Full wwPDB X-ray Structure Validation Report (i)

Mar 11, 2024 – 01:58 PM EDT

PDB ID	:	8TQ8
Title	:	Crystal structure of Fab.34.5.8 in complex with MHC-I (H2-Dd)
Authors	:	Jiang, J.; Boyd, L.F.; Natarajan, K.; Margulies, D.H.
Deposited on	:	2023-08-06
Resolution	:	2.69 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 (1)) were used in the production of this report:

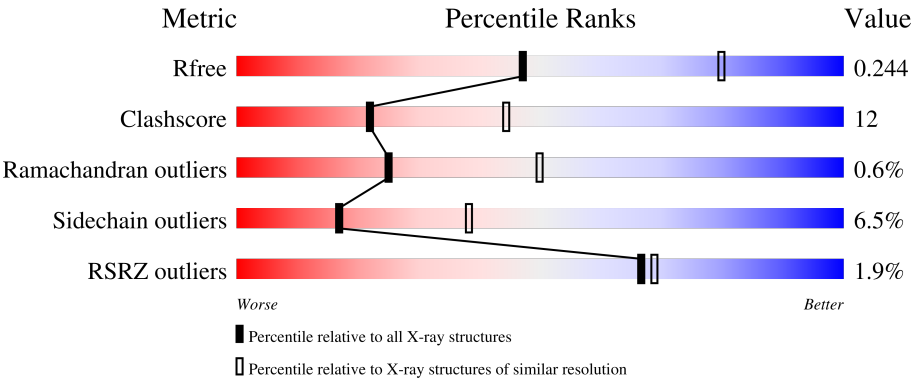
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	74% 25% .
1	C	273	75% 24% .
2	B	99	68% 30% .
2	D	99	73% 22% . .
3	E	10	80% 20%

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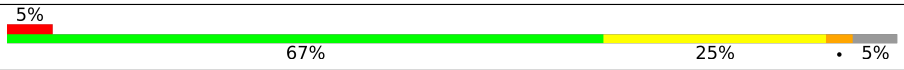
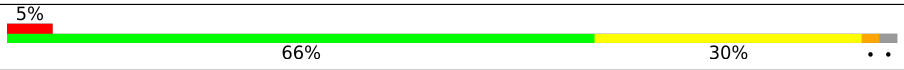
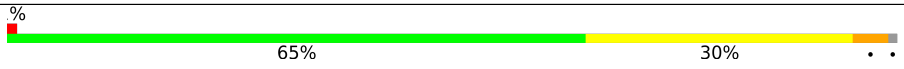
Mol	Chain	Length	Quality of chain
3	P	10	
4	F	219	
4	H	219	
5	G	219	
5	L	219	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12558 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	1	0	0
			2231	1403	405	414	9			
1	C	273	Total	C	N	O	S	1	0	0
			2236	1404	405	418	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	0	0	0
			817	523	138	149	7			
2	D	98	Total	C	N	O	S	0	0	0
			812	519	137	150	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	engineered mutation	UNP P01887
D	85	ASP	ALA	engineered mutation	UNP P01887

- Molecule 3 is a protein called Transmembrane protein gp41.

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

- Molecule 4 is a protein called Fab.34.5.8 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	207	Total	C	N	O	S	27	0	0
			1482	939	239	296	8			

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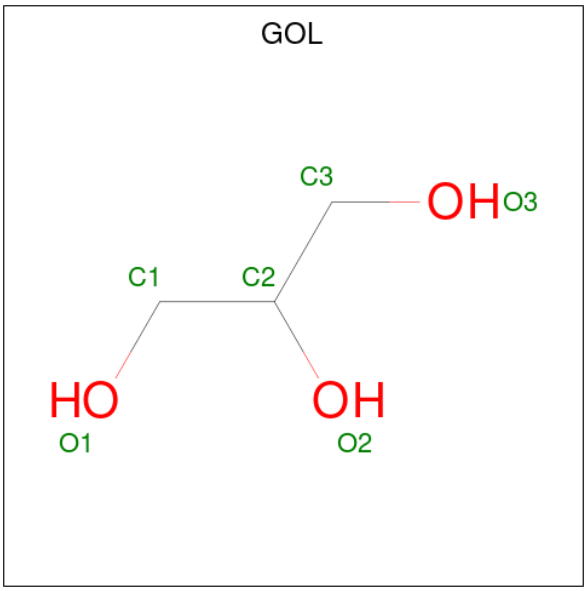
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	201	Total	C	N	O	S	9	0	0
			1462	930	234	289	9			

- Molecule 5 is a protein called Fab.34.5.8 Light chain.

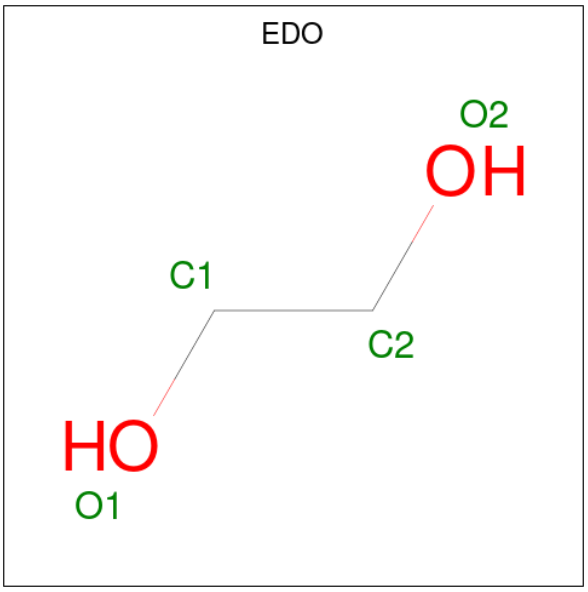
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	217	Total	C	N	O	S	6	0	0
			1628	1010	283	328	7			
5	G	215	Total	C	N	O	S	20	0	0
			1573	970	277	320	6			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	33	Total O 33 33	0	0
8	B	8	Total O 8 8	0	0
8	H	12	Total O 12 12	0	0
8	L	9	Total O 9 9	0	0
8	C	25	Total O 25 25	0	0
8	D	14	Total O 14 14	0	0
8	E	1	Total O 1 1	0	0
8	F	18	Total O 18 18	0	0
8	G	3	Total O 3 3	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

