



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 10:19 pm GMT

PDB ID : 5MER  
Title : Human Leukocyte Antigen A02 presenting ILAKFLHEL  
Authors : Rizkallah, P.J.; Lloyd, A.; Crowther, M.; Cole, D.K.; Sewell, A.K.  
Deposited on : 2016-11-16  
Resolution : 1.88 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](mailto: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>.

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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)  
Xtriage (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

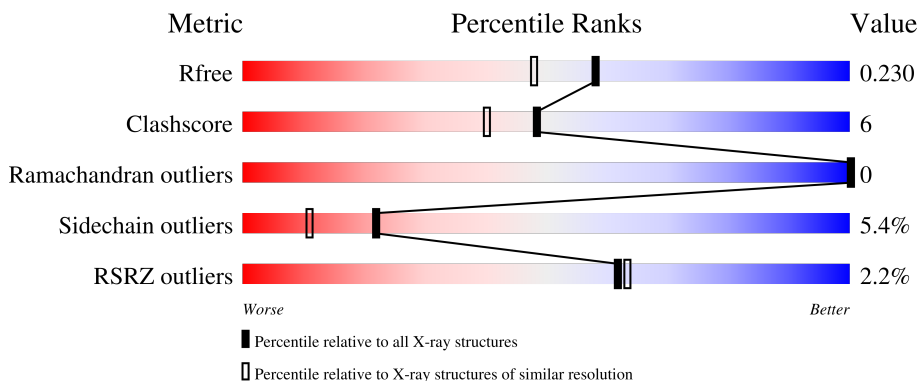
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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  $\geq 3$ , 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	3% 86% 13%
1	D	276	0% 82% 15%
2	B	100	3% 80% 16%
2	E	100	2% 86% 14%
3	C	9	67% 11% 22%

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Mol	Chain	Length	Quality of chain
3	F	9	 78% 11% 11%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7032 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	1	0
			2266	1417	411	429	9			
1	D	276	Total	C	N	O	S	0	2	0
			2272	1420	412	430	10			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	2	0
			851	542	143	162	4			
2	E	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
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ILE-LEU-ALA-LYS-PHE-LEU-HIS-GLU-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	Total	C	N	O	0	0	0
			77	53	12	12			
3	F	9	Total	C	N	O	0	0	0
			77	53	12	12			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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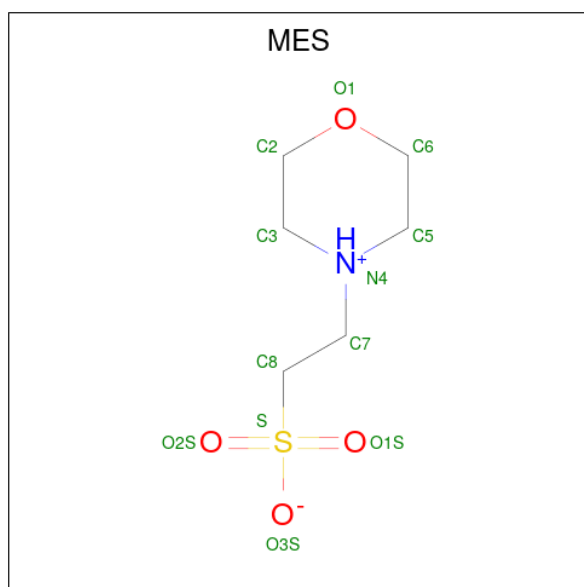
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



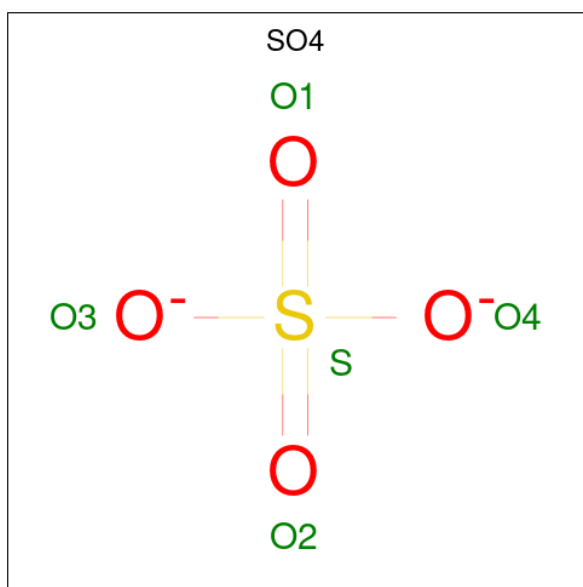
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	Total 12	C 6	N 1	O 4	S 1	0	0
6	D	1	Total 12	C 6	N 1	O 4	S 1	0	0
6	E	1	Total 12	C 6	N 1	O 4	S 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



