



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:10 PM UTC

PDB ID : 7PBE / pdb_00007pbe
Title : Emergence of immune escape at dominant SARS-CoV-2 killer T-cell epitope
Authors : Rizkallah, P.J.; Sewell, A.K.; Wall, A.; Fuller, A.
Deposited on : 2021-08-02
Resolution : 3.00 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

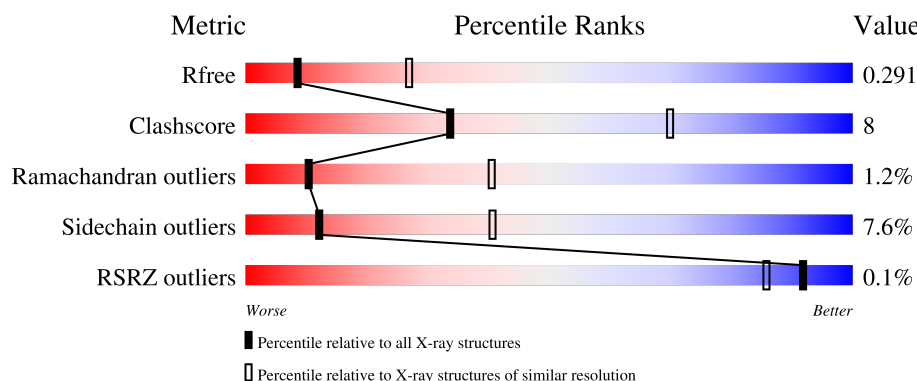
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	276	77% 21% .
1	F	276	75% 24% .
2	B	100	% 76% 23% .
2	G	100	% 75% 24% .
3	C	9	78% 22%

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Mol	Chain	Length	Quality of chain
3	H	9	 44% 44% 11%
4	D	203	 71% 24% . .
4	I	203	 70% 23% . .
5	E	243	 75% 23% .
5	J	243	 79% 20% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13403 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	F	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			82	56	13	13			
3	H	9	Total	C	N	O	0	0	0
			82	56	13	13			

- Molecule 4 is a protein called Human T-cell Receptor YLQ36, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1564	977	259	319	9			

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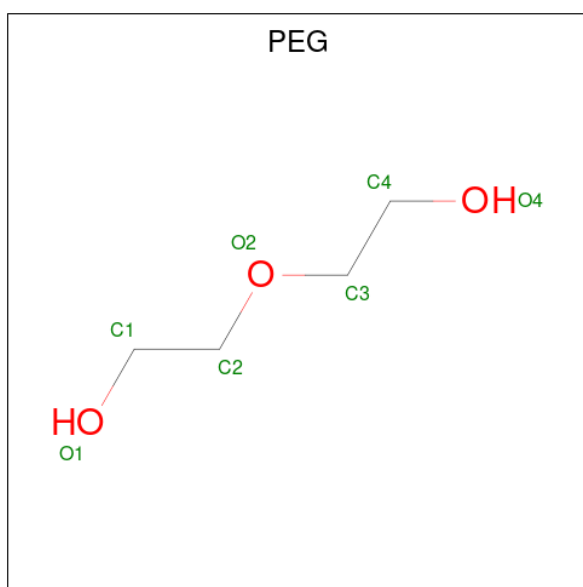
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	199	Total	C	N	O	S	0	0	0
			1564	977	259	319	9			

- Molecule 5 is a protein called Human T-cell Receptor YLQ36, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1945	1217	345	377	6			
5	J	242	Total	C	N	O	S	0	0	0
			1945	1217	345	377	6			