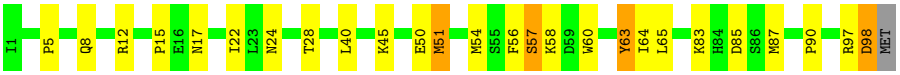
Chain C:

• Molecule 2: Beta-2-microglobulin

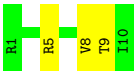
Chain B:

• Molecule 2: Beta-2-microglobulin

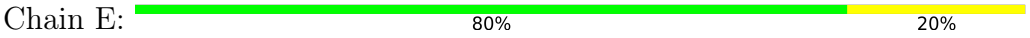
Chain D:



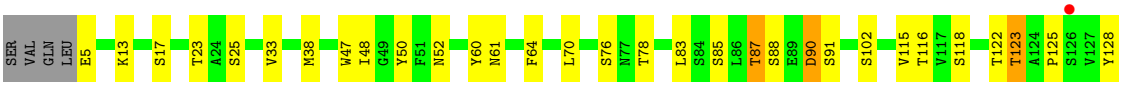
• Molecule 3: Transmembrane protein gp41

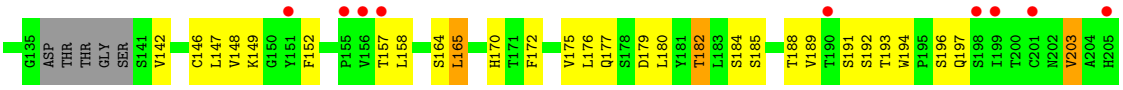


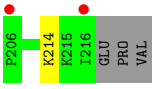
• Molecule 3: Transmembrane protein gp41



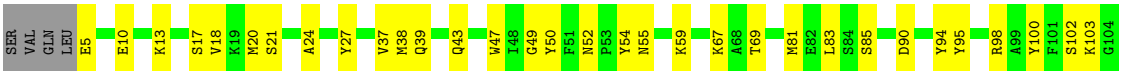
• Molecule 4: Fab.34.5.8 Heavy chain

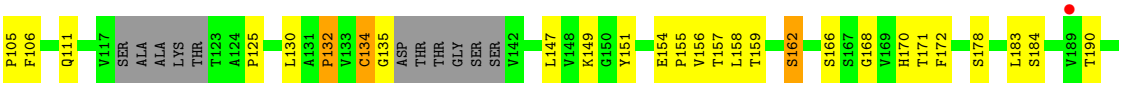


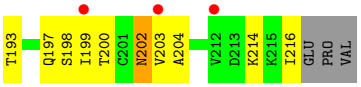




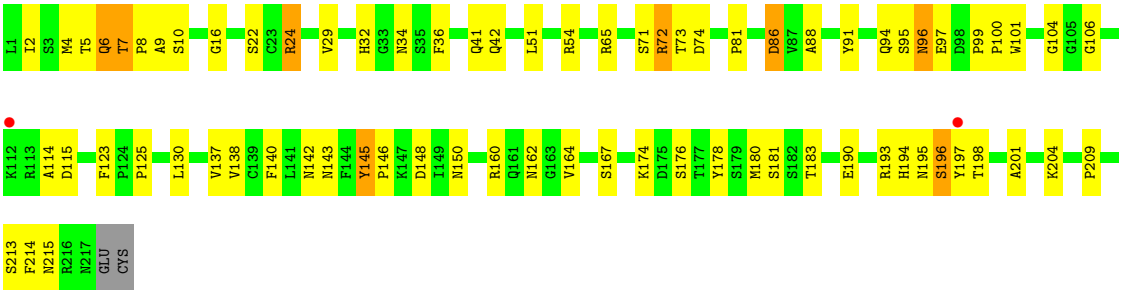
• Molecule 4: Fab.34.5.8 Heavy chain





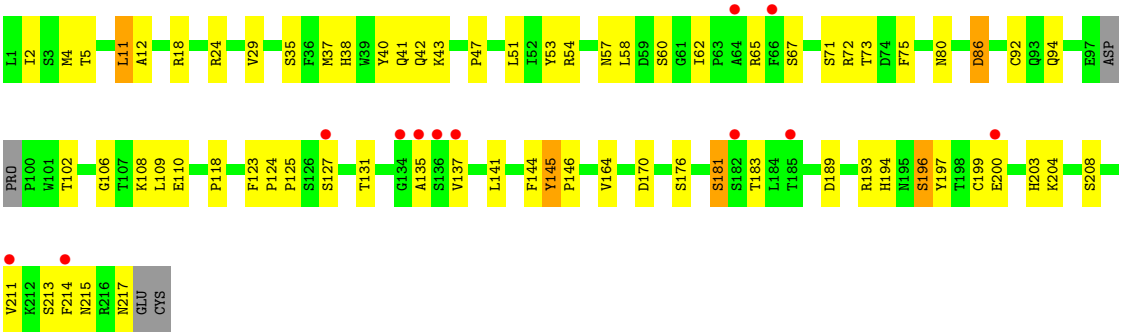


• Molecule 5: Fab.34.5.8 Light chain



• Molecule 5: Fab.34.5.8 Light chain

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	87.09Å 50.89Å 224.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.09 – 2.69 87.09 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.4 (87.09-2.69) 97.4 (87.09-2.69)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.201 , 0.242 0.213 , 0.244	Depositor DCC
R_{free} test set	2706 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.410 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12558	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: GOL, EDO

