Full wwPDB X-ray Structure Validation Report (i)

Apr 19, 2022 – 01:03 pm BST

PDB ID	:	7PBE
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

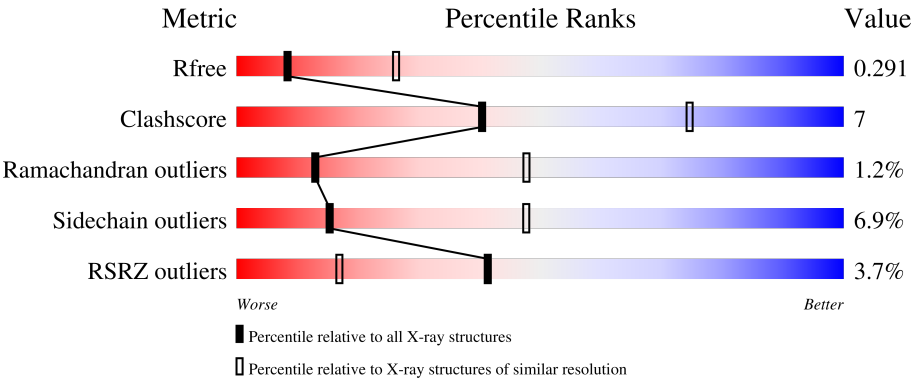
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	6% 79% 20%
1	F	276	6% 76% 22%
2	B	100	79% 20%
2	G	100	% 78% 21%
3	C	9	89% 11%

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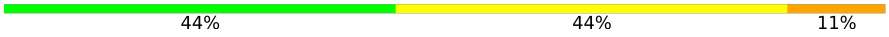
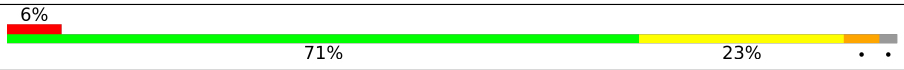
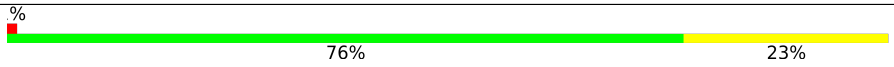
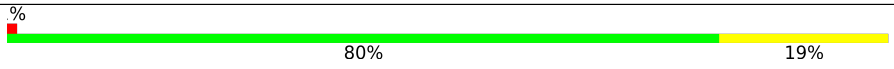
Mol	Chain	Length	Quality of chain
3	H	9	
4	D	203	
4	I	203	
5	E	243	
5	J	243	

2 Entry composition

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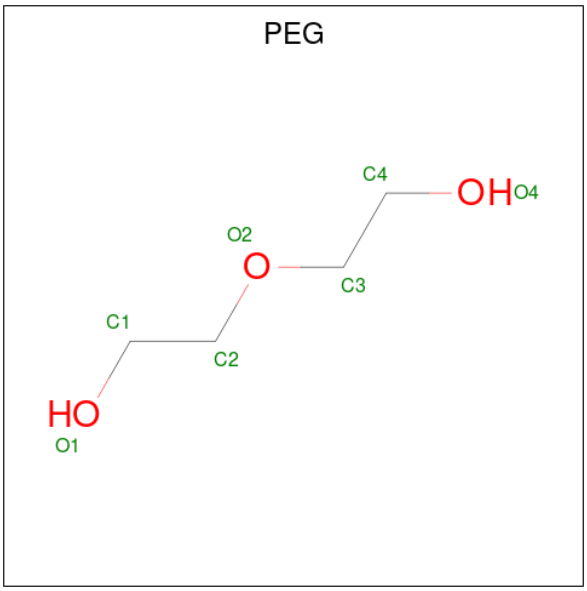
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	199	Total	C	N	O	S	0	0	0
			1564	977	259	319	9			

