Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 04:26 pm BST

PDB ID	:	2R29
Title	:	Neutralization of dengue virus by a serotype cross-reactive antibody elucidated by cryoelectron microscopy and x-ray crystallography
Authors	:	Lok, S.M.; Kostyuchenko, V.K.; Nybakken, G.E.; Holdaway, H.A.; Battisti, A.J.; Sukupolvi-petty, S.; Sedlak, D.; Fremont, D.H.; Chipman, P.R.; Roehrig, J.T.; Diamond, M.S.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2007-08-24
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

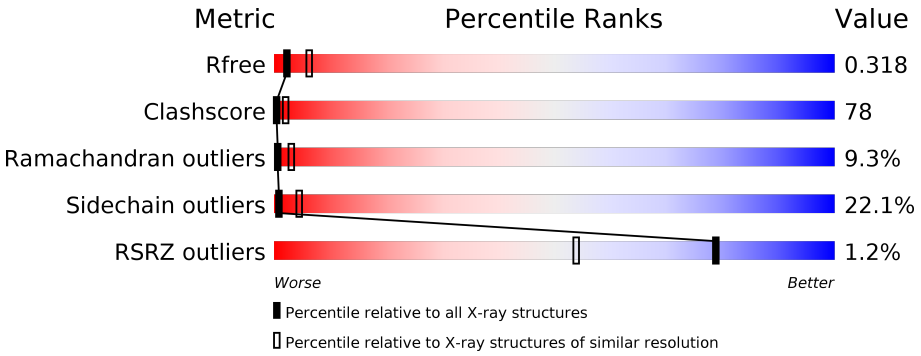
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	97	18% 57% 21% 5%
2	H	216	2% 21% 61% 17%
3	L	217	% 19% 52% 21% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4234 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			768	495	126	143	4			

- Molecule 2 is a protein called Heavy chain of Fab 1A1D-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1625	1028	266	326	5			

- Molecule 3 is a protein called Light chain of Fab 1A1D-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	204	Total	C	N	O	S	0	0	0
			1587	994	271	316	6			

- Molecule 4 is water.

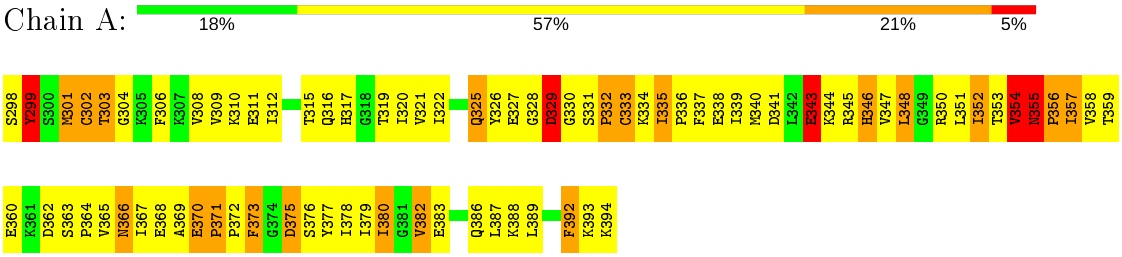
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	H	97	Total	O	0	0
			97	97		
4	L	98	Total	O	0	0
			98	98		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

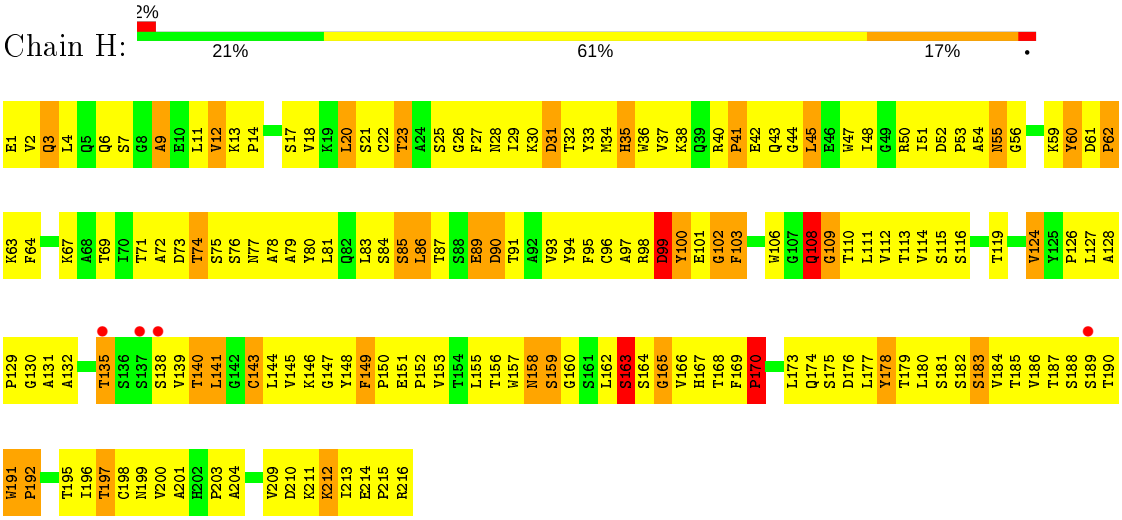
- Molecule 1: Envelope protein E

Chain A:



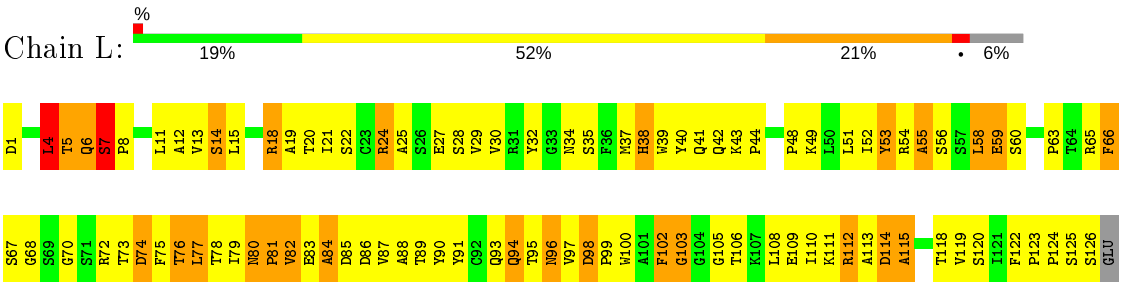
- Molecule 2: Heavy chain of Fab 1A1D-2

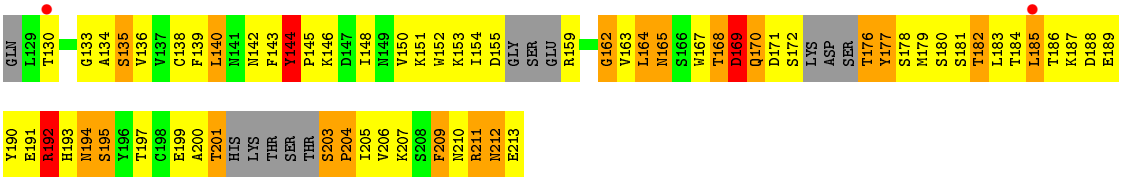
Chain H:



- Molecule 3: Light chain of Fab 1A1D-2

Chain L:




GLN L129 T130 G133 A134 S135 V136 V137 C138 F139 L140 N141 N142 F143 Y144 P145 K146 D147 I148 N149 V150 K151 W152 K153 I154 D155 GLY SER GLU R159 G162 V163 L164 N165 S166 W167 T168 D169 Q170 D171 S172 LYS ASP SER T176 Y177 S178 M179 S180 S181 T182 L183 T184 L185 T186 K187 D188 E189
Y190 E191 R192 H193 N194 S195 Y196 T197 C198 E199 A200 T201 HIS LYS THR SER THR S203 P204 I205 V206 K207 S208 F209 N210 R211 N212 E213

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.12Å 58.66Å 78.19Å 90.00° 114.41° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 46.90 – 2.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 56.6 (46.90-2.83)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.321 0.258 , 0.318	Depositor DCC
R_{free} test set	1125 reflections (10.28%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	4234	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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