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	0.31	0/2294	0.57	0/3116
1	C	0.33	0/2299	0.56	0/3124
2	B	0.29	0/843	0.53	0/1144
2	D	0.27	0/838	0.52	0/1138
3	E	0.27	0/77	0.61	0/101
3	P	0.30	0/77	0.64	0/101
4	F	0.28	0/1501	0.51	0/2049
4	H	0.28	0/1519	0.51	0/2075
5	G	0.27	0/1610	0.55	0/2199
5	L	0.39	0/1668	0.62	0/2277
All	All	0.31	0/12726	0.55	0/17324

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	2231	0	2094	50	0
1	C	2236	0	2096	46	0
2	B	817	0	794	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	812	0	787	14	0
3	E	76	0	82	2	0
3	P	76	0	82	5	0
4	F	1462	0	1348	37	0
4	H	1482	0	1380	44	0
5	G	1573	0	1397	45	0
5	L	1628	0	1503	59	0
6	A	12	0	16	0	0
6	D	12	0	16	0	0
6	H	6	0	8	0	0
7	B	4	0	6	0	0
7	C	4	0	6	0	0
7	F	4	0	6	0	0
8	A	33	0	0	4	0
8	B	8	0	0	0	0
8	C	25	0	0	3	0
8	D	14	0	0	1	0
8	E	1	0	0	0	0
8	F	18	0	0	0	0
8	G	3	0	0	0	0
8	H	12	0	0	2	0
8	L	9	0	0	0	0
All	All	12558	0	11621	282	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (282) 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)
5:L:24:ARG:HB3	5:L:24:ARG:HH11	1.12	1.10
5:G:4:MET:HA	5:G:24:ARG:O	1.56	1.04
5:G:196:SER:HA	5:G:214:PHE:O	1.68	0.93
5:L:196:SER:HA	5:L:214:PHE:O	1.70	0.89
5:L:24:ARG:HB3	5:L:24:ARG:NH1	1.88	0.88
5:L:96:ASN:O	5:L:96:ASN:ND2	2.08	0.85
5:L:29:VAL:HG12	5:L:94:GLN:HG3	1.60	0.84
5:L:201:ALA:O	5:L:209:PRO:HA	1.81	0.80
1:C:44:ARG:HD2	1:C:64:THR:HG21	1.63	0.80
5:L:24:ARG:HH11	5:L:24:ARG:CB	1.95	0.79
4:H:50:TYR:HE2	5:L:97:GLU:OE2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:193:THR:HG23	4:F:197:GLN:HB2	1.66	0.77
5:L:2:ILE:HG13	5:L:99:PRO:HG2	1.67	0.77
5:L:7:THR:HG23	5:L:22:SER:HB3	1.66	0.76
4:F:154:GLU:OE1	4:F:155:PRO:HA	1.86	0.75
5:G:118:PRO:HB3	5:G:144:PHE:HB3	1.67	0.75
5:G:65:ARG:NH1	5:G:86:ASP:OD2	2.20	0.74
4:H:50:TYR:CE2	5:L:97:GLU:OE2	2.41	0.73
2:D:28:THR:HG22	2:D:63:TYR:HB2	1.71	0.73
5:L:6:GLN:HE22	5:L:91:TYR:HA	1.51	0.73
4:F:5:GLU:HA	4:F:111:GLN:HE22	1.54	0.72
4:F:159:THR:OG1	4:F:202:ASN:ND2	2.22	0.71
2:D:24:ASN:HB3	2:D:65:LEU:HD21	1.73	0.70
5:G:200:GLU:HG2	5:G:211:VAL:HG12	1.74	0.70
5:L:198:THR:HG23	5:L:213:SER:HB3	1.74	0.70
1:A:35:ARG:HD3	1:A:48:ARG:HH11	1.56	0.70
1:A:124:ILE:HD11	1:A:133:TRP:HB3	1.72	0.70
1:C:77:ASP:OD2	3:E:5:ARG:NH1	2.25	0.69
1:A:133:TRP:HB2	1:A:144:ARG:HG3	1.76	0.68
2:B:41:LYS:NZ	2:B:76:ASP:OD1	2.26	0.68
4:H:176:LEU:HD12	4:H:179:ASP:HA	1.76	0.68
4:H:158:LEU:HD23	4:H:203:VAL:HG13	1.76	0.68
5:G:41:GLN:HB2	5:G:51:LEU:HD11	1.76	0.67
5:G:125:PRO:HD3	5:G:137:VAL:HG22	1.77	0.67
1:C:45:TYR:HE2	1:C:67:ALA:HB2	1.60	0.67
4:F:125:PRO:HB3	4:F:151:TYR:HB3	1.77	0.66
1:C:131:LYS:NZ	8:C:402:HOH:O	2.29	0.65
4:H:175:VAL:HG22	4:H:182:THR:HG22	1.79	0.64
4:H:33:VAL:HG12	4:H:52:ASN:HA	1.80	0.64
1:C:45:TYR:CE2	1:C:67:ALA:HB2	2.33	0.64
2:D:83:LYS:HG3	2:D:90:PRO:HG3	1.80	0.64
4:H:142:VAL:O	4:H:188:THR:HA	1.97	0.63
2:D:98:ASP:N	2:D:98:ASP:OD1	2.32	0.63
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.30	0.62
1:A:170:ARG:NH1	8:A:404:HOH:O	2.32	0.62
4:F:17:SER:HA	4:F:83:LEU:O	2.00	0.61
4:F:52:ASN:ND2	4:F:55:ASN:OD1	2.31	0.61
5:L:41:GLN:HB2	5:L:51:LEU:HD11	1.82	0.61
4:H:61:ASN:HB3	4:H:64:PHE:HD2	1.64	0.61
2:B:16:GLU:HB2	2:B:19:LYS:HE2	1.82	0.61
1:C:194:ARG:HD3	1:C:198:ASP:HB2	1.83	0.60
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:7:THR:CG2	5:L:22:SER:HB3	2.31	0.60
4:H:87:THR:OG1	4:H:88:SER:N	2.34	0.59
4:F:132:PRO:HG3	5:G:123:PHE:HA	1.83	0.59
4:H:147:LEU:HD22	5:L:138:VAL:HG21	1.85	0.59
1:C:173:LYS:NZ	1:C:174:ASN:OD1	2.23	0.59
