Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 06:21 PM BST

PDB ID	:	6QD6
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 following versions of software and data (see references ①) were used in the production of this report:

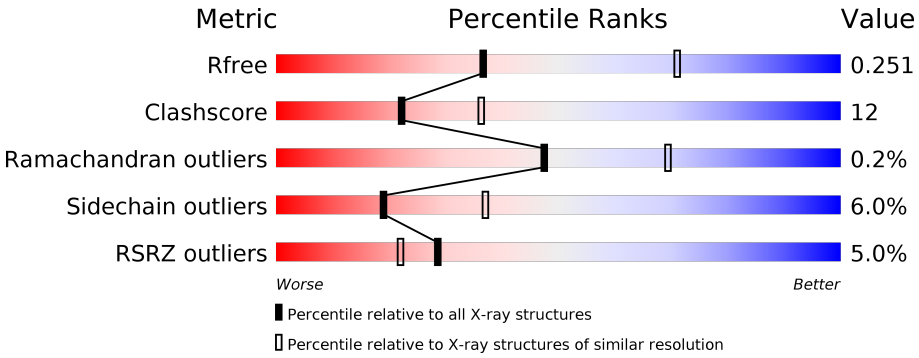
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (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 on 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 <=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% 69% 13% • 17%
1	B	542	5% 68% 13% • 18%
1	C	542	3% 59% 19% • 20%
1	D	542	2% 68% 13% • 18%
1	E	542	4% 64% 17% • 17%
1	F	542	3% 65% 18% • 16%

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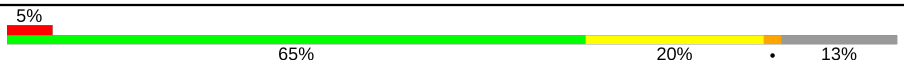
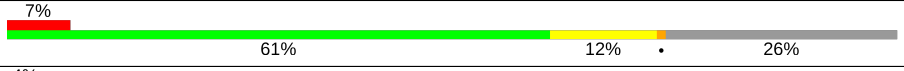
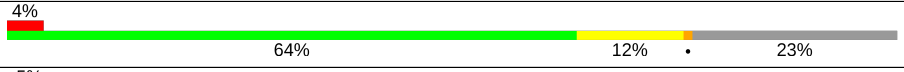
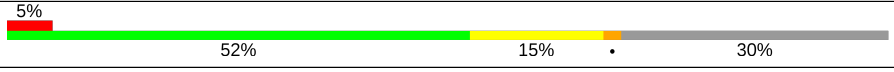
Mol	Chain	Length	Quality of chain
1	G	542	
1	H	542	
1	I	542	
1	J	542	

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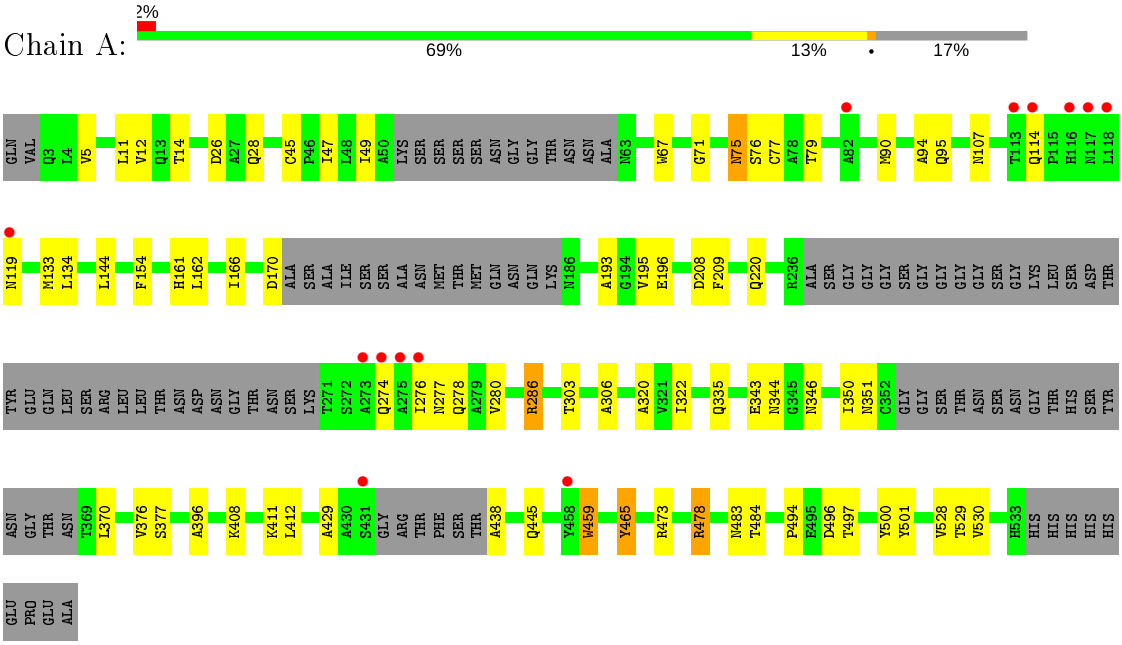
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	15	Total O 15 15	0	0
3	C	11	Total O 11 11	0	0
3	D	12	Total O 12 12	0	0
3	E	8	Total O 8 8	0	0
3	F	14	Total O 14 14	0	0
3	G	14	Total O 14 14	0	0
3	H	5	Total O 5 5	0	0
3	I	12	Total O 12 12	0	0
3	J	5	Total O 5 5	0	0

3 Residue-property plots (i)

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.

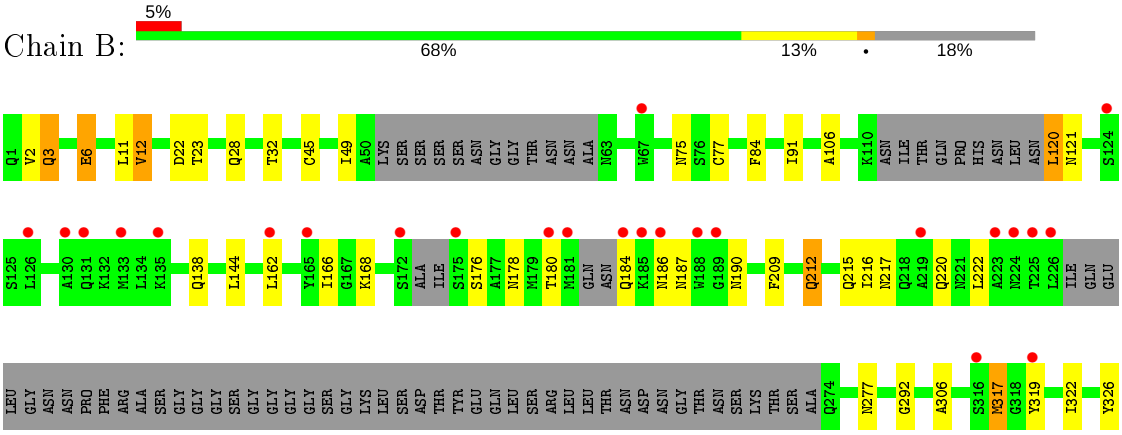
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207