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	0.60	0/785	1.07	5/1060 (0.5%)
2	H	0.45	0/1667	0.91	3/2279 (0.1%)
3	L	0.48	0/1621	1.02	7/2200 (0.3%)
All	All	0.50	0/4073	0.99	15/5539 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	4	LEU	CA-CB-CG	-7.36	98.36	115.30
1	A	346	HIS	N-CA-C	6.83	129.46	111.00
3	L	115	ALA	N-CA-C	6.83	129.43	111.00
3	L	66	PHE	N-CA-C	-6.54	93.33	111.00
1	A	352	ILE	O-C-N	-6.13	112.89	122.70
1	A	343	GLU	N-CA-C	-6.04	94.68	111.00
2	H	163	SER	N-CA-C	-5.88	95.13	111.00
2	H	165	GLY	N-CA-C	-5.84	98.50	113.10
3	L	170	GLN	N-CA-C	5.75	126.53	111.00
1	A	299	TYR	N-CA-C	5.30	125.32	111.00
2	H	99	ASP	N-CA-C	5.29	125.28	111.00
3	L	7	SER	C-N-CD	5.26	139.44	128.40
1	A	352	ILE	CG1-CB-CG2	-5.16	100.06	111.40
3	L	6	GLN	N-CA-C	-5.09	97.24	111.00
3	L	7	SER	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	144	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	768	0	780	125	0
2	H	1625	0	1584	241	0
3	L	1587	0	1527	282	0
4	A	59	0	0	9	0
4	H	97	0	0	4	0
4	L	98	0	0	9	0
All	All	4234	0	3891	612	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 78.