4:H:125:PRO:HA	4:H:149:LYS:O	2.03	0.59
4:F:199:ILE:O	4:F:216:ILE:C	2.42	0.59
5:G:127:SER:O	5:G:131:THR:HG23	2.02	0.58
1:C:141:GLN:NE2	8:C:405:HOH:O	2.36	0.58
5:L:145:TYR:HD1	5:L:146:PRO:HA	1.68	0.58
1:C:194:ARG:HH11	1:C:198:ASP:HB2	1.68	0.58
2:D:15:PRO:HG3	2:D:97:ARG:HB3	1.86	0.58
3:P:5:ARG:HH22	3:P:9:THR:HA	1.69	0.57
4:F:166:SER:O	4:F:166:SER:OG	2.22	0.57
2:B:7:ILE:HG12	2:B:82:VAL:HG21	1.86	0.57
5:L:2:ILE:CG1	5:L:99:PRO:HG2	2.33	0.57
1:C:218:GLN:HA	1:C:223:GLU:HA	1.87	0.57
1:C:234:ARG:NH1	2:D:8:GLN:OE1	2.30	0.57
5:L:65:ARG:NH2	5:L:86:ASP:OD1	2.38	0.56
5:L:95:SER:OG	5:L:95:SER:O	2.15	0.56
4:H:192:SER:O	4:H:196:SER:OG	2.23	0.56
1:A:266:LEU:HD13	1:A:270:LEU:HD13	1.87	0.56
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.87	0.56
4:H:5:GLU:N	8:H:401:HOH:O	2.38	0.56
1:A:242:GLN:HE22	2:B:12:ARG:HA	1.71	0.56
5:L:123:PHE:HB2	5:L:138:VAL:HG22	1.88	0.56
5:L:196:SER:H	5:L:215:ASN:HA	1.70	0.56
1:C:214:THR:HB	1:C:262:GLU:HB2	1.87	0.56
1:C:219:LEU:HD11	1:C:256:LYS:HE2	1.88	0.56
2:D:51:MET:HG3	2:D:64:ILE:HD11	1.88	0.55
4:H:76:SER:OG	4:H:78:THR:OG1	2.21	0.55
5:L:36:PHE:HD2	5:L:96:ASN:OD1	1.90	0.55
1:C:191:HIS:NE2	1:C:199:VAL:HG11	2.22	0.55
4:F:39:GLN:HE21	5:G:42:GLN:HE22	1.55	0.55
4:H:17:SER:HA	4:H:83:LEU:O	2.07	0.55
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.89	0.54
1:A:187:ALA:HA	1:A:204:TRP:O	2.07	0.54
4:F:162:SER:H	4:F:202:ASN:HD21	1.54	0.54
5:L:140:PHE:CE1	5:L:181:SER:HB2	2.43	0.54
5:L:29:VAL:CG1	5:L:94:GLN:HG3	2.33	0.54
1:A:224:LEU:HD21	1:A:227:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:O	1:A:149:GLN:HG2	2.09	0.53
2:D:12:ARG:HG2	2:D:22:ILE:HD12	1.90	0.53
1:A:206:LEU:HD13	2:B:14:PRO:HD3	1.90	0.53
5:G:38:HIS:HD2	5:G:54:ARG:H	1.55	0.53
5:G:118:PRO:HB2	5:G:141:LEU:HD12	1.91	0.53
5:G:196:SER:H	5:G:215:ASN:HA	1.73	0.53
2:B:29:GLN:HA	2:B:61:SER:HB2	1.91	0.52
5:L:145:TYR:CD1	5:L:146:PRO:HA	2.44	0.52
4:F:157:THR:O	4:F:203:VAL:HA	2.09	0.52
4:H:193:THR:HG23	4:H:197:GLN:HB3	1.90	0.52
4:H:170:HIS:HB3	4:H:172:PHE:CZ	2.45	0.52
1:C:78:LEU:HG	1:C:95:LEU:HD12	1.92	0.52
1:A:206:LEU:HD23	1:A:242:GLN:HG2	1.92	0.52
1:C:71:GLU:O	1:C:75:ARG:HG3	2.10	0.52
1:C:110:LEU:HD12	4:F:102:SER:HB3	1.91	0.52
5:G:29:VAL:HG22	5:G:94:GLN:HG3	1.93	0.51
4:H:128:TYR:HB2	4:H:147:LEU:HD23	1.92	0.51
5:L:6:GLN:OE1	5:L:106:GLY:N	2.36	0.51
1:A:252:GLY:O	1:A:255:GLN:NE2	2.40	0.51
1:A:21:ARG:NH2	1:A:37:ASP:OD2	2.42	0.51
5:L:16:GLY:HA2	5:L:81:PRO:HB2	1.92	0.51
1:C:169:ARG:NH1	8:C:403:HOH:O	2.35	0.51
1:A:14:ARG:NH2	8:A:410:HOH:O	2.45	0.50
5:G:215:ASN:ND2	5:G:217:ASN:O	2.44	0.50
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.50
1:C:187:ALA:HA	1:C:204:TRP:O	2.10	0.50
4:F:111:GLN:HA	5:G:47:PRO:HG3	1.93	0.50
4:H:123:THR:HG21	4:H:152:PHE:HB3	1.93	0.50
4:F:37:VAL:HG23	4:F:95:TYR:HB2	1.94	0.50
4:F:20:MET:HG2	4:F:81:MET:O	2.11	0.50
4:F:147:LEU:HD21	4:F:149:LYS:HD2	1.94	0.50
5:L:95:SER:HA	5:L:101:TRP:CD1	2.47	0.49
1:C:231:VAL:O	1:C:243:LYS:NZ	2.31	0.49
5:L:160:ARG:HH21	5:L:162:ASN:HB2	1.77	0.49
4:F:52:ASN:HD21	4:F:54:TYR:HB3	1.77	0.49
1:A:9:VAL:HG13	1:A:24:GLU:HG3	1.93	0.49
5:G:41:GLN:HE22	5:G:43:LYS:HE3	1.78	0.49
5:G:194:HIS:HB3	5:G:197:TYR:HE1	1.77	0.49
4:F:67:LYS:NZ	4:F:85:SER:O	2.42	0.49
5:G:2:ILE:H	5:G:102:THR:HG21	1.77	0.49
1:A:218:GLN:OE1	1:A:260:HIS:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:NE2	8:A:407:HOH:O	2.34	0.49
4:F:156:VAL:HA	4:F:204:ALA:O	2.13	0.49
5:L:42:GLN:O	5:L:88:ALA:HB1	2.13	0.49
5:G:53:TYR:O	5:G:57:ASN:HB2	2.12	0.48