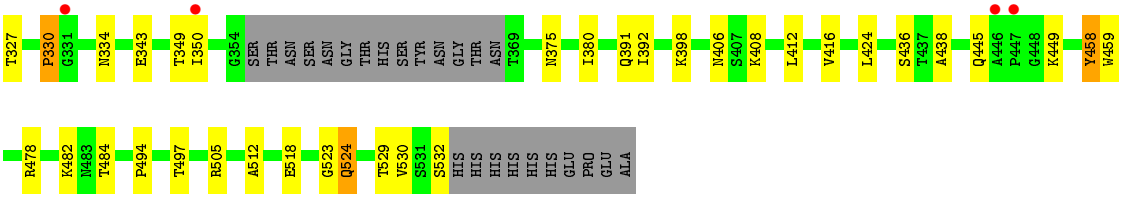
Chain A:

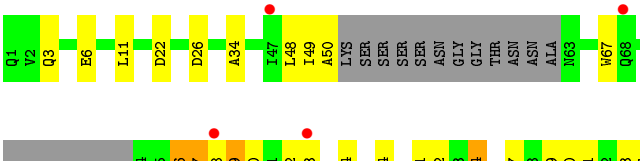


• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207

Chain B:





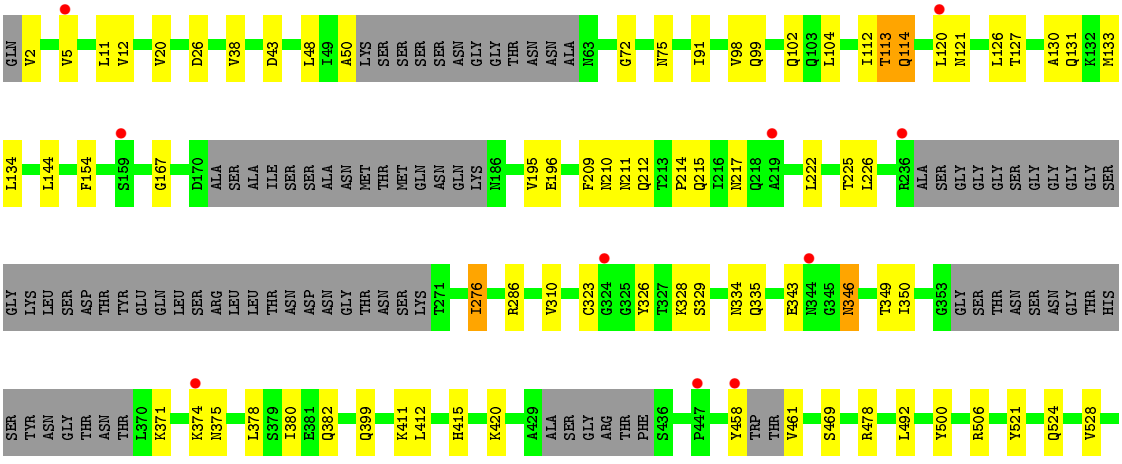


• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain C:

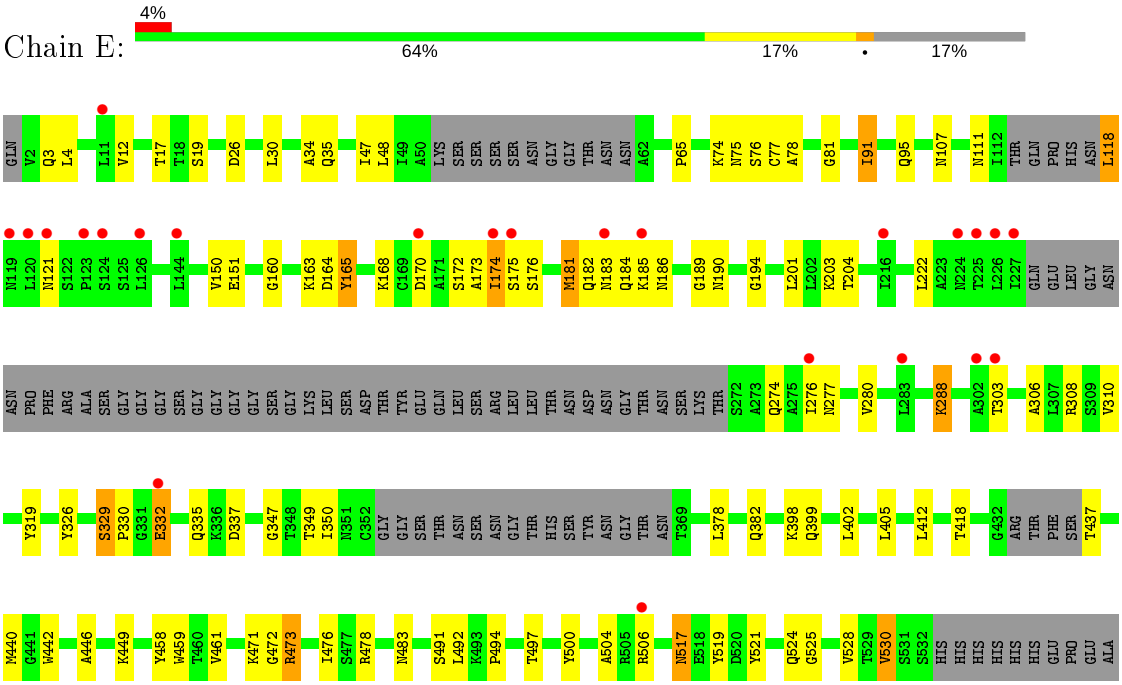
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain D:



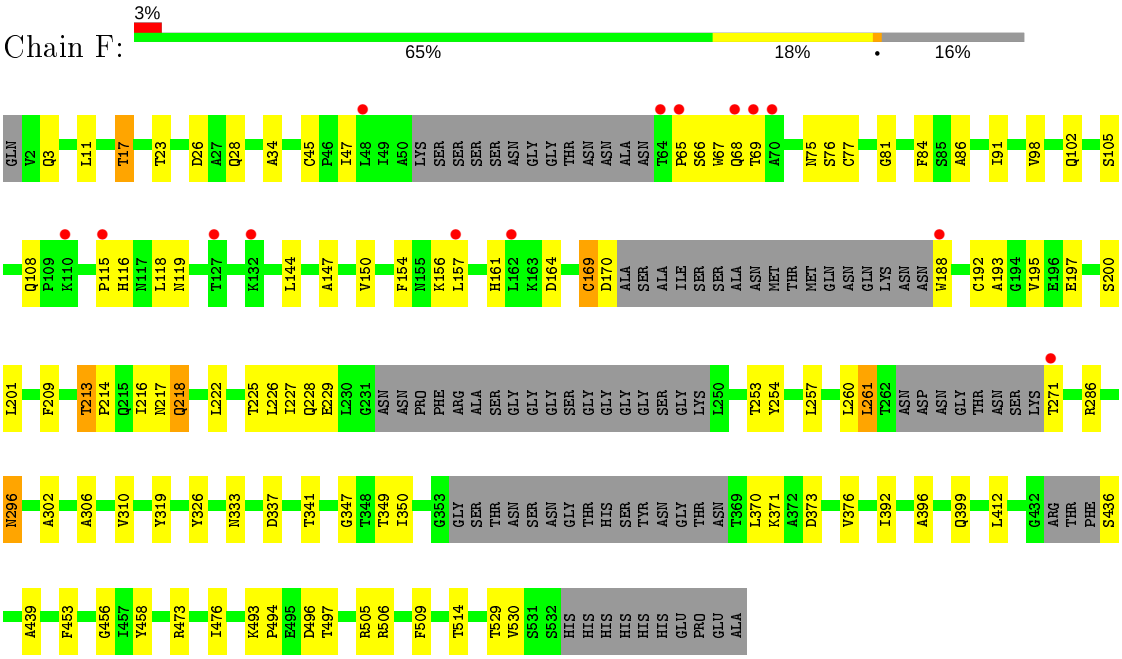
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain E:



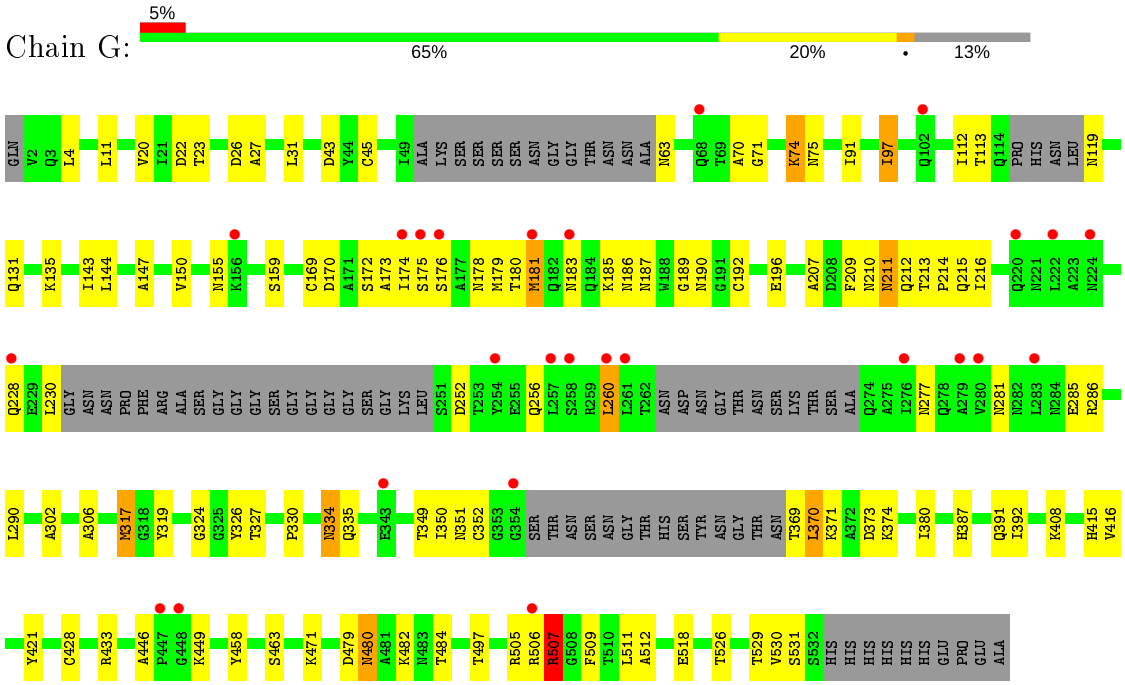
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain F:



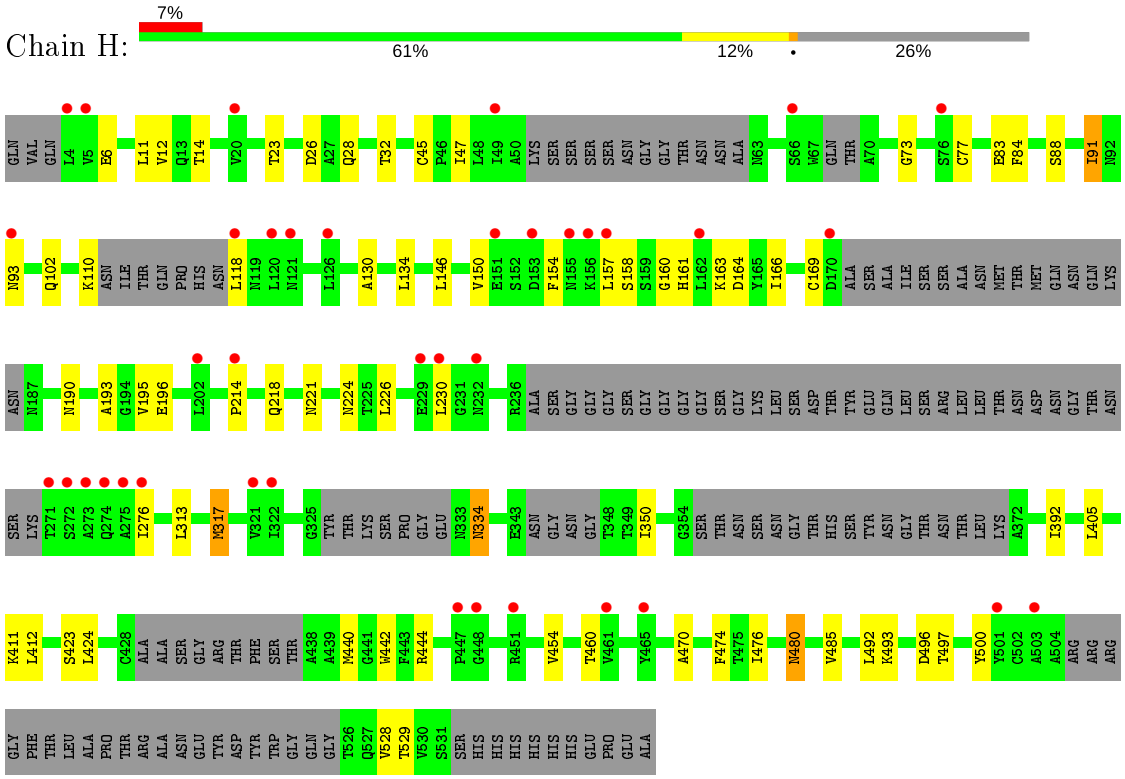
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain G:



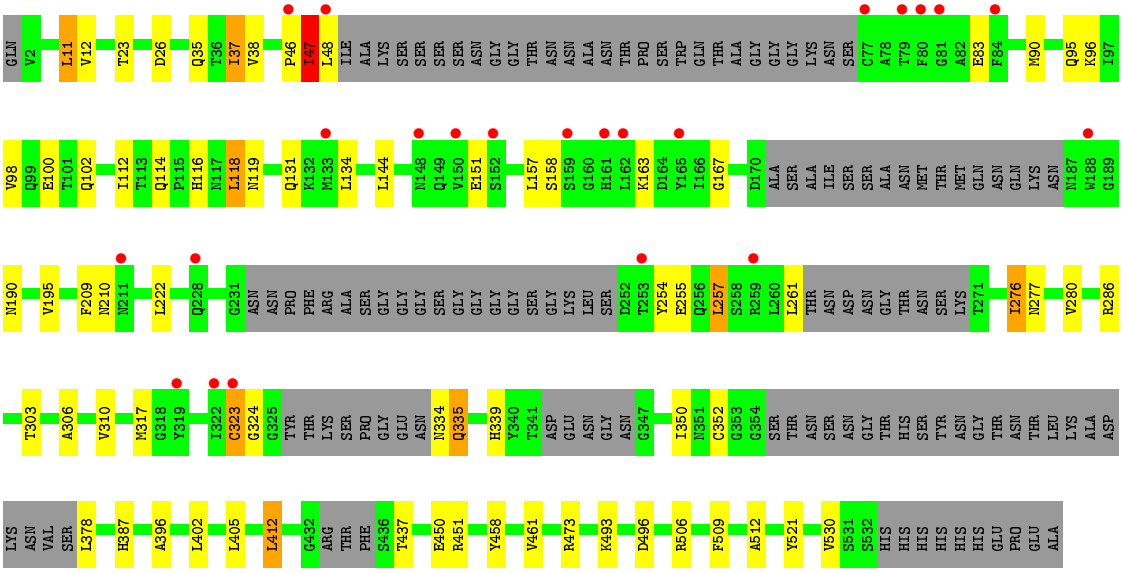
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain H:



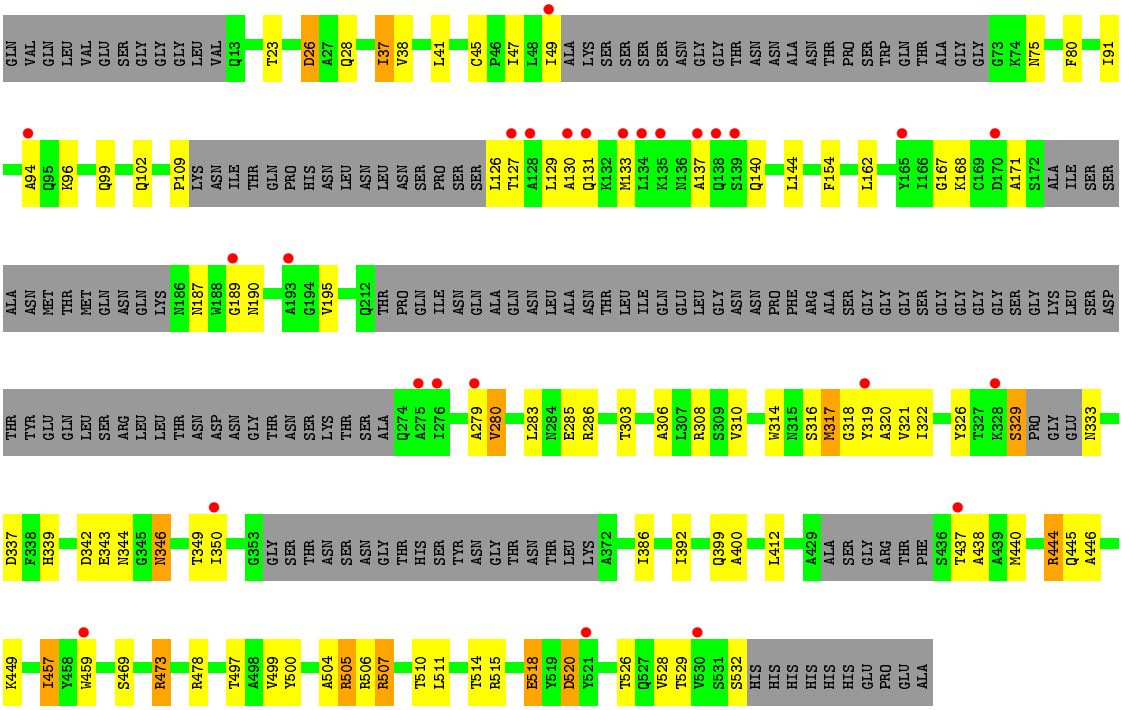
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain I:



• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane pr otein,Mb-cHopQ-Nb207

Chain J:



4 Data and refinement statistics (i)

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 44.77 – 2.84	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.45-2.84) 95.4 (44.77-2.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.204 , 0.239 0.225 , 0.251	Depositor DCC
R_{free} test set	6538 reflections (5.06%)	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 , 72.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.50	0/3461	0.73	0/4690
1	B	0.56	0/3419	0.74	0/4625
1	C	0.55	0/3310	0.77	0/4479
1	D	0.51	0/3432	0.74	0/4647
1	E	0.50	0/3453	0.73	0/4676
1	F	0.55	0/3514	0.74	0/4760
1	G	0.52	0/3610	0.74	0/4887
1	H	0.48	0/3051	0.72	0/4124
1	I	0.48	0/3229	0.72	0/4369
1	J	0.53	0/2939	0.73	0/3971
All	All	0.52	0/33418	0.74	0/45228

There are no bond length outliers.

There are no bond angle outliers.

