Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:46 pm BST

PDB ID	:	6FRA
Title	:	F11 T-Cell Receptor Recognising PKYVKQNTLKLAT Peptide Presented by HLA-DR*0101
Authors	:	Rizkallah, P.J.; Cole, D.K.
Deposited on	:	2018-02-15
Resolution	:	1.73 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:

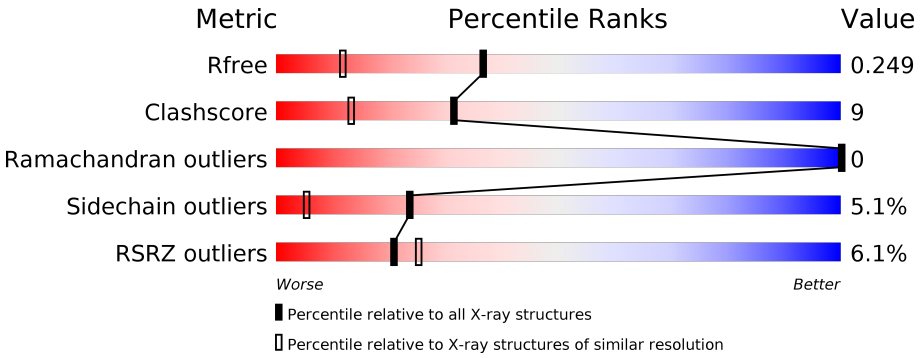
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	201	5% 86% 12%
2	B	240	7% 82% 16%

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
3	EDO	A	301	-	-	X	-
3	EDO	A	302	-	-	X	-
4	SO4	A	309	-	-	-	X
4	SO4	B	305	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3710 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.

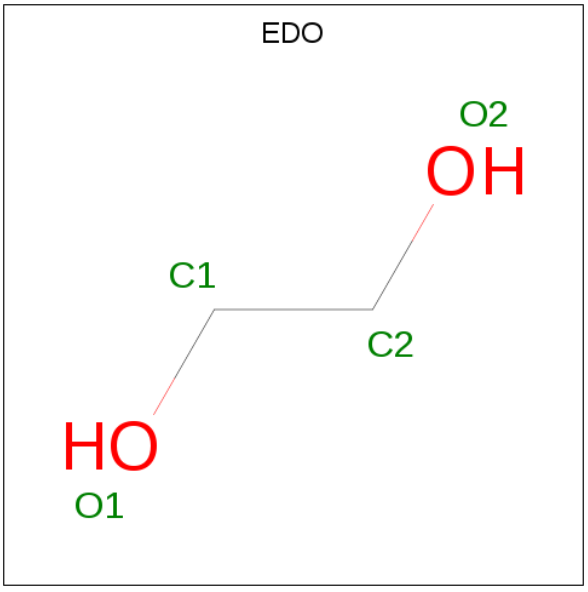
- Molecule 1 is a protein called Human T-Cell Receptor F11 alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	2	0
			1579	998	257	313	11			

- Molecule 2 is a protein called Human T-Cell Receptor F11 beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	4	0
			1934	1213	338	373	10			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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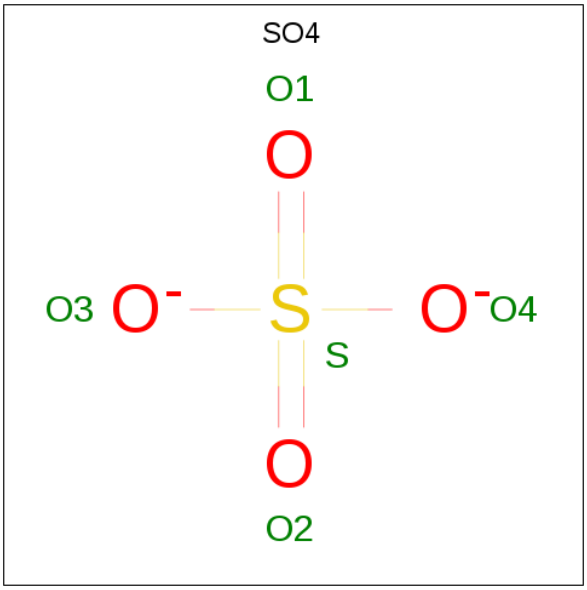
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

