



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:00 am BST

PDB ID : 4GKS
Title : A2-MHC Complex carrying FLTGIITV
Authors : Sewell, A.K.; Rizkallah, P.J.; Cole, D.K.; Wooldridge, L.; Price, D.A.
Deposited on : 2012-08-13
Resolution : 2.35 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

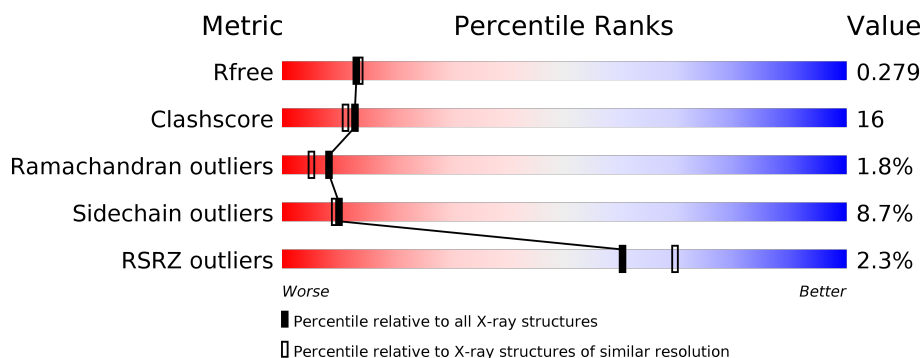
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 $\leq 5\%$. 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	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div></div> </div> <div></div> </div>
1	D	276	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div></div> </div> <div></div> </div>
2	B	100	<div> <div></div> <div> <div></div> <div>61%</div> <div>37%</div> <div></div> </div> <div></div> </div>
2	E	100	<div> <div></div> <div> <div></div> <div>60%</div> <div>30%</div> <div>9%</div> </div> <div></div> </div>
3	C	10	<div> <div></div> <div> <div></div> <div>70%</div> <div>30%</div> </div> </div>
3	F	10	<div> <div></div> <div> <div></div> <div>70%</div> <div>30%</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6535 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	0	0
			2254	1408	410	427	9			
1	D	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	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	1	0
			846	539	143	160	4			
2	E	100	Total	C	N	O	S	0	3	0
			867	549	150	164	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769
E	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called FLT Cognate peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			73	50	10	13			
3	F	10	Total	C	N	O	0	0	0
			73	50	10	13			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

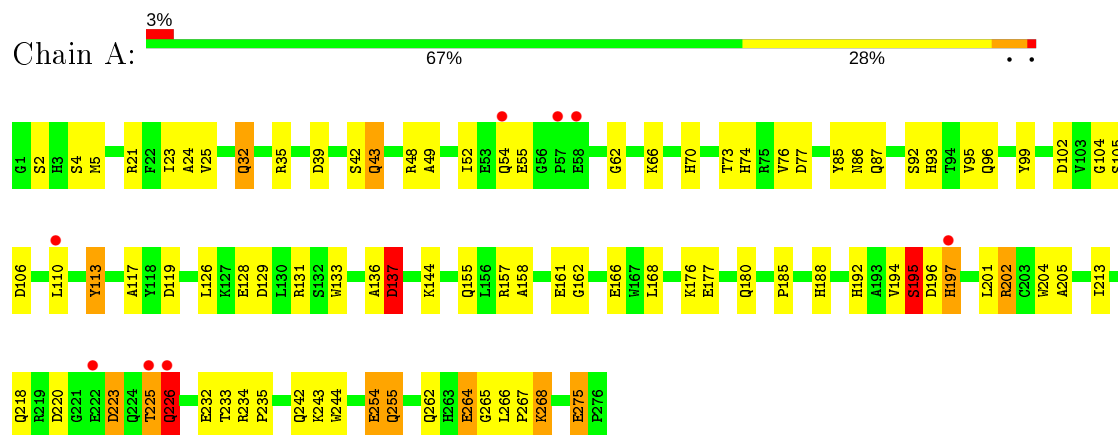
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total 35	O 35	0	0
7	B	17	Total 17	O 17	0	0
7	C	1	Total 1	O 1	0	0
7	D	33	Total 33	O 33	0	0
7	E	14	Total 14	O 14	0	0

