
1:F:154:PHE:CZ	1:F:195:VAL:CG1	2.89	0.56
1:G:179:MET:HG3	1:G:180:THR:N	2.20	0.56
1:F:91:ILE:HD13	1:F:306:ALA:HB1	1.87	0.55
1:G:131:GLN:HB3	1:G:135:LYS:HZ1	1.71	0.55
1:E:47:ILE:CG2	1:E:48:LEU:N	2.69	0.55
1:E:170:ASP:H	1:E:190:ASN:HD22	1.54	0.55
1:A:500:TYR:HD1	1:A:528:VAL:HG13	1.68	0.55
1:G:210:ASN:O	1:G:213:THR:HG23	2.07	0.55
1:E:184:GLN:C	1:E:185:LYS:HG2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:LEU:HD23	1:J:133:MET:HG2	1.88	0.55
1:I:167:GLY:HA2	1:I:195:VAL:HG22	1.88	0.55
1:C:71:GLY:HA3	1:C:79:THR:OG1	2.06	0.55
1:G:176:SER:HB3	1:G:319:TYR:HD2	1.72	0.55
1:G:352:CYS:CB	1:G:380:ILE:CD1	2.84	0.55
1:J:91:ILE:HD13	1:J:306:ALA:HB1	1.89	0.55
1:A:459:TRP:HD1	1:A:459:TRP:O	1.90	0.55
1:B:216:ILE:HG13	1:B:217:ASN:N	2.22	0.55
1:D:99:GLN:O	1:D:102:GLN:HB2	2.06	0.55
1:E:506:ARG:HD3	1:E:521:TYR:HE2	1.71	0.55
1:G:45:CYS:O	1:G:75:ASN:HB2	2.07	0.55
1:D:154:PHE:CE1	1:D:195:VAL:HG22	2.41	0.55
1:G:207:ALA:O	1:G:210:ASN:HB3	2.07	0.55
1:J:505:ARG:CD	1:J:518:GLU:O	2.55	0.55
1:E:471:LYS:HD2	1:E:472:GLY:N	2.22	0.54
1:A:344:ASN:HB2	1:A:346:ASN:HD21	1.72	0.54
1:H:489:MET:HE2	1:H:492:LEU:HD21	1.89	0.54
1:C:394:SER:O	1:C:398:LYS:HG3	2.06	0.54
1:G:326:TYR:CG	1:G:330:PRO:HA	2.43	0.54
1:J:167:GLY:HA2	1:J:195:VAL:HG12	1.89	0.54
1:A:12:VAL:CG1	1:A:530:VAL:HG22	2.37	0.54
1:B:326:TYR:CE2	1:B:330:PRO:HG3	2.42	0.54
1:C:91:ILE:HD13	1:C:306:ALA:HB1	1.90	0.54
1:D:343:GLU:CD	1:D:399:GLN:HE21	2.15	0.54
1:E:500:TYR:HD1	1:E:528:VAL:HG13	1.67	0.54
1:A:154:PHE:CZ	1:A:195:VAL:CG1	2.90	0.54
1:D:98:VAL:O	1:D:102:GLN:HG2	2.08	0.53
1:B:212:GLN:HG3	1:B:215:GLN:CD	2.33	0.53
1:D:20:VAL:HG22	1:D:415:HIS:HD2	1.73	0.53
1:I:46:PRO:HG2	1:I:378:LEU:HB2	1.91	0.53
1:G:230:LEU:HD13	1:G:252:ASP:OD2	2.08	0.53
1:G:212:GLN:HB2	1:G:286:ARG:HE	1.74	0.53
1:G:369:THR:HG23	1:G:370:LEU:HD22	1.91	0.53
1:A:396:ALA:CB	1:A:412:LEU:HD11	2.38	0.53
1:E:91:ILE:HD12	1:E:306:ALA:HB1	1.90	0.53
1:E:446:ALA:HB3	1:E:449:LYS:HD3	1.91	0.53
1:G:497:THR:HG22	1:G:529:THR:HA	1.90	0.53
1:J:444:ARG:NH1	1:J:500:TYR:OH	2.29	0.53
1:D:112:ILE:HG23	1:D:121:ASN:HD21	1.74	0.53
1:E:151:GLU:OE1	1:E:203:LYS:HE3	2.09	0.53
1:J:399:GLN:HG2	1:J:400:ALA:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:506:ARG:O	1:J:506:ARG:HG3	2.07	0.53
1:D:212:GLN:HB3	1:D:286:ARG:HH11	1.74	0.53
1:G:446:ALA:HB3	1:G:449:LYS:HD2	1.91	0.53
1:E:107:ASN:HD21	1:F:3:GLN:HE22	1.56	0.52
1:I:167:GLY:HA2	1:I:195:VAL:CG2	2.39	0.52
1:F:154:PHE:HE1	1:F:195:VAL:HG11	1.75	0.52
1:G:324:GLY:HA2	1:G:380:ILE:CD1	2.39	0.52
1:C:3:GLN:H	1:C:431:SER:HB2	1.73	0.52
1:C:127:THR:HG23	1:C:128:ALA:N	2.22	0.52
1:E:440:MET:HE3	1:E:504:ALA:HB2	1.91	0.52
1:C:457:ILE:HG23	1:C:457:ILE:O	2.09	0.52
1:F:326:TYR:CD2	1:F:370:LEU:C	2.88	0.52
1:G:212:GLN:OE1	1:G:286:ARG:HG3	2.10	0.52
1:J:507:ARG:CD	1:J:507:ARG:N	2.73	0.52
1:F:45:CYS:SG	1:F:77:CYS:SG	0.52	0.52
1:G:169:CYS:SG	1:G:192:CYS:CB	2.82	0.52
1:G:326:TYR:CB	1:G:330:PRO:HA	2.40	0.52
1:E:184:GLN:O	1:E:185:LYS:CG	2.57	0.52
1:F:154:PHE:CE1	1:F:195:VAL:HG11	2.44	0.52
1:H:317:MET:SD	1:H:317:MET:C	2.93	0.52
1:J:37:ILE:HG13	1:J:38:VAL:N	2.24	0.52
1:B:317:MET:SD	1:B:317:MET:C	2.93	0.52
1:D:334:ASN:O	1:D:380:ILE:HD11	2.10	0.52
1:I:41:LEU:HD21	1:I:317:MET:HE1	1.91	0.52
1:F:193:ALA:HB3	1:F:195:VAL:HG23	1.91	0.52
1:I:35:GLN:HE22	1:I:95:GLN:NE2	2.05	0.52
1:A:322:ILE:HD11	1:A:376:VAL:O	2.10	0.51
1:F:326:TYR:OH	1:F:371:LYS:HB2	2.10	0.51
1:G:370:LEU:CD2	1:G:370:LEU:N	2.73	0.51
1:F:216:ILE:HD12	1:F:286:ARG:HH12	1.75	0.51
1:G:509:PHE:HD2	1:G:511:LEU:C	2.18	0.51
1:J:26:ASP:OD1	1:J:28:GLN:N	2.43	0.51
1:A:445:GLN:HG2	1:A:501:TYR:HE2	1.75	0.51
1:C:497:THR:HG22	1:C:529:THR:HA	1.92	0.51
1:D:126:LEU:HD12	1:D:226:LEU:HD22	1.92	0.51
1:F:326:TYR:CE2	1:F:371:LYS:CA	2.93	0.51
1:F:497:THR:HG22	1:F:529:THR:HA	1.92	0.51
1:J:317:MET:C	1:J:317:MET:SD	2.93	0.51
