



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 08:41 pm GMT

PDB ID : 5NMF
Title : 868 TCR in complex with HLA A02 presenting SLYNTIATL
Authors : Rizkallah, P.J.; Cole, D.K.; Fuller, A.; Sewell, A.K.
Deposited on : 2017-04-05
Resolution : 2.89 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

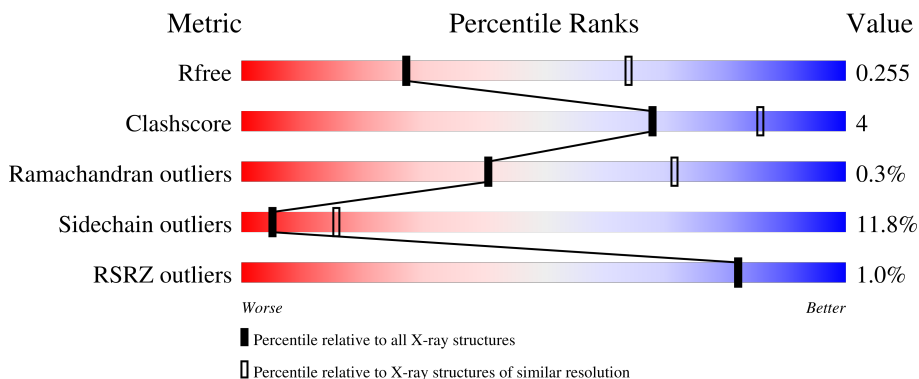
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	 84% 13% .
1	F	276	 80% 16% .
2	B	100	 6% 70% 26% ..
2	G	100	 75% 23% .
3	C	9	 78% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	9	 67% 22% 11%
4	D	200	 2% 82% 16%
5	E	240	 84% 15%
5	J	240	 85% 13%
6	I	201	 2% 83% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	SO4	E	307	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13511 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
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 Gag protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	Total	C	N	O	0	0	0
			70	45	10	15			
3	H	9	Total	C	N	O	0	0	0
			70	45	10	15			

- Molecule 4 is a protein called HUman T-cell receptor Alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	200	Total	C	N	O	S	0	0	0
			1560	976	259	317	8			

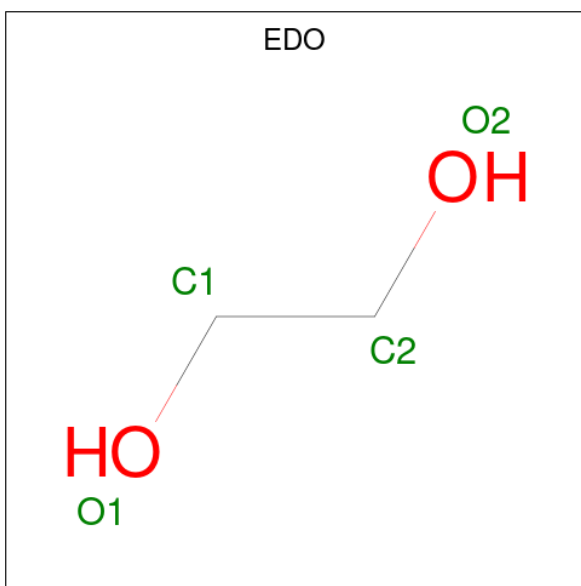
- Molecule 5 is a protein called Human T-cell receptor Beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	239	Total	C	N	O	S	0	0	0
			1917	1208	334	370	5			
5	J	240	Total	C	N	O	S	0	0	0
			1922	1211	335	371	5			

- Molecule 6 is a protein called HUman T-cell receptor Alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	I	201	Total	C	N	O	S	0	0	0
			1567	981	260	318	8			

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	J	1	Total	O	S	0	0
			5	4	1		
9	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total	O	0	0
			3	3		
10	B	3	Total	O	0	0
			3	3		
10	D	9	Total	O	0	0
			9	9		
10	E	7	Total	O	0	0
			7	7		
10	F	19	Total	O	0	0
			19	19		
10	G	5	Total	O	0	0
			5	5		
10	H	1	Total	O	0	0
			1	1		
10	I	10	Total	O	0	0
			10	10		

Continued on next page...

