Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:05 pm BST

PDB ID	:	6ET9
Title	:	Structure of the acetoacetyl-CoA-thiolase/HMG-CoA-synthase complex from Methanothermococcus thermolithotrophicus at 2.75 A
Authors	:	Engilberge, S.; Voegeli, B.; Girard, E.; Riobe, F.; Maury, O.; Erb, T.J.; Shima, S.; Wagner, T.
Deposited on	:	2017-10-25
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

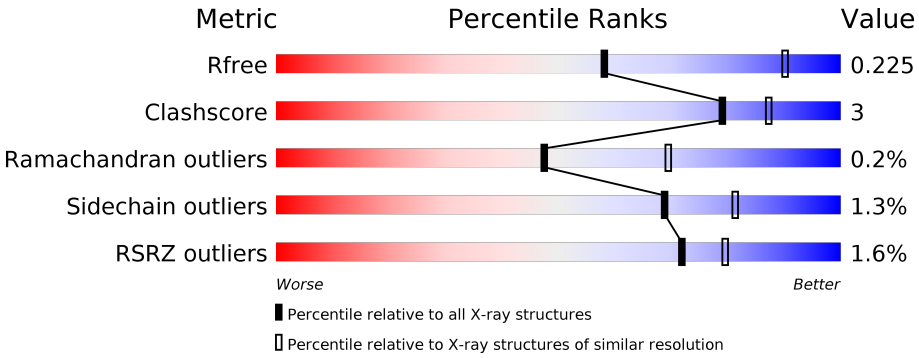
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	3% 89% 11%
1	B	392	% 92% 8%
1	C	392	2% 91% 7%
1	D	392	93% 7%
2	E	130	2% 95%
2	F	130	% 96%

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Mol	Chain	Length	Quality of chain
2	G	130	2% 91% 8%
2	H	130	13% 94% 5%
3	I	349	94% 5%
3	J	349	91% 7%
3	K	349	92% 7%
3	L	349	2% 91% 7%

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
9	GOL	I	405	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26928 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 Acetyl-CoA acetyltransferase thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			2932	1839	496	578	19			
1	B	392	Total	C	N	O	S	0	0	0
			2932	1839	496	578	19			
1	C	389	Total	C	N	O	S	0	0	0
			2905	1821	490	575	19			
1	D	392	Total	C	N	O	S	0	0	0
			2932	1839	496	578	19			

- Molecule 2 is a protein called Pfam DUF35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	128	Total	C	N	O	S	0	0	0
			1028	662	176	184	6			
2	F	128	Total	C	N	O	S	0	0	0
			1028	662	176	184	6			
2	G	128	Total	C	N	O	S	0	0	0
			1028	662	176	184	6			
2	H	128	Total	C	N	O	S	0	0	0
			1028	662	176	184	6			

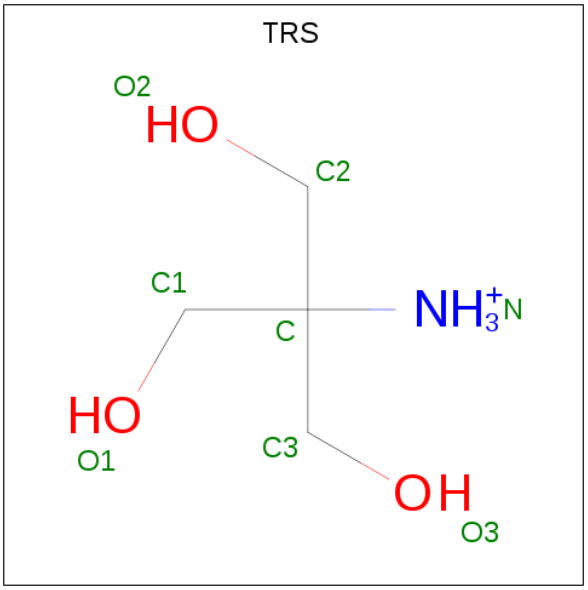
- Molecule 3 is a protein called HydroxyMethylGlutaryl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	347	Total	C	N	O	S	0	0	0
			2623	1674	435	505	9			
3	J	348	Total	C	N	O	S	0	0	0
			2632	1680	437	506	9			
3	K	347	Total	C	N	O	S	0	0	0
			2623	1674	435	505	9			
3	L	347	Total	C	N	O	S	0	0	0
			2623	1674	435	505	9			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 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
5	A	1	Total C N O 8 4 1 3	0	0
5	A	1	Total C N O 8 4 1 3	0	0
5	A	1	Total C N O 8 4 1 3	0	0
5	B	1	Total C N O 8 4 1 3	0	0
5	B	1	Total C N O 8 4 1 3	0	0
5	C	1	Total C N O 8 4 1 3	0	0
5	C	1	Total C N O 8 4 1 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N O 8 4 1 3	0	0
5	F	1	Total C N O 8 4 1 3	0	0
5	G	1	Total C N O 8 4 1 3	0	0
5	H	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	K	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0
6	I	2	Total K 2 2	0	0
6	C	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0

