Full wwPDB X-ray Structure Validation Report (i)

Mar 11, 2024 – 01:52 PM EDT

PDB ID	:	8TQ7
Title	:	Crystal structure of Fab.34.2.12 in complex with MHC-I (H2-Dd)
Authors	:	Jiang, J.; Boyd, L.F.; Natarajan, K.; Margulies, D.H.
Deposited on	:	2023-08-06
Resolution	:	2.80 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:

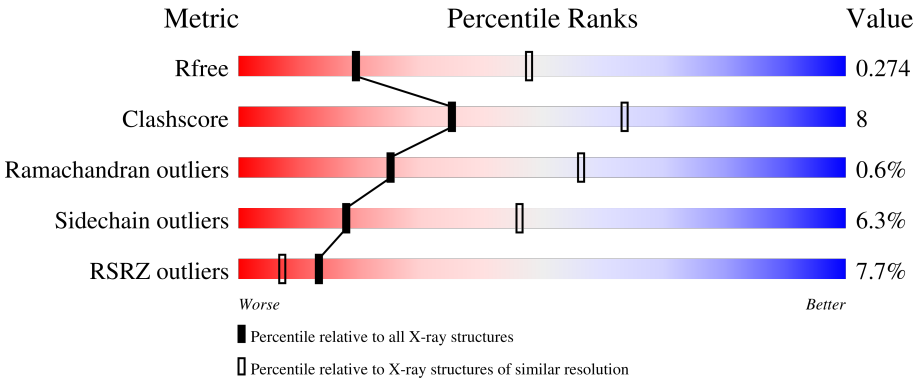
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	A	273	78% 20% .
1	C	273	3% 75% 23% .
2	B	99	79% 19% .
2	D	99	11% 78% 19% .
3	E	10	90% 10%

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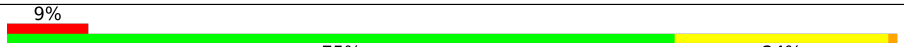
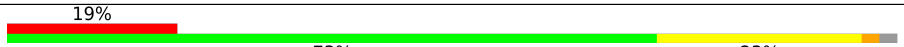
Mol	Chain	Length	Quality of chain
3	P	10	
4	F	215	
4	H	215	
5	G	213	
5	L	213	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12530 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 H-2 class I histocompatibility antigen, D-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2224	1399	400	416	9			
1	C	273	Total	C	N	O	S	0	0	0
			2148	1355	382	402	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	1	0	0
			805	515	136	147	7			
2	D	99	Total	C	N	O	S	0	0	0
			794	510	134	144	6			

- Molecule 3 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			76	48	16	12			
3	P	10	Total	C	N	O	0	0	0
			76	48	16	12			

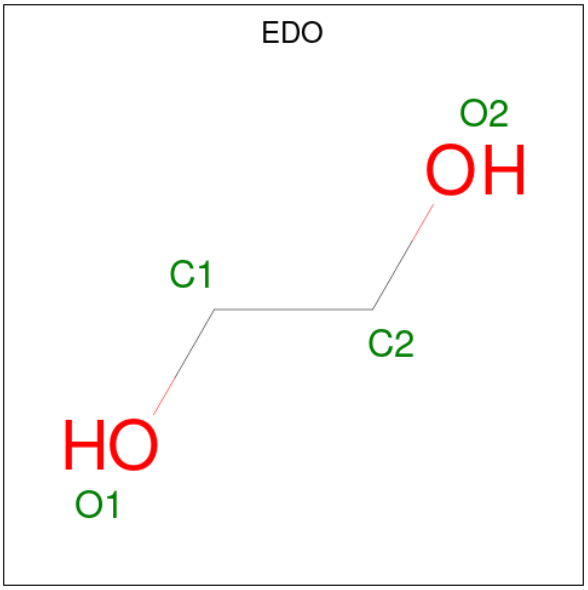
- Molecule 4 is a protein called Fab.34.2.12 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	211	Total	C	N	O	S	0	0	0
			1575	998	263	308	6			
4	H	206	Total	C	N	O	S	12	0	0
			1531	971	258	296	6			

- Molecule 5 is a protein called Fab 34.2.12 Light Chain.

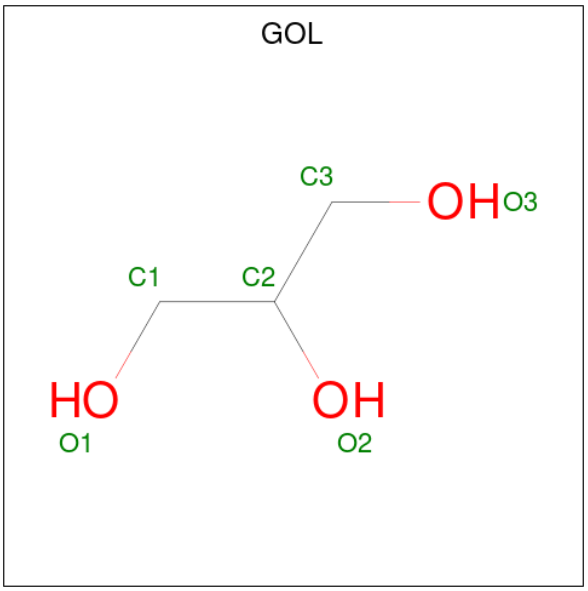
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	213	Total	C	N	O	S	1	0	0
			1630	1011	276	337	6			
5	L	209	Total	C	N	O	S	18	0	0
			1531	954	258	313	6			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