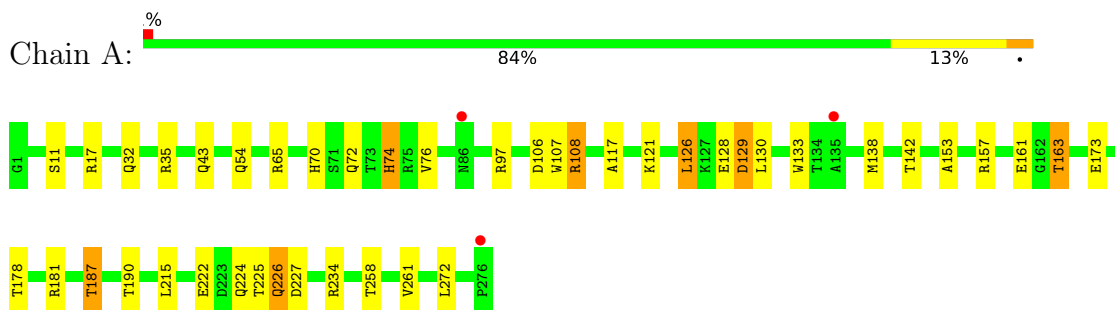
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	J	20	Total	O	0	0
			20	20		

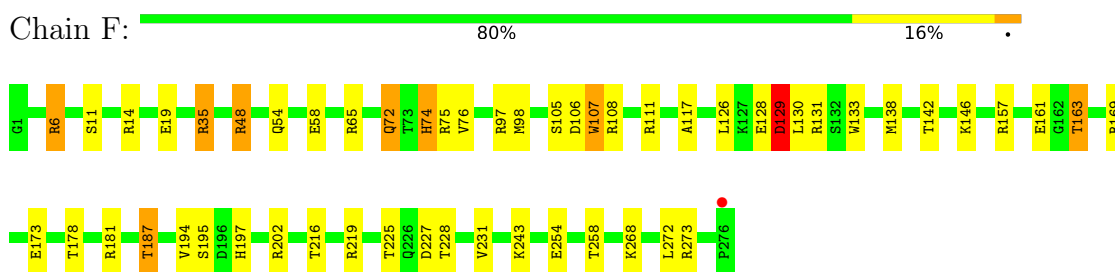
3 Residue-property plots [i](#)

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.

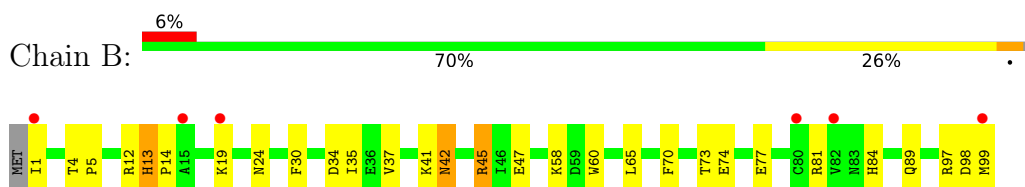
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



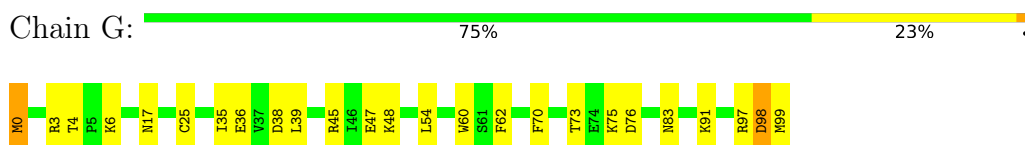
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain




- Molecule 2: Beta-2-microglobulin

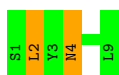


- Molecule 2: Beta-2-microglobulin



- Molecule 3: Gag protein

Chain C:  78% 22%




- Molecule 3: Gag protein

Chain H:  67% 22% 11%




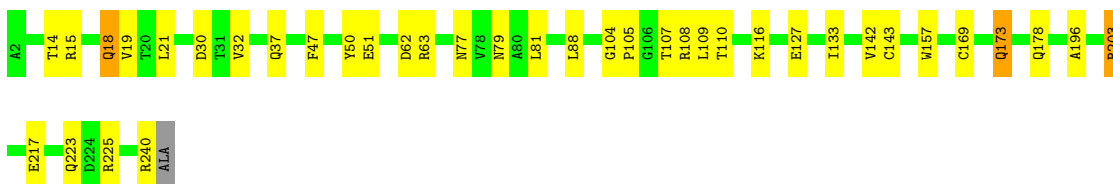
- Molecule 4: HUman T-cell receptor Alpha chain

Chain D:  2% 82% 16%




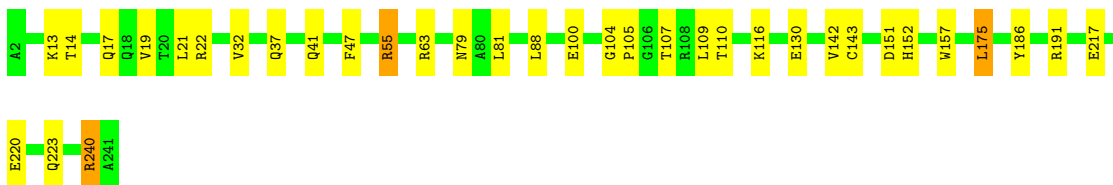
- Molecule 5: Human T-cell receptor Beta chain