All (612) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:4:LEU:HD13	3:L:103:GLY:HA2	1.22	1.17
3:L:115:ALA:CB	3:L:144:TYR:H	1.60	1.15
3:L:58:LEU:HD22	3:L:58:LEU:H	1.12	1.15
3:L:115:ALA:HB2	3:L:144:TYR:N	1.63	1.12
1:A:353:THR:HG22	1:A:356:PRO:HG2	1.35	1.08
2:H:40:ARG:HB3	2:H:41:PRO:HD2	1.32	1.06
1:A:355:ASN:N	1:A:356:PRO:HD2	1.69	1.04
3:L:115:ALA:HB2	3:L:144:TYR:H	0.90	1.04
1:A:343:GLU:HG3	1:A:344:LYS:H	1.17	1.04
3:L:77:LEU:HD12	3:L:78:THR:H	1.22	1.02
3:L:112:ARG:NH2	3:L:113:ALA:HB3	1.74	1.01
3:L:55:ALA:O	3:L:68:GLY:HA3	1.61	1.00
1:A:353:THR:CG2	1:A:356:PRO:HG2	1.90	1.00
3:L:96:ASN:C	3:L:96:ASN:HD22	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191:TRP:HB3	2:H:192:PRO:HD3	1.46	0.98
2:H:170:PRO:HD2	3:L:167:TRP:O	1.64	0.97
3:L:58:LEU:HD22	3:L:58:LEU:N	1.79	0.97
3:L:58:LEU:H	3:L:58:LEU:CD2	1.79	0.96
3:L:140:LEU:H	3:L:140:LEU:HD12	1.31	0.95
3:L:4:LEU:CD1	3:L:103:GLY:HA2	1.97	0.94
2:H:187:THR:HB	2:H:190:THR:OG1	1.67	0.94
2:H:100:TYR:O	3:L:95:THR:HG21	1.68	0.94
2:H:212:LYS:HA	4:H:281:HOH:O	1.67	0.92
3:L:150:VAL:HG13	3:L:199:GLU:O	1.68	0.92
2:H:140:THR:HB	2:H:185:THR:HG22	1.52	0.91
3:L:4:LEU:HD13	3:L:103:GLY:CA	1.99	0.91
3:L:41:GLN:HB2	3:L:51:LEU:HD21	1.50	0.91
3:L:30:VAL:HG23	3:L:72:ARG:HA	1.49	0.91
3:L:77:LEU:HD12	3:L:78:THR:N	1.85	0.90
3:L:12:ALA:HB1	3:L:111:LYS:HE3	1.51	0.90
3:L:80:ASN:HB3	3:L:81:PRO:HD3	1.52	0.90
1:A:352:ILE:O	1:A:352:ILE:HG22	1.71	0.89
1:A:355:ASN:ND2	1:A:355:ASN:O	2.05	0.89
1:A:355:ASN:N	1:A:356:PRO:CD	2.35	0.88
3:L:18:ARG:HB3	3:L:18:ARG:NH1	1.88	0.88
2:H:129:PRO:HG3	3:L:122:PHE:HE2	1.38	0.87
2:H:200:VAL:HB	2:H:209:VAL:HG13	1.54	0.87
3:L:200:ALA:HB3	3:L:205:ILE:HG23	1.56	0.86
1:A:343:GLU:HG3	1:A:344:LYS:N	1.85	0.86
1:A:353:THR:HG22	1:A:356:PRO:CG	2.06	0.85
3:L:97:VAL:HG12	3:L:99:PRO:HD2	1.59	0.84
3:L:179:MET:HG2	3:L:180:SER:H	1.43	0.84
3:L:4:LEU:O	3:L:4:LEU:HD12	1.78	0.84
3:L:102:PHE:N	3:L:102:PHE:HD2	1.74	0.84
3:L:119:VAL:HB	3:L:207:LYS:HD3	1.57	0.84
2:H:50:ARG:HH11	2:H:50:ARG:HG3	1.40	0.83
3:L:5:THR:HG23	3:L:24:ARG:CB	2.08	0.83
2:H:11:LEU:HD11	2:H:115:SER:HB3	1.61	0.83
2:H:200:VAL:HB	2:H:209:VAL:CG1	2.08	0.83
3:L:115:ALA:HB1	3:L:143:PHE:HA	1.61	0.82
3:L:40:TYR:HB2	3:L:91:TYR:HB2	1.62	0.82
2:H:37:VAL:HG11	2:H:45:LEU:HD23	1.61	0.82
2:H:166:VAL:HG13	2:H:183:SER:O	1.80	0.81
2:H:14:PRO:HG3	2:H:114:VAL:HG12	1.63	0.81
3:L:102:PHE:N	3:L:102:PHE:CD2	2.48	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:GLN:OE1	3:L:164:LEU:HD22	1.80	0.81
2:H:6:GLN:HG2	2:H:96:CYS:SG	2.21	0.81
3:L:200:ALA:HB3	3:L:205:ILE:CG2	2.10	0.80
3:L:162:GLY:O	3:L:183:LEU:HA	1.80	0.80
1:A:344:LYS:C	1:A:346:HIS:H	1.84	0.80
1:A:306:PHE:O	1:A:387:LEU:HD21	1.83	0.79
2:H:45:LEU:HD21	3:L:48:PRO:HG2	1.64	0.79
3:L:28:SER:HA	3:L:73:THR:OG1	1.83	0.79
3:L:159:ARG:NH2	3:L:189:GLU:HG2	1.96	0.79
3:L:96:ASN:HD22	3:L:97:VAL:N	1.81	0.78
2:H:4:LEU:HD21	2:H:27:PHE:HZ	1.49	0.78
2:H:9:ALA:HB3	2:H:203:PRO:HB2	1.66	0.78
1:A:366:ASN:HD22	1:A:367:ILE:H	1.32	0.78
1:A:319:THR:HG21	1:A:368:GLU:OE2	1.84	0.78
2:H:29:ILE:HG12	2:H:53:PRO:HG2	1.64	0.77
2:H:40:ARG:HB3	2:H:41:PRO:CD	2.12	0.77
1:A:350:ARG:HB3	1:A:370:GLU:HB3	1.64	0.77
1:A:352:ILE:CG2	1:A:352:ILE:O	2.33	0.77
3:L:112:ARG:HH21	3:L:113:ALA:HB3	1.49	0.77
1:A:340:MET:HE3	1:A:346:HIS:HA	1.67	0.77
3:L:163:VAL:C	3:L:164:LEU:HD23	2.05	0.77
1:A:344:LYS:HE3	4:A:425:HOH:O	1.84	0.77
3:L:140:LEU:HD12	3:L:140:LEU:N	1.99	0.77
3:L:183:LEU:HG	3:L:185:LEU:HD21	1.67	0.76
3:L:155:ASP:HA	3:L:195:SER:O	1.86	0.76
2:H:29:ILE:HG13	2:H:34:MET:CE	2.16	0.75
3:L:84:ALA:HA	3:L:110:ILE:HD12	1.68	0.75
2:H:170:PRO:CD	3:L:167:TRP:O	2.34	0.75
3:L:140:LEU:HD13	3:L:179:MET:HB3	1.67	0.75
1:A:366:ASN:HD22	1:A:367:ILE:N	1.85	0.75
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.68	0.75
3:L:192:ARG:HH11	3:L:192:ARG:HG3	1.52	0.75
2:H:127:LEU:HD11	2:H:144:LEU:HB2	1.66	0.74
2:H:40:ARG:CB	2:H:41:PRO:HD2	2.14	0.74
2:H:129:PRO:HG3	3:L:122:PHE:CE2	2.22	0.74
2:H:162:LEU:O	2:H:164:SER:N	2.21	0.74
3:L:95:THR:O	3:L:95:THR:HG22	1.88	0.74
1:A:369:ALA:O	1:A:371:PRO:HD3	1.88	0.73
2:H:2:VAL:HG13	2:H:27:PHE:CD2	2.23	0.73
3:L:96:ASN:C	3:L:96:ASN:ND2	2.38	0.73
3:L:58:LEU:HD11	4:L:245:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:VAL:HG22	1:A:365:VAL:HG21	1.71	0.72
1:A:354:VAL:C	1:A:356:PRO:CD	2.57	0.72
1:A:366:ASN:C	1:A:367:ILE:HD12	2.09	0.72
2:H:29:ILE:HG13	2:H:34:MET:HE1	1.71	0.72
2:H:149:PHE:HB3	2:H:150:PRO:HD3	1.71	0.72
2:H:191:TRP:CD1	2:H:196:ILE:HG13	2.26	0.71
2:H:97:ALA:HB3	2:H:103:PHE:HD1	1.55	0.71
3:L:187:LYS:HG2	3:L:187:LYS:O	1.89	0.71
2:H:33:TYR:O	2:H:98:ARG:O	2.09	0.71
2:H:124:VAL:HG22	2:H:211:LYS:HG3	1.73	0.70
2:H:139:VAL:HG21	4:H:283:HOH:O	1.91	0.70
2:H:169:PHE:CD2	3:L:180:SER:HB2	2.26	0.70
2:H:166:VAL:HG12	2:H:167:HIS:N	2.05	0.70
3:L:4:LEU:HD22	3:L:102:PHE:C	2.12	0.70
2:H:47:TRP:HB2	3:L:102:PHE:HE2	1.56	0.70
3:L:213:GLU:HB2	4:L:299:HOH:O	1.92	0.70
3:L:18:ARG:HA	3:L:80:ASN:HA	1.74	0.70
3:L:13:VAL:HG11	3:L:82:VAL:HG21	1.74	0.69
2:H:99:ASP:HB2	2:H:102:GLY:O	1.92	0.69
1:A:365:VAL:HA	4:A:450:HOH:O	1.92	0.69
2:H:2:VAL:HA	2:H:25:SER:OG	1.92	0.69
3:L:30:VAL:CG2	3:L:72:ARG:HA	2.22	0.69
2:H:102:GLY:N	3:L:38:HIS:ND1	2.40	0.69
2:H:29:ILE:HG12	2:H:53:PRO:CG	2.22	0.69
3:L:179:MET:HG2	3:L:180:SER:N	2.06	0.69
2:H:190:THR:HG22	2:H:190:THR:O	1.93	0.69
3:L:183:LEU:HG	3:L:185:LEU:CD2	2.23	0.69
3:L:18:ARG:HH11	3:L:18:ARG:HB3	1.58	0.69
2:H:184:VAL:HG13	2:H:184:VAL:O	1.92	0.68
3:L:28:SER:HA	3:L:73:THR:HG1	1.56	0.68
3:L:150:VAL:HG12	3:L:151:LYS:N	2.09	0.68
3:L:80:ASN:O	3:L:82:VAL:N	2.27	0.68
3:L:15:LEU:HD23	3:L:83:GLU:HA	1.76	0.68
3:L:11:LEU:H	3:L:11:LEU:HD23	1.59	0.68
2:H:30:LYS:HA	2:H:53:PRO:HB2	1.74	0.68
3:L:5:THR:CG2	3:L:24:ARG:HB3	2.24	0.68
2:H:17:SER:HB2	2:H:84:SER:HB2	1.76	0.67
2:H:67:LYS:NZ	2:H:86:LEU:HA	2.10	0.67
3:L:13:VAL:HG12	3:L:14:SER:N	2.10	0.67
3:L:70:GLY:HA3	3:L:75:PHE:CD1	2.30	0.67
1:A:353:THR:HG21	1:A:356:PRO:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:ASP:O	2:H:76:SER:O	2.13	0.67
1:A:376:SER:H	1:A:392:PHE:HA	1.60	0.67
2:H:102:GLY:H	3:L:38:HIS:CE1	2.12	0.67
3:L:5:THR:HG22	3:L:24:ARG:O	1.95	0.67
3:L:6:GLN:NE2	3:L:90:TYR:O	2.27	0.67
1:A:315:THR:HG22	1:A:317:HIS:H	1.60	0.66
3:L:194:ASN:O	3:L:211:ARG:HG3	1.95	0.66
2:H:71:THR:HG22	2:H:72:ALA:N	2.10	0.66
3:L:115:ALA:CB	3:L:144:TYR:N	2.38	0.66
2:H:111:LEU:HD13	2:H:152:PRO:HG3	1.77	0.65
2:H:191:TRP:HB3	2:H:192:PRO:CD	2.24	0.65
3:L:95:THR:HG23	3:L:100:TRP:CE3	2.32	0.65
3:L:115:ALA:CB	3:L:143:PHE:HA	2.26	0.65
3:L:49:LYS:HB2	3:L:49:LYS:NZ	2.12	0.65
3:L:96:ASN:ND2	3:L:97:VAL:N	2.45	0.65
