Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 10:34 PM EDT

PDB ID : 3FMG

Title : Structure of rotavirus outer capsid protein VP7 trimer in complex with a neutralizing Fab

Authors : Aoki, S.T.; Settembre, E.C.; Trask, S.D.; Greenberg, H.B.; Harrison, S.C.; Dormitzer, P.R.

Deposited on : 2008-12-22

Resolution : 3.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35
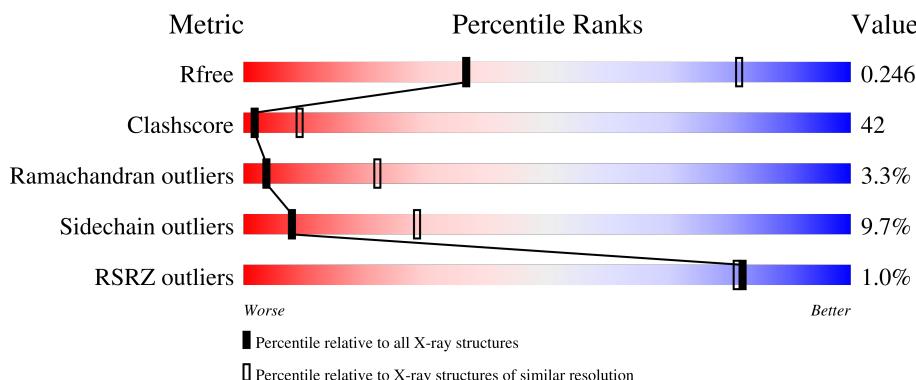
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
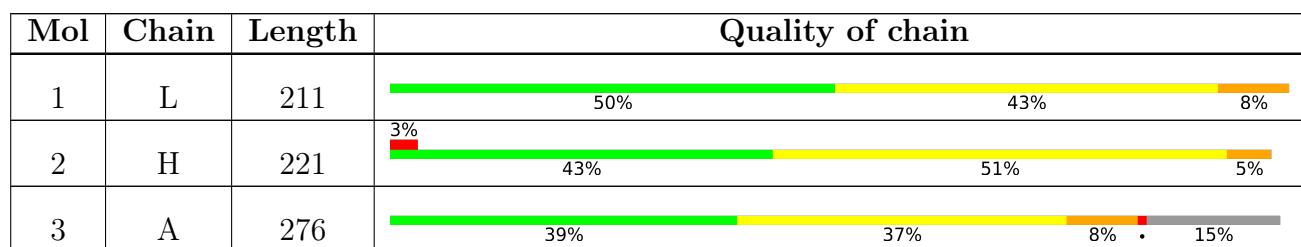
The reported resolution of this entry is 3.40 Å.

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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	L	211	50% 43% 8%
2	H	221	3% / 43% 51% 5%
3	A	276	39% 37% 8% · 15%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5166 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 Fab of neutralizing antibody 4F8, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1636	1025	277	328	6			

- Molecule 2 is a protein called Fab of neutralizing antibody 4F8, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1668	1055	277	328	8			

- Molecule 3 is a protein called Glycoprotein VP7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	235	Total	C	N	O	S	0	0	0
			1860	1184	292	369	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	THR	ALA	SEE REMARK 999	UNP P12476
A	324	TYR	ASN	SEE REMARK 999	UNP P12476

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
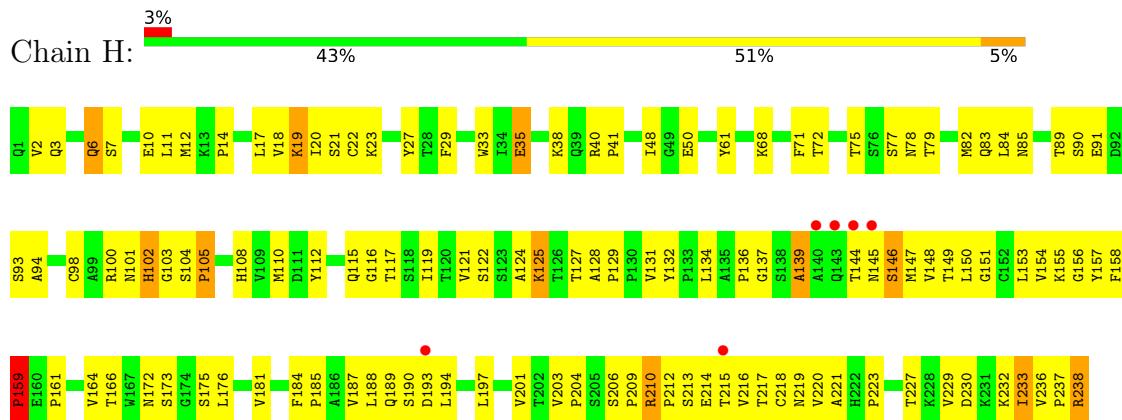
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
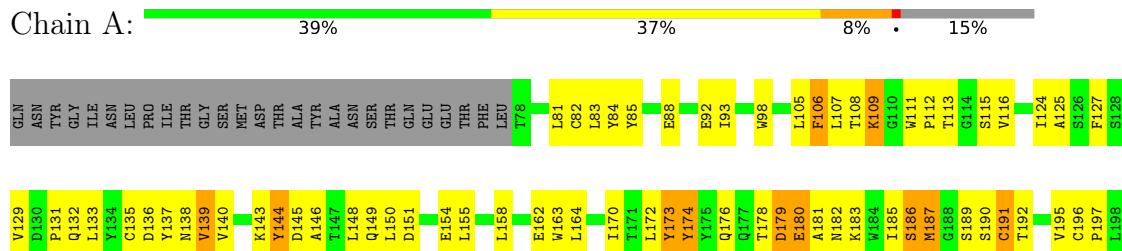
• Molecule 1: Fab of neutralizing antibody 4F8, light chain
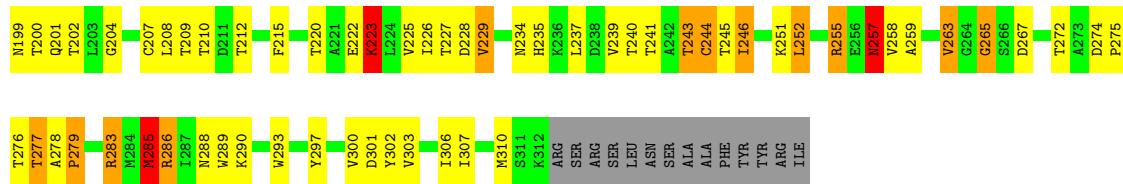
Chain L:

• Molecule 2: Fab of neutralizing antibody 4F8, heavy chain

Chain H:

• Molecule 3: Glycoprotein VP7

Chain A:

N199 T200 Q201 T202 L203 G204 C207 L208 T209 T210 D211 T212 F215 T220 A221 E222 K223 L224 V225 I226 T227 D228 V229 N234 H235 K236 L237 D238 V239 T240 T241 A242 T243 C244 T245 I246 K251 L252 R255 E256 N257 V258 A259 V263 G264 G265 S266 D267 T272 A273 D274 P275

T276 T277 A278 P279 R283 M284 M285 R286 I287 N288 W289 K290 W293 Y297 V300 D301 Y302 V303 I306 I307 M310 S311 K312 ARG SER ARG SER LEU ASN SER ALA ALA PHE TYR TYR ARG ILE

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	244.18Å 244.18Å 244.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.61 – 3.40	Depositor EDS
% Data completeness (in resolution range)	82.8 (30.00-3.40) 97.8 (29.61-3.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.238 0.231 , 0.246	Depositor DCC
R_{free} test set	3380 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	89.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 54.3	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5166	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	L	0.39	0/1677	0.71	1/2276 (0.0%)
2	H	0.40	0/1714	0.71	0/2341
3	A	0.64	4/1899 (0.2%)	0.92	8/2596 (0.3%)
All	All	0.50	4/5290 (0.1%)	0.79	9/7213 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	286	ARG	N-CA	10.31	1.67	1.46
3	A	285	MET	C-N	10.22	1.57	1.34
3	A	245	THR	CB-OG1	6.34	1.55	1.43
3	A	246	ILE	CB-CG2	6.10	1.71	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	ILE	CA-CB-CG2	-7.88	95.14	110.90
3	A	286	ARG	CB-CA-C	-7.18	96.04	110.40
3	A	223	LYS	CD-CE-NZ	6.16	125.86	111.70
3	A	286	ARG	N-CA-CB	6.05	121.49	110.60
3	A	245	THR	CA-CB-OG1	-6.01	96.38	109.00
3	A	244	CYS	CA-CB-SG	-5.86	103.45	114.00
1	L	29	ILE	N-CA-C	-5.24	96.86	111.00
3	A	257	ASN	CB-CA-C	-5.20	100.01	110.40
3	A	285	MET	C-N-CA	5.02	134.26	121.70

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	L	1636	0	1582	129	0
2	H	1668	0	1625	164	0
3	A	1860	0	1819	149	1
4	A	2	0	0	0	0
All	All	5166	0	5026	431	1

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 42.