Chain E:  84% 15%




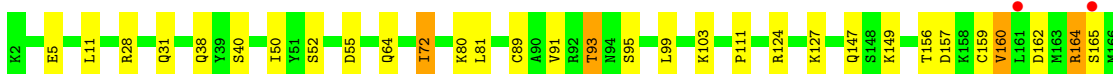
- Molecule 5: Human T-cell receptor Beta chain

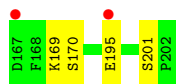
Chain J:  85% 13%



- Molecule 6: HUman T-cell receptor Alpha chain

Chain I:  2% 83% 15%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	207.59Å 84.71Å 112.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.12 – 2.89 112.12 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (112.12-2.89) 99.9 (112.12-2.89)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.193 , 0.255 0.196 , 0.255	Depositor DCC
R_{free} test set	2277 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13511	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, 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	0.75	0/2320	0.90	2/3149 (0.1%)
1	F	0.85	0/2320	1.01	11/3149 (0.3%)
2	B	0.70	0/852	0.91	1/1152 (0.1%)
2	G	0.85	0/860	0.97	3/1162 (0.3%)
3	C	0.81	0/70	1.03	0/94
3	H	0.98	0/70	1.35	0/94
4	D	0.79	0/1593	0.95	0/2155
5	E	0.81	0/1972	0.93	3/2688 (0.1%)
5	J	0.85	1/1977 (0.1%)	0.96	4/2695 (0.1%)
6	I	0.81	0/1601	0.95	2/2167 (0.1%)
All	All	0.81	1/13635 (0.0%)	0.95	26/18505 (0.1%)

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
2	G	0	1
4	D	0	2
6	I	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	100	GLU	CD-OE1	5.82	1.32	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	38	ASP	CB-CG-OD1	7.65	125.18	118.30
5	J	22	ARG	NE-CZ-NH1	-7.59	116.50	120.30
6	I	28	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	107	TRP	CA-CB-CG	7.18	127.34	113.70
1	F	111	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	F	138	MET	CG-SD-CE	6.34	110.35	100.20
5	J	55	ARG	CG-CD-NE	-6.32	98.53	111.80
1	F	106	ASP	CB-CG-OD1	6.18	123.86	118.30
5	J	191	ARG	CG-CD-NE	5.90	124.19	111.80
1	F	129	ASP	CB-CG-OD1	5.76	123.48	118.30
1	F	75	ARG	NE-CZ-NH2	5.71	123.16	120.30
2	G	3	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	F	219	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	108	ARG	NE-CZ-NH1	5.44	123.02	120.30
5	E	108	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	157	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	108	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	B	12	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	F	202	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	G	76	ASP	CB-CG-OD1	5.13	122.91	118.30
5	E	225	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	F	6	ARG	CG-CD-NE	5.08	122.47	111.80
1	F	157	ARG	NE-CZ-NH1	5.08	122.84	120.30
5	E	203	ARG	NE-CZ-NH1	5.08	122.84	120.30
5	J	240	ARG	NE-CZ-NH2	5.07	122.83	120.30
6	I	164	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	130	ASP	Peptide
4	D	195	GLU	Peptide
2	G	0	MET	Peptide
6	I	201	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2103	22	0
1	F	2254	0	2103	18	0
2	B	829	0	794	15	0
2	G	837	0	803	7	0
3	C	70	0	74	3	0
3	H	70	0	74	3	0
4	D	1560	0	1486	13	0
5	E	1917	0	1798	14	0
5	J	1922	0	1803	12	0
6	I	1567	0	1493	16	0
7	A	4	0	6	0	0
7	D	4	0	6	0	0
7	E	12	0	18	0	0
7	F	24	0	36	0	0
7	I	8	0	12	0	0
7	J	24	0	36	2	0
8	A	6	0	8	0	0
8	D	6	0	8	0	0
8	I	6	0	8	0	0
9	A	20	0	0	1	0
9	E	20	0	0	2	0
9	F	10	0	0	0	0
9	J	10	0	0	0	0
10	A	3	0	0	0	0
10	B	3	0	0	0	0
10	D	9	0	0	0	0
10	E	7	0	0	0	0
10	F	19	0	0	0	0
10	G	5	0	0	0	0
10	H	1	0	0	0	0
10	I	10	0	0	1	0
10	J	20	0	0	0	0
All	All	13511	0	12669	99	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 4.

