



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:32 PM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

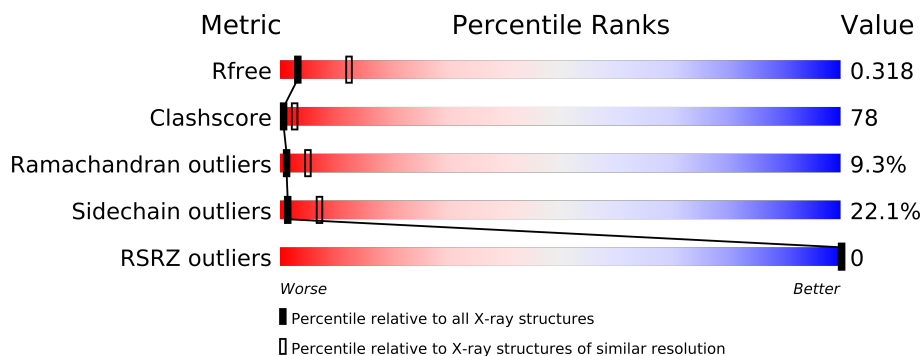
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	97	
2	H	216	
3	L	217	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4234 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

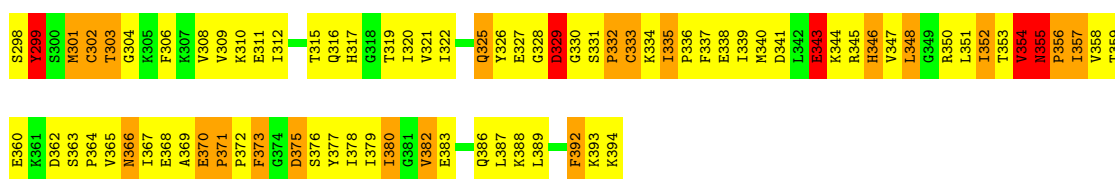
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	H	97	Total	O	0	0
			97	97		
4	L	98	Total	O	0	0
			98	98		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

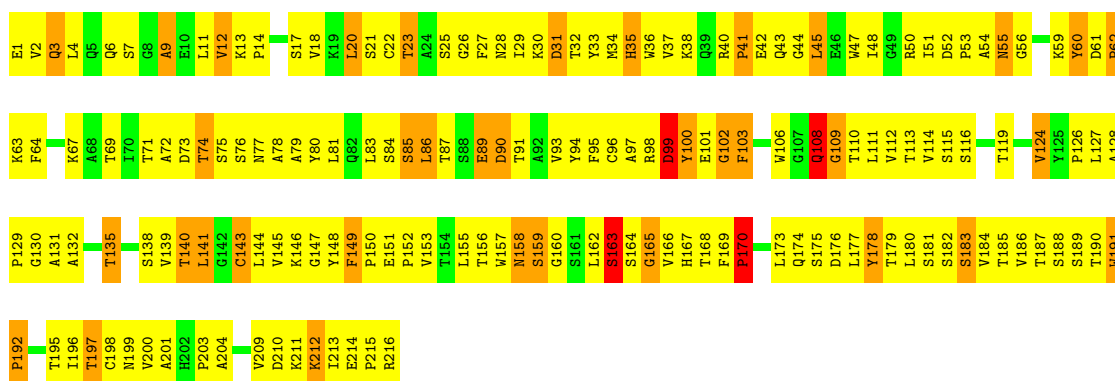
• Molecule 1: Envelope protein E

Chain A:



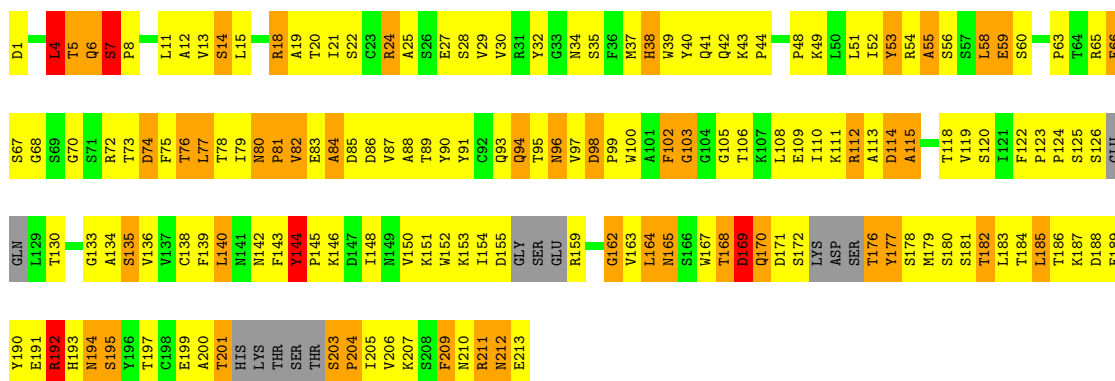
• Molecule 2: Heavy chain of Fab 1A1D-2

Chain H:



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

Chain L:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	1087 reflections (10.29%)	DCC
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 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 10945 reflections	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 78.

All (612) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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:100:TYR:O	3:L:95:THR:HG21	1.68	0.94
2:H:187:THR:HB	2:H:190:THR:OG1	1.67	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:4:LEU:O	3:L:4:LEU:HD12	1.78	0.84
3:L:179:MET:HG2	3:L:180:SER:H	1.43	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
3:L:102:PHE:N	3:L:102:PHE:CD2	2.48	0.81
2:H:14:PRO:HG3	2:H:114:VAL:HG12	1.63	0.81
2:H:6:GLN:HG2	2:H:96:CYS:SG	2.21	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:174:GLN:OE1	3:L:164:LEU:HD22	1.80	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
2:H:45:LEU:HD21	3:L:48:PRO:HG2	1.64	0.79
1:A:306:PHE:O	1:A:387:LEU:HD21	1.83	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:319:THR:HG21	1:A:368:GLU:OE2	1.84	0.78
1:A:366:ASN:HD22	1:A:367:ILE:H	1.32	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
3:L:112:ARG:HH21	3:L:113:ALA:HB3	1.49	0.77
1:A:352:ILE:CG2	1:A:352:ILE:O	2.33	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:HG3	3:L:192:ARG:HH11	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:169:PHE:CD2	3:L:180:SER:HB2	2.26	0.70
2:H:139:VAL:HG21	4:H:283:HOH:O	1.91	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:18:ARG:HA	3:L:80:ASN:HA	1.74	0.70
3:L:213:GLU:HB2	4:L:299:HOH:O	1.92	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
3:L:30:VAL:CG2	3:L:72:ARG:HA	2.22	0.69
2:H:2:VAL:HA	2:H:25:SER:OG	1.92	0.69
1:A:365:VAL:HA	4:A:450:HOH:O	1.92	0.69
2:H:102:GLY:N	3:L:38:HIS:ND1	2.40	0.69
3:L:179:MET:HG2	3:L:180:SER:N	2.06	0.69
2:H:29:ILE:HG12	2:H:53:PRO:CG	2.22	0.69
2:H:190:THR:HG22	2:H:190:THR:O	1.93	0.69
3:L:18:ARG:HH11	3:L:18:ARG:HB3	1.58	0.69
3:L:183:LEU:HG	3:L:185:LEU:CD2	2.23	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:80:ASN:O	3:L:82:VAL:N	2.27	0.68
3:L:150:VAL:HG12	3:L:151:LYS:N	2.09	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
3:L:5:THR:CG2	3:L:24:ARG:HB3	2.24	0.68
2:H:30:LYS:HA	2:H:53:PRO:HB2	1.74	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
2:H:73:ASP:O	2:H:76:SER:O	2.13	0.67
2:H:102:GLY:H	3:L:38:HIS:CE1	2.12	0.67
3:L:6:GLN:NE2	3:L:90:TYR:O	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:5:THR:HG22	3:L:24:ARG:O	1.95	0.67
1:A:376:SER:H	1:A:392:PHE:HA	1.60	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:115:ALA:CB	3:L:143:PHE:HA	2.26	0.65
3:L:95:THR:HG23	3:L:100:TRP:CE3	2.32	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:141:LEU:HA	3:L:122:PHE:CZ	2.31	0.65
2:H:216:ARG:CD	3:L:126:SER:OG	2.44	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
3:L:5:THR:HG23	3:L:24:ARG:HB3	1.79	0.64