5:G:108:LYS:HD2	5:G:109:LEU:N	2.28	0.48
5:L:71:SER:OG	5:L:72:ARG:N	2.46	0.48
2:D:57:SER:OG	2:D:58:LYS:N	2.46	0.48
4:F:132:PRO:HG3	5:G:124:PRO:HD3	1.95	0.48
1:A:176:ASN:OD1	1:A:180:LEU:HD12	2.13	0.48
5:G:71:SER:O	5:G:73:THR:N	2.46	0.48
4:H:147:LEU:HD13	5:L:140:PHE:HZ	1.79	0.48
1:C:9:VAL:HG22	1:C:24:GLU:HG2	1.96	0.48
4:H:147:LEU:HD13	5:L:140:PHE:CZ	2.49	0.47
5:G:196:SER:O	5:G:196:SER:OG	2.30	0.47
1:A:106:ASP:HB2	4:H:52:ASN:ND2	2.29	0.47
1:C:25:VAL:HG21	2:D:54:MET:O	2.14	0.47
5:L:114:ALA:HB1	5:L:204:LYS:HD3	1.94	0.47
1:C:191:HIS:CD2	1:C:199:VAL:HG11	2.50	0.47
1:C:182:THR:O	1:C:182:THR:OG1	2.31	0.47
4:F:134:CYS:SG	4:F:135:GLY:N	2.87	0.47
3:P:5:ARG:NH1	3:P:8:VAL:O	2.35	0.47
1:A:199:VAL:HG23	1:A:251:LEU:HD23	1.97	0.47
4:F:193:THR:O	4:F:197:GLN:N	2.39	0.47
5:G:118:PRO:CB	5:G:144:PHE:HB3	2.39	0.47
5:G:196:SER:CA	5:G:214:PHE:O	2.53	0.47
1:A:193:ARG:HB3	1:C:17:PHE:CD1	2.50	0.47
4:H:90:ASP:N	4:H:90:ASP:OD1	2.47	0.47
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.50	0.46
5:L:7:THR:HG23	5:L:22:SER:CB	2.40	0.46
1:A:217:TRP:NE1	1:A:245:ALA:O	2.44	0.46
1:C:66:ARG:NH1	3:E:3:PRO:O	2.44	0.46
5:L:125:PRO:HD3	5:L:137:VAL:HG22	1.97	0.46
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.50	0.46
4:H:164:SER:OG	4:H:165:LEU:N	2.47	0.46
4:F:105:PRO:HB3	5:G:38:HIS:CD2	2.51	0.46
1:A:49:ALA:O	1:A:52:ILE:HG22	2.16	0.46
1:C:132:THR:HG21	5:G:60:SER:HB3	1.98	0.46
5:G:58:LEU:HD22	5:G:62:ILE:HB	1.98	0.46
1:A:71:GLU:O	1:A:75:ARG:HG3	2.17	0.45
1:C:203:CYS:O	1:C:244:TRP:HA	2.15	0.45
2:D:5:PRO:HD2	2:D:87:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.97	0.45
2:B:33:PRO:HB3	2:B:62:PHE:CZ	2.51	0.45
4:H:170:HIS:O	4:H:185:SER:HA	2.16	0.45
5:L:8:PRO:HB2	5:L:9:ALA:H	1.63	0.45
1:C:198:ASP:HB3	1:C:248:VAL:HG13	1.96	0.45
5:G:18:ARG:HG3	5:G:80:ASN:ND2	2.32	0.45
2:B:4:THR:HA	2:B:86:SER:OG	2.16	0.45
5:L:71:SER:O	5:L:73:THR:N	2.50	0.45
5:L:195:ASN:O	5:L:196:SER:OG	2.30	0.45
1:C:14:ARG:HB3	1:C:17:PHE:HB2	1.98	0.45
4:H:172:PHE:CZ	5:L:142:ASN:HB3	2.51	0.45
1:A:108:ARG:HB3	4:H:102:SER:HB2	1.99	0.45
2:D:40:LEU:HD23	2:D:45:LYS:HA	1.98	0.45
1:A:112:GLY:O	8:A:401:HOH:O	2.20	0.45
4:H:148:VAL:HG21	4:H:203:VAL:HG11	1.98	0.45
4:F:158:LEU:HA	4:F:202:ASN:O	2.17	0.45
1:C:176:ASN:HA	1:C:180:LEU:HD12	1.98	0.44
5:L:196:SER:CA	5:L:214:PHE:O	2.55	0.44
1:C:196:GLU:OE1	1:C:196:GLU:N	2.50	0.44
5:G:12:ALA:HA	5:G:110:GLU:O	2.18	0.44
5:G:38:HIS:CD2	5:G:54:ARG:H	2.34	0.44
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.82	0.44
4:H:85:SER:O	4:H:85:SER:OG	2.34	0.44
5:L:164:VAL:HA	5:L:183:THR:O	2.17	0.44
1:C:193:ARG:HG3	1:C:199:VAL:HG22	1.99	0.44
1:A:106:ASP:OD2	1:A:108:ARG:NH2	2.48	0.44
4:H:38:MET:HB3	4:H:48:ILE:HD11	1.99	0.44
4:H:214:LYS:HA	4:H:214:LYS:HD3	1.62	0.44
5:G:164:VAL:HA	5:G:183:THR:O	2.17	0.44
2:B:17:ASN:HD21	2:B:74:GLU:N	2.16	0.44
4:H:142:VAL:HB	4:H:189:VAL:HG22	1.99	0.44
5:L:2:ILE:HG13	5:L:99:PRO:CG	2.44	0.44
1:C:185:PRO:HB3	1:C:208:PHE:HB3	1.99	0.44
5:L:174:LYS:HE2	5:L:174:LYS:HB3	1.90	0.44
1:A:130:LEU:HD13	1:A:157:ARG:HG3	2.00	0.43
4:H:175:VAL:CG2	5:L:167:SER:HB2	2.48	0.43
4:F:38:MET:HB2	4:F:94:TYR:CE2	2.53	0.43
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.53	0.43
4:H:61:ASN:ND2	8:H:402:HOH:O	2.50	0.43
1:C:253:LYS:O	1:C:256:LYS:HB2	2.19	0.43
4:F:106:PHE:O	5:G:40:TYR:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:HB3	1:A:113:TYR:HE1	1.82	0.43
1:A:77:ASP:OD1	3:P:9:THR:HB	2.19	0.43
1:A:76:VAL:HG11	3:P:9:THR:HG21	2.01	0.43