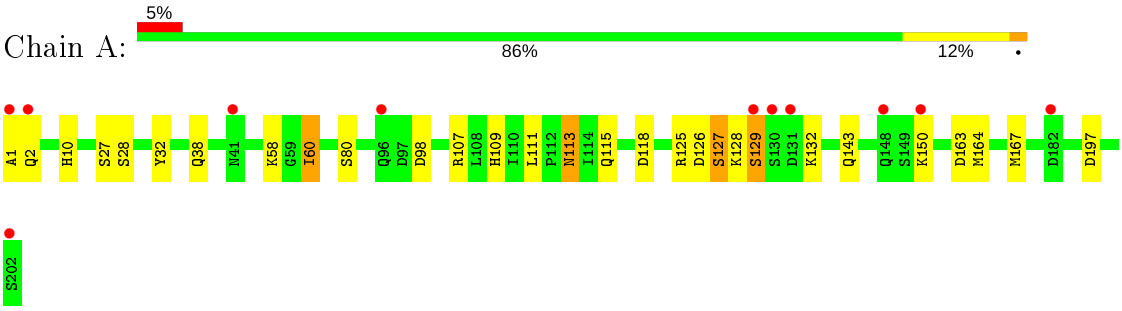
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	67	Total O 67 67	0	0
5	B	65	Total O 65 65	0	0

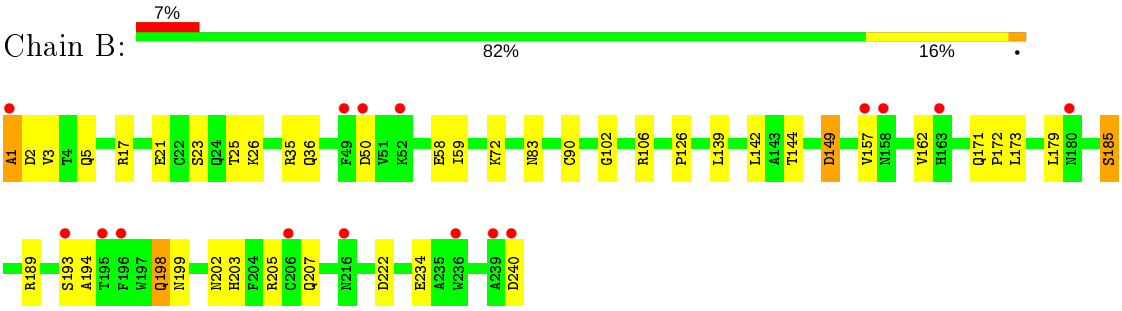
3 Residue-property plots (i)

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: Human T-Cell Receptor F11 alpha Chain