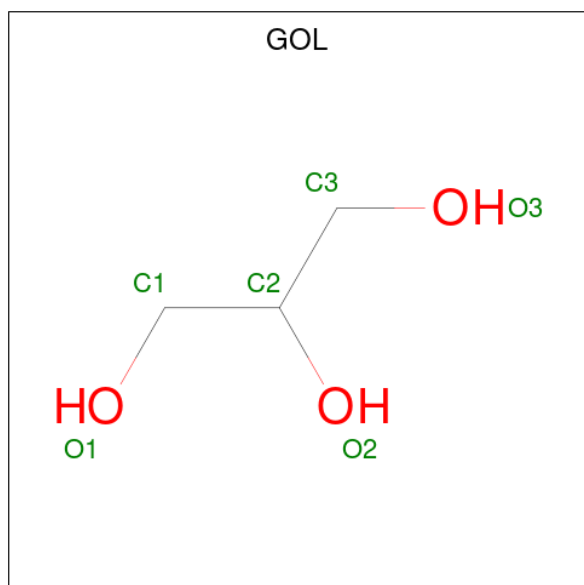
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	B	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0
7	C	1	Total 5	O 4	S 1	0	0
7	D	1	Total 5	O 4	S 1	0	0
7	D	1	Total 5	O 4	S 1	0	0
7	D	1	Total 5	O 4	S 1	0	0
7	D	1	Total 5	O 4	S 1	0	0
7	D	1	Total 5	O 4	S 1	0	0

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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	140	Total O 140 140	0	0
9	B	77	Total O 77 77	0	0
9	C	7	Total O 7 7	0	0
9	D	163	Total O 163 163	0	0

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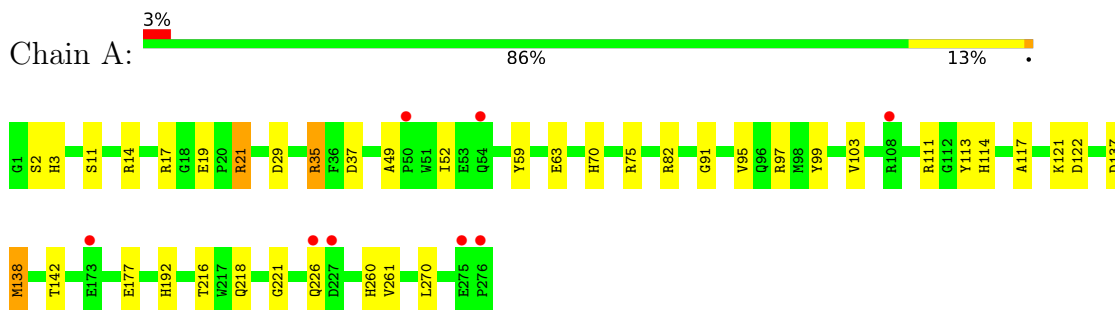
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
9	E	58	Total O 58 58	0	0
9	F	9	Total O 9 9	0	0

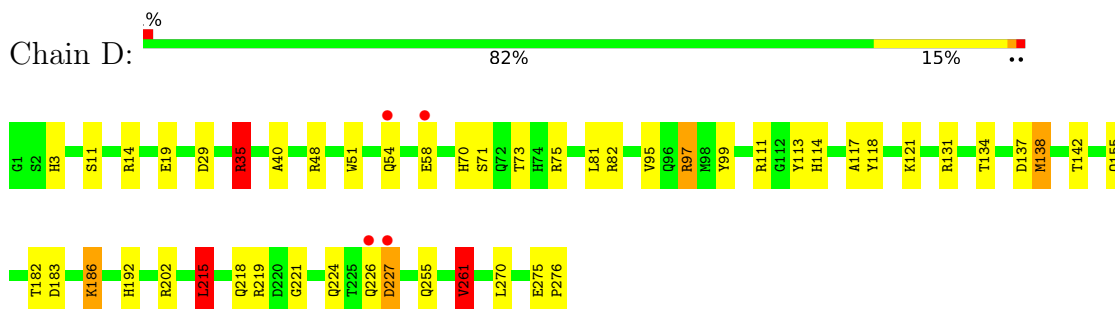
### 3 Residue-property plots [i](#)

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.