1:J:337:ASP:HB3	1:J:349:THR:HG23	1.92	0.51
1:H:454:VAL:HG11	1:H:474:PHE:HD2	1.74	0.51
1:A:12:VAL:HG11	1:A:530:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:THR:HB	1:B:349:THR:CG2	2.41	0.51
1:B:91:ILE:HD13	1:B:306:ALA:HB1	1.93	0.51
1:C:396:ALA:HB2	1:C:412:LEU:HD11	1.93	0.51
1:F:197:GLU:O	1:F:201:LEU:HD13	2.10	0.51
1:J:506:ARG:HA	1:J:507:ARG:NH1	2.25	0.51
1:E:517:ASN:H	1:E:517:ASN:ND2	1.97	0.51
1:I:493:LYS:C	1:I:530:VAL:HG11	2.36	0.51
1:A:154:PHE:CE1	1:A:195:VAL:HG11	2.46	0.50
1:H:440:MET:SD	1:H:485:VAL:HG21	2.50	0.50
1:H:12:VAL:HG22	1:H:424:LEU:CD1	2.41	0.50
1:J:90:MET:HE2	1:J:306:ALA:HA	1.93	0.50
1:C:22:ASP:OD1	1:C:413:GLU:HG3	2.11	0.50
1:E:173:ALA:HB1	1:E:185:LYS:NZ	2.25	0.50
1:G:170:ASP:N	1:G:190:ASN:ND2	2.42	0.50
1:I:396:ALA:HB2	1:I:412:LEU:HD21	1.92	0.50
1:B:334:ASN:O	1:B:380:ILE:CD1	2.58	0.50
1:E:332:GLU:N	1:E:332:GLU:OE1	2.45	0.50
1:G:326:TYR:CD1	1:G:326:TYR:C	2.89	0.50
1:I:23:THR:HG23	1:I:412:LEU:CD1	2.38	0.50
1:J:109:PRO:HB2	1:J:280:VAL:HG22	1.93	0.50
1:C:107:ASN:HD22	1:C:132:LYS:HG2	1.77	0.50
1:C:458:TYR:CE2	1:C:512:ALA:HB1	2.46	0.50
1:C:473:ARG:HH22	1:C:496:ASP:CG	2.19	0.50
1:A:438:ALA:C	1:A:459:TRP:HB2	2.37	0.50
1:B:6:GLU:OE2	1:B:523:GLY:HA3	2.11	0.50
1:B:138:GLN:HE21	1:B:220:GLN:NE2	2.09	0.50
1:B:176:SER:HB2	1:B:319:TYR:HD2	1.76	0.50
1:H:226:LEU:CD2	1:H:230:LEU:HD12	2.41	0.50
1:B:438:ALA:HB1	1:B:505:ARG:O	2.12	0.50
1:E:48:LEU:CD1	1:E:76:SER:HA	2.38	0.50
1:B:292:GLY:CA	1:B:406:ASN:ND2	2.75	0.50
1:F:227:ILE:C	1:F:229:GLU:N	2.67	0.50
1:F:337:ASP:HB3	1:F:349:THR:HG21	1.94	0.50
1:F:396:ALA:HA	1:F:412:LEU:HD22	1.94	0.50
1:I:257:LEU:HD13	1:I:257:LEU:C	2.35	0.50
1:D:378:LEU:HD22	1:D:382:GLN:HB3	1.94	0.49
1:G:370:LEU:N	1:G:370:LEU:HD23	2.25	0.49
1:G:479:ASP:CG	1:G:482:LYS:HD3	2.37	0.49
1:G:91:ILE:HD13	1:G:306:ALA:HB1	1.93	0.49
1:G:509:PHE:CD2	1:G:511:LEU:O	2.65	0.49
1:J:41:LEU:HD21	1:J:314:TRP:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ALA:O	1:G:150:VAL:HG22	2.13	0.49
1:I:412:LEU:HD12	1:I:412:LEU:O	2.12	0.49
1:A:473:ARG:HH22	1:A:496:ASP:CG	2.20	0.49
1:C:49:ILE:HG22	1:C:50:ALA:N	2.27	0.49
1:I:118:LEU:CD1	1:I:257:LEU:HD23	2.42	0.49
1:B:180:THR:HB	1:B:349:THR:HG22	1.94	0.49
1:B:391:GLN:HB2	1:B:416:VAL:HG22	1.93	0.49
1:D:524:GLN:HB2	3:D:610:HOH:O	2.12	0.49
1:G:174:ILE:O	1:G:174:ILE:HG13	2.13	0.49
1:A:193:ALA:HB3	1:A:195:VAL:HG23	1.94	0.49
1:F:396:ALA:HB2	1:F:412:LEU:HD21	1.95	0.49
1:F:439:ALA:HB3	1:F:505:ARG:HB3	1.94	0.49
1:I:473:ARG:HH22	1:I:496:ASP:CG	2.21	0.49
1:J:140:GLN:HB3	1:J:286:ARG:HH11	1.77	0.49
1:J:189:GLY:HA2	1:J:316:SER:O	2.13	0.49
1:A:114:GLN:HG3	1:A:114:GLN:O	2.12	0.49
1:E:440:MET:CE	1:E:504:ALA:HB2	2.43	0.49
1:I:412:LEU:C	1:I:412:LEU:CD1	2.85	0.49
1:E:19:SER:OG	1:F:17:THR:HB	2.13	0.49
1:D:50:ALA:HB2	1:D:72:GLY:HA3	1.95	0.49
1:B:292:GLY:HA3	1:B:406:ASN:HD21	1.77	0.48
1:F:458:TYR:HB3	1:F:509:PHE:HZ	1.78	0.48
1:B:6:GLU:OE2	1:B:523:GLY:C	2.56	0.48
1:I:23:THR:CG2	1:I:412:LEU:CD1	2.89	0.48
1:A:277:ASN:HA	1:A:280:VAL:CG1	2.43	0.48
1:G:256:GLN:O	1:G:260:LEU:HB2	2.14	0.48
1:B:168:LYS:NZ	1:B:190:ASN:HD21	2.11	0.48
1:A:274:GLN:OE1	1:A:274:GLN:HA	2.14	0.48
1:A:335:GLN:HG3	1:A:351:ASN:OD1	2.14	0.48
1:D:210:ASN:C	1:D:212:GLN:H	2.21	0.48
1:D:212:GLN:OE1	1:D:286:ARG:HG3	2.13	0.48
1:F:473:ARG:HH22	1:F:496:ASP:CG	2.22	0.48
1:J:438:ALA:HB2	1:J:507:ARG:HB3	1.95	0.48
1:A:154:PHE:HE1	1:A:195:VAL:HG11	1.77	0.48
1:A:370:LEU:CD1	1:A:376:VAL:HG22	2.44	0.48
1:B:292:GLY:CA	1:B:406:ASN:HD21	2.26	0.48
1:D:326:TYR:HB3	1:D:371:LYS:HE3	1.95	0.48
1:D:75:ASN:ND2	1:D:375:ASN:OD1	2.43	0.48
1:H:476:ILE:HD11	1:H:485:VAL:HG11	1.94	0.48
1:B:445:GLN:HG3	1:B:449:LYS:O	2.14	0.48
1:E:184:GLN:O	1:E:185:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:TYR:CZ	1:B:330:PRO:HG3	2.49	0.48
1:F:76:SER:HG	1:F:84:PHE:HE2	1.60	0.48