All (99) 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)
2:B:35:ILE:HD11	2:B:84:HIS:CD2	1.87	1.09
4:D:38:GLN:HE22	5:E:37:GLN:HE22	1.11	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:38:GLN:HE22	5:J:37:GLN:HE22	0.96	0.91
1:A:234:ARG:NH1	2:B:99:MET:SD	2.55	0.78
6:I:38:GLN:HE22	5:J:37:GLN:NE2	1.80	0.72
6:I:38:GLN:NE2	5:J:37:GLN:HE22	1.80	0.71
1:F:163:THR:CG2	6:I:31:GLN:HE21	2.02	0.71
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.40	0.69
1:F:74:HIS:HE1	1:F:97:ARG:HE	1.41	0.68
1:F:163:THR:HG21	6:I:31:GLN:HE21	1.58	0.68
5:E:18:GLN:NE2	5:E:77:ASN:HD21	1.91	0.68
1:A:163:THR:CG2	4:D:31:GLN:HE21	2.09	0.66
5:J:151:ASP:HB3	5:J:186:TYR:CE2	2.34	0.63
4:D:110:THR:HG23	4:D:141:SER:CB	2.29	0.62
1:A:72:GLN:NE2	5:E:51:GLU:OE2	2.33	0.61
2:B:35:ILE:HG22	2:B:37:VAL:HG23	1.83	0.61
6:I:156:THR:HG22	5:J:175:LEU:HD21	1.82	0.60
5:E:15:ARG:NH2	9:E:307:SO4:O1	2.36	0.59
1:A:70:HIS:CE1	3:C:2:LEU:HD23	2.38	0.59
2:B:13:HIS:CG	2:B:14:PRO:HD2	2.39	0.58
5:J:21:LEU:HD22	5:J:107:THR:HG21	1.86	0.57
5:J:13:LYS:HD2	5:J:17:GLN:NE2	2.20	0.57
4:D:38:GLN:NE2	5:E:37:GLN:HE22	1.93	0.56
1:F:163:THR:HG21	6:I:31:GLN:NE2	2.20	0.56
1:F:35:ARG:HD2	1:F:48:ARG:CZ	2.35	0.56
1:A:163:THR:HG21	4:D:31:GLN:HE21	1.70	0.55
4:D:110:THR:HG23	4:D:141:SER:HB3	1.88	0.55
5:E:173:GLN:HE21	5:E:173:GLN:HA	1.71	0.55
1:A:70:HIS:CE1	3:C:2:LEU:CD2	2.91	0.54
1:F:231:VAL:O	1:F:243:LYS:NZ	2.37	0.53
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.43	0.53
4:D:38:GLN:HE22	5:E:37:GLN:NE2	1.94	0.53
5:J:223:GLN:HE21	7:J:303:EDO:H11	1.75	0.52
1:A:187:THR:HB	1:A:272:LEU:HD21	1.91	0.52
1:A:129:ASP:C	1:A:130:LEU:HG	2.29	0.52
6:I:55:ASP:OD1	6:I:64:GLN:HG3	2.11	0.51
5:E:21:LEU:HD22	5:E:107:THR:HG21	1.93	0.51
1:F:272:LEU:N	1:F:272:LEU:HD12	2.25	0.50
5:E:30:ASP:OD2	5:E:50:TYR:HE1	1.92	0.50
4:D:21:LEU:HD22	4:D:87:TYR:HB2	1.93	0.50
1:F:146:LYS:HE3	3:H:9:LEU:OXT	2.12	0.49
1:F:72:GLN:HG3	7:J:306:EDO:O2	2.12	0.49
6:I:162:ASP:HB3	6:I:164:ARG:HE	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:HE21	1:A:226:GLN:HA	1.77	0.49
1:F:129:ASP:C	1:F:130:LEU:HG	2.33	0.49
3:H:6:ILE:HG23	3:H:6:ILE:O	2.13	0.48
1:A:121:LYS:HD3	2:B:1:ILE:HG21	1.96	0.48
1:F:163:THR:HG23	6:I:31:GLN:HE21	1.75	0.48
5:J:151:ASP:HB3	5:J:186:TYR:CD2	2.49	0.48
2:B:34:ASP:O	2:B:35:ILE:HD13	2.14	0.48
2:G:36:GLU:HG2	2:G:83:ASN:HB3	1.96	0.47
1:F:126:LEU:HD13	1:F:133:TRP:CZ3	2.50	0.47
6:I:149:LYS:NZ	10:I:401:HOH:O	2.47	0.47
2:B:5:PRO:HD3	2:B:84:HIS:CD2	2.50	0.47
1:F:128:GLU:C	1:F:129:ASP:O	2.50	0.46
2:B:41:LYS:O	2:B:42:ASN:ND2	2.48	0.46
1:A:153:ALA:HB3	9:A:305:SO4:O3	2.15	0.46
4:D:22:ASN:ND2	4:D:73:SER:OG	2.49	0.46
1:F:187:THR:HB	1:F:272:LEU:HD21	1.98	0.46
4:D:6:GLN:O	4:D:103:LYS:HE2	2.15	0.45
5:J:104:GLY:C	5:J:105:PRO:O	2.53	0.45
1:A:190:THR:HG21	2:B:98:ASP:OD1	2.16	0.45