2:H:216:ARG:CD	3:L:126:SER:OG	2.44	0.65
2:H:141:LEU:HA	3:L:122:PHE:CZ	2.31	0.65
2:H:173:LEU:HD11	2:H:176:ASP:HA	1.77	0.65
3:L:98:ASP:O	3:L:100:TRP:N	2.28	0.65
3:L:148:ILE:HG23	3:L:201:THR:OG1	1.97	0.65
3:L:115:ALA:HB1	3:L:143:PHE:CA	2.27	0.65
3:L:155:ASP:OD1	3:L:194:ASN:ND2	2.30	0.64
2:H:89:GLU:C	2:H:91:THR:H	2.00	0.64
2:H:140:THR:CB	2:H:185:THR:HG22	2.27	0.64
1:A:382:VAL:O	1:A:386:GLN:HB2	1.97	0.64
3:L:5:THR:HG23	3:L:24:ARG:HB3	1.79	0.64
1:A:359:THR:O	1:A:359:THR:CG2	2.45	0.64
1:A:354:VAL:C	1:A:356:PRO:HD3	2.17	0.64
2:H:169:PHE:O	2:H:180:LEU:HG	1.98	0.64
1:A:343:GLU:CG	1:A:344:LYS:N	2.60	0.64
2:H:126:PRO:HG3	2:H:212:LYS:O	1.98	0.64
3:L:21:ILE:HD12	3:L:21:ILE:N	2.12	0.64
1:A:394:LYS:HD3	4:A:415:HOH:O	1.97	0.63
3:L:136:VAL:HG12	3:L:152:TRP:CH2	2.33	0.63
2:H:157:TRP:HZ3	2:H:213:ILE:CD1	2.11	0.63
1:A:317:HIS:NE2	4:A:427:HOH:O	2.30	0.63
2:H:213:ILE:HG22	2:H:213:ILE:O	1.99	0.63
2:H:4:LEU:HD21	2:H:27:PHE:CZ	2.33	0.63
2:H:71:THR:CG2	2:H:72:ALA:N	2.60	0.63
2:H:186:VAL:HG23	2:H:187:THR:O	1.99	0.63
3:L:134:ALA:HB3	3:L:185:LEU:HG	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:C	1:A:356:PRO:HD2	2.19	0.63
2:H:111:LEU:HD23	2:H:112:VAL:N	2.14	0.63
2:H:2:VAL:HG13	2:H:27:PHE:HD2	1.62	0.63
2:H:45:LEU:CD2	3:L:48:PRO:HG2	2.28	0.62
3:L:84:ALA:HA	3:L:110:ILE:CD1	2.28	0.62
1:A:382:VAL:HG12	1:A:383:GLU:H	1.64	0.62
2:H:97:ALA:CB	2:H:103:PHE:HD1	2.12	0.62
2:H:166:VAL:CG1	2:H:167:HIS:H	2.13	0.62
2:H:20:LEU:HD23	2:H:20:LEU:N	2.15	0.61
3:L:138:CYS:O	3:L:138:CYS:SG	2.58	0.61
2:H:97:ALA:HB3	2:H:103:PHE:CD1	2.35	0.61
3:L:12:ALA:HB1	3:L:111:LYS:CE	2.29	0.61
3:L:169:ASP:OD1	3:L:169:ASP:N	2.32	0.61
3:L:164:LEU:HD23	3:L:164:LEU:N	2.15	0.61
3:L:140:LEU:H	3:L:140:LEU:CD1	2.11	0.61
3:L:38:HIS:CD2	3:L:53:TYR:O	2.54	0.61
2:H:166:VAL:CG1	2:H:167:HIS:N	2.63	0.60
2:H:40:ARG:HG2	2:H:91:THR:O	2.00	0.60
3:L:191:GLU:C	3:L:193:HIS:H	2.05	0.60
1:A:346:HIS:O	1:A:347:VAL:HG23	2.01	0.60
3:L:59:GLU:OE2	3:L:60:SER:N	2.27	0.60
3:L:94:GLN:HG2	3:L:95:THR:N	2.15	0.60
1:A:315:THR:HB	1:A:319:THR:HG23	1.83	0.60
1:A:340:MET:CE	1:A:346:HIS:HA	2.32	0.60
2:H:126:PRO:HA	2:H:143:CYS:HB2	1.83	0.60
3:L:142:ASN:HA	3:L:176:THR:OG1	2.02	0.60
1:A:378:ILE:HG22	1:A:379:ILE:H	1.67	0.59
2:H:143:CYS:N	2:H:182:SER:OG	2.35	0.59
1:A:344:LYS:C	1:A:346:HIS:N	2.54	0.59
2:H:36:TRP:NE1	2:H:80:TYR:O	2.34	0.59
3:L:114:ASP:OD1	3:L:114:ASP:N	2.35	0.59
1:A:321:VAL:HG12	1:A:366:ASN:HD21	1.68	0.59
3:L:11:LEU:HD23	3:L:11:LEU:N	2.16	0.59
2:H:157:TRP:CZ3	2:H:213:ILE:HD11	2.38	0.58
2:H:91:THR:HG23	2:H:113:THR:HA	1.85	0.58
3:L:5:THR:HG23	3:L:24:ARG:HB2	1.85	0.58
3:L:4:LEU:HD22	3:L:103:GLY:HA2	1.85	0.58
3:L:150:VAL:HG12	3:L:151:LYS:O	2.03	0.58
2:H:169:PHE:CD2	3:L:168:THR:HG23	2.38	0.58
3:L:73:THR:HG22	3:L:73:THR:O	2.02	0.58
3:L:19:ALA:HB3	3:L:79:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASP:HB3	1:A:392:PHE:HB2	1.85	0.58
3:L:79:ILE:HD11	3:L:90:TYR:HE2	1.66	0.58
2:H:211:LYS:NZ	2:H:212:LYS:HE3	2.18	0.58
2:H:166:VAL:HG12	2:H:167:HIS:H	1.69	0.58
2:H:191:TRP:CB	2:H:192:PRO:HD3	2.30	0.58
1:A:359:THR:O	1:A:359:THR:HG22	2.04	0.57
3:L:188:ASP:C	3:L:188:ASP:OD1	2.42	0.57
1:A:312:ILE:HG23	1:A:322:ILE:HG12	1.85	0.57
2:H:103:PHE:HD2	2:H:103:PHE:N	2.03	0.57
2:H:52:ASP:OD2	2:H:54:ALA:HB3	2.05	0.57
2:H:153:VAL:HA	2:H:201:ALA:O	2.04	0.57
3:L:42:GLN:O	3:L:88:ALA:HB1	2.04	0.57
3:L:28:SER:HB3	3:L:72:ARG:HG2	1.87	0.57
1:A:331:SER:N	1:A:332:PRO:HD3	2.19	0.57
3:L:12:ALA:CB	3:L:111:LYS:HE3	2.31	0.57
2:H:124:VAL:CG1	2:H:209:VAL:HG21	2.34	0.57
3:L:153:LYS:HB2	3:L:197:THR:HB	1.85	0.57
2:H:140:THR:HA	2:H:185:THR:HA	1.86	0.57
3:L:159:ARG:HH22	3:L:189:GLU:HG2	1.70	0.57
3:L:19:ALA:HB2	3:L:82:VAL:CG2	2.35	0.57
2:H:102:GLY:N	3:L:38:HIS:CE1	2.73	0.57
1:A:348:LEU:HD22	1:A:372:PRO:HG3	1.87	0.57
2:H:126:PRO:O	2:H:127:LEU:HD23	2.05	0.57
2:H:157:TRP:HZ2	2:H:182:SER:HB2	1.69	0.57
1:A:319:THR:OG1	1:A:368:GLU:HG3	2.05	0.56
1:A:320:ILE:HG13	1:A:320:ILE:O	2.05	0.56
1:A:357:ILE:HD13	1:A:357:ILE:H	1.69	0.56
3:L:108:LEU:HD12	3:L:109:GLU:N	2.20	0.56
3:L:164:LEU:HG	3:L:182:THR:OG1	2.04	0.56
2:H:50:ARG:HG3	2:H:50:ARG:NH1	2.16	0.56
3:L:80:ASN:HB3	3:L:81:PRO:CD	2.29	0.56
1:A:327:GLU:HG3	4:A:404:HOH:O	2.05	0.56
2:H:36:TRP:CE3	2:H:95:PHE:O	2.59	0.56
3:L:115:ALA:CB	3:L:143:PHE:CA	2.83	0.56
2:H:216:ARG:HD2	3:L:126:SER:OG	2.05	0.56
2:H:196:ILE:HG22	2:H:197:THR:N	2.21	0.56
3:L:7:SER:O	3:L:8:PRO:C	2.35	0.56
1:A:359:THR:O	1:A:360:GLU:HG3	2.06	0.56
1:A:387:LEU:HD21	3:L:54:ARG:HH22	1.71	0.56
2:H:144:LEU:HD23	2:H:145:VAL:N	2.21	0.56
2:H:211:LYS:HZ3	2:H:212:LYS:HE3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:PRO:HB2	2:H:213:ILE:HA	1.88	0.56
3:L:65:ARG:HB2	3:L:81:PRO:HD2	1.88	0.56
3:L:4:LEU:CG	3:L:103:GLY:HA2	2.36	0.55
2:H:187:THR:CB	2:H:190:THR:OG1	2.50	0.55
2:H:191:TRP:HZ2	2:H:213:ILE:O	1.88	0.55
1:A:355:ASN:H	1:A:356:PRO:HD2	1.65	0.55
2:H:157:TRP:O	2:H:158:ASN:HB2	2.06	0.55
2:H:60:TYR:N	2:H:60:TYR:CD1	2.73	0.55
2:H:129:PRO:CG	3:L:122:PHE:HE2	2.14	0.55
1:A:301:MET:HB2	1:A:336:PRO:HG3	1.88	0.55
1:A:392:PHE:HD1	1:A:392:PHE:O	1.89	0.55
2:H:108:GLN:O	2:H:109:GLY:C	2.45	0.55
1:A:310:LYS:HE2	2:H:52:ASP:OD1	2.07	0.55
3:L:95:THR:HG23	3:L:100:TRP:CZ3	2.41	0.55
1:A:333:CYS:O	1:A:357:ILE:HB	2.06	0.55
3:L:37:MET:CE	3:L:93:GLN:O	2.55	0.55
3:L:70:GLY:HA3	3:L:75:PHE:HD1	1.72	0.55
3:L:120:SER:O	3:L:138:CYS:HA	2.06	0.55
3:L:6:GLN:HA	3:L:22:SER:O	2.06	0.55
2:H:143:CYS:O	2:H:182:SER:OG	2.24	0.55
3:L:144:TYR:O	3:L:145:PRO:C	2.43	0.55
3:L:38:HIS:N	3:L:38:HIS:CD2	2.72	0.55
2:H:12:VAL:HG21	2:H:18:VAL:CG1	2.37	0.55
3:L:112:ARG:CZ	3:L:113:ALA:HB3	2.37	0.54
3:L:133:GLY:HA3	3:L:185:LEU:O	2.07	0.54
1:A:339:ILE:HG23	1:A:377:TYR:O	2.07	0.54
2:H:6:GLN:HA	2:H:21:SER:O	2.06	0.54
3:L:41:GLN:CB	3:L:51:LEU:HD21	2.32	0.54
1:A:387:LEU:CD2	3:L:54:ARG:NH2	2.71	0.54
1:A:333:CYS:HB3	4:A:433:HOH:O	2.07	0.54
1:A:378:ILE:HG22	1:A:379:ILE:N	2.22	0.54
2:H:103:PHE:CD2	2:H:103:PHE:N	2.74	0.54
2:H:144:LEU:HD21	2:H:146:LYS:HB3	1.88	0.54
2:H:89:GLU:C	2:H:91:THR:N	2.60	0.54
1:A:350:ARG:NH1	1:A:370:GLU:OE1	2.41	0.54
2:H:59:LYS:HD3	3:L:98:ASP:CG	2.28	0.54
3:L:212:ASN:O	3:L:213:GLU:O	2.26	0.54
3:L:18:ARG:HG2	3:L:80:ASN:ND2	2.23	0.53
1:A:299:TYR:N	1:A:299:TYR:CD2	2.76	0.53
2:H:127:LEU:HG	2:H:143:CYS:HA	1.91	0.53
3:L:203:SER:OG	3:L:204:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:O	1:A:309:VAL:HG23	2.09	0.53
3:L:124:PRO:HG3	3:L:135:SER:H	1.73	0.53
2:H:45:LEU:H	2:H:45:LEU:HD12	1.72	0.53
3:L:168:THR:OG1	3:L:178:SER:O	2.25	0.53
3:L:192:ARG:HH11	3:L:192:ARG:CG	2.17	0.53
1:A:331:SER:H	1:A:332:PRO:HD3	1.74	0.53