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

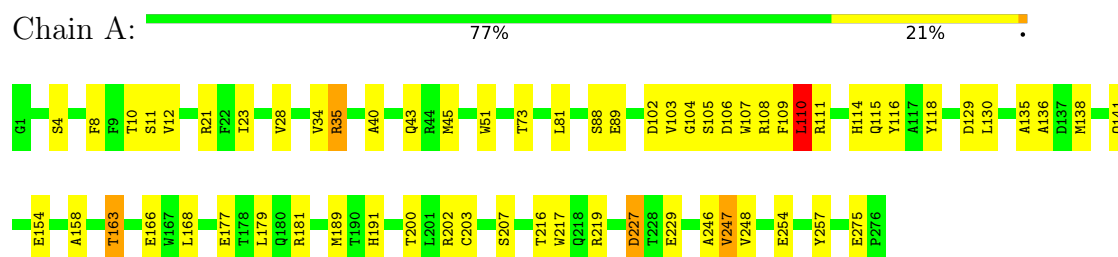


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	I	1	Total	O	S	0	0
			5	4	1		

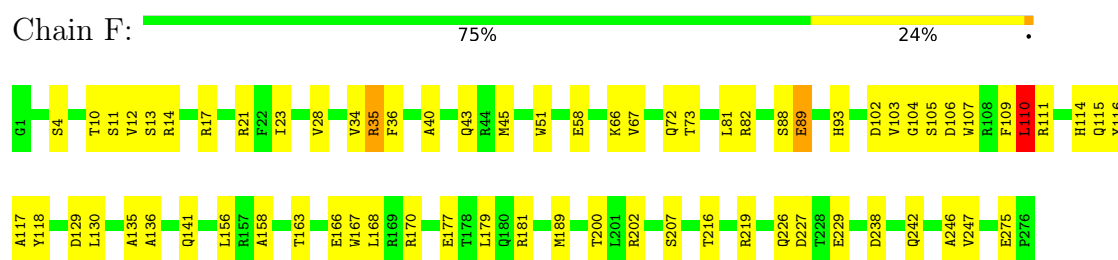
3 Residue-property plots

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.

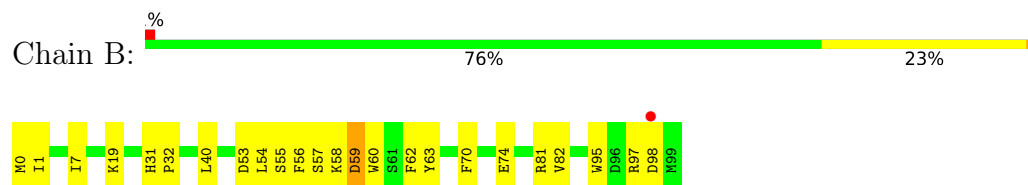
• Molecule 1: MHC class I antigen



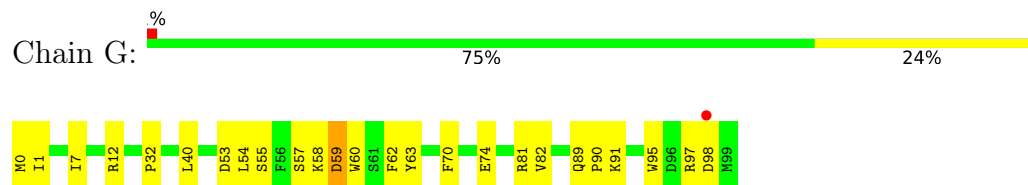
• Molecule 1: MHC class I antigen



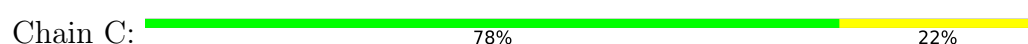
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 3: Spike protein S1





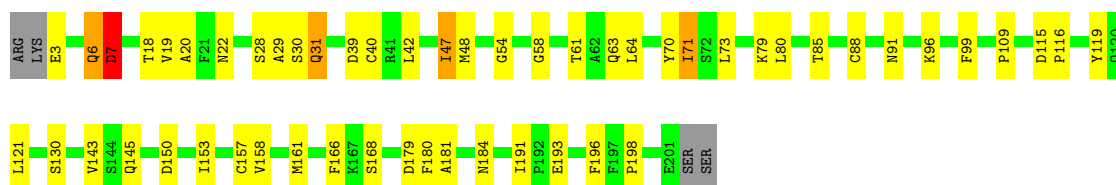
- Molecule 3: Spike protein S1

Chain H: 44% 44% 11%



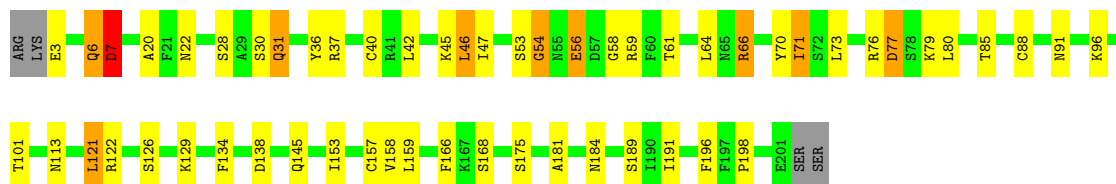
- Molecule 4: Human T-cell Receptor YLQ36, alpha chain

Chain D: 71% 24% . .



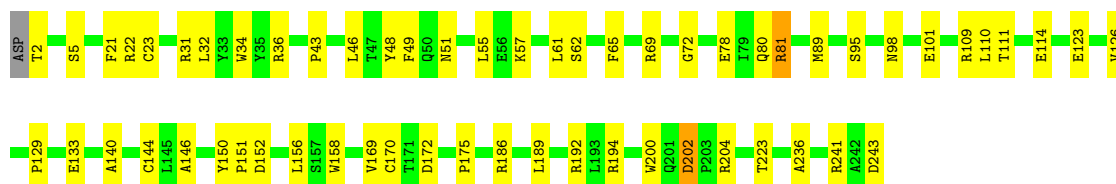
- Molecule 4: Human T-cell Receptor YLQ36, alpha chain

Chain I: 70% 23% . .



