Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 09:44 PM JST

PDB ID	:	4ZFZ
Title	:	Crystal structure of rhesus macaque MHC class I molecule Mamu-B*098 complexed with myristoylated 5-mer lipopeptide derived from SIV Nef protein
Authors	:	Morita, D.; Sugita, M.
Deposited on	:	2015-04-22
Resolution	:	1.76 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

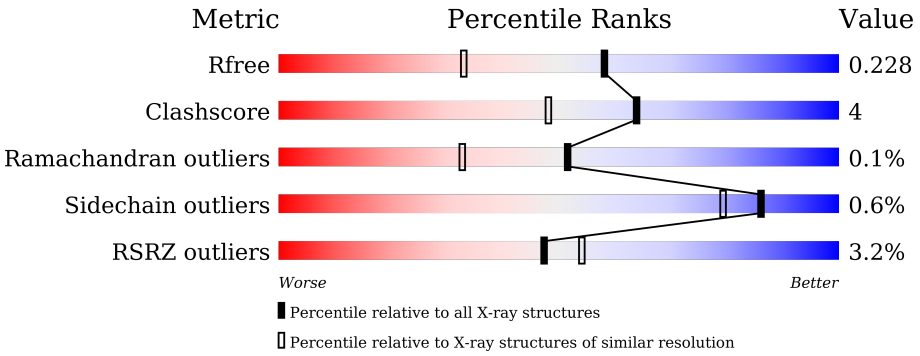
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	277	2% 94% 6%
1	D	277	.% 93% 7%
1	G	277	3% 91% 9%
1	J	277	2% 92% 8%
2	B	100	3% 88% 10% ••
2	E	100	4% 87% 13%

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Mol	Chain	Length	Quality of chain
2	H	100	6% 89% 9%
2	K	100	4% 89% 10%
3	C	5	40% 100%
3	F	5	60% 80% 20%
3	I	5	60% 80% 20%
3	L	5	60% 80% 20%

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
5	EDO	J	306	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 13805 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 Major histocompatibility complex class I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2275	1410	410	447	8	0	5	0
1	D	277	2253	1397	405	443	8	0	3	0
1	G	277	2305	1428	416	452	9	0	8	0
1	J	277	2287	1421	410	447	9	0	7	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	849	539	144	162	4	0	3	0
2	E	100	835	533	141	157	4	0	2	0
2	H	100	845	537	143	161	4	0	3	0
2	K	100	849	540	144	161	4	0	3	0

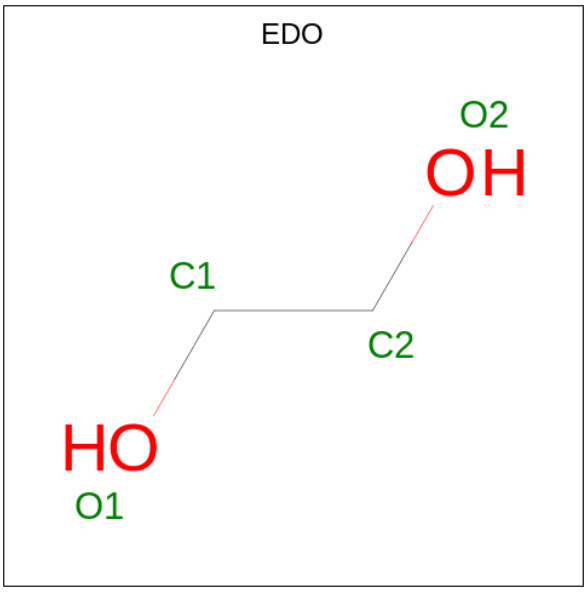
- Molecule 3 is a protein called 5-mer lipopeptide from Protein Nef.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	28	16	5	7	0	0	0
3	F	5	28	16	5	7	0	0	0
3	I	5	28	16	5	7	0	0	0
3	L	5	28	16	5	7	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Zn 4 4	0	0
4	B	2	Total Zn 2 2	0	0
4	D	3	Total Zn 3 3	0	0
4	E	2	Total Zn 2 2	0	0
4	G	2	Total Zn 2 2	0	0
4	H	1	Total Zn 1 1	0	0
4	J	2	Total Zn 2 2	0	0
4	K	2	Total Zn 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	H	1	4	2	2	0	0
			Total	C	O		
5	H	1	4	2	2	0	0
			Total	C	O		
5	H	1	4	2	2	0	0

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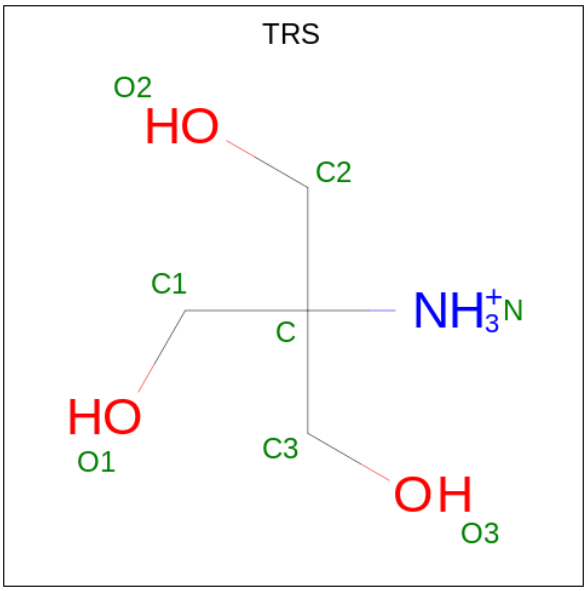
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	H	1	4	2	2	0	0
			Total	C	O		
5	H	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	K	1	4	2	2	0	0
			Total	C	O		
5	K	1	4	2	2	0	0
			Total	C	O		
5	K	1	4	2	2	0	0
			Total	C	O		
5	K	1	4	2	2	0	0
			Total	C	O		
5	K	1	4	2	2	0	0
			Total	C	O		
5	K	1	4	2	2	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

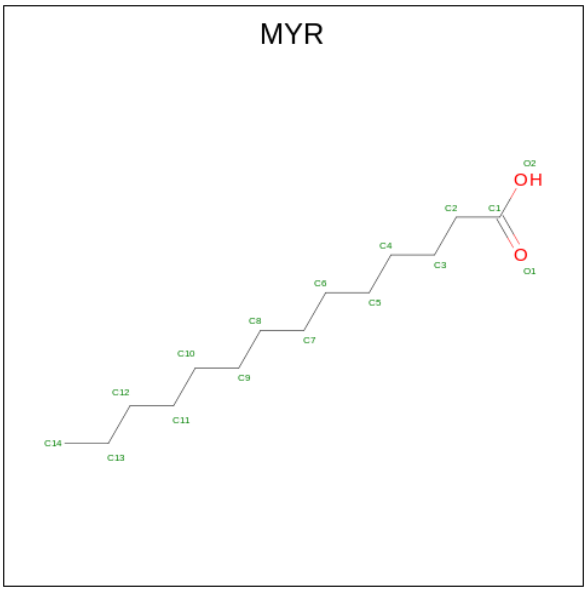


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	8	4	1	3	0	0
			Total	C	N	O		
6	D	1	8	4	1	3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	A	1	1	1	0	0
			Total	Cl		
7	G	1	1	1	0	0
			Total	Cl		
7	J	1	1	1	0	0

- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	C	1	15	14	1	0	0
			Total	C	O		
8	F	1	15	14	1	0	0
			Total	C	O		
8	I	1	15	14	1	0	0
			Total	C	O		
8	L	1	15	14	1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	158	169	169	0	10
			Total	O		
9	B	58	59	59	0	1
			Total	O		
9	C	3	3	3	0	0
			Total	O		
9	D	161	167	167	0	6
			Total	O		
9	E	58	59	59	0	1
			Total	O		
9	G	134	135	135	0	1
			Total	O		
9	H	45	46	46	0	1
			Total	O		
9	I	1	1	1	0	0

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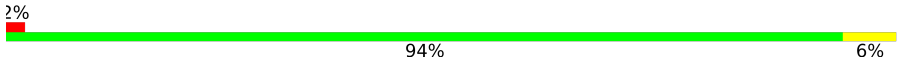
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	J	145	148	148	0	3
			Total	O		
9	K	46	49	49	0	3
			Total	O		
9	L	1	2	2	0	1

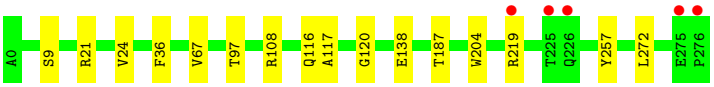
3 Residue-property plots (i)

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: Major histocompatibility complex class I

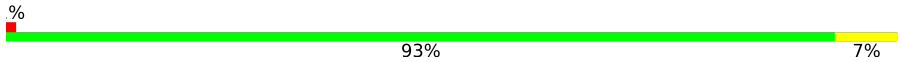
Chain A:





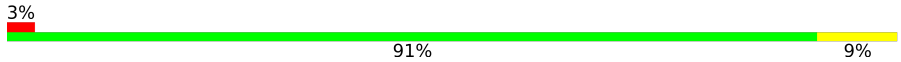
• Molecule 1: Major histocompatibility complex class I

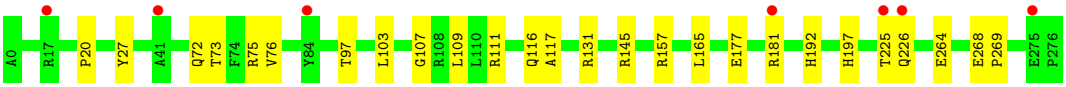
Chain D:



• Molecule 1: Major histocompatibility complex class I

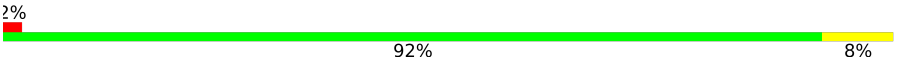
Chain G:

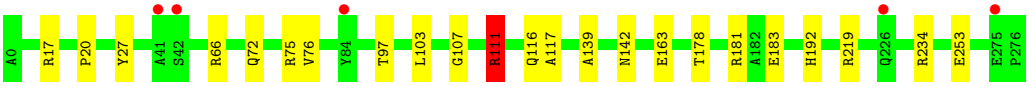




• Molecule 1: Major histocompatibility complex class I

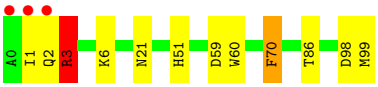
Chain J:





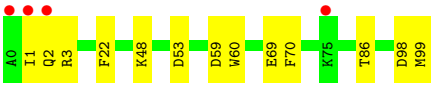
• Molecule 2: Beta-2-microglobulin

Chain B:



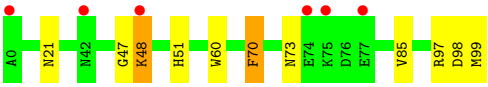
• Molecule 2: Beta-2-microglobulin

Chain E:



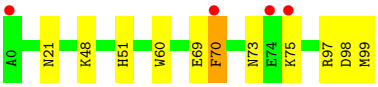
- Molecule 2: Beta-2-microglobulin

Chain H:



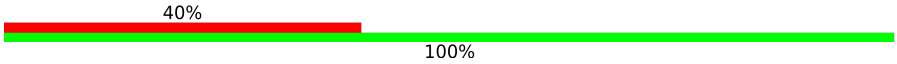
- Molecule 2: Beta-2-microglobulin

Chain K:



- Molecule 3: 5-mer lipopeptide from Protein Nef

Chain C:



- Molecule 3: 5-mer lipopeptide from Protein Nef

Chain F:

- Molecule 3: 5-mer lipopeptide from Protein Nef

Chain I:

- Molecule 3: 5-mer lipopeptide from Protein Nef

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	46.40Å 85.18Å 127.99Å 89.20° 79.57° 90.02°	Depositor
Resolution (Å)	31.18 – 1.76 31.18 – 1.76	Depositor EDS
% Data completeness (in resolution range)	95.9 (31.18-1.76) 95.9 (31.18-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.195 , 0.228 0.196 , 0.228	Depositor DCC
R_{free} test set	9078 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,-k,h-l 0.014 for -h,k,-l 0.013 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13805	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MYR, ZN, TRS, CL

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	0.40	0/2339	0.55	0/3179
1	D	0.39	0/2317	0.56	0/3148
1	G	0.37	0/2370	0.53	0/3217
1	J	0.42	0/2358	0.59	0/3202
2	B	0.40	0/874	0.56	1/1185 (0.1%)
2	E	0.42	0/866	0.56	0/1174
2	H	0.38	0/873	0.53	0/1182
2	K	0.38	0/874	0.51	0/1184
3	C	0.30	0/27	0.39	0/33
3	F	0.30	0/27	0.67	0/33
3	I	0.27	0/27	0.36	0/33
3	L	0.25	0/27	0.33	0/33
All	All	0.39	0/12979	0.55	1/17603 (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	J	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	ARG	NE-CZ-NH1	6.52	123.56	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	111[A]	ARG	Mainchain
1	J	111[B]	ARG	Mainchain

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	2275	0	2111	13	0
1	D	2253	0	2091	17	0
1	G	2305	0	2133	17	0
1	J	2287	0	2128	19	0
2	B	849	0	806	16	0
2	E	835	0	804	13	0
2	H	845	0	804	9	0
2	K	849	0	807	9	0
3	C	28	0	26	0	0
3	F	28	0	26	1	0
3	I	28	0	26	2	0
3	L	28	0	26	1	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	D	3	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
5	A	36	0	54	2	0
5	B	28	0	41	5	0
5	D	32	0	48	2	0
5	E	28	0	41	3	0
5	G	44	0	65	1	0
5	H	20	0	29	0	0
5	J	48	0	71	7	0
5	K	24	0	36	2	0
6	A	8	0	12	0	0
6	D	8	0	12	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	1	0	0	0	0
8	C	15	0	27	1	0
8	F	15	0	27	3	0
8	I	15	0	27	0	0
8	L	15	0	27	0	0
9	A	169	0	0	2	0
9	B	59	0	0	1	0
9	C	3	0	0	0	0
9	D	167	0	0	3	0
9	E	59	0	0	1	0
9	G	135	0	0	3	0
9	H	46	0	0	3	0
9	I	1	0	0	0	0
9	J	148	0	0	2	0
9	K	49	0	0	2	0
9	L	2	0	0	0	0
All	All	13805	0	12305	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (106) 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:1:ILE:HD13	2:B:3:ARG:NH1	1.24	1.51
2:B:1:ILE:CD1	2:B:3:ARG:NH1	1.94	1.30
1:G:145:ARG:NH1	9:G:401:HOH:O	1.97	0.95
2:B:1:ILE:CD1	2:B:3:ARG:HH12	1.69	0.92
2:B:1:ILE:HD13	2:B:3:ARG:HH11	0.80	0.82
2:B:1:ILE:HD11	2:B:3:ARG:HH12	1.46	0.81
2:B:1:ILE:HD11	2:B:3:ARG:NH1	1.98	0.79
1:D:120:GLY:HA3	2:E:1:ILE:HD11	1.64	0.78
1:D:121:ARG:HH12	2:E:1:ILE:HG23	1.47	0.78
1:A:24[B]:VAL:HG22	1:A:36:PHE:HB3	1.69	0.73
1:A:204:TRP:HZ2	2:B:99:MET:HB2	1.53	0.73
1:G:73:THR:HG23	3:I:5:ILE:HG12	1.75	0.68
1:J:234:ARG:HH22	5:J:306:EDO:H21	1.58	0.68
2:K:98:ASP:OD1	9:K:201:HOH:O	2.11	0.68
1:G:72:GLN:OE1	1:G:75:ARG:NH1	2.27	0.67
1:D:204:TRP:HZ2	2:E:99:MET:HB2	1.59	0.67
1:J:72:GLN:OE1	1:J:75:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:GLU:HG3	1:G:269:PRO:HD2	1.78	0.65
2:B:98:ASP:OD1	9:B:201:HOH:O	2.15	0.65
2:H:47:GLY:O	2:H:48:LYS:HB2	1.97	0.64
1:A:97:THR:HG22	1:A:116:GLN:HG2	1.80	0.64
1:A:219:ARG:NH1	1:A:257:TYR:OH	2.30	0.62
1:D:219:ARG:NH1	1:D:257:TYR:OH	2.32	0.62
2:E:3:ARG:NH1	2:E:59:ASP:O	2.26	0.62
2:K:73:ASN:O	2:K:97:ARG:NH1	2.29	0.61
2:K:48:LYS:HE3	2:K:69:GLU:OE1	2.01	0.61
1:A:138:GLU:OE2	9:A:401:HOH:O	2.16	0.60
1:D:67:VAL:HG12	8:F:101:MYR:H122	1.83	0.60
2:B:3:ARG:NH2	2:B:59:ASP:O	2.36	0.59
1:D:21:ARG:HH22	5:E:108:EDO:H22	1.68	0.59
5:D:306:EDO:H12	8:F:101:MYR:H82	1.86	0.57
2:B:2:GLN:HB3	2:B:86:THR:HG22	1.89	0.54
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.43	0.54
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.44	0.53
2:H:98:ASP:OD1	9:H:801:HOH:O	2.19	0.53
1:G:97:THR:HG22	1:G:116:GLN:HG2	1.90	0.53
2:E:1:ILE:HD13	2:E:3:ARG:HH21	1.74	0.52
1:D:39:ASP:OD2	9:D:401:HOH:O	2.19	0.52
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.45	0.52
2:K:21:ASN:HB3	2:K:70:PHE:CE1	2.44	0.52
2:E:99:MET:OXT	5:E:105:EDO:O2	2.27	0.52
2:E:98:ASP:OD1	9:E:201:HOH:O	2.19	0.51
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.46	0.51
5:J:306:EDO:H12	5:K:107:EDO:H12	1.93	0.51
1:G:225:THR:HG23	1:G:226:GLN:HG3	1.93	0.51
1:D:177[B]:GLU:H	1:D:177[B]:GLU:CD	2.15	0.50
1:D:214[B]:THR:OG1	1:D:262:GLN:HB2	2.11	0.50
1:A:36:PHE:CG	1:A:67:VAL:HG11	2.47	0.49
1:G:177:GLU:OE1	1:G:181:ARG:NH1	2.46	0.49
1:J:27:TYR:CD2	5:J:303:EDO:H22	2.47	0.49
1:D:235:PRO:HG3	5:D:309:EDO:H11	1.93	0.49
9:A:404:HOH:O	2:B:6:LYS:HD2	2.13	0.48
2:E:53:ASP:HA	5:E:107:EDO:H12	1.96	0.48
2:H:51:HIS:HE1	9:H:839:HOH:O	1.96	0.48
1:G:27:TYR:CD2	5:G:305:EDO:H22	2.49	0.47
1:G:20:PRO:HD2	1:G:75:ARG:HD3	1.97	0.47
1:A:9:SER:HB2	1:A:24[B]:VAL:HG12	1.97	0.47
2:K:51:HIS:HE1	9:K:239:HOH:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:HIS:ND1	9:G:403:HOH:O	2.35	0.46
1:J:234:ARG:NH2	5:J:306:EDO:H21	2.28	0.46
1:A:120:GLY:HA3	2:B:1:ILE:HD11	1.98	0.46
2:H:73:ASN:O	2:H:97:ARG:NH1	2.48	0.46
2:B:99:MET:OXT	5:B:106:EDO:O2	2.32	0.46
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.51	0.45
1:G:131:ARG:HG2	1:G:157:ARG:NH1	2.31	0.45
1:J:178:THR:O	1:J:181:ARG:NH2	2.42	0.45
1:J:66:ARG:NH1	1:J:163:GLU:OE2	2.37	0.45
1:D:177[B]:GLU:HG2	9:D:438:HOH:O	2.17	0.44
1:D:183:GLU:OE2	9:D:402:HOH:O	2.21	0.44
2:E:2:GLN:HB3	2:E:86:THR:HG22	1.98	0.44
1:A:21:ARG:HH22	5:B:109:EDO:H11	1.81	0.44
1:D:97:THR:HG22	1:D:116:GLN:HG2	1.99	0.44
3:F:2:GLY:HA2	8:F:101:MYR:H22	1.55	0.44
2:K:75:LYS:HB3	2:K:75:LYS:HE3	1.55	0.44
5:J:309:EDO:H21	9:J:421:HOH:O	2.17	0.44
2:H:48:LYS:HE2	2:H:48:LYS:HB3	1.70	0.43
1:J:76[A]:VAL:HG12	3:L:5:ILE:HG21	1.99	0.43
1:J:72:GLN:O	1:J:76[B]:VAL:HG12	2.18	0.43
1:J:181:ARG:HG3	1:J:183:GLU:HG2	2.01	0.43
1:A:108:ARG:HA	5:A:310:EDO:H22	2.01	0.43
1:J:20:PRO:HD2	1:J:75:ARG:HD3	2.01	0.43
1:G:109:LEU:HB2	1:G:165:LEU:HD11	2.01	0.43
1:G:192:HIS:NE2	2:H:99:MET:OXT	2.50	0.43
1:D:121:ARG:NH1	2:E:1:ILE:HG23	2.24	0.43
1:J:139:ALA:O	1:J:142:ASN:HB3	2.18	0.43
2:K:51:HIS:CD2	5:K:108:EDO:H21	2.52	0.43
1:J:103:LEU:HD11	1:J:107:GLY:HA2	2.01	0.43
2:B:51:HIS:CE1	5:B:109:EDO:H12	2.54	0.42
5:B:108:EDO:O1	1:D:197:HIS:CE1	2.71	0.42
1:J:192:HIS:NE2	2:K:99:MET:O	2.45	0.42
2:E:22:PHE:CE2	2:E:69:GLU:HG2	2.55	0.42
1:G:103:LEU:HD11	1:G:107:GLY:HA2	2.02	0.42
1:J:181:ARG:O	5:J:310:EDO:O1	2.38	0.42
1:A:187:THR:HB	1:A:272:LEU:HD21	2.01	0.42
1:G:264[B]:GLU:HG2	9:G:434:HOH:O	2.20	0.42
5:A:307:EDO:H21	8:C:101:MYR:C8	2.50	0.42
1:J:97:THR:HG22	1:J:116:GLN:HG2	2.01	0.42
1:J:219:ARG:HH21	1:J:253:GLU:CD	2.23	0.41
1:D:129:ASP:O	1:D:131:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:234:ARG:HH22	5:J:306:EDO:C2	2.30	0.41
2:E:48:LYS:N	2:E:48:LYS:CD	2.84	0.41
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.55	0.41
1:A:21:ARG:NH1	5:B:104:EDO:H21	2.35	0.41
2:H:85[B]:VAL:HG23	9:H:812:HOH:O	2.20	0.40
1:G:76:VAL:HG12	3:I:5:ILE:HG21	2.03	0.40
1:J:17:ARG:NH2	9:J:401:HOH:O	2.30	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	280/277 (101%)	277 (99%)	3 (1%)	0	100	100
1	D	278/277 (100%)	274 (99%)	4 (1%)	0	100	100
1	G	283/277 (102%)	281 (99%)	2 (1%)	0	100	100
1	J	282/277 (102%)	277 (98%)	3 (1%)	2 (1%)	22	8
2	B	101/100 (101%)	100 (99%)	1 (1%)	0	100	100
2	E	100/100 (100%)	99 (99%)	1 (1%)	0	100	100
2	H	101/100 (101%)	100 (99%)	1 (1%)	0	100	100
2	K	101/100 (101%)	99 (98%)	2 (2%)	0	100	100
3	C	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
3	F	3/5 (60%)	3 (100%)	0	0	100	100
3	I	3/5 (60%)	3 (100%)	0	0	100	100
3	L	3/5 (60%)	3 (100%)	0	0	100	100
All	All	1538/1528 (101%)	1518 (99%)	18 (1%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	111[A]	ARG
1	J	111[B]	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/231 (102%)	236 (100%)	0	100	100
1	D	234/231 (101%)	234 (100%)	0	100	100
1	G	239/231 (104%)	237 (99%)	2 (1%)	81	72
1	J	238/231 (103%)	236 (99%)	2 (1%)	81	72
2	B	96/93 (103%)	94 (98%)	2 (2%)	53	31
2	E	95/93 (102%)	94 (99%)	1 (1%)	73	60
2	H	96/93 (103%)	94 (98%)	2 (2%)	53	31
2	K	96/93 (103%)	95 (99%)	1 (1%)	76	63
3	C	2/2 (100%)	2 (100%)	0	100	100
3	F	2/2 (100%)	2 (100%)	0	100	100
3	I	2/2 (100%)	2 (100%)	0	100	100
3	L	2/2 (100%)	2 (100%)	0	100	100
All	All	1338/1304 (103%)	1328 (99%)	10 (1%)	86	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3	ARG
2	B	70	PHE
2	E	70	PHE
1	G	111[A]	ARG
1	G	111[B]	ARG
2	H	48	LYS
2	H	70	PHE
1	J	111[A]	ARG
1	J	111[B]	ARG

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Mol	Chain	Res	Type
2	K	70	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 92 ligands modelled in this entry, 21 are monoatomic - leaving 71 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	$\#\|Z\| > 2$
5	EDO	B	104	-	3,3,3	0.39	0	2,2,2	0.63	0
5	EDO	G	312	-	3,3,3	0.48	0	2,2,2	0.28	0
5	EDO	K	106	-	3,3,3	0.43	0	2,2,2	0.41	0
5	EDO	A	309	-	3,3,3	0.43	0	2,2,2	0.42	0
5	EDO	G	311	4	3,3,3	0.42	0	2,2,2	0.42	0
5	EDO	A	311	-	3,3,3	0.52	0	2,2,2	0.54	0
5	EDO	G	307	-	3,3,3	0.47	0	2,2,2	0.45	0
5	EDO	J	310	-	3,3,3	0.48	0	2,2,2	0.16	0
5	EDO	D	304	-	3,3,3	0.51	0	2,2,2	0.35	0
5	EDO	B	105	-	3,3,3	0.58	0	2,2,2	0.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	J	311	-	3,3,3	0.49	0	2,2,2	0.61	0
8	MYR	C	101	3	14,14,15	0.42	0	13,13,15	0.45	0
5	EDO	J	308	-	3,3,3	0.45	0	2,2,2	0.45	0
5	EDO	D	310	-	3,3,3	0.40	0	2,2,2	0.54	0
5	EDO	E	106	-	3,3,3	0.54	0	2,2,2	0.29	0
5	EDO	J	314	4	3,3,3	0.48	0	2,2,2	0.11	0
5	EDO	H	102	-	3,3,3	0.55	0	2,2,2	0.17	0
5	EDO	B	109	4	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	G	306	-	3,3,3	0.56	0	2,2,2	0.06	0
5	EDO	H	103	-	3,3,3	0.53	0	2,2,2	0.32	0
5	EDO	J	306	-	3,3,3	0.46	0	2,2,2	0.18	0
5	EDO	D	307	-	3,3,3	0.52	0	2,2,2	0.52	0
5	EDO	K	103	-	3,3,3	0.53	0	2,2,2	0.31	0
5	EDO	B	106	-	3,3,3	0.49	0	2,2,2	0.33	0
5	EDO	G	305	-	3,3,3	0.41	0	2,2,2	0.51	0
5	EDO	J	305	-	3,3,3	0.52	0	2,2,2	0.18	0
5	EDO	E	103	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	J	304	-	3,3,3	0.49	0	2,2,2	0.13	0
5	EDO	B	107	-	3,3,3	0.43	0	2,2,2	0.44	0
5	EDO	K	105	-	3,3,3	0.60	0	2,2,2	0.05	0
5	EDO	G	309	-	3,3,3	0.52	0	2,2,2	0.19	0
5	EDO	H	106	4	3,3,3	0.47	0	2,2,2	0.27	0
5	EDO	E	107	-	3,3,3	0.52	0	2,2,2	0.19	0
5	EDO	D	306	-	3,3,3	0.44	0	2,2,2	0.57	0
5	EDO	H	105	-	3,3,3	0.45	0	2,2,2	0.44	0
5	EDO	G	313	-	3,3,3	0.54	0	2,2,2	0.12	0
5	EDO	G	303	-	3,3,3	0.45	0	2,2,2	0.49	0
5	EDO	E	104	-	3,3,3	0.42	0	2,2,2	0.48	0
5	EDO	J	313	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	A	310	-	3,3,3	0.46	0	2,2,2	0.35	0
8	MYR	F	101	3	14,14,15	0.43	0	13,13,15	0.62	0
5	EDO	G	310	-	3,3,3	0.48	0	2,2,2	0.22	0
5	EDO	B	103	-	3,3,3	0.46	0	2,2,2	0.17	0
5	EDO	D	308	-	3,3,3	0.52	0	2,2,2	0.23	0
5	EDO	E	105	-	3,3,3	0.48	0	2,2,2	0.37	0
5	EDO	G	308	-	3,3,3	0.54	0	2,2,2	0.15	0
5	EDO	J	309	-	3,3,3	0.49	0	2,2,2	0.29	0
5	EDO	A	308	-	3,3,3	0.60	0	2,2,2	0.18	0
5	EDO	A	307	-	3,3,3	0.44	0	2,2,2	0.59	0
5	EDO	A	312	-	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	J	312	-	3,3,3	0.48	0	2,2,2	0.46	0
6	TRS	D	312	-	7,7,7	0.24	0	9,9,9	0.48	0
5	EDO	K	104	-	3,3,3	0.42	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	D	309	-	3,3,3	0.45	0	2,2,2	0.56	0
5	EDO	E	109	4	3,3,3	0.61	0	2,2,2	0.08	0
5	EDO	K	108	-	3,3,3	0.48	0	2,2,2	0.37	0
5	EDO	K	107	-	3,3,3	0.44	0	2,2,2	0.41	0
5	EDO	J	303	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	D	311	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	H	104	-	3,3,3	0.44	0	2,2,2	0.44	0
8	MYR	I	101	3	14,14,15	0.41	0	13,13,15	0.60	0
5	EDO	A	305	-	3,3,3	0.52	0	2,2,2	0.31	0
8	MYR	L	101	3	14,14,15	0.40	0	13,13,15	0.69	0
5	EDO	E	108	-	3,3,3	0.49	0	2,2,2	0.33	0
5	EDO	A	306	-	3,3,3	0.57	0	2,2,2	0.14	0
5	EDO	J	307	-	3,3,3	0.56	0	2,2,2	0.30	0
5	EDO	G	304	-	3,3,3	0.50	0	2,2,2	0.02	0
5	EDO	A	313	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	B	108	4	3,3,3	0.43	0	2,2,2	0.55	0
6	TRS	A	314	-	7,7,7	0.25	0	9,9,9	0.34	0
5	EDO	D	305	-	3,3,3	0.59	0	2,2,2	0.23	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
5	EDO	B	104	-	-	1/1/1/1	-
5	EDO	G	312	-	-	0/1/1/1	-
5	EDO	K	106	-	-	0/1/1/1	-
5	EDO	A	309	-	-	0/1/1/1	-
5	EDO	G	311	4	-	1/1/1/1	-
5	EDO	A	311	-	-	1/1/1/1	-
5	EDO	G	307	-	-	1/1/1/1	-
5	EDO	J	310	-	-	1/1/1/1	-
5	EDO	D	304	-	-	0/1/1/1	-
5	EDO	B	105	-	-	0/1/1/1	-
5	EDO	J	311	-	-	1/1/1/1	-
8	MYR	C	101	3	-	7/11/12/13	-
5	EDO	J	308	-	-	0/1/1/1	-
5	EDO	D	310	-	-	0/1/1/1	-
5	EDO	E	106	-	-	1/1/1/1	-
5	EDO	J	314	4	-	0/1/1/1	-
5	EDO	H	102	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	109	4	-	0/1/1/1	-
5	EDO	G	306	-	-	0/1/1/1	-
5	EDO	H	103	-	-	0/1/1/1	-
5	EDO	J	306	-	-	0/1/1/1	-
5	EDO	D	307	-	-	1/1/1/1	-
5	EDO	K	103	-	-	0/1/1/1	-
5	EDO	B	106	-	-	1/1/1/1	-
5	EDO	G	305	-	-	0/1/1/1	-
5	EDO	J	305	-	-	0/1/1/1	-
5	EDO	E	103	-	-	0/1/1/1	-
5	EDO	J	304	-	-	0/1/1/1	-
5	EDO	B	107	-	-	1/1/1/1	-
5	EDO	K	105	-	-	1/1/1/1	-
5	EDO	G	309	-	-	0/1/1/1	-
5	EDO	H	106	4	-	0/1/1/1	-
5	EDO	E	107	-	-	0/1/1/1	-
5	EDO	D	306	-	-	1/1/1/1	-
5	EDO	H	105	-	-	0/1/1/1	-
5	EDO	G	313	-	-	0/1/1/1	-
5	EDO	G	303	-	-	0/1/1/1	-
5	EDO	E	104	-	-	0/1/1/1	-
5	EDO	J	313	-	-	0/1/1/1	-
5	EDO	A	310	-	-	1/1/1/1	-
8	MYR	F	101	3	-	7/11/12/13	-
5	EDO	G	310	-	-	0/1/1/1	-
5	EDO	B	103	-	-	0/1/1/1	-
5	EDO	D	308	-	-	1/1/1/1	-
5	EDO	E	105	-	-	0/1/1/1	-
5	EDO	G	308	-	-	0/1/1/1	-
5	EDO	J	309	-	-	1/1/1/1	-
5	EDO	A	308	-	-	1/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-
5	EDO	A	312	-	-	0/1/1/1	-
5	EDO	J	312	-	-	1/1/1/1	-
6	TRS	D	312	-	-	0/9/9/9	-
5	EDO	K	104	-	-	0/1/1/1	-
5	EDO	D	309	-	-	0/1/1/1	-
5	EDO	E	109	4	-	1/1/1/1	-
5	EDO	K	108	-	-	0/1/1/1	-
5	EDO	K	107	-	-	1/1/1/1	-
5	EDO	J	303	-	-	0/1/1/1	-
5	EDO	D	311	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	H	104	-	-	1/1/1/1	-
8	MYR	I	101	3	-	6/11/12/13	-
5	EDO	A	305	-	-	0/1/1/1	-
8	MYR	L	101	3	-	2/11/12/13	-
5	EDO	E	108	-	-	0/1/1/1	-
5	EDO	A	306	-	-	0/1/1/1	-
5	EDO	J	307	-	-	0/1/1/1	-
5	EDO	G	304	-	-	0/1/1/1	-
5	EDO	A	313	-	-	0/1/1/1	-
5	EDO	B	108	4	-	0/1/1/1	-
6	TRS	A	314	-	-	0/9/9/9	-
5	EDO	D	305	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	101	MYR	C1-C2-C3-C4
5	D	306	EDO	O1-C1-C2-O2
8	F	101	MYR	C11-C10-C9-C8
8	I	101	MYR	C5-C6-C7-C8
8	C	101	MYR	C2-C3-C4-C5
8	F	101	MYR	C4-C5-C6-C7
8	L	101	MYR	C10-C11-C12-C13
8	C	101	MYR	C11-C10-C9-C8
8	I	101	MYR	C11-C10-C9-C8
5	A	307	EDO	O1-C1-C2-O2
5	D	305	EDO	O1-C1-C2-O2
5	D	307	EDO	O1-C1-C2-O2
5	E	109	EDO	O1-C1-C2-O2
5	G	311	EDO	O1-C1-C2-O2
5	H	104	EDO	O1-C1-C2-O2
5	J	309	EDO	O1-C1-C2-O2
8	C	101	MYR	C6-C7-C8-C9
8	C	101	MYR	C4-C5-C6-C7
8	F	101	MYR	C6-C7-C8-C9
8	I	101	MYR	C11-C12-C13-C14
8	I	101	MYR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	308	EDO	O1-C1-C2-O2
5	A	311	EDO	O1-C1-C2-O2
5	G	307	EDO	O1-C1-C2-O2
8	F	101	MYR	C5-C6-C7-C8
8	L	101	MYR	C6-C7-C8-C9
8	C	101	MYR	C9-C10-C11-C12
5	J	312	EDO	O1-C1-C2-O2
8	F	101	MYR	C10-C11-C12-C13
8	F	101	MYR	C9-C10-C11-C12
8	I	101	MYR	C3-C4-C5-C6
5	B	104	EDO	O1-C1-C2-O2
5	B	106	EDO	O1-C1-C2-O2
5	A	310	EDO	O1-C1-C2-O2
5	B	107	EDO	O1-C1-C2-O2
8	C	101	MYR	C3-C4-C5-C6
8	C	101	MYR	C7-C8-C9-C10
5	D	308	EDO	O1-C1-C2-O2
5	E	106	EDO	O1-C1-C2-O2
5	J	310	EDO	O1-C1-C2-O2
5	J	311	EDO	O1-C1-C2-O2
5	K	105	EDO	O1-C1-C2-O2
5	K	107	EDO	O1-C1-C2-O2
8	I	101	MYR	C4-C5-C6-C7

There are no ring outliers.

20 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	104	EDO	1	0
5	J	310	EDO	1	0
8	C	101	MYR	1	0
5	B	109	EDO	2	0
5	J	306	EDO	4	0
5	B	106	EDO	1	0
5	G	305	EDO	1	0
5	E	107	EDO	1	0
5	D	306	EDO	1	0
5	A	310	EDO	1	0
8	F	101	MYR	3	0
5	E	105	EDO	1	0
5	J	309	EDO	1	0
5	A	307	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	309	EDO	1	0
5	K	108	EDO	1	0
5	K	107	EDO	1	0
5	J	303	EDO	1	0
5	E	108	EDO	1	0
5	B	108	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	277/277 (100%)	0.13	5 (1%)	68	76	15, 29, 48, 74	0
1	D	277/277 (100%)	0.05	4 (1%)	75	82	15, 29, 49, 74	0
1	G	277/277 (100%)	0.11	7 (2%)	57	63	18, 30, 48, 67	0
1	J	277/277 (100%)	0.07	5 (1%)	68	76	18, 30, 47, 65	0
2	B	100/100 (100%)	0.25	3 (3%)	50	56	19, 31, 53, 62	0
2	E	100/100 (100%)	0.17	4 (4%)	38	45	19, 31, 54, 64	0
2	H	100/100 (100%)	0.39	6 (6%)	21	27	19, 39, 66, 79	0
2	K	100/100 (100%)	0.51	4 (4%)	38	45	20, 40, 63, 78	0
3	C	5/5 (100%)	1.67	2 (40%)	0	0	35, 41, 59, 62	0
3	F	5/5 (100%)	2.98	3 (60%)	0	0	36, 42, 61, 62	0
3	I	5/5 (100%)	4.85	3 (60%)	0	0	40, 45, 67, 70	0
3	L	5/5 (100%)	3.67	3 (60%)	0	0	39, 46, 68, 72	0
All	All	1528/1528 (100%)	0.19	49 (3%)	47	54	15, 31, 55, 79	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	2	GLY	12.0
2	E	0	ALA	7.7
2	E	1	ILE	7.0
3	L	3	GLY	6.6
3	I	4	ALA	6.4
3	F	3	GLY	6.3
3	F	2	GLY	5.1
1	D	225	THR	5.0
1	D	276	PRO	4.9
3	L	2	GLY	4.9
1	A	276	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	4.4
2	K	75	LYS	4.2
1	A	226	GLN	4.2
3	I	3	GLY	4.1
3	L	4	ALA	4.0
2	K	0	ALA	3.9
2	B	0	ALA	3.9
3	C	2	GLY	3.9
2	H	74	GLU	3.6
2	B	2	GLN	3.4
3	F	4	ALA	3.2
1	D	226	GLN	3.1
1	D	223	ASP	3.0
1	G	181	ARG	2.9
1	A	219	ARG	2.9
2	E	75	LYS	2.9
1	J	226	GLN	2.9
2	K	74	GLU	2.7
1	G	41	ALA	2.7
1	J	84[A]	TYR	2.6
1	A	275	GLU	2.6
1	G	17	ARG	2.6
1	G	225	THR	2.5
1	G	226	GLN	2.4
1	J	42	SER	2.4
2	H	42	ASN	2.3
1	J	275	GLU	2.3
1	J	41	ALA	2.3
2	H	77	GLU	2.3
2	H	0	ALA	2.2
1	G	84[A]	TYR	2.2
2	H	75	LYS	2.2
1	G	275	GLU	2.2
1	A	225	THR	2.2
2	H	48	LYS	2.1
2	E	2	GLN	2.1
3	C	4	ALA	2.0
2	K	70	PHE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MYR	I	101	15/16	0.57	0.21	34,51,71,73	0
4	ZN	K	101	1/1	0.65	0.10	93,93,93,93	0
5	EDO	B	109	4/4	0.67	0.25	55,60,61,64	0
8	MYR	L	101	15/16	0.72	0.20	34,50,68,71	0
5	EDO	A	308	4/4	0.74	0.18	33,34,36,43	0
8	MYR	F	101	15/16	0.76	0.16	41,46,53,56	0
8	MYR	C	101	15/16	0.77	0.17	36,44,53,53	0
5	EDO	G	313	4/4	0.78	0.13	37,38,39,40	0
5	EDO	J	309	4/4	0.78	0.20	43,43,44,55	0
5	EDO	D	305	4/4	0.79	0.16	32,33,36,42	0
5	EDO	K	108	4/4	0.79	0.29	54,62,66,68	0
5	EDO	K	105	4/4	0.80	0.12	33,37,42,42	0
5	EDO	D	307	4/4	0.80	0.18	33,34,42,45	0
5	EDO	E	108	4/4	0.80	0.15	51,53,55,57	0
5	EDO	H	103	4/4	0.82	0.15	37,39,40,44	0
5	EDO	A	312	4/4	0.82	0.11	45,46,46,50	0
5	EDO	G	309	4/4	0.83	0.11	32,32,37,43	0
5	EDO	A	311	4/4	0.83	0.17	33,33,37,39	0
5	EDO	G	305	4/4	0.84	0.18	36,36,38,38	0
5	EDO	J	313	4/4	0.84	0.12	41,42,43,48	0
5	EDO	E	106	4/4	0.84	0.15	30,34,36,47	0
5	EDO	J	303	4/4	0.84	0.17	35,35,36,37	0
5	EDO	D	308	4/4	0.85	0.15	37,42,42,55	0
5	EDO	J	311	4/4	0.85	0.15	40,47,48,56	0
5	EDO	A	307	4/4	0.85	0.18	23,32,39,40	0
5	EDO	J	307	4/4	0.86	0.17	34,34,38,40	0
5	EDO	A	313	4/4	0.86	0.12	40,42,43,43	0
5	EDO	G	310	4/4	0.87	0.16	42,48,55,63	0
4	ZN	H	101	1/1	0.87	0.05	80,80,80,80	0
5	EDO	G	307	4/4	0.87	0.10	38,41,47,49	0
5	EDO	E	109	4/4	0.87	0.14	37,50,51,51	0
5	EDO	J	304	4/4	0.87	0.12	32,32,35,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	E	105	4/4	0.88	0.20	27,40,45,55	0
5	EDO	A	310	4/4	0.88	0.17	36,39,50,52	0
4	ZN	E	101	1/1	0.88	0.05	75,75,75,75	0
5	EDO	D	311	4/4	0.88	0.24	44,44,45,54	0
5	EDO	J	306	4/4	0.88	0.18	33,41,41,55	0
4	ZN	G	301	1/1	0.89	0.11	87,87,87,87	0
5	EDO	J	310	4/4	0.90	0.13	32,34,35,44	0
5	EDO	D	306	4/4	0.90	0.11	24,35,40,40	0
5	EDO	K	106	4/4	0.90	0.15	39,43,47,49	0
5	EDO	J	312	4/4	0.90	0.13	34,45,45,49	0
4	ZN	B	101	1/1	0.91	0.06	75,75,75,75	0
5	EDO	G	312	4/4	0.92	0.13	28,36,36,44	0
5	EDO	E	104	4/4	0.92	0.12	28,28,36,41	0
5	EDO	G	311	4/4	0.92	0.15	27,30,45,55	0
7	CL	J	315	1/1	0.92	0.14	66,66,66,66	0
6	TRS	D	312	8/8	0.93	0.12	25,30,31,32	0
5	EDO	K	104	4/4	0.93	0.12	29,33,39,45	0
5	EDO	G	303	4/4	0.93	0.10	30,36,37,38	0
4	ZN	K	102	1/1	0.93	0.04	73,73,73,73	0
5	EDO	K	107	4/4	0.93	0.13	49,49,50,55	0
5	EDO	D	309	4/4	0.93	0.11	31,33,37,43	0
5	EDO	K	103	4/4	0.94	0.08	22,28,31,31	0
5	EDO	H	106	4/4	0.94	0.20	60,61,62,70	0
5	EDO	G	308	4/4	0.94	0.11	29,33,36,39	0
5	EDO	D	304	4/4	0.94	0.13	26,27,29,30	0
5	EDO	J	305	4/4	0.94	0.12	28,31,34,38	0
5	EDO	A	305	4/4	0.94	0.10	26,26,30,31	0
6	TRS	A	314	8/8	0.94	0.14	23,28,32,34	0
5	EDO	A	306	4/4	0.94	0.15	29,29,29,32	0
7	CL	A	315	1/1	0.94	0.06	63,63,63,63	0
7	CL	G	314	1/1	0.94	0.10	61,61,61,61	0
5	EDO	G	304	4/4	0.94	0.09	34,35,35,37	0
5	EDO	B	105	4/4	0.94	0.11	32,32,35,41	0
4	ZN	D	302	1/1	0.94	0.07	76,76,76,76	0
5	EDO	H	104	4/4	0.94	0.10	31,32,38,46	0
5	EDO	H	105	4/4	0.94	0.12	40,43,47,49	0
4	ZN	A	303	1/1	0.95	0.04	69,69,69,69	0
5	EDO	B	106	4/4	0.95	0.11	29,39,42,50	0
5	EDO	J	314	4/4	0.95	0.12	28,33,40,60	0
5	EDO	E	103	4/4	0.95	0.12	26,29,30,36	0
5	EDO	A	309	4/4	0.95	0.09	29,31,31,32	0
5	EDO	B	104	4/4	0.95	0.08	35,37,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	D	310	4/4	0.96	0.15	30,31,34,37	0
5	EDO	B	107	4/4	0.96	0.13	27,29,35,42	0
5	EDO	J	308	4/4	0.96	0.09	31,34,36,37	0
5	EDO	H	102	4/4	0.96	0.08	24,28,29,33	0
5	EDO	G	306	4/4	0.96	0.10	29,29,29,35	0
5	EDO	E	107	4/4	0.96	0.08	30,40,46,48	0
5	EDO	B	108	4/4	0.97	0.12	27,39,42,49	0
4	ZN	A	301	1/1	0.97	0.07	26,26,26,26	0
4	ZN	G	302	1/1	0.97	0.04	33,33,33,33	0
4	ZN	B	102	1/1	0.97	0.04	37,37,37,37	0
4	ZN	J	302	1/1	0.98	0.05	32,32,32,32	0
5	EDO	B	103	4/4	0.98	0.09	26,28,32,35	0
4	ZN	J	301	1/1	0.99	0.08	24,24,24,24	0
4	ZN	A	304	1/1	0.99	0.11	23,23,23,23	0
4	ZN	E	102	1/1	0.99	0.03	38,38,38,38	0
4	ZN	D	301	1/1	0.99	0.06	26,26,26,26	0
4	ZN	A	302	1/1	0.99	0.12	24,24,24,24	0
4	ZN	D	303	1/1	0.99	0.09	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.