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	64	0
1	B	3372	0	3291	62	0
1	C	3263	0	3181	77	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	96	0
1	F	3465	0	3388	85	0
1	G	3561	0	3477	122	0
1	H	3015	0	2948	57	0
1	I	3187	0	3118	56	0
1	J	2900	0	2817	104	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	761	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 (761) 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: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
1:E:497:THR:HG22	1:E:530:VAL:H	1.15	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:I:47:ILE:HD12	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:C:127:THR:HG22	1:C:128:ALA:N	1.87	0.90
1:F:118:LEU:HD22	1:F:253:THR:HG22	1.53	0.89
1:G:143:ILE:HG21	1:G:290:LEU:HD11	1.55	0.88
1:H:130:ALA:HB2	1:H:226:LEU:HD22	1.57	0.87
1:A:370:LEU:HD11	1:A:377:SER:HB2	1.56	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:H:84:PHE:CE1	1:H:317:MET:CE	2.60	0.84
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:H	1:E:517:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:181:MET:CE	1:G:186:ASN:OD1	2.28	0.82
1:G:326:TYR:CD2	1:G:330:PRO:CB	2.60	0.81
1:E:3:GLN:CG	1:E:4:LEU:H	1.94	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: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:H:84:PHE:HE1	1:H:317:MET:HE3	1.47	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:J:133:MET:HE1	1:J:279:ALA:O	1.84	0.78
1:I:11:LEU:HD21	3:I:601:HOH:O	1.84	0.77
1:E:288:LYS:HE2	1:E:288:LYS:HA	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:I:83:GLU:HB3	1:I:157:LEU:CD1	2.14	0.77
1:J:507:ARG:NE	1:J:507:ARG:H	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
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:D:113:THR:C	1:D:114:GLN:HG2	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:SER:OG	1:G:181:MET:CE	2.36	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: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:H:214:PRO:O	1:H:218:GLN:HG3	1.87	0.73
1:G:181:MET:HE2	1:G:186:ASN:OD1	1.88	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:N	1:D:346:ASN:OD1	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: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:HG2	1:F:228:GLN:O	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:J:133:MET:HE2	1:J:279:ALA:O	1.91	0.70
1:F:341:THR:HA	1:F:347:GLY:HA2	1.73	0.70
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:J:133:MET:HE3	1:J:283:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:I:257:LEU:HD13	1.93	0.69
1:F:119:ASN:ND2	1:G:471:LYS:HE2	2.07	0.69
1:I:335:GLN:HE21	1:I:335:GLN:C	1.96	0.69
1:H:440:MET:SD	1:H:485:VAL:CG2	2.80	0.69
1:J:440:MET:HG3	1:J:459:TRP:CE3	2.27	0.69
1:G:369:THR:HG23	1:G:370:LEU:CD2	2.22	0.69
1:G:144:LEU:HD21	1:G:209:PHE:HB3	1.75	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:O	1:A:478:ARG:HD2	1.93	0.68
1:G:181:MET:HE3	1:G:186:ASN:OD1	1.92	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: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
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: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:B:84:PHE:HE1	1:B:317:MET:HE2	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:497:THR:HG22	1:E:530:VAL:N	2.00	0.66
1:H:84:PHE:CZ	1:H:317:MET:HE1	2.30	0.66
1:J:440:MET:HG3	1:J:459:TRP:CZ3	2.31	0.66
1:C:164:ASP:N	1:C:164:ASP:OD1	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:J:342:ASP:CG	1:J:346:ASN:OD1	2.35	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:CE	1:E:288:LYS:HA	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:227:ILE:C	1:F:229:GLU:H	2.03	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:F:229:GLU:HA	1:F:229:GLU:OE1	2.01	0.61
1:A:370:LEU:C	1:A:370:LEU:HD12	2.21	0.61
1:E:398:LYS:HG3	1:E:399:GLN:HG3	1.83	0.61
1:H:84:PHE:CE1	1:H:317:MET:HE1	2.34	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:E:471:LYS:HD2	1:E:472:GLY:H	1.66	0.60
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: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:J:133:MET:HE1	1:J:283:LEU:HB2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:458:TYR:HB3	1:I:509:PHE:CZ	2.37	0.59
1:J:507:ARG:CD	1:J:507:ARG:H	2.11	0.59
1:E:517:ASN:H	1:E:517:ASN:ND2	1.97	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: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: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:I:412:LEU:HD12	1:I:412:LEU:C	2.24	0.58
1:I:47:ILE:N	1:I:47:ILE:HD12	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:507:ARG:H	1:J:507:ARG:HE	1.48	0.58
1:J:437:THR:CG2	1:J:507:ARG:NH2	2.49	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
1:G:326:TYR:CD2	1:G:370:LEU:C	2.76	0.58
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: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:E:165:TYR:N	1:E:165:TYR:CD1	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CD1	1:A:465:TYR:N	2.72	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: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:E:170:ASP:H	1:E:190:ASN:HD22	1.54	0.55
1:E:47:ILE:CG2	1:E:48:LEU:N	2.69	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:HD13	1:C:306:ALA:HB1	1.90	0.54
1:E:500:TYR:HD1	1:E:528:VAL:HG13	1.67	0.54
1:D:113:THR:C	1:D:114:GLN:CG	2.76	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: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:F:326:TYR:CE2	1:F:370:LEU:C	2.82	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:G:326:TYR:CE2	1:G:370:LEU:C	2.81	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
1:J:506:ARG:HG3	1:J:506:ARG:O	2.07	0.53
1:D:212:GLN:HB3	1:D:286:ARG:HH11	1.74	0.53
1:J:506:ARG:HB3	1:J:520:ASP:CG	2.29	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:127:THR:HG23	1:C:128:ALA:N	2.22	0.52
1:C:3:GLN:H	1:C:431:SER:HB2	1.73	0.52
1:C:457:ILE:O	1:C:457:ILE:HG23	2.09	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:J:37:ILE:HG13	1:J:38:VAL:N	2.24	0.52
1:D:334:ASN:O	1:D:380:ILE:HD11	2.10	0.52
1:B:84:PHE:CE1	1:B:317:MET:HE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:E:184:GLN:C	1:E:185:LYS:HG2	2.31	0.50
1:H:12:VAL:HG22	1:H:424:LEU:CD1	2.41	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:OE1	1:E:332:GLU:N	2.45	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: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:B:6:GLU:OE2	1:B:523:GLY:HA3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:D:343:GLU:CD	1:D:399:GLN:HE21	2.15	0.49
1:G:147:ALA:O	1:G:150:VAL:HG22	2.13	0.49
1:I:412:LEU:O	1:I:412:LEU:HD12	2.12	0.49
1:B:212:GLN:HG3	1:B:215:GLN:CD	2.33	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: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:O	1:A:114:GLN:HG3	2.12	0.49
1:E:440:MET:CE	1:E:504:ALA:HB2	2.43	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:G:131:GLN:HB3	1:G:135:LYS:HZ1	1.77	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:HA	1:A:274:GLN:OE1	2.14	0.48
1:A:335:GLN:HG3	1:A:351:ASN:OD1	2.14	0.48
1:D:212:GLN:OE1	1:D:286:ARG:HG3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:326:TYR:CZ	1:B:330:PRO:HG3	2.49	0.48
1:A:28:GLN:HE22	1:A:95:GLN:HG2	1.79	0.47
1:F:76:SER:HG	1:F:84:PHE:HE2	1.61	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:G:352:CYS:HB2	1:G:380:ILE:HD12	1.96	0.47
1:H:226:LEU:HD23	1:H:230:LEU:HD12	1.94	0.47
1:H:47:ILE:CG2	1:H:73:GLY:HA2	2.43	0.47
1:J:444:ARG:HG3	1:J:444:ARG:O	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:411:LYS:H	1:H:411:LYS:HG2	1.38	0.47
1:H:12:VAL:HG21	1:H:492:LEU:HD13	1.96	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:F:326:TYR:CD2	1:F:370:LEU:C	2.88	0.47
1:H:317:MET:C	1:H:317:MET:SD	2.93	0.47
1:H:440:MET:CB	1:H:485:VAL:HG21	2.44	0.47
1:B:317:MET:SD	1:B:317:MET:C	2.93	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:E:164:ASP:O	1:E:168:LYS:HD3	2.14	0.47
1:E:517:ASN:N	1:E:517:ASN:ND2	2.62	0.47
1:G:180:THR:HB	1:G:349:THR:CG2	2.45	0.47
1:J:162:LEU:HD22	1:J:316:SER:HB3	1.97	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:HG22	1.97	0.47
1:J:129:LEU:HD21	1:J:280:VAL:CG2	2.45	0.47
1:J:445:GLN:HB3	1:J:499:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:77:CYS:O	1:F:81:GLY:N	2.48	0.47
1:A:45:CYS:SG	1:A:77:CYS:CB	2.85	0.47
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:133:MET:HB3	1:A:133:MET:HE2	1.59	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:J:317:MET:SD	1:J:317:MET:C	2.93	0.47
1:D:500:TYR:CD1	1:D:528:VAL:CG1	2.96	0.46
1:J:80:PHE:CE2	1:J:317:MET:HG3	2.49	0.46
1:J:45:CYS:HB3	1:J:75:ASN:HD22	1.80	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:I:493:LYS:C	1:I:530:VAL:HG11	2.36	0.46
1:B:327:THR:O	1:B:327:THR:HG22	2.15	0.46
1:C:129:LEU:HG	1:C:129:LEU:O	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:C:175:SER:HB3	1:C:181:MET:HE1	1.98	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:G:509:PHE:HD2	1:G:511:LEU:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG12	1:A:320:ALA:HA	1.99	0.45
1:D:130:ALA:HA	1:D:133:MET:CE	2.46	0.45
1:F:23:THR:HG23	1:F:412:LEU:HD11	1.98	0.45
1:G:326:TYR:C	1:G:326:TYR:CD1	2.89	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:C:473:ARG:HH22	1:C:496:ASP:CG	2.19	0.45
1:A:438:ALA:C	1:A:459:TRP:HB2	2.37	0.45
1:F:227:ILE:C	1:F:229:GLU:N	2.67	0.45
1:G:22:ASP:HB2	1:H:14:THR:OG1	2.17	0.45
1:I:257:LEU:HD13	1:I:257:LEU:C	2.35	0.45
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: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:CD1	1:A:459:TRP:O	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:G:479:ASP:CG	1:G:482:LYS:HD3	2.37	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: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: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:C:74:LYS:HG2	1:C:75:ASN:N	2.32	0.45
1:G:70:ALA:O	1:G:74:LYS:CE	2.65	0.44
1:I:473:ARG:HH22	1:I:496:ASP:CG	2.21	0.44
1:I:412:LEU:C	1:I:412:LEU:CD1	2.85	0.44
1:C:175:SER:CB	1:C:181:MET:CE	2.95	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:A:473:ARG:HH22	1:A:496:ASP:CG	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:84:PHE:HZ	1:H:317:MET:HE1	1.82	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:175:SER:HB3	1:C:181:MET:CE	2.48	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:B:6:GLU:OE2	1:B:523:GLY:C	2.56	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
1:G:317:MET:C	1:G:317:MET:CE	2.86	0.44
1:B:391:GLN:CB	1:B:416:VAL:HG22	2.47	0.44
1:E:440:MET:HE2	1:E:504:ALA:HB2	2.00	0.44
1:I:458:TYR:CE2	1:I:512:ALA:HB1	2.53	0.44
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:J:133:MET:CE	1:J:283:LEU:HD22	2.47	0.43
1:B:505:ARG:HD2	1:B:518:GLU:O	2.18	0.43
1:D:210:ASN:C	1:D:212:GLN:H	2.21	0.43
1:F:473:ARG:HH22	1:F:496:ASP:CG	2.22	0.43
1:H:313:LEU:O	1:H:317:MET:HG3	2.18	0.43
1:A:45:CYS:HB3	1:A:77:CYS:SG	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:214:PRO:O	1:F:218:GLN:HB2	2.18	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: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
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: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:G:317:MET:HB2	1:G:317:MET:HE2	1.35	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:133:MET:HE1	1:J:283:LEU:CB	2.46	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: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: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:90:MET:HE2	1:A:306:ALA:HA	2.02	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:I:530:VAL:HG12	1:I:530:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:130:ALA:HA	1:D:133:MET:HE2	2.01	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:80:PHE:CZ	1:J:317:MET:HG3	2.55	0.42
1:J:49:ILE:HG22	1:J:320:ALA:HA	2.01	0.42
1:B:45:CYS:O	1:B:75:ASN:HB2	2.20	0.41
1:C:129:LEU:HD23	1:C:129:LEU:C	2.40	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:HD2	1:J:473:ARG:H	1.84	0.41
1:C:130:ALA:HB1	1:C:133:MET:CE	2.50	0.41
1:D:506:ARG:HB2	1:D:521:TYR:HE2	1.84	0.41
1:E:175:SER:OG	1:E:181:MET:CE	2.68	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:318:GLY:O	1:J:321:VAL:HB	2.20	0.41
1:J:47:ILE:HA	1:J:75:ASN:HA	2.02	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:175:SER:CB	1:C:181:MET:HE1	2.50	0.41
1:C:428:CYS:O	1:C:484:THR:HA	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:90:MET:HE2	1:I:306:ALA:HA	2.03	0.41
1:B:212:GLN:HG3	1:B:215:GLN:NE2	2.36	0.41
1:C:349:THR:O	1:C:349:THR:HG23	2.21	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:116:HIS:CE1	1:F:261:LEU:HD22	2.56	0.41
1:F:45:CYS:O	1:F:75:ASN:HB2	2.20	0.41
1:G:23:THR:HG21	1:G:392:ILE:HG23	2.02	0.41
1:A:429:ALA:HA	1:A:484:THR:HG22	2.03	0.41
1:E:12:VAL:HG21	1:E:492:LEU:HD13	2.03	0.41
1:E:517:ASN:C	1:E:519:TYR:H	2.24	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:D:12:VAL:HG11	1:D: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:J:129:LEU:CD2	1:J:133:MET:HG2	2.51	0.41
1:E:288:LYS:CA	1:E:288:LYS:CE	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:ALA:HB1	1:J:303:THR:HG22	2.04	0.40
1:A:67:TRP:HB3	1:A:161:HIS:HB3	2.03	0.40
1:A:14:THR:OG1	1:B:22:ASP:HB2	2.21	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/542 (80%)	417 (96%)	19 (4%)	0	100	100
1	B	432/542 (80%)	412 (95%)	19 (4%)	1 (0%)	47	69
1	C	421/542 (78%)	398 (94%)	21 (5%)	2 (0%)	29	51
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%)	47	69
1	G	457/542 (84%)	441 (96%)	15 (3%)	1 (0%)	47	69
1	H	377/542 (70%)	364 (97%)	12 (3%)	1 (0%)	41	61
1	I	401/542 (74%)	388 (97%)	12 (3%)	1 (0%)	47	69
1	J	364/542 (67%)	350 (96%)	14 (4%)	0	100	100
All	All	4202/5420 (78%)	4033 (96%)	162 (4%)	7 (0%)	47	69