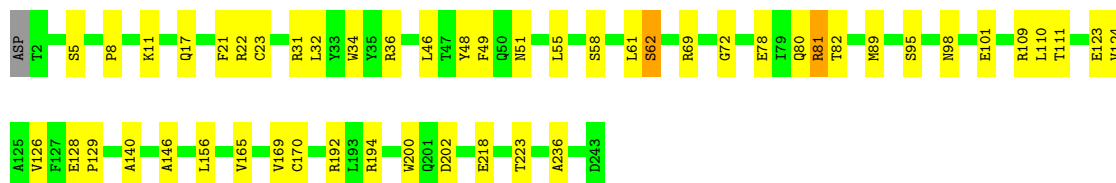
- Molecule 5: Human T-cell Receptor YLQ36, beta chain

Chain E: 75% 23% .



- Molecule 5: Human T-cell Receptor YLQ36, beta chain

Chain J: 79% 20% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.24Å 46.45Å 184.72Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	113.83 – 3.00 113.83 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (113.83-3.00) 99.3 (113.83-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.228 , 0.296 0.229 , 0.291	Depositor DCC
R_{free} test set	2670 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13403	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6801e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4

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	1.01	0/2320	1.32	0/3149
1	F	1.02	0/2320	1.32	0/3149
2	B	0.98	0/860	1.15	0/1162
2	G	0.97	0/860	1.15	0/1162
3	C	0.97	0/84	1.07	0/112
3	H	0.93	0/84	1.15	0/112
4	D	1.06	0/1598	1.27	0/2170
4	I	1.08	0/1598	1.26	0/2170
5	E	0.99	0/1995	1.23	0/2706
5	J	1.00	0/1995	1.22	0/2706
All	All	1.02	0/13714	1.26	0/18598

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
4	D	0	1
4	I	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	LEU	Peptide
4	D	3	GLU	Peptide
1	F	110	LEU	Peptide
4	I	3	GLU	Peptide
4	I	47	ILE	Peptide