1:A:215:LEU:HD12	1:A:261:VAL:HG22	1.97	0.45
2:B:35:ILE:CD1	2:B:84:HIS:CD2	2.79	0.45
6:I:81:LEU:HD21	6:I:111:PRO:HB3	1.99	0.45
1:A:163:THR:HG23	4:D:31:GLN:HE21	1.79	0.45
6:I:93:THR:HG22	6:I:95:SER:H	1.81	0.45
1:A:126:LEU:HD13	1:A:133:TRP:CZ3	2.52	0.44
5:E:143:CYS:HB2	5:E:157:TRP:CZ2	2.53	0.44
5:E:104:GLY:C	5:E:105:PRO:O	2.53	0.44
2:G:17:ASN:OD1	2:G:97:ARG:NH1	2.49	0.44
1:A:106:ASP:O	1:A:106:ASP:CG	2.54	0.44
2:B:45:ARG:NH1	2:B:47:GLU:OE1	2.50	0.44
2:G:35:ILE:O	2:G:35:ILE:HG23	2.17	0.44
5:E:133:ILE:HG23	5:E:196:ALA:HB1	1.99	0.43
1:A:128:GLU:C	1:A:129:ASP:O	2.53	0.43
4:D:192:ILE:HD13	4:D:192:ILE:O	2.19	0.43
6:I:111:PRO:HG3	6:I:160:VAL:HG21	2.01	0.43
1:A:215:LEU:CD1	1:A:261:VAL:HG22	2.48	0.43
1:A:126:LEU:HD23	1:A:130:LEU:HD22	2.00	0.43
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.99	0.42
6:I:103:LYS:HG2	5:J:41:GLN:HE22	1.84	0.42
2:B:35:ILE:HD11	2:B:84:HIS:CG	2.46	0.42
1:A:106:ASP:O	1:A:106:ASP:OD1	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:LEU:HD23	1:F:130:LEU:HD22	2.00	0.42
3:C:4:ASN:H	3:C:4:ASN:HD22	1.66	0.42
5:J:143:CYS:HB2	5:J:157:TRP:CZ2	2.55	0.42
4:D:75:LEU:HD22	4:D:75:LEU:N	2.35	0.41
5:E:15:ARG:NH2	9:E:307:SO4:S	2.94	0.41
3:H:6:ILE:O	3:H:6:ILE:CG2	2.68	0.41
6:I:72:ILE:HD13	6:I:89:CYS:SG	2.61	0.41
2:G:54:LEU:HD11	2:G:62:PHE:HB3	2.02	0.41
1:F:194:VAL:HG12	1:F:195:SER:N	2.36	0.41
2:B:30:PHE:HB2	2:B:84:HIS:NE2	2.36	0.41
1:F:169:ARG:O	1:F:173:GLU:HG3	2.21	0.41
2:G:25:CYS:HB2	2:G:39:LEU:HD21	2.02	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40
2:G:98:ASP:O	2:G:99:MET:HG2	2.21	0.40
5:E:18:GLN:HE21	5:E:18:GLN:HB2	1.67	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%)	257 (94%)	15 (6%)	2 (1%)	22	54
1	F	274/276 (99%)	260 (95%)	13 (5%)	1 (0%)	34	66
2	B	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
2	G	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/200 (99%)	185 (93%)	12 (6%)	1 (0%)	29	61
5	E	237/240 (99%)	229 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	238/240 (99%)	230 (97%)	7 (3%)	1 (0%)	34	66
6	I	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
All	All	1629/1651 (99%)	1540 (94%)	84 (5%)	5 (0%)	41	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	167	ASP
1	A	107	TRP
1	A	129	ASP
1	F	129	ASP
5	J	63	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%)	207 (89%)	25 (11%)	6	20
1	F	232/232 (100%)	201 (87%)	31 (13%)	4	11
2	B	94/95 (99%)	81 (86%)	13 (14%)	3	10
2	G	95/95 (100%)	84 (88%)	11 (12%)	5	16
3	C	8/8 (100%)	6 (75%)	2 (25%)	0	2
3	H	8/8 (100%)	6 (75%)	2 (25%)	0	2
4	D	178/178 (100%)	152 (85%)	26 (15%)	3	9
5	E	209/209 (100%)	187 (90%)	22 (10%)	7	21
5	J	209/209 (100%)	191 (91%)	18 (9%)	10	30
6	I	179/179 (100%)	159 (89%)	20 (11%)	6	18
All	All	1444/1445 (100%)	1274 (88%)	170 (12%)	5	16