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 (i)

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%)	351 (96%)	15 (4%)	30	56
1	B	361/438 (82%)	342 (95%)	19 (5%)	22	43
1	C	349/438 (80%)	325 (93%)	24 (7%)	15	31
1	D	364/438 (83%)	342 (94%)	22 (6%)	19	37
1	E	365/438 (83%)	346 (95%)	19 (5%)	23	44
1	F	373/438 (85%)	354 (95%)	19 (5%)	24	45
1	G	384/438 (88%)	359 (94%)	25 (6%)	17	33
1	H	325/438 (74%)	305 (94%)	20 (6%)	18	35
1	I	342/438 (78%)	318 (93%)	24 (7%)	15	30
1	J	309/438 (70%)	284 (92%)	25 (8%)	11	24
All	All	3538/4380 (81%)	3326 (94%)	212 (6%)	19	37

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	26	ASP
1	A	75	ASN
1	A	119	ASN
1	A	134	LEU
1	A	170	ASP
1	A	196	GLU

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Mol	Chain	Res	Type
1	A	220	GLN
1	A	276	ILE
1	A	278	GLN
1	A	286	ARG
1	A	350	ILE
1	A	459	TRP
1	A	465	TYR
1	A	478	ARG
1	B	2	VAL
1	B	3	GLN
1	B	6	GLU
1	B	11	LEU
1	B	12	VAL
1	B	120	LEU
1	B	184	GLN
1	B	186	ASN
1	B	187	ASN
1	B	212	GLN
1	B	222	LEU
1	B	277	ASN
1	B	317	MET
1	B	375	ASN
1	B	408	LYS
1	B	412	LEU
1	B	458	TYR
1	B	524	GLN
1	B	532	SER
1	C	11	LEU
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	186	ASN
1	C	208	ASP
1	C	216	ILE
1	C	217	ASN
1	C	317	MET
1	C	350	ILE
1	C	410	GLU
1	C	412	LEU