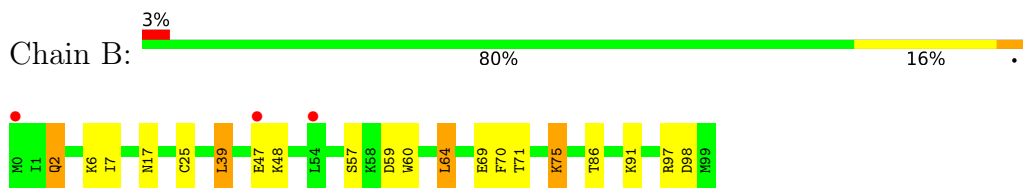
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



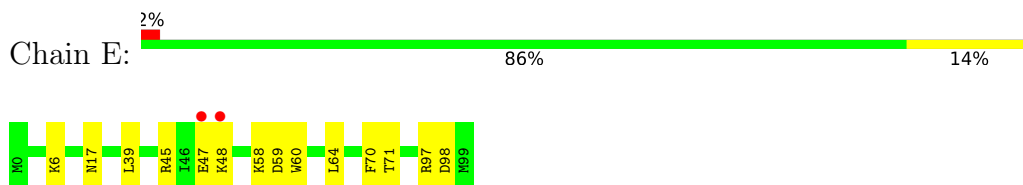
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin




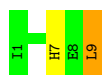
- Molecule 3: ILE-LEU-ALA-LYS-PHE-LEU-HIS-GLU-LEU

Chain C:  67% 11% 22%



• Molecule 3: ILE-LEU-ALA-LYS-PHE-LEU-HIS-GLU-LEU

Chain F:  78% 11% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.97Å 170.28Å 45.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.06 – 1.88 33.35 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.06-1.88) 99.9 (33.35-1.88)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 1.88Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.184 , 0.224 0.193 , 0.230	Depositor DCC
$R_{free}$ test set	3797 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtrriage
Anisotropy	0.372	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0315e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.91	0/2333	1.02	9/3167 (0.3%)
1	D	0.92	1/2339 (0.0%)	1.02	11/3175 (0.3%)
2	B	1.08	1/874 (0.1%)	1.03	2/1181 (0.2%)
2	E	1.00	0/860	1.01	1/1162 (0.1%)
3	C	0.95	0/78	1.38	2/102 (2.0%)
3	F	0.95	0/78	1.06	0/102
All	All	0.95	2/6562 (0.0%)	1.02	25/8889 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	GLU	CG-CD	6.04	1.61	1.51
1	D	71	SER	CB-OG	-5.12	1.35	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ARG	NE-CZ-NH2	10.95	125.78	120.30
1	A	35	ARG	NE-CZ-NH1	-9.57	115.52	120.30
1	D	219	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	14	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	D	219	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	D	35	ARG	NE-CZ-NH2	-7.21	116.70	120.30
2	B	59	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	261	VAL	CG1-CB-CG2	6.64	121.53	110.90
1	D	14	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	82	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	E	59	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	138	MET	CG-SD-CE	6.39	110.42	100.20
1	A	137	ASP	CB-CG-OD1	6.25	123.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	VAL	CG1-CB-CG2	6.19	120.81	110.90
1	D	138	MET	CG-SD-CE	6.00	109.80	100.20
1	A	17	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	202	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	97	ARG	NE-CZ-NH2	5.69	123.14	120.30
3	C	6	LEU	CB-CG-CD1	5.43	120.23	111.00
1	A	17	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	137	ASP	CB-CG-OD1	5.33	123.10	118.30
3	C	9	LEU	CB-CA-C	-5.22	100.29	110.20
1	D	131	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	D	215	LEU	CA-CB-CG	5.03	126.88	115.30
2	B	64	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2266	0	2111	25	0
1	D	2272	0	2114	28	0
2	B	851	0	817	16	0
2	E	837	0	803	7	0
3	C	77	0	86	4	0
3	F	77	0	86	6	0
4	A	8	0	12	1	0
4	B	28	0	42	1	0
4	C	4	0	6	0	0
4	D	16	0	24	1	0
4	E	20	0	30	0	0
4	F	4	0	6	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	12	0	13	2	0
6	B	12	0	13	1	0
6	D	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	12	0	13	1	0
7	B	10	0	0	1	0
7	C	5	0	0	0	0
7	D	30	0	0	1	0
7	E	5	0	0	0	0
8	C	6	0	8	0	0
8	D	6	0	8	3	0
8	E	6	0	8	0	0
9	A	140	0	0	3	0
9	B	77	0	0	2	1
9	C	7	0	0	0	0
9	D	163	0	0	9	0
9	E	58	0	0	0	1
9	F	9	0	0	2	0
All	All	7032	0	6213	77	1

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 6.