1:A:382:VAL:O	1:A:386:GLN:HB2	1.97	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:N	3:L:21:ILE:HD12	2.12	0.64
3:L:136:VAL:HG12	3:L:152:TRP:CH2	2.33	0.63
1:A:394:LYS:HD3	4:A:415:HOH:O	1.97	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:84:ALA:HA	3:L:110:ILE:CD1	2.28	0.62
2:H:97:ALA:CB	2:H:103:PHE:HD1	2.12	0.62
1:A:382:VAL:HG12	1:A:383:GLU:H	1.64	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:SG	3:L:138:CYS:O	2.58	0.61
3:L:12:ALA:HB1	3:L:111:LYS:CE	2.29	0.61
2:H:97:ALA:HB3	2:H:103:PHE:CD1	2.35	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:94:GLN:HG2	3:L:95:THR:N	2.15	0.60
3:L:59:GLU:OE2	3:L:60:SER:N	2.27	0.60
1:A:340:MET:CE	1:A:346:HIS:HA	2.32	0.60
1:A:315:THR:HB	1:A:319:THR:HG23	1.83	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:91:THR:HG23	2:H:113:THR:HA	1.85	0.58
2:H:157:TRP:CZ3	2:H:213:ILE:HD11	2.38	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
2:H:169:PHE:CD2	3:L:168:THR:HG23	2.38	0.58
3:L:150:VAL:HG12	3:L:151:LYS:O	2.03	0.58
3:L:73:THR:O	3:L:73:THR:HG22	2.02	0.58
3:L:19:ALA:HB3	3:L:79:ILE:HB	1.85	0.58
3:L:79:ILE:HD11	3:L:90:TYR:HE2	1.66	0.58
1:A:375:ASP:HB3	1:A:392:PHE:HB2	1.85	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:188:ASP:C	3:L:188:ASP:OD1	2.42	0.57
1:A:359:THR:O	1:A:359:THR:HG22	2.04	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
1:A:312:ILE:HG23	1:A:322:ILE:HG12	1.85	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
3:L:12:ALA:CB	3:L:111:LYS:HE3	2.31	0.57
1:A:331:SER:N	1:A:332:PRO:HD3	2.19	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:102:GLY:N	3:L:38:HIS:CE1	2.73	0.57
3:L:19:ALA:HB2	3:L:82:VAL:CG2	2.35	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
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:348:LEU:HD22	1:A:372:PRO:HG3	1.87	0.57
1:A:319:THR:OG1	1:A:368:GLU:HG3	2.05	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
1:A:357:ILE:HD13	1:A:357:ILE:H	1.69	0.56
1:A:320:ILE:HG13	1:A:320:ILE:O	2.05	0.56
3:L:80:ASN:HB3	3:L:81:PRO:CD	2.29	0.56
2:H:50:ARG:HG3	2:H:50:ARG:NH1	2.16	0.56
3:L:115:ALA:CB	3:L:143:PHE:CA	2.83	0.56
2:H:36:TRP:CE3	2:H:95:PHE:O	2.59	0.56
2:H:216:ARG:HD2	3:L:126:SER:OG	2.05	0.56
1:A:327:GLU:HG3	4:A:404:HOH:O	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: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
1:A:359:THR:O	1:A:360:GLU:HG3	2.06	0.56
3:L:65:ARG:HB2	3:L:81:PRO:HD2	1.88	0.56
2:H:126:PRO:HB2	2:H:213:ILE:HA	1.88	0.56
3:L:4:LEU:CG	3:L:103:GLY:HA2	2.36	0.55
2:H:191:TRP:HZ2	2:H:213:ILE:O	1.88	0.55
2:H:187:THR:CB	2:H:190:THR:OG1	2.50	0.55
1:A:355:ASN:H	1:A:356:PRO:HD2	1.65	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:157:TRP:O	2:H:158:ASN:HB2	2.06	0.55
2:H:129:PRO:CG	3:L:122:PHE:HE2	2.14	0.55
2:H:60:TYR:N	2:H:60:TYR:CD1	2.73	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:301:MET:HB2	1:A:336:PRO:HG3	1.88	0.55
3:L:95:THR:HG23	3:L:100:TRP:CZ3	2.41	0.55
1:A:310:LYS:HE2	2:H:52:ASP:OD1	2.07	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