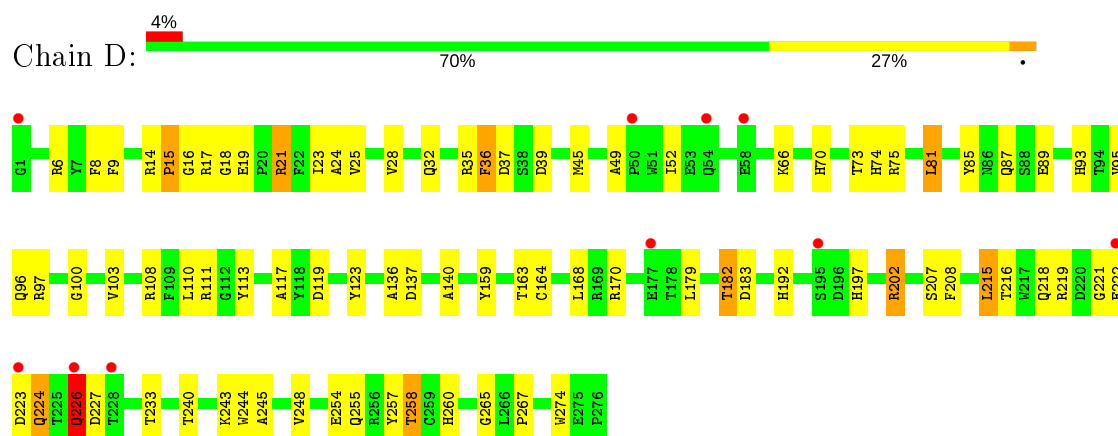
3 Residue-property plots [i](#)

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.

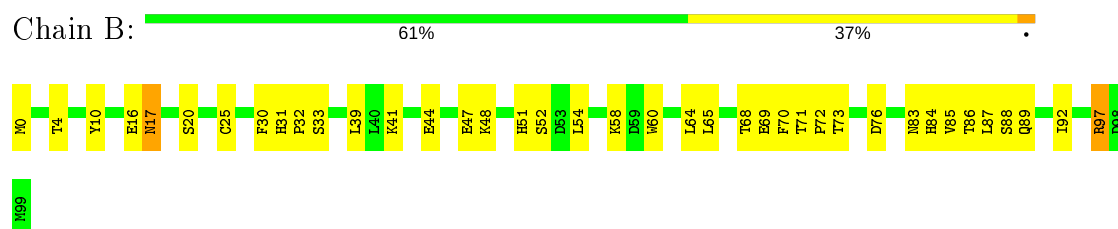
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



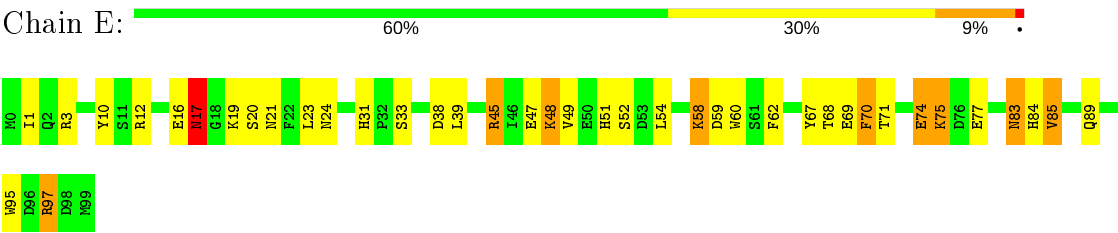
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



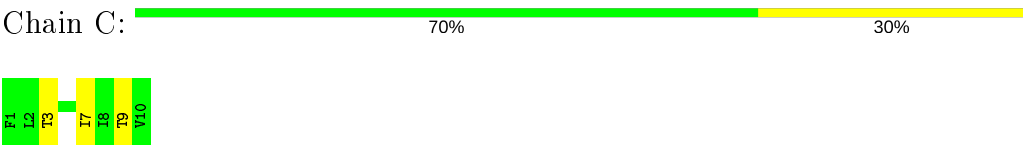
- Molecule 2: Beta-2-microglobulin



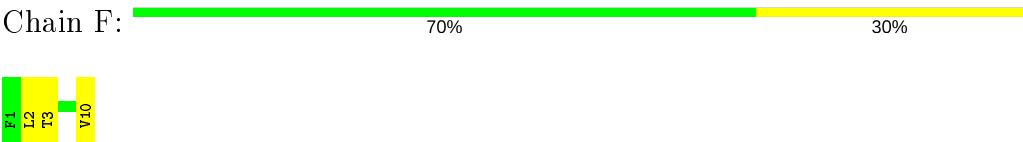
● Molecule 2: Beta-2-microglobulin



● Molecule 3: FLT Cognate peptide



● Molecule 3: FLT Cognate peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.54Å 46.78Å 115.86Å 90.00° 121.66° 90.00°	Depositor
Resolution (Å)	39.05 – 2.35 39.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.05-2.35) 92.1 (39.05-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.285 0.209 , 0.279	Depositor DCC
R_{free} test set	1798 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6535	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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, 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	0.75	0/2320	0.81	2/3149 (0.1%)
1	D	0.76	0/2319	0.89	2/3149 (0.1%)
2	B	0.77	0/869	0.85	0/1173
2	E	0.77	0/890	0.81	0/1201
3	C	0.74	0/73	0.73	0/97
3	F	0.72	0/73	0.67	0/97
All	All	0.76	0/6544	0.84	4/8866 (0.0%)