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

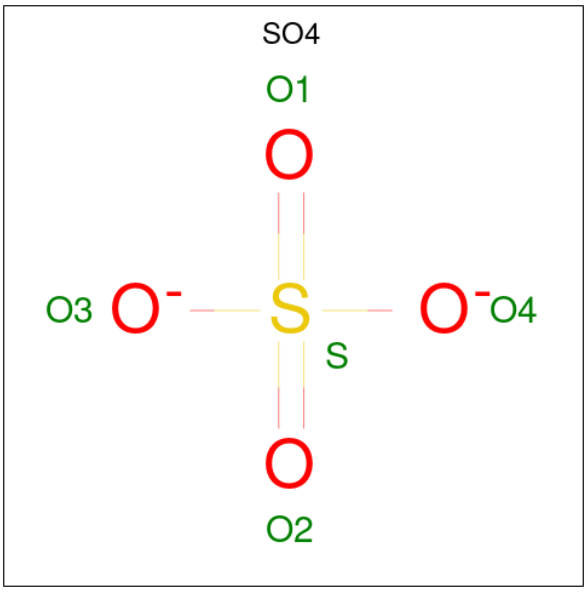
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1945	1217	345	377	6			
5	J	242	Total	C	N	O	S	0	0	0
			1945	1217	345	377	6			

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: 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 (three-letter code: SO4) (formula: O_4S).



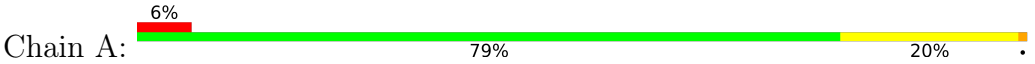
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	I	1	Total	O	S	0	0
			5	4	1		

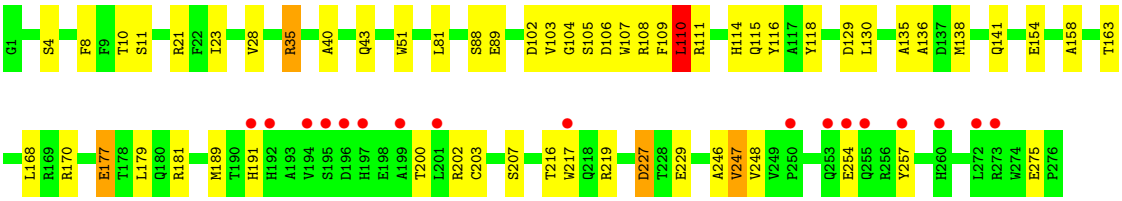
3 Residue-property plots (i)

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: MHC class I antigen

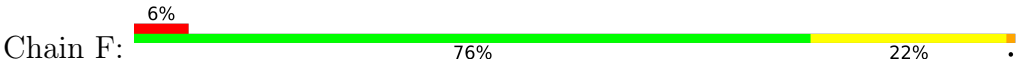
Chain A:

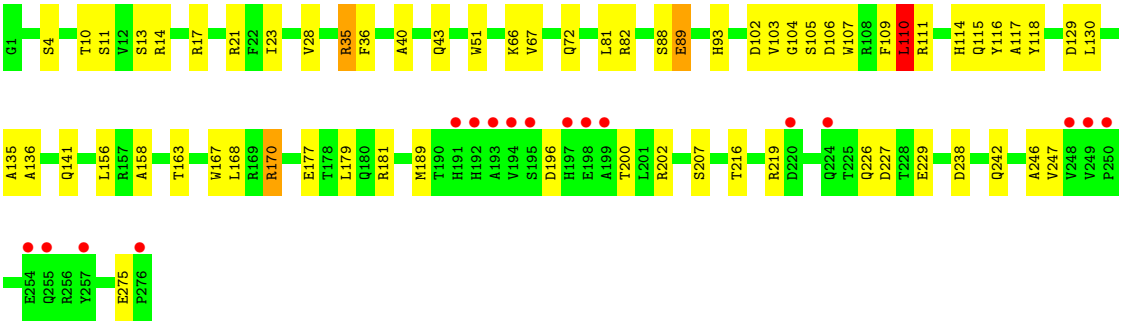




• Molecule 1: MHC class I antigen

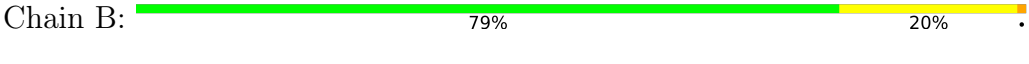
Chain F:





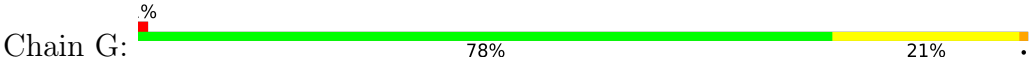
• Molecule 2: Beta-2-microglobulin

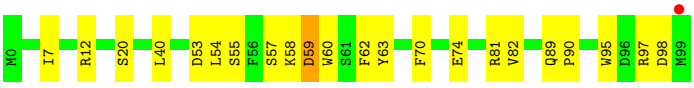
Chain B:



• Molecule 2: Beta-2-microglobulin

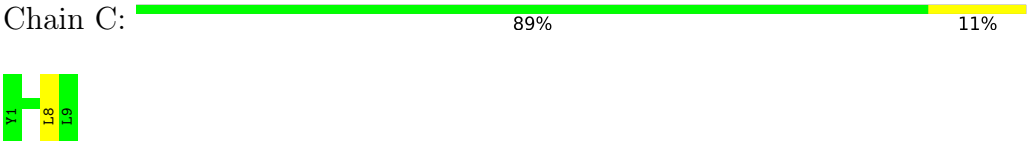
Chain G:





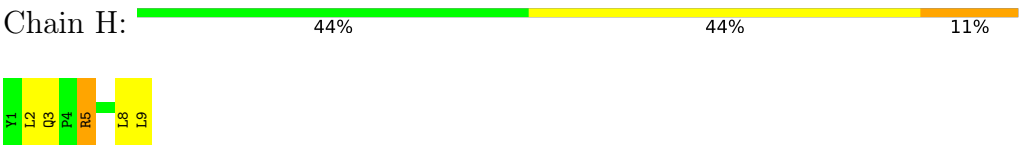
• Molecule 3: Spike protein S1

Chain C:



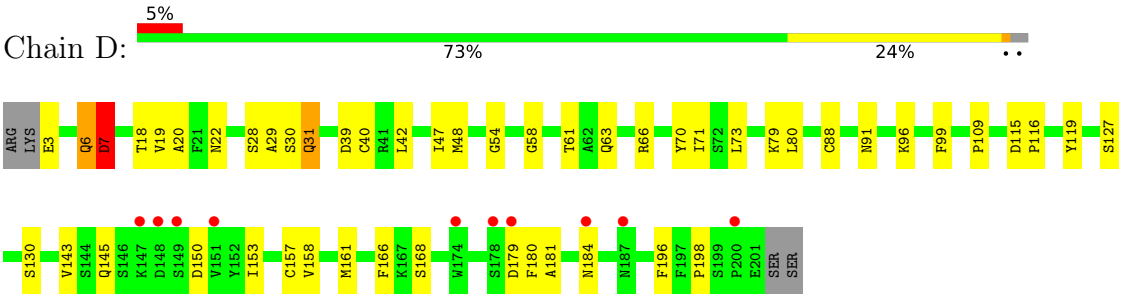
• Molecule 3: Spike protein S1

Chain H:



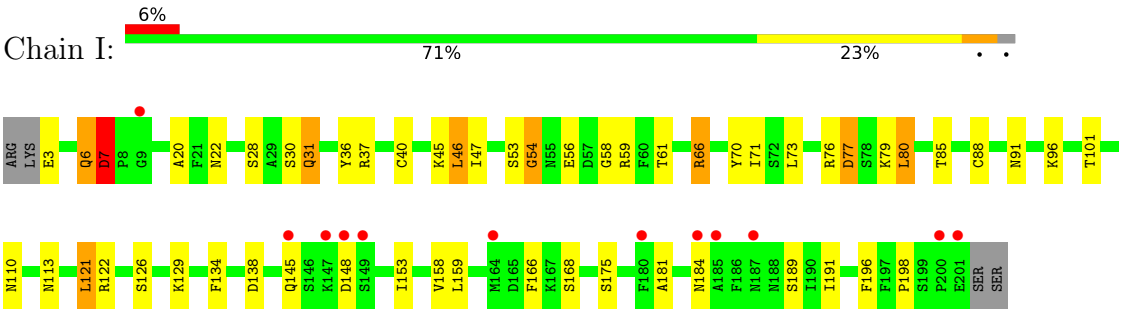
• Molecule 4: Human T-cell Receptor YLQ36, alpha chain

Chain D:



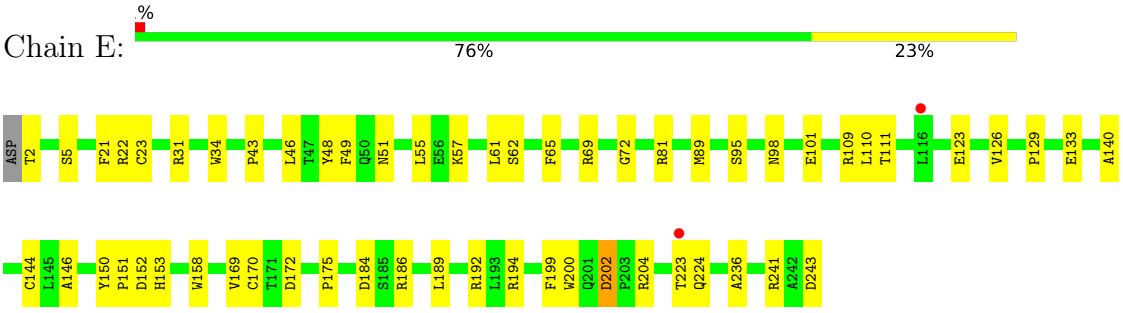
• Molecule 4: Human T-cell Receptor YLQ36, alpha chain

Chain I:



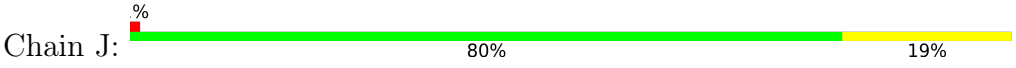
• Molecule 5: Human T-cell Receptor YLQ36, beta chain

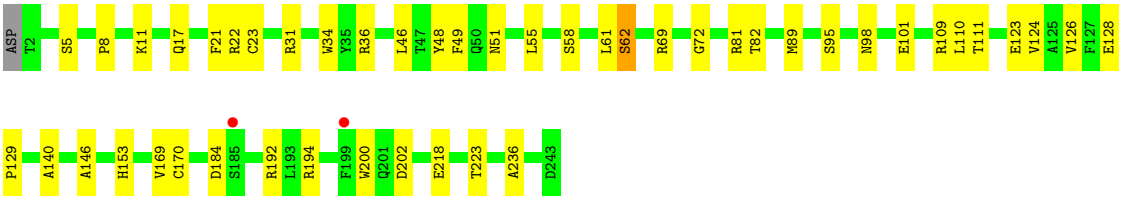
Chain E:



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

Chain J:




ASP T2 S5 P8 K11 Q17 F21 R22 C23 R31 W34 Y35 R36 L46 T47 Y48 F49 Q50 N51 L55 S58 L61 S62 R69 G72 R81 T82 M89 S95 N98 E101 R109 L110 T111 E123 V124 A125 V126 F127 E128
P129 A140 A146 H153 V169 C170 D184 S185 R192 L193 R194 F199 W200 Q201 D202 E218 T223 A236 D243

4 Data and refinement statistics (i)

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 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (113.83-3.00) 99.1 (113.83-2.68)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	2666 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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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.*

[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: 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	0.68	0/2320	0.68	0/3149
1	F	0.68	0/2320	0.68	0/3149
2	B	0.66	0/860	0.67	0/1162
2	G	0.65	0/860	0.66	0/1162
3	C	0.62	0/84	0.62	0/112
3	H	0.60	0/84	0.82	0/112
4	D	0.70	0/1598	0.69	0/2170
4	I	0.71	0/1598	0.70	0/2170
5	E	0.65	0/1995	0.69	0/2706
5	J	0.65	0/1995	0.68	0/2706
All	All	0.67	0/13714	0.68	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	31	0
1	F	2254	0	2103	39	0
2	B	837	0	803	9	0
2	G	837	0	803	13	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	25	0
5	E	1945	0	1841	35	0
5	J	1945	0	1841	27	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	188	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 7.