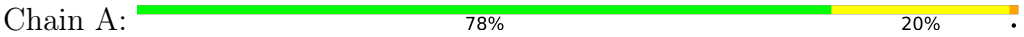
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	23	Total O 23 23	0	0
8	B	19	Total O 19 19	0	0
8	C	13	Total O 13 13	0	0
8	D	3	Total O 3 3	0	0
8	E	3	Total O 3 3	0	0
8	F	26	Total O 26 26	0	0
8	G	3	Total O 3 3	0	0
8	H	34	Total O 34 34	0	0
8	L	6	Total O 6 6	0	0

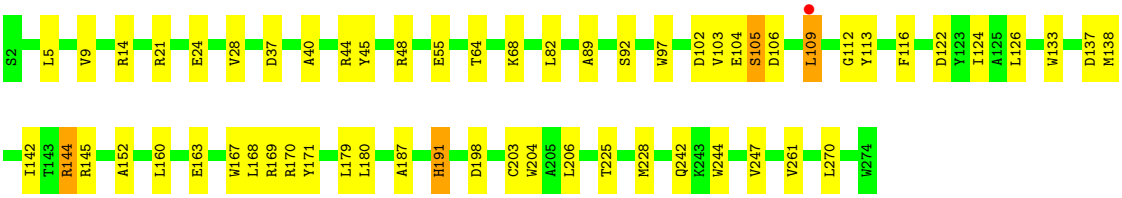
3 Residue-property plots (i)

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

• Molecule 1: H-2 class I histocompatibility antigen, D-D alpha chain

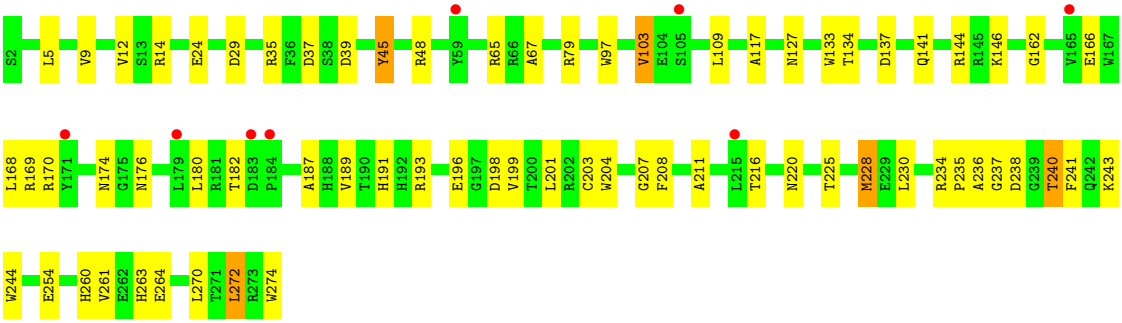
Chain A:





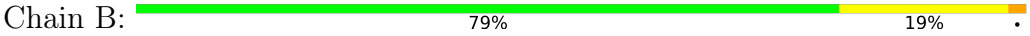
• Molecule 1: H-2 class I histocompatibility antigen, D-D alpha chain

Chain C:



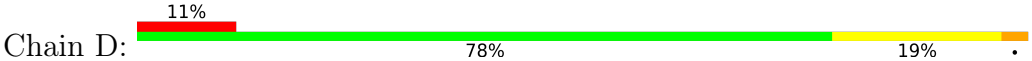
• Molecule 2: Beta-2-microglobulin

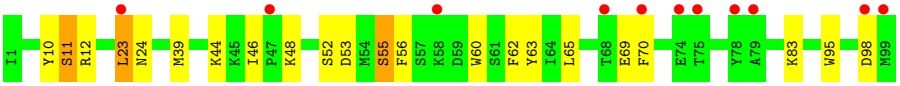
Chain B:



• Molecule 2: Beta-2-microglobulin

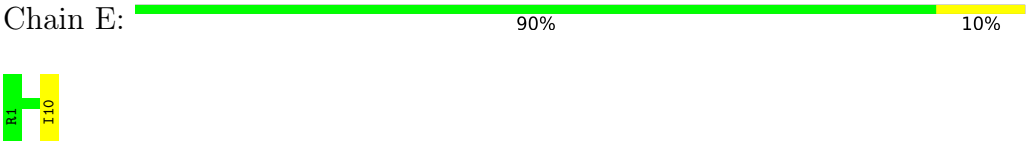
Chain D:





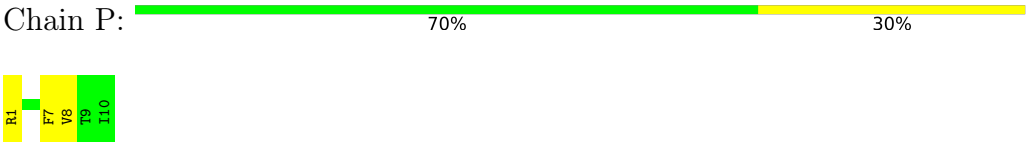
• Molecule 3: Transmembrane protein gp41

Chain E:



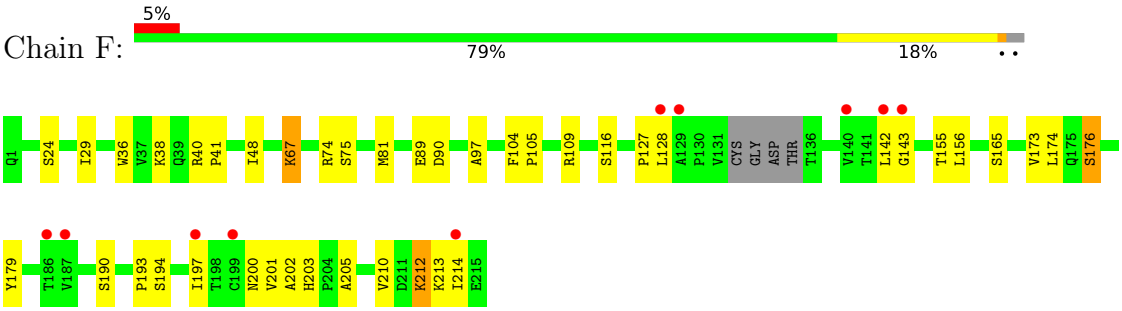
• Molecule 3: Transmembrane protein gp41

Chain P:



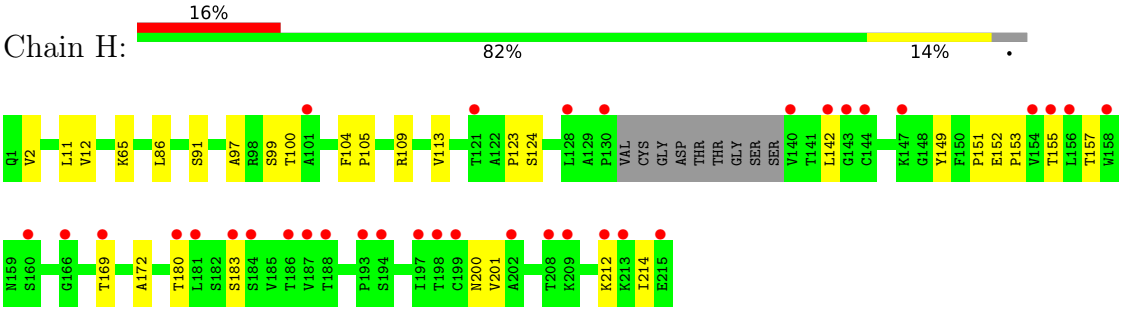
• Molecule 4: Fab.34.2.12 Heavy Chain

Chain F:



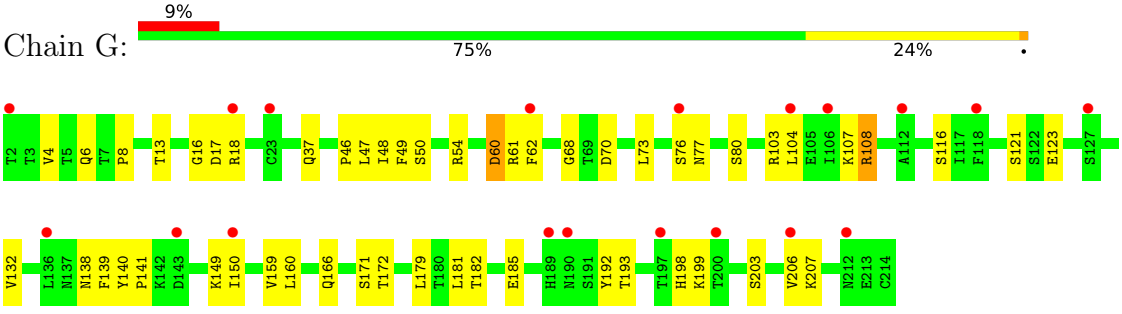
• Molecule 4: Fab.34.2.12 Heavy Chain

Chain H:



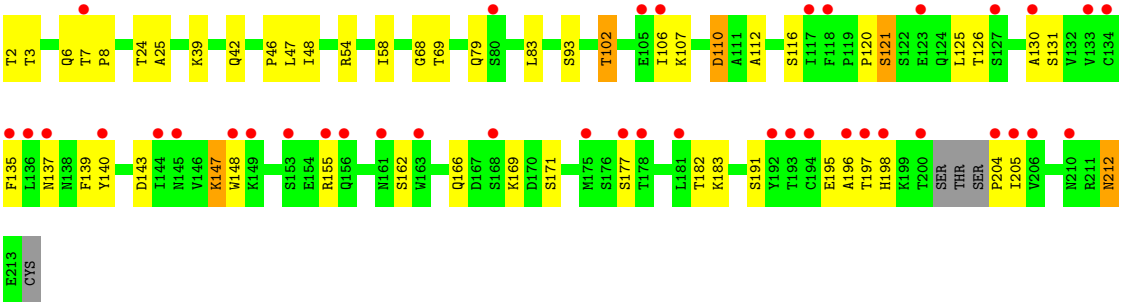
• Molecule 5: Fab 34.2.12 Light Chain

Chain G:



• Molecule 5: Fab 34.2.12 Light Chain

Chain L:


T2 T3 Q6 T7 P8 T24 A25 K39 Q42 P46 L47 I48 R54 I58 G68 T69 Q79 S80 L83 S93 T102 E105 I106 K107 D110 A111 A112 S116 I117 F118 P119 P120 S121 S122 E123 Q124 L125 T126 S127 A130 S131 V132 V133 C134
F135 L136 N137 N138 F139 Y140 D143 I144 N145 V146 K147 W148 K149 S153 E154 R155 Q156 N161 S162 W163 Q166 D167 S168 K169 D170 S171 M175 S176 S177 T178 L181 T182 K183 S191 Y192 T193 C194 E195 A196 T197 H198 K199 T200 SER THR SER P204 I205 V206 N210 R211 M212
E213 CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.59Å 113.33Å 196.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.62 – 2.80 56.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (56.62-2.80) 97.0 (56.62-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.271 0.226 , 0.274	Depositor DCC
R_{free} test set	2374 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12530	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.27	0/2287	0.54	0/3109
1	C	0.30	0/2210	0.56	0/3014
2	B	0.24	0/831	0.49	0/1131
2	D	0.27	0/820	0.50	0/1116
3	E	0.27	0/77	0.64	0/101
3	P	0.27	0/77	0.64	0/101
4	F	0.26	0/1618	0.50	0/2212
4	H	0.26	0/1572	0.50	0/2146
5	G	0.28	0/1669	0.56	0/2273
5	L	0.31	0/1567	0.54	0/2138
All	All	0.28	0/12728	0.53	0/17341