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	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ARG	NE-CZ-NH1	-14.52	113.04	120.30
1	D	202	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	202	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	A	110	LEU	CA-CB-CG	5.36	127.63	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	221	GLY	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	79	0
1	D	2253	0	2103	62	0
2	B	846	0	815	32	0
2	E	867	0	830	35	0
3	C	73	0	84	7	0
3	F	73	0	84	4	0
4	A	8	0	12	0	0
4	B	20	0	30	5	0
4	D	16	0	24	1	0
4	E	8	0	12	2	0
5	A	5	0	0	0	0
6	A	6	0	8	1	0
6	D	6	0	8	1	0
7	A	35	0	0	6	0
7	B	17	0	0	1	0
7	C	1	0	0	0	0
7	D	33	0	0	3	0
7	E	14	0	0	2	0
All	All	6535	0	6113	207	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 16.

All (207) 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:64:LEU:HD21	4:B:105:EDO:H11	1.24	1.15
3:C:3:THR:CG2	3:C:7:ILE:HD11	1.85	1.05
2:E:97[B]:ARG:H	2:E:97[B]:ARG:HD2	1.22	1.05
1:D:226:GLN:HG3	1:D:227:ASP:H	1.19	1.04
3:C:3:THR:HG23	3:C:7:ILE:HD11	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:THR:OG1	1:A:243:LYS:HE2	1.63	0.97
2:B:20:SER:HA	2:B:71:THR:HG22	1.47	0.96
1:D:226:GLN:HG3	1:D:227:ASP:N	1.83	0.92
1:D:258:THR:HG22	7:D:415:HOH:O	1.71	0.89
1:D:16:GLY:O	1:D:18:GLY:N	2.06	0.88
1:D:66:LYS:O	1:D:70:HIS:HD2	1.58	0.85
1:A:25:VAL:HG23	1:A:32:GLN:NE2	1.92	0.84
2:E:39:LEU:HD13	2:E:68:THR:HG22	1.60	0.83
1:A:194:VAL:O	1:A:195:SER:HB3	1.80	0.81
3:C:3:THR:HG23	3:C:7:ILE:CD1	2.11	0.80
2:B:97:ARG:HH11	4:B:101:EDO:H21	1.48	0.79
1:A:225:THR:O	1:A:226:GLN:HB2	1.82	0.78
1:A:96:GLN:HE22	2:B:31:HIS:HE1	1.28	0.78
1:A:21:ARG:HH21	1:A:39:ASP:HB2	1.48	0.78
1:D:182:THR:HG21	1:D:265:GLY:HA2	1.67	0.76
1:D:226:GLN:CG	1:D:227:ASP:H	1.99	0.75
1:D:36:PHE:CD2	1:D:37:ASP:N	2.55	0.75
1:D:218:GLN:HB2	1:D:258:THR:HG23	1.67	0.74
1:A:74:HIS:HD2	1:A:95:VAL:HG11	1.51	0.74
1:D:14:ARG:HB3	1:D:15:PRO:HD2	1.69	0.74
1:D:66:LYS:O	1:D:70:HIS:CD2	2.41	0.74
2:E:97[B]:ARG:N	2:E:97[B]:ARG:HD2	2.02	0.74
1:A:233:THR:OG1	1:A:243:LYS:CE	2.38	0.71
1:A:218:GLN:HG2	1:A:223:ASP:HB2	1.74	0.69
2:E:58:LYS:H	2:E:58:LYS:CD	2.04	0.69
1:D:93:HIS:HD2	1:D:119:ASP:OD1	1.76	0.67
4:E:101:EDO:H11	7:E:214:HOH:O	1.94	0.66
2:E:69:GLU:CD	2:E:69:GLU:H	1.98	0.65
1:D:108:ARG:HB3	6:D:305:GOL:O3	1.97	0.65
2:E:16:GLU:O	2:E:17:ASN:CB	2.44	0.65
1:A:267:PRO:HB2	1:A:268:LYS:HE3	1.79	0.64
2:B:4:THR:HG22	2:B:86:THR:HB	1.79	0.64
1:A:96:GLN:NE2	2:B:31:HIS:HE1	1.96	0.64
1:D:202:ARG:NH1	1:D:244:TRP:CZ3	2.64	0.64
1:A:129:ASP:O	1:A:131:ARG:HG3	1.99	0.62
1:D:197:HIS:HB3	7:D:430:HOH:O	1.99	0.62