1:A:28:GLN:HE22	1:A:95:GLN:HG2	1.79	0.47
1:B:458:TYR:CZ	1:B:512:ALA:HB1	2.49	0.47
1:G:369:THR:HG23	1:G:370:LEU:HD23	1.95	0.47
1:H:226:LEU:CD2	1:H:230:LEU:CD1	2.92	0.47
1:D:38:VAL:HG21	1:D:91:ILE:CD1	2.44	0.47
1:F:326:TYR:CZ	1:F:371:LYS:CB	2.97	0.47
1:F:426:LEU:HG	1:F:489:MET:HE2	1.96	0.47
1:G:352:CYS:HB2	1:G:380:ILE:HD12	1.96	0.47
1:H:47:ILE:CG2	1:H:73:GLY:HA2	2.43	0.47
1:H:226:LEU:HD23	1:H:230:LEU:HD12	1.94	0.47
1:J:444:ARG:O	1:J:444:ARG:HG3	2.14	0.47
1:J:506:ARG:HA	1:J:507:ARG:CZ	2.43	0.47
1:J:506:ARG:HD3	1:J:520:ASP:OD1	2.15	0.47
1:A:94:ALA:HB1	1:A:303:THR:HG22	1.96	0.47
1:B:45:CYS:HB3	1:B:75:ASN:HD22	1.78	0.47
1:G:170:ASP:H	1:G:190:ASN:HD22	1.53	0.47
1:H:12:VAL:HG21	1:H:492:LEU:HD13	1.96	0.47
1:H:84:PHE:HZ	1:H:317:MET:HE1	1.78	0.47
1:H:411:LYS:H	1:H:411:LYS:HG2	1.38	0.47
1:J:326:TYR:CB	1:J:329:SER:CB	2.92	0.47
1:J:497:THR:HG23	1:J:529:THR:HA	1.96	0.47
1:C:332:GLU:O	1:C:334:ASN:N	2.43	0.47
1:H:440:MET:CB	1:H:485:VAL:HG21	2.44	0.47
1:G:150:VAL:HG21	1:G:302:ALA:CB	2.43	0.47
1:G:326:TYR:OH	1:G:371:LYS:HB2	2.14	0.47
1:B:84:PHE:HE1	1:B:317:MET:HE3	1.79	0.47
1:E:164:ASP:O	1:E:168:LYS:HD3	2.14	0.47
1:E:517:ASN:ND2	1:E:517:ASN:N	2.62	0.47
1:F:188:TRP:CD2	1:F:319:TYR:HB3	2.50	0.47
1:G:20:VAL:HG23	1:G:415:HIS:CD2	2.50	0.47
1:G:180:THR:HB	1:G:349:THR:CG2	2.45	0.47
1:G:180:THR:HB	1:G:349:THR:HG22	1.97	0.47
1:J:129:LEU:HD21	1:J:280:VAL:CG2	2.45	0.47
1:J:162:LEU:HD22	1:J:316:SER:HB3	1.97	0.47
1:J:445:GLN:HB3	1:J:499:VAL:HG23	1.95	0.47
1:F:77:CYS:O	1:F:81:GLY:N	2.48	0.47
1:F:226:LEU:O	1:F:229:GLU:CB	2.59	0.47
1:F:456:GLY:O	1:F:476:ILE:HG21	2.14	0.47
1:A:45:CYS:SG	1:A:77:CYS:CB	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:436:SER:O	1:F:506:ARG:HG2	2.15	0.47
1:J:514:THR:HB	1:J:515:ARG:HH11	1.80	0.47
1:A:500:TYR:CD1	1:A:528:VAL:CG1	2.96	0.47
1:C:49:ILE:CG2	1:C:50:ALA:N	2.77	0.47
1:H:493:LYS:HG2	1:H:496:ASP:OD2	2.14	0.47
1:D:500:TYR:CD1	1:D:528:VAL:CG1	2.96	0.46
1:J:45:CYS:HB3	1:J:75:ASN:HD22	1.80	0.46
1:J:80:PHE:CE2	1:J:317:MET:HG3	2.49	0.46
1:A:408:LYS:HA	1:A:408:LYS:HD3	1.42	0.46
1:E:26:ASP:O	1:E:30:LEU:HG	2.15	0.46
1:I:47:ILE:HB	1:I:48:LEU:H	1.57	0.46
1:J:339:HIS:N	1:J:339:HIS:CD2	2.82	0.46
1:G:334:ASN:OD1	1:G:380:ILE:HG12	2.15	0.46
1:B:327:THR:O	1:B:327:THR:HG22	2.15	0.46
1:C:129:LEU:O	1:C:129:LEU:HG	2.15	0.46
1:C:173:ALA:HA	1:C:185:LYS:HB3	1.96	0.46
1:B:12:VAL:HG23	1:B:424:LEU:HG	1.97	0.46
1:D:167:GLY:HA2	1:D:195:VAL:HG12	1.98	0.46
1:F:67:TRP:HB3	1:F:161:HIS:HB3	1.97	0.46
1:E:201:LEU:HA	1:E:204:THR:HG22	1.98	0.46
1:C:505:ARG:HD2	1:C:518:GLU:O	2.16	0.46
1:D:326:TYR:HD1	1:D:334:ASN:ND2	2.13	0.46
1:F:28:GLN:HG2	1:F:98:VAL:HG11	1.98	0.46
1:H:47:ILE:HG23	1:H:73:GLY:HA2	1.98	0.46
1:J:510:THR:HG23	1:J:511:LEU:H	1.80	0.46
1:E:77:CYS:O	1:E:81:GLY:N	2.47	0.46
1:F:147:ALA:O	1:F:150:VAL:HG22	2.16	0.46
1:H:28:GLN:O	1:H:32:THR:HG23	2.16	0.46
1:H:454:VAL:CG1	1:H:474:PHE:HD2	2.29	0.46
1:F:86:ALA:HB2	1:F:156:LYS:HD3	1.98	0.46
1:E:65:PRO:CG	1:E:174:ILE:HD12	2.46	0.45
1:H:6:GLU:OE1	1:H:500:TYR:O	2.33	0.45
1:A:49:ILE:HG12	1:A:320:ALA:HA	1.99	0.45
1:C:129:LEU:C	1:C:129:LEU:HD23	2.40	0.45
1:D:130:ALA:HA	1:D:133:MET:CE	2.46	0.45
1:E:517:ASN:C	1:E:519:TYR:H	2.24	0.45
1:F:23:THR:HG23	1:F:412:LEU:HD11	1.98	0.45
1:J:37:ILE:HB	1:J:386:ILE:HG23	1.98	0.45
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.78	0.45
1:E:489:MET:HE2	1:E:492:LEU:HD21	1.99	0.45
1:G:22:ASP:HB2	1:H:14:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:TYR:CE2	1:D:328:LYS:HB2	2.52	0.45
1:E:337:ASP:HB3	1:E:349:THR:HG21	1.99	0.45
1:E:398:LYS:CG	1:E:399:GLN:HG3	2.44	0.45
1:E:500:TYR:CD1	1:E:528:VAL:CG1	2.96	0.45
1:F:222:LEU:HD11	1:F:271:THR:HA	1.98	0.45
1:I:424:LEU:HB2	1:I:489:MET:HE3	1.99	0.45
1:A:107:ASN:HD21	1:B:3:GLN:NE2	2.14	0.45