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2224	0	2081	34	0
1	C	2148	0	1952	50	0
2	B	805	0	771	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	794	0	758	15	0
3	E	76	0	82	1	0
3	P	76	0	82	2	0
4	F	1575	0	1518	24	0
4	H	1531	0	1470	15	0
5	G	1630	0	1503	35	0
5	L	1531	0	1372	27	0
6	C	4	0	6	0	0
7	F	6	0	8	0	0
8	A	23	0	0	0	0
8	B	19	0	0	0	0
8	C	13	0	0	0	0
8	D	3	0	0	0	0
8	E	3	0	0	0	0
8	F	26	0	0	1	0
8	G	3	0	0	0	0
8	H	34	0	0	0	0
8	L	6	0	0	0	0
All	All	12530	0	11603	197	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 8.

All (197) 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:C:237:GLY:O	2:D:12:ARG:NH2	2.02	0.90
1:C:216:THR:HA	1:C:228:MET:HE1	1.68	0.76
1:C:45:TYR:HE1	1:C:67:ALA:HB2	1.51	0.76
1:C:208:PHE:HB2	1:C:263:HIS:HE1	1.54	0.73
1:C:234:ARG:O	1:C:241:PHE:HD1	1.74	0.69
5:G:140:TYR:CD1	5:G:141:PRO:HA	2.28	0.69
5:G:103:ARG:HG2	5:G:103:ARG:HH11	1.59	0.68
5:G:181:LEU:HD13	5:G:185:GLU:HG2	1.74	0.68
1:C:211:ALA:HB2	1:C:241:PHE:CE2	2.29	0.67
5:G:108:ARG:H	5:G:140:TYR:HE2	1.43	0.67
1:C:207:GLY:HA2	1:C:240:THR:HG23	1.76	0.67
4:H:212:LYS:HA	4:H:212:LYS:HE2	1.77	0.65
1:C:187:ALA:HA	1:C:204:TRP:O	1.97	0.65
5:L:120:PRO:HB3	5:L:131:SER:H	1.60	0.65
4:F:105:PRO:HA	5:G:46:PRO:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:18:ARG:HG2	5:G:76:SER:HA	1.79	0.64
5:G:140:TYR:HD1	5:G:141:PRO:HA	1.61	0.64
1:A:82:LEU:HD21	1:A:89:ALA:HA	1.78	0.64
4:F:173:VAL:HB	5:G:160:LEU:HD23	1.80	0.64
4:F:156:LEU:HD13	4:F:201:VAL:HG22	1.80	0.63
1:C:208:PHE:HB2	1:C:263:HIS:CE1	2.33	0.63
1:C:9:VAL:HB	1:C:97:TRP:HB3	1.78	0.63
4:H:11:LEU:HB2	4:H:151:PRO:HG3	1.80	0.62
2:B:57:SER:OG	2:B:58:LYS:N	2.32	0.62
5:G:150:ILE:HG23	5:G:192:TYR:HE1	1.63	0.62
5:G:6:GLN:OE1	5:G:6:GLN:N	2.32	0.62
5:G:149:LYS:HB2	5:G:193:THR:HB	1.82	0.62
1:A:9:VAL:HG22	1:A:24:GLU:HG2	1.82	0.61
1:C:141:GLN:OE1	1:C:144:ARG:NH1	2.32	0.61
4:H:152:GLU:OE1	4:H:153:PRO:HA	2.01	0.61
1:C:9:VAL:HG22	1:C:24:GLU:HG2	1.83	0.60
4:H:105:PRO:HA	5:L:46:PRO:HG3	1.83	0.60
5:L:6:GLN:NE2	5:L:24:THR:O	2.34	0.60
4:F:176:SER:O	4:F:176:SER:OG	2.17	0.59
2:B:7:ILE:HD12	2:B:91:LYS:HE3	1.84	0.59
5:G:60:ASP:OD1	5:G:60:ASP:N	2.34	0.59
4:H:123:PRO:HB3	4:H:149:TYR:HB3	1.85	0.59
5:L:148:TRP:HE1	5:L:177:SER:HG	1.48	0.59
1:C:230:LEU:HD22	1:C:243:LYS:HE3	1.85	0.58
1:C:103:VAL:CG2	1:C:168:LEU:HD23	2.33	0.58
5:G:16:GLY:HA2	5:G:77:ASN:HD22	1.69	0.58
1:C:103:VAL:HG23	1:C:168:LEU:HD23	1.84	0.58
1:A:206:LEU:HD23	1:A:242:GLN:HB3	1.86	0.57
1:C:207:GLY:HA2	1:C:240:THR:CG2	2.34	0.57
1:A:225:THR:HA	1:A:228:MET:HE3	1.87	0.57
5:L:83:LEU:HD11	5:L:166:GLN:HB3	1.86	0.57
4:F:212:LYS:NZ	5:G:123:GLU:OE2	2.38	0.57
1:C:133:TRP:HB2	1:C:144:ARG:HG3	1.86	0.56
1:C:220:ASN:OD1	4:F:74:ARG:NH2	2.38	0.56
1:C:5:LEU:HB2	1:C:168:LEU:HD13	1.86	0.56
1:C:263:HIS:CD2	1:C:264:GLU:H	2.23	0.56
1:C:24:GLU:OE1	1:C:45:TYR:OH	2.20	0.56
4:H:172:ALA:HA	4:H:180:THR:O	2.06	0.56
1:C:235:PRO:HD2	2:D:10:TYR:OH	2.06	0.56
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.40	0.55
5:L:106:ILE:N	5:L:166:GLN:OE1	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:212:ASN:OD1	5:L:212:ASN:N	2.39	0.55
4:H:12:VAL:HG11	4:H:86:LEU:HD12	1.89	0.55
4:F:142:LEU:HD13	4:F:214:ILE:HD13	1.89	0.55
4:F:201:VAL:HB	4:F:210:VAL:HG23	1.87	0.54
5:G:54:ARG:HH11	5:G:54:ARG:HB2	1.72	0.54
1:A:116:PHE:HB2	1:A:124:ILE:HG22	1.90	0.54
1:C:127:ASN:OD1	1:C:134:THR:OG1	2.24	0.54
1:C:225:THR:HA	1:C:228:MET:CE	2.38	0.54
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.88	0.54
5:G:206:VAL:O	5:G:207:LYS:HD2	2.07	0.53
5:G:150:ILE:HG23	5:G:192:TYR:CE1	2.43	0.53