- Molecule 2: Human T-Cell Receptor F11 beta Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.71Å 114.63Å 50.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 1.73 47.64 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.64-1.73) 99.9 (47.64-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.203 , 0.243 0.211 , 0.249	Depositor DCC
R_{free} test set	2690 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3710	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: 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	0.99	1/1624 (0.1%)	1.06	9/2200 (0.4%)
2	B	0.96	1/1994 (0.1%)	1.01	7/2707 (0.3%)
All	All	0.97	2/3618 (0.1%)	1.04	16/4907 (0.3%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	185	SER	CB-OG	-5.78	1.34	1.42
1	A	80	SER	CB-OG	-5.68	1.34	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	106	ARG	NE-CZ-NH2	8.49	124.55	120.30
2	B	2	ASP	N-CA-C	-8.45	88.17	111.00
1	A	164	MET	CG-SD-CE	-7.14	88.78	100.20
2	B	222	ASP	CB-CG-OD1	7.00	124.61	118.30
2	B	149	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	A	107	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	98	ASP	CB-CG-OD1	6.06	123.75	118.30
2	B	17	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	A	197	ASP	CB-CG-OD1	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	ASP	CB-CG-OD1	5.43	123.19	118.30
2	B	72	LYS	CD-CE-NZ	5.09	123.41	111.70
1	A	164	MET	CA-CB-CG	5.07	121.92	113.30
1	A	143	GLN	CA-CB-CG	-5.01	102.37	113.40
2	B	106	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	A	98	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	32	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	ALA	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	1579	0	1514	26	0
2	B	1934	0	1858	36	0
3	A	28	0	40	13	3
3	B	12	0	18	2	0
4	A	10	0	0	0	0
4	B	15	0	0	2	0
5	A	67	0	0	4	0
5	B	65	0	0	1	0
All	All	3710	0	3430	63	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:HE22	2:B:36:GLN:HE22	1.07	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:ALA:HB1	5:B:428:HOH:O	1.67	0.95
3:A:302:EDO:C1	5:A:406:HOH:O	2.17	0.92
3:A:302:EDO:H11	5:A:406:HOH:O	1.73	0.88
3:A:301:EDO:O1	3:A:302:EDO:H12	1.78	0.82
2:B:126:PRO:HD3	2:B:139:LEU:CD2	2.10	0.81
1:A:109:HIS:HD2	5:A:466:HOH:O	1.67	0.77
1:A:167:MET:CE	2:B:193:SER:HB3	2.16	0.76
3:A:301:EDO:C1	3:A:302:EDO:H12	2.15	0.76
1:A:126:ASP:CG	1:A:129:SER:HB2	2.09	0.72
3:A:301:EDO:H12	3:A:302:EDO:C1	2.19	0.72
1:A:126:ASP:OD2	1:A:129:SER:HB2	1.92	0.67
1:A:113:ASN:HD21	1:A:115:GLN:HE21	1.43	0.67
1:A:60:ILE:HD13	1:A:60:ILE:H	1.59	0.67
3:A:301:EDO:H12	3:A:302:EDO:H12	1.75	0.67
3:A:302:EDO:H12	5:A:406:HOH:O	1.90	0.64
2:B:83:ASN:OD1	3:B:302:EDO:H12	1.98	0.64
2:B:58:GLU:HG3	2:B:59:ILE:HG23	1.81	0.63
1:A:126:ASP:CB	1:A:129:SER:HB2	2.28	0.63
1:A:113:ASN:ND2	1:A:115:GLN:HE21	1.97	0.62
1:A:126:ASP:HB3	1:A:129:SER:HB2	1.81	0.62
2:B:1:ALA:H2	2:B:25:THR:H	1.49	0.60
2:B:23:SER:OG	4:B:305:SO4:O4	2.17	0.60
1:A:167:MET:HE1	2:B:193:SER:HB3	1.84	0.58
1:A:38:GLN:HE22	2:B:36:GLN:NE2	1.90	0.58
1:A:167:MET:HE1	2:B:193:SER:CB	2.34	0.57
2:B:35:ARG:HD3	2:B:59:ILE:HD12	1.87	0.57
1:A:126:ASP:HB3	1:A:129:SER:CB	2.35	0.57
2:B:1:ALA:HB3	2:B:26:LYS:HD2	1.87	0.56
2:B:1:ALA:N	2:B:25:THR:H	2.04	0.55
1:A:167:MET:CE	2:B:193:SER:CB	2.83	0.55
1:A:10:HIS:ND1	1:A:109:HIS:HE1	2.06	0.54
3:A:301:EDO:H12	3:A:302:EDO:C2	2.38	0.54
1:A:167:MET:HE2	2:B:193:SER:HB3	1.91	0.53
2:B:162:VAL:HB	3:B:303:EDO:H21	1.90	0.52
2:B:5:GLN:HA	4:B:305:SO4:O1	2.10	0.52
1:A:113:ASN:HD21	1:A:115:GLN:NE2	2.08	0.51
1:A:38:GLN:NE2	2:B:36:GLN:HE22	1.91	0.51
2:B:173:LEU:C	2:B:173:LEU:HD12	2.31	0.51
2:B:126:PRO:HG3	2:B:139:LEU:HD23	1.93	0.49
1:A:163:ASP:OD2	3:A:302:EDO:H21	2.13	0.48
2:B:126:PRO:HD3	2:B:139:LEU:HD22	1.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:GLN:HE21	2:B:102:GLY:HA3	1.79	0.47
1:A:1:ALA:HA	1:A:27:SER:HB2	1.96	0.47
2:B:5:GLN:NE2	2:B:90[B]:CYS:H	2.12	0.47
2:B:5:GLN:NE2	2:B:90[A]:CYS:H	2.13	0.46
1:A:126:ASP:OD1	1:A:127:SER:N	2.49	0.46
2:B:149:ASP:OD1	2:B:172:PRO:HG3	2.16	0.45
2:B:126:PRO:CD	2:B:139:LEU:CD2	2.91	0.45
1:A:163:ASP:OD2	3:A:302:EDO:C2	2.64	0.44
2:B:5:GLN:HE22	2:B:90[B]:CYS:H	1.64	0.44
2:B:199:ASN:HB3	2:B:202:ASN:ND2	2.33	0.43
3:A:301:EDO:HO1	3:A:302:EDO:H12	1.78	0.43
1:A:113:ASN:C	1:A:113:ASN:HD22	2.22	0.42
2:B:144:THR:HG22	2:B:185:SER:HB2	2.00	0.42
2:B:157:VAL:O	2:B:203:HIS:O	2.38	0.42
2:B:5:GLN:HE22	2:B:90[A]:CYS:H	1.67	0.42
1:A:163:ASP:OD2	3:A:302:EDO:O2	2.33	0.42
2:B:126:PRO:HD3	2:B:139:LEU:HD23	1.98	0.42
1:A:111:LEU:O	3:A:305:EDO:C2	2.68	0.41
2:B:205:ARG:NH1	2:B:207:GLN:HB2	2.35	0.41
2:B:194:ALA:O	2:B:198:GLN:HB2	2.20	0.40
2:B:1:ALA:HA	2:B:3:VAL:HG23	2.03	0.40