1:A:438:ALA:N	1:A:459:TRP:HE3	2.13	0.45
1:A:459:TRP:O	1:A:459:TRP:CD1	2.70	0.45
1:E:303:THR:HG23	1:E:402:LEU:HD21	1.98	0.45
1:G:391:GLN:HG3	1:G:416:VAL:HG22	1.98	0.45
1:H:83:GLU:OE1	1:H:160:GLY:HA3	2.17	0.45
1:J:446:ALA:HB3	1:J:449:LYS:HB2	1.99	0.45
1:G:75:ASN:HD22	1:G:375:ASN:CG	2.25	0.45
1:G:178:ASN:OD1	1:G:178:ASN:N	2.50	0.45
1:E:277:ASN:HD22	1:E:277:ASN:HA	1.57	0.45
1:F:493:LYS:HD3	1:F:494:PRO:HD2	1.98	0.45
1:J:23:THR:HG21	1:J:392:ILE:HG23	1.98	0.45
1:C:74:LYS:HG2	1:C:75:ASN:N	2.32	0.45
1:C:167:GLY:HA2	1:C:195:VAL:CG1	2.46	0.45
1:C:173:ALA:HA	1:C:185:LYS:HD2	1.98	0.45
1:C:289:THR:O	1:C:297:SER:HB2	2.18	0.45
1:G:70:ALA:O	1:G:74:LYS:CE	2.65	0.44
1:G:479:ASP:CG	1:G:482:LYS:CD	2.91	0.44
1:D:130:ALA:HA	1:D:133:MET:HE3	1.99	0.44
1:C:436:SER:O	1:C:459:TRP:O	2.35	0.44
1:J:438:ALA:CB	1:J:507:ARG:HA	2.46	0.44
1:B:12:VAL:CG1	1:B:530:VAL:HG13	2.47	0.44
1:J:154:PHE:HE1	1:J:195:VAL:HG21	1.81	0.44
1:B:49:ILE:CD1	1:B:322:ILE:HG13	2.48	0.44
1:C:106:ALA:CB	1:D:5:VAL:HG21	2.47	0.44
1:D:335:GLN:O	1:D:420:LYS:HG3	2.18	0.44
1:I:209:PHE:CE2	1:I:286:ARG:HG2	2.53	0.44
1:J:326:TYR:CE1	1:J:329:SER:CB	2.94	0.44
1:C:154:PHE:HE1	1:C:195:VAL:HG21	1.83	0.44
1:G:505:ARG:HG3	1:G:518:GLU:O	2.17	0.44
1:H:221:ASN:HA	1:H:224:ASN:HD22	1.81	0.44
1:J:187:ASN:OD1	1:J:342:ASP:CG	2.60	0.44
1:D:214:PRO:HA	1:D:217:ASN:HB2	1.98	0.44
1:E:194:GLY:HA3	1:E:308:ARG:HH11	1.83	0.44
1:F:213:THR:HA	1:F:216:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLN:CB	1:B:416:VAL:HG22	2.47	0.44
1:I:458:TYR:CE2	1:I:512:ALA:HB1	2.53	0.44
1:B:188:TRP:C	1:B:190:ASN:H	2.26	0.43
1:F:257:LEU:HD12	1:G:463:SER:OG	2.18	0.43
1:G:43:ASP:O	1:G:374:LYS:HE2	2.18	0.43
1:J:47:ILE:HG13	1:J:322:ILE:CD1	2.44	0.43
1:A:344:ASN:HB2	1:A:346:ASN:ND2	2.31	0.43
1:D:222:LEU:HD11	1:D:276:ILE:HG22	2.00	0.43
1:E:182:GLN:CB	3:E:608:HOH:O	2.66	0.43
1:G:212:GLN:HA	1:G:215:GLN:NE2	2.33	0.43
1:B:505:ARG:HD2	1:B:518:GLU:O	2.18	0.43
1:H:313:LEU:O	1:H:317:MET:HG3	2.18	0.43
1:I:257:LEU:C	1:I:257:LEU:CD1	2.91	0.43
1:A:45:CYS:HB3	1:A:77:CYS:SG	2.55	0.43
1:B:473:ARG:HH22	1:B:496:ASP:CG	2.25	0.43
1:E:174:ILE:HD11	1:E:189:GLY:HA3	2.00	0.43
1:H:423:SER:O	1:H:424:LEU:HD12	2.18	0.43
1:J:137:ALA:HB2	1:J:283:LEU:HD21	1.99	0.43
1:G:175:SER:HA	1:G:179:MET:HE3	2.00	0.43
1:H:45:CYS:CB	1:H:77:CYS:HG	2.28	0.43
1:I:47:ILE:H	1:I:47:ILE:CD1	2.03	0.43
1:E:118:LEU:HA	1:E:121:ASN:HD22	1.83	0.43
1:E:182:GLN:HB2	3:E:608:HOH:O	2.19	0.43
1:G:169:CYS:CA	1:G:192:CYS:SG	3.05	0.43
1:G:326:TYR:CG	1:G:330:PRO:CA	3.02	0.43
1:G:326:TYR:CD1	1:G:330:PRO:HB3	2.53	0.43
1:H:154:PHE:CE1	1:H:195:VAL:HG12	2.51	0.43
1:G:212:GLN:HA	1:G:215:GLN:HE21	1.83	0.43
1:G:326:TYR:CE1	1:G:371:LYS:CD	2.99	0.43
1:I:339:HIS:O	1:I:387:HIS:HE1	2.00	0.43
1:C:332:GLU:C	1:C:334:ASN:H	2.27	0.43
1:F:214:PRO:O	1:F:218:GLN:HB2	2.18	0.43
1:C:436:SER:O	1:C:459:TRP:C	2.61	0.43
1:E:47:ILE:HG23	1:E:74:LYS:O	2.19	0.43
1:E:494:PRO:HA	1:E:530:VAL:O	2.18	0.43
1:I:131:GLN:HA	1:I:134:LEU:HG	2.00	0.43
1:J:326:TYR:HB2	1:J:329:SER:CA	2.49	0.43
1:A:343:GLU:C	1:A:344:ASN:CG	2.87	0.42
1:B:6:GLU:OE2	1:B:524:GLN:N	2.52	0.42
1:E:329:SER:HB2	1:E:330:PRO:CD	2.49	0.42
1:H:454:VAL:HG11	1:H:474:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:497:THR:HG23	1:H:529:THR:HA	2.01	0.42
1:B:28:GLN:O	1:B:32:THR:HG23	2.19	0.42
1:C:41:LEU:CD1	1:C:317:MET:HE1	2.49	0.42
1:D:2:VAL:HG22	1:D:521:TYR:CD1	2.53	0.42
1:E:437:THR:HA	1:E:506:ARG:HA	2.00	0.42
1:H:23:THR:HG21	1:H:392:ILE:HG23	2.01	0.42
1:B:45:CYS:SG	1:B:77:CYS:HB2	2.59	0.42
1:B:497:THR:HG23	1:B:529:THR:HA	2.01	0.42
1:I:116:HIS:HA	1:I:257:LEU:HD11	2.00	0.42
1:I:324:GLY:HA2	1:I:334:ASN:HD21	1.83	0.42
1:J:37:ILE:HG12	1:J:310:VAL:CG1	2.49	0.42
1:H:158:SER:O	1:H:163:LYS:HA	2.20	0.42
1:I:158:SER:O	1:I:163:LYS:HA	2.19	0.42
1:J:326:TYR:HB2	1:J:329:SER:N	2.34	0.42