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	17	ARG
1	A	32	GLN
1	A	35	ARG
1	A	43	GLN
1	A	54	GLN
1	A	65	ARG
1	A	74	HIS
1	A	76	VAL
1	A	108	ARG
1	A	126	LEU
1	A	138	MET
1	A	142	THR
1	A	161	GLU
1	A	163	THR
1	A	173	GLU
1	A	178	THR
1	A	181	ARG
1	A	187	THR
1	A	222	GLU
1	A	224	GLN
1	A	225	THR
1	A	226	GLN
1	A	227	ASP
1	A	258	THR
2	B	4	THR
2	B	13	HIS
2	B	19	LYS
2	B	42	ASN
2	B	45	ARG
2	B	58	LYS
2	B	70	PHE
2	B	73	THR
2	B	74	GLU
2	B	77	GLU
2	B	81	ARG
2	B	89	GLN
2	B	97	ARG
3	C	2	LEU
3	C	4	ASN
4	D	2	LYS
4	D	3	GLU
4	D	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	12	SER
4	D	40	SER
4	D	42	LYS
4	D	50	ILE
4	D	52	SER
4	D	64	GLN
4	D	72	ILE
4	D	75	LEU
4	D	91	VAL
4	D	99	LEU
4	D	110	THR
4	D	114	GLN
4	D	122	GLN
4	D	124	ARG
4	D	127	LYS
4	D	147	GLN
4	D	158	LYS
4	D	160	VAL
4	D	170	SER
4	D	186	ASN
4	D	192	ILE
4	D	193	ILE
4	D	195	GLU
5	E	14	THR
5	E	18	GLN
5	E	19	VAL
5	E	32	VAL
5	E	47	PHE
5	E	62	ASP
5	E	63	ARG
5	E	79	ASN
5	E	81	LEU
5	E	88	LEU
5	E	109	LEU
5	E	110	THR
5	E	116	LYS
5	E	127	GLU
5	E	142	VAL
5	E	169	CYS
5	E	173	GLN
5	E	178	GLN
5	E	203	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	217	GLU
5	E	223	GLN
5	E	240	ARG
1	F	6	ARG
1	F	11	SER
1	F	14	ARG
1	F	19	GLU
1	F	35	ARG
1	F	48	ARG
1	F	54	GLN
1	F	58	GLU
1	F	65	ARG
1	F	72	GLN
1	F	74	HIS
1	F	76	VAL
1	F	98	MET
1	F	105	SER
1	F	107	TRP
1	F	131	ARG
1	F	142	THR
1	F	161	GLU
1	F	163	THR
1	F	178	THR
1	F	181	ARG
1	F	187	THR
1	F	197	HIS
1	F	216	THR
1	F	225	THR
1	F	227	ASP
1	F	228	THR
1	F	254	GLU
1	F	258	THR
1	F	268	LYS
1	F	273	ARG
2	G	0	MET
2	G	4	THR
2	G	6	LYS
2	G	45	ARG
2	G	47	GLU
2	G	48	LYS
2	G	70	PHE
2	G	73	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	75	LYS
2	G	91	LYS
2	G	98	ASP
3	H	2	LEU
3	H	9	LEU
6	I	5	GLU
6	I	11	LEU
6	I	40	SER
6	I	50	ILE
6	I	52	SER
6	I	72	ILE
6	I	80	LYS
6	I	91	VAL
6	I	93	THR
6	I	99	LEU
6	I	124	ARG
6	I	127	LYS
6	I	147	GLN
6	I	157	ASP
6	I	159	CYS
6	I	160	VAL
6	I	165	SER
6	I	169	LYS
6	I	170	SER
6	I	195	GLU
5	J	14	THR
5	J	19	VAL
5	J	32	VAL
5	J	47	PHE
5	J	55	ARG
5	J	79	ASN
5	J	81	LEU
5	J	88	LEU
5	J	109	LEU
5	J	110	THR
5	J	116	LYS
5	J	130	GLU
5	J	142	VAL
5	J	152	HIS
5	J	175	LEU
5	J	217	GLU
5	J	220	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	J	240	ARG