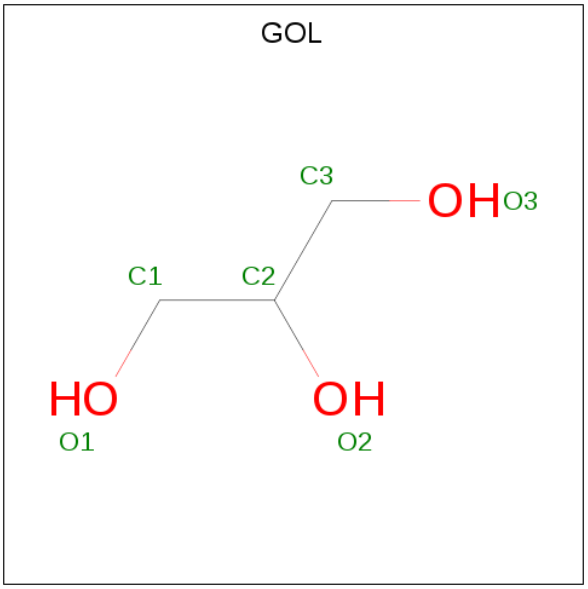
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total Cl 1 1	0	0
7	G	1	Total Cl 1 1	0	0
7	I	1	Total Cl 1 1	0	0
7	C	1	Total Cl 1 1	0	0
7	E	2	Total Cl 2 2	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	0
9	K	1	Total C O 6 3 3	0	0
9	L	1	Total C O 6 3 3	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total Zn 1 1	0	0
10	G	1	Total Zn 1 1	0	0
10	F	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total Zn 1 1	0	0

- Molecule 11 is water.

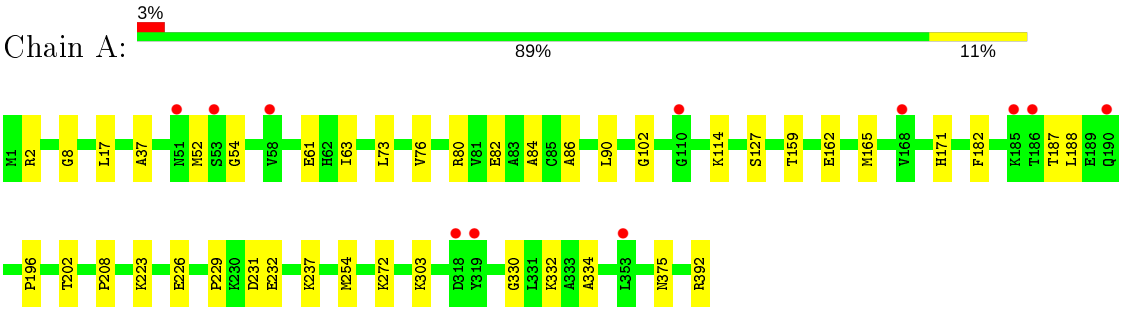
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	30	Total O 30 30	0	0
11	B	66	Total O 66 66	0	0
11	C	23	Total O 23 23	0	0
11	D	66	Total O 66 66	0	0
11	E	28	Total O 28 28	0	0
11	F	20	Total O 20 20	0	0
11	G	35	Total O 35 35	0	0
11	H	8	Total O 8 8	0	0
11	I	71	Total O 71 71	0	0
11	J	43	Total O 43 43	0	0
11	K	47	Total O 47 47	0	0
11	L	31	Total O 31 31	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