3:L:150:VAL:CG1	3:L:151:LYS:N	2.72	0.53
3:L:58:LEU:HD21	4:L:245:HOH:O	2.07	0.53
3:L:144:TYR:HB3	3:L:145:PRO:HD3	1.90	0.53
3:L:159:ARG:NH1	3:L:185:LEU:HD22	2.23	0.53
2:H:13:LYS:HA	2:H:115:SER:O	2.09	0.53
3:L:163:VAL:HA	3:L:182:THR:O	2.09	0.53
3:L:136:VAL:CG1	3:L:152:TRP:CH2	2.91	0.53
3:L:4:LEU:HD22	3:L:103:GLY:N	2.24	0.53
3:L:79:ILE:HD11	3:L:90:TYR:CE2	2.43	0.53
2:H:149:PHE:O	2:H:150:PRO:C	2.46	0.52
2:H:201:ALA:O	2:H:203:PRO:HD3	2.08	0.52
2:H:191:TRP:CH2	2:H:215:PRO:HA	2.43	0.52
1:A:379:ILE:O	1:A:380:ILE:HG12	2.08	0.52
2:H:17:SER:HB2	2:H:84:SER:CB	2.39	0.52
2:H:197:THR:HG23	2:H:198:CYS:N	2.25	0.52
2:H:36:TRP:HE3	2:H:95:PHE:O	1.91	0.52
3:L:185:LEU:HD12	3:L:190:TYR:HB2	1.91	0.52
3:L:4:LEU:HD11	4:L:219:HOH:O	2.08	0.52
2:H:157:TRP:CZ3	2:H:213:ILE:CD1	2.92	0.52
3:L:8:PRO:HB2	3:L:11:LEU:HD22	1.92	0.52
3:L:154:ILE:O	3:L:195:SER:O	2.28	0.52
3:L:37:MET:HA	3:L:37:MET:CE	2.40	0.52
3:L:63:PRO:HG2	3:L:66:PHE:HE2	1.75	0.52
3:L:18:ARG:CG	3:L:80:ASN:ND2	2.73	0.52
3:L:18:ARG:CZ	3:L:18:ARG:CB	2.87	0.52
2:H:20:LEU:HB2	2:H:81:LEU:HB3	1.91	0.52
3:L:37:MET:HG2	3:L:75:PHE:CD2	2.43	0.52
3:L:93:GLN:HG2	3:L:94:GLN:N	2.25	0.52
2:H:52:ASP:O	2:H:56:GLY:N	2.43	0.52
2:H:33:TYR:CE2	2:H:52:ASP:OD1	2.63	0.52
1:A:360:GLU:HB3	1:A:362:ASP:H	1.74	0.52
2:H:144:LEU:CD2	2:H:146:LYS:HB3	2.40	0.52
3:L:52:ILE:HD11	3:L:67:SER:HA	1.92	0.51
3:L:30:VAL:HA	3:L:35:SER:HA	1.91	0.51
2:H:155:LEU:HD21	2:H:157:TRP:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:LYS:HZ2	3:L:199:GLU:CD	2.14	0.51
2:H:71:THR:CG2	2:H:72:ALA:H	2.22	0.51
2:H:2:VAL:O	2:H:3:GLN:HG3	2.11	0.51
2:H:200:VAL:CB	2:H:209:VAL:HG13	2.34	0.51
1:A:376:SER:H	1:A:392:PHE:CA	2.23	0.51
1:A:376:SER:N	1:A:392:PHE:HB3	2.27	0.51
3:L:4:LEU:CD2	3:L:103:GLY:HA2	2.40	0.51
1:A:337:PHE:C	1:A:338:GLU:CG	2.78	0.50
2:H:135:THR:HG21	2:H:139:VAL:HA	1.92	0.50
2:H:157:TRP:CD1	2:H:166:VAL:HG21	2.46	0.50
2:H:141:LEU:HA	3:L:122:PHE:HZ	1.76	0.50
2:H:152:PRO:O	2:H:203:PRO:HD2	2.11	0.50
2:H:143:CYS:H	2:H:182:SER:HG	1.59	0.50
3:L:12:ALA:HA	3:L:109:GLU:O	2.11	0.50
3:L:136:VAL:CG1	3:L:152:TRP:CZ3	2.94	0.50
3:L:146:LYS:HD2	3:L:167:TRP:CZ3	2.47	0.50
2:H:28:ASN:ND2	2:H:30:LYS:HB2	2.27	0.50
3:L:27:GLU:O	3:L:73:THR:HG23	2.11	0.50
3:L:95:THR:HA	3:L:100:TRP:CG	2.47	0.50
3:L:194:ASN:HA	3:L:211:ARG:HD3	1.93	0.50
1:A:382:VAL:HG12	1:A:383:GLU:N	2.26	0.50
2:H:12:VAL:HG11	2:H:18:VAL:HG12	1.93	0.50
2:H:106:TRP:HZ2	3:L:40:TYR:CE2	2.29	0.50
1:A:340:MET:HE3	1:A:346:HIS:CA	2.37	0.49
1:A:353:THR:HG22	1:A:354:VAL:N	2.27	0.49
2:H:67:LYS:HZ2	2:H:86:LEU:HA	1.75	0.49
3:L:138:CYS:HB3	3:L:152:TRP:HZ2	1.77	0.49
3:L:29:VAL:HG22	3:L:72:ARG:O	2.12	0.49
1:A:304:GLY:HA3	1:A:328:GLY:HA3	1.94	0.49
3:L:12:ALA:HB3	3:L:111:LYS:NZ	2.26	0.49
3:L:40:TYR:HA	3:L:49:LYS:O	2.11	0.49
1:A:367:ILE:HD12	1:A:367:ILE:N	2.27	0.49
1:A:380:ILE:HB	1:A:387:LEU:HB2	1.93	0.49
2:H:148:TYR:HE1	2:H:151:GLU:HA	1.78	0.49
2:H:162:LEU:HG	2:H:163:SER:H	1.77	0.49
3:L:209:PHE:CD1	3:L:209:PHE:C	2.86	0.49
3:L:111:LYS:HG2	3:L:144:TYR:OH	2.13	0.49
3:L:18:ARG:CZ	3:L:18:ARG:HB3	2.40	0.49
3:L:210:ASN:O	3:L:212:ASN:N	2.45	0.49
3:L:86:ASP:O	3:L:108:LEU:HD23	2.13	0.49
2:H:93:VAL:HA	2:H:111:LEU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:13:VAL:CG1	3:L:14:SER:N	2.74	0.49
3:L:49:LYS:HB2	3:L:49:LYS:HZ2	1.77	0.49
1:A:353:THR:CG2	1:A:356:PRO:CG	2.75	0.49
3:L:109:GLU:OE2	3:L:177:TYR:OH	2.31	0.49
2:H:35:HIS:N	2:H:35:HIS:CD2	2.81	0.49
1:A:303:THR:HG23	1:A:329:ASP:HB2	1.95	0.49
3:L:54:ARG:O	3:L:56:SER:N	2.46	0.49
3:L:30:VAL:HB	3:L:72:ARG:HG3	1.94	0.49
3:L:81:PRO:O	3:L:83:GLU:HG3	2.13	0.49
3:L:151:LYS:HB2	3:L:199:GLU:HB3	1.95	0.48
3:L:191:GLU:O	3:L:193:HIS:N	2.45	0.48
3:L:146:LYS:HD2	3:L:167:TRP:CH2	2.48	0.48
3:L:1:ASP:HA	4:L:268:HOH:O	2.12	0.48
1:A:337:PHE:CE2	1:A:339:ILE:HG13	2.49	0.48
2:H:124:VAL:HA	2:H:144:LEU:O	2.14	0.48
2:H:101:GLU:HA	3:L:38:HIS:CE1	2.49	0.48
3:L:75:PHE:C	3:L:76:THR:HG22	2.32	0.48
1:A:302:CYS:HB2	1:A:336:PRO:HD3	1.95	0.48
1:A:387:LEU:HD22	3:L:54:ARG:NH2	2.29	0.48
1:A:365:VAL:HG12	1:A:367:ILE:HD11	1.96	0.48
3:L:5:THR:CG2	3:L:24:ARG:O	2.61	0.48
2:H:3:GLN:O	2:H:25:SER:HB3	2.13	0.48
1:A:302:CYS:SG	1:A:326:TYR:CZ	3.07	0.48
2:H:14:PRO:HG3	2:H:114:VAL:CG1	2.40	0.48
3:L:18:ARG:NH2	4:L:218:HOH:O	2.47	0.48
3:L:192:ARG:NH1	3:L:192:ARG:CG	2.77	0.48
3:L:43:LYS:HB3	3:L:44:PRO:HD2	1.96	0.48
3:L:80:ASN:CB	3:L:81:PRO:HD3	2.33	0.48
1:A:303:THR:HA	1:A:382:VAL:HG21	1.95	0.48
1:A:357:ILE:HD13	1:A:357:ILE:N	2.29	0.48
2:H:157:TRP:HZ3	2:H:213:ILE:HD11	1.76	0.48
2:H:36:TRP:HA	2:H:95:PHE:O	2.13	0.47
2:H:108:GLN:O	2:H:108:GLN:OE1	2.32	0.47
2:H:162:LEU:C	2:H:164:SER:N	2.67	0.47
2:H:83:LEU:HD11	2:H:94:TYR:CD2	2.49	0.47
3:L:195:SER:HB2	3:L:210:ASN:OD1	2.14	0.47
3:L:4:LEU:HD22	3:L:103:GLY:CA	2.43	0.47
3:L:140:LEU:HD21	3:L:150:VAL:HG21	1.95	0.47
2:H:9:ALA:O	2:H:204:ALA:HA	2.14	0.47
3:L:89:THR:HA	3:L:106:THR:O	2.14	0.47
2:H:141:LEU:HD23	2:H:141:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:20:THR:C	3:L:21:ILE:HD12	2.35	0.47
2:H:72:ALA:HA	2:H:79:ALA:HA	1.95	0.47
1:A:306:PHE:CZ	1:A:335:ILE:HG13	2.49	0.47
2:H:157:TRP:CZ2	2:H:182:SER:HB2	2.50	0.47
2:H:89:GLU:O	2:H:91:THR:N	2.35	0.47
3:L:168:THR:OG1	3:L:178:SER:C	2.53	0.47
2:H:130:GLY:HA3	4:L:216:HOH:O	2.14	0.47
3:L:95:THR:HG23	3:L:100:TRP:CD2	2.50	0.47
3:L:207:LYS:NZ	4:L:278:HOH:O	2.48	0.47
3:L:43:LYS:HB3	3:L:44:PRO:CD	2.45	0.47
3:L:63:PRO:HG2	3:L:66:PHE:CE2	2.49	0.47
3:L:123:PRO:HB3	3:L:209:PHE:CZ	2.50	0.46
3:L:119:VAL:CB	3:L:207:LYS:HD3	2.39	0.46
3:L:66:PHE:CD1	3:L:79:ILE:HG12	2.50	0.46
2:H:184:VAL:CG1	2:H:184:VAL:O	2.60	0.46
2:H:62:PRO:C	2:H:64:PHE:H	2.18	0.46
3:L:191:GLU:HG3	3:L:192:ARG:HD3	1.97	0.46
1:A:321:VAL:HA	1:A:367:ILE:O	2.14	0.46
1:A:337:PHE:O	1:A:338:GLU:HG2	2.16	0.46
2:H:42:GLU:O	2:H:42:GLU:HG2	2.14	0.46
3:L:13:VAL:HG12	3:L:14:SER:H	1.79	0.46
3:L:187:LYS:HB3	3:L:187:LYS:HE2	1.64	0.46
1:A:360:GLU:HB2	1:A:363:SER:HB2	1.98	0.46
2:H:135:THR:OG1	2:H:138:SER:O	2.33	0.46
2:H:51:ILE:HG12	2:H:52:ASP:N	2.30	0.46
3:L:115:ALA:HB1	3:L:143:PHE:CB	2.46	0.46
1:A:326:TYR:HE2	1:A:330:GLY:O	1.99	0.46
2:H:29:ILE:O	2:H:53:PRO:HG2	2.15	0.46
2:H:174:GLN:CD	3:L:164:LEU:HD22	2.35	0.46
2:H:124:VAL:HG13	2:H:209:VAL:HG21	1.98	0.46
2:H:151:GLU:HG2	2:H:151:GLU:O	2.16	0.46
2:H:12:VAL:O	2:H:114:VAL:HA	2.15	0.46
2:H:124:VAL:O	2:H:211:LYS:HE3	2.16	0.46
2:H:21:SER:HA	2:H:80:TYR:HA	1.97	0.46
3:L:37:MET:HE2	3:L:93:GLN:O	2.16	0.46
1:A:306:PHE:HE2	1:A:335:ILE:HD11	1.80	0.46
2:H:216:ARG:NH2	4:H:269:HOH:O	2.48	0.46
3:L:59:GLU:CD	3:L:60:SER:H	2.15	0.46
1:A:353:THR:CG2	1:A:354:VAL:N	2.79	0.46
2:H:214:GLU:HA	2:H:215:PRO:HD3	1.52	0.46