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	72	GLN
1	A	74	HIS
1	A	93	HIS
1	A	115	GLN
1	A	174	ASN
1	A	226	GLN
1	A	262	GLN
2	B	42	ASN
3	C	4	ASN
4	D	6	GLN
4	D	22	ASN
4	D	31	GLN
5	E	10	HIS
5	E	18	GLN
5	E	37	GLN
5	E	79	ASN
5	E	117	ASN
5	E	137	GLN
5	E	173	GLN
5	E	205	HIS
1	F	72	GLN
1	F	74	HIS
1	F	93	HIS
1	F	115	GLN
1	F	174	ASN
1	F	262	GLN
6	I	6	GLN
6	I	31	GLN
6	I	70	GLN
6	I	122	GLN
6	I	147	GLN
5	J	17	GLN
5	J	37	GLN
5	J	41	GLN
5	J	79	ASN
5	J	117	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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	$\# Z > 2$
7	EDO	J	302	-	3,3,3	0.42	0	2,2,2	0.41	0
9	SO4	F	308	-	4,4,4	0.43	0	6,6,6	0.36	0
7	EDO	F	303	-	3,3,3	0.57	0	2,2,2	0.15	0
7	EDO	E	302	-	3,3,3	0.43	0	2,2,2	0.38	0
7	EDO	F	305	-	3,3,3	0.53	0	2,2,2	0.32	0
7	EDO	E	301	-	3,3,3	0.48	0	2,2,2	0.51	0
8	GOL	I	303	-	5,5,5	0.47	0	5,5,5	0.59	0
9	SO4	A	303	-	4,4,4	0.32	0	6,6,6	0.40	0
7	EDO	F	302	-	3,3,3	0.45	0	2,2,2	0.38	0
7	EDO	J	305	-	3,3,3	0.56	0	2,2,2	0.17	0
7	EDO	F	306	-	3,3,3	0.53	0	2,2,2	0.28	0
7	EDO	I	301	-	3,3,3	0.52	0	2,2,2	0.27	0
9	SO4	A	304	-	4,4,4	0.36	0	6,6,6	0.21	0
7	EDO	J	304	-	3,3,3	0.58	0	2,2,2	0.26	0
9	SO4	E	307	-	4,4,4	0.27	0	6,6,6	0.47	0
7	EDO	J	306	-	3,3,3	0.52	0	2,2,2	0.43	0
7	EDO	I	302	-	3,3,3	0.46	0	2,2,2	0.29	0
7	EDO	A	301	-	3,3,3	0.62	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	E	305	-	4,4,4	0.38	0	6,6,6	0.24	0
7	EDO	F	301	-	3,3,3	0.39	0	2,2,2	0.53	0
7	EDO	D	301	-	3,3,3	0.57	0	2,2,2	0.28	0
7	EDO	F	304	-	3,3,3	0.43	0	2,2,2	0.45	0
9	SO4	A	305	-	4,4,4	0.40	0	6,6,6	0.22	0
9	SO4	J	307	-	4,4,4	0.40	0	6,6,6	0.19	0
9	SO4	A	306	-	4,4,4	0.36	0	6,6,6	0.19	0
8	GOL	D	302	-	5,5,5	0.53	0	5,5,5	0.25	0
9	SO4	E	304	-	4,4,4	0.41	0	6,6,6	0.18	0
9	SO4	J	308	-	4,4,4	0.31	0	6,6,6	0.51	0
9	SO4	E	306	-	4,4,4	0.39	0	6,6,6	0.30	0
7	EDO	J	303	-	3,3,3	0.64	0	2,2,2	0.06	0
9	SO4	F	307	-	4,4,4	0.54	0	6,6,6	0.48	0
7	EDO	E	303	-	3,3,3	0.49	0	2,2,2	0.23	0
7	EDO	J	301	-	3,3,3	0.48	0	2,2,2	0.37	0
8	GOL	A	302	-	5,5,5	0.55	0	5,5,5	0.53	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
7	EDO	J	302	-	-	0/1/1/1	-
7	EDO	F	303	-	-	0/1/1/1	-
7	EDO	E	302	-	-	0/1/1/1	-
7	EDO	F	305	-	-	1/1/1/1	-
7	EDO	E	301	-	-	1/1/1/1	-
8	GOL	I	303	-	-	2/4/4/4	-
7	EDO	F	302	-	-	1/1/1/1	-
7	EDO	J	305	-	-	0/1/1/1	-
7	EDO	F	306	-	-	1/1/1/1	-
7	EDO	I	301	-	-	1/1/1/1	-
7	EDO	J	304	-	-	1/1/1/1	-
7	EDO	J	306	-	-	1/1/1/1	-
7	EDO	I	302	-	-	1/1/1/1	-
7	EDO	A	301	-	-	0/1/1/1	-
7	EDO	F	301	-	-	0/1/1/1	-
7	EDO	D	301	-	-	0/1/1/1	-
7	EDO	F	304	-	-	0/1/1/1	-
8	GOL	D	302	-	-	3/4/4/4	-
7	EDO	J	303	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	E	303	-	-	1/1/1/1	-
7	EDO	J	301	-	-	0/1/1/1	-
8	GOL	A	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	302	GOL	C1-C2-C3-O3
8	D	302	GOL	O1-C1-C2-O2
8	D	302	GOL	O1-C1-C2-C3
8	I	303	GOL	O1-C1-C2-C3
8	D	302	GOL	C1-C2-C3-O3
7	J	304	EDO	O1-C1-C2-O2
7	J	306	EDO	O1-C1-C2-O2
8	A	302	GOL	O2-C2-C3-O3
8	I	303	GOL	O1-C1-C2-O2
