Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:44 pm BST

PDB ID	:	5NME
Title	:	868 TCR in complex with HLA A02 presenting SLYNTVATL
Authors	:	Rizkallah, P.J.; Cole, D.K.; Fuller, A.; Sewell, A.K.
Deposited on	:	2017-04-05
Resolution	:	2.94 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 following versions of software and data (see references ⓘ) were used in the production of this report:

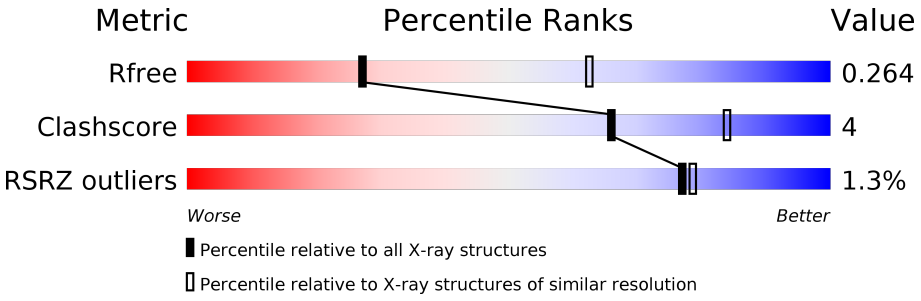
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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 on 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	88% 12%
1	F	276	89% 11%
2	B	100	87% 13%
2	G	100	8% 85% 15%
3	C	9	67% 33%
3	H	9	11% 89% 11%
4	D	201	93% 7%
4	I	201	91% 8%

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Mol	Chain	Length	Quality of chain
5	E	242	88% 12%
5	J	242	2% 91% 8%

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
7	SO4	J	305	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13441 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
1	A	276	Total	C	N	O	S	0	1	0
			2264	1414	413	428	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 Gag protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			69	44	10	15			
3	H	9	Total	C	N	O	0	0	0
			69	44	10	15			

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

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

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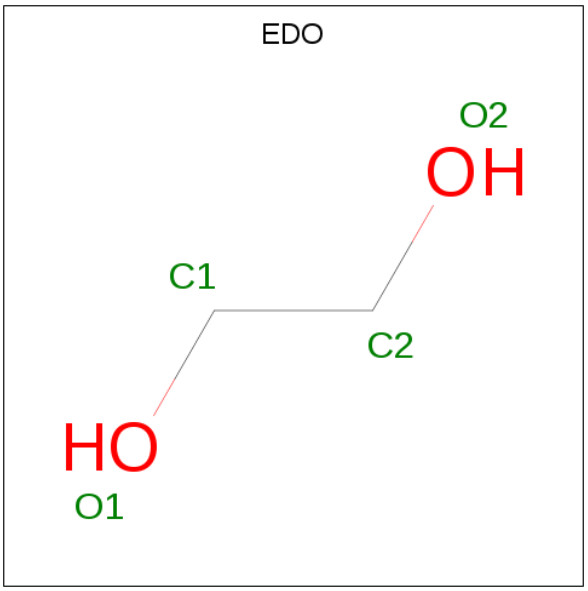
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	200	Total	C	N	O	S	0	0	0
			1560	976	259	317	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	0	0
			1939	1219	337	378	5			
5	J	241	Total	C	N	O	S	0	0	0
			1930	1215	336	374	5			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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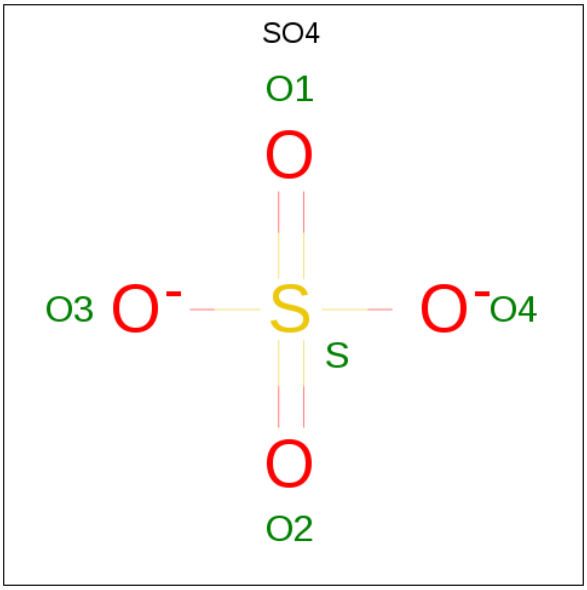
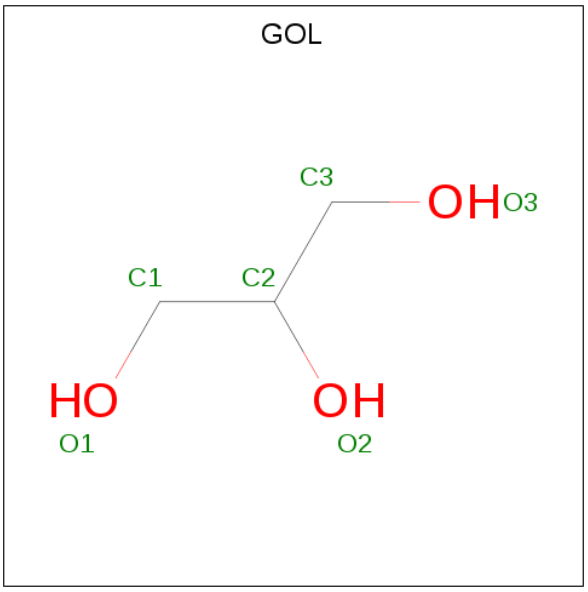
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 4 2 2	0	0
6	J	1	Total C O 4 2 2	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is water.