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	2254	0	2103	33	0
1	F	2254	0	2103	40	0
2	B	837	0	803	11	0
2	G	837	0	803	14	0
3	C	82	0	88	1	0
3	H	82	0	88	6	0
4	D	1564	0	1473	26	0
4	I	1564	0	1473	26	0
5	E	1945	0	1841	38	0
5	J	1945	0	1841	31	0
6	A	7	0	10	0	0
6	F	7	0	10	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	E	5	0	0	0	0
7	F	5	0	0	0	0
7	I	5	0	0	0	0
All	All	13403	0	12636	201	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 (201) 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)
4:D:47:ILE:HG22	4:D:48:MET:HB2	1.60	0.82
1:F:35:ARG:NH2	2:G:53:ASP:OD2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5:ARG:HG2	3:H:5:ARG:HH21	1.45	0.80
4:D:71:ILE:HD11	4:D:88:CYS:SG	2.25	0.76
4:I:71:ILE:HD11	4:I:88:CYS:SG	2.26	0.76
1:A:203:CYS:HB2	1:A:217:TRP:HZ3	1.51	0.74
4:I:66:ARG:HD3	4:I:66:ARG:N	2.03	0.73
1:A:35:ARG:NH2	2:B:53:ASP:OD2	2.22	0.72
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.24	0.68
1:F:156:LEU:HD23	3:H:3:GLN:HE22	1.59	0.68
2:G:59:ASP:OD1	2:G:60:TRP:N	2.27	0.68
1:F:21:ARG:CZ	1:F:23:ILE:HD11	2.24	0.68
2:B:59:ASP:OD1	2:B:60:TRP:N	2.28	0.66
4:I:158:VAL:O	5:J:170:CYS:SG	2.54	0.65
1:A:227:ASP:HB3	1:A:248:VAL:HG12	1.79	0.64
2:G:89:GLN:HG3	2:G:90:PRO:HD2	1.81	0.63
4:D:47:ILE:HG22	4:D:48:MET:CB	2.27	0.63
3:H:5:ARG:HH21	3:H:5:ARG:CG	2.11	0.63
4:D:158:VAL:O	5:E:170:CYS:SG	2.56	0.62
4:D:181:ALA:HB1	4:D:184:ASN:HB3	1.81	0.61
1:F:135:ALA:HB3	1:F:141:GLN:HE21	1.64	0.61
4:I:36:TYR:CZ	4:I:46:LEU:HD23	2.37	0.60
4:I:66:ARG:N	4:I:66:ARG:CD	2.65	0.59
1:A:135:ALA:HB3	1:A:141:GLN:HE21	1.67	0.59
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.38	0.58
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.40	0.57
1:F:177:GLU:O	1:F:181:ARG:HB3	2.05	0.57
1:A:177:GLU:O	1:A:181:ARG:HB3	2.04	0.56
4:D:6:GLN:O	4:D:7:ASP:C	2.47	0.56
4:I:6:GLN:O	4:I:7:ASP:C	2.48	0.56
1:F:17:ARG:NE	1:F:17:ARG:HA	2.21	0.55
5:E:69:ARG:CZ	5:E:72:GLY:O	2.55	0.55
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.88	0.55
5:J:21:PHE:HZ	5:J:110:LEU:HB2	1.72	0.55
5:E:21:PHE:HZ	5:E:110:LEU:HB2	1.72	0.55
2:G:54:LEU:HD11	2:G:62:PHE:HB3	1.88	0.54
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.89	0.54
1:F:28:VAL:HG11	1:F:179:LEU:HD13	1.89	0.54
5:J:51:ASN:HD22	5:J:51:ASN:N	2.05	0.54
2:B:95:TRP:CZ2	2:B:97:ARG:HB3	2.42	0.54
4:I:54:GLY:O	4:I:56:GLU:HG2	2.07	0.54
5:E:51:ASN:N	5:E:51:ASN:HD22	2.06	0.53
4:I:181:ALA:HB3	4:I:184:ASN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TRP:NE1	1:A:247:VAL:HG11	2.23	0.53
4:D:22:ASN:ND2	4:D:70:TYR:OH	2.42	0.53
1:F:219:ARG:CG	1:F:219:ARG:O	2.57	0.53
4:I:122:ARG:HB2	4:I:126:SER:OG	2.09	0.52
1:F:21:ARG:NH2	1:F:23:ILE:HD11	2.25	0.52
4:I:22:ASN:ND2	4:I:70:TYR:OH	2.42	0.52
4:I:126:SER:HB2	4:I:129:LYS:O	2.10	0.52
3:H:8:LEU:H	5:J:98:ASN:HD21	1.58	0.51
4:I:166:PHE:CE2	4:I:168:SER:HB3	2.45	0.51
4:D:166:PHE:CE2	4:D:168:SER:HB3	2.46	0.51
1:A:109:PHE:CG	1:A:110:LEU:N	2.79	0.51
1:A:203:CYS:HB2	1:A:217:TRP:CZ3	2.41	0.51
4:D:145:GLN:N	4:D:145:GLN:OE1	2.42	0.51
5:E:48:TYR:OH	5:E:55:LEU:HD12	2.11	0.51
5:E:129:PRO:HD2	5:E:200:TRP:CZ2	2.45	0.51
1:F:109:PHE:CG	1:F:110:LEU:N	2.78	0.51
2:G:95:TRP:CZ2	2:G:97:ARG:HB3	2.46	0.51
5:J:8:PRO:HG3	5:J:11:LYS:HD3	1.93	0.51
