



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:06 PM UTC

PDB ID : 8TQ7 / pdb_00008tq7
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

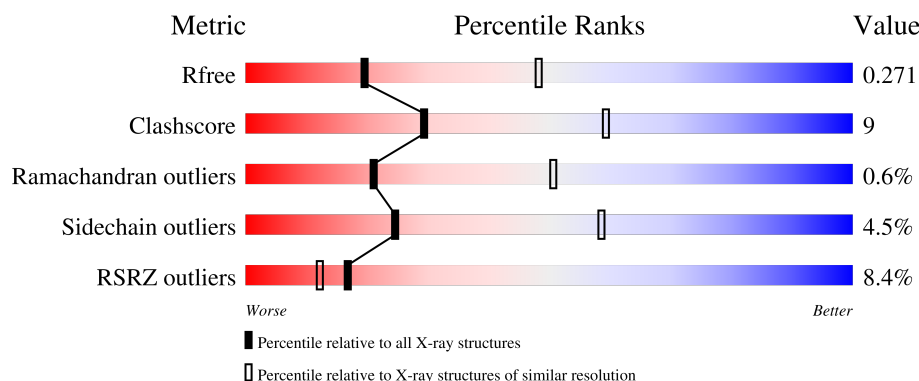
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	
1	C	273	
2	B	99	
2	D	99	
3	E	10	

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Mol	Chain	Length	Quality of chain
3	P	10	80%20%
4	F	215	7% 80%17%
4	H	215	8% 83%13%
5	G	213	9% 75%23%
5	L	213	23% 73%23%

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.

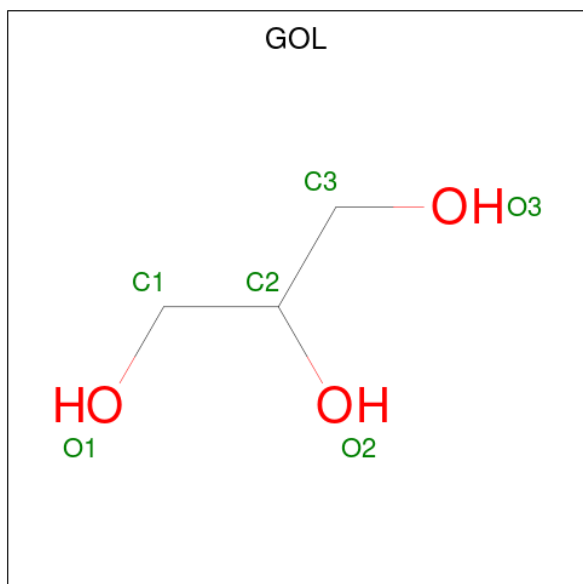
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	213	Total	C	N	O	S	1	0	0
			1630	1011	276	337	6			
5	L	209	Total	C	N	O	S	18	0	0
			1531	954	258	313	6			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

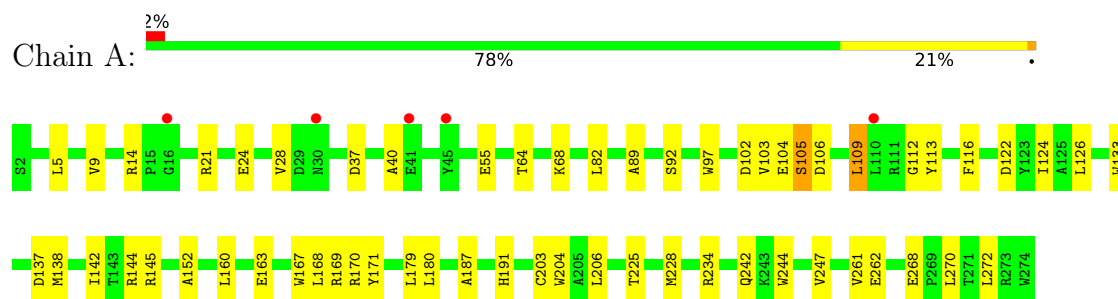
- Molecule 8 is water.