1:A:25:VAL:CG2	1:A:32:GLN:NE2	2.62	0.61
2:B:84:HIS:ND1	2:B:86:THR:OG1	2.23	0.61
1:D:258:THR:CG2	7:D:415:HOH:O	2.39	0.61
1:D:255:GLN:NE2	1:D:274:TRP:O	2.28	0.61
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HD2	1:A:204:TRP:NE1	2.16	0.61
3:C:3:THR:HG21	3:C:7:ILE:HD11	1.80	0.61
1:A:93:HIS:CE1	7:A:430:HOH:O	2.54	0.60
1:A:93:HIS:HE1	7:A:430:HOH:O	1.83	0.60
1:A:234:ARG:HH21	1:A:242:GLN:NE2	1.99	0.60
1:A:218:GLN:HG2	1:A:223:ASP:CB	2.31	0.60
2:B:4:THR:CG2	2:B:86:THR:HB	2.30	0.60
1:D:45:MET:HE1	3:F:2:LEU:HD11	1.84	0.59
1:D:159:TYR:CZ	1:D:164:CYS:HB2	2.38	0.58
1:D:25:VAL:HG21	1:D:32:GLN:HE21	1.68	0.58
2:E:58:LYS:H	2:E:58:LYS:HD3	1.68	0.58
1:A:21:ARG:HH21	1:A:39:ASP:CB	2.15	0.58
1:D:36:PHE:CD2	1:D:36:PHE:C	2.77	0.58
2:E:47:GLU:HG3	2:E:48:LYS:H	1.68	0.57
1:A:104:GLY:O	1:A:106:ASP:N	2.37	0.57
1:D:202:ARG:NH1	1:D:244:TRP:CE3	2.72	0.57
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.87	0.57
1:D:216:THR:HG23	1:D:260:HIS:HB2	1.87	0.57
2:E:51:HIS:HD2	2:E:52:SER:O	1.86	0.57
1:A:23:ILE:HD12	2:B:54:LEU:HD23	1.86	0.56
1:A:162:GLY:O	1:A:166:GLU:HG3	2.05	0.56
2:E:38:ASP:OD1	2:E:45:ARG:NH1	2.39	0.56
1:D:85:TYR:OH	1:D:137:ASP:OD1	2.19	0.55
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.89	0.55
1:A:70:HIS:HE1	1:A:99:TYR:OH	1.88	0.55
1:D:219:ARG:HD3	1:D:257:TYR:CZ	2.42	0.54
1:A:66:LYS:O	1:A:70:HIS:CD2	2.59	0.54
2:B:47:GLU:HG3	2:B:48:LYS:N	2.22	0.54
1:D:207:SER:HA	1:D:240:THR:HB	1.90	0.54
1:A:177:GLU:HA	1:D:267:PRO:HB3	1.90	0.54
1:A:220:ASP:HA	7:A:409:HOH:O	2.07	0.53
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.43	0.53
2:E:10:TYR:O	2:E:24:ASN:HB2	2.09	0.53
2:E:58:LYS:HD3	2:E:58:LYS:N	2.24	0.52
1:A:42:SER:O	1:A:43:GLN:HB2	2.09	0.52
2:E:83:ASN:HD22	2:E:84:HIS:H	1.57	0.52
1:A:223:ASP:OD1	1:A:225:THR:HG22	2.10	0.52
1:A:255:GLN:CD	1:A:255:GLN:H	2.11	0.52
1:D:233:THR:OG1	1:D:243:LYS:HE2	2.08	0.52
1:D:192:HIS:ND1	4:D:302:EDO:O1	2.37	0.52
1:D:28:VAL:HG11	1:D:179:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ARG:HD3	1:D:100:GLY:HA3	1.92	0.52
1:D:21:ARG:HH11	1:D:39:ASP:HB2	1.75	0.52
1:A:188:HIS:HD2	7:A:428:HOH:O	1.93	0.52
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.57	0.51
2:E:33:SER:HB2	2:E:54:LEU:HD21	1.90	0.51
2:B:17:ASN:HB2	2:B:73:THR:HA	1.91	0.51
1:D:218:GLN:CD	1:D:260:HIS:CE1	2.84	0.51
1:A:202:ARG:NH1	1:A:244:TRP:CZ3	2.79	0.51
2:B:20:SER:CA	2:B:71:THR:HG22	2.31	0.51
1:A:232:GLU:HG2	7:B:204:HOH:O	2.09	0.51
2:B:97:ARG:NH1	4:B:101:EDO:H21	2.19	0.51
1:D:49:ALA:O	1:D:52:ILE:HG22	2.11	0.51
2:E:95:TRP:CH2	2:E:97[B]:ARG:HG3	2.46	0.51