1:A:386:GLN:O	1:A:388:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:ASN:HD21	2:H:30:LYS:HD2	1.80	0.45
2:H:34:MET:HE3	2:H:79:ALA:HB2	1.97	0.45
3:L:188:ASP:O	3:L:192:ARG:HD3	2.17	0.45
1:A:348:LEU:CD2	1:A:372:PRO:HG3	2.45	0.45
2:H:115:SER:HG	2:H:149:PHE:HE2	1.62	0.45
3:L:12:ALA:CB	3:L:111:LYS:NZ	2.79	0.45
2:H:45:LEU:HD21	3:L:48:PRO:CG	2.42	0.45
3:L:123:PRO:HB3	3:L:209:PHE:CE1	2.51	0.45
3:L:165:ASN:HA	3:L:180:SER:O	2.16	0.45
3:L:95:THR:CG2	3:L:95:THR:O	2.59	0.45
1:A:331:SER:N	1:A:332:PRO:CD	2.79	0.45
2:H:22:CYS:O	2:H:78:ALA:HB1	2.16	0.45
2:H:84:SER:OG	2:H:85:SER:N	2.49	0.45
3:L:183:LEU:CG	3:L:185:LEU:HD21	2.43	0.45
3:L:146:LYS:HD3	4:L:253:HOH:O	2.17	0.45
3:L:151:LYS:HZ1	3:L:199:GLU:HG2	1.82	0.45
3:L:194:ASN:OD1	3:L:195:SER:HB3	2.15	0.45
3:L:4:LEU:HD22	3:L:102:PHE:O	2.17	0.45
4:A:396:HOH:O	3:L:58:LEU:CD2	2.64	0.45
2:H:166:VAL:HG22	2:H:184:VAL:HG23	1.99	0.45
3:L:30:VAL:CG2	3:L:72:ARG:HG3	2.46	0.45
3:L:83:GLU:C	3:L:85:ASP:H	2.20	0.45
2:H:180:LEU:HD23	2:H:181:SER:N	2.32	0.45
2:H:91:THR:HG23	2:H:112:VAL:O	2.16	0.45
2:H:45:LEU:HD22	3:L:102:PHE:HE1	1.81	0.45
1:A:326:TYR:CE2	1:A:330:GLY:O	2.70	0.45
2:H:11:LEU:HD22	2:H:119:THR:HG22	1.99	0.45
2:H:158:ASN:C	2:H:160:GLY:H	2.20	0.45
2:H:67:LYS:HZ3	2:H:86:LEU:HA	1.81	0.45
2:H:28:ASN:O	2:H:31:ASP:HB2	2.17	0.45
2:H:2:VAL:O	2:H:3:GLN:CG	2.65	0.45
3:L:188:ASP:HA	3:L:191:GLU:HG2	1.98	0.45
2:H:11:LEU:CD2	2:H:119:THR:HG22	2.47	0.44
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.52	0.44
2:H:128:ALA:HA	2:H:129:PRO:HD3	1.81	0.44
2:H:126:PRO:CG	2:H:212:LYS:O	2.64	0.44
2:H:2:VAL:O	2:H:3:GLN:CB	2.65	0.44
2:H:32:THR:OG1	2:H:33:TYR:N	2.47	0.44
3:L:12:ALA:CB	3:L:111:LYS:CE	2.94	0.44
3:L:19:ALA:HB2	3:L:82:VAL:HG21	1.99	0.44
3:L:191:GLU:C	3:L:193:HIS:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:PHE:HA	2:H:170:PRO:HD3	1.87	0.44
2:H:167:HIS:NE2	3:L:142:ASN:OD1	2.49	0.44
3:L:87:VAL:HG11	3:L:170:GLN:HB2	1.98	0.44
3:L:49:LYS:NZ	3:L:49:LYS:CB	2.79	0.44
1:A:333:CYS:N	4:A:433:HOH:O	2.51	0.44
1:A:394:LYS:CD	4:A:415:HOH:O	2.61	0.44
2:H:40:ARG:O	2:H:41:PRO:C	2.56	0.44
1:A:337:PHE:HD1	1:A:380:ILE:CD1	2.31	0.44
2:H:176:ASP:O	2:H:177:LEU:HD23	2.18	0.44
2:H:2:VAL:HG13	2:H:27:PHE:CE2	2.53	0.44
3:L:144:TYR:C	3:L:144:TYR:CD1	2.91	0.44
1:A:312:ILE:HG23	1:A:322:ILE:CG1	2.48	0.44
2:H:108:GLN:O	2:H:109:GLY:O	2.36	0.44
2:H:85:SER:O	2:H:85:SER:OG	2.33	0.44
3:L:39:TRP:CG	3:L:77:LEU:HD22	2.53	0.44
1:A:306:PHE:CE2	1:A:335:ILE:HD11	2.53	0.43
2:H:25:SER:OG	2:H:26:GLY:N	2.51	0.43
3:L:49:LYS:HB2	3:L:49:LYS:HZ3	1.81	0.43
1:A:389:LEU:HD23	1:A:389:LEU:N	2.33	0.43
2:H:158:ASN:C	2:H:160:GLY:N	2.70	0.43
2:H:162:LEU:CG	2:H:163:SER:H	2.30	0.43
2:H:2:VAL:CA	2:H:25:SER:OG	2.63	0.43
2:H:163:SER:C	2:H:165:GLY:H	2.22	0.43
3:L:108:LEU:HD12	3:L:109:GLU:H	1.81	0.43
2:H:167:HIS:CE1	3:L:172:SER:HB2	2.54	0.43
3:L:37:MET:C	3:L:38:HIS:HD2	2.21	0.43
2:H:216:ARG:CZ	4:H:269:HOH:O	2.66	0.43
2:H:61:ASP:O	2:H:62:PRO:C	2.56	0.43
2:H:37:VAL:HG11	2:H:45:LEU:HB3	2.01	0.43
1:A:364:PRO:CD	2:H:31:ASP:OD1	2.67	0.43
2:H:149:PHE:HB3	2:H:150:PRO:CD	2.44	0.43
1:A:337:PHE:HD1	1:A:380:ILE:HD11	1.84	0.42
3:L:12:ALA:O	3:L:111:LYS:NZ	2.46	0.42
1:A:341:ASP:OD1	1:A:343:GLU:O	2.37	0.42
1:A:376:SER:H	1:A:392:PHE:HB3	1.84	0.42
2:H:197:THR:CG2	2:H:198:CYS:N	2.79	0.42
3:L:130:THR:HG22	3:L:130:THR:O	2.18	0.42
1:A:387:LEU:CD2	3:L:54:ARG:HH22	2.32	0.42
1:A:387:LEU:HD21	3:L:54:ARG:NH2	2.32	0.42
1:A:337:PHE:CD2	1:A:351:LEU:HD13	2.55	0.42
2:H:147:GLY:N	2:H:178:TYR:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:GLU:O	2:H:42:GLU:CG	2.67	0.42
3:L:150:VAL:HG12	3:L:151:LYS:H	1.81	0.42
3:L:152:TRP:HE1	3:L:181:SER:HG	1.67	0.42
1:A:392:PHE:CD1	1:A:392:PHE:O	2.70	0.42
2:H:167:HIS:O	2:H:183:SER:HB3	2.18	0.42
3:L:12:ALA:HB3	3:L:111:LYS:HZ1	1.84	0.42
2:H:124:VAL:HG11	2:H:209:VAL:HG21	2.02	0.42
2:H:169:PHE:CE2	3:L:180:SER:HB2	2.54	0.42
3:L:32:TYR:C	3:L:34:ASN:H	2.23	0.42
2:H:20:LEU:CD2	2:H:20:LEU:N	2.82	0.42
3:L:28:SER:CA	3:L:73:THR:OG1	2.63	0.42
1:A:387:LEU:HD23	1:A:387:LEU:N	2.34	0.42
2:H:135:THR:OG1	2:H:138:SER:N	2.52	0.42
2:H:188:SER:C	2:H:190:THR:H	2.22	0.42
1:A:376:SER:H	1:A:392:PHE:CB	2.32	0.42
3:L:98:ASP:C	3:L:100:TRP:N	2.74	0.42
2:H:6:GLN:HE22	2:H:110:THR:H	1.68	0.41
2:H:111:LEU:HB3	2:H:152:PRO:HG2	2.02	0.41
2:H:30:LYS:O	2:H:31:ASP:C	2.58	0.41
3:L:30:VAL:HG23	3:L:72:ARG:CA	2.35	0.41
1:A:340:MET:HE3	1:A:346:HIS:CG	2.55	0.41
1:A:337:PHE:CD1	1:A:380:ILE:HD11	2.56	0.41
2:H:4:LEU:HA	2:H:23:THR:O	2.20	0.41
3:L:5:THR:HG23	3:L:24:ARG:CA	2.50	0.41
3:L:90:TYR:CD1	3:L:90:TYR:N	2.88	0.41
3:L:94:GLN:NE2	3:L:99:PRO:O	2.54	0.41
1:A:310:LYS:HB3	1:A:311:GLU:H	1.28	0.41
3:L:22:SER:HA	3:L:76:THR:HA	2.01	0.41
3:L:87:VAL:HG22	3:L:110:ILE:HG12	2.01	0.41
1:A:353:THR:HG22	1:A:356:PRO:CD	2.49	0.41
2:H:196:ILE:CG2	2:H:197:THR:N	2.83	0.41
2:H:212:LYS:HG3	2:H:212:LYS:H	1.41	0.41
3:L:150:VAL:CG1	3:L:151:LYS:H	2.33	0.41
1:A:353:THR:CG2	1:A:354:VAL:H	2.34	0.41
1:A:375:ASP:HA	1:A:392:PHE:CA	2.50	0.41
2:H:34:MET:CE	2:H:79:ALA:HB2	2.50	0.41
3:L:25:ALA:HB3	3:L:73:THR:HG23	2.02	0.41
1:A:340:MET:HE3	1:A:346:HIS:ND1	2.35	0.41
2:H:52:ASP:HB3	2:H:55:ASN:ND2	2.36	0.41
2:H:97:ALA:CB	2:H:103:PHE:CD1	2.98	0.41
2:H:99:ASP:HB3	2:H:100:TYR:H	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:136:VAL:HB	3:L:183:LEU:HB3	2.02	0.41
3:L:24:ARG:HG2	3:L:74:ASP:CG	2.41	0.41
1:A:334:LYS:O	1:A:336:PRO:HD3	2.21	0.41
1:A:364:PRO:HD3	2:H:31:ASP:OD1	2.21	0.41
2:H:74:THR:O	2:H:75:SER:C	2.60	0.41
3:L:6:GLN:NE2	3:L:105:GLY:HA2	2.36	0.41
2:H:197:THR:HG23	2:H:210:ASP:OD1	2.21	0.41
3:L:194:ASN:HA	3:L:211:ARG:CD	2.51	0.41
2:H:148:TYR:O	2:H:178:TYR:HB2	2.21	0.40
2:H:191:TRP:CD1	2:H:196:ILE:CG1	3.00	0.40
3:L:179:MET:CG	3:L:180:SER:N	2.80	0.40
1:A:316:GLN:CG	1:A:316:GLN:O	2.69	0.40
1:A:339:ILE:HG22	1:A:340:MET:N	2.36	0.40
2:H:158:ASN:O	2:H:159:SER:HB2	2.20	0.40
2:H:151:GLU:HG3	2:H:178:TYR:CD1	2.57	0.40
2:H:62:PRO:O	2:H:64:PHE:N	2.55	0.40
3:L:97:VAL:O	3:L:99:PRO:N	2.54	0.40
1:A:375:ASP:HA	1:A:392:PHE:HB2	2.03	0.40
2:H:130:GLY:O	2:H:132:ALA:N	2.54	0.40
3:L:37:MET:HA	3:L:37:MET:HE3	2.04	0.40
1:A:325:GLN:HB3	1:A:325:GLN:HE21	1.58	0.40
2:H:182:SER:O	2:H:183:SER:HB2	2.22	0.40
1:A:375:ASP:CA	1:A:392:PHE:HB2	2.52	0.40
3:L:58:LEU:N	3:L:58:LEU:CD2	2.48	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	95/97 (98%)	65 (68%)	19 (20%)	11 (12%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	214/216 (99%)	157 (73%)	36 (17%)	21 (10%)	0 2
3	L	194/217 (89%)	142 (73%)	37 (19%)	15 (8%)	1 5
All	All	503/530 (95%)	364 (72%)	92 (18%)	47 (9%)	0 3