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

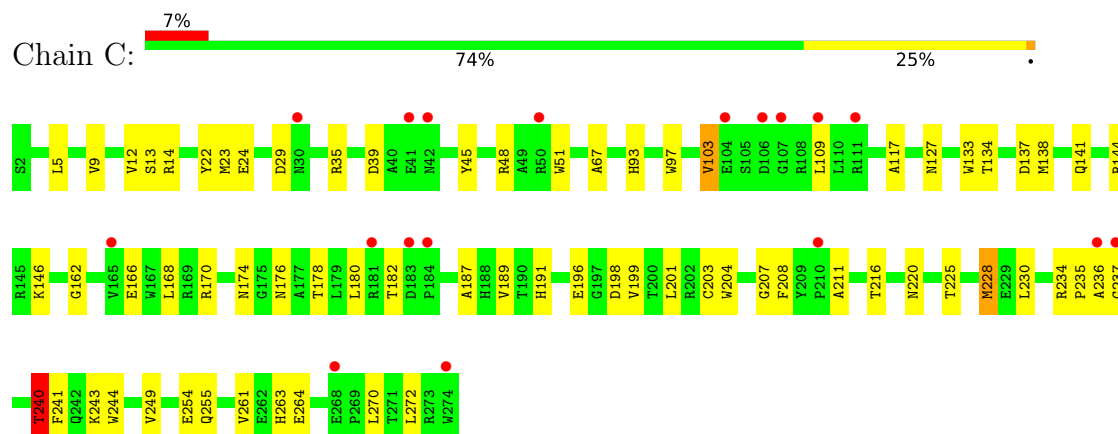
3 Residue-property plots

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.

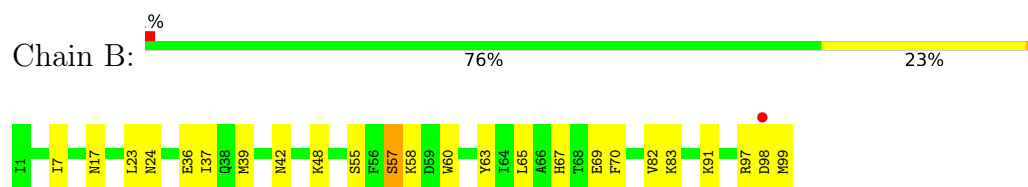
- Molecule 1: H-2 class I histocompatibility antigen, D-D alpha chain



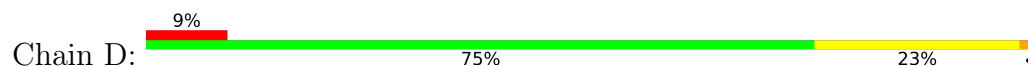
- Molecule 1: H-2 class I histocompatibility antigen, D-D alpha chain

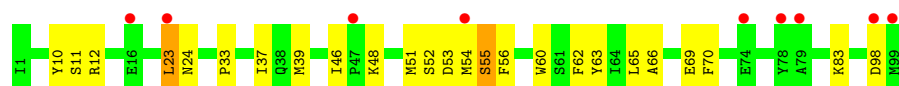


- Molecule 2: Beta-2-microglobulin

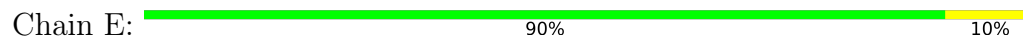


- Molecule 2: Beta-2-microglobulin

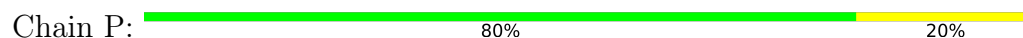




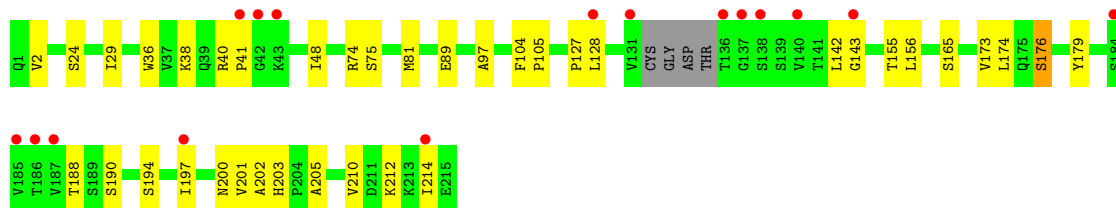
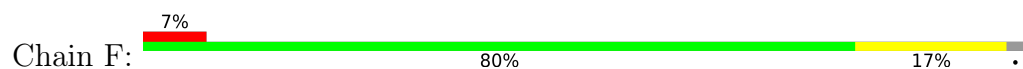
- Molecule 3: Transmembrane protein gp41