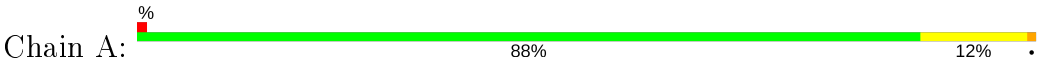
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	13	Total O 13 13	0	0
9	B	4	Total O 4 4	0	0
9	D	5	Total O 5 5	0	0
9	E	4	Total O 4 4	0	0
9	F	5	Total O 5 5	0	0
9	G	1	Total O 1 1	0	0
9	I	5	Total O 5 5	0	0
9	J	5	Total O 5 5	0	0

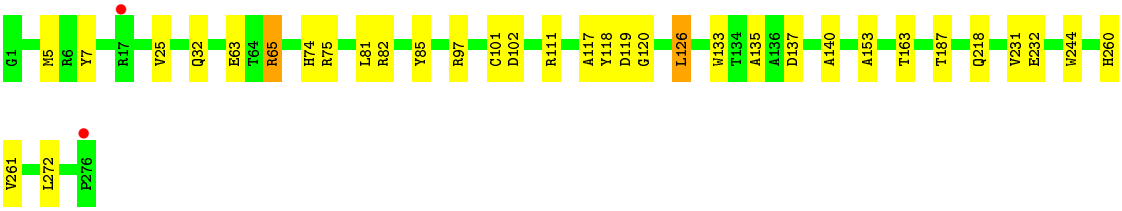
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

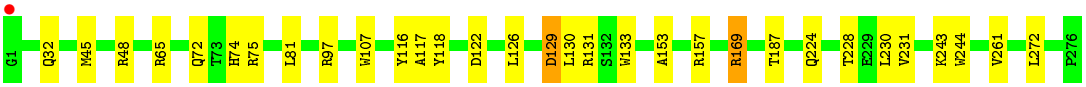
Chain A:





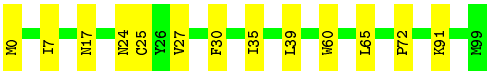
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain F:



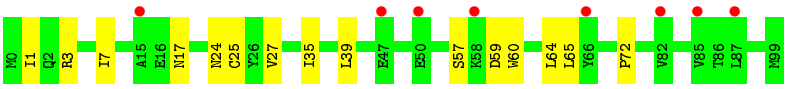
- Molecule 2: Beta-2-microglobulin

Chain B:



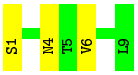
- Molecule 2: Beta-2-microglobulin

Chain G:



- Molecule 3: Gag protein

Chain C:

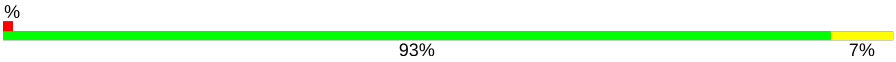


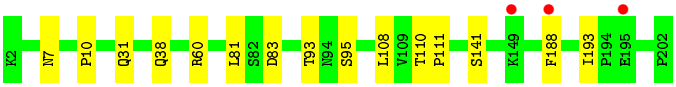
• Molecule 3: Gag protein

Chain H:

• Molecule 4: T-cell receptor Alpha chain

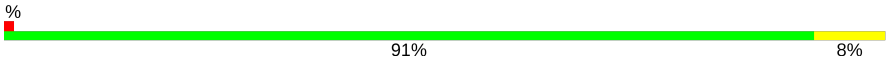
Chain D:

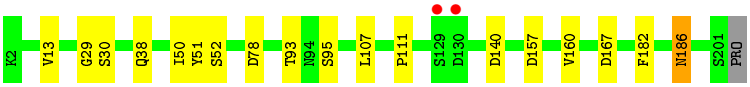




• Molecule 4: T-cell receptor Alpha chain

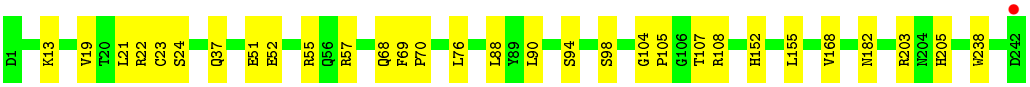
Chain I:





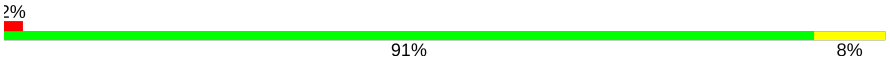
• Molecule 5: Human T-cell receptor beta chain

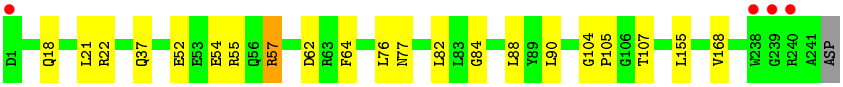
Chain E:



• Molecule 5: Human T-cell receptor beta chain

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	211.14Å 85.14Å 113.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.76 – 2.94 64.76 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (64.76-2.94) 99.0 (64.76-2.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.263 0.199 , 0.264	Depositor DCC
R_{free} test set	2212 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13441	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.94	4/2331 (0.2%)	1.03	8/3164 (0.3%)
1	F	0.78	0/2320	0.93	1/3149 (0.0%)
2	B	0.83	0/860	0.98	1/1162 (0.1%)
2	G	0.66	0/860	0.88	0/1162
3	C	1.37	0/69	1.35	0/93
3	H	0.79	0/69	1.05	0/93
4	D	0.92	0/1601	0.99	0/2167
4	I	0.96	1/1593 (0.1%)	1.03	3/2155 (0.1%)
5	E	0.94	1/1994 (0.1%)	1.04	10/2717 (0.4%)
5	J	0.88	0/1985	1.03	7/2706 (0.3%)
All	All	0.89	6/13682 (0.0%)	1.00	30/18568 (0.2%)