All (3) 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)
3:A:307:EDO:O2	3:A:307:EDO:O2[2_555]	1.30	0.90
3:A:307:EDO:C2	3:A:307:EDO:O2[2_555]	2.15	0.05
3:A:307:EDO:C2	3:A:307:EDO:C2[2_555]	2.17	0.03

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	200/201 (100%)	190 (95%)	10 (5%)	0	100	100
2	B	242/240 (101%)	233 (96%)	9 (4%)	0	100	100
All	All	442/441 (100%)	423 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	182/179 (102%)	171 (94%)	11 (6%)	19	4
2	B	214/210 (102%)	205 (96%)	9 (4%)	30	9
All	All	396/389 (102%)	376 (95%)	20 (5%)	24	5

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	28	SER
1	A	58	LYS
1	A	60	ILE
1	A	113	ASN
1	A	125	ARG
1	A	127	SER
1	A	128	LYS
1	A	129	SER
1	A	132	LYS
1	A	150	LYS
2	B	21	GLU
2	B	50	ASP
2	B	142	LEU
2	B	171	GLN
2	B	179	LEU
2	B	189	ARG
2	B	198	GLN

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Mol	Chain	Res	Type
2	B	234	GLU
2	B	240	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	82	HIS
1	A	109	HIS
1	A	113	ASN
1	A	190	ASN
2	B	5	GLN
2	B	68	GLN
2	B	221	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