All (77) 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:216:THR:HG22	9:A:490:HOH:O	1.64	0.96
1:D:19:GLU:OE1	1:D:75:ARG:NH1	1.98	0.95
1:A:19:GLU:OE1	1:A:75:ARG:NH1	1.98	0.94
3:F:7:HIS:HD2	9:F:208:HOH:O	1.57	0.87
1:A:142:THR:OG1	6:A:304:MES:H51	1.79	0.82
1:A:192:HIS:HE1	2:B:98:ASP:OD2	1.62	0.82
1:D:118:TYR:HB3	4:D:305:EDO:H21	1.63	0.81
1:D:82:ARG:NH1	9:D:401:HOH:O	2.17	0.76
2:B:39[B]:LEU:HD22	2:B:39[B]:LEU:N	2.04	0.73
2:B:2:GLN:HG2	2:B:86:THR:HG22	1.73	0.71
1:D:155:GLN:HE22	3:F:7:HIS:HE1	1.39	0.71
2:B:17:ASN:HD21	2:B:97:ARG:HH12	1.40	0.70
1:D:3:HIS:HE1	9:D:544:HOH:O	1.74	0.70
1:D:192:HIS:HE1	2:E:98:ASP:OD2	1.75	0.69
1:D:186:LYS:HE2	9:D:449:HOH:O	1.92	0.69
2:E:17:ASN:HD21	2:E:97:ARG:HH22	1.41	0.68
1:D:97:ARG:HH21	1:D:114:HIS:HE1	1.43	0.67
1:D:3:HIS:HD2	1:D:29:ASP:OD2	1.77	0.67
2:E:58:LYS:HG3	6:E:107:MES:O1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:301:GOL:C1	9:D:481:HOH:O	2.42	0.66
8:D:301:GOL:H11	9:D:481:HOH:O	1.97	0.64
2:B:2:GLN:HG2	2:B:86:THR:CG2	2.28	0.64
1:A:59:TYR:CE2	3:C:1:ILE:CD1	2.81	0.64
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.81	0.63
1:A:97:ARG:HH11	1:A:114:HIS:HE1	1.47	0.63
1:D:97:ARG:HH21	1:D:114:HIS:CE1	2.19	0.60
1:D:226:GLN:H	1:D:226:GLN:CD	2.07	0.58
1:A:111:ARG:HD3	1:A:113[A]:TYR:OH	2.04	0.58
1:D:155:GLN:NE2	3:F:7:HIS:HE1	2.00	0.57
1:D:183:ASP:OD1	9:D:402:HOH:O	2.18	0.57
2:B:75:LYS:HD3	9:B:223:HOH:O	2.06	0.56
2:B:75:LYS:CD	9:B:223:HOH:O	2.54	0.56
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.87	0.56
1:A:216:THR:HG23	1:A:260:HIS:HB2	1.88	0.55
1:D:121:LYS:HG2	9:D:477:HOH:O	2.05	0.55
1:A:70:HIS:HE1	1:A:99:TYR:OH	1.90	0.55
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.72	0.54
1:D:70:HIS:HE1	1:D:99:TYR:OH	1.91	0.54
1:A:97:ARG:HH11	1:A:114:HIS:CE1	2.25	0.54
1:D:227:ASP:N	1:D:227:ASP:OD1	2.41	0.53
2:B:25:CYS:HB2	2:B:39[B]:LEU:HD11	1.91	0.53
1:D:218:GLN:HE21	1:D:221:GLY:HA2	1.74	0.52
3:F:7:HIS:CD2	9:F:208:HOH:O	2.43	0.52
2:E:47:GLU:H	2:E:47:GLU:CD	2.14	0.51
1:A:2:SER:HB2	1:A:103:VAL:O	2.12	0.49
2:B:47:GLU:H	2:B:47:GLU:CD	2.15	0.49
1:A:91:GLY:C	9:A:402:HOH:O	2.51	0.49
9:A:480:HOH:O	6:B:108:MES:H32	2.13	0.49
1:D:35:ARG:NH2	7:D:311:SO4:O2	2.44	0.49
1:A:177:GLU:H	1:A:177:GLU:CD	2.15	0.49
1:D:142:THR:OG1	6:D:307:MES:H52	2.12	0.49
2:B:6:LYS:HB3	4:B:107:EDO:H22	1.95	0.48
1:A:63:GLU:OE1	3:C:1:ILE:HG13	2.14	0.48
8:D:301:GOL:H12	2:E:6:LYS:HD3	1.95	0.48
2:B:39[B]:LEU:N	2:B:39[B]:LEU:CD2	2.75	0.47
1:D:111:ARG:HD3	1:D:113[A]:TYR:OH	2.15	0.47
1:A:142:THR:HG1	6:A:304:MES:H51	1.77	0.47
1:D:81:LEU:HD11	3:F:9:LEU:HD11	1.98	0.46
1:A:122:ASP:H	4:A:302:EDO:H12	1.80	0.45
1:D:275:GLU:C	1:D:276:PRO:O	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:NH1	1:A:37:ASP:OD2	2.50	0.45
2:B:57:SER:HB3	7:B:109:SO4:O3	2.16	0.44
2:B:17:ASN:HD21	2:B:97:ARG:NH1	2.12	0.44
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.53	0.44
1:D:186:LYS:CE	9:D:449:HOH:O	2.58	0.43
1:A:59:TYR:CE2	3:C:1:ILE:HD11	2.52	0.43
1:D:11:SER:HB3	1:D:95:VAL:CG2	2.49	0.43
1:A:192:HIS:CE1	2:B:98:ASP:OD2	2.54	0.42
1:D:51:TRP:O	1:D:54:GLN:HG2	2.19	0.42
3:F:9:LEU:C	3:F:9:LEU:HD23	2.39	0.42
1:D:40:ALA:HB3	9:D:478:HOH:O	2.20	0.41
1:A:59:TYR:CE2	3:C:1:ILE:HD12	2.54	0.41
1:A:49:ALA:O	1:A:52:ILE:HG22	2.21	0.41
1:D:215:LEU:HD12	1:D:261:VAL:HB	2.03	0.41
1:A:11:SER:HB3	1:A:95:VAL:CG2	2.51	0.41
2:E:17:ASN:HD21	2:E:97:ARG:NH2	2.12	0.41
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.56	0.40