1:A:333:CYS:O	1:A:357:ILE:HB	2.06	0.55
3:L:6:GLN:HA	3:L:22:SER:O	2.06	0.55
3:L:120:SER:O	3:L:138:CYS:HA	2.06	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:143:CYS:O	2:H:182:SER:OG	2.24	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
1:A:387:LEU:CD2	3:L:54:ARG:NH2	2.71	0.54
3:L:41:GLN:CB	3:L:51:LEU:HD21	2.32	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:89:GLU:C	2:H:91:THR:N	2.60	0.54
2:H:144:LEU:HD21	2:H:146:LYS:HB3	1.88	0.54
2:H:59:LYS:HD3	3:L:98:ASP:CG	2.28	0.54
1:A:350:ARG:NH1	1:A:370:GLU:OE1	2.41	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
3:L:124:PRO:HG3	3:L:135:SER:H	1.73	0.53
1:A:309:VAL:O	1:A:309:VAL:HG23	2.09	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
3:L:58:LEU:HD21	4:L:245:HOH:O	2.07	0.53
3:L:150:VAL:CG1	3:L:151:LYS:N	2.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:331:SER:H	1:A:332:PRO:HD3	1.74	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: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
3:L:136:VAL:CG1	3:L:152:TRP:CH2	2.91	0.53
2:H:201:ALA:O	2:H:203:PRO:HD3	2.08	0.52
2:H:149:PHE:O	2:H:150:PRO:C	2.46	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
3:L:4:LEU:HD11	4:L:219:HOH:O	2.08	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
2:H:17:SER:HB2	2:H:84:SER:CB	2.39	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
2:H:157:TRP:CZ3	2:H:213:ILE:CD1	2.92	0.52
3:L:154:ILE:O	3:L:195:SER:O	2.28	0.52
3:L:8:PRO:HB2	3:L:11:LEU:HD22	1.92	0.52
3:L:18:ARG:CB	3:L:18:ARG:CZ	2.87	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:20:LEU:HB2	2:H:81:LEU:HB3	1.91	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
2:H:144:LEU:CD2	2:H:146:LYS:HB3	2.40	0.52
1:A:360:GLU:HB3	1:A:362:ASP:H	1.74	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
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
3:L:4:LEU:CD2	3:L:103:GLY:HA2	2.40	0.51
1:A:376:SER:N	1:A:392:PHE:HB3	2.27	0.51
1:A:337:PHE:C	1:A:338:GLU:CG	2.78	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:135:THR:HG21	2:H:139:VAL:HA	1.92	0.50
2:H:152:PRO:O	2:H:203:PRO:HD2	2.11	0.50
3:L:12:ALA:HA	3:L:109:GLU:O	2.11	0.50
2:H:143:CYS:H	2:H:182:SER:HG	1.59	0.50
3:L:146:LYS:HD2	3:L:167:TRP:CZ3	2.47	0.50
3:L:136:VAL:CG1	3:L:152:TRP:CZ3	2.94	0.50
3:L:95:THR:HA	3:L:100:TRP:CG	2.47	0.50
3:L:27:GLU:O	3:L:73:THR:HG23	2.11	0.50
2:H:28:ASN:ND2	2:H:30:LYS:HB2	2.27	0.50
3:L:194:ASN:HA	3:L:211:ARG:HD3	1.93	0.50
2:H:106:TRP:HZ2	3:L:40:TYR:CE2	2.29	0.50
2:H:12:VAL:HG11	2:H:18:VAL:HG12	1.93	0.50
1:A:382:VAL:HG12	1:A:383:GLU:N	2.26	0.50
1:A:353:THR:HG22	1:A:354:VAL:N	2.27	0.49
1:A:340:MET:HE3	1:A:346:HIS:CA	2.37	0.49
3:L:29:VAL:HG22	3:L:72:ARG:O	2.12	0.49
3:L:138:CYS:HB3	3:L:152:TRP:HZ2	1.77	0.49
2:H:67:LYS:HZ2	2:H:86:LEU:HA	1.75	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:304:GLY:HA3	1:A:328:GLY:HA3	1.94	0.49
1:A:380:ILE:HB	1:A:387:LEU:HB2	1.93	0.49
1:A:367:ILE:HD12	1:A:367:ILE:N	2.27	0.49
2:H:162:LEU:HG	2:H:163:SER:H	1.77	0.49