5:J:48:TYR:OH	5:J:55:LEU:HD12	2.11	0.51
4:D:145:GLN:HB3	4:D:153:ILE:HB	1.94	0.50
4:I:66:ARG:CD	4:I:66:ARG:H	2.25	0.50
5:E:202:ASP:OD2	5:E:204:ARG:HG3	2.12	0.50
1:F:34:VAL:HB	1:F:45:MET:HE3	1.94	0.50
1:A:104:GLY:N	1:A:109:PHE:HB3	2.28	0.49
5:E:57:LYS:HE3	5:E:61:LEU:HD23	1.94	0.49
5:J:169:VAL:HA	5:J:192:ARG:O	2.13	0.49
5:E:61:LEU:HG	5:E:65:PHE:HB2	1.95	0.49
1:A:21:ARG:NH2	1:A:23:ILE:HD11	2.26	0.49
1:A:163:THR:HG21	4:D:29:ALA:HA	1.93	0.49
4:D:157:CYS:C	5:E:170:CYS:SG	2.96	0.49
2:G:7:ILE:HG12	2:G:82:VAL:HG21	1.95	0.49
1:A:106:ASP:O	1:A:107:TRP:HB2	2.13	0.48
1:F:106:ASP:O	1:F:107:TRP:HB2	2.13	0.48
4:D:39:ASP:HB2	4:D:42:LEU:HD12	1.94	0.48
4:I:56:GLU:HA	4:I:61:THR:HG22	1.95	0.48
5:E:169:VAL:HA	5:E:192:ARG:O	2.14	0.48
2:G:0:MET:HE1	2:G:32:PRO:HG3	1.94	0.48
5:J:129:PRO:HD2	5:J:200:TRP:CZ2	2.48	0.48
4:D:130:SER:HB2	4:D:180:PHE:CZ	2.48	0.48
1:A:158:ALA:HB3	4:D:31:GLN:HB3	1.95	0.48
1:F:40:ALA:O	1:F:43:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:H	1:A:109:PHE:HB3	1.79	0.47
1:F:189:MET:HA	1:F:202:ARG:O	2.14	0.47
4:I:91:ASN:HA	4:I:96:LYS:O	2.13	0.47
1:A:34:VAL:CG2	1:A:45:MET:HE3	2.43	0.47
1:F:135:ALA:HB3	1:F:141:GLN:NE2	2.30	0.47
1:A:40:ALA:O	1:A:43:GLN:NE2	2.47	0.47
1:F:14:ARG:NH1	1:F:21:ARG:HB2	2.30	0.47
1:F:102:ASP:HB2	1:F:111:ARG:HB3	1.97	0.47
1:F:104:GLY:N	1:F:109:PHE:HB3	2.30	0.46
2:G:58:LYS:C	2:G:59:ASP:O	2.59	0.46
5:E:126:VAL:HG23	5:E:236:ALA:HB3	1.96	0.46
1:F:219:ARG:O	1:F:219:ARG:HG2	2.15	0.46
5:J:51:ASN:HD22	5:J:51:ASN:H	1.63	0.46
3:C:8:LEU:H	5:E:98:ASN:HD21	1.62	0.46
1:A:34:VAL:HB	1:A:45:MET:HE3	1.98	0.46
1:A:114:HIS:CE1	1:A:116:TYR:HE1	2.34	0.46
5:J:126:VAL:HG23	5:J:236:ALA:HB3	1.98	0.46
4:I:20:ALA:HA	4:I:73:LEU:O	2.16	0.46
2:B:7:ILE:HG12	2:B:82:VAL:HG21	1.98	0.45
5:E:51:ASN:HD22	5:E:51:ASN:H	1.64	0.45
1:F:226:GLN:O	1:F:227:ASP:HB2	2.15	0.45
1:A:189:MET:HA	1:A:202:ARG:O	2.15	0.45
5:E:129:PRO:CG	5:E:140:ALA:HB1	2.47	0.45
1:F:34:VAL:CG2	1:F:45:MET:HE3	2.47	0.45
4:D:91:ASN:HA	4:D:96:LYS:O	2.15	0.45
5:E:34:TRP:O	5:E:46:LEU:HB2	2.15	0.45
5:E:123:GLU:O	5:E:146:ALA:HA	2.16	0.45
1:A:103:VAL:HG22	1:A:168:LEU:HD21	1.97	0.45
1:F:104:GLY:H	1:F:109:PHE:HB3	1.81	0.45
1:F:229:GLU:HB3	1:F:246:ALA:HB3	1.98	0.45
5:J:129:PRO:CG	5:J:140:ALA:HB1	2.46	0.45
1:A:229:GLU:HB3	1:A:246:ALA:HB3	1.97	0.45
5:J:34:TRP:O	5:J:46:LEU:HB2	2.16	0.45
5:E:31:ARG:HA	5:E:49:PHE:O	2.16	0.45
5:E:69:ARG:NH2	5:E:72:GLY:O	2.50	0.44
2:B:97:ARG:HG3	2:B:98:ASP:N	2.32	0.44
4:D:109:PRO:HD3	4:D:158:VAL:HG21	1.99	0.44
1:F:158:ALA:HB3	4:I:31:GLN:HB3	1.98	0.44
5:E:129:PRO:HD2	5:E:200:TRP:CE2	2.53	0.44
5:J:80:GLN:O	5:J:81:ARG:C	2.61	0.44
5:J:89:MET:SD	5:J:109:ARG:HG2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:ASP:O	5:E:175:PRO:HG2	2.18	0.44
4:I:76:ARG:HD2	4:I:76:ARG:HA	1.85	0.44
1:A:104:GLY:C	1:A:106:ASP:N	2.74	0.44
5:E:21:PHE:CZ	5:E:110:LEU:HB2	2.53	0.44
5:E:80:GLN:O	5:E:81:ARG:C	2.60	0.44
4:D:20:ALA:HA	4:D:73:LEU:O	2.18	0.43
1:F:66:LYS:HE3	3:H:2:LEU:HB2	1.99	0.43
5:J:61:LEU:O	5:J:62:SER:O	2.36	0.43
1:F:36:PHE:HB2	1:F:67:VAL:HG21	2.00	0.43
1:F:51:TRP:CZ2	1:F:179:LEU:HD11	2.53	0.43
1:F:103:VAL:HG22	1:F:168:LEU:HD21	2.00	0.43
1:F:114:HIS:CE1	1:F:116:TYR:HE1	2.35	0.43
2:G:97:ARG:HG3	2:G:98:ASP:N	2.33	0.43