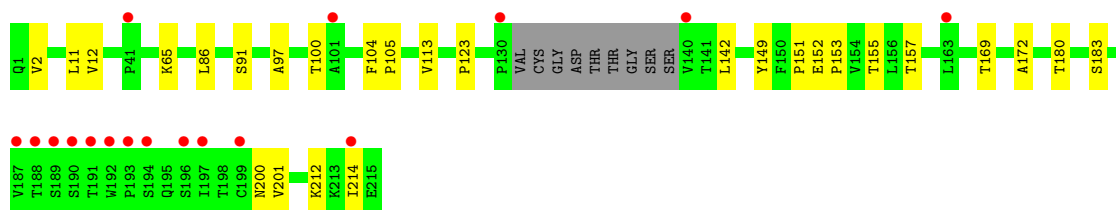
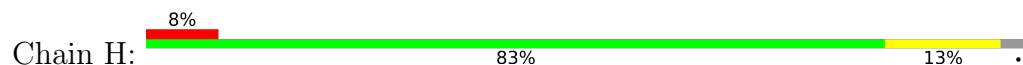
- Molecule 3: Transmembrane protein gp41



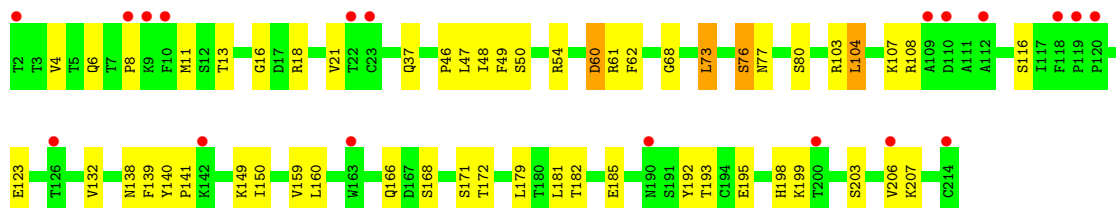
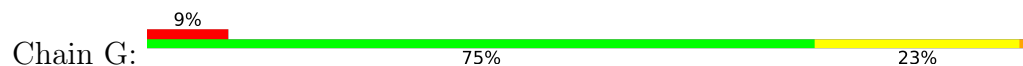
- Molecule 4: Fab.34.2.12 Heavy Chain