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	I	0	2
5	E	0	1
5	J	0	1
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	94	SER	CB-OG	7.55	1.52	1.42
1	A	101	CYS	CB-SG	-6.99	1.70	1.82
4	I	78	ASP	CB-CG	6.80	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	CG-CD	6.49	1.61	1.51
1	A	119	ASP	C-O	5.52	1.33	1.23
1	A	63	GLU	CD-OE1	5.05	1.31	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	62	ASP	CB-CG-OD1	7.76	125.28	118.30
4	I	186	ASN	CB-CA-C	-7.35	95.70	110.40
1	A	119	ASP	CB-CA-C	7.32	125.04	110.40
1	A	101	CYS	CB-CA-C	-7.28	95.83	110.40
5	E	57	ARG	NE-CZ-NH2	7.28	123.94	120.30
5	E	57	ARG	NE-CZ-NH1	-6.98	116.81	120.30
5	E	55	ARG	NE-CZ-NH1	-6.86	116.87	120.30
5	J	62	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	65	ARG	NE-CZ-NH1	6.68	123.64	120.30
5	E	22	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	A	65	ARG	CG-CD-NE	6.16	124.73	111.80
5	J	22	ARG	NE-CZ-NH2	6.09	123.35	120.30
5	E	108	ARG	NE-CZ-NH1	-5.93	117.33	120.30
4	I	78	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	126	LEU	CA-CB-CG	5.71	128.44	115.30
5	E	55	ARG	NE-CZ-NH2	5.67	123.14	120.30
5	E	108	ARG	NE-CZ-NH2	5.64	123.12	120.30
5	J	52	GLU	CA-CB-CG	5.59	125.69	113.40
1	A	5	MET	CG-SD-CE	5.58	109.12	100.20
1	F	169	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	B	0	MET	CG-SD-CE	5.47	108.95	100.20
5	E	98	SER	C-N-CA	-5.42	108.15	121.70
5	E	203	ARG	NE-CZ-NH1	5.42	123.01	120.30
5	J	57	ARG	NE-CZ-NH2	5.24	122.92	120.30
5	J	82	LEU	CB-CG-CD1	5.19	119.83	111.00
5	E	152	HIS	N-CA-CB	5.11	119.79	110.60
4	I	140	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	232	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	82	ARG	NE-CZ-NH1	-5.02	117.79	120.30
5	J	55	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	GLY	Peptide
5	E	168	VAL	Peptide
1	F	129	ASP	Peptide
4	I	167	ASP	Peptide
4	I	29	GLY	Peptide
5	J	168	VAL	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	2264	0	2109	23	0
1	F	2254	0	2103	20	0
2	B	837	0	803	8	0
2	G	837	0	803	11	0
3	C	69	0	72	8	0
3	H	69	0	72	1	0
4	D	1567	0	1493	11	0
4	I	1560	0	1486	10	0
5	E	1939	0	1814	16	0
5	J	1930	0	1810	10	0
6	A	8	0	12	2	0
6	D	4	0	6	0	0
6	E	4	0	6	0	0
6	I	12	0	18	0	0
6	J	4	0	6	0	0
7	A	5	0	0	0	0
7	E	10	0	0	0	0
7	J	20	0	0	1	5
8	F	6	0	8	0	0
9	A	13	0	0	0	0
9	B	4	0	0	0	0
9	D	5	0	0	1	0
9	E	4	0	0	0	0
9	F	5	0	0	0	0
9	G	1	0	0	0	0
9	I	5	0	0	0	0
9	J	5	0	0	0	0
All	All	13441	0	12621	105	5