1:A:95:LEU:HD23	1:A:117:ALA:O	2.18	0.43
1:A:207:GLY:HA2	2:B:12:ARG:HH12	1.84	0.43
1:C:138:MET:HA	1:C:141:GLN:HG3	2.00	0.43
5:G:11:LEU:HD23	5:G:11:LEU:HA	1.84	0.43
4:H:5:GLU:N	4:H:23:THR:O	2.52	0.43
5:L:190:GLU:HG2	5:L:193:ARG:HH21	1.83	0.43
1:C:5:LEU:HB2	1:C:168:LEU:HD13	2.00	0.43
1:C:155:ARG:NE	1:C:156:ASP:OD1	2.52	0.43
5:L:6:GLN:HE22	5:L:91:TYR:CA	2.24	0.42
4:H:177:GLN:O	4:H:180:LEU:HB2	2.19	0.42
4:F:52:ASN:ND2	4:F:55:ASN:H	2.17	0.42
1:A:218:GLN:HB3	1:A:223:GLU:HA	2.01	0.42
2:B:40:LEU:HD11	2:B:81:ARG:HB2	2.01	0.42
4:H:184:SER:HB2	5:L:140:PHE:CD1	2.55	0.42
5:G:37:MET:HE1	5:G:92:CYS:HB2	2.00	0.42
1:C:14:ARG:CB	1:C:17:PHE:HB2	2.49	0.42
5:G:35:SER:O	5:G:54:ARG:HD3	2.19	0.42
5:L:194:HIS:HB2	5:L:197:TYR:HE1	1.84	0.42
4:F:24:ALA:HB1	4:F:27:TYR:CE1	2.54	0.42
5:G:145:TYR:HD1	5:G:146:PRO:HA	1.85	0.42
1:A:185:PRO:HB3	1:A:208:PHE:HB3	2.01	0.42
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.79	0.42
3:P:5:ARG:NH2	3:P:9:THR:HA	2.35	0.42
1:C:216:THR:OG1	1:C:260:HIS:HB2	2.19	0.42
5:G:203:HIS:CG	5:G:204:LYS:N	2.87	0.42
1:A:234:ARG:NH2	2:B:8:GLN:HB3	2.35	0.41
5:L:4:MET:O	5:L:104:GLY:HA2	2.20	0.41
1:C:55:GLU:OE2	1:C:170:ARG:NH2	2.40	0.41
4:F:199:ILE:HG22	4:F:200:THR:H	1.84	0.41
5:G:125:PRO:HB3	5:G:135:ALA:HA	2.02	0.41
4:H:47:TRP:CZ3	5:L:100:PRO:HB2	2.55	0.41
1:C:13:SER:HA	1:C:20:PRO:HB3	2.01	0.41
1:C:24:GLU:HB2	1:C:36:PHE:HB3	2.00	0.41
4:F:10:GLU:HB3	4:F:18:VAL:HG11	2.01	0.41
2:B:79:ALA:HB2	2:B:94:TYR:CD1	2.54	0.41
4:H:147:LEU:HD22	5:L:138:VAL:CG2	2.49	0.41
5:L:180:MET:HG3	5:L:181:SER:N	2.35	0.41
4:H:175:VAL:HG21	5:L:167:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:OE2	5:L:54:ARG:NH1	2.54	0.41
2:B:83:LYS:HD2	2:B:90:PRO:HG3	2.03	0.41
5:L:148:ASP:OD1	5:L:148:ASP:N	2.54	0.41
4:F:43:GLN:NE2	5:G:106:GLY:O	2.53	0.41
5:G:189:ASP:O	5:G:193:ARG:HB2	2.21	0.41
1:A:108:ARG:HE	1:A:108:ARG:HB2	1.71	0.41
2:B:33:PRO:HB3	2:B:62:PHE:CE2	2.55	0.41
4:H:76:SER:O	4:H:78:THR:HG23	2.20	0.41
5:L:32:HIS:C	5:L:34:ASN:H	2.25	0.41
1:C:49:ALA:O	1:C:52:ILE:HG22	2.20	0.41
4:F:172:PHE:CZ	5:G:181:SER:HB3	2.56	0.41
5:G:4:MET:CA	5:G:24:ARG:O	2.46	0.41
1:A:111:ARG:HB3	1:A:113:TYR:CE1	2.56	0.41
4:H:60:TYR:CE1	4:H:70:LEU:HG	2.56	0.41
2:B:75:THR:HA	1:C:76:VAL:HG13	2.03	0.40
4:H:184:SER:HB2	5:L:140:PHE:CE1	2.56	0.40
2:D:12:ARG:NH1	8:D:204:HOH:O	2.54	0.40
1:A:231:VAL:HG21	1:A:234:ARG:NH2	2.36	0.40
4:F:50:TYR:CE2	4:F:59:LYS:HB3	2.56	0.40
4:F:183:LEU:HD23	4:F:184:SER:N	2.36	0.40
1:A:124:ILE:HD12	1:A:134:THR:O	2.22	0.40
4:H:91:SER:HA	4:H:115:VAL:O	2.21	0.40
4:F:47:TRP:CZ2	4:F:49:GLY:HA2	2.57	0.40
1:A:116:PHE:O	1:A:123:TYR:HB3	2.21	0.40
5:G:37:MET:HG3	5:G:75:PHE:CZ	2.55	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%)	263 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	271/273 (99%)	264 (97%)	7 (3%)	0	100	100
2	B	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	15	37
2	D	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
3	E	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	P	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	F	195/219 (89%)	175 (90%)	17 (9%)	3 (2%)	10	26
4	H	203/219 (93%)	170 (84%)	31 (15%)	2 (1%)	15	37
5	G	211/219 (96%)	196 (93%)	13 (6%)	2 (1%)	17	40
5	L	215/219 (98%)	195 (91%)	18 (8%)	2 (1%)	17	40
All	All	1575/1640 (96%)	1464 (93%)	101 (6%)	10 (1%)	25	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	122	THR
5	G	72	ARG
5	L	72	ARG
4	F	134	CYS
5	L	196	SER
2	B	47	PRO
4	H	194	TRP
5	G	196	SER
4	F	132	PRO
4	F	168	GLY