1:A:192:HIS:HA	6:A:304:GOL:H12	1.92	0.50
2:B:41:LYS:O	2:B:44:GLU:HG2	2.12	0.50
1:A:226:GLN:HA	1:A:226:GLN:HE21	1.77	0.50
2:B:39:LEU:CD1	2:B:68:THR:HG22	2.40	0.50
2:E:20:SER:HA	2:E:71:THR:HG22	1.92	0.50
2:B:17:ASN:HB2	2:B:72:PRO:O	2.12	0.50
1:A:234:ARG:HE	1:A:242:GLN:NE2	2.09	0.50
1:D:254:GLU:H	1:D:254:GLU:CD	2.15	0.49
1:D:36:PHE:HD2	1:D:37:ASP:N	2.06	0.49
2:E:23:LEU:O	2:E:67:TYR:HA	2.13	0.49
1:A:225:THR:HG23	1:A:225:THR:O	2.13	0.49
1:A:93:HIS:HD2	1:A:119:ASP:OD1	1.96	0.49
3:F:3:THR:O	3:F:3:THR:HG23	2.11	0.49
2:B:51:HIS:HD2	2:B:52:SER:O	1.96	0.49
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.48	0.49
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.31	0.49
2:E:69:GLU:CD	2:E:69:GLU:N	2.66	0.49
1:A:185:PRO:HB3	1:A:205:ALA:HB1	1.95	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.48	0.48
1:A:49:ALA:O	1:A:52:ILE:HG22	2.13	0.48
1:A:35:ARG:HE	1:A:48:ARG:HH11	1.62	0.48
1:A:66:LYS:O	1:A:70:HIS:HD2	1.97	0.47
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.96	0.47
1:D:81:LEU:CD2	3:F:10:VAL:HG21	2.45	0.47
1:A:223:ASP:OD1	1:A:223:ASP:C	2.54	0.46
1:A:264:GLU:HG3	1:A:265:GLY:N	2.30	0.46
1:D:224:GLN:NE2	1:D:224:GLN:HA	2.30	0.46
1:D:182:THR:CG2	1:D:265:GLY:HA2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD22	3:F:10:VAL:HG21	1.97	0.46
2:B:88:SER:H	4:B:104:EDO:H12	1.80	0.46
1:A:137:ASP:OD1	1:A:137:ASP:C	2.54	0.46
2:E:17:ASN:HB2	2:E:97[A]:ARG:NH1	2.30	0.46
1:D:74:HIS:HD2	1:D:95:VAL:HG11	1.81	0.46
2:E:38:ASP:CG	2:E:45:ARG:NH1	2.69	0.46
1:A:225:THR:O	1:A:226:GLN:CB	2.59	0.46
1:D:111:ARG:HD2	1:D:113:TYR:OH	2.16	0.46
1:A:55:GLU:HA	1:A:55:GLU:OE1	2.17	0.45
1:A:70:HIS:CE1	1:A:99:TYR:OH	2.69	0.45
2:B:87:LEU:HA	4:B:104:EDO:H21	1.98	0.45
1:A:201:LEU:HD11	1:A:254:GLU:CB	2.46	0.45
3:C:7:ILE:N	3:C:7:ILE:HD12	2.32	0.45
1:A:54:GLN:HE21	1:A:54:GLN:HB2	1.59	0.45
1:A:234:ARG:HH21	1:A:242:GLN:HE22	1.65	0.45
1:D:9:PHE:HA	1:D:23:ILE:O	2.17	0.45
1:D:103:VAL:HG13	1:D:168:LEU:HD23	1.99	0.45
1:D:215:LEU:HD12	1:D:245:ALA:CB	2.47	0.45
1:D:25:VAL:HG21	1:D:32:GLN:NE2	2.30	0.45
1:A:62:GLY:O	1:A:66:LYS:HG3	2.17	0.44
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.52	0.44
2:B:39:LEU:HD13	2:B:68:THR:HG22	1.99	0.44
2:B:4:THR:HG22	2:B:86:THR:CB	2.46	0.44
2:B:10:TYR:CD2	2:B:10:TYR:N	2.85	0.44
1:A:24:ALA:O	1:A:35:ARG:HA	2.17	0.44
2:E:16:GLU:O	2:E:17:ASN:HB2	2.15	0.44
2:B:31:HIS:CD2	2:B:32:PRO:HA	2.53	0.44
1:D:36:PHE:HD2	1:D:36:PHE:C	2.19	0.44
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.84	0.44
1:A:275:GLU:CB	7:A:431:HOH:O	2.65	0.44
1:D:8:PHE:O	1:D:24:ALA:HA	2.16	0.44