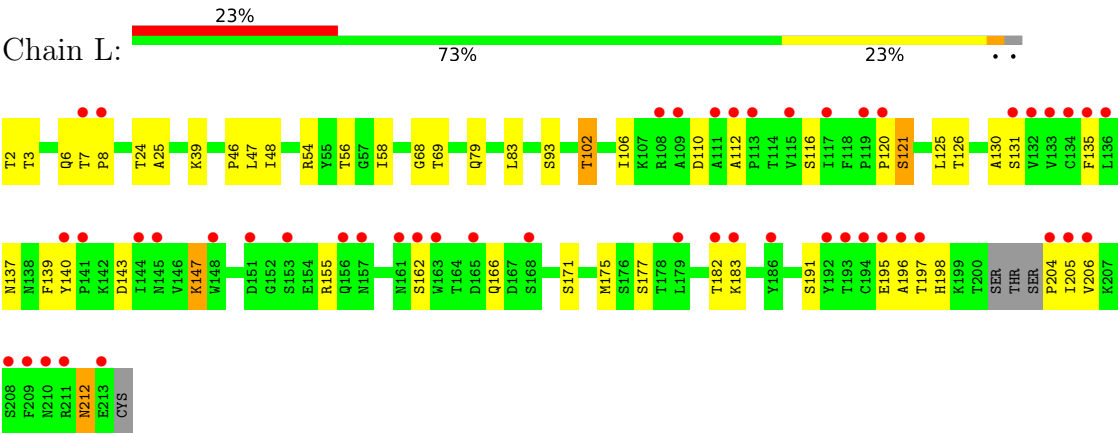
- Molecule 4: Fab.34.2.12 Heavy Chain



- Molecule 5: Fab 34.2.12 Light Chain



● Molecule 5: Fab 34.2.12 Light Chain



4 Data and refinement statistics

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) 96.9 (56.62-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 0.225 , 0.271	Depositor DCC
R_{free} test set	2374 reflections (4.86%)	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)	0.31 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.17	0/2287	0.37	0/3109
1	C	0.32	0/2210	0.49	1/3014 (0.0%)
2	B	0.11	0/831	0.35	0/1131
2	D	0.21	0/820	0.38	0/1116
3	E	0.11	0/77	0.27	0/101
3	P	0.12	0/77	0.28	0/101
4	F	0.14	0/1618	0.34	0/2212
4	H	0.13	0/1572	0.35	0/2146
5	G	0.16	0/1669	0.40	0/2273
5	L	0.28	0/1567	0.48	0/2138
All	All	0.21	0/12728	0.41	1/17341 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	THR	CB-CA-C	5.61	122.83	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2224	0	2081	35	0
1	C	2148	0	1952	55	0
2	B	805	0	771	13	0
2	D	794	0	758	17	0
3	E	76	0	82	1	0
3	P	76	0	82	2	0
4	F	1575	0	1518	22	0
4	H	1531	0	1470	15	0
5	G	1630	0	1503	37	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	0	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	206	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 9.

All (206) 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:45:TYR:HE1	1:C:67:ALA:HB2	1.51	0.76
1:C:216:THR:HA	1:C:228:MET:HE1	1.68	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:225:THR:HA	1:A:228:MET:HE3	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
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
1:C:51:TRP:CD1	1:C:178:THR:HG1	2.20	0.59
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
1:C:24:GLU:OE1	1:C:45:TYR:OH	2.20	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
1:C:230:LEU:HD22	1:C:243:LYS:HE3	1.85	0.58
2:B:57:SER:OG	2:B:58:LYS:N	2.32	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:225:THR:HA	1:C:228:MET:HE3	1.90	0.54
5:G:54:ARG:HH11	5:G:54:ARG:HB2	1.72	0.54
5:G:166:GLN:HE21	5:G:171:SER:C	2.15	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
5:L:175:MET:HE1	5:L:177:SER:HB2	1.90	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
2:D:37:ILE:HB	2:D:51:MET:HE1	1.91	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
5:G:11:MET:HE1	5:G:21:VAL:HA	1.91	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
4:F:36:TRP:HB3	4:F:81:MET:HE2	1.94	0.50
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
1:C:13:SER:HG	1:C:93:HIS:H	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
5:G:47:LEU:C	5:G:48:ILE:HG13	2.38	0.47
1:C:176:ASN:O	1:C:180:LEU:HB2	2.14	0.47
2:B:23:LEU:HD23	2:B:39:MET:HE2	1.96	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:G:149:LYS:NZ	5:G:195:GLU:OE2	2.44	0.46
5:L:120:PRO:HG2	5:L:125:LEU:HD21	1.96	0.46
1:C:22:TYR:OH	1:C:24:GLU:OE2	2.32	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
1:A:191:HIS:CD2	1:A:191:HIS:C	2.94	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:14:ARG:HH12	1:C:39:ASP:CG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:23:MET:HE3	1:C:23:MET:HB2	1.84	0.43
2:D:39:MET:HE2	2:D:66:ALA:HB1	2.00	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
5:L:110:ASP:OD1	5:L:110:ASP:N	2.52	0.42
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.50	0.42
1:A:171:TYR:OH	3:P:1:ARG:N	2.45	0.42
1:C:255:GLN:H	1:C:255:GLN:CD	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:G:13:THR:HG22	5:G:104:LEU:HD21	2.02	0.41
1:A:234:ARG:HH12	2:B:99:MET:HE1	1.85	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
5:L:7:THR:HG21	5:L:102:THR:OG1	2.21	0.41
1:C:138:MET:HE3	1:C:138:MET:HB3	1.73	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
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
2:D:33:PRO:HB2	2:D:54:MET:HE3	2.03	0.40
5:L:147:LYS:NZ	5:L:204:PRO:HG2	2.37	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/273 (99%)	259 (96%)	11 (4%)	1 (0%)	30	60
1	C	271/273 (99%)	254 (94%)	16 (6%)	1 (0%)	30	60
2	B	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	12	38
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
4	F	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	24	55
4	H	202/215 (94%)	192 (95%)	10 (5%)	0	100	100
5	G	211/213 (99%)	197 (93%)	11 (5%)	3 (1%)	9	30
5	L	205/213 (96%)	193 (94%)	9 (4%)	3 (2%)	8	28
All	All	1577/1620 (97%)	1493 (95%)	74 (5%)	10 (1%)	21	51