4:F:40:ARG:NH1	4:F:89:GLU:OE1	2.42	0.53
5:G:16:GLY:HA2	5:G:77:ASN:ND2	2.23	0.53
1:A:163:GLU:HG3	1:A:167:TRP:HD1	1.73	0.53
1:A:126:LEU:HB2	1:A:133:TRP:CZ3	2.44	0.52
4:F:38:LYS:NZ	8:F:402:HOH:O	2.43	0.52
5:G:54:ARG:HB2	5:G:54:ARG:NH1	2.25	0.52
2:B:37:ILE:HG12	2:B:82:VAL:HG22	1.91	0.52
5:L:83:LEU:CD1	5:L:166:GLN:HB3	2.40	0.51
2:D:11:SER:HG	2:D:95:TRP:HZ2	1.59	0.51
2:D:55:SER:HB2	2:D:63:TYR:CZ	2.45	0.51
5:L:137:ASN:N	5:L:137:ASN:HD22	2.09	0.51
5:L:135:PHE:HB3	5:L:137:ASN:HD21	1.76	0.51
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.94	0.50
1:C:170:ARG:O	1:C:174:ASN:HB2	2.11	0.50
1:A:103:VAL:HG23	1:A:109:LEU:HA	1.92	0.50
5:G:108:ARG:NH2	5:G:172:THR:HG22	2.26	0.50
5:G:37:GLN:HB2	5:G:47:LEU:HD11	1.93	0.50
5:L:54:ARG:HG3	5:L:58:ILE:HB	1.93	0.50
4:H:91:SER:HA	4:H:113:VAL:O	2.11	0.49
5:G:166:GLN:HE21	5:G:171:SER:C	2.15	0.49
4:H:142:LEU:HD13	4:H:214:ILE:HG12	1.94	0.49
5:L:121:SER:O	5:L:125:LEU:HD23	2.13	0.49
1:C:35:ARG:CZ	2:D:53:ASP:HB3	2.43	0.49
5:L:120:PRO:HG3	5:L:130:ALA:HB1	1.93	0.49
1:C:235:PRO:HA	1:C:241:PHE:CD1	2.48	0.48
5:L:25:ALA:O	5:L:69:THR:OG1	2.31	0.48
5:G:159:VAL:HG23	5:G:179:LEU:HD23	1.95	0.48
4:F:36:TRP:CE3	4:F:81:MET:HE2	2.49	0.48
2:B:17:ASN:OD1	2:B:97:ARG:NH2	2.47	0.48
1:C:162:GLY:O	1:C:166:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:PRO:HA	1:C:241:PHE:CE1	2.48	0.48
5:L:106:ILE:HB	5:L:171:SER:OG	2.14	0.48
1:C:137:ASP:O	1:C:141:GLN:HG2	2.14	0.48
4:F:142:LEU:HD22	4:F:214:ILE:HG21	1.95	0.48
1:C:176:ASN:O	1:C:180:LEU:HB2	2.14	0.47
2:D:24:ASN:HB3	2:D:65:LEU:HD21	1.97	0.47
5:G:108:ARG:HD2	5:G:140:TYR:HD2	1.79	0.47
1:A:64:THR:O	1:A:68:LYS:HG2	2.14	0.47
1:A:152:ALA:HB2	3:P:8:VAL:HG11	1.96	0.47
5:L:196:ALA:O	5:L:204:PRO:HA	2.14	0.47
1:C:236:ALA:O	2:D:24:ASN:ND2	2.48	0.47
5:L:139:PHE:HB2	5:L:198:HIS:CE1	2.49	0.47
1:A:14:ARG:CZ	1:A:21:ARG:HB2	2.45	0.46
5:L:120:PRO:HG2	5:L:125:LEU:HD21	1.96	0.46
4:F:128:LEU:HD12	4:F:143:GLY:HA3	1.97	0.46
5:L:195:GLU:HA	5:L:205:ILE:O	2.16	0.46
5:G:103:ARG:HG2	5:G:103:ARG:NH1	2.25	0.45
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.97	0.45
4:F:174:LEU:HB2	4:F:179:TYR:CE1	2.52	0.45
4:H:11:LEU:HD22	4:H:151:PRO:HD3	1.97	0.45
1:A:9:VAL:HB	1:A:97:TRP:HB3	1.97	0.45
2:D:23:LEU:HB3	2:D:70:PHE:CE1	2.51	0.45
4:H:97:ALA:HB1	4:H:104:PHE:HB3	1.98	0.45
5:L:147:LYS:HD2	5:L:197:THR:OG1	2.17	0.45
1:C:45:TYR:CE1	1:C:67:ALA:HB2	2.40	0.45
1:C:196:GLU:HG3	5:G:49:PHE:CE2	2.52	0.45
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.85	0.45
1:A:169:ARG:HH11	1:A:169:ARG:HG3	1.81	0.45
4:H:212:LYS:HA	4:H:212:LYS:CE	2.44	0.45
1:C:103:VAL:HG13	1:C:109:LEU:HA	1.98	0.44
5:G:132:VAL:HG13	5:G:179:LEU:HB3	1.97	0.44
4:H:155:THR:O	4:H:201:VAL:HA	2.18	0.44
1:A:102:ASP:OD2	1:A:113:TYR:HE2	2.01	0.44
1:A:163:GLU:HG3	1:A:167:TRP:CD1	2.50	0.44
1:C:191:HIS:CE1	1:C:199:VAL:HG11	2.52	0.44
1:C:261:VAL:HB	1:C:270:LEU:HB3	1.99	0.44
1:A:124:ILE:HD11	1:A:144:ARG:HB3	1.99	0.44
5:L:47:LEU:O	5:L:48:ILE:HD12	2.17	0.44
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.98	0.44
4:F:155:THR:HG22	4:F:202:ALA:HB3	2.00	0.44
2:B:36:GLU:HG2	2:B:83:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:67:LYS:NZ	4:F:90:ASP:OD2	2.49	0.44
5:L:8:PRO:O	5:L:102:THR:HG23	2.18	0.43
5:G:138:ASN:HA	5:G:172:THR:OG1	2.19	0.43
1:A:203:CYS:O	1:A:244:TRP:HA	2.19	0.43
1:C:146:LYS:NZ	3:E:10:ILE:O	2.51	0.43
1:A:171:TYR:OH	3:P:1:ARG:N	2.45	0.43
5:G:47:LEU:C	5:G:48:ILE:HG13	2.38	0.43
5:G:139:PHE:HE1	5:G:141:PRO:O	2.02	0.43
4:H:65:LYS:HB3	4:H:65:LYS:HE3	1.88	0.43
5:L:110:ASP:N	5:L:110:ASP:OD1	2.52	0.43