1:D:202:ARG:HG3	1:D:202:ARG:HH11	1.82	0.44
2:E:39:LEU:HD12	2:E:49:VAL:HG22	2.00	0.43
1:A:4:SER:HB3	1:A:102:ASP:OD1	2.19	0.43
2:E:75:LYS:HG3	2:E:75:LYS:O	2.19	0.43
1:A:218:GLN:HA	1:A:223:ASP:HA	2.01	0.43
1:D:182:THR:CG2	1:D:265:GLY:CA	2.97	0.43
2:E:12:ARG:HH11	4:E:102:EDO:H21	1.83	0.43
1:A:74:HIS:CD2	1:A:95:VAL:HG11	2.41	0.43
1:D:215:LEU:HD21	1:D:243:LYS:CD	2.49	0.43
1:D:96:GLN:OE1	2:E:31:HIS:HE1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HG2	1:A:244:TRP:N	2.34	0.42
1:A:85:TYR:O	1:A:87:GLN:HG3	2.19	0.42
2:B:48:LYS:O	2:B:48:LYS:HG2	2.18	0.42
2:B:97:ARG:HG3	2:B:97:ARG:H	1.42	0.42
2:B:73:THR:OG1	2:B:76:ASP:HB2	2.19	0.42
2:E:16:GLU:O	2:E:17:ASN:HB3	2.18	0.42
1:D:218:GLN:HB2	1:D:258:THR:CG2	2.42	0.42
1:A:202:ARG:HD2	1:A:204:TRP:CE2	2.55	0.42
1:A:235:PRO:HG2	2:B:65:LEU:HD13	2.02	0.42
1:D:16:GLY:C	1:D:18:GLY:H	2.09	0.42
1:D:215:LEU:HA	1:D:260:HIS:O	2.20	0.42
1:A:4:SER:CB	1:A:102:ASP:OD1	2.68	0.41
1:A:155:GLN:NE2	7:A:420:HOH:O	2.44	0.41
1:A:77:ASP:OD1	3:C:9:THR:HA	2.19	0.41
1:D:202:ARG:HH11	1:D:202:ARG:CG	2.33	0.41
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.38	0.41
1:A:213:ILE:HG13	1:A:262:GLN:O	2.20	0.41
2:B:47:GLU:CG	2:B:48:LYS:N	2.83	0.41
2:E:47:GLU:HG3	2:E:48:LYS:N	2.34	0.41
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.01	0.41
2:E:16:GLU:HB2	2:E:19:LYS:HB2	2.02	0.41
2:E:85:VAL:HG22	7:E:213:HOH:O	2.20	0.41
2:B:30:PHE:HZ	2:B:64:LEU:CD1	2.33	0.41
1:A:266:LEU:HA	1:A:267:PRO:HD3	1.94	0.41
2:E:3[A]:ARG:NH1	2:E:59:ASP:O	2.54	0.41
2:E:97[A]:ARG:H	2:E:97[A]:ARG:HG3	1.67	0.41
1:A:195:SER:OG	1:A:197:HIS:N	2.53	0.41
2:E:74:GLU:HG3	2:E:74:GLU:O	2.20	0.41
1:D:183:ASP:O	1:D:208:PHE:HA	2.21	0.41
1:D:19:GLU:OE2	1:D:75:ARG:HD3	2.21	0.41
2:E:31:HIS:CE1	2:E:62:PHE:CE2	3.09	0.41
1:A:157:ARG:O	1:A:158:ALA:C	2.59	0.41
1:A:35:ARG:HE	1:A:48:ARG:NH1	2.19	0.41
1:A:76:VAL:CG1	3:C:9:THR:HG21	2.50	0.41
1:A:136:ALA:O	1:A:137:ASP:CB	2.69	0.40
1:D:85:TYR:O	1:D:87:GLN:HG3	2.20	0.40
1:A:195:SER:OG	1:A:196:ASP:N	2.53	0.40
2:B:0:MET:HG3	2:B:0:MET:O	2.21	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%)	18 (7%)	7 (3%)	5	2
1	D	274/276 (99%)	254 (93%)	14 (5%)	6 (2%)	6	4
2	B	99/100 (99%)	96 (97%)	3 (3%)	0	100	100
2	E	101/100 (101%)	96 (95%)	4 (4%)	1 (1%)	15	14
3	C	8/10 (80%)	8 (100%)	0	0	100	100
3	F	8/10 (80%)	8 (100%)	0	0	100	100
All	All	764/772 (99%)	711 (93%)	39 (5%)	14 (2%)	8	5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ASP
1	A	195	SER
1	A	225	THR
1	D	15	PRO
1	D	17	ARG
1	D	163	THR
1	D	223	ASP
1	D	226	GLN
1	A	105	SER
1	A	226	GLN
2	E	17	ASN
1	A	264	GLU
1	A	43	GLN
1	D	136	ALA