2:B:63:TYR:O	2:B:63:TYR:CD1	2.71	0.43
4:D:99:PHE:CB	5:E:43:PRO:HD2	2.48	0.43
1:A:102:ASP:HB2	1:A:111:ARG:HB3	2.00	0.43
4:D:196:PHE:CE2	4:D:198:PRO:HB3	2.53	0.43
4:D:119:TYR:CE2	5:E:133:GLU:HG3	2.54	0.43
5:J:22:ARG:HG3	5:J:23:CYS:N	2.34	0.43
2:B:40:LEU:HD11	2:B:81:ARG:HB2	2.01	0.43
2:G:40:LEU:HD11	2:G:81:ARG:HB2	2.01	0.43
1:F:72:GLN:HG2	5:J:55:LEU:HD21	2.00	0.43
5:E:89:MET:SD	5:E:109:ARG:HG2	2.57	0.43
2:G:63:TYR:O	2:G:63:TYR:CD1	2.71	0.43
1:A:219:ARG:CG	1:A:257:TYR:CE1	3.02	0.42
1:F:82:ARG:HH11	1:F:89:GLU:HG3	1.84	0.42
4:D:119:TYR:CE1	5:E:133:GLU:HA	2.54	0.42
1:F:156:LEU:HD23	3:H:3:GLN:NE2	2.28	0.42
5:J:123:GLU:O	5:J:146:ALA:HA	2.19	0.42
5:J:21:PHE:CZ	5:J:110:LEU:HB2	2.52	0.42
5:J:156:LEU:C	5:J:156:LEU:HD23	2.44	0.42
4:D:109:PRO:HG3	4:D:158:VAL:HG13	2.01	0.42
1:F:238:ASP:HB3	2:G:12:ARG:HD3	2.01	0.42
1:A:129:ASP:O	1:A:130:LEU:HB2	2.20	0.42
5:E:32:LEU:HD23	5:E:32:LEU:C	2.44	0.42
4:I:79:LYS:HG2	4:I:80:LEU:HD23	2.00	0.42
5:J:31:ARG:HA	5:J:49:PHE:O	2.19	0.42
5:E:241:ARG:HB2	5:E:243:ASP:OD1	2.20	0.42
4:D:115:ASP:N	4:D:116:PRO:HD3	2.35	0.42
1:F:104:GLY:C	1:F:106:ASP:N	2.75	0.42
4:I:196:PHE:CE2	4:I:198:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.54	0.42
5:E:150:TYR:HB2	5:E:186:ARG:HG2	2.01	0.42
5:E:172:ASP:HB2	5:E:189:LEU:HD12	2.01	0.42
4:I:134:PHE:CE2	4:I:191:ILE:CD1	3.03	0.42
5:J:95:SER:HA	5:J:101:GLU:O	2.20	0.42
1:F:242:GLN:NE2	2:G:12:ARG:O	2.52	0.41
5:J:129:PRO:HD2	5:J:200:TRP:CE2	2.55	0.41
2:B:58:LYS:C	2:B:59:ASP:O	2.60	0.41
1:F:117:ALA:HB2	2:G:60:TRP:CD2	2.56	0.41
5:J:69:ARG:CZ	5:J:72:GLY:O	2.68	0.41
5:E:156:LEU:HD23	5:E:156:LEU:C	2.46	0.41
5:J:32:LEU:HD23	5:J:32:LEU:C	2.45	0.41
1:F:167:TRP:CE3	1:F:170:ARG:HD2	2.55	0.41
4:I:159:LEU:HD21	5:J:194:ARG:HB3	2.02	0.41
4:D:79:LYS:HG2	4:D:80:LEU:HD23	2.02	0.41
5:E:22:ARG:HG3	5:E:23:CYS:N	2.35	0.41
4:I:121:LEU:HD22	5:J:128:GLU:O	2.21	0.41
5:J:124:VAL:HG12	5:J:236:ALA:CB	2.50	0.41
1:F:129:ASP:O	1:F:130:LEU:HB2	2.20	0.41
2:B:31:HIS:HA	2:B:32:PRO:C	2.45	0.41
4:I:145:GLN:HA	4:I:153:ILE:HD12	2.01	0.41
1:A:138:MET:O	1:A:141:GLN:HB2	2.20	0.41
4:D:161:MET:CE	5:E:194:ARG:HD3	2.51	0.41
5:E:95:SER:HA	5:E:101:GLU:O	2.21	0.41
5:E:144:CYS:HB2	5:E:158:TRP:CZ2	2.56	0.41
1:F:13:SER:HG	1:F:93:HIS:H	1.68	0.41
5:J:17:GLN:O	5:J:82:THR:OG1	2.29	0.41
5:E:46:LEU:HD22	5:E:61:LEU:HD13	2.03	0.41
1:A:8:PHE:HD2	2:B:56:PHE:CE1	2.38	0.40
5:E:150:TYR:HA	5:E:151:PRO:HA	1.91	0.40
4:I:59:ARG:NH2	4:I:77:ASP:O	2.53	0.40
4:I:157:CYS:C	5:J:170:CYS:SG	3.04	0.40
1:A:106:ASP:OD2	1:A:108:ARG:O	2.40	0.40
1:A:191:HIS:O	1:A:191:HIS:CG	2.72	0.40
5:J:129:PRO:HG2	5:J:140:ALA:HB1	2.03	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	274/276 (99%)	249 (91%)	23 (8%)	2 (1%)	18	53
1	F	274/276 (99%)	245 (89%)	27 (10%)	2 (1%)	18	53
2	B	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	12	45
2	G	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	12	45
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	197/203 (97%)	170 (86%)	22 (11%)	5 (2%)	4	23
4	I	197/203 (97%)	169 (86%)	24 (12%)	4 (2%)	6	28
5	E	240/243 (99%)	225 (94%)	13 (5%)	2 (1%)	16	50
5	J	240/243 (99%)	227 (95%)	11 (5%)	2 (1%)	16	50
All	All	1632/1662 (98%)	1486 (91%)	127 (8%)	19 (1%)	10	40