1:A:138:MET:O	1:A:142:ILE:HG13	2.18	0.43
2:B:23:LEU:HB2	2:B:70:PHE:CE1	2.54	0.43
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.54	0.42
2:D:48:LYS:HE3	2:D:69:GLU:HG3	2.01	0.42
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.50	0.42
4:F:38:LYS:HB2	4:F:48:ILE:HD11	2.01	0.42
2:D:39:MET:O	2:D:46:ILE:HG22	2.19	0.42
2:B:24:ASN:HD22	2:B:67:HIS:HB3	1.85	0.42
4:F:127:PRO:HG3	4:F:212:LYS:HE2	2.00	0.42
4:F:190:SER:O	4:F:194:SER:OG	2.31	0.42
4:F:197:ILE:O	4:F:214:ILE:HD12	2.19	0.42
5:G:107:LYS:HA	5:G:140:TYR:OH	2.20	0.42
1:A:137:ASP:OD1	1:A:138:MET:N	2.52	0.42
2:B:24:ASN:HB3	2:B:65:LEU:HD21	2.01	0.42
1:C:48:ARG:NH1	2:D:53:ASP:OD2	2.45	0.42
1:C:225:THR:HA	1:C:228:MET:HE3	2.02	0.42
5:G:54:ARG:NH2	5:G:62:PHE:O	2.46	0.42
2:B:48:LYS:HD2	2:B:48:LYS:HA	1.70	0.42
5:G:198:HIS:CD2	5:G:199:LYS:H	2.38	0.42
1:C:199:VAL:HG12	1:C:201:LEU:HD22	2.00	0.42
4:H:169:THR:HG23	4:H:183:SER:HB2	2.02	0.42
1:A:104:GLU:HG3	1:A:105:SER:N	2.34	0.41
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.94	0.41
1:C:225:THR:HA	1:C:228:MET:HE2	2.02	0.41
5:G:13:THR:HG22	5:G:104:LEU:HD21	2.02	0.41
1:C:189:VAL:HG23	1:C:272:LEU:HD12	2.02	0.41
1:A:104:GLU:O	1:A:106:ASP:N	2.48	0.41
1:C:201:LEU:HD11	1:C:254:GLU:HB3	2.02	0.41
2:D:56:PHE:HB3	2:D:62:PHE:CD2	2.55	0.41
5:L:155:ARG:HD2	5:L:155:ARG:HA	1.90	0.41
1:C:204:TRP:HZ2	2:D:98:ASP:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:7:THR:HG21	5:L:102:THR:OG1	2.21	0.41
4:F:24:SER:HB3	4:F:29:ILE:HG23	2.03	0.41
4:F:97:ALA:HB1	4:F:104:PHE:HB3	2.03	0.41
4:F:203:HIS:CE1	4:F:205:ALA:HB3	2.56	0.41
5:G:48:ILE:HD12	5:G:73:LEU:HD21	2.03	0.41
1:A:191:HIS:CD2	1:A:191:HIS:C	2.94	0.41
4:F:155:THR:CG2	4:F:202:ALA:HB3	2.50	0.41
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.87	0.40
1:A:187:ALA:HA	1:A:204:TRP:O	2.21	0.40
1:C:203:CYS:O	1:C:244:TRP:HA	2.21	0.40
1:A:112:GLY:HA3	1:A:160:LEU:HD13	2.02	0.40
1:A:102:ASP:OD2	1:A:113:TYR:CE2	2.75	0.40
2:B:55:SER:HB2	2:B:63:TYR:CZ	2.57	0.40
5:L:147:LYS:NZ	5:L:204:PRO:HG2	2.37	0.40
1:C:14:ARG:HH12	1:C:39:ASP:CG	2.25	0.40
1:C:220:ASN:N	1:C:220:ASN:HD22	2.18	0.40
2:D:83:LYS:HA	2:D:83:LYS:HD2	1.77	0.40
5:L:140:TYR:H	5:L:198:HIS:HE1	1.68	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	271/273 (99%)	259 (96%)	11 (4%)	1 (0%)	34	66
1	C	271/273 (99%)	254 (94%)	16 (6%)	1 (0%)	34	66
2	B	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	44
2	D	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
3	E	8/10 (80%)	8 (100%)	0	0	100	100
3	P	8/10 (80%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	F	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	29 61
4	H	202/215 (94%)	192 (95%)	10 (5%)	0	100 100
5	G	211/213 (99%)	197 (93%)	11 (5%)	3 (1%)	11 34
5	L	205/213 (96%)	193 (94%)	9 (4%)	3 (2%)	10 33
All	All	1577/1620 (97%)	1493 (95%)	74 (5%)	10 (1%)	25 56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	4	VAL
5	L	143	ASP
5	G	68	GLY
5	L	68	GLY
1	A	105	SER
2	B	42	ASN
5	G	8	PRO
5	L	112	ALA
1	C	29	ASP
4	F	41	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	225/229 (98%)	215 (96%)	10 (4%)	28 61
1	C	207/229 (90%)	191 (92%)	16 (8%)	13 35
2	B	90/93 (97%)	87 (97%)	3 (3%)	38 72
2	D	87/93 (94%)	82 (94%)	5 (6%)	20 50
3	E	7/7 (100%)	7 (100%)	0	100 100
3	P	7/7 (100%)	6 (86%)	1 (14%)	3 10
4	F	173/182 (95%)	163 (94%)	10 (6%)	20 50
4	H	164/182 (90%)	157 (96%)	7 (4%)	29 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	G	182/189 (96%)	171 (94%)	11 (6%)	19 48
5	L	160/189 (85%)	141 (88%)	19 (12%)	5 16
All	All	1302/1400 (93%)	1220 (94%)	82 (6%)	18 46