All (431) 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:L:108:ARG:HD3	1:L:140:TYR:CD1	1.42	1.53
2:H:23:LYS:CE	2:H:79:THR:HG21	1.18	1.53
1:L:108:ARG:CD	1:L:140:TYR:CD1	1.90	1.53
2:H:23:LYS:CE	2:H:79:THR:CG2	1.82	1.52
2:H:23:LYS:HE3	2:H:79:THR:CG2	1.37	1.50
1:L:108:ARG:HD2	1:L:140:TYR:CE1	1.49	1.45
2:H:23:LYS:CD	2:H:79:THR:HG21	1.46	1.44
3:A:82:CYS:HB2	3:A:135:CYS:SG	1.56	1.44
3:A:229:VAL:HG11	3:A:235:HIS:CE1	1.50	1.42
2:H:23:LYS:CD	2:H:79:THR:CG2	1.94	1.42
3:A:191:CYS:HA	3:A:244:CYS:SG	1.66	1.34
3:A:82:CYS:CB	3:A:135:CYS:SG	2.15	1.32
3:A:229:VAL:CG1	3:A:235:HIS:HE1	1.49	1.25
3:A:105:LEU:O	3:A:108:THR:HG22	1.33	1.21
3:A:82:CYS:SG	3:A:135:CYS:HB3	1.83	1.18
2:H:125:LYS:HD3	2:H:125:LYS:N	1.58	1.15
2:H:23:LYS:CG	2:H:79:THR:HG22	1.77	1.15
2:H:125:LYS:H	2:H:125:LYS:HE2	1.08	1.14
3:A:191:CYS:CA	3:A:244:CYS:SG	2.35	1.14
2:H:23:LYS:HD2	2:H:79:THR:CG2	1.73	1.12
2:H:131:VAL:HG21	2:H:220:VAL:HG11	1.32	1.11
2:H:210:ARG:HH11	2:H:210:ARG:HB3	1.07	1.11
1:L:108:ARG:CD	1:L:140:TYR:CE1	2.19	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:HD2	1:L:140:TYR:CD1	1.66	1.10
2:H:125:LYS:N	2:H:125:LYS:CD	2.15	1.09
2:H:23:LYS:NZ	2:H:79:THR:HG21	1.67	1.06
2:H:125:LYS:H	2:H:125:LYS:CE	1.68	1.06
3:A:229:VAL:CG1	3:A:235:HIS:CE1	2.27	1.05
2:H:23:LYS:CD	2:H:79:THR:HG22	1.74	1.04
3:A:82:CYS:SG	3:A:135:CYS:CB	2.46	1.03
2:H:19:LYS:O	2:H:19:LYS:HG2	1.22	1.00
3:A:288:ASN:OD1	3:A:290:LYS:NZ	1.96	0.99
2:H:124:ALA:C	2:H:125:LYS:HD3	1.81	0.99
3:A:300:VAL:O	3:A:303:VAL:HG23	1.60	0.99
2:H:23:LYS:HD2	2:H:79:THR:HG21	1.35	0.98
2:H:23:LYS:HG3	2:H:79:THR:HG22	1.42	0.98
2:H:124:ALA:HB2	2:H:193:ASP:OD1	1.63	0.98
1:L:108:ARG:CD	1:L:140:TYR:HD1	1.48	0.97
2:H:23:LYS:HE3	2:H:79:THR:HG23	0.99	0.96
1:L:107:LYS:HA	1:L:140:TYR:OH	1.66	0.96
2:H:19:LYS:O	2:H:19:LYS:CG	2.12	0.95
2:H:20:ILE:HD11	2:H:119:ILE:HD11	1.47	0.94
1:L:108:ARG:HB3	1:L:140:TYR:CE1	2.03	0.94
2:H:210:ARG:HD2	2:H:212:PRO:HA	1.49	0.92
1:L:108:ARG:HD2	1:L:140:TYR:HE1	1.16	0.90
2:H:210:ARG:HB3	2:H:210:ARG:NH1	1.85	0.90
2:H:210:ARG:NH2	2:H:237:PRO:HG3	1.87	0.90
3:A:170:ILE:HD12	3:A:237:LEU:HB2	1.54	0.90
2:H:206:SER:HB2	2:H:209:PRO:HD3	1.54	0.88
2:H:125:LYS:N	2:H:125:LYS:HE2	1.88	0.87
3:A:133:LEU:CD1	3:A:258:VAL:CG1	2.53	0.87
1:L:61:ARG:H	1:L:61:ARG:HD2	1.37	0.87
3:A:133:LEU:HD11	3:A:258:VAL:CG1	2.04	0.87
3:A:183:LYS:HE2	3:A:228:ASP:OD2	1.74	0.87
3:A:81:LEU:HB3	3:A:116:VAL:HG22	1.57	0.86
3:A:143:LYS:HA	3:A:263:VAL:HG23	1.57	0.86
3:A:191:CYS:CB	3:A:244:CYS:SG	2.64	0.85
3:A:82:CYS:N	3:A:135:CYS:SG	2.50	0.85
3:A:133:LEU:HD11	3:A:258:VAL:HG11	1.60	0.84
3:A:191:CYS:CB	3:A:244:CYS:HG	1.91	0.83
1:L:107:LYS:CA	1:L:140:TYR:OH	2.26	0.83
1:L:140:TYR:HB3	1:L:141:PRO:HD3	1.59	0.82
2:H:10:GLU:HB3	2:H:12:MET:HE1	1.62	0.81
1:L:47:LEU:HD23	1:L:48:VAL:HG23	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:277:THR:HG22	3:A:279:PRO:HD3	1.63	0.80
1:L:106:LEU:HB3	1:L:166:GLN:HE22	1.42	0.80
3:A:229:VAL:HG11	3:A:235:HIS:ND1	1.97	0.80
3:A:300:VAL:O	3:A:303:VAL:CG2	2.30	0.79
1:L:118:PHE:HB3	2:H:134:LEU:HD12	1.65	0.79
3:A:105:LEU:O	3:A:108:THR:CG2	2.24	0.79
2:H:210:ARG:HH11	2:H:210:ARG:CB	1.93	0.79
2:H:23:LYS:CG	2:H:79:THR:CG2	2.46	0.79
3:A:112:PRO:HG2	3:A:115:SER:HB2	1.65	0.79
3:A:144:TYR:HD1	3:A:265:GLY:HA3	1.47	0.78
2:H:20:ILE:HD12	2:H:117:THR:HG21	1.66	0.78
1:L:54:LEU:HB3	1:L:58:VAL:HG11	1.64	0.78
2:H:124:ALA:HB2	2:H:193:ASP:CG	2.04	0.78
3:A:283:ARG:HG2	3:A:283:ARG:HH11	1.48	0.77
2:H:129:PRO:HB3	2:H:157:TYR:HB3	1.67	0.76
3:A:158:LEU:HD21	3:A:185:ILE:HD13	1.66	0.76
1:L:107:LYS:C	1:L:140:TYR:OH	2.25	0.75
2:H:11:LEU:HD12	2:H:11:LEU:O	1.86	0.75
3:A:293:TRP:CE3	3:A:297:TYR:CE1	2.74	0.75
2:H:124:ALA:CB	2:H:193:ASP:OD1	2.33	0.75
1:L:166:GLN:HE21	1:L:171:SER:HB3	1.52	0.75
1:L:108:ARG:HG2	1:L:109:ALA:N	2.00	0.74