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Mol	Chain	Res	Type
1	C	413	GLU
1	C	433	ARG
1	C	434	THR
1	C	451	ARG
1	C	458	TYR
1	C	460	THR
1	C	461	VAL
1	C	524	GLN
1	C	530	VAL
1	D	11	LEU
1	D	26	ASP
1	D	104	LEU
1	D	113	THR
1	D	114	GLN
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	323	CYS
1	D	346	ASN
1	D	349	THR
1	D	350	ILE
1	D	411	LYS
1	D	412	LEU
1	D	458	TYR
1	D	461	VAL
1	D	469	SER
1	D	478	ARG
1	E	91	ILE
1	E	118	LEU
1	E	150	VAL
1	E	165	TYR
1	E	174	ILE
1	E	181	MET
1	E	186	ASN
1	E	274	GLN
1	E	280	VAL
1	E	288	LYS
1	E	329	SER

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Mol	Chain	Res	Type
1	E	332	GLU
1	E	350	ILE
1	E	412	LEU
1	E	473	ARG
1	E	478	ARG
1	E	483	ASN
1	E	517	ASN
1	E	530	VAL
1	F	11	LEU
1	F	17	THR
1	F	26	ASP
1	F	102	GLN
1	F	157	LEU
1	F	164	ASP
1	F	169	CYS
1	F	170	ASP
1	F	213	THR
1	F	217	ASN
1	F	218	GLN
1	F	254	TYR
1	F	260	LEU
1	F	261	LEU
1	F	296	ASN
1	F	350	ILE
1	F	373	ASP
1	F	376	VAL
1	F	399	GLN
1	G	11	LEU
1	G	26	ASP
1	G	74	LYS
1	G	97	ILE
1	G	113	THR
1	G	119	ASN
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	228	GLN
1	G	260	LEU
1	G	317	MET

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Mol	Chain	Res	Type
1	G	327	THR
1	G	334	ASN
1	G	350	ILE
1	G	370	LEU
1	G	373	ASP
1	G	408	LYS
1	G	458	TYR
1	G	480	ASN
1	G	507	ARG
1	G	526	THR
1	H	11	LEU
1	H	26	ASP
1	H	91	ILE
1	H	102	GLN
1	H	110	LYS
1	H	118	LEU
1	H	134	LEU
1	H	157	LEU
1	H	164	ASP
1	H	166	ILE
1	H	196	GLU
1	H	276	ILE
1	H	317	MET
1	H	334	ASN
1	H	350	ILE
1	H	405	LEU
1	H	412	LEU
1	H	460	THR
1	H	480	ASN
1	H	528	VAL
1	I	11	LEU
1	I	26	ASP
1	I	37	ILE
1	I	47	ILE
1	I	114	GLN
1	I	118	LEU
1	I	119	ASN
1	I	151	GLU
1	I	190	ASN
1	I	210	ASN
1	I	254	TYR
1	I	255	GLU

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Mol	Chain	Res	Type
1	I	257	LEU
1	I	261	LEU
1	I	276	ILE
1	I	317	MET
1	I	323	CYS
1	I	335	GLN
1	I	350	ILE
1	I	412	LEU
1	I	437	THR
1	I	450	GLU
1	I	451	ARG
1	I	461	VAL
1	J	26	ASP
1	J	37	ILE
1	J	102	GLN
1	J	126	LEU
1	J	131	GLN
1	J	144	LEU
1	J	280	VAL
1	J	285	GLU
1	J	308	ARG
1	J	317	MET
1	J	329	SER
1	J	333	ASN
1	J	346	ASN
1	J	350	ILE
1	J	412	LEU
1	J	444	ARG
1	J	457	ILE
1	J	473	ARG
1	J	478	ARG
1	J	505	ARG
1	J	507	ARG
1	J	518	GLU
1	J	520	ASP
1	J	528	VAL
1	J	532	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	119	ASN
1	A	149	GLN
1	A	220	GLN
1	A	346	ASN
1	A	375	ASN
1	B	3	GLN
1	B	35	GLN
1	B	75	ASN
1	B	107	ASN
1	B	149	GLN
1	B	186	ASN
1	B	190	ASN
1	B	210	ASN
1	B	212	GLN
1	B	215	GLN
1	B	220	GLN
1	B	301	GLN
1	B	315	ASN
1	B	399	GLN
1	B	445	GLN
1	B	517	ASN
1	C	3	GLN
1	C	28	GLN
1	C	35	GLN
1	C	75	ASN
1	C	102	GLN
1	C	107	ASN
1	C	186	ASN
1	C	190	ASN
1	C	215	GLN
1	C	315	ASN
1	C	333	ASN
1	C	517	ASN
1	D	28	GLN
1	D	35	GLN
1	D	39	ASN
1	D	103	GLN
1	D	107	ASN
1	D	108	GLN
1	D	111	ASN
1	D	121	ASN

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Mol	Chain	Res	Type
1	D	131	GLN
1	D	155	ASN
1	D	187	ASN
1	D	190	ASN
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	415	HIS
1	D	488	GLN
1	E	28	GLN
1	E	35	GLN
1	E	103	GLN
1	E	183	ASN
1	E	186	ASN
1	E	190	ASN
1	E	277	ASN
1	E	278	GLN
1	E	315	ASN
1	E	335	GLN
1	E	375	ASN
1	E	517	ASN
1	F	3	GLN
1	F	35	GLN
1	F	68	GLN
1	F	107	ASN
1	F	108	GLN
1	F	199	GLN
1	F	217	ASN
1	F	224	ASN
1	F	375	ASN
1	F	387	HIS
1	F	445	GLN
1	G	39	ASN
1	G	111	ASN
1	G	131	GLN
1	G	190	ASN
1	G	215	GLN
1	G	256	GLN
1	G	277	ASN