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%)	216 (96%)	9 (4%)	31	60
1	C	227/229 (99%)	219 (96%)	8 (4%)	36	65
2	B	93/94 (99%)	89 (96%)	4 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	93/94 (99%)	85 (91%)	8 (9%)	10 24
3	E	7/7 (100%)	7 (100%)	0	100 100
3	P	7/7 (100%)	7 (100%)	0	100 100
4	F	151/184 (82%)	135 (89%)	16 (11%)	6 15
4	H	154/184 (84%)	141 (92%)	13 (8%)	11 25
5	G	161/193 (83%)	150 (93%)	11 (7%)	16 36
5	L	176/193 (91%)	161 (92%)	15 (8%)	10 24
All	All	1294/1414 (92%)	1210 (94%)	84 (6%)	17 38

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	TYR
1	A	88	SER
1	A	103	VAL
1	A	132	THR
1	A	193	ARG
1	A	229	GLU
1	A	231	VAL
1	A	234	ARG
1	A	255	GLN
2	B	17	ASN
2	B	56	PHE
2	B	70	PHE
2	B	74	GLU
4	H	13	LYS
4	H	25	SER
4	H	87	THR
4	H	90	ASP
4	H	116	THR
4	H	118	SER
4	H	123	THR
4	H	146	CYS
4	H	157	THR
4	H	165	LEU
4	H	182	THR
4	H	191	SER
4	H	203	VAL
5	L	5	THR
5	L	6	GLN