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	45	TYR
1	A	48	ARG
1	A	92	SER
1	A	109	LEU
1	A	144	ARG
1	A	180	LEU
1	A	191	HIS
1	A	198	ASP
1	A	247	VAL
2	B	57	SER
2	B	70	PHE
2	B	98	ASP
1	C	12	VAL
1	C	37	ASP
1	C	45	TYR
1	C	65	ARG
1	C	79	ARG
1	C	103	VAL
1	C	169	ARG
1	C	182	THR
1	C	193	ARG
1	C	198	ASP
1	C	228	MET
1	C	238	ASP
1	C	240	THR
1	C	260	HIS
1	C	272	LEU
1	C	274	TRP
2	D	11	SER
2	D	23	LEU
2	D	44	LYS
2	D	52	SER
2	D	55	SER

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Mol	Chain	Res	Type
4	F	67	LYS
4	F	75	SER
4	F	109	ARG
4	F	116	SER
4	F	165	SER
4	F	176	SER
4	F	193	PRO
4	F	200	ASN
4	F	212	LYS
4	F	213	LYS
5	G	17	ASP
5	G	50	SER
5	G	60	ASP
5	G	61	ARG
5	G	70	ASP
5	G	80	SER
5	G	108	ARG
5	G	116	SER
5	G	121	SER
5	G	182	THR
5	G	203	SER
4	H	2	VAL
4	H	99	SER
4	H	100	THR
4	H	109	ARG
4	H	124	SER
4	H	157	THR
4	H	200	ASN
5	L	2	THR
5	L	3	THR
5	L	39	LYS
5	L	42	GLN
5	L	79	GLN
5	L	93	SER
5	L	102	THR
5	L	107	LYS
5	L	110	ASP
5	L	116	SER
5	L	121	SER
5	L	126	THR
5	L	147	LYS
5	L	162	SER

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Mol	Chain	Res	Type
5	L	169	LYS
5	L	182	THR
5	L	183	LYS
5	L	191	SER
5	L	212	ASN
3	P	7	PHE

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

Mol	Chain	Res	Type
1	A	191	HIS
2	B	24	ASN
1	C	191	HIS
1	C	263	HIS
5	G	42	GLN
5	G	77	ASN
5	G	210	ASN
5	L	92	HIS
5	L	137	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	C	301	-	3,3,3	0.46	0	2,2,2	0.29	0
7	GOL	F	301	-	5,5,5	0.85	0	5,5,5	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	301	-	-	0/1/1/1	-
7	GOL	F	301	-	-	0/4/4/4	-