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Mol	Chain	Res	Type
1	G	346	ASN
1	G	351	ASN
1	G	415	HIS
1	H	93	ASN
1	H	224	ASN
1	H	334	ASN
1	H	415	HIS
1	I	35	GLN
1	I	315	ASN
1	I	334	ASN
1	I	335	GLN
1	I	387	HIS
1	I	445	GLN
1	I	517	ASN
1	J	28	GLN
1	J	35	GLN
1	J	75	ASN
1	J	107	ASN
1	J	136	ASN
1	J	190	ASN
1	J	315	ASN
1	J	333	ASN
1	J	344	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 monosaccharides 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, 95^{th} 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%)	0.27	13 (2%) 51 45	56, 89, 132, 163	0
1	B	446/542 (82%)	0.30	29 (6%) 18 13	47, 89, 149, 197	0
1	C	431/542 (79%)	0.19	14 (3%) 47 41	46, 88, 138, 187	0
1	D	446/542 (82%)	0.28	10 (2%) 62 57	54, 89, 135, 160	0
1	E	451/542 (83%)	0.26	24 (5%) 26 20	61, 103, 160, 179	0
1	F	457/542 (84%)	0.18	14 (3%) 49 42	55, 88, 130, 157	0
1	G	469/542 (86%)	0.27	26 (5%) 25 18	59, 95, 144, 178	0
1	H	399/542 (73%)	0.45	38 (9%) 8 4	76, 110, 152, 175	0
1	I	419/542 (77%)	0.35	23 (5%) 25 18	63, 107, 151, 183	0
1	J	380/542 (70%)	0.35	26 (6%) 17 11	69, 110, 152, 184	0
All	All	4346/5420 (80%)	0.29	217 (4%) 28 22	46, 97, 146, 197	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	THR	6.3
1	B	185	LYS	6.1
1	H	272	SER	6.1
1	G	176	SER	6.0
1	B	184	GLN	5.4
1	E	126	LEU	5.3
1	I	165	TYR	5.3
1	B	319	TYR	5.2
1	J	521	TYR	5.2
1	H	5	VAL	5.1
1	H	276	ILE	5.1
1	I	80	PHE	5.0
1	G	254	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	79	THR	4.9
1	A	273	ALA	4.9
1	C	133	MET	4.6
1	C	319	TYR	4.6
1	G	506	ARG	4.6
1	I	46	PRO	4.5
1	C	175	SER	4.3
1	J	319	TYR	4.3
1	B	186	ASN	4.2
1	B	130	ALA	4.2
1	G	276	ILE	4.2
1	H	273	ALA	4.2
1	J	133	MET	4.2
1	I	81	GLY	4.1
1	F	70	ALA	4.1
1	E	121	ASN	4.0
1	B	219	ALA	4.0
1	I	322	ILE	4.0
1	B	447	PRO	3.8
1	D	120	LEU	3.8
1	F	271	THR	3.8
1	H	214	PRO	3.7
1	I	77	CYS	3.7
1	G	260	LEU	3.6
1	B	223	ALA	3.6
1	F	65	PRO	3.6
1	J	137	ALA	3.5
1	F	69	THR	3.5
1	J	131	GLN	3.5
1	D	344	ASN	3.5
1	H	461	VAL	3.5
1	B	181	MET	3.5
1	H	322	ILE	3.4
1	J	135	LYS	3.4
1	B	131	GLN	3.4
1	B	224	ASN	3.4
1	H	230	LEU	3.4
1	J	189	GLY	3.4
1	C	128	ALA	3.4
1	C	179	MET	3.4
1	G	448	GLY	3.3
1	G	257	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	177	ALA	3.3
1	B	124	SER	3.2
1	G	175	SER	3.2
1	J	139	SER	3.2
1	B	226	LEU	3.2
1	H	118	LEU	3.2
1	F	68	GLN	3.2
1	C	446	ALA	3.2
1	G	258	SER	3.2
1	A	119	ASN	3.2
1	B	331	GLY	3.2
1	I	159	SER	3.1
1	G	447	PRO	3.1
1	E	174	ILE	3.1
1	G	222	LEU	3.0
1	C	68	GLN	3.0
1	B	446	ALA	3.0
1	B	316	SER	3.0
1	B	67	TRP	3.0
1	E	303	THR	3.0
1	G	220	GLN	3.0
1	J	276	ILE	3.0
1	A	458	TYR	3.0
1	G	228	GLN	2.9
1	F	64	THR	2.9
1	H	121	ASN	2.9
1	A	276	ILE	2.9
1	E	227	ILE	2.9
1	A	116	HIS	2.9
1	G	181	MET	2.9
1	H	126	LEU	2.9
1	G	280	VAL	2.9
1	E	123	PRO	2.9
1	E	302	ALA	2.9
1	H	76	SER	2.9
1	F	157	LEU	2.9
1	F	48	LEU	2.8
1	I	161	HIS	2.8
1	H	49	ILE	2.8
1	I	84	PHE	2.8
1	E	183	ASN	2.8
1	E	216	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	321	VAL	2.8
1	E	276	ILE	2.8
1	H	156	LYS	2.8
1	E	224	ASN	2.8
1	H	274	GLN	2.7
1	H	4	LEU	2.7
1	B	126	LEU	2.7
1	I	323	CYS	2.7
1	H	465	TYR	2.7
1	H	151	GLU	2.7
1	J	165	TYR	2.7
1	I	228	GLN	2.6
1	J	279	ALA	2.6
1	H	232	ASN	2.6
1	H	229	GLU	2.6
1	J	170	ASP	2.6
1	B	189	GLY	2.6
1	E	226	LEU	2.6
1	B	133	MET	2.6
1	G	354	GLY	2.6
1	I	150	VAL	2.6
1	E	124	SER	2.5
1	H	120	LEU	2.5
1	B	135	LYS	2.5
1	A	118	LEU	2.5
1	D	374	LYS	2.5
1	B	175	SER	2.5
1	E	283	LEU	2.5
1	H	202	LEU	2.5
1	D	324	GLY	2.5
1	E	175	SER	2.4
1	H	93	ASN	2.4
1	A	274	GLN	2.4
1	E	120	LEU	2.4
1	E	144	LEU	2.4
1	F	188	TRP	2.4
1	G	174	ILE	2.4
1	F	110	LYS	2.4
1	B	165	TYR	2.4
1	A	82	ALA	2.4
1	G	343	GLU	2.4
1	F	115	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	501	TYR	2.4
1	H	448	GLY	2.4
1	G	183	ASN	2.4
1	H	503	ALA	2.4
1	E	332	GLU	2.3
1	I	188	TRP	2.3
1	D	5	VAL	2.3
1	J	530	VAL	2.3
1	G	156	LYS	2.3
1	D	159	SER	2.3
1	H	66	SER	2.3
1	I	152	SER	2.3
1	J	459	TRP	2.3
1	A	114	GLN	2.3
1	D	447	PRO	2.3
1	H	447	PRO	2.3
1	B	350	ILE	2.3
1	H	170	ASP	2.3
1	B	162	LEU	2.3
1	I	259	ARG	2.3
1	J	350	ILE	2.2
1	H	275	ALA	2.2
1	J	128	ALA	2.2
1	E	170	ASP	2.2
1	H	271	THR	2.2
1	G	279	ALA	2.2
1	H	157	LEU	2.2
1	C	47	ILE	2.2
1	J	130	ALA	2.2
1	H	155	ASN	2.2
1	G	261	LEU	2.2
1	J	275	ALA	2.2
1	F	132	LYS	2.2
1	E	225	THR	2.2
1	I	48	LEU	2.2
1	J	134	LEU	2.2
1	G	68	GLN	2.2
1	D	458	TYR	2.2
1	E	119	ASN	2.2
1	G	283	LEU	2.2
1	I	211	ASN	2.2
1	A	113	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	447	PRO	2.2
1	H	20	VAL	2.2
1	F	127	THR	2.2
1	J	127	THR	2.2
1	E	506	ARG	2.2
1	D	219	ALA	2.1
1	C	369	THR	2.1
1	H	451	ARG	2.1
1	A	431	SER	2.1
1	H	153	ASP	2.1
1	J	138	GLN	2.1
1	A	117	ASN	2.1
1	I	148	ASN	2.1
1	B	172	SER	2.1
1	I	253	THR	2.1
1	J	193	ALA	2.1
1	D	236	ARG	2.1
1	E	11	LEU	2.1
1	A	275	ALA	2.1
1	E	185	LYS	2.1
1	I	162	LEU	2.1
1	I	133	MET	2.1
1	J	328	LYS	2.1
1	J	437	THR	2.1
1	B	180	THR	2.1
1	C	322	ILE	2.1
1	I	319	TYR	2.1
1	J	49	ILE	2.1
1	C	320	ALA	2.0
1	B	188	TRP	2.0
1	J	94	ALA	2.0
1	C	183	ASN	2.0
1	G	224	ASN	2.0
1	F	162	LEU	2.0
1	G	102	GLN	2.0
1	H	162	LEU	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 monosaccharides 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, 95^{th} 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	0.84	0.25	91,91,91,91	0

6.5 Other polymers (i)

There are no such residues in this entry.