1:A:494:PRO:HA	1:A:530:VAL:HB	2.02	0.42
1:B:45:CYS:O	1:B:46:PRO:C	2.60	0.42
1:G:213:THR:HG1	1:G:214:PRO:HD3	1.81	0.42
1:G:428:CYS:O	1:G:484:THR:HA	2.20	0.42
1:I:46:PRO:CG	1:I:378:LEU:HD13	2.46	0.42
1:J:168:LYS:HD3	1:J:190:ASN:HD21	1.84	0.42
1:J:187:ASN:OD1	1:J:342:ASP:OD2	2.38	0.42
1:B:482:LYS:HB2	1:B:484:THR:HG23	2.02	0.42
1:E:165:TYR:O	1:E:166:ILE:C	2.62	0.42
1:G:174:ILE:HD11	1:G:189:GLY:HA3	2.01	0.42
1:H:154:PHE:HE1	1:H:195:VAL:HG11	1.85	0.42
1:J:507:ARG:NE	1:J:507:ARG:N	2.59	0.42
1:A:497:THR:HG23	1:A:529:THR:HA	2.02	0.42
1:B:524:GLN:H	1:B:524:GLN:HG2	1.50	0.42
1:C:169:CYS:HB2	1:C:192:CYS:HA	2.01	0.42
1:C:332:GLU:C	1:C:334:ASN:N	2.76	0.42
1:I:530:VAL:O	1:I:530:VAL:HG12	2.20	0.42
1:J:154:PHE:CE1	1:J:195:VAL:HG21	2.55	0.42
1:A:370:LEU:HD13	1:A:376:VAL:HG21	2.01	0.42
1:B:23:THR:HG21	1:B:392:ILE:HG23	2.01	0.42
1:B:319:TYR:HA	1:B:350:ILE:CD1	2.49	0.42
1:C:75:ASN:HD21	1:C:375:ASN:HA	1.85	0.42
1:D:127:THR:O	1:D:131:GLN:HG2	2.20	0.42
1:G:172:SER:O	1:G:185:LYS:HB3	2.20	0.42
1:G:326:TYR:CG	1:G:330:PRO:CB	2.92	0.42
1:G:421:TYR:HE1	1:G:531:SER:O	2.02	0.42
1:G:506:ARG:O	1:G:507:ARG:CB	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:ARG:HB2	1:H:454:VAL:CG2	2.49	0.42
1:C:67:TRP:HB3	1:C:161:HIS:HB3	2.02	0.42
1:E:442:TRP:HD1	1:E:476:ILE:HD12	1.84	0.42
1:G:4:LEU:HB3	1:G:428:CYS:SG	2.59	0.42
1:J:49:ILE:HG22	1:J:320:ALA:HA	2.01	0.42
1:J:80:PHE:CZ	1:J:317:MET:HG3	2.55	0.42
1:B:45:CYS:O	1:B:75:ASN:HB2	2.20	0.41
1:E:329:SER:HB2	1:E:330:PRO:HD2	2.02	0.41
1:F:326:TYR:CE2	1:F:371:LYS:HA	2.55	0.41
1:J:437:THR:HG21	1:J:504:ALA:HB1	2.02	0.41
1:J:473:ARG:H	1:J:473:ARG:HD2	1.84	0.41
1:D:506:ARG:HB2	1:D:521:TYR:HE2	1.84	0.41
1:C:162:LEU:HD22	1:C:316:SER:HB3	2.02	0.41
1:F:326:TYR:CD2	1:F:370:LEU:O	2.73	0.41
1:J:167:GLY:HA2	1:J:195:VAL:CG1	2.50	0.41
1:B:436:SER:O	1:B:459:TRP:O	2.39	0.41
1:F:66:SER:O	1:F:69:THR:HG22	2.21	0.41
1:G:97:ILE:HG22	1:G:143:ILE:HA	2.02	0.41
1:J:47:ILE:HA	1:J:75:ASN:HA	2.02	0.41
1:J:318:GLY:O	1:J:321:VAL:HB	2.20	0.41
1:B:334:ASN:HB2	1:B:380:ILE:CD1	2.50	0.41
1:C:126:LEU:HG	1:C:129:LEU:HB3	2.01	0.41
1:C:428:CYS:O	1:C:484:THR:HA	2.21	0.41
1:E:184:GLN:C	1:E:185:LYS:CG	2.92	0.41
1:B:162:LEU:HB3	1:B:166:ILE:HG13	2.02	0.41
1:F:115:PRO:O	1:F:257:LEU:HD22	2.20	0.41
1:J:129:LEU:HD21	1:J:280:VAL:HG23	2.01	0.41
1:C:376:VAL:HG23	1:C:377:SER:N	2.35	0.41
1:C:445:GLN:HG3	1:C:449:LYS:O	2.21	0.41
1:E:17:THR:CG2	1:E:418:THR:OG1	2.68	0.41
1:G:479:ASP:OD2	1:G:482:LYS:HD2	2.21	0.41
1:H:146:LEU:O	1:H:150:VAL:HG23	2.20	0.41
1:B:212:GLN:HG3	1:B:215:GLN:NE2	2.36	0.41
1:C:98:VAL:HG12	1:C:405:LEU:HD22	2.02	0.41
1:D:43:ASP:O	1:D:374:LYS:HG3	2.21	0.41
1:D:48:LEU:O	1:D:72:GLY:O	2.38	0.41
1:E:35:GLN:HE22	1:E:95:GLN:HE22	1.69	0.41
1:F:23:THR:HG21	1:F:392:ILE:HG23	2.03	0.41
1:F:45:CYS:O	1:F:75:ASN:HB2	2.20	0.41
1:F:116:HIS:CE1	1:F:261:LEU:HD22	2.56	0.41
1:G:23:THR:HG21	1:G:392:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:C	1:A:370:LEU:CD1	2.92	0.41
1:A:429:ALA:HA	1:A:484:THR:HG22	2.03	0.41
1:D:12:VAL:HG11	1:D:492:LEU:HD13	2.03	0.41
1:E:12:VAL:HG21	1:E:492:LEU:HD13	2.03	0.41
1:E:378:LEU:HD22	1:E:382:GLN:HB3	2.03	0.41
1:E:437:THR:HG23	1:E:459:TRP:CD1	2.56	0.41
1:H:88:SER:O	1:H:91:ILE:HG13	2.21	0.41
1:I:37:ILE:HG12	1:I:310:VAL:CG1	2.50	0.41
1:J:129:LEU:CD2	1:J:133:MET:HG2	2.51	0.41
1:E:288:LYS:CE	1:E:288:LYS:CA	2.92	0.41
1:C:210:ASN:HA	1:C:213:THR:HG23	2.02	0.40
1:G:174:ILE:O	1:G:174:ILE:CG1	2.69	0.40
1:G:210:ASN:O	1:G:213:THR:CG2	2.69	0.40
1:J:505:ARG:HD2	1:J:518:GLU:O	2.19	0.40
1:B:120:LEU:HD23	1:B:120:LEU:N	2.36	0.40
1:C:335:GLN:HG3	1:C:353:GLY:HA3	2.03	0.40
1:F:453:PHE:HB2	1:F:514:THR:O	2.21	0.40
1:F:458:TYR:HB3	1:F:509:PHE:CZ	2.55	0.40
1:G:479:ASP:OD2	1:G:482:LYS:CD	2.69	0.40
1:I:12:VAL:CG1	1:I:530:VAL:HG22	2.51	0.40