2:H:148:TYR:HE1	2:H:151:GLU:HA	1.78	0.49
3:L:209:PHE:CD1	3:L:209:PHE:C	2.86	0.49
3:L:86:ASP:O	3:L:108:LEU:HD23	2.13	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
2:H:93:VAL:HA	2:H:111:LEU:HA	1.94	0.49
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
3:L:109:GLU:OE2	3:L:177:TYR:OH	2.31	0.49
1:A:353:THR:CG2	1:A:356:PRO:CG	2.75	0.49
2:H:35:HIS:CD2	2:H:35:HIS:N	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:81:PRO:O	3:L:83:GLU:HG3	2.13	0.49
3:L:30:VAL:HB	3:L:72:ARG:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:387:LEU:HD22	3:L:54:ARG:NH2	2.29	0.48
1:A:302:CYS:HB2	1:A:336:PRO:HD3	1.95	0.48
3:L:5:THR:CG2	3:L:24:ARG:O	2.61	0.48
1:A:365:VAL:HG12	1:A:367:ILE:HD11	1.96	0.48
2:H:3:GLN:O	2:H:25:SER:HB3	2.13	0.48
3:L:18:ARG:NH2	4:L:218:HOH:O	2.47	0.48
3:L:80:ASN:CB	3:L:81:PRO:HD3	2.33	0.48
2:H:14:PRO:HG3	2:H:114:VAL:CG1	2.40	0.48
3:L:192:ARG:NH1	3:L:192:ARG:CG	2.77	0.48
1:A:302:CYS:SG	1:A:326:TYR:CZ	3.07	0.48
3:L:43:LYS:HB3	3:L:44:PRO:HD2	1.96	0.48
2:H:157:TRP:HZ3	2:H:213:ILE:HD11	1.76	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:36:TRP:HA	2:H:95:PHE:O	2.13	0.47
3:L:4:LEU:HD22	3:L:103:GLY:CA	2.43	0.47
3:L:195:SER:HB2	3:L:210:ASN:OD1	2.14	0.47
2:H:162:LEU:C	2:H:164:SER:N	2.67	0.47
2:H:108:GLN:OE1	2:H:108:GLN:O	2.32	0.47
2:H:83:LEU:HD11	2:H:94:TYR:CD2	2.49	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
3:L:20:THR:C	3:L:21:ILE:HD12	2.35	0.47
2:H:89:GLU:O	2:H:91:THR:N	2.35	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
3:L:168:THR:OG1	3:L:178:SER:C	2.53	0.47
2:H:72:ALA:HA	2:H:79:ALA:HA	1.95	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:63:PRO:HG2	3:L:66:PHE:CE2	2.49	0.47
3:L:207:LYS:NZ	4:L:278:HOH:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:43:LYS:HB3	3:L:44:PRO:CD	2.45	0.47
3:L:66:PHE:CD1	3:L:79:ILE:HG12	2.50	0.46
3:L:119:VAL:CB	3:L:207:LYS:HD3	2.39	0.46
3:L:123:PRO:HB3	3:L:209:PHE:CZ	2.50	0.46
2:H:184:VAL:CG1	2:H:184:VAL:O	2.60	0.46
3:L:191:GLU:HG3	3:L:192:ARG:HD3	1.97	0.46
2:H:62:PRO:C	2:H:64:PHE:H	2.18	0.46
1:A:337:PHE:O	1:A:338:GLU:HG2	2.16	0.46
3:L:13:VAL:HG12	3:L:14:SER:H	1.79	0.46
1:A:321:VAL:HA	1:A:367:ILE:O	2.14	0.46
3:L:187:LYS:HB3	3:L:187:LYS:HE2	1.64	0.46
2:H:42:GLU:O	2:H:42:GLU:HG2	2.14	0.46
3:L:115:ALA:HB1	3:L:143:PHE:CB	2.46	0.46
2:H:51:ILE:HG12	2:H:52:ASP:N	2.30	0.46
2:H:135:THR:OG1	2:H:138:SER:O	2.33	0.46
1:A:360:GLU:HB2	1:A:363:SER:HB2	1.98	0.46
2:H:174:GLN:CD	3:L:164:LEU:HD22	2.35	0.46
2:H:29:ILE:O	2:H:53:PRO:HG2	2.15	0.46
1:A:326:TYR:HE2	1:A:330:GLY:O	1.99	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
3:L:37:MET:HE2	3:L:93:GLN:O	2.16	0.46
2:H:124:VAL:O	2:H:211:LYS:HE3	2.16	0.46
2:H:12:VAL:O	2:H:114:VAL:HA	2.15	0.46
2:H:21:SER:HA	2:H:80:TYR:HA	1.97	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
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:386:GLN:O	1:A:388:LYS:HG3	2.17	0.45
3:L:12:ALA:CB	3:L:111:LYS:NZ	2.79	0.45
2:H:115:SER:HG	2:H:149:PHE:HE2	1.62	0.45