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 (105) 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:38:GLN:HE22	5:E:37:GLN:HE22	1.12	0.96
5:E:21:LEU:HD22	5:E:107:THR:HG21	1.57	0.85
3:C:4:ASN:HD22	3:C:4:ASN:H	1.23	0.85
4:I:38:GLN:HE22	5:J:37:GLN:HE22	1.23	0.83
4:I:50:ILE:HD11	4:I:52:SER:O	1.81	0.80
1:A:7:TYR:CZ	3:C:1:SER:O	2.35	0.79
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.05	0.75
1:A:74:HIS:HE1	1:A:97:ARG:HE	1.38	0.70
2:B:27:VAL:HG21	2:B:35:ILE:HD13	1.72	0.70
1:F:131:ARG:HH21	1:F:153:ALA:HB3	1.55	0.69
2:G:7:ILE:N	2:G:7:ILE:HD13	2.07	0.69
1:F:74:HIS:HE1	1:F:97:ARG:HE	1.39	0.68
4:D:7:ASN:ND2	9:D:401:HOH:O	2.27	0.66
5:J:21:LEU:HD22	5:J:107:THR:HG21	1.78	0.66
4:I:182:PHE:HA	4:I:186:ASN:HD22	1.62	0.65
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.15	0.64
3:C:4:ASN:HD22	3:C:4:ASN:N	1.92	0.64
4:D:93:THR:HG23	4:D:95:SER:H	1.63	0.63
5:J:84:GLY:N	7:J:305:SO4:O1	2.24	0.63
1:F:74:HIS:CE1	1:F:97:ARG:HE	2.16	0.63
1:F:230:LEU:HD12	1:F:243:LYS:HE3	1.81	0.61
4:D:10:PRO:HB3	4:D:108:LEU:HD23	1.82	0.61
2:B:7:ILE:HD12	2:B:91:LYS:HE3	1.82	0.61
2:G:35:ILE:HD11	2:G:64:LEU:HD12	1.83	0.59
1:F:129:ASP:OD2	1:F:129:ASP:N	2.36	0.59
1:F:130:LEU:HB2	1:F:157:ARG:HG3	1.84	0.59
4:D:60:ARG:NH2	4:D:83:ASP:OD2	2.36	0.58
5:E:182:ASN:HD22	5:E:182:ASN:C	2.07	0.58
4:I:182:PHE:HA	4:I:186:ASN:ND2	2.19	0.57
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.41	0.56
3:C:4:ASN:H	3:C:4:ASN:ND2	1.99	0.55
4:D:110:THR:HG23	4:D:141:SER:HB3	1.89	0.55
1:F:224:GLN:O	1:F:228:THR:OG1	2.25	0.55
1:A:7:TYR:OH	3:C:1:SER:O	2.22	0.53
1:A:7:TYR:CE1	3:C:1:SER:O	2.61	0.53
5:J:155:LEU:C	5:J:155:LEU:HD23	2.30	0.53
5:J:21:LEU:HD12	5:J:76:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:205:HIS:HB2	5:E:238:TRP:CE3	2.45	0.52
4:I:111:PRO:HG3	4:I:160:VAL:HG21	1.91	0.52
5:E:52:GLU:H	5:E:68:GLN:NE2	2.07	0.52
5:E:155:LEU:C	5:E:155:LEU:HD23	2.29	0.51
1:A:135:ALA:HB1	1:A:140:ALA:HB1	1.92	0.51
5:J:88:LEU:HD13	5:J:90:LEU:HD21	1.93	0.51
1:A:218:GLN:OE1	1:A:260:HIS:ND1	2.44	0.51
5:J:104:GLY:C	5:J:105:PRO:O	2.49	0.50
1:F:116:TYR:O	1:F:122:ASP:O	2.29	0.50
2:B:27:VAL:HG21	2:B:35:ILE:CD1	2.42	0.50
5:E:21:LEU:HD12	5:E:76:LEU:HD23	1.94	0.50
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.93	0.50
5:E:205:HIS:HB2	5:E:238:TRP:CZ3	2.48	0.49
2:B:27:VAL:HG23	2:B:30:PHE:CE1	2.49	0.48
1:F:117:ALA:HB2	2:G:60:TRP:CZ2	2.49	0.48
1:A:163:THR:HG23	4:D:31:GLN:HE21	1.77	0.48
5:J:54:GLU:OE1	5:J:57:ARG:NH2	2.46	0.47
4:I:50:ILE:HD12	4:I:51:TYR:N	2.28	0.47
2:G:57:SER:O	2:G:59:ASP:O	2.32	0.47
5:E:182:ASN:ND2	5:E:182:ASN:C	2.68	0.47
5:E:13:LYS:HD2	5:E:19:VAL:HG23	1.96	0.47
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.96	0.47
1:A:126:LEU:HD13	1:A:133:TRP:CZ3	2.50	0.47
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.98	0.46
5:E:104:GLY:C	5:E:105:PRO:O	2.52	0.46
1:F:32:GLN:HE21	1:F:48:ARG:HG3	1.80	0.46
4:I:13:VAL:HG21	4:I:107:LEU:HD11	1.98	0.46
2:B:17:ASN:HA	2:B:72:PRO:O	2.15	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.51	0.46
4:I:157:ASP:OD1	4:I:157:ASP:N	2.47	0.46
4:D:81:LEU:HD21	4:D:111:PRO:HB3	1.98	0.46
1:F:272:LEU:HD12	1:F:272:LEU:N	2.31	0.46