All (1) 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)
9:B:272:HOH:O	9:E:233:HOH:O[4_456]	2.11	0.09

## 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	275/276 (100%)	271 (98%)	4 (2%)	0	100 100
1	D	276/276 (100%)	271 (98%)	5 (2%)	0	100 100
2	B	100/100 (100%)	100 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	98/100 (98%)	98 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	763/770 (99%)	754 (99%)	9 (1%)	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	233/232 (100%)	227 (97%)	6 (3%)	46	36
1	D	234/232 (101%)	220 (94%)	14 (6%)	19	8
2	B	97/95 (102%)	89 (92%)	8 (8%)	11	4
2	E	95/95 (100%)	89 (94%)	6 (6%)	18	7
3	C	8/8 (100%)	6 (75%)	2 (25%)	0	0
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	1
All	All	675/670 (101%)	638 (94%)	37 (6%)	22	10

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	35	ARG
1	A	121	LYS
1	A	138	MET
1	A	226	GLN
1	A	270	LEU
2	B	2	GLN
2	B	39[A]	LEU
2	B	39[B]	LEU
2	B	48	LYS

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Mol	Chain	Res	Type
2	B	64	LEU
2	B	70	PHE
2	B	71	THR
2	B	75	LYS
3	C	1	ILE
3	C	6	LEU
1	D	35	ARG
1	D	48	ARG
1	D	58	GLU
1	D	73	THR
1	D	134	THR
1	D	138	MET
1	D	182	THR
1	D	186	LYS
1	D	215	LEU
1	D	224	GLN
1	D	227	ASP
1	D	255	GLN
1	D	261	VAL
1	D	270	LEU
2	E	39	LEU
2	E	45	ARG
2	E	48	LYS
2	E	64	LEU
2	E	70	PHE
2	E	71	THR
3	F	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	70	HIS
1	A	72	GLN
1	A	114	HIS
1	A	141	GLN
1	A	192	HIS
1	A	197	HIS
1	A	218	GLN
1	A	253	GLN
2	B	17	ASN
1	D	3	HIS

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Mol	Chain	Res	Type
1	D	70	HIS
1	D	72	GLN
1	D	114	HIS
1	D	115	GLN
1	D	141	GLN
1	D	155	GLN
1	D	192	HIS
1	D	218	GLN
1	D	224	GLN
1	D	253	GLN
2	E	17	ASN
3	F	7	HIS

### 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](#)

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 for Mogul analysis.