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	41	PRO
2	H	45	LEU
2	H	99	ASP
2	H	108	GLN
2	H	191	TRP
3	L	55	ALA
3	L	169	ASP
1	A	299	TYR
1	A	373	PHE
1	A	382	VAL
2	H	3	GLN
2	H	44	GLY
2	H	62	PRO
2	H	63	LYS
2	H	109	GLY
2	H	178	TYR
3	L	98	ASP
3	L	192	ARG
3	L	211	ARG
3	L	212	ASN
1	A	329	ASP
1	A	333	CYS
1	A	354	VAL
1	A	355	ASN
1	A	356	PRO
2	H	9	ALA
2	H	183	SER
3	L	59	GLU
3	L	84	ALA
3	L	162	GLY
1	A	348	LEU
2	H	149	PHE
3	L	14	SER
3	L	18	ARG

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Mol	Chain	Res	Type
1	A	332	PRO
1	A	370	GLU
2	H	163	SER
2	H	170	PRO
2	H	69	THR
2	H	90	ASP
2	H	131	ALA
2	H	102	GLY
2	H	192	PRO
3	L	103	GLY
3	L	144	TYR
3	L	81	PRO
3	L	80	ASN

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	87/87 (100%)	66 (76%)	21 (24%)	0	3
2	H	181/181 (100%)	143 (79%)	38 (21%)	1	5
3	L	179/191 (94%)	139 (78%)	40 (22%)	1	4
All	All	447/459 (97%)	348 (78%)	99 (22%)	1	4