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Mol	Chain	Res	Type
5	L	7	THR
5	L	10	SER
5	L	24	ARG
5	L	74	ASP
5	L	86	ASP
5	L	96	ASN
5	L	115	ASP
5	L	130	LEU
5	L	143	ASN
5	L	145	TYR
5	L	150	ASN
5	L	176	SER
5	L	178	TYR
1	C	6	ARG
1	C	45	TYR
1	C	86	ASN
1	C	146	LYS
1	C	155	ARG
1	C	182	THR
1	C	212	ASP
1	C	271	THR
2	D	17	ASN
2	D	50	GLU
2	D	51	MET
2	D	56	PHE
2	D	57	SER
2	D	63	TYR
2	D	85	ASP
2	D	98	ASP
4	F	13	LYS
4	F	21	SER
4	F	69	THR
4	F	90	ASP
4	F	98	ARG
4	F	100	TYR
4	F	103	LYS
4	F	130	LEU
4	F	162	SER
4	F	170	HIS
4	F	171	THR
4	F	178	SER
4	F	190	THR

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Mol	Chain	Res	Type
4	F	198	SER
4	F	202	ASN
4	F	214	LYS
5	G	5	THR
5	G	11	LEU
5	G	67	SER
5	G	86	ASP
5	G	145	TYR
5	G	170	ASP
5	G	176	SER
5	G	181	SER
5	G	199	CYS
5	G	208	SER
5	G	213	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
2	B	29	GLN
5	L	41	GLN
1	C	115	GLN
1	C	176	ASN
1	C	218	GLN
4	F	39	GLN
4	F	52	ASN
4	F	111	GLN
4	F	202	ASN
5	G	38	HIS
5	G	42	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	GOL	A	302	-	5,5,5	0.93	0	5,5,5	0.96	0
6	GOL	D	102	-	5,5,5	1.03	0	5,5,5	0.89	0
7	EDO	B	101	-	3,3,3	0.45	0	2,2,2	0.38	0
7	EDO	F	301	-	3,3,3	0.47	0	2,2,2	0.28	0
6	GOL	A	301	-	5,5,5	0.86	0	5,5,5	1.03	0
7	EDO	C	301	-	3,3,3	0.57	0	2,2,2	0.12	0
6	GOL	D	101	-	5,5,5	0.97	0	5,5,5	0.96	0
6	GOL	H	301	-	5,5,5	0.07	0	5,5,5	0.36	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	GOL	A	302	-	-	0/4/4/4	-
6	GOL	D	102	-	-	4/4/4/4	-
7	EDO	B	101	-	-	1/1/1/1	-
7	EDO	F	301	-	-	0/1/1/1	-
6	GOL	A	301	-	-	1/4/4/4	-
7	EDO	C	301	-	-	1/1/1/1	-
6	GOL	D	101	-	-	0/4/4/4	-
6	GOL	H	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	301	GOL	C1-C2-C3-O3
6	D	102	GOL	O1-C1-C2-C3
6	H	301	GOL	O1-C1-C2-C3
6	D	102	GOL	C1-C2-C3-O3
6	H	301	GOL	O2-C2-C3-O3
6	D	102	GOL	O1-C1-C2-O2
6	D	102	GOL	O2-C2-C3-O3
6	H	301	GOL	O1-C1-C2-O2
7	C	301	EDO	O1-C1-C2-O2
7	B	101	EDO	O1-C1-C2-O2
6	A	301	GOL	O1-C1-C2-C3

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%)	-0.37	1 (0%) 92 93	32, 48, 78, 110	1 (0%)
1	C	273/273 (100%)	-0.41	0 100 100	31, 47, 75, 96	0
2	B	99/99 (100%)	-0.45	0 100 100	33, 48, 65, 76	0
2	D	98/99 (98%)	-0.42	0 100 100	33, 50, 70, 81	0
3	E	10/10 (100%)	-0.28	0 100 100	30, 41, 50, 55	0
3	P	10/10 (100%)	-0.39	0 100 100	34, 41, 46, 47	0
4	F	199/219 (90%)	-0.04	4 (2%) 65 67	33, 66, 103, 120	0
4	H	204/219 (93%)	0.09	12 (5%) 22 21	33, 68, 103, 120	4 (1%)
5	G	212/219 (96%)	0.12	12 (5%) 23 22	41, 76, 111, 123	2 (0%)
5	L	216/219 (98%)	-0.17	2 (0%) 84 85	31, 70, 92, 106	1 (0%)
All	All	1594/1640 (97%)	-0.19	31 (1%) 66 69	30, 58, 100, 123	8 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	190	THR	4.6
5	G	66	PHE	4.5
4	H	206	PRO	4.5
4	H	201	CYS	4.4
4	F	212	VAL	4.2
4	H	156	VAL	3.8
4	F	203	VAL	3.6
5	G	137	VAL	3.4
5	L	112	LYS	3.4
1	A	197	GLY	3.3
5	G	136	SER	3.2
5	G	211	VAL	3.0
4	H	199	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
5	G	200	GLU	2.9
4	H	216	ILE	2.9
4	H	126	SER	2.9
5	G	127	SER	2.6
4	H	151	TYR	2.6
5	G	134	GLY	2.5
4	F	189	VAL	2.5
4	H	157	THR	2.4
5	G	64	ALA	2.4
5	G	135	ALA	2.4
5	G	185	THR	2.4
5	G	182	SER	2.2
5	G	214	PHE	2.1
4	H	155	PRO	2.1
4	H	205	HIS	2.1
4	H	198	SER	2.1
4	F	199	ILE	2.1
5	L	197	TYR	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	EDO	F	301	4/4	0.86	0.12	53,56,58,58	0
6	GOL	A	302	6/6	0.91	0.11	26,36,40,70	0
7	EDO	C	301	4/4	0.92	0.15	26,27,29,29	0
6	GOL	D	101	6/6	0.92	0.19	16,25,27,80	0
6	GOL	A	301	6/6	0.93	0.12	17,21,25,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	D	102	6/6	0.94	0.16	14,30,31,38	0
6	GOL	H	301	6/6	0.96	0.08	25,25,25,25	0
7	EDO	B	101	4/4	0.96	0.13	13,24,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.