15 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	$\#\|Z\|>2$
4	SO4	B	304	-	4,4,4	0.50	0	6,6,6	0.88	0
3	EDO	B	303	-	3,3,3	0.25	0	2,2,2	0.76	0
4	SO4	B	305	-	4,4,4	0.37	0	6,6,6	0.20	0
3	EDO	A	306	-	3,3,3	0.78	0	2,2,2	0.39	0
3	EDO	B	302	-	3,3,3	0.27	0	2,2,2	0.85	0
3	EDO	A	302	-	3,3,3	0.79	0	2,2,2	0.36	0
4	SO4	B	306	-	4,4,4	0.54	0	6,6,6	0.30	0
4	SO4	A	308	-	4,4,4	0.62	0	6,6,6	0.57	0
4	SO4	A	309	-	4,4,4	0.60	0	6,6,6	0.32	0
3	EDO	A	307	-	3,3,3	0.35	0	2,2,2	1.27	0
3	EDO	B	301	-	3,3,3	0.25	0	2,2,2	0.84	0
3	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	305	-	3,3,3	0.86	0	2,2,2	0.27	0
3	EDO	A	301	-	3,3,3	1.01	0	2,2,2	1.47	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
3	EDO	B	303	-	-	1/1/1/1	-
3	EDO	A	306	-	-	0/1/1/1	-
3	EDO	B	302	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	A	307	-	-	1/1/1/1	-
3	EDO	B	301	-	-	1/1/1/1	-
3	EDO	A	303	-	-	1/1/1/1	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	A	305	-	-	0/1/1/1	-
3	EDO	A	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	EDO	O1-C1-C2-O2
3	A	307	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	301	EDO	O1-C1-C2-O2
3	A	301	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2
3	B	303	EDO	O1-C1-C2-O2
3	A	303	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	EDO	1	0
4	B	305	SO4	2	0
3	B	302	EDO	1	0
3	A	302	EDO	12	0
3	A	307	EDO	0	3
3	A	305	EDO	1	0
3	A	301	EDO	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	99:LYS	C	101:ILE	N	4.02

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	201/201 (100%)	0.43	11 (5%)	25	30	16, 25, 57, 89	0
2	B	240/240 (100%)	0.30	16 (6%)	17	22	15, 26, 53, 92	0
All	All	441/441 (100%)	0.36	27 (6%)	21	25	15, 26, 56, 92	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	SER	11.1
1	A	182	ASP	6.8
2	B	239	ALA	6.2
1	A	1	ALA	4.8
1	A	129	SER	4.5
2	B	240	ASP	4.5
2	B	52	LYS	4.4
2	B	49	PHE	3.9
2	B	195	THR	3.8
1	A	202	SER	3.6
1	A	2	GLN	3.5
2	B	196	PHE	3.4
1	A	131	ASP	2.9
1	A	41	ASN	2.9
1	A	148	GLN	2.9
2	B	216	ASN	2.8
2	B	163	HIS	2.6
2	B	193	SER	2.5
2	B	157	VAL	2.4
1	A	150	LYS	2.4
2	B	236	TRP	2.3
2	B	180	ASN	2.3
2	B	1	ALA	2.1
2	B	206[A]	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	50	ASP	2.0
2	B	158	ASN	2.0
1	A	96	GLN	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
4	SO4	A	309	5/5	0.63	0.56	69,71,74,83	0
3	EDO	A	306	4/4	0.72	0.17	24,25,28,29	0
3	EDO	A	301	4/4	0.73	0.16	25,28,29,31	0
4	SO4	A	308	5/5	0.80	0.55	55,64,72,77	0
4	SO4	B	306	5/5	0.84	0.34	64,68,72,73	0
4	SO4	B	305	5/5	0.84	0.65	75,79,88,90	0
3	EDO	B	303	4/4	0.85	0.20	42,44,44,44	0
3	EDO	B	301	4/4	0.87	0.19	37,37,37,45	0
3	EDO	B	302	4/4	0.87	0.25	41,43,45,50	0
3	EDO	A	304	4/4	0.91	0.10	29,33,38,39	0
3	EDO	A	302	4/4	0.91	0.20	32,32,35,38	0
4	SO4	B	304	5/5	0.92	0.76	57,60,72,74	0
3	EDO	A	303	4/4	0.93	0.13	37,47,48,51	0
3	EDO	A	305	4/4	0.94	0.22	28,31,36,36	0
3	EDO	A	307	4/4	0.94	0.34	38,44,47,143	0

6.5 Other polymers (i)

There are no such residues in this entry.