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	273/273 (100%)	0.07	1 (0%) 92 91	25, 62, 109, 145	1 (0%)
1	C	273/273 (100%)	0.22	8 (2%) 51 41	42, 67, 110, 139	0
2	B	99/99 (100%)	-0.01	0 100 100	30, 50, 69, 89	1 (1%)
2	D	99/99 (100%)	0.64	11 (11%) 5 3	48, 88, 133, 160	0
3	E	10/10 (100%)	-0.11	0 100 100	47, 54, 65, 81	0
3	P	10/10 (100%)	0.15	0 100 100	55, 59, 71, 72	0
4	F	211/215 (98%)	0.20	10 (4%) 31 22	28, 49, 128, 172	0
4	H	206/215 (95%)	0.61	34 (16%) 1 1	24, 43, 124, 161	5 (2%)
5	G	213/213 (100%)	0.67	19 (8%) 9 5	53, 91, 125, 152	3 (1%)
5	L	206/213 (96%)	0.90	40 (19%) 1 0	39, 98, 141, 177	2 (0%)
All	All	1600/1620 (98%)	0.40	123 (7%) 13 7	24, 70, 127, 177	12 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	187	VAL	4.7
4	H	198	THR	4.1
5	G	106	ILE	4.1
5	L	117	ILE	4.1
4	H	166	GLY	3.9
5	G	200	THR	3.8
2	D	99	MET	3.7
5	L	137	ASN	3.7
5	L	175	MET	3.7
5	G	112	ALA	3.6
5	L	204	PRO	3.6
4	F	143	GLY	3.6
4	H	215	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
4	H	130	PRO	3.5
5	L	198	HIS	3.4
4	H	213	LYS	3.4
4	H	183	SER	3.4
4	H	142	LEU	3.3
4	F	186	THR	3.3
4	H	158	TRP	3.3
5	L	196	ALA	3.2
5	G	190	ASN	3.2
1	C	184	PRO	3.2
4	F	214	ILE	3.2
4	F	128	LEU	3.1
1	C	165	VAL	3.1
4	H	194	SER	3.1
2	D	79	ALA	3.1
5	L	193	THR	3.1
5	G	212	ASN	3.1
2	D	23	LEU	3.1
5	L	181	LEU	3.1
4	H	188	THR	3.1
5	L	144	ILE	3.0
5	L	177	SER	3.0
5	L	130	ALA	3.0
5	L	192	TYR	3.0
5	L	194	CYS	3.0
4	H	197	ILE	3.0
4	H	193	PRO	2.9
5	L	134	CYS	2.9
1	C	171	TYR	2.9
2	D	78	TYR	2.9
5	L	127	SER	2.9
1	A	109	LEU	2.9
4	F	187	VAL	2.9
4	F	199	CYS	2.9
4	F	197	ILE	2.9
5	L	106	ILE	2.8
4	H	199	CYS	2.8
5	L	140	TYR	2.8
4	H	208	THR	2.8
1	C	183	ASP	2.7
5	L	156	GLN	2.7
5	L	148	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
5	L	135	PHE	2.7
5	L	136	LEU	2.7
5	L	105	GLU	2.6
5	G	197	THR	2.6
5	L	155	ARG	2.6
5	L	80	SER	2.6
5	G	104	LEU	2.6
5	L	168	SER	2.6
4	H	186	THR	2.6
5	G	150	ILE	2.6
5	L	161	ASN	2.6
4	H	169	THR	2.5
4	H	184	SER	2.5
5	G	62	PHE	2.5
5	G	189	HIS	2.5
2	D	70	PHE	2.5
4	H	143	GLY	2.5
4	H	140	VAL	2.5
5	L	118	PHE	2.5
4	H	155	THR	2.4
4	H	154	VAL	2.4
5	L	210	ASN	2.4
4	H	144	CYS	2.4
5	L	206	VAL	2.4
5	L	200	THR	2.4
4	H	156	LEU	2.4
5	G	23	CYS	2.4
1	C	59	TYR	2.3
2	D	47	PRO	2.3
5	G	127	SER	2.3
5	L	145	ASN	2.3
5	G	206	VAL	2.3
5	G	136	LEU	2.3
5	L	123	GLU	2.3
4	F	142	LEU	2.3
4	H	128	LEU	2.3
2	D	74	GLU	2.3
2	D	68	THR	2.2
5	L	153	SER	2.2
5	L	197	THR	2.2
4	H	212	LYS	2.2
4	H	202	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
5	G	76	SER	2.2
5	L	7	THR	2.2
5	L	163	TRP	2.2
5	G	18	ARG	2.2
2	D	58	LYS	2.2
5	G	118	PHE	2.2
2	D	75	THR	2.2
4	F	140	VAL	2.2
5	L	149	LYS	2.2
4	H	121	THR	2.2
4	H	180	THR	2.1
2	D	98	ASP	2.1
5	G	2	THR	2.1
1	C	179	LEU	2.1
4	H	147	LYS	2.1
5	L	133	VAL	2.1
1	C	105	SER	2.1
5	G	143	ASP	2.1
4	H	209	LYS	2.0
4	H	181	LEU	2.0
4	H	101	ALA	2.0
5	L	205	ILE	2.0
4	F	129	ALA	2.0
4	H	160	SER	2.0
5	L	178	THR	2.0
1	C	215	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	F	301	6/6	0.71	0.33	41,44,50,50	0
6	EDO	C	301	4/4	0.92	0.12	62,64,66,68	0

6.5 Other polymers (i)

There are no such residues in this entry.