All (188) 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:HH21	3:H:5:ARG:HG2	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:N	4:I:66:ARG:HD3	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ARG:CG	1:F:219:ARG:O	2.57	0.53
4:D:6:GLN:O	4:D:7:ASP:C	2.47	0.52
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:6:GLN:O	4:I:7:ASP:C	2.48	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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
4:D:157:CYS:C	5:E:170:CYS:SG	2.96	0.44
5:J:89:MET:SD	5:J:109:ARG:HG2	2.57	0.44
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
5:E:21:PHE:CZ	5:E:110:LEU:HB2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	2:B:63:TYR:O	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:CD1	2:G:63:TYR:O	2.71	0.43
1:A:191:HIS:O	1:A:191:HIS:CG	2.72	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
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
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
4:I:196:PHE:CE2	4:I:198:PRO:HB3	2.54	0.42
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
2:G:58:LYS:C	2:G:59:ASP:O	2.59	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
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
1:A:104:GLY:C	1:A:106:ASP:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:35:ARG:O	1:F:35:ARG:HG2	2.21	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
1:F:104:GLY:C	1:F:106:ASP:N	2.75	0.40
4:I:59:ARG:NH2	4:I:77:ASP:O	2.53	0.40
1:A:106:ASP:OD2	1:A:108:ARG:O	2.40	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 (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	274/276 (99%)	249 (91%)	23 (8%)	2 (1%)	22	60
1	F	274/276 (99%)	245 (89%)	27 (10%)	2 (1%)	22	60
2	B	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	15	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	15 53
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%)	5 28
4	I	197/203 (97%)	169 (86%)	24 (12%)	4 (2%)	7 34
5	E	240/243 (99%)	225 (94%)	13 (5%)	2 (1%)	19 57
5	J	240/243 (99%)	227 (95%)	11 (5%)	2 (1%)	19 57
All	All	1632/1662 (98%)	1486 (91%)	127 (8%)	19 (1%)	13 48

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
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 (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	232/232 (100%)	214 (92%)	18 (8%)	12 42
1	F	232/232 (100%)	216 (93%)	16 (7%)	15 48
2	B	95/95 (100%)	88 (93%)	7 (7%)	13 44
2	G	95/95 (100%)	90 (95%)	5 (5%)	22 58
3	C	9/9 (100%)	9 (100%)	0	100 100
3	H	9/9 (100%)	7 (78%)	2 (22%)	1 4
4	D	181/185 (98%)	168 (93%)	13 (7%)	14 45
4	I	181/185 (98%)	160 (88%)	21 (12%)	5 23
5	E	212/213 (100%)	203 (96%)	9 (4%)	30 66
5	J	212/213 (100%)	203 (96%)	9 (4%)	30 66
All	All	1458/1468 (99%)	1358 (93%)	100 (7%)	15 48

All (100) 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	35	ARG
1	A	88	SER
1	A	89	GLU
1	A	110	LEU
1	A	115	GLN
1	A	154	GLU
1	A	170	ARG
1	A	177	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	20	SER
2	B	55	SER
2	B	57	SER
2	B	70	PHE

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Mol	Chain	Res	Type
2	B	74	GLU
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	61	THR
4	D	63	GLN
4	D	66	ARG
4	D	127	SER
4	D	143	VAL
4	D	179	ASP
5	E	2	THR
5	E	5	SER
5	E	111	THR
5	E	153	HIS
5	E	184	ASP
5	E	199	PHE
5	E	202	ASP
5	E	223	THR
5	E	224	GLN
1	F	4	SER
1	F	10	THR
1	F	11	SER
1	F	35	ARG
1	F	88	SER
1	F	89	GLU
1	F	110	LEU
1	F	115	GLN
1	F	163	THR
1	F	170	ARG
1	F	196	ASP
1	F	200	THR
1	F	207	SER
1	F	216	THR
1	F	247	VAL
1	F	275	GLU
2	G	20	SER
2	G	55	SER
2	G	57	SER

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Mol	Chain	Res	Type
2	G	70	PHE
2	G	74	GLU
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	45	LYS
4	I	46	LEU
4	I	53	SER
4	I	66	ARG
4	I	77	ASP
4	I	80	LEU
4	I	85	THR
4	I	101	THR
4	I	110	ASN
4	I	113	ASN
4	I	121	LEU
4	I	138	ASP
4	I	148	ASP
4	I	175	SER
4	I	189	SER
5	J	5	SER
5	J	36	ARG
5	J	58	SER
5	J	111	THR
5	J	153	HIS
5	J	184	ASP
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 (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	87	GLN
1	A	141	GLN
4	D	22	ASN

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Mol	Chain	Res	Type
4	D	65	ASN
4	D	69	GLN
4	D	112	GLN
4	D	142	ASN
5	E	41	GLN
5	E	51	ASN
5	E	98	ASN
5	E	174	GLN
5	E	183	ASN
5	E	212	GLN
1	F	74	HIS
1	F	87	GLN
1	F	141	GLN
1	F	151	HIS
3	H	3	GLN
4	I	22	ASN
4	I	55	ASN
4	I	65	ASN
4	I	69	GLN
4	I	142	ASN
4	I	184	ASN
4	I	188	ASN
5	J	41	GLN
5	J	50	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	212	GLN
5	J	224	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)