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	SO4	D	312	-	4,4,4	0.47	0	6,6,6	0.12	0
4	EDO	B	102	-	3,3,3	0.51	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	E	108	-	4,4,4	0.46	0	6,6,6	1.22	1 (16%)
8	GOL	E	101	-	5,5,5	0.76	0	5,5,5	0.28	0
4	EDO	F	101	-	3,3,3	0.46	0	2,2,2	0.26	0
6	MES	E	107	-	12,12,12	1.93	1 (8%)	14,16,16	2.24	4 (28%)
7	SO4	D	309	-	4,4,4	0.45	0	6,6,6	0.96	0
4	EDO	C	102	-	3,3,3	0.63	0	2,2,2	0.78	0
7	SO4	B	109	-	4,4,4	0.36	0	6,6,6	0.91	0
4	EDO	E	103	-	3,3,3	0.78	0	2,2,2	0.73	0
4	EDO	E	104	-	3,3,3	0.74	0	2,2,2	1.18	0
8	GOL	D	301	-	5,5,5	0.64	0	5,5,5	1.18	0
4	EDO	B	106	-	3,3,3	0.14	0	2,2,2	0.97	0
4	EDO	E	106	-	3,3,3	0.30	0	2,2,2	0.19	0
6	MES	B	108	-	12,12,12	1.77	1 (8%)	14,16,16	3.88	6 (42%)
4	EDO	B	101	-	3,3,3	0.51	0	2,2,2	0.20	0
4	EDO	B	107	-	3,3,3	0.50	0	2,2,2	0.14	0
4	EDO	E	102	-	3,3,3	0.37	0	2,2,2	0.87	0
8	GOL	C	101	-	5,5,5	0.93	0	5,5,5	1.59	1 (20%)
4	EDO	D	305	-	3,3,3	0.64	0	2,2,2	0.95	0
4	EDO	D	302	-	3,3,3	0.59	0	2,2,2	0.41	0
4	EDO	D	304	-	3,3,3	0.22	0	2,2,2	0.94	0
4	EDO	A	301	-	3,3,3	0.23	0	2,2,2	1.52	1 (50%)
4	EDO	B	103	-	3,3,3	0.69	0	2,2,2	0.18	0
7	SO4	C	103	-	4,4,4	0.45	0	6,6,6	0.64	0
7	SO4	D	308	-	4,4,4	0.68	0	6,6,6	0.46	0
7	SO4	D	310	-	4,4,4	0.54	0	6,6,6	0.64	0
4	EDO	B	105	-	3,3,3	0.63	0	2,2,2	0.45	0
7	SO4	B	110	-	4,4,4	0.41	0	6,6,6	0.58	0
7	SO4	D	311	-	4,4,4	0.34	0	6,6,6	0.42	0
4	EDO	A	302	-	3,3,3	0.31	0	2,2,2	0.50	0
7	SO4	D	313	-	4,4,4	0.46	0	6,6,6	0.25	0
4	EDO	B	104	-	3,3,3	1.05	0	2,2,2	0.89	0
6	MES	A	304	-	12,12,12	1.86	2 (16%)	14,16,16	2.80	6 (42%)
6	MES	D	307	-	12,12,12	2.02	1 (8%)	14,16,16	2.25	5 (35%)
4	EDO	D	303	-	3,3,3	0.45	0	2,2,2	0.25	0
4	EDO	E	105	-	3,3,3	0.75	0	2,2,2	0.33	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	102	-	-	1/1/1/1	-
8	GOL	E	101	-	-	0/4/4/4	-
4	EDO	F	101	-	-	0/1/1/1	-
6	MES	E	107	-	-	4/6/14/14	0/1/1/1
4	EDO	C	102	-	-	0/1/1/1	-
4	EDO	E	103	-	-	1/1/1/1	-
4	EDO	E	104	-	-	1/1/1/1	-
8	GOL	D	301	-	-	1/4/4/4	-
4	EDO	B	106	-	-	0/1/1/1	-
4	EDO	E	106	-	-	0/1/1/1	-
6	MES	B	108	-	-	6/6/14/14	0/1/1/1
4	EDO	B	101	-	-	0/1/1/1	-
4	EDO	B	107	-	-	0/1/1/1	-
4	EDO	E	102	-	-	1/1/1/1	-
8	GOL	C	101	-	-	4/4/4/4	-
4	EDO	D	305	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	D	304	-	-	1/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	B	103	-	-	1/1/1/1	-
4	EDO	B	105	-	-	1/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	B	104	-	-	1/1/1/1	-
6	MES	A	304	-	-	2/6/14/14	0/1/1/1
6	MES	D	307	-	-	5/6/14/14	0/1/1/1
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	E	105	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	307	MES	C8-S	-6.66	1.68	1.77
6	E	107	MES	C8-S	-6.25	1.68	1.77
6	A	304	MES	C8-S	-5.70	1.69	1.77
6	B	108	MES	C8-S	-5.34	1.69	1.77
6	A	304	MES	O2S-S	2.02	1.51	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	108	MES	O2S-S-C8	8.53	117.19	106.92
6	B	108	MES	O1S-S-C8	8.04	116.59	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	304	MES	C6-C5-N4	6.70	120.27	110.10
6	B	108	MES	O1-C2-C3	-5.69	99.27	111.80
6	A	304	MES	O2S-S-C8	5.14	113.11	106.92
6	D	307	MES	O3S-S-C8	4.84	113.60	105.77
6	E	107	MES	O1-C6-C5	-4.25	102.42	111.80
6	B	108	MES	O3S-S-C8	-4.18	99.01	105.77
6	D	307	MES	O2S-S-C8	4.08	111.83	106.92
6	E	107	MES	O3S-S-C8	3.95	112.15	105.77
6	E	107	MES	O1S-S-C8	3.79	111.48	106.92
6	B	108	MES	O2S-S-O1S	-3.41	102.13	113.95
6	A	304	MES	O1-C2-C3	-3.19	104.77	111.80
6	A	304	MES	O3S-S-C8	3.19	110.93	105.77
6	E	107	MES	O1-C2-C3	-3.03	105.13	111.80
6	D	307	MES	O3S-S-O2S	-2.60	104.91	111.27
6	A	304	MES	C2-C3-N4	-2.41	106.46	110.10
6	A	304	MES	O3S-S-O2S	-2.36	105.51	111.27
8	C	101	GOL	C3-C2-C1	2.29	120.60	111.70
7	E	108	SO4	O4-S-O3	2.21	118.48	109.06
6	B	108	MES	C6-C5-N4	-2.13	106.88	110.10
6	D	307	MES	C5-N4-C3	2.12	113.59	108.83
4	A	301	EDO	O1-C1-C2	-2.11	96.70	111.91
6	D	307	MES	C7-N4-C5	-2.00	106.12	111.23

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	102	EDO	O1-C1-C2-O2
6	A	304	MES	N4-C7-C8-S
6	B	108	MES	N4-C7-C8-S
6	D	307	MES	N4-C7-C8-S
6	D	307	MES	C7-C8-S-O1S
6	D	307	MES	C7-C8-S-O3S
6	E	107	MES	N4-C7-C8-S
8	C	101	GOL	O1-C1-C2-C3
8	C	101	GOL	O2-C2-C3-O3
6	B	108	MES	C7-C8-S-O3S
8	C	101	GOL	C1-C2-C3-O3
8	D	301	GOL	C1-C2-C3-O3
4	D	304	EDO	O1-C1-C2-O2
6	E	107	MES	C7-C8-S-O3S
8	C	101	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	E	105	EDO	O1-C1-C2-O2
6	B	108	MES	C8-C7-N4-C3
6	B	108	MES	C8-C7-N4-C5
4	A	302	EDO	O1-C1-C2-O2
6	B	108	MES	C7-C8-S-O1S
6	B	108	MES	C7-C8-S-O2S
6	D	307	MES	C7-C8-S-O2S
6	E	107	MES	C7-C8-S-O1S
6	E	107	MES	C7-C8-S-O2S
4	B	105	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
4	E	103	EDO	O1-C1-C2-O2
6	A	304	MES	C7-C8-S-O3S
4	E	102	EDO	O1-C1-C2-O2
4	B	103	EDO	O1-C1-C2-O2
4	B	104	EDO	O1-C1-C2-O2
4	D	305	EDO	O1-C1-C2-O2
4	E	104	EDO	O1-C1-C2-O2
6	D	307	MES	C8-C7-N4-C5

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	107	MES	1	0
7	B	109	SO4	1	0
8	D	301	GOL	3	0
6	B	108	MES	1	0
4	B	107	EDO	1	0
4	D	305	EDO	1	0
7	D	311	SO4	1	0
4	A	302	EDO	1	0
6	A	304	MES	2	0
6	D	307	MES	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/276 (100%)	0.05	8 (2%) 51 53	16, 33, 55, 73	0
1	D	276/276 (100%)	0.08	4 (1%) 75 77	16, 32, 52, 70	0
2	B	100/100 (100%)	0.02	3 (3%) 50 51	14, 27, 48, 61	0
2	E	100/100 (100%)	0.05	2 (2%) 65 67	14, 26, 46, 58	0
3	C	9/9 (100%)	0.49	0 100 100	26, 31, 41, 43	0
3	F	9/9 (100%)	0.19	0 100 100	25, 28, 42, 43	0
All	All	770/770 (100%)	0.06	17 (2%) 62 63	14, 30, 52, 73	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	ASP	3.9
1	A	226	GLN	3.2
1	A	50	PRO	3.1
1	D	226	GLN	2.9
1	D	54	GLN	2.8
2	E	47	GLU	2.6
2	E	48	LYS	2.4
1	A	54	GLN	2.4
1	D	227	ASP	2.3
2	B	47	GLU	2.2
1	A	173	GLU	2.2
1	A	276	PRO	2.1
1	D	58	GLU	2.1
1	A	108	ARG	2.1
2	B	54	LEU	2.1
1	A	275	GLU	2.1
2	B	0	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	MES	D	307	12/12	0.68	0.27	59,64,113,118	0
6	MES	A	304	12/12	0.77	0.32	49,60,96,101	0
7	SO4	E	108	5/5	0.77	0.26	78,79,99,105	0
7	SO4	D	312	5/5	0.78	0.34	47,85,90,95	0
7	SO4	C	103	5/5	0.79	0.27	68,93,98,102	0
8	GOL	C	101	6/6	0.79	0.23	45,46,53,56	0
4	EDO	A	301	4/4	0.80	0.38	48,49,52,56	0
4	EDO	E	105	4/4	0.80	0.20	40,55,57,57	0
6	MES	E	107	12/12	0.81	0.24	47,66,111,119	0
6	MES	B	108	12/12	0.82	0.20	35,52,85,90	0
8	GOL	E	101	6/6	0.82	0.19	39,42,51,54	0
4	EDO	B	105	4/4	0.83	0.20	38,40,43,54	0
4	EDO	D	304	4/4	0.85	0.21	45,48,53,59	0
8	GOL	D	301	6/6	0.86	0.27	29,50,56,62	0
4	EDO	D	305	4/4	0.86	0.20	37,42,42,45	0
4	EDO	B	102	4/4	0.87	0.14	37,43,47,48	0
7	SO4	D	313	5/5	0.87	0.20	61,74,80,84	0
7	SO4	B	110	5/5	0.89	0.32	98,98,102,106	0
4	EDO	D	302	4/4	0.89	0.21	43,44,50,52	0
4	EDO	B	101	4/4	0.90	0.11	36,42,44,45	0
4	EDO	B	107	4/4	0.91	0.19	43,50,51,55	0
4	EDO	A	302	4/4	0.91	0.20	46,47,48,58	0
4	EDO	D	303	4/4	0.91	0.23	39,45,51,51	0
7	SO4	D	308	5/5	0.92	0.22	64,67,69,78	0
4	EDO	B	106	4/4	0.93	0.14	23,27,30,36	0
5	CA	D	306	1/1	0.93	0.29	62,62,62,62	0
4	EDO	E	102	4/4	0.93	0.14	22,24,28,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	D	310	5/5	0.94	0.15	45,50,60,62	0
7	SO4	D	311	5/5	0.94	0.20	66,71,75,84	0
4	EDO	E	103	4/4	0.94	0.13	30,38,38,42	0
4	EDO	C	102	4/4	0.94	0.11	25,25,27,28	0
4	EDO	B	103	4/4	0.95	0.10	32,40,41,45	0
4	EDO	E	106	4/4	0.95	0.13	38,39,40,49	0
5	CA	A	303	1/1	0.96	0.29	57,57,57,57	0
7	SO4	B	109	5/5	0.97	0.10	52,59,63,64	0
4	EDO	B	104	4/4	0.97	0.09	19,20,23,29	0
4	EDO	F	101	4/4	0.97	0.13	21,23,24,28	0
4	EDO	E	104	4/4	0.98	0.08	18,20,23,27	0
7	SO4	D	309	5/5	0.98	0.21	35,47,50,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.