1:I:90:MET:HE2	1:I:306:ALA:HA	2.04	0.40
1:J:96:LYS:HA	1:J:99:GLN:HG2	2.03	0.40
1:A:5:VAL:HG11	1:B:106:ALA:CB	2.51	0.40
1:E:47:ILE:HA	1:E:75:ASN:HA	2.04	0.40
1:G:70:ALA:O	1:G:74:LYS:NZ	2.49	0.40
1:I:303:THR:HG23	1:I:402:LEU:HD21	2.03	0.40
1:J:94:ALA:HB1	1:J:303:THR:HG22	2.04	0.40
1:F:254:TYR:C	1:F:254:TYR:CD1	3.00	0.40
1:A:14:THR:OG1	1:B:22:ASP:HB2	2.21	0.40
1:A:67:TRP:HB3	1:A:161:HIS:HB3	2.03	0.40
1:D:154:PHE:CE1	1:D:195:VAL:HG21	2.57	0.40
1:E:17:THR:HG23	1:E:418:THR:OG1	2.22	0.40
1:H:93:ASN:HD22	1:H:146:LEU:HD23	1.86	0.40
1:I:506:ARG:HD3	1:I:521:TYR:OH	2.22	0.40
1:J:499:VAL:HA	1:J:526:THR:O	2.22	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	436/542 (80%)	417 (96%)	19 (4%)	0	100	100
1	B	432/542 (80%)	412 (95%)	19 (4%)	1 (0%)	43	62
1	C	421/542 (78%)	398 (94%)	21 (5%)	2 (0%)	24	43
1	D	432/542 (80%)	417 (96%)	15 (4%)	0	100	100
1	E	439/542 (81%)	422 (96%)	17 (4%)	0	100	100
1	F	443/542 (82%)	424 (96%)	18 (4%)	1 (0%)	43	62
1	G	457/542 (84%)	441 (96%)	15 (3%)	1 (0%)	43	62
1	H	377/542 (70%)	364 (97%)	12 (3%)	1 (0%)	36	55
1	I	401/542 (74%)	388 (97%)	12 (3%)	1 (0%)	43	62
1	J	364/542 (67%)	350 (96%)	14 (4%)	0	100	100
All	All	4202/5420 (78%)	4033 (96%)	162 (4%)	7 (0%)	43	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	161	HIS
1	I	47	ILE
1	C	75	ASN
1	F	333	ASN
1	G	507	ARG
1	C	171	ALA
1	B	330	PRO

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	366/438 (84%)	346 (94%)	20 (6%)	19	40
1	B	361/438 (82%)	330 (91%)	31 (9%)	10	21
1	C	349/438 (80%)	314 (90%)	35 (10%)	7	16
1	D	364/438 (83%)	336 (92%)	28 (8%)	12	26
1	E	365/438 (83%)	336 (92%)	29 (8%)	11	25
1	F	373/438 (85%)	349 (94%)	24 (6%)	16	33
1	G	384/438 (88%)	352 (92%)	32 (8%)	10	23
1	H	325/438 (74%)	305 (94%)	20 (6%)	16	34
1	I	342/438 (78%)	314 (92%)	28 (8%)	10	23
1	J	309/438 (70%)	287 (93%)	22 (7%)	13	29
All	All	3538/4380 (81%)	3269 (92%)	269 (8%)	12	26

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	VAL
1	A	26	ASP
1	A	49	ILE
1	A	75	ASN
1	A	91	ILE
1	A	134	LEU
1	A	170	ASP
1	A	220	GLN
1	A	276	ILE
1	A	278	GLN
1	A	286	ARG
1	A	321	VAL
1	A	350	ILE
1	A	376	VAL
1	A	398	LYS
1	A	465	TYR
1	A	478	ARG
1	A	511	LEU
1	A	528	VAL
1	B	2	VAL
1	B	3	GLN
1	B	6	GLU

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Mol	Chain	Res	Type
1	B	11	LEU
1	B	12	VAL
1	B	49	ILE
1	B	103	GLN
1	B	110	LYS
1	B	120	LEU
1	B	132	LYS
1	B	168	LYS
1	B	187	ASN
1	B	196	GLU
1	B	212	GLN
1	B	222	LEU
1	B	277	ASN
1	B	317	MET
1	B	321	VAL
1	B	370	LEU
1	B	375	ASN
1	B	380	ILE
1	B	408	LYS
1	B	411	LYS
1	B	412	LEU
1	B	449	LYS
1	B	458	TYR
1	B	461	VAL
1	B	484	THR
1	B	524	GLN
1	B	530	VAL
1	B	532	SER
1	C	5	VAL
1	C	11	LEU
1	C	12	VAL
1	C	26	ASP
1	C	104	LEU
1	C	126	LEU
1	C	127	THR
1	C	129	LEU
1	C	164	ASP
1	C	196	GLU
1	C	197	GLU
1	C	216	ILE
1	C	217	ASN
1	C	278	GLN

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Mol	Chain	Res	Type
1	C	317	MET
1	C	321	VAL
1	C	333	ASN
1	C	335	GLN
1	C	350	ILE
1	C	382	GLN
1	C	399	GLN
1	C	408	LYS
1	C	410	GLU
1	C	411	LYS
1	C	412	LEU
1	C	413	GLU
1	C	433	ARG
1	C	434	THR
1	C	451	ARG
1	C	460	THR
1	C	461	VAL
1	C	511	LEU
1	C	520	ASP
1	C	524	GLN
1	C	530	VAL
1	D	2	VAL
1	D	11	LEU
1	D	12	VAL
1	D	26	ASP
1	D	104	LEU
1	D	112	ILE
1	D	113	THR
1	D	114	GLN
1	D	116	HIS
1	D	120	LEU
1	D	134	LEU
1	D	196	GLU
1	D	211	ASN
1	D	215	GLN
1	D	225	THR
1	D	276	ILE
1	D	321	VAL
1	D	322	ILE
1	D	323	CYS
1	D	346	ASN
1	D	349	THR

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Mol	Chain	Res	Type
1	D	350	ILE
1	D	376	VAL
1	D	380	ILE
1	D	412	LEU
1	D	461	VAL
1	D	469	SER
1	D	528	VAL
1	E	11	LEU
1	E	49	ILE
1	E	91	ILE
1	E	102	GLN
1	E	110	LYS
1	E	118	LEU
1	E	144	LEU
1	E	150	VAL
1	E	174	ILE
1	E	176	SER
1	E	181	MET
1	E	182	GLN
1	E	201	LEU
1	E	203	LYS
1	E	216	ILE
1	E	274	GLN
1	E	280	VAL
1	E	288	LYS
1	E	321	VAL
1	E	329	SER
1	E	332	GLU
1	E	350	ILE