1:A:348:LEU:CD2	1:A:372:PRO:HG3	2.45	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:95:THR:CG2	3:L:95:THR:O	2.59	0.45
3:L:165:ASN:HA	3:L:180:SER:O	2.16	0.45
3:L:183:LEU:CG	3:L:185:LEU:HD21	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:84:SER:OG	2:H:85:SER:N	2.49	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
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
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:83:GLU:C	3:L:85:ASP:H	2.20	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
2:H:45:LEU:HD22	3:L:102:PHE:HE1	1.81	0.45
2:H:91:THR:HG23	2:H:112:VAL:O	2.16	0.45
2:H:180:LEU:HD23	2:H:181:SER:N	2.32	0.45
2:H:158:ASN:C	2:H:160:GLY:H	2.20	0.45
2:H:11:LEU:HD22	2:H:119:THR:HG22	1.99	0.45
2:H:67:LYS:HZ3	2:H:86:LEU:HA	1.81	0.45
1:A:326:TYR:CE2	1:A:330:GLY:O	2.70	0.45
2:H:2:VAL:O	2:H:3:GLN:CG	2.65	0.45
2:H:28:ASN:O	2:H:31:ASP:HB2	2.17	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
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
2:H:126:PRO:CG	2:H:212:LYS:O	2.64	0.44
2:H:128:ALA:HA	2:H:129:PRO:HD3	1.81	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:191:GLU:C	3:L:193:HIS:N	2.71	0.44
2:H:167:HIS:NE2	3:L:142:ASN:OD1	2.49	0.44
2:H:169:PHE:HA	2:H:170:PRO:HD3	1.87	0.44
3:L:49:LYS:NZ	3:L:49:LYS:CB	2.79	0.44
3:L:87:VAL:HG11	3:L:170:GLN:HB2	1.98	0.44
2:H:40:ARG:O	2:H:41:PRO:C	2.56	0.44
1:A:394:LYS:CD	4:A:415:HOH:O	2.61	0.44
1:A:333:CYS:N	4:A:433:HOH:O	2.51	0.44
3:L:144:TYR:C	3:L:144:TYR:CD1	2.91	0.44
1:A:337:PHE:HD1	1:A:380:ILE:CD1	2.31	0.44
2:H:2:VAL:HG13	2:H:27:PHE:CE2	2.53	0.44
2:H:176:ASP:O	2:H:177:LEU:HD23	2.18	0.44
3:L:39:TRP:CG	3:L:77:LEU:HD22	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:85:SER:O	2:H:85:SER:OG	2.33	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
1:A:306:PHE:CE2	1:A:335:ILE:HD11	2.53	0.43
3:L:49:LYS:HB2	3:L:49:LYS:HZ3	1.81	0.43
2:H:25:SER:OG	2:H:26:GLY:N	2.51	0.43
2:H:158:ASN:C	2:H:160:GLY:N	2.70	0.43
1:A:389:LEU:HD23	1:A:389:LEU:N	2.33	0.43
2:H:2:VAL:CA	2:H:25:SER:OG	2.63	0.43
2:H:162:LEU:CG	2:H:163:SER:H	2.30	0.43
3:L:108:LEU:HD12	3:L:109:GLU:H	1.81	0.43
2:H:163:SER:C	2:H:165:GLY:H	2.22	0.43
3:L:37:MET:C	3:L:38:HIS:HD2	2.21	0.43
2:H:167:HIS:CE1	3:L:172:SER:HB2	2.54	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
2:H:149:PHE:HB3	2:H:150:PRO:CD	2.44	0.43
1:A:364:PRO:CD	2:H:31:ASP:OD1	2.67	0.43
3:L:12:ALA:O	3:L:111:LYS:NZ	2.46	0.42
1:A:337:PHE:HD1	1:A:380:ILE:HD11	1.84	0.42
1:A:341:ASP:OD1	1:A:343:GLU:O	2.37	0.42
1:A:387:LEU:CD2	3:L:54:ARG:HH22	2.32	0.42
2:H:197:THR:CG2	2:H:198:CYS:N	2.79	0.42
1:A:376:SER:H	1:A:392:PHE:HB3	1.84	0.42
3:L:130:THR:HG22	3:L:130:THR:O	2.18	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
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
2:H:147:GLY:N	2:H:178:TYR:O	2.47	0.42
2:H:42:GLU:O	2:H:42:GLU:CG	2.67	0.42
3:L:12:ALA:HB3	3:L:111:LYS:HZ1	1.84	0.42
2:H:167:HIS:O	2:H:183:SER:HB3	2.18	0.42