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	F	301	-	6,6,6	0.17	0	5,5,5	0.06	0
7	SO4	E	301	-	4,4,4	0.37	0	6,6,6	0.05	0
7	SO4	A	302	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	F	302	-	4,4,4	0.37	0	6,6,6	0.04	0
7	SO4	B	101	-	4,4,4	0.38	0	6,6,6	0.05	0
6	PEG	A	301	-	6,6,6	0.20	0	5,5,5	0.08	0
7	SO4	I	301	-	4,4,4	0.38	0	6,6,6	0.05	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	A	301	-	-	2/4/4/4	-
6	PEG	F	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

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Mol	Chain	Res	Type	Atoms
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

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	276/276 (100%)	-0.10	17 (6%) 20 7	55, 102, 222, 250	0
1	F	276/276 (100%)	-0.10	17 (6%) 20 7	54, 106, 211, 231	0
2	B	100/100 (100%)	-0.56	0 100 100	57, 84, 130, 149	0
2	G	100/100 (100%)	-0.62	1 (1%) 82 59	62, 88, 136, 156	0
3	C	9/9 (100%)	-0.56	0 100 100	60, 65, 69, 74	0
3	H	9/9 (100%)	-0.38	0 100 100	60, 65, 73, 85	0
4	D	199/203 (98%)	-0.13	10 (5%) 28 10	64, 117, 182, 234	0
4	I	199/203 (98%)	-0.13	12 (6%) 21 7	65, 119, 180, 236	0
5	E	242/243 (99%)	-0.38	2 (0%) 86 65	60, 104, 153, 188	0
5	J	242/243 (99%)	-0.42	2 (0%) 86 65	58, 106, 161, 198	0
All	All	1652/1662 (99%)	-0.26	61 (3%) 41 17	54, 105, 188, 250	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	HIS	11.1
4	I	148	ASP	10.5
1	F	194	VAL	8.8
1	A	194	VAL	8.0
1	A	195	SER	7.3
1	F	197	HIS	6.9
1	F	193	ALA	6.7
1	F	195	SER	6.3
1	A	254	GLU	6.1
1	F	192	HIS	5.8
1	F	250	PRO	5.2
1	F	191	HIS	4.9
4	D	179	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	191	HIS	4.8
4	D	148	ASP	4.8
1	F	199	ALA	4.7
4	I	145	GLN	4.4
4	I	149	SER	4.3
5	E	223	THR	4.3
1	F	220	ASP	4.3
1	A	250	PRO	4.2
4	I	180	PHE	4.2
1	A	196	ASP	4.0
1	A	257	TYR	4.0
1	A	272	LEU	3.9
1	A	199	ALA	3.8
4	D	147	LYS	3.6
1	A	192	HIS	3.6
4	D	178	SER	3.5
1	F	255	GLN	3.4
4	I	185	ALA	3.4
1	F	249	VAL	3.4
4	D	200	PRO	3.3
4	I	200	PRO	3.2
4	D	149	SER	3.1
4	D	184	ASN	3.1
2	G	99	MET	3.0
4	I	201	GLU	3.0
4	I	164	MET	3.0
1	A	260	HIS	2.9
1	A	255	GLN	2.9
4	D	187	ASN	2.9
5	J	185	SER	2.8
4	I	147	LYS	2.8
1	F	248	VAL	2.7
1	F	254	GLU	2.7
1	F	276	PRO	2.7
1	F	257	TYR	2.6
1	A	273	ARG	2.5
1	F	224	GLN	2.5
4	D	151	VAL	2.5
4	I	184	ASN	2.5
4	I	187	ASN	2.4
1	A	217	TRP	2.3
4	I	9	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
5	J	199	PHE	2.2
1	A	253	GLN	2.2
1	A	201	LEU	2.1
5	E	116	LEU	2.1
4	D	174	TRP	2.1
1	F	198	GLU	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	SO4	E	301	5/5	0.73	0.22	157,160,176,183	0
6	PEG	F	301	7/7	0.78	0.23	97,108,119,123	0
7	SO4	A	302	5/5	0.82	0.27	140,141,152,155	0
6	PEG	A	301	7/7	0.82	0.23	97,101,111,114	0
7	SO4	I	301	5/5	0.84	0.15	157,157,159,162	0
7	SO4	B	101	5/5	0.90	0.10	173,175,176,179	0
7	SO4	F	302	5/5	0.95	0.08	113,127,131,132	0

6.5 Other polymers (i)

There are no such residues in this entry.