3:A:212:THR:HA	3:A:215:PHE:CD1	2.21	0.74
3:A:277:THR:CG2	3:A:279:PRO:HD3	2.18	0.74
1:L:108:ARG:HB3	1:L:140:TYR:HE1	1.45	0.74
3:A:293:TRP:HE3	3:A:297:TYR:CE1	2.06	0.74
2:H:125:LYS:N	2:H:125:LYS:CE	2.38	0.74
2:H:23:LYS:HG3	2:H:79:THR:CG2	2.12	0.73
3:A:135:CYS:SG	3:A:137:TYR:O	2.46	0.73
1:L:193:THR:HG22	1:L:208:SER:CB	2.19	0.73
1:L:193:THR:HG22	1:L:208:SER:HB2	1.70	0.73
2:H:188:LEU:HD21	2:H:193:ASP:H	1.53	0.72
1:L:150:ILE:HG13	1:L:192:TYR:CE2	2.24	0.72
3:A:229:VAL:HG12	3:A:235:HIS:HE1	1.52	0.72
1:L:198:HIS:CD2	1:L:199:LYS:H	2.08	0.72
3:A:83:LEU:HD23	3:A:139:VAL:HG13	1.71	0.72
1:L:106:LEU:HB3	1:L:166:GLN:NE2	2.04	0.71
1:L:108:ARG:HD3	1:L:140:TYR:HD1	1.12	0.71
2:H:23:LYS:HZ2	2:H:79:THR:HG21	1.56	0.70
1:L:108:ARG:CB	1:L:140:TYR:CE1	2.75	0.70
2:H:2:VAL:HG13	2:H:27:TYR:HD2	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:ILE:O	3:A:246:ILE:HG23	1.91	0.70
3:A:82:CYS:HG	3:A:135:CYS:HB3	1.57	0.69
3:A:108:THR:HG23	3:A:109:LYS:N	2.07	0.69
1:L:140:TYR:O	1:L:141:PRO:C	2.31	0.69
3:A:293:TRP:CE3	3:A:297:TYR:HE1	2.11	0.68
3:A:150:LEU:HD21	3:A:223:LYS:HB3	1.75	0.68
3:A:293:TRP:O	3:A:297:TYR:HD1	1.77	0.68
2:H:100:ARG:HH12	2:H:112:TYR:HD1	1.41	0.68
2:H:204:PRO:O	2:H:209:PRO:HD2	1.93	0.68
2:H:23:LYS:HD2	2:H:79:THR:HG22	1.54	0.68
2:H:14:PRO:HG3	2:H:121:VAL:HG12	1.75	0.67
3:A:151:ASP:HB3	3:A:154:GLU:HG3	1.74	0.67
2:H:217:THR:HG23	2:H:232:LYS:HD3	1.76	0.67
3:A:234:ASN:O	3:A:235:HIS:HD2	1.75	0.67
2:H:10:GLU:HB3	2:H:12:MET:CE	2.25	0.67
3:A:178:THR:H	3:A:182:ASN:HD22	1.41	0.67
3:A:195:VAL:HG22	3:A:237:LEU:CD2	2.25	0.67
2:H:176:LEU:HD11	2:H:203:VAL:HG11	1.78	0.66
2:H:136:PRO:HD3	2:H:150:LEU:HD13	1.76	0.66
2:H:212:PRO:HB3	2:H:237:PRO:HG2	1.77	0.66
3:A:189:SER:HB2	3:A:243:THR:HB	1.78	0.66
2:H:193:ASP:OD1	2:H:193:ASP:O	2.13	0.66
3:A:140:VAL:HG12	3:A:259:ALA:O	1.96	0.66
3:A:133:LEU:HD13	3:A:258:VAL:CG1	2.26	0.65
3:A:82:CYS:CA	3:A:135:CYS:SG	2.85	0.65
1:L:136:LEU:N	1:L:136:LEU:HD12	2.11	0.64
1:L:89:GLN:HB3	1:L:98:PHE:CD1	2.34	0.63
3:A:163:TRP:CZ2	3:A:251:LYS:HD3	2.34	0.63
3:A:277:THR:CG2	3:A:278:ALA:N	2.58	0.63
1:L:106:LEU:CB	1:L:166:GLN:HE22	2.12	0.63
2:H:18:VAL:HG22	2:H:19:LYS:N	2.13	0.63
2:H:209:PRO:O	2:H:214:GLU:HG2	1.99	0.62
2:H:156:GLY:HA2	2:H:194:LEU:HB3	1.82	0.62
2:H:144:THR:CG2	2:H:148:VAL:HG22	2.30	0.62
3:A:307:ILE:HD13	3:A:310:MET:CE	2.30	0.62
2:H:129:PRO:HB2	2:H:154:VAL:HG12	1.82	0.61
1:L:142:LYS:HD2	1:L:173:TYR:OH	2.00	0.61
1:L:170:ASP:O	1:L:171:SER:HB2	1.99	0.61
1:L:115:VAL:HA	1:L:135:PHE:O	1.99	0.61
3:A:307:ILE:HD13	3:A:310:MET:HE3	1.81	0.61
2:H:18:VAL:HG11	2:H:119:ILE:HD13	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:221:ALA:O	2:H:223:PRO:HD3	2.01	0.61
3:A:144:TYR:CD1	3:A:265:GLY:HA3	2.34	0.61
3:A:143:LYS:CA	3:A:263:VAL:HG23	2.31	0.60
3:A:148:LEU:HD11	3:A:223:LYS:HE3	1.82	0.60
2:H:217:THR:CG2	2:H:232:LYS:HD3	2.31	0.60
3:A:202:THR:HG22	3:A:202:THR:O	2.01	0.60
1:L:140:TYR:HB3	1:L:141:PRO:CD	2.29	0.60
1:L:162:SER:HB2	2:H:187:VAL:HG21	1.82	0.60
1:L:160:LEU:HB2	2:H:189:GLN:NE2	2.17	0.60
3:A:144:TYR:HD2	3:A:145:ASP:N	2.00	0.59
1:L:122:SER:OG	2:H:238:ARG:NH2	2.36	0.59
1:L:148:TRP:HE1	1:L:177:SER:HB3	1.67	0.59
1:L:4:MET:HE2	1:L:23:CYS:SG	2.42	0.59
2:H:124:ALA:HB2	2:H:193:ASP:OD2	2.01	0.59
1:L:124:GLN:HG2	1:L:129:GLY:O	2.02	0.59
2:H:124:ALA:CA	2:H:125:LYS:HD3	2.32	0.59
2:H:210:ARG:HE	2:H:233:ILE:HD13	1.67	0.59
2:H:217:THR:OG1	2:H:232:LYS:HD2	2.02	0.59
3:A:172:LEU:HB2	3:A:173:TYR:CE1	2.37	0.59
1:L:2:ILE:HD12	1:L:2:ILE:H	1.67	0.59
1:L:108:ARG:N	1:L:140:TYR:OH	2.36	0.59
3:A:185:ILE:HG12	3:A:226:ILE:HG12	1.85	0.59
3:A:307:ILE:HA	3:A:310:MET:HE3	1.84	0.59
1:L:150:ILE:HG23	1:L:150:ILE:O	2.03	0.58
2:H:153:LEU:CD1	2:H:155:LYS:HB2	2.32	0.58
3:A:172:LEU:HB2	3:A:173:TYR:CD1	2.38	0.58