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ALA
2	B	59	ASP
4	D	54	GLY
4	D	58	GLY
4	D	150	ASP
5	E	62	SER
1	F	136	ALA
2	G	59	ASP
4	I	58	GLY
5	J	62	SER
1	A	105	SER
4	I	54	GLY
5	E	81	ARG
1	F	105	SER

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Mol	Chain	Res	Type
4	D	7	ASP
4	D	30	SER
4	I	7	ASP
4	I	30	SER
5	J	81	ARG

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	232/232 (100%)	212 (91%)	20 (9%)	10	36
1	F	232/232 (100%)	214 (92%)	18 (8%)	11	39
2	B	95/95 (100%)	88 (93%)	7 (7%)	13	42
2	G	95/95 (100%)	89 (94%)	6 (6%)	16	48
3	C	9/9 (100%)	8 (89%)	1 (11%)	6	25
3	H	9/9 (100%)	7 (78%)	2 (22%)	1	5
4	D	181/185 (98%)	163 (90%)	18 (10%)	7	30
4	I	181/185 (98%)	159 (88%)	22 (12%)	5	21
5	E	212/213 (100%)	204 (96%)	8 (4%)	29	63
5	J	212/213 (100%)	203 (96%)	9 (4%)	26	61
All	All	1458/1468 (99%)	1347 (92%)	111 (8%)	12	41

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	10	THR
1	A	11	SER
1	A	12	VAL
1	A	35	ARG
1	A	73	THR
1	A	88	SER
1	A	89	GLU

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Mol	Chain	Res	Type
1	A	110	LEU
1	A	115	GLN
1	A	154	GLU
1	A	163	THR
1	A	166	GLU
1	A	200	THR
1	A	207	SER
1	A	216	THR
1	A	227	ASP
1	A	247	VAL
1	A	254	GLU
1	A	275	GLU
2	B	0	MET
2	B	1	ILE
2	B	19	LYS
2	B	55	SER
2	B	57	SER
2	B	70	PHE
2	B	74	GLU
3	C	9	LEU
4	D	6	GLN
4	D	7	ASP
4	D	18	THR
4	D	19	VAL
4	D	28	SER
4	D	31	GLN
4	D	40	CYS
4	D	47	ILE
4	D	61	THR
4	D	63	GLN
4	D	64	LEU
4	D	71	ILE
4	D	85	THR
4	D	121	LEU
4	D	143	VAL
4	D	179	ASP
4	D	191	ILE
4	D	193	GLU
5	E	2	THR
5	E	5	SER
5	E	36	ARG
5	E	78	GLU

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Mol	Chain	Res	Type
5	E	111	THR
5	E	114	GLU
5	E	202	ASP
5	E	223	THR
1	F	4	SER
1	F	10	THR
1	F	11	SER
1	F	12	VAL
1	F	35	ARG
1	F	58	GLU
1	F	73	THR
1	F	88	SER
1	F	89	GLU
1	F	110	LEU
1	F	115	GLN
1	F	163	THR
1	F	166	GLU
1	F	200	THR
1	F	207	SER
1	F	216	THR
1	F	247	VAL
1	F	275	GLU
2	G	1	ILE
2	G	55	SER
2	G	57	SER
2	G	70	PHE
2	G	74	GLU
2	G	91	LYS
3	H	5	ARG
3	H	9	LEU
4	I	6	GLN
4	I	7	ASP
4	I	28	SER
4	I	31	GLN
4	I	37	ARG
4	I	40	CYS
4	I	42	LEU
4	I	45	LYS
4	I	46	LEU
4	I	53	SER
4	I	56	GLU
4	I	64	LEU