1	E	408	LYS
1	E	412	LEU
1	E	473	ARG
1	E	483	ASN
1	E	517	ASN
1	E	528	VAL
1	E	530	VAL
1	F	2	VAL
1	F	11	LEU
1	F	12	VAL
1	F	17	THR
1	F	26	ASP
1	F	102	GLN

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Mol	Chain	Res	Type
1	F	107	ASN
1	F	110	LYS
1	F	157	LEU
1	F	162	LEU
1	F	169	CYS
1	F	170	ASP
1	F	213	THR
1	F	218	GLN
1	F	226	LEU
1	F	260	LEU
1	F	261	LEU
1	F	296	ASN
1	F	321	VAL
1	F	328	LYS
1	F	350	ILE
1	F	376	VAL
1	F	399	GLN
1	F	461	VAL
1	G	2	VAL
1	G	11	LEU
1	G	12	VAL
1	G	26	ASP
1	G	74	LYS
1	G	97	ILE
1	G	113	THR
1	G	134	LEU
1	G	166	ILE
1	G	179	MET
1	G	181	MET
1	G	183	ASN
1	G	187	ASN
1	G	196	GLU
1	G	211	ASN
1	G	216	ILE
1	G	222	LEU
1	G	260	LEU
1	G	317	MET
1	G	321	VAL
1	G	327	THR
1	G	334	ASN
1	G	350	ILE
1	G	370	LEU

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Mol	Chain	Res	Type
1	G	373	ASP
1	G	376	VAL
1	G	408	LYS
1	G	458	TYR
1	G	480	ASN
1	G	507	ARG
1	G	514	THR
1	G	526	THR
1	H	26	ASP
1	H	91	ILE
1	H	102	GLN
1	H	103	GLN
1	H	118	LEU
1	H	120	LEU
1	H	134	LEU
1	H	157	LEU
1	H	166	ILE
1	H	202	LEU
1	H	276	ILE
1	H	317	MET
1	H	334	ASN
1	H	350	ILE
1	H	405	LEU
1	H	411	LYS
1	H	412	LEU
1	H	460	THR
1	H	480	ASN
1	H	528	VAL
1	I	11	LEU
1	I	12	VAL
1	I	26	ASP
1	I	37	ILE
1	I	47	ILE
1	I	83	GLU
1	I	114	GLN
1	I	118	LEU
1	I	134	LEU
1	I	151	GLU
1	I	155	ASN
1	I	190	ASN
1	I	210	ASN
1	I	217	ASN

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Mol	Chain	Res	Type
1	I	255	GLU
1	I	257	LEU
1	I	260	LEU
1	I	261	LEU
1	I	276	ILE
1	I	317	MET
1	I	321	VAL
1	I	323	CYS
1	I	335	GLN
1	I	350	ILE
1	I	412	LEU
1	I	437	THR
1	I	451	ARG
1	I	461	VAL
1	J	26	ASP
1	J	37	ILE
1	J	102	GLN
1	J	131	GLN
1	J	144	LEU
1	J	202	LEU
1	J	276	ILE
1	J	280	VAL
1	J	283	LEU
1	J	285	GLU
1	J	308	ARG
1	J	317	MET
1	J	333	ASN
1	J	346	ASN
1	J	349	THR
1	J	350	ILE
1	J	412	LEU
1	J	457	ILE
1	J	473	ARG
1	J	507	ARG
1	J	518	GLU
1	J	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	63	ASN

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Mol	Chain	Res	Type
1	A	117	ASN
1	A	119	ASN
1	A	149	GLN
1	A	161	HIS
1	A	211	ASN
1	A	220	GLN
1	A	224	ASN
1	A	346	ASN
1	B	3	GLN
1	B	29	ASN
1	B	75	ASN
1	B	107	ASN
1	B	121	ASN
1	B	149	GLN
1	B	190	ASN
1	B	215	GLN
1	B	218	GLN
1	B	220	GLN
1	B	301	GLN
1	B	315	ASN
1	B	375	ASN
1	B	399	GLN
1	B	445	GLN
1	B	517	ASN
1	C	3	GLN
1	C	13	GLN
1	C	28	GLN
1	C	29	ASN
1	C	102	GLN
1	C	107	ASN
1	C	186	ASN
1	C	190	ASN
1	C	215	GLN
1	C	281	ASN
1	C	315	ASN
1	C	333	ASN
1	C	375	ASN
1	C	517	ASN
1	C	524	GLN
1	D	28	GLN
1	D	103	GLN
1	D	107	ASN

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Mol	Chain	Res	Type
1	D	108	GLN
1	D	117	ASN
1	D	121	ASN
1	D	131	GLN
1	D	155	ASN
1	D	161	HIS
1	D	187	ASN
1	D	190	ASN
1	D	215	GLN
1	D	221	ASN
1	D	224	ASN
1	D	281	ASN
1	D	301	GLN
1	D	335	GLN
1	D	351	ASN
1	D	391	GLN
1	D	399	GLN
1	D	415	HIS
1	D	488	GLN
1	D	527	GLN
1	E	28	GLN
1	E	35	GLN
1	E	103	GLN
1	E	107	ASN
1	E	183	ASN
1	E	186	ASN
1	E	187	ASN
1	E	190	ASN
1	E	220	GLN
1	E	277	ASN
1	E	278	GLN
1	E	315	ASN
1	E	335	GLN
1	E	344	ASN
1	E	346	ASN
1	E	375	ASN
1	E	445	GLN
1	E	480	ASN
1	E	488	GLN
1	E	517	ASN
1	E	527	GLN
1	F	68	GLN

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Mol	Chain	Res	Type
1	F	75	ASN
1	F	107	ASN
1	F	108	GLN
1	F	114	GLN
1	F	121	ASN
1	F	199	GLN
1	F	211	ASN
1	F	212	GLN
1	F	217	ASN
1	F	221	ASN
1	F	346	ASN
1	F	387	HIS
1	G	13	GLN
1	G	39	ASN
1	G	95	GLN
1	G	111	ASN
1	G	131	GLN
1	G	161	HIS
1	G	187	ASN
1	G	190	ASN
1	G	215	GLN
1	G	224	ASN
1	G	256	GLN
1	G	277	ASN
1	G	281	ASN
1	G	351	ASN
1	G	415	HIS
1	H	75	ASN
1	H	93	ASN
1	H	103	GLN
1	H	119	ASN
1	H	217	ASN
1	H	224	ASN
1	H	232	ASN
1	H	233	ASN
1	H	281	ASN
1	H	334	ASN
1	H	415	HIS
1	I	29	ASN
1	I	92	ASN
1	I	95	GLN
1	I	99	GLN

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Mol	Chain	Res	Type
1	I	116	HIS
1	I	119	ASN
1	I	187	ASN
1	I	211	ASN