3:A:124:ILE:HD13	3:A:155:LEU:HD13	1.84	0.58
3:A:144:TYR:C	3:A:144:TYR:CD2	2.76	0.58
3:A:222:GLU:HB2	3:A:225:VAL:HG23	1.84	0.58
3:A:173:TYR:CD1	3:A:173:TYR:N	2.72	0.58
3:A:246:ILE:O	3:A:246:ILE:CG2	2.51	0.58
1:L:181:LEU:HD22	1:L:185:GLU:HG3	1.86	0.57
2:H:115:GLN:HG2	2:H:116:GLY:N	2.19	0.57
2:H:166:THR:OG1	2:H:219:ASN:HB2	2.04	0.57
1:L:74:LYS:O	1:L:74:LYS:HG2	2.04	0.57
3:A:195:VAL:HG22	3:A:237:LEU:HD22	1.84	0.57
3:A:300:VAL:HA	3:A:303:VAL:HG22	1.86	0.57
2:H:89:THR:HG22	2:H:91:GLU:H	1.68	0.57
2:H:172:ASN:CB	2:H:175:SER:HB3	2.34	0.57
2:H:172:ASN:HB3	2:H:175:SER:HB3	1.87	0.57
3:A:84:TYR:HB2	3:A:140:VAL:HG23	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:124:ILE:HG23	3:A:125:ALA:N	2.19	0.56
3:A:208:LEU:C	3:A:210:THR:H	2.08	0.56
1:L:206:VAL:HG22	1:L:207:LYS:N	2.20	0.56
3:A:93:ILE:HG23	3:A:293:TRP:NE1	2.20	0.56
3:A:170:ILE:HD11	3:A:237:LEU:HD12	1.86	0.56
1:L:28:ASN:ND2	1:L:68:GLY:HA2	2.20	0.56
3:A:108:THR:CG2	3:A:109:LYS:N	2.69	0.56
3:A:109:LYS:HG3	3:A:300:VAL:O	2.06	0.56
1:L:142:LYS:H	1:L:142:LYS:HD3	1.71	0.55
2:H:129:PRO:HB2	2:H:154:VAL:CG1	2.36	0.55
3:A:138:ASN:HD22	3:A:257:ASN:HB2	1.71	0.55
3:A:162:GLU:OE1	3:A:162:GLU:HA	2.07	0.55
3:A:277:THR:HG23	3:A:278:ALA:N	2.22	0.55
1:L:54:LEU:HB3	1:L:58:VAL:CG1	2.35	0.55
1:L:205:ILE:O	1:L:205:ILE:HG23	2.07	0.54
3:A:180:GLU:HG3	3:A:180:GLU:O	2.07	0.54
3:A:283:ARG:HG2	3:A:283:ARG:NH1	2.18	0.54
3:A:82:CYS:HG	3:A:135:CYS:CB	2.18	0.54
1:L:120:PRO:HG2	1:L:130:ALA:HB1	1.89	0.54
1:L:155:ARG:HG2	1:L:156:GLN:N	2.23	0.54
3:A:285:MET:HE2	3:A:306:ILE:HG12	1.89	0.53
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.44	0.53
1:L:79:GLN:HB3	1:L:80:PRO:HD2	1.88	0.53
3:A:272:THR:HG21	3:A:277:THR:CG2	2.38	0.53
2:H:172:ASN:ND2	2:H:217:THR:H	2.06	0.53
3:A:133:LEU:CD1	3:A:258:VAL:HG12	2.39	0.53
3:A:133:LEU:HD13	3:A:258:VAL:HG12	1.90	0.53
2:H:238:ARG:OXT	2:H:238:ARG:HD2	2.09	0.53
1:L:6:GLN:HG3	1:L:88:CYS:SG	2.49	0.53
2:H:33:TRP:HB2	2:H:101:ASN:HB3	1.91	0.53
2:H:134:LEU:HB2	2:H:151:GLY:O	2.08	0.53
1:L:163:TRP:CD1	1:L:175:MET:HG3	2.44	0.53
2:H:237:PRO:O	2:H:238:ARG:CB	2.57	0.52
1:L:108:ARG:HH21	1:L:172:THR:HG23	1.75	0.52
2:H:210:ARG:CZ	2:H:237:PRO:HG3	2.37	0.52
3:A:81:LEU:HD13	3:A:307:ILE:HD11	1.91	0.52
3:A:197:PRO:HA	3:A:235:HIS:CD2	2.44	0.52
1:L:185:GLU:HA	1:L:188:ARG:HE	1.74	0.52
2:H:77:SER:O	2:H:78:ASN:HB2	2.08	0.52
3:A:234:ASN:O	3:A:235:HIS:CD2	2.60	0.52
2:H:227:THR:HG22	2:H:229:VAL:HG23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ILE:HD12	1:L:2:ILE:N	2.25	0.52
2:H:206:SER:HB2	2:H:209:PRO:CD	2.33	0.52
1:L:62:PHE:CE2	1:L:75:ILE:HG12	2.45	0.52
2:H:104:SER:N	2:H:105:PRO:CD	2.73	0.51
3:A:133:LEU:CD1	3:A:258:VAL:HG13	2.38	0.51
1:L:11:LEU:HD21	1:L:19:VAL:HB	1.92	0.51
2:H:134:LEU:HB2	2:H:151:GLY:C	2.30	0.51
2:H:68:LYS:HE2	2:H:85:ASN:O	2.10	0.51
2:H:104:SER:O	2:H:105:PRO:C	2.48	0.51
3:A:208:LEU:O	3:A:210:THR:N	2.44	0.51
1:L:67:SER:HA	1:L:71:PHE:CE2	2.46	0.51
1:L:155:ARG:NH1	1:L:155:ARG:HG3	2.26	0.51
1:L:47:LEU:CD2	1:L:48:VAL:HG23	2.39	0.51
2:H:7:SER:HB3	2:H:21:SER:OG	2.10	0.51
2:H:18:VAL:CG2	2:H:19:LYS:N	2.74	0.51
2:H:238:ARG:HH11	2:H:238:ARG:HG2	1.76	0.51
1:L:13:ALA:HB1	1:L:17:GLU:OE2	2.11	0.51
1:L:89:GLN:HB3	1:L:98:PHE:CE1	2.46	0.51
1:L:118:PHE:CD2	2:H:134:LEU:HB3	2.46	0.50
3:A:272:THR:HG21	3:A:277:THR:HG22	1.93	0.50
1:L:14:SER:OG	1:L:107:LYS:HB3	2.11	0.50
2:H:27:TYR:CE1	2:H:29:PHE:HA	2.46	0.50
2:H:17:LEU:H	2:H:17:LEU:HD23	1.75	0.50
2:H:50:GLU:OE1	2:H:108:HIS:HE1	1.95	0.50
1:L:150:ILE:HG13	1:L:192:TYR:HE2	1.73	0.50
1:L:156:GLN:O	1:L:159:VAL:HG12	2.12	0.50
1:L:155:ARG:HG3	1:L:155:ARG:HH11	1.76	0.49
2:H:40:ARG:HB3	2:H:41:PRO:HD2	1.93	0.49
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.40	0.49
2:H:136:PRO:HD3	2:H:150:LEU:CD1	2.41	0.49
2:H:22:CYS:O	2:H:79:THR:HA	2.13	0.49