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	SER
1	A	299	TYR
1	A	301	MET
1	A	302	CYS
1	A	303	THR
1	A	308	VAL
1	A	325	GLN
1	A	329	ASP
1	A	335	ILE

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Mol	Chain	Res	Type
1	A	343	GLU
1	A	345	ARG
1	A	354	VAL
1	A	355	ASN
1	A	357	ILE
1	A	366	ASN
1	A	371	PRO
1	A	373	PHE
1	A	375	ASP
1	A	380	ILE
1	A	392	PHE
1	A	393	LYS
2	H	1	GLU
2	H	7	SER
2	H	12	VAL
2	H	20	LEU
2	H	23	THR
2	H	31	ASP
2	H	35	HIS
2	H	43	GLN
2	H	55	ASN
2	H	60	TYR
2	H	74	THR
2	H	77	ASN
2	H	85	SER
2	H	86	LEU
2	H	87	THR
2	H	89	GLU
2	H	90	ASP
2	H	100	TYR
2	H	103	PHE
2	H	108	GLN
2	H	116	SER
2	H	124	VAL
2	H	135	THR
2	H	140	THR
2	H	141	LEU
2	H	143	CYS
2	H	156	THR
2	H	158	ASN
2	H	159	SER
2	H	168	THR

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Mol	Chain	Res	Type
2	H	170	PRO
2	H	175	SER
2	H	179	THR
2	H	189	SER
2	H	195	THR
2	H	197	THR
2	H	199	ASN
2	H	212	LYS
3	L	4	LEU
3	L	5	THR
3	L	7	SER
3	L	24	ARG
3	L	38	HIS
3	L	53	TYR
3	L	58	LEU
3	L	74	ASP
3	L	76	THR
3	L	77	LEU
3	L	82	VAL
3	L	94	GLN
3	L	96	ASN
3	L	102	PHE
3	L	112	ARG
3	L	114	ASP
3	L	118	THR
3	L	125	SER
3	L	135	SER
3	L	139	PHE
3	L	140	LEU
3	L	164	LEU
3	L	165	ASN
3	L	168	THR
3	L	169	ASP
3	L	171	ASP
3	L	176	THR
3	L	177	TYR
3	L	182	THR
3	L	184	THR
3	L	185	LEU
3	L	186	THR
3	L	192	ARG
3	L	194	ASN

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Mol	Chain	Res	Type
3	L	195	SER
3	L	201	THR
3	L	203	SER
3	L	204	PRO
3	L	206	VAL
3	L	209	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
1	A	366	ASN
1	A	390	ASN
2	H	55	ASN
2	H	108	GLN
3	L	38	HIS
3	L	41	GLN
3	L	96	ASN
3	L	141	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	97/97 (100%)	-0.23	0 100 100	7, 43, 60, 66	0
2	H	216/216 (100%)	-0.33	4 (1%) 66 37	10, 33, 58, 66	0
3	L	204/217 (94%)	-0.28	2 (0%) 82 59	18, 43, 56, 65	0
All	All	517/530 (97%)	-0.29	6 (1%) 79 54	7, 40, 59, 66	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	189	SER	2.7
2	H	135	THR	2.6
3	L	130	THR	2.4
2	H	138	SER	2.3
2	H	137	SER	2.2
3	L	185	LEU	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.