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 ⓘ

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%)	218 (97%)	7 (3%)	35	70
1	C	207/229 (90%)	200 (97%)	7 (3%)	32	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	90/93 (97%)	87 (97%)	3 (3%)	33	69
2	D	87/93 (94%)	83 (95%)	4 (5%)	24	58
3	E	7/7 (100%)	7 (100%)	0	100	100
3	P	7/7 (100%)	7 (100%)	0	100	100
4	F	173/182 (95%)	167 (96%)	6 (4%)	32	67
4	H	164/182 (90%)	160 (98%)	4 (2%)	43	77
5	G	182/189 (96%)	171 (94%)	11 (6%)	17	47
5	L	160/189 (85%)	143 (89%)	17 (11%)	6	22
All	All	1302/1400 (93%)	1243 (96%)	59 (4%)	24	58

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	109	LEU
1	A	180	LEU
1	A	247	VAL
1	A	262	GLU
1	A	268	GLU
1	A	272	LEU
2	B	57	SER
2	B	69	GLU
2	B	98	ASP
1	C	12	VAL
1	C	103	VAL
1	C	182	THR
1	C	198	ASP
1	C	228	MET
1	C	240	THR
1	C	249	VAL
2	D	11	SER
2	D	23	LEU
2	D	52	SER
2	D	55	SER
4	F	2	VAL
4	F	75	SER
4	F	165	SER
4	F	176	SER
4	F	188	THR

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Mol	Chain	Res	Type
4	F	200	ASN
5	G	50	SER
5	G	60	ASP
5	G	61	ARG
5	G	73	LEU
5	G	76	SER
5	G	80	SER
5	G	104	LEU
5	G	116	SER
5	G	168	SER
5	G	182	THR
5	G	203	SER
4	H	2	VAL
4	H	100	THR
4	H	157	THR
4	H	200	ASN
5	L	2	THR
5	L	3	THR
5	L	39	LYS
5	L	56	THR
5	L	79	GLN
5	L	93	SER
5	L	102	THR
5	L	116	SER
5	L	121	SER
5	L	126	THR
5	L	147	LYS
5	L	162	SER
5	L	182	THR
5	L	183	LYS
5	L	191	SER
5	L	206	VAL
5	L	212	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	HIS
1	A	226	GLN
2	B	6	GLN
2	B	24	ASN
1	C	191	HIS

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Mol	Chain	Res	Type
1	C	263	HIS
2	D	13	HIS
5	G	38	GLN
5	G	42	GLN
5	G	77	ASN
5	G	138	ASN
5	G	166	GLN
5	G	210	ASN
5	L	37	GLN
5	L	79	GLN
5	L	92	HIS
5	L	137	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.43	0	2,2,2	0.34	0
7	GOL	F	301	-	5,5,5	0.88	0	5,5,5	1.11	1 (20%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	301	GOL	C3-C2-C1	-2.05	104.29	111.80