3:A:208:LEU:C	3:A:210:THR:N	2.66	0.49
3:A:148:LEU:CD1	3:A:223:LYS:HE3	2.43	0.49
1:L:118:PHE:CB	2:H:134:LEU:HD12	2.37	0.49
2:H:238:ARG:HD2	2:H:238:ARG:C	2.33	0.49
3:A:190:SER:O	3:A:243:THR:OG1	2.31	0.49
1:L:108:ARG:NH2	1:L:172:THR:HG23	2.27	0.49
1:L:155:ARG:HG2	1:L:156:GLN:H	1.78	0.49
2:H:164:VAL:HA	2:H:219:ASN:O	2.13	0.49
3:A:108:THR:HG23	3:A:109:LYS:H	1.78	0.49
3:A:131:PRO:O	3:A:133:LEU:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:46:LEU:HD11	1:L:49:TYR:HD2	1.78	0.48
2:H:124:ALA:HB3	2:H:158:PHE:CZ	2.47	0.48
2:H:176:LEU:HD11	2:H:203:VAL:CG1	2.43	0.48
1:L:170:ASP:O	1:L:171:SER:CB	2.61	0.48
1:L:193:THR:HG22	1:L:208:SER:OG	2.12	0.48
1:L:133:VAL:HG12	1:L:134:CYS:N	2.29	0.48
2:H:188:LEU:CD2	2:H:193:ASP:H	2.24	0.48
2:H:236:VAL:O	2:H:236:VAL:HG13	2.13	0.48
1:L:108:ARG:CG	1:L:140:TYR:CE1	2.94	0.48
1:L:139:PHE:HB2	1:L:198:HIS:CE1	2.48	0.48
3:A:144:TYR:HD2	3:A:144:TYR:C	2.13	0.48
1:L:105:GLU:HB3	1:L:142:LYS:HZ2	1.78	0.48
2:H:124:ALA:HA	2:H:125:LYS:HD3	1.95	0.48
3:A:129:VAL:HG21	3:A:187:MET:CE	2.43	0.48
1:L:206:VAL:CG2	1:L:207:LYS:N	2.77	0.47
1:L:207:LYS:HD3	1:L:207:LYS:HA	1.73	0.47
1:L:39:LYS:NZ	1:L:81:GLU:O	2.45	0.47
2:H:82:MET:CE	2:H:84:LEU:HD21	2.44	0.47
2:H:27:TYR:CE2	2:H:100:ARG:HD3	2.50	0.47
2:H:237:PRO:O	2:H:238:ARG:HB3	2.13	0.47
2:H:146:SER:HB2	2:H:147:MET:HE3	1.96	0.47
3:A:106:PHE:HE2	3:A:303:VAL:CG2	2.27	0.47
3:A:204:GLY:HA3	3:A:207:CYS:O	2.14	0.47
2:H:20:ILE:HG22	2:H:21:SER:N	2.29	0.47
2:H:100:ARG:NH1	2:H:112:TYR:CD1	2.75	0.47
2:H:188:LEU:HD21	2:H:193:ASP:N	2.27	0.47
3:A:191:CYS:HG	3:A:244:CYS:CB	2.27	0.47
3:A:222:GLU:HB2	3:A:225:VAL:CG2	2.45	0.47
1:L:21:ILE:HG12	1:L:102:THR:HG21	1.97	0.47
2:H:35:GLU:O	2:H:98:CYS:HA	2.14	0.47
2:H:18:VAL:O	2:H:83:GLN:HG3	2.15	0.46
3:A:108:THR:CG2	3:A:109:LYS:H	2.28	0.46
3:A:124:ILE:CG2	3:A:125:ALA:N	2.78	0.46
3:A:164:LEU:HB2	3:A:252:LEU:HD21	1.97	0.46
3:A:201:GLN:O	3:A:202:THR:HB	2.16	0.46
1:L:142:LYS:HD2	1:L:173:TYR:CZ	2.50	0.46
2:H:2:VAL:HB	2:H:112:TYR:CE2	2.50	0.46
3:A:106:PHE:HE2	3:A:303:VAL:HG21	1.80	0.46
3:A:180:GLU:O	3:A:180:GLU:CG	2.63	0.46
3:A:186:SER:HB3	3:A:246:ILE:HG13	1.98	0.46
1:L:61:ARG:HD2	1:L:61:ARG:N	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:148:VAL:HG12	2:H:149:THR:N	2.30	0.46
1:L:113:PRO:HD3	1:L:198:HIS:ND1	2.30	0.46
3:A:192:THR:HG23	3:A:220:THR:HA	1.97	0.46
2:H:29:PHE:CD2	2:H:78:ASN:HA	2.51	0.46
2:H:134:LEU:HD21	2:H:153:LEU:HB2	1.98	0.46
2:H:217:THR:HG22	2:H:218:CYS:N	2.31	0.46
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.51	0.46
1:L:108:ARG:HH21	1:L:170:ASP:HB2	1.81	0.46
3:A:239:VAL:HG12	3:A:240:THR:N	2.30	0.46
1:L:121:SER:OG	2:H:132:TYR:HB3	2.16	0.46
2:H:181:VAL:HG22	2:H:201:VAL:HB	1.97	0.46
1:L:166:GLN:HE21	1:L:171:SER:CB	2.24	0.46
3:A:199:ASN:HD21	3:A:201:GLN:HG2	1.81	0.46
3:A:83:LEU:CD2	3:A:139:VAL:HG13	2.44	0.46
1:L:118:PHE:HZ	2:H:149:THR:HG22	1.81	0.45
1:L:160:LEU:HD11	2:H:187:VAL:HB	1.97	0.45
3:A:252:LEU:N	3:A:252:LEU:HD23	2.30	0.45
1:L:140:TYR:O	1:L:142:LYS:N	2.50	0.45
3:A:149:GLN:O	3:A:149:GLN:HG2	2.16	0.45
3:A:301:ASP:OD1	3:A:301:ASP:O	2.34	0.45
1:L:105:GLU:HB3	1:L:142:LYS:NZ	2.31	0.45
3:A:307:ILE:HA	3:A:310:MET:CE	2.46	0.45
1:L:89:GLN:O	1:L:89:GLN:HG3	2.15	0.45
2:H:6:GLN:HA	2:H:21:SER:O	2.16	0.45
2:H:190:SER:O	2:H:193:ASP:HB3	2.17	0.45
2:H:209:PRO:HB3	2:H:214:GLU:HG3	1.98	0.45
3:A:174:TYR:CD1	3:A:174:TYR:C	2.90	0.45
3:A:275:PRO:HD2	3:A:276:THR:H	1.82	0.45
1:L:46:LEU:HD22	1:L:47:LEU:N	2.32	0.45
1:L:173:TYR:N	1:L:173:TYR:CD2	2.84	0.45
1:L:108:ARG:NE	1:L:140:TYR:HD1	2.08	0.44
2:H:20:ILE:HD11	2:H:119:ILE:CD1	2.34	0.44
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.99	0.44
2:H:127:THR:HG22	2:H:128:ALA:N	2.31	0.44
1:L:31:SER:H	1:L:32:TYR:HD1	1.65	0.44
2:H:144:THR:HG23	2:H:148:VAL:HG22	1.99	0.44