1:A:153:ALA:HB3	6:A:301:EDO:C1	2.47	0.45
1:A:102:ASP:OD2	1:A:111:ARG:NH1	2.50	0.45
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.97	0.45
1:A:25:VAL:HB	1:A:32:GLN:HE21	1.82	0.45
2:G:7:ILE:N	2:G:7:ILE:CD1	2.76	0.45
2:G:17:ASN:HA	2:G:72:PRO:O	2.17	0.44
1:A:272:LEU:N	1:A:272:LEU:HD12	2.33	0.44
5:E:88:LEU:HD13	5:E:90:LEU:HD21	2.00	0.44
5:J:57:ARG:NH1	5:J:64:PHE:O	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG11	1:A:244:TRP:CZ2	2.53	0.43
1:F:231:VAL:HG11	1:F:244:TRP:CZ2	2.53	0.43
1:F:187:THR:HG21	1:F:261:VAL:HG21	2.00	0.43
4:I:30:SER:HA	4:I:93:THR:HG22	2.01	0.43
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.54	0.43
2:G:25:CYS:HB2	2:G:39:LEU:HD21	1.99	0.43
2:G:1:ILE:HD11	2:G:3:ARG:NH1	2.33	0.43
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.53	0.43
5:E:23:CYS:SG	5:E:24:SER:N	2.92	0.43
3:C:6:VAL:O	3:C:6:VAL:HG13	2.20	0.42
1:A:163:THR:CG2	4:D:31:GLN:HE21	2.32	0.42
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.32	0.42
4:D:93:THR:CG2	4:D:95:SER:HB2	2.48	0.42
1:A:153:ALA:HB3	6:A:301:EDO:H12	2.01	0.42
1:F:45:MET:CE	3:H:2:LEU:HD11	2.49	0.42
1:F:65:ARG:NH1	4:I:95:SER:O	2.53	0.42
1:F:107:TRP:HB2	1:F:169:ARG:HD3	2.02	0.42
1:F:72:GLN:HG2	1:F:75:ARG:HH11	1.84	0.42
1:F:126:LEU:HD13	1:F:133:TRP:CZ3	2.56	0.41
3:C:4:ASN:N	3:C:4:ASN:ND2	2.64	0.41
4:D:188:PHE:HB3	4:D:193:ILE:HD11	2.02	0.41
5:E:69:PHE:HB3	5:E:70:PRO:HD2	2.03	0.41
5:J:18:GLN:HE21	5:J:77:ASN:HD21	1.69	0.40
1:A:75:ARG:HH12	5:E:51:GLU:HG2	1.86	0.40
5:E:52:GLU:H	5:E:68:GLN:HE21	1.68	0.40
2:G:7:ILE:HD12	2:G:27:VAL:HG13	2.04	0.40
1:A:74:HIS:HE1	1:A:97:ARG:NE	2.14	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:305:SO4:O2	7:J:305:SO4:O2[2_655]	1.18	1.02
7:J:305:SO4:O4	7:J:305:SO4:O4[2_655]	1.41	0.79
7:J:305:SO4:S	7:J:305:SO4:O4[2_655]	1.65	0.55
7:J:305:SO4:O3	7:J:305:SO4:O4[2_655]	1.71	0.49
7:J:305:SO4:S	7:J:305:SO4:O2[2_655]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	A	301	-	3,3,3	0.44	0	2,2,2	0.54	0
6	EDO	I	302	-	3,3,3	0.48	0	2,2,2	0.39	0
6	EDO	E	301	-	3,3,3	0.48	0	2,2,2	0.51	0
7	SO4	E	302	-	4,4,4	0.37	0	6,6,6	0.66	0
7	SO4	J	302	-	4,4,4	0.34	0	6,6,6	0.40	0
8	GOL	F	301	-	5,5,5	0.29	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	302	-	3,3,3	0.56	0	2,2,2	0.18	0
6	EDO	I	303	-	3,3,3	0.46	0	2,2,2	0.41	0
6	EDO	J	301	-	3,3,3	0.52	0	2,2,2	0.37	0
7	SO4	E	303	-	4,4,4	0.42	0	6,6,6	0.27	0
7	SO4	J	303	-	4,4,4	0.38	0	6,6,6	0.34	0
7	SO4	A	303	-	4,4,4	0.33	0	6,6,6	0.31	0
6	EDO	I	301	-	3,3,3	0.48	0	2,2,2	0.43	0
6	EDO	D	301	-	3,3,3	0.60	0	2,2,2	0.22	0
7	SO4	J	305	-	4,4,4	0.35	0	6,6,6	0.70	0
7	SO4	J	304	-	4,4,4	0.39	0	6,6,6	0.27	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	EDO	A	301	-	-	1/1/1/1	-
6	EDO	I	302	-	-	1/1/1/1	-
6	EDO	E	301	-	-	1/1/1/1	-
8	GOL	F	301	-	-	1/4/4/4	-
6	EDO	J	301	-	-	0/1/1/1	-
6	EDO	I	303	-	-	0/1/1/1	-
6	EDO	A	302	-	-	0/1/1/1	-
6	EDO	I	301	-	-	0/1/1/1	-
6	EDO	D	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	EDO	O1-C1-C2-O2
6	I	302	EDO	O1-C1-C2-O2
6	D	301	EDO	O1-C1-C2-O2
8	F	301	GOL	O1-C1-C2-C3
6	E	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	EDO	2	0
7	J	305	SO4	1	5