7	I	301	EDO	O1-C1-C2-O2
7	I	302	EDO	O1-C1-C2-O2
7	E	301	EDO	O1-C1-C2-O2
7	F	302	EDO	O1-C1-C2-O2
7	F	305	EDO	O1-C1-C2-O2
7	F	306	EDO	O1-C1-C2-O2
7	J	303	EDO	O1-C1-C2-O2
7	E	303	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	307	SO4	2	0
7	J	306	EDO	1	0
9	A	305	SO4	1	0
7	J	303	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.15	3 (1%) 80 80	43, 70, 107, 143	0
1	F	276/276 (100%)	-0.13	1 (0%) 92 93	26, 47, 86, 125	0
2	B	99/100 (99%)	0.65	6 (6%) 21 17	63, 95, 123, 128	0
2	G	100/100 (100%)	-0.23	0 100 100	28, 48, 73, 82	0
3	C	9/9 (100%)	0.36	0 100 100	45, 50, 62, 71	0
3	H	9/9 (100%)	-0.14	0 100 100	28, 30, 35, 41	0
4	D	200/200 (100%)	0.03	3 (1%) 73 73	33, 53, 106, 137	0
5	E	239/240 (99%)	-0.13	0 100 100	31, 50, 76, 109	0
5	J	240/240 (100%)	-0.19	0 100 100	26, 43, 71, 102	0
6	I	201/201 (100%)	-0.01	4 (1%) 65 63	27, 51, 102, 119	0
All	All	1649/1651 (99%)	-0.01	17 (1%) 82 82	26, 54, 102, 143	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	129	SER	4.2
2	B	19	LYS	3.5
6	I	195	GLU	3.4
2	B	1	ILE	3.2
1	A	276	PRO	3.1
4	D	130	ASP	3.0
2	B	15	ALA	2.8
1	F	276	PRO	2.7
6	I	165	SER	2.7
6	I	161	LEU	2.5
6	I	167	ASP	2.4
2	B	82	VAL	2.3
2	B	80	CYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	86	ASN	2.2
1	A	135	ALA	2.1
2	B	99	MET	2.1
4	D	152	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 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, 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
8	GOL	D	302	6/6	0.56	0.27	87,93,97,97	0
7	EDO	A	301	4/4	0.74	0.23	61,63,65,65	0
7	EDO	I	302	4/4	0.79	0.23	72,80,80,81	0
7	EDO	J	305	4/4	0.80	0.22	57,60,62,63	0
8	GOL	A	302	6/6	0.80	0.23	63,67,69,69	0
7	EDO	F	305	4/4	0.80	0.23	51,57,60,60	0
9	SO4	A	306	5/5	0.84	0.34	109,109,112,116	0
7	EDO	F	302	4/4	0.85	0.16	57,60,62,64	0
7	EDO	J	302	4/4	0.86	0.20	53,53,54,55	0
7	EDO	F	304	4/4	0.87	0.21	69,75,77,78	0
7	EDO	J	306	4/4	0.88	0.50	48,53,54,55	0
7	EDO	J	301	4/4	0.88	0.20	63,67,70,72	0
8	GOL	I	303	6/6	0.89	0.19	55,59,62,64	0
9	SO4	A	304	5/5	0.89	0.16	98,104,110,113	0
7	EDO	F	303	4/4	0.89	0.16	57,58,59,61	0
9	SO4	J	307	5/5	0.89	0.27	87,88,92,93	0
7	EDO	J	303	4/4	0.90	0.25	41,49,55,61	0
7	EDO	J	304	4/4	0.91	0.12	54,54,56,56	0
7	EDO	E	302	4/4	0.91	0.18	38,42,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	E	303	4/4	0.91	0.16	65,66,67,69	0
9	SO4	A	305	5/5	0.92	0.23	95,95,101,102	0
9	SO4	E	304	5/5	0.93	0.18	80,81,84,85	0
9	SO4	E	305	5/5	0.93	0.20	100,100,101,107	0
7	EDO	E	301	4/4	0.93	0.20	52,54,55,55	0
7	EDO	F	306	4/4	0.94	0.14	57,58,58,60	0
9	SO4	F	307	5/5	0.94	0.12	58,58,65,70	0
7	EDO	I	301	4/4	0.94	0.12	50,51,52,52	0
7	EDO	F	301	4/4	0.95	0.17	46,46,47,49	0
9	SO4	A	303	5/5	0.96	0.19	66,72,76,78	0
7	EDO	D	301	4/4	0.96	0.12	39,42,44,44	0
9	SO4	J	308	5/5	0.96	0.12	61,64,66,71	0
9	SO4	E	306	5/5	0.97	0.10	52,54,57,60	0
9	SO4	F	308	5/5	0.97	0.15	57,63,65,66	0
9	SO4	E	307	5/5	0.99	0.13	37,37,39,40	5

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.