3:A:170:ILE:HG23	3:A:237:LEU:O	2.17	0.44
3:A:178:THR:N	3:A:182:ASN:HD22	2.13	0.44
2:H:17:LEU:HD23	2:H:17:LEU:N	2.32	0.44
2:H:89:THR:HG22	2:H:90:SER:N	2.32	0.44
3:A:127:PHE:HE2	3:A:140:VAL:HG21	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:179:ASP:C	3:A:181:ALA:H	2.19	0.44
3:A:196:CYS:HA	3:A:197:PRO:HD2	1.83	0.44
1:L:47:LEU:O	1:L:48:VAL:HG23	2.18	0.44
2:H:150:LEU:HD12	2:H:233:ILE:HB	2.00	0.44
1:L:149:LYS:HB2	1:L:193:THR:OG1	2.18	0.44
1:L:182:THR:HB	1:L:185:GLU:H	1.82	0.44
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.83	0.43
2:H:61:TYR:HE2	2:H:71:PHE:CE2	2.35	0.43
2:H:158:PHE:HA	2:H:159:PRO:HA	1.66	0.43
2:H:137:GLY:C	2:H:139:ALA:H	2.22	0.43
1:L:116:SER:HB2	1:L:118:PHE:HE1	1.84	0.43
1:L:162:SER:HB2	2:H:187:VAL:CG2	2.48	0.43
2:H:172:ASN:HB2	2:H:175:SER:HB3	1.99	0.43
3:A:107:LEU:HD23	3:A:111:TRP:O	2.18	0.43
3:A:138:ASN:O	3:A:258:VAL:HA	2.19	0.43
3:A:178:THR:HB	3:A:179:ASP:OD1	2.18	0.43
3:A:186:SER:HB3	3:A:246:ILE:CB	2.49	0.43
2:H:18:VAL:CG2	2:H:19:LYS:H	2.32	0.43
2:H:40:ARG:HG2	2:H:94:ALA:HB2	2.01	0.43
2:H:102:HIS:CG	2:H:103:GLY:N	2.87	0.43
2:H:2:VAL:HB	2:H:112:TYR:CD2	2.54	0.43
2:H:237:PRO:O	2:H:238:ARG:CG	2.67	0.43
3:A:92:GLU:O	3:A:92:GLU:HG2	2.19	0.43
2:H:219:ASN:N	2:H:219:ASN:HD22	2.17	0.43
1:L:159:VAL:HG22	1:L:160:LEU:N	2.34	0.42
3:A:144:TYR:CE2	3:A:146:ALA:HB2	2.54	0.42
3:A:285:MET:CE	3:A:306:ILE:HG23	2.49	0.42
2:H:93:SER:O	2:H:94:ALA:HB2	2.19	0.42
1:L:32:TYR:CD1	1:L:32:TYR:N	2.88	0.42
1:L:160:LEU:C	1:L:161:ASN:HD22	2.22	0.42
1:L:33:LEU:HD11	1:L:88:CYS:HB2	2.02	0.42
1:L:124:GLN:HE22	1:L:131:SER:CB	2.31	0.42
1:L:75:ILE:HD11	1:L:86:TYR:CE2	2.54	0.42
2:H:129:PRO:HB3	2:H:157:TYR:CB	2.44	0.42
1:L:47:LEU:O	1:L:48:VAL:CG2	2.68	0.42
1:L:141:PRO:HG2	1:L:199:LYS:HD3	2.01	0.42
2:H:127:THR:CG2	2:H:128:ALA:N	2.83	0.42
3:A:289:TRP:CD1	3:A:289:TRP:C	2.93	0.42
1:L:160:LEU:HB2	2:H:189:GLN:HE21	1.80	0.42
3:A:106:PHE:CE2	3:A:303:VAL:HG21	2.54	0.42
3:A:136:ASP:O	3:A:257:ASN:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:285:MET:CE	3:A:306:ILE:HA	2.49	0.42
3:A:303:VAL:O	3:A:307:ILE:HG12	2.20	0.42
2:H:18:VAL:HG22	2:H:19:LYS:H	1.85	0.42
2:H:102:HIS:CG	2:H:103:GLY:H	2.37	0.42
3:A:85:TYR:CZ	3:A:98:TRP:CH2	3.08	0.42
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.94	0.42
3:A:302:TYR:O	3:A:306:ILE:HG13	2.19	0.42
1:L:36:TYR:N	1:L:36:TYR:CD2	2.87	0.41
1:L:108:ARG:CG	1:L:108:ARG:HH11	2.31	0.41
2:H:17:LEU:HD12	2:H:83:GLN:NE2	2.35	0.41
3:A:191:CYS:N	3:A:244:CYS:SG	2.91	0.41
1:L:21:ILE:HG22	1:L:22:THR:N	2.35	0.41
1:L:36:TYR:HE2	1:L:89:GLN:HG2	1.86	0.41
2:H:103:GLY:C	2:H:105:PRO:HD2	2.40	0.41
2:H:104:SER:N	2:H:105:PRO:HD2	2.36	0.41
2:H:233:ILE:HD12	2:H:233:ILE:O	2.20	0.41
3:A:255:ARG:HB3	3:A:258:VAL:HG22	2.02	0.41
3:A:93:ILE:HG23	3:A:293:TRP:HE1	1.85	0.41
1:L:17:GLU:O	1:L:76:SER:O	2.38	0.41
3:A:170:ILE:HD12	3:A:237:LEU:CB	2.39	0.41
3:A:283:ARG:NH1	3:A:283:ARG:CG	2.77	0.41
1:L:147:LYS:HD2	1:L:154:GLU:OE1	2.21	0.41
2:H:2:VAL:HG12	2:H:3:GLN:N	2.36	0.41
2:H:61:TYR:CE2	2:H:71:PHE:CE2	3.09	0.41
2:H:172:ASN:HD21	2:H:217:THR:H	1.69	0.41
1:L:61:ARG:H	1:L:61:ARG:CD	2.21	0.41
1:L:105:GLU:CB	1:L:142:LYS:NZ	2.84	0.41
2:H:122:SER:C	2:H:124:ALA:H	2.25	0.41
2:H:210:ARG:NE	2:H:233:ILE:HD13	2.33	0.40
1:L:108:ARG:N	1:L:140:TYR:CZ	2.89	0.40
2:H:184:PHE:HA	2:H:185:PRO:HD3	1.77	0.40
2:H:215:THR:HG22	2:H:215:THR:O	2.21	0.40
2:H:219:ASN:N	2:H:219:ASN:ND2	2.69	0.40
3:A:201:GLN:O	3:A:202:THR:CB	2.69	0.40
2:H:18:VAL:HG11	2:H:119:ILE:CD1	2.48	0.40
3:A:162:GLU:OE1	3:A:162:GLU:CA	2.70	0.40
1:L:150:ILE:O	1:L:151:ASP:HB2	2.21	0.40
2:H:173:SER:N	2:H:219:ASN:OD1	2.50	0.40
3:A:234:ASN:C	3:A:235:HIS:CD2	2.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:151:ASP:OD2	3:A:288:ASN:OD1[8_555]	2.16	0.04