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/273 (100%)	0.26	5 (1%) 67 58	25, 62, 109, 145	1 (0%)
1	C	273/273 (100%)	0.52	18 (6%) 24 18	42, 67, 110, 139	0
2	B	99/99 (100%)	-0.06	1 (1%) 79 72	30, 50, 69, 77	1 (1%)
2	D	99/99 (100%)	0.97	9 (9%) 15 11	48, 88, 133, 160	0
3	E	10/10 (100%)	-0.21	0 100 100	47, 54, 65, 81	0
3	P	10/10 (100%)	0.01	0 100 100	55, 59, 71, 72	0
4	F	211/215 (98%)	0.33	16 (7%) 20 14	28, 49, 128, 172	0
4	H	206/215 (95%)	0.43	17 (8%) 17 12	11, 41, 123, 161	5 (2%)
5	G	213/213 (100%)	0.96	19 (8%) 15 11	53, 91, 123, 152	3 (1%)
5	L	206/213 (96%)	1.16	49 (23%) 2 1	39, 98, 141, 177	2 (0%)
All	All	1600/1620 (98%)	0.56	134 (8%) 17 12	11, 69, 126, 177	12 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	188	THR	9.2
4	H	197	ILE	8.2
5	G	214	CYS	7.8
4	H	192	TRP	5.8
4	H	187	VAL	5.7
5	L	141	PRO	4.6
4	H	196	SER	4.3
2	D	99	MET	4.2
5	G	119	PRO	4.1
5	G	2	THR	4.0
5	L	192	TYR	3.9
4	H	190	SER	3.9
5	L	196	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
5	L	8	PRO	3.7
5	L	157	ASN	3.7
5	L	206	VAL	3.7
4	H	193	PRO	3.6
1	C	107	GLY	3.6
1	C	42	ASN	3.6
4	F	136	THR	3.5
4	H	101	ALA	3.5
5	L	144	ILE	3.4
4	F	131	VAL	3.4
4	F	41	PRO	3.3
5	L	119	PRO	3.3
5	L	205	ILE	3.3
5	G	109	ALA	3.3
5	G	23	CYS	3.2
2	D	98	ASP	3.2
5	L	153	SER	3.1
4	F	197	ILE	3.1
5	L	163	TRP	3.1
5	L	111	ALA	3.1
5	L	210	ASN	3.1
5	G	8	PRO	3.1
5	L	209	PHE	3.0
1	C	50	ARG	3.0
1	A	41	GLU	3.0
4	F	214	ILE	2.9
5	G	206	VAL	2.9
1	C	109	LEU	2.9
5	L	140	TYR	2.9
5	L	112	ALA	2.9
4	H	163	LEU	2.9
5	G	9	LYS	2.8
1	A	16	GLY	2.8
5	G	120	PRO	2.8
2	D	47	PRO	2.8
5	L	211	ARG	2.7
1	A	110	LEU	2.7
5	L	7	THR	2.7
1	C	41	GLU	2.7
1	A	30	ASN	2.7
5	G	110	ASP	2.7
4	H	140	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
5	L	213	GLU	2.7
5	L	179	LEU	2.7
4	H	189	SER	2.7
4	H	214	ILE	2.6
5	L	168	SER	2.6
1	C	104	GLU	2.6
5	L	133	VAL	2.6
5	L	195	GLU	2.6
5	G	10	PHE	2.6
5	L	109	ALA	2.6
1	A	45	TYR	2.6
5	G	190	ASN	2.6
1	C	210	PRO	2.6
5	L	204	PRO	2.6
1	C	165	VAL	2.6
5	L	108	ARG	2.5
5	L	148	TRP	2.5
2	D	74	GLU	2.5
5	L	134	CYS	2.5
5	L	186	TYR	2.5
1	C	30	ASN	2.5
5	L	145	ASN	2.5
4	F	184	SER	2.5
1	C	184	PRO	2.4
5	L	117	ILE	2.4
4	F	187	VAL	2.4
5	L	197	THR	2.4
1	C	106	ASP	2.4
5	L	151	ASP	2.4
5	L	132	VAL	2.4
4	F	42	GLY	2.4
1	C	236	ALA	2.4
5	G	126	THR	2.4
5	L	136	LEU	2.4
4	F	143	GLY	2.4
2	D	79	ALA	2.4
5	G	22	THR	2.4
4	H	130	PRO	2.4
5	G	163	TRP	2.3
2	D	23	LEU	2.3
5	G	118	PHE	2.3
5	L	162	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	186	THR	2.3
5	L	193	THR	2.3
5	G	142	LYS	2.3
1	C	183	ASP	2.3
5	L	156	GLN	2.3
5	L	115	VAL	2.3
1	C	268	GLU	2.3
4	F	128	LEU	2.2
4	H	41	PRO	2.2
5	L	208	SER	2.2
1	C	237	GLY	2.2
2	D	54	MET	2.2
5	L	161	ASN	2.2
4	H	191	THR	2.2
5	G	112	ALA	2.2
5	L	113	PRO	2.2
4	F	138	SER	2.2
5	L	182	THR	2.2
4	H	194	SER	2.2
5	L	165	ASP	2.1
2	D	78	TYR	2.1
1	C	181	ARG	2.1
2	D	16	GLU	2.1
4	F	43	LYS	2.1
5	G	200	THR	2.1
4	F	185	VAL	2.1
5	L	120	PRO	2.1
5	L	183	LYS	2.1
1	C	111	ARG	2.1
1	C	274	TRP	2.1
5	L	131	SER	2.1
4	F	137	GLY	2.1
2	B	98	ASP	2.1
4	H	199	CYS	2.0
5	L	135	PHE	2.0
5	L	194	CYS	2.0
4	F	140	VAL	2.0

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 [i](#)

There are no oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
6	EDO	C	301	4/4	0.80	0.15	62,64,66,68	0
7	GOL	F	301	6/6	0.81	0.21	41,44,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.