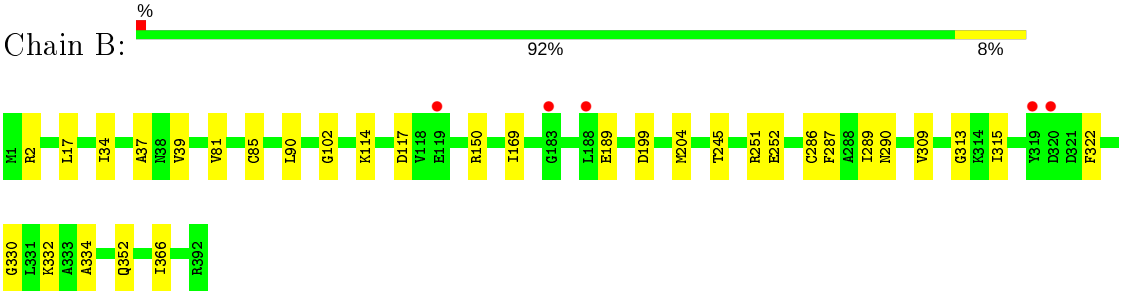
- Molecule 1: Acetyl-CoA acetyltransferase thiolase

Chain A:



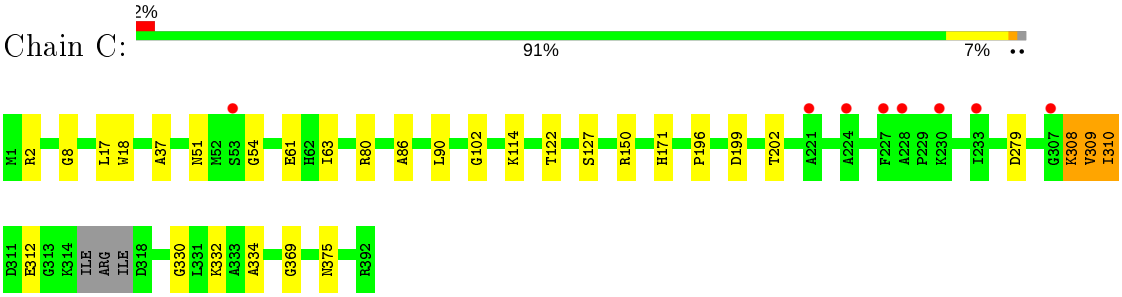
- Molecule 1: Acetyl-CoA acetyltransferase thiolase

Chain B:



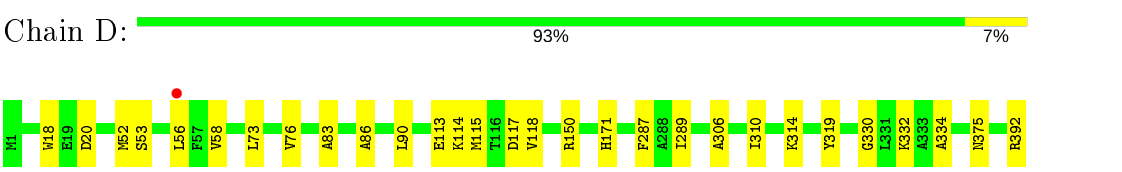
- Molecule 1: Acetyl-CoA acetyltransferase thiolase

Chain C:



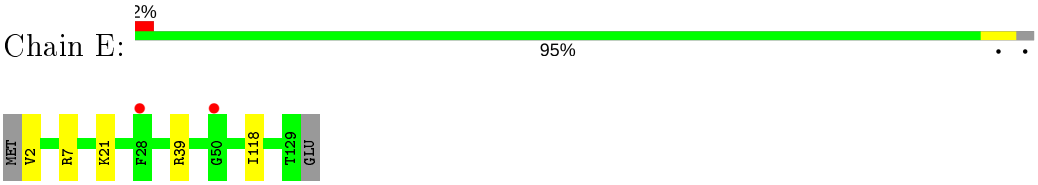
- Molecule 1: Acetyl-CoA acetyltransferase thiolase