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	L	209/211 (99%)	170 (81%)	33 (16%)	6 (3%)	4	24
2	H	219/221 (99%)	184 (84%)	26 (12%)	9 (4%)	3	18
3	A	233/276 (84%)	206 (88%)	20 (9%)	7 (3%)	4	23
All	All	661/708 (93%)	560 (85%)	79 (12%)	22 (3%)	4	22

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	102	HIS
2	H	145	ASN
2	H	146	SER
3	A	132	GLN
3	A	267	ASP
2	H	139	ALA
3	A	265	GLY
1	L	140	TYR
1	L	156	GLN
2	H	105	PRO
3	A	200	THR
3	A	209	THR
3	A	241	THR
1	L	138	ASN
2	H	213	SER
1	L	55	PRO
1	L	59	PRO
1	L	78	VAL
2	H	233	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	279	PRO
2	H	159	PRO
2	H	161	PRO

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	187/187 (100%)	170 (91%)	17 (9%)	9	32
2	H	188/188 (100%)	175 (93%)	13 (7%)	15	45
3	A	212/247 (86%)	185 (87%)	27 (13%)	4	16
All	All	587/622 (94%)	530 (90%)	57 (10%)	8	28

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	22	THR
1	L	46	LEU
1	L	61	ARG
1	L	72	SER
1	L	81	GLU
1	L	106	LEU
1	L	108	ARG
1	L	115	VAL
1	L	117	ILE
1	L	142	LYS
1	L	151	ASP
1	L	164	THR
1	L	170	ASP
1	L	175	MET
1	L	181	LEU
1	L	184	ASP
1	L	207	LYS
2	H	6	GLN
2	H	19	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	35	GLU
2	H	72	THR
2	H	75	THR
2	H	110	MET
2	H	125	LYS
2	H	159	PRO
2	H	197	LEU
2	H	210	ARG
2	H	216	VAL
2	H	230	ASP
2	H	238	ARG
3	A	88	GLU
3	A	106	PHE
3	A	109	LYS
3	A	113	THR
3	A	139	VAL
3	A	144	TYR
3	A	173	TYR
3	A	174	TYR
3	A	176	GLN
3	A	179	ASP
3	A	180	GLU
3	A	186	SER
3	A	187	MET
3	A	191	CYS
3	A	223	LYS
3	A	227	THR
3	A	229	VAL
3	A	243	THR
3	A	252	LEU
3	A	255	ARG
3	A	257	ASN
3	A	263	VAL
3	A	274	ASP
3	A	277	THR
3	A	283	ARG
3	A	285	MET
3	A	286	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	28	ASN
1	L	38	GLN
1	L	70	HIS
1	L	90	HIS
1	L	91	HIS
1	L	92	ASN
1	L	124	GLN
1	L	161	ASN
1	L	166	GLN
1	L	198	HIS
2	H	1	GLN
2	H	39	GLN
2	H	83	GLN
2	H	108	HIS
2	H	145	ASN
2	H	172	ASN
2	H	189	GLN
3	A	161	ASN
3	A	176	GLN
3	A	182	ASN
3	A	235	HIS
3	A	248	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	211/211 (100%)	-0.01	1 (0%)	91	90	51, 92, 128, 151	0
2	H	221/221 (100%)	0.18	6 (2%)	54	53	50, 96, 160, 183	0
3	A	235/276 (85%)	-0.18	0	100	100	43, 74, 128, 187	0
All	All	667/708 (94%)	-0.01	7 (1%)	82	81	43, 85, 147, 187	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	145	ASN	3.4
2	H	144	THR	2.9
2	H	193	ASP	2.6
2	H	215	THR	2.6
2	H	143	GLN	2.4
2	H	140	ALA	2.4
1	L	152	GLY	2.3

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 monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	327	1/1	0.98	0.18	89,89,89,89	0
4	CA	A	328	1/1	0.98	0.16	75,75,75,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.