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Mol	Chain	Res	Type
4	I	66	ARG
4	I	71	ILE
4	I	77	ASP
4	I	85	THR
4	I	101	THR
4	I	113	ASN
4	I	121	LEU
4	I	138	ASP
4	I	175	SER
4	I	189	SER
5	J	5	SER
5	J	36	ARG
5	J	58	SER
5	J	78	GLU
5	J	111	THR
5	J	165	VAL
5	J	202	ASP
5	J	218	GLU
5	J	223	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	87	GLN
1	A	141	GLN
1	A	151	HIS
1	A	218	GLN
4	D	22	ASN
4	D	55	ASN
4	D	65	ASN
4	D	69	GLN
4	D	112	GLN
4	D	142	ASN
4	D	169	ASN
5	E	29	HIS
5	E	41	GLN
5	E	51	ASN
5	E	84	GLN
5	E	98	ASN
5	E	161	ASN
5	E	174	GLN

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Mol	Chain	Res	Type
5	E	183	ASN
5	E	212	GLN
5	E	232	GLN
1	F	3	HIS
1	F	87	GLN
1	F	141	GLN
1	F	151	HIS
1	F	218	GLN
2	G	2	GLN
3	H	3	GLN
4	I	22	ASN
4	I	27	ASN
4	I	55	ASN
4	I	65	ASN
4	I	142	ASN
4	I	169	ASN
4	I	187	ASN
4	I	188	ASN
5	J	29	HIS
5	J	41	GLN
5	J	51	ASN
5	J	84	GLN
5	J	98	ASN
5	J	161	ASN
5	J	174	GLN
5	J	183	ASN
5	J	206	HIS
5	J	212	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 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	PEG	A	301	-	6,6,6	0.21	0	5,5,5	0.08	0
7	SO4	I	301	-	4,4,4	0.34	0	6,6,6	0.08	0
7	SO4	F	302	-	4,4,4	0.32	0	6,6,6	0.07	0
6	PEG	F	301	-	6,6,6	0.17	0	5,5,5	0.06	0
7	SO4	E	301	-	4,4,4	0.32	0	6,6,6	0.08	0
7	SO4	B	101	-	4,4,4	0.34	0	6,6,6	0.08	0
7	SO4	A	302	-	4,4,4	0.34	0	6,6,6	0.07	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	PEG	F	301	-	-	2/4/4/4	-
6	PEG	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	PEG	O2-C3-C4-O4
6	A	301	PEG	C1-C2-O2-C3
6	F	301	PEG	O1-C1-C2-O2
6	F	301	PEG	O2-C3-C4-O4

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	276/276 (100%)	-0.27	0	100	100	55, 102, 222, 250	0
1	F	276/276 (100%)	-0.26	0	100	100	54, 106, 211, 231	0
2	B	100/100 (100%)	-0.38	1 (1%)	79	59	57, 84, 130, 149	0
2	G	100/100 (100%)	-0.43	1 (1%)	79	59	62, 88, 136, 156	0
3	C	9/9 (100%)	-0.69	0	100	100	60, 65, 69, 74	0
3	H	9/9 (100%)	-0.54	0	100	100	60, 65, 73, 85	0
4	D	199/203 (98%)	0.08	0	100	100	64, 117, 182, 234	0
4	I	199/203 (98%)	-0.02	0	100	100	65, 119, 180, 236	0
5	E	242/243 (99%)	-0.40	0	100	100	60, 104, 153, 188	0
5	J	242/243 (99%)	-0.34	0	100	100	58, 106, 161, 198	0
All	All	1652/1662 (99%)	-0.25	2 (0%)	92	86	54, 105, 188, 250	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	98	ASP	2.5
2	G	98	ASP	2.1

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 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(Å ²)	Q<0.9
7	SO4	B	101	5/5	0.64	0.07	173,175,176,179	0
7	SO4	I	301	5/5	0.65	0.08	157,157,159,162	0
7	SO4	E	301	5/5	0.72	0.14	157,160,176,183	0
7	SO4	A	302	5/5	0.74	0.08	140,141,152,155	0
7	SO4	F	302	5/5	0.75	0.07	113,127,131,132	0
6	PEG	A	301	7/7	0.75	0.16	97,101,111,114	0
6	PEG	F	301	7/7	0.87	0.14	97,108,119,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.