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%)	-0.09	2 (0%) 87 88	39, 66, 112, 147	0
1	F	276/276 (100%)	0.16	1 (0%) 92 93	59, 92, 125, 144	0
2	B	100/100 (100%)	-0.18	0 100 100	43, 61, 89, 107	0
2	G	100/100 (100%)	0.62	8 (8%) 12 10	71, 101, 130, 154	0
3	C	9/9 (100%)	-0.04	0 100 100	41, 43, 59, 64	0
3	H	9/9 (100%)	0.38	1 (11%) 5 5	62, 66, 79, 95	0
4	D	201/201 (100%)	-0.02	3 (1%) 73 75	37, 66, 114, 137	0
4	I	200/201 (99%)	-0.04	2 (1%) 82 83	41, 64, 103, 136	0
5	E	242/242 (100%)	-0.17	1 (0%) 92 93	35, 59, 93, 126	0
5	J	241/242 (99%)	-0.03	4 (1%) 70 71	45, 63, 97, 149	0
All	All	1654/1656 (99%)	0.00	22 (1%) 77 78	35, 69, 117, 154	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	1	ASP	7.9
5	J	238	TRP	5.1
3	H	9	LEU	4.3
5	E	242	ASP	3.9
1	A	17	ARG	3.4
1	A	276	PRO	3.3
5	J	240	ARG	3.2
4	I	129	SER	3.1
2	G	85	VAL	2.7
4	D	149	LYS	2.6
4	D	195	GLU	2.5
5	J	239	GLY	2.4
4	I	130	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	1	GLY	2.2
2	G	82	VAL	2.2
4	D	188	PHE	2.1
2	G	50	GLU	2.1
2	G	15	ALA	2.1
2	G	47	GLU	2.0
2	G	58	LYS	2.0
2	G	66	TYR	2.0
2	G	87	LEU	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 carbohydrates 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
8	GOL	F	301	6/6	0.81	0.21	75,90,93,98	0
6	EDO	D	301	4/4	0.82	0.31	69,75,75,77	0
6	EDO	I	303	4/4	0.83	0.27	84,85,87,91	0
6	EDO	A	302	4/4	0.83	0.21	72,72,72,74	0
6	EDO	E	301	4/4	0.87	0.20	66,73,74,81	0
6	EDO	I	302	4/4	0.88	0.29	70,71,73,74	0
6	EDO	A	301	4/4	0.89	0.22	61,62,62,65	0
6	EDO	I	301	4/4	0.90	0.31	71,75,80,82	0
6	EDO	J	301	4/4	0.92	0.22	64,66,71,72	0
7	SO4	A	303	5/5	0.93	0.17	96,99,102,103	0
7	SO4	E	303	5/5	0.93	0.16	93,94,96,104	0
7	SO4	E	302	5/5	0.96	0.11	72,78,82,84	0
7	SO4	J	304	5/5	0.97	0.21	89,91,97,98	0
7	SO4	J	303	5/5	0.97	0.11	67,69,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	J	302	5/5	0.97	0.12	63,69,71,84	0
7	SO4	J	305	5/5	0.99	0.16	48,75,153,165	1

6.5 Other polymers (i)

There are no such residues in this entry.