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%)	213 (92%)	19 (8%)	11	11
1	D	232/232 (100%)	217 (94%)	15 (6%)	17	19
2	B	96/95 (101%)	85 (88%)	11 (12%)	5	4
2	E	98/95 (103%)	84 (86%)	14 (14%)	3	3
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
All	All	674/670 (101%)	615 (91%)	59 (9%)	10	9

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	32	GLN
1	A	73	THR
1	A	86	ASN
1	A	92	SER
1	A	113	TYR
1	A	128	GLU
1	A	137	ASP
1	A	161	GLU
1	A	176	LYS
1	A	180	GLN
1	A	195	SER
1	A	197	HIS
1	A	223	ASP
1	A	226	GLN
1	A	254	GLU
1	A	255	GLN
1	A	268	LYS
1	A	275	GLU
2	B	16	GLU
2	B	17	ASN
2	B	33	SER
2	B	58	LYS
2	B	69	GLU
2	B	70	PHE
2	B	83	ASN
2	B	85	VAL

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Mol	Chain	Res	Type
2	B	89	GLN
2	B	92	ILE
2	B	97	ARG
1	D	21	ARG
1	D	35	ARG
1	D	36	PHE
1	D	73	THR
1	D	81	LEU
1	D	89	GLU
1	D	110	LEU
1	D	170	ARG
1	D	182	THR
1	D	215	LEU
1	D	222	GLU
1	D	224	GLN
1	D	226	GLN
1	D	248	VAL
1	D	258	THR
2	E	1	ILE
2	E	17	ASN
2	E	45	ARG
2	E	48	LYS
2	E	58	LYS
2	E	70	PHE
2	E	74	GLU
2	E	75	LYS
2	E	77	GLU
2	E	83	ASN
2	E	85	VAL
2	E	89	GLN
2	E	97[A]	ARG
2	E	97[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	54	GLN
1	A	70	HIS
1	A	74	HIS
1	A	93	HIS
1	A	96	GLN

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Mol	Chain	Res	Type
1	A	141	GLN
1	A	145	HIS
1	A	155	GLN
1	A	180	GLN
1	A	188	HIS
1	A	226	GLN
1	A	242	GLN
2	B	8	GLN
2	B	17	ASN
2	B	31	HIS
2	B	51	HIS
2	B	83	ASN
1	D	32	GLN
1	D	43	GLN
1	D	70	HIS
1	D	87	GLN
1	D	93	HIS
1	D	191	HIS
1	D	226	GLN
1	D	260	HIS
2	E	8	GLN
2	E	31	HIS
2	E	51	HIS
2	E	83	ASN
2	E	89	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