1	I	212	GLN
1	I	220	GLN
1	I	315	ASN
1	I	334	ASN
1	I	335	GLN
1	I	387	HIS
1	J	29	ASN
1	J	75	ASN
1	J	107	ASN
1	J	108	GLN
1	J	190	ASN
1	J	281	ASN
1	J	282	ASN
1	J	315	ASN
1	J	333	ASN
1	J	344	ASN
1	J	351	ASN
1	J	480	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/542 (82%)	0.16	11 (2%) 58 49	56, 89, 132, 163	0
1	B	446/542 (82%)	0.21	25 (5%) 30 23	47, 89, 149, 197	0
1	C	431/542 (79%)	0.23	15 (3%) 47 37	46, 88, 138, 186	0
1	D	446/542 (82%)	0.16	10 (2%) 62 53	54, 89, 135, 160	0
1	E	451/542 (83%)	0.34	19 (4%) 40 32	61, 103, 160, 179	0
1	F	457/542 (84%)	0.22	16 (3%) 47 37	55, 88, 130, 157	0
1	G	469/542 (86%)	0.21	6 (1%) 75 69	59, 95, 144, 178	0
1	H	399/542 (73%)	0.39	19 (4%) 35 29	76, 110, 152, 175	0
1	I	419/542 (77%)	0.34	14 (3%) 49 39	63, 107, 151, 183	0
1	J	380/542 (70%)	0.44	22 (5%) 29 22	69, 110, 152, 184	0
All	All	4346/5420 (80%)	0.27	157 (3%) 46 37	46, 97, 146, 197	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	TYR	6.8
1	J	133	MET	4.8
1	G	506	ARG	4.6
1	J	496	ASP	4.5
1	B	316	SER	4.4
1	C	321	VAL	4.4
1	B	369	THR	4.2
1	E	306	ALA	4.1
1	D	333	ASN	4.0
1	F	351	ASN	4.0
1	J	137	ALA	3.9
1	I	432	GLY	3.9
1	E	303	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	319	TYR	3.9
1	C	322	ILE	3.8
1	A	458	TYR	3.8
1	H	438	ALA	3.8
1	H	5	VAL	3.7
1	J	429	ALA	3.7
1	C	177	ALA	3.7
1	C	179	MET	3.7
1	B	189	GLY	3.6
1	J	353	GLY	3.6
1	B	50	ALA	3.6
1	E	349	THR	3.6
1	C	320	ALA	3.5
1	E	369	THR	3.5
1	B	219	ALA	3.5
1	E	34	ALA	3.5
1	C	175	SER	3.4
1	C	133	MET	3.4
1	E	98	VAL	3.4
1	E	302	ALA	3.3
1	H	127	THR	3.3
1	F	188	TRP	3.2
1	I	78	ALA	3.1
1	A	120	LEU	3.1
1	H	20	VAL	3.0
1	D	70	ALA	3.0
1	J	276	ILE	3.0
1	I	231	GLY	3.0
1	A	159	SER	3.0
1	H	19	SER	2.9
1	J	139	SER	2.9
1	F	68	GLN	2.9
1	E	126	LEU	2.9
1	D	324	GLY	2.9
1	B	184	GLN	2.9
1	A	216	ILE	2.9
1	I	322	ILE	2.9
1	G	40	THR	2.8
1	H	397	LEU	2.8
1	J	510	THR	2.8
1	I	194	GLY	2.8
1	E	62	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	2.8
1	J	172	SER	2.8
1	J	350	ILE	2.8
1	F	262	THR	2.8
1	J	460	THR	2.8
1	I	323	CYS	2.7
1	D	344	ASN	2.7
1	C	276	ILE	2.7
1	F	195	VAL	2.7
1	C	128	ALA	2.6
1	I	87	ALA	2.6
1	B	354	GLY	2.6
1	G	251	SER	2.6
1	B	447	PRO	2.6
1	F	253	THR	2.6
1	G	176	SER	2.6
1	A	273	ALA	2.6
1	B	448	GLY	2.6
1	J	319	TYR	2.6
1	A	333	ASN	2.6
1	I	19	SER	2.5
1	I	198	THR	2.5
1	I	150	VAL	2.5
1	B	446	ALA	2.5
1	B	331	GLY	2.5
1	B	185	LYS	2.5
1	H	276	ILE	2.5
1	A	166	ILE	2.4
1	H	504	ALA	2.4
1	B	178	ASN	2.4
1	E	305	LEU	2.4
1	A	276	ILE	2.4
1	H	354	GLY	2.4
1	J	521	TYR	2.4
1	B	181	MET	2.4
1	B	350	ILE	2.4
1	E	174	ILE	2.4
1	H	70	ALA	2.4
1	E	146	LEU	2.4
1	J	126	LEU	2.4
1	H	461	VAL	2.3
1	C	446	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	188	TRP	2.3
1	A	369	THR	2.3
1	D	458	TYR	2.3
1	E	310	VAL	2.3
1	C	130	ALA	2.3
1	F	193	ALA	2.3
1	H	67	TRP	2.3
1	I	47	ILE	2.3
1	J	530	VAL	2.3
1	J	189	GLY	2.3
1	D	334	ASN	2.3
1	F	343	GLU	2.3
1	J	94	ALA	2.3
1	E	460	THR	2.3
1	F	349	THR	2.3
1	H	71	GLY	2.3
1	H	333	ASN	2.3
1	F	147	ALA	2.3
1	F	369	THR	2.3
1	C	189	GLY	2.3
1	F	70	ALA	2.2
1	G	369	THR	2.2
1	F	76	SER	2.2
1	G	72	GLY	2.2
1	H	118	LEU	2.2
1	B	143	ILE	2.2
1	J	37	ILE	2.2
1	B	286	ARG	2.2
1	J	79	THR	2.2
1	B	166	ILE	2.2
1	H	216	ILE	2.2
1	B	40	THR	2.2
1	F	115	PRO	2.2
1	H	502	CYS	2.2
1	J	463	SER	2.2
1	B	315	ASN	2.1
1	J	280	VAL	2.1
1	A	490	ASP	2.1
1	E	179	MET	2.1
1	F	8	GLY	2.1
1	C	166	ILE	2.1
1	C	103	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	5	VAL	2.1
1	I	517	ASN	2.1
1	D	71	GLY	2.1
1	B	275	ALA	2.1
1	D	159	SER	2.1
1	F	77	CYS	2.1
1	H	232	ASN	2.1
1	E	31	LEU	2.1
1	E	307	LEU	2.1
1	E	73	GLY	2.1
1	E	94	ALA	2.1
1	J	275	ALA	2.1
1	B	179	MET	2.0
1	D	471	LYS	2.0
1	H	226	LEU	2.0
1	I	80	PHE	2.0
1	I	354	GLY	2.0
1	A	343	GLU	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	601	1/1	0.92	0.11	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.