1:A:392:PHE:CD1	1:A:392:PHE:O	2.70	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
3:L:28:SER:CA	3:L:73:THR:OG1	2.63	0.42
2:H:20:LEU:CD2	2:H:20:LEU:N	2.82	0.42
1:A:387:LEU:HD23	1:A:387:LEU:N	2.34	0.42
2:H:188:SER:C	2:H:190:THR:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:135:THR:OG1	2:H:138:SER:N	2.52	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:111:LEU:HB3	2:H:152:PRO:HG2	2.02	0.41
3:L:30:VAL:HG23	3:L:72:ARG:CA	2.35	0.41
2:H:6:GLN:HE22	2:H:110:THR:H	1.68	0.41
2:H:30:LYS:O	2:H:31:ASP:C	2.58	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
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
3:L:5:THR:HG23	3:L:24:ARG:CA	2.50	0.41
2:H:4:LEU:HA	2:H:23:THR:O	2.20	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:310:LYS:HB3	1:A:311:GLU:H	1.28	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:H	2:H:212:LYS:HG3	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
3:L:25:ALA:HB3	3:L:73:THR:HG23	2.02	0.41
2:H:34:MET:CE	2:H:79:ALA:HB2	2.50	0.41
1:A:375:ASP:HA	1:A:392:PHE:CA	2.50	0.41
1:A:340:MET:HE3	1:A:346:HIS:ND1	2.35	0.41
2:H:97:ALA:CB	2:H:103:PHE:CD1	2.98	0.41
2:H:52:ASP:HB3	2:H:55:ASN:ND2	2.36	0.41
2:H:99:ASP:HB3	2:H:100:TYR:H	1.57	0.41
3:L:24:ARG:HG2	3:L:74:ASP:CG	2.41	0.41
3:L:136:VAL:HB	3:L:183:LEU:HB3	2.02	0.41
3:L:6:GLN:NE2	3:L:105:GLY:HA2	2.36	0.41
1:A:364:PRO:HD3	2:H:31:ASP:OD1	2.21	0.41
1:A:334:LYS:O	1:A:336:PRO:HD3	2.21	0.41
2:H:74:THR:O	2:H:75:SER:C	2.60	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: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
2:H:148:TYR:O	2:H:178:TYR:HB2	2.21	0.40
1:A:339:ILE:HG22	1:A:340:MET:N	2.36	0.40
3:L:97:VAL:O	3:L:99:PRO:N	2.54	0.40
2:H:158:ASN:O	2:H:159:SER:HB2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:316:GLN:CG	1:A:316:GLN:O	2.69	0.40
3:L:37:MET:HE3	3:L:37:MET:HA	2.04	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
2:H:182:SER:O	2:H:183:SER:HB2	2.22	0.40
1:A:325:GLN:HB3	1:A:325:GLN:HE21	1.58	0.40
3:L:58:LEU:N	3:L:58:LEU:CD2	2.48	0.40
1:A:375:ASP:CA	1:A:392:PHE:HB2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/97 (98%)	65 (68%)	19 (20%)	11 (12%)	1	3
2	H	214/216 (99%)	157 (73%)	36 (17%)	21 (10%)	1	4
3	L	194/217 (89%)	142 (73%)	37 (19%)	15 (8%)	1	7
All	All	503/530 (95%)	364 (72%)	92 (18%)	47 (9%)	1	5

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 ⓘ

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%)	1	5
2	H	181/181 (100%)	143 (79%)	38 (21%)	1	8
3	L	179/191 (94%)	139 (78%)	40 (22%)	1	7
All	All	447/459 (97%)	348 (78%)	99 (22%)	1	7

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	141	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	97/97 (100%)	-0.19	0 100 100	7, 43, 60, 66	0
2	H	216/216 (100%)	-0.25	0 100 100	10, 33, 58, 66	0
3	L	204/217 (94%)	-0.20	0 100 100	18, 43, 56, 65	0
All	All	517/530 (97%)	-0.22	0 100 100	7, 40, 59, 66	0

There are no RSRZ outliers to report.

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 ⓘ

There are no such residues in this entry.