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	$\# Z > 2$
4	EDO	B	103	-	3,3,3	0.49	0	2,2,2	0.17	0
4	EDO	A	301	-	3,3,3	0.37	0	2,2,2	0.72	0
4	EDO	B	102	-	3,3,3	0.43	0	2,2,2	0.73	0
4	EDO	D	303	-	3,3,3	0.48	0	2,2,2	0.50	0
4	EDO	D	302	-	3,3,3	0.46	0	2,2,2	0.69	0
4	EDO	A	302	-	3,3,3	0.61	0	2,2,2	0.22	0
4	EDO	E	102	-	3,3,3	0.46	0	2,2,2	0.64	0
4	EDO	D	301	-	3,3,3	0.41	0	2,2,2	1.21	0
4	EDO	B	101	-	3,3,3	0.55	0	2,2,2	0.23	0
4	EDO	B	105	-	3,3,3	0.43	0	2,2,2	0.50	0
5	SO4	A	303	-	4,4,4	0.20	0	6,6,6	0.41	0
6	GOL	A	304	-	5,5,5	0.33	0	5,5,5	1.55	1 (20%)
4	EDO	D	304	-	3,3,3	0.52	0	2,2,2	0.34	0
6	GOL	D	305	-	5,5,5	0.42	0	5,5,5	0.74	0
4	EDO	B	104	-	3,3,3	0.42	0	2,2,2	0.69	0
4	EDO	E	101	-	3,3,3	0.43	0	2,2,2	0.85	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
4	EDO	B	103	-	-	1/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	B	102	-	-	0/1/1/1	-
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	E	102	-	-	1/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	101	-	-	1/1/1/1	-
4	EDO	B	105	-	-	1/1/1/1	-
6	GOL	A	304	-	-	2/4/4/4	-
4	EDO	D	304	-	-	1/1/1/1	-
6	GOL	D	305	-	-	4/4/4/4	-
4	EDO	B	104	-	-	0/1/1/1	-
4	EDO	E	101	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	A	304	GOL	C3-C2-C1	-2.27	102.89	111.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	304	GOL	C1-C2-C3-O3
6	D	305	GOL	C1-C2-C3-O3
6	A	304	GOL	O2-C2-C3-O3
6	D	305	GOL	O1-C1-C2-O2
6	D	305	GOL	O1-C1-C2-C3
4	D	304	EDO	O1-C1-C2-O2
4	E	102	EDO	O1-C1-C2-O2
4	A	302	EDO	O1-C1-C2-O2
6	D	305	GOL	O2-C2-C3-O3
4	B	105	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
4	B	103	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
4	B	101	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	EDO	1	0
4	E	102	EDO	1	0
4	B	101	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	105	EDO	1	0
6	A	304	GOL	1	0
6	D	305	GOL	1	0
4	B	104	EDO	2	0
4	E	101	EDO	1	0

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, 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%)	0.14	8 (2%) 51 61	21, 46, 82, 97	0
1	D	276/276 (100%)	0.16	10 (3%) 42 53	23, 46, 77, 89	0
2	B	100/100 (100%)	-0.16	0 100 100	20, 40, 64, 77	0
2	E	100/100 (100%)	-0.14	0 100 100	20, 38, 64, 75	0
3	C	10/10 (100%)	0.10	0 100 100	30, 35, 43, 48	0
3	F	10/10 (100%)	0.36	0 100 100	33, 37, 45, 48	0
All	All	772/772 (100%)	0.07	18 (2%) 60 69	20, 43, 77, 97	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	GLU	3.8
1	A	54	GLN	3.7
1	A	222	GLU	3.1
1	A	226	GLN	3.1
1	D	58	GLU	2.8
1	D	1	GLY	2.8
1	D	226	GLN	2.7
1	D	50	PRO	2.4
1	D	195	SER	2.4
1	D	222	GLU	2.2
1	D	54	GLN	2.2
1	D	223	ASP	2.2
1	A	225	THR	2.2
1	D	228	THR	2.2
1	A	57	PRO	2.2
1	A	197	HIS	2.1
1	A	110	LEU	2.0
1	D	177	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 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, 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(\AA^2)	Q<0.9
4	EDO	B	101	4/4	0.79	0.12	49,52,52,56	0
6	GOL	D	305	6/6	0.80	0.20	60,66,67,68	0
4	EDO	A	302	4/4	0.86	0.17	52,57,57,59	0
4	EDO	D	304	4/4	0.88	0.10	47,51,58,58	0
4	EDO	B	103	4/4	0.90	0.13	63,66,68,69	0
4	EDO	A	301	4/4	0.91	0.13	51,55,56,59	0
4	EDO	B	102	4/4	0.91	0.20	45,47,49,49	0
4	EDO	E	102	4/4	0.92	0.10	39,47,48,52	0
4	EDO	E	101	4/4	0.92	0.10	35,40,44,49	0
4	EDO	D	303	4/4	0.93	0.13	53,54,55,55	0
4	EDO	D	301	4/4	0.93	0.28	33,39,52,57	0
4	EDO	B	104	4/4	0.94	0.20	58,58,63,65	0
6	GOL	A	304	6/6	0.95	0.15	27,40,42,46	0
5	SO4	A	303	5/5	0.96	0.12	56,62,73,73	0
4	EDO	D	302	4/4	0.96	0.19	33,38,44,44	0
4	EDO	B	105	4/4	0.96	0.15	43,47,51,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.