Chain D:



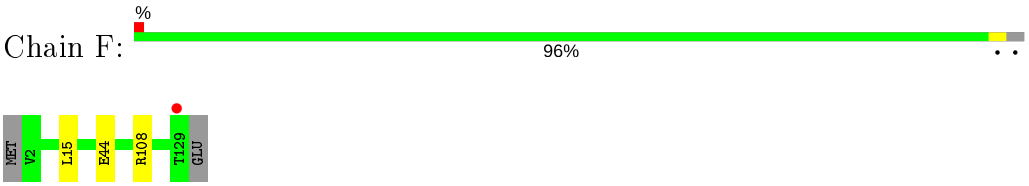
- Molecule 2: Pfam DUF35

Chain E:



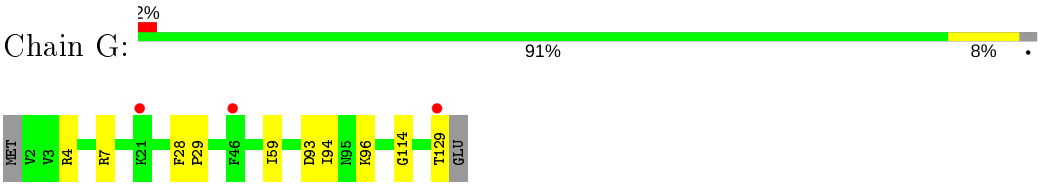
- Molecule 2: Pfam DUF35

Chain F:



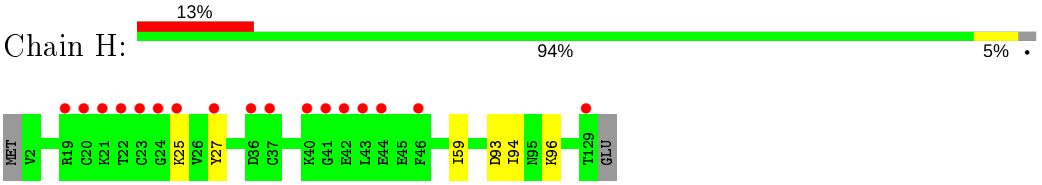
- Molecule 2: Pfam DUF35

Chain G:



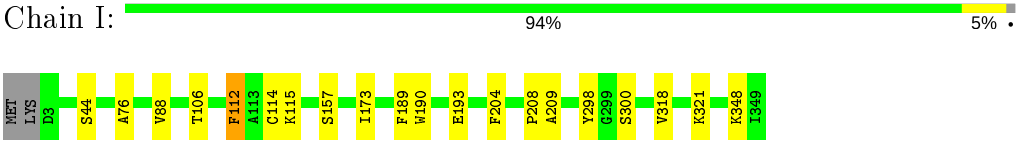
- Molecule 2: Pfam DUF35

Chain H:



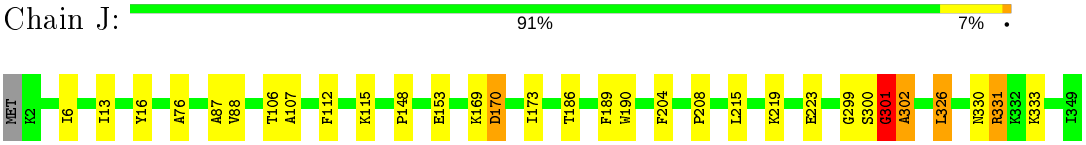
- Molecule 3: HydroxyMethylGlutaryl-CoA synthase

Chain I:



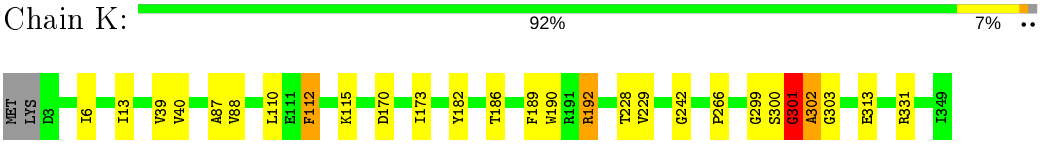
- Molecule 3: HydroxyMethylGlutaryl-CoA synthase

Chain J:



