



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 07:22 AM EDT

PDB ID : 3T80
Title : Crystal structure of 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase from *Salmonella typhimurium* bound to cytidine
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID); Staker, B.L.; Edwards, T.E.
Deposited on : 2011-07-31
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35
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) : 2.35

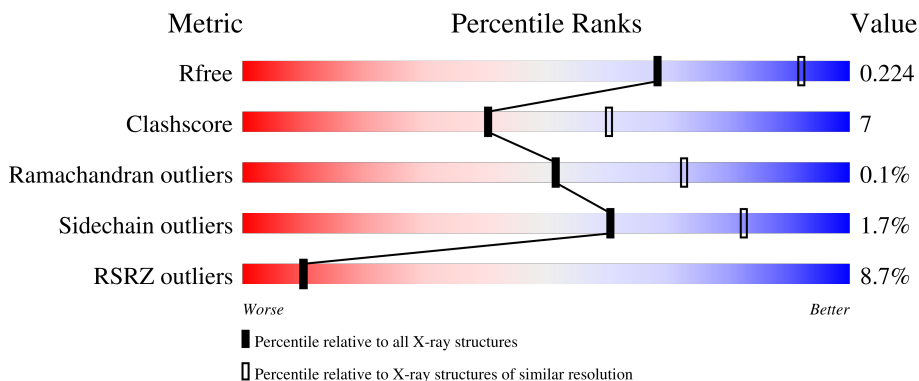
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	162	 10% 83% 13% ..
1	B	162	 7% 79% 12% 9%
1	C	162	 10% 84% 9% 7%
1	D	162	 7% 86% 10% ..
1	E	162	 8% 78% 18% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	162	

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
6	EDO	B	161	-	-	-	X
6	EDO	D	161	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6999 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	157	Total 1156	C 733	N 205	O 211	S 7	0	0	0
1	B	147	Total 1076	C 680	N 193	O 197	S 6	0	0	0
1	C	151	Total 1109	C 704	N 197	O 201	S 7	0	0	0
1	D	157	Total 1152	C 731	N 203	O 212	S 6	0	0	0
1	E	157	Total 1127	C 716	N 197	O 208	S 6	0	0	0
1	F	146	Total 1073	C 680	N 192	O 194	S 7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8ZMF7
A	-1	ASN	-	expression tag	UNP Q8ZMF7
A	0	ALA	-	expression tag	UNP Q8ZMF7
B	-2	SER	-	expression tag	UNP Q8ZMF7
B	-1	ASN	-	expression tag	UNP Q8ZMF7
B	0	ALA	-	expression tag	UNP Q8ZMF7
C	-2	SER	-	expression tag	UNP Q8ZMF7
C	-1	ASN	-	expression tag	UNP Q8ZMF7
C	0	ALA	-	expression tag	UNP Q8ZMF7
D	-2	SER	-	expression tag	UNP Q8ZMF7
D	-1	ASN	-	expression tag	UNP Q8ZMF7
D	0	ALA	-	expression tag	UNP Q8ZMF7
E	-2	SER	-	expression tag	UNP Q8ZMF7
E	-1	ASN	-	expression tag	UNP Q8ZMF7
E	0	ALA	-	expression tag	UNP Q8ZMF7
F	-2	SER	-	expression tag	UNP Q8ZMF7
F	-1	ASN	-	expression tag	UNP Q8ZMF7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q8ZMF7

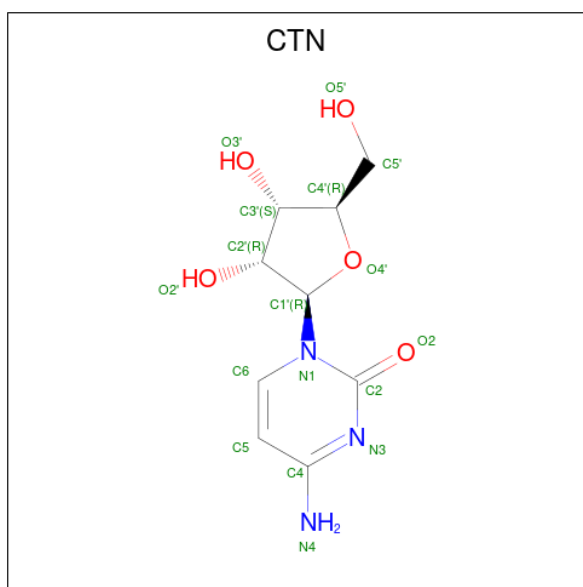
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

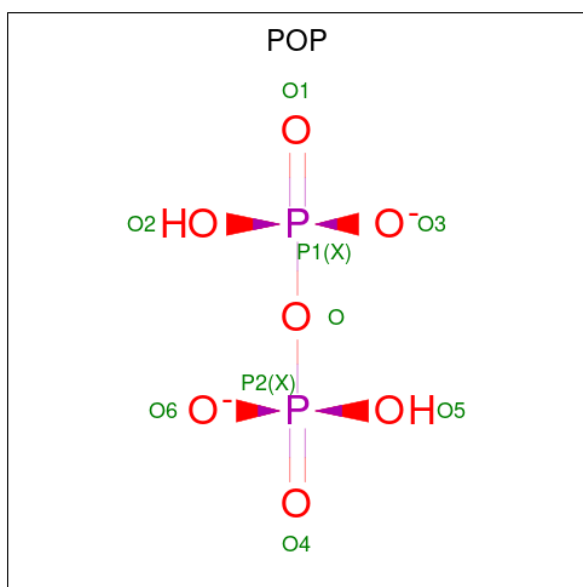
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	2	Total Mg 2 2	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is 4-AMINO-1-BETA-D-RIBOFURANOSYL-2(1H)-PYRIMIDINONE (three-letter code: CTN) (formula: C₉H₁₃N₃O₅).



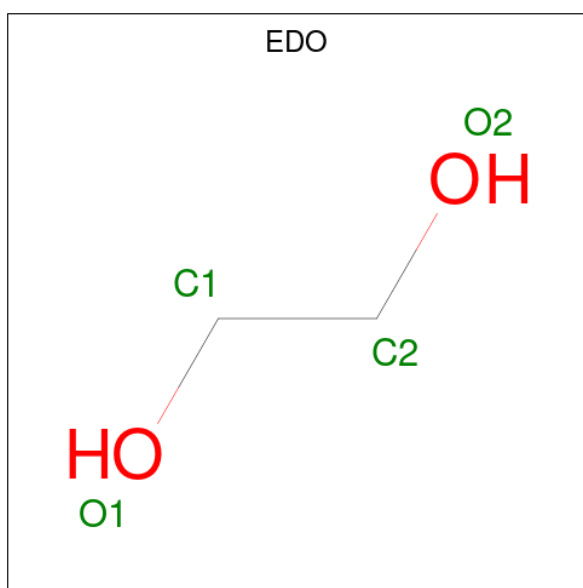
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			17	9	3	5		
4	B	1	Total	C	N	O	0	0
			17	9	3	5		
4	C	1	Total	C	N	O	0	0
			17	9	3	5		
4	D	1	Total	C	N	O	0	0
			17	9	3	5		
4	E	1	Total	C	N	O	0	0
			17	9	3	5		
4	F	1	Total	C	N	O	0	0
			17	9	3	5		

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 9 7 2	0	0
5	E	1	Total O P 9 7 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

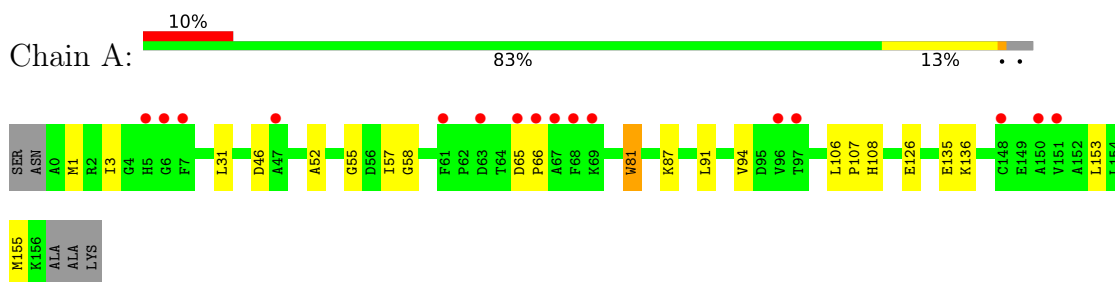
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	26	Total O 26 26	0	0
7	B	19	Total O 19 19	0	0
7	C	19	Total O 19 19	0	0
7	D	21	Total O 21 21	0	0
7	E	9	Total O 9 9	0	0
7	F	22	Total O 22 22	0	0

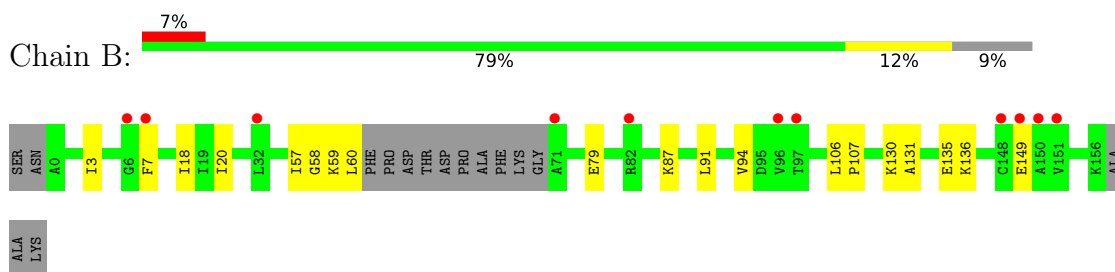
3 Residue-property plots [i](#)

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.

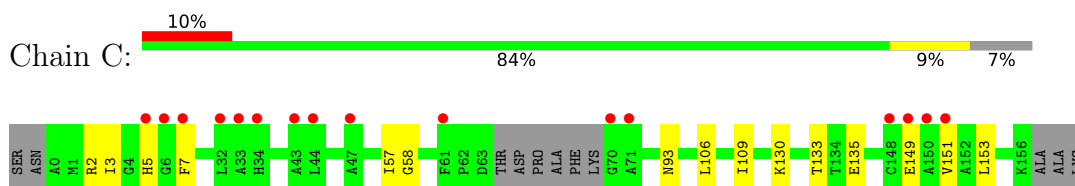
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



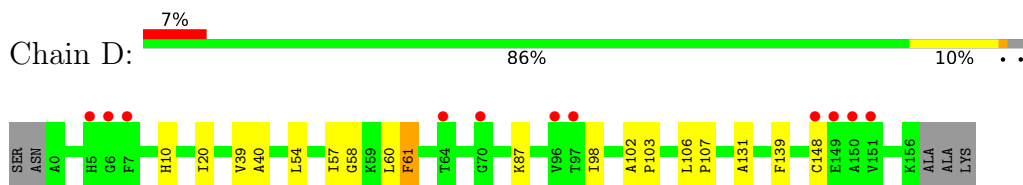
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



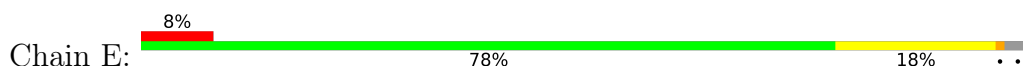
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

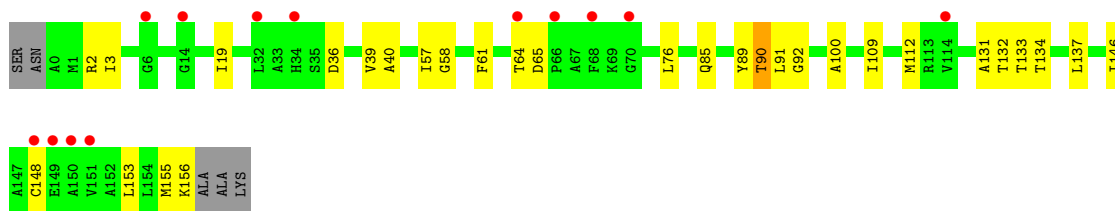


- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

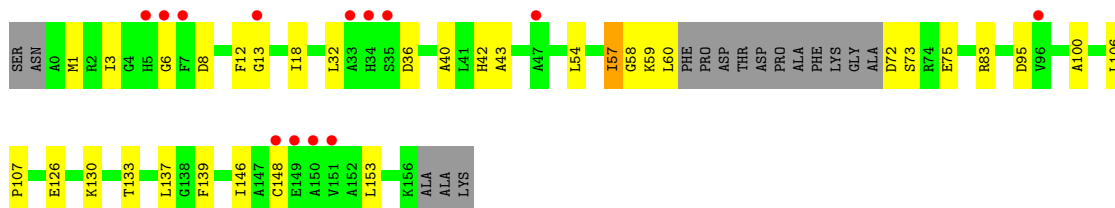


- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase





● Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.01Å 147.66Å 56.92Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.50) 98.8 (29.44-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.211 , 0.245 0.196 , 0.224	Depositor DCC
R_{free} test set	2748 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6999	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, POP, MG, CTN, 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	0.76	1/1178 (0.1%)	0.95	0/1594
1	B	0.74	0/1092	0.95	0/1475
1	C	0.74	0/1127	0.98	0/1522
1	D	0.74	0/1173	0.95	0/1589
1	E	0.74	0/1149	0.97	0/1562
1	F	0.75	0/1089	0.98	0/1470
All	All	0.75	1/6808 (0.0%)	0.96	0/9212

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	TRP	CD2-CE2	5.25	1.47	1.41

There are no bond angle outliers.

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	1156	0	1149	20	0
1	B	1076	0	1082	16	0
1	C	1109	0	1119	11	0
1	D	1152	0	1149	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1127	0	1095	20	0
1	F	1073	0	1089	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	17	0	13	0	0
4	B	17	0	13	2	0
4	C	17	0	13	1	0
4	D	17	0	13	1	0
4	E	17	0	13	4	0
4	F	17	0	13	1	0
5	A	9	0	0	0	0
5	E	9	0	0	0	0
6	A	12	0	18	0	0
6	B	16	0	24	0	0
6	C	8	0	12	0	0
6	D	8	0	12	0	0
6	E	4	0	6	0	0
6	F	8	0	12	0	0
7	A	26	0	0	1	0
7	B	19	0	0	0	0
7	C	19	0	0	0	0
7	D	21	0	0	0	0
7	E	9	0	0	0	0
7	F	22	0	0	1	0
All	All	6999	0	6845	99	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 7.

All (99) 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:B:18:ILE:HD12	1:B:20:ILE:HD11	1.63	0.80
1:A:1:MET:HE3	1:A:155:MET:SD	2.25	0.75
1:F:13:GLY:HA3	1:F:32:LEU:HG	1.68	0.75
1:A:65:ASP:OD1	1:A:66:PRO:HD2	1.87	0.75
1:C:3:ILE:HG22	1:C:153:LEU:HD13	1.75	0.68
1:E:39:VAL:HG12	1:E:148:CYS:HB3	1.77	0.66
1:B:57:ILE:C	1:B:59:LYS:H	1.98	0.66
1:F:59:LYS:C	1:F:60:LEU:HD12	2.16	0.65
4:E:401:CTN:C5'	4:E:401:CTN:H6	2.29	0.63
1:F:57:ILE:HG22	1:F:58:GLY:N	2.15	0.60
1:D:131:ALA:O	4:D:401:CTN:H2'	2.02	0.60
1:B:18:ILE:HD12	1:B:20:ILE:CD1	2.29	0.60
1:D:54:LEU:HD21	1:D:87:LYS:HD2	1.85	0.59
4:B:401:CTN:O3'	1:C:58:GLY:HA3	2.03	0.58
1:D:106:LEU:N	1:D:107:PRO:HD2	2.18	0.58
1:A:1:MET:HE3	1:A:155:MET:CG	2.34	0.58
1:C:7:PHE:HD1	1:C:149:GLU:HG2	1.69	0.58
1:B:57:ILE:C	1:B:59:LYS:N	2.58	0.58
1:A:1:MET:HE1	1:A:153:LEU:HD21	1.85	0.57
1:A:58:GLY:HA3	4:C:401:CTN:O3'	2.05	0.57
1:B:18:ILE:CD1	1:B:20:ILE:HD11	2.34	0.56
1:B:57:ILE:O	1:B:60:LEU:N	2.37	0.56
1:B:18:ILE:CD1	1:B:20:ILE:CD1	2.84	0.56
1:B:57:ILE:O	1:B:59:LYS:N	2.38	0.56
1:D:57:ILE:HG12	1:D:61:PHE:HD2	1.70	0.55
1:F:95:ASP:OD1	1:F:130:LYS:NZ	2.40	0.55
1:E:137:LEU:HD13	1:F:139:PHE:CD1	2.42	0.54
1:E:132:THR:OG1	1:E:133:THR:N	2.40	0.54
1:E:2:ARG:O	1:E:153:LEU:HD12	2.08	0.53
1:F:100:ALA:HB2	1:F:146:ILE:HG23	1.91	0.53
1:E:91:LEU:HG	1:E:92:GLY:N	2.24	0.52
1:C:3:ILE:HG22	1:C:153:LEU:CD1	2.38	0.52
1:D:139:PHE:CD2	1:F:137:LEU:HD13	2.45	0.52
1:D:39:VAL:HG12	1:D:148:CYS:HB2	1.91	0.52
1:A:108:HIS:HD2	7:F:163:HOH:O	1.93	0.51
1:A:1:MET:HE3	1:A:155:MET:HG3	1.92	0.51
1:A:91:LEU:HD11	1:A:94:VAL:HG13	1.93	0.51
1:B:7:PHE:HD1	1:B:149:GLU:HG2	1.76	0.51
1:F:106:LEU:HB3	1:F:107:PRO:HD3	1.93	0.50
1:E:19:ILE:HD12	1:E:36:ASP:HB2	1.93	0.50
1:F:100:ALA:O	1:F:133:THR:HG22	2.11	0.50
1:F:40:ALA:HA	1:F:148:CYS:SG	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:HIS:HD2	1:D:39:VAL:HG22	1.77	0.49
1:F:8:ASP:OD2	1:F:42:HIS:ND1	2.38	0.49
1:A:3:ILE:HG13	1:B:3:ILE:HD12	1.94	0.49
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.93	0.49
1:F:12:PHE:CZ	1:F:146:ILE:HG13	2.48	0.48
1:D:57:ILE:HG12	1:D:61:PHE:CD2	2.48	0.48
1:F:36:ASP:OD1	1:F:73:SER:OG	2.30	0.48
1:D:102:ALA:HB1	1:D:103:PRO:HA	1.97	0.47
4:E:401:CTN:H6	4:E:401:CTN:H5'2	1.96	0.47
1:D:20:ILE:HG21	1:D:98:ILE:HD13	1.96	0.47
1:C:2:ARG:O	1:C:153:LEU:HD12	2.14	0.46
1:E:134:THR:O	1:E:137:LEU:HB2	2.15	0.46
1:F:1:MET:CE	1:F:153:LEU:HD21	2.46	0.46
1:A:135:GLU:O	1:A:136:LYS:HB2	2.15	0.46
1:F:72:ASP:HB3	1:F:75:GLU:OE1	2.15	0.46
1:D:40:ALA:HA	1:D:148:CYS:SG	2.57	0.45
1:D:60:LEU:HD12	1:D:60:LEU:N	2.31	0.45
1:A:81:TRP:CH2	1:A:91:LEU:HB2	2.52	0.45
1:A:52:ALA:O	1:A:87:LYS:NZ	2.42	0.45
1:A:3:ILE:HD13	1:C:151:VAL:HB	1.99	0.45
1:F:60:LEU:HD12	1:F:60:LEU:N	2.31	0.44
1:E:89:TYR:CE1	1:E:156:LYS:CB	3.01	0.44
1:F:106:LEU:HB3	1:F:107:PRO:CD	2.48	0.44
1:E:3:ILE:HD11	1:F:3:ILE:HD11	1.99	0.44
1:A:1:MET:CE	1:A:155:MET:HG3	2.48	0.43
1:B:91:LEU:HD11	1:B:94:VAL:HG13	2.00	0.43
1:E:57:ILE:HG13	1:E:58:GLY:H	1.83	0.43
1:D:58:GLY:HA3	4:F:401:CTN:O3'	2.18	0.43
1:B:130:LYS:HE3	1:C:5:HIS:O	2.18	0.43
1:C:133:THR:HG21	1:C:135:GLU:OE1	2.19	0.43
1:D:10:HIS:CD2	1:D:39:VAL:HG22	2.53	0.43
1:E:133:THR:HG23	4:E:401:CTN:H5	2.01	0.43
1:D:39:VAL:HG12	1:D:148:CYS:CB	2.48	0.42
1:F:6:GLY:HA3	1:F:43:ALA:O	2.18	0.42
1:B:18:ILE:CD1	1:B:20:ILE:HD12	2.49	0.42
1:A:108:HIS:HE1	7:A:169:HOH:O	2.02	0.42
1:A:55:GLY:O	1:C:130:LYS:HG2	2.20	0.42
1:E:40:ALA:HA	1:E:148:CYS:SG	2.60	0.42
1:E:64:THR:OG1	1:E:65:ASP:N	2.53	0.42
1:E:131:ALA:O	4:E:401:CTN:H3'	2.20	0.42
1:E:90:THR:CG2	1:E:155:MET:O	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:HA	1:C:109:ILE:HD12	2.02	0.41
1:A:46:ASP:OD1	1:A:57:ILE:N	2.49	0.41
1:E:90:THR:OG1	1:E:91:LEU:N	2.53	0.41
1:E:109:ILE:O	1:E:112:MET:HB2	2.21	0.41
1:A:65:ASP:OD1	1:A:66:PRO:CD	2.63	0.41
1:B:106:LEU:N	1:B:107:PRO:CD	2.83	0.41
1:E:65:ASP:OD1	1:E:65:ASP:C	2.59	0.41
1:E:100:ALA:HB2	1:E:146:ILE:HG23	2.03	0.41
1:F:54:LEU:HD23	1:F:54:LEU:HA	1.91	0.41
1:D:60:LEU:N	1:D:60:LEU:CD1	2.84	0.41
1:E:61:PHE:CD2	1:E:76:LEU:HD22	2.56	0.41
1:B:135:GLU:O	1:B:136:LYS:CB	2.69	0.40
1:B:131:ALA:O	4:B:401:CTN:H2'	2.22	0.40
1:F:60:LEU:HD23	1:F:83:ARG:HD2	2.04	0.40
1:C:7:PHE:HD1	1:C:149:GLU:CG	2.33	0.40
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.89	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	155/162 (96%)	150 (97%)	5 (3%)	0	100	100
1	B	143/162 (88%)	138 (96%)	4 (3%)	1 (1%)	22	39
1	C	147/162 (91%)	144 (98%)	3 (2%)	0	100	100
1	D	155/162 (96%)	151 (97%)	4 (3%)	0	100	100
1	E	155/162 (96%)	150 (97%)	5 (3%)	0	100	100
1	F	142/162 (88%)	135 (95%)	7 (5%)	0	100	100
All	All	897/972 (92%)	868 (97%)	28 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	GLY

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	112/120 (93%)	111 (99%)	1 (1%)	78	92
1	B	104/120 (87%)	102 (98%)	2 (2%)	57	80
1	C	108/120 (90%)	106 (98%)	2 (2%)	57	80
1	D	112/120 (93%)	111 (99%)	1 (1%)	78	92
1	E	106/120 (88%)	104 (98%)	2 (2%)	57	80
1	F	105/120 (88%)	102 (97%)	3 (3%)	42	69
All	All	647/720 (90%)	636 (98%)	11 (2%)	60	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLU
1	B	79	GLU
1	B	87	LYS
1	C	57	ILE
1	C	93	ASN
1	D	61	PHE
1	E	85	GLN
1	E	90	THR
1	F	18	ILE
1	F	57	ILE
1	F	126	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	10	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 36 ligands modelled in this entry, 14 are monoatomic - leaving 22 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$
6	EDO	A	164	-	3,3,3	0.60	0	2,2,2	0.20	0
6	EDO	B	162	-	3,3,3	0.48	0	2,2,2	0.20	0
6	EDO	E	161	-	3,3,3	0.52	0	2,2,2	0.23	0
6	EDO	F	160	-	3,3,3	0.47	0	2,2,2	0.26	0
6	EDO	B	161	-	3,3,3	0.47	0	2,2,2	0.28	0
5	POP	A	161	-	6,8,8	0.86	0	13,13,13	1.36	2 (15%)
6	EDO	B	163	-	3,3,3	0.54	0	2,2,2	0.19	0
5	POP	E	160	-	6,8,8	0.79	0	13,13,13	1.30	2 (15%)
6	EDO	C	160	-	3,3,3	0.45	0	2,2,2	0.23	0
6	EDO	D	162	-	3,3,3	0.56	0	2,2,2	0.22	0
4	CTN	F	401	-	15,18,18	1.00	2 (13%)	17,26,26	1.36	2 (11%)
4	CTN	E	401	-	15,18,18	1.17	2 (13%)	17,26,26	1.77	7 (41%)
4	CTN	C	401	-	15,18,18	1.33	3 (20%)	17,26,26	1.46	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CTN	A	401	-	15,18,18	1.32	2 (13%)	17,26,26	1.44	2 (11%)
6	EDO	B	164	-	3,3,3	0.47	0	2,2,2	0.24	0
6	EDO	F	161	-	3,3,3	0.48	0	2,2,2	0.22	0
6	EDO	C	161	-	3,3,3	0.59	0	2,2,2	0.19	0
4	CTN	D	401	-	15,18,18	0.99	1 (6%)	17,26,26	1.25	2 (11%)
4	CTN	B	401	-	15,18,18	1.15	2 (13%)	17,26,26	1.57	3 (17%)
6	EDO	A	163	-	3,3,3	0.50	0	2,2,2	0.18	0
6	EDO	A	162	-	3,3,3	0.50	0	2,2,2	0.14	0
6	EDO	D	161	-	3,3,3	0.45	0	2,2,2	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	164	-	-	1/1/1/1	-
6	EDO	B	162	-	-	1/1/1/1	-
6	EDO	E	161	-	-	1/1/1/1	-
6	EDO	F	160	-	-	0/1/1/1	-
6	EDO	B	161	-	-	1/1/1/1	-
5	POP	A	161	-	-	2/6/6/6	-
6	EDO	B	163	-	-	1/1/1/1	-
5	POP	E	160	-	-	1/6/6/6	-
6	EDO	C	160	-	-	1/1/1/1	-
6	EDO	D	162	-	-	1/1/1/1	-
4	CTN	F	401	-	-	4/4/22/22	0/2/2/2
4	CTN	E	401	-	-	1/4/22/22	0/2/2/2
4	CTN	C	401	-	-	0/4/22/22	0/2/2/2
4	CTN	A	401	-	-	2/4/22/22	0/2/2/2
6	EDO	B	164	-	-	1/1/1/1	-
6	EDO	F	161	-	-	1/1/1/1	-
6	EDO	C	161	-	-	1/1/1/1	-
4	CTN	D	401	-	-	0/4/22/22	0/2/2/2
4	CTN	B	401	-	-	4/4/22/22	0/2/2/2
6	EDO	A	163	-	-	1/1/1/1	-
6	EDO	A	162	-	-	1/1/1/1	-
6	EDO	D	161	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	CTN	C2'-C1'	-2.97	1.49	1.53
4	C	401	CTN	C6-N1	-2.79	1.32	1.35
4	E	401	CTN	C6-N1	-2.74	1.32	1.35
4	E	401	CTN	C2'-C1'	-2.67	1.49	1.53
4	A	401	CTN	C6-N1	-2.39	1.32	1.35
4	C	401	CTN	C2-N3	-2.37	1.33	1.38
4	B	401	CTN	C6-N1	-2.32	1.33	1.35
4	B	401	CTN	C2-N3	-2.27	1.33	1.38
4	F	401	CTN	C6-N1	-2.26	1.33	1.35
4	C	401	CTN	C2'-C1'	-2.24	1.50	1.53
4	F	401	CTN	C2-N3	-2.17	1.33	1.38
4	D	401	CTN	C6-N1	-2.14	1.33	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	CTN	C5'-C4'-C3'	-4.09	105.23	115.09
4	C	401	CTN	C3'-C2'-C1'	3.83	106.74	100.98
4	A	401	CTN	C3'-C2'-C1'	3.80	106.70	100.98
4	E	401	CTN	N4-C4-N3	3.34	121.76	116.49
4	B	401	CTN	C3'-C2'-C1'	3.20	105.80	100.98
4	E	401	CTN	C3'-C2'-C1'	3.11	105.66	100.98
4	A	401	CTN	C4-N3-C2	2.97	119.35	116.34
5	A	161	POP	O5-P2-O	2.93	114.47	104.64
5	E	160	POP	P2-O-P1	-2.64	123.77	132.83
4	C	401	CTN	C4-N3-C2	2.61	118.98	116.34
4	D	401	CTN	C4-N3-C2	2.60	118.97	116.34
5	A	161	POP	P2-O-P1	-2.48	124.33	132.83
4	E	401	CTN	C4-N3-C2	2.45	118.83	116.34
4	F	401	CTN	C3'-C2'-C1'	2.45	104.67	100.98
4	E	401	CTN	O4'-C4'-C5'	2.44	114.49	109.21
4	D	401	CTN	C3'-C2'-C1'	2.37	104.55	100.98
4	E	401	CTN	C2'-C3'-C4'	2.37	107.25	102.64
4	C	401	CTN	C5'-C4'-C3'	-2.31	109.51	115.09
5	E	160	POP	O2-P1-O	2.24	112.13	104.64
4	F	401	CTN	C5'-C4'-C3'	-2.23	109.72	115.09
4	E	401	CTN	C5-C4-N4	-2.18	117.36	121.14
4	E	401	CTN	C5'-C4'-C3'	-2.14	109.92	115.09
4	B	401	CTN	C4-N3-C2	2.10	118.47	116.34

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	CTN	O4'-C4'-C5'-O5'
4	A	401	CTN	C3'-C4'-C5'-O5'
4	B	401	CTN	O4'-C1'-N1-C6
4	B	401	CTN	C2'-C1'-N1-C6
4	F	401	CTN	O4'-C1'-N1-C6
4	F	401	CTN	C2'-C1'-N1-C6
5	A	161	POP	P1-O-P2-O5
4	B	401	CTN	O4'-C4'-C5'-O5'
4	B	401	CTN	C3'-C4'-C5'-O5'
4	F	401	CTN	C3'-C4'-C5'-O5'
4	F	401	CTN	O4'-C4'-C5'-O5'
6	A	164	EDO	O1-C1-C2-O2
6	B	161	EDO	O1-C1-C2-O2
6	B	163	EDO	O1-C1-C2-O2
6	B	164	EDO	O1-C1-C2-O2
6	C	160	EDO	O1-C1-C2-O2
6	D	161	EDO	O1-C1-C2-O2
6	D	162	EDO	O1-C1-C2-O2
6	F	161	EDO	O1-C1-C2-O2
6	A	163	EDO	O1-C1-C2-O2
6	A	162	EDO	O1-C1-C2-O2
5	E	160	POP	P1-O-P2-O5
6	E	161	EDO	O1-C1-C2-O2
4	E	401	CTN	O4'-C4'-C5'-O5'
5	A	161	POP	P1-O-P2-O4
6	B	162	EDO	O1-C1-C2-O2
6	C	161	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	401	CTN	1	0
4	E	401	CTN	4	0
4	C	401	CTN	1	0
4	D	401	CTN	1	0
4	B	401	CTN	2	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, 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	157/162 (96%)	0.31	16 (10%) 6 6	34, 44, 84, 119	0
1	B	147/162 (90%)	0.07	11 (7%) 14 14	36, 47, 68, 85	0
1	C	151/162 (93%)	0.29	16 (10%) 6 5	37, 47, 76, 100	0
1	D	157/162 (96%)	0.03	11 (7%) 16 16	38, 49, 68, 84	0
1	E	157/162 (96%)	0.26	13 (8%) 11 11	46, 66, 94, 102	0
1	F	146/162 (90%)	0.18	13 (8%) 9 9	38, 51, 74, 88	0
All	All	915/972 (94%)	0.19	80 (8%) 10 10	34, 50, 80, 119	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	GLY	6.5
1	A	66	PRO	5.1
1	A	67	ALA	4.2
1	E	150	ALA	4.0
1	E	64	THR	4.0
1	C	71	ALA	3.7
1	B	97	THR	3.7
1	B	148	CYS	3.6
1	C	61	PHE	3.5
1	A	61	PHE	3.5
1	C	6	GLY	3.5
1	A	96	VAL	3.4
1	F	151	VAL	3.4
1	A	65	ASP	3.3
1	B	6	GLY	3.3
1	A	68	PHE	3.3
1	D	6	GLY	3.3
1	E	68	PHE	3.3
1	C	150	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	148	CYS	3.2
1	F	150	ALA	3.2
1	E	66	PRO	3.2
1	A	151	VAL	3.2
1	B	151	VAL	3.2
1	A	69	LYS	3.1
1	D	148	CYS	3.0
1	F	34	HIS	3.0
1	D	96	VAL	3.0
1	A	97	THR	2.8
1	C	151	VAL	2.8
1	D	7	PHE	2.7
1	F	7	PHE	2.7
1	A	6	GLY	2.7
1	C	34	HIS	2.7
1	E	14	GLY	2.7
1	D	149	GLU	2.7
1	E	34	HIS	2.7
1	C	5	HIS	2.6
1	A	150	ALA	2.6
1	E	32	LEU	2.6
1	B	149	GLU	2.5
1	F	6	GLY	2.5
1	B	150	ALA	2.5
1	D	5	HIS	2.4
1	F	33	ALA	2.4
1	B	32	LEU	2.4
1	E	149	GLU	2.4
1	F	149	GLU	2.4
1	D	150	ALA	2.4
1	E	114	VAL	2.4
1	E	148	CYS	2.4
1	F	47	ALA	2.4
1	B	96	VAL	2.4
1	C	47	ALA	2.3
1	D	64	THR	2.3
1	E	6	GLY	2.3
1	C	149	GLU	2.3
1	C	43	ALA	2.3
1	F	148	CYS	2.3
1	E	70	GLY	2.3
1	C	33	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	5	HIS	2.2
1	B	71	ALA	2.2
1	B	82	ARG	2.2
1	D	97	THR	2.2
1	F	35	SER	2.2
1	C	32	LEU	2.1
1	C	44	LEU	2.1
1	E	151	VAL	2.1
1	D	70	GLY	2.1
1	F	13	GLY	2.1
1	F	96	VAL	2.1
1	A	63	ASP	2.1
1	D	151	VAL	2.0
1	C	7	PHE	2.0
1	C	148	CYS	2.0
1	A	7	PHE	2.0
1	A	47	ALA	2.0
1	F	5	HIS	2.0
1	B	7	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
6	EDO	B	163	4/4	0.36	0.30	85,87,89,90	0
3	MG	A	302	1/1	0.60	0.20	57,57,57,57	0
6	EDO	B	161	4/4	0.71	0.57	73,75,75,79	0
6	EDO	D	161	4/4	0.72	0.64	83,85,86,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	C	161	4/4	0.73	0.19	61,63,64,66	0
6	EDO	C	160	4/4	0.75	0.40	71,73,74,78	0
3	MG	A	160	1/1	0.76	0.34	66,66,66,66	0
6	EDO	E	161	4/4	0.78	0.39	67,69,70,72	0
6	EDO	B	162	4/4	0.79	0.22	62,64,65,65	0
6	EDO	D	162	4/4	0.82	0.13	75,76,77,79	0
6	EDO	A	162	4/4	0.82	0.64	74,77,77,79	0
6	EDO	A	164	4/4	0.83	0.20	72,73,75,76	0
2	ZN	F	301	1/1	0.84	0.33	102,102,102,102	0
6	EDO	F	160	4/4	0.84	0.78	80,81,83,84	0
3	MG	D	302	1/1	0.85	0.26	50,50,50,50	0
2	ZN	C	301	1/1	0.88	0.17	81,81,81,81	0
6	EDO	B	164	4/4	0.88	0.12	61,65,65,66	0
6	EDO	A	163	4/4	0.90	0.08	73,79,80,81	0
3	MG	C	302	1/1	0.90	0.25	58,58,58,58	0
2	ZN	B	301	1/1	0.91	0.22	86,86,86,86	0
3	MG	E	302	1/1	0.92	0.35	50,50,50,50	0
4	CTN	E	401	17/17	0.92	0.23	41,45,49,50	0
3	MG	D	160	1/1	0.92	0.29	45,45,45,45	0
3	MG	F	302	1/1	0.93	0.14	62,62,62,62	0
2	ZN	A	301	1/1	0.94	0.13	80,80,80,80	0
5	POP	E	160	9/9	0.95	0.16	54,58,85,85	0
4	CTN	A	401	17/17	0.95	0.18	33,38,46,48	0
6	EDO	F	161	4/4	0.95	0.10	66,67,67,67	0
3	MG	B	160	1/1	0.96	0.20	39,39,39,39	0
4	CTN	F	401	17/17	0.96	0.23	38,45,49,52	0
5	POP	A	161	9/9	0.96	0.15	43,51,74,74	0
4	CTN	B	401	17/17	0.96	0.15	38,43,55,60	0
4	CTN	C	401	17/17	0.96	0.14	38,45,60,61	0
4	CTN	D	401	17/17	0.96	0.20	39,44,48,49	0
2	ZN	E	301	1/1	0.97	0.12	71,71,71,71	0
2	ZN	D	301	1/1	0.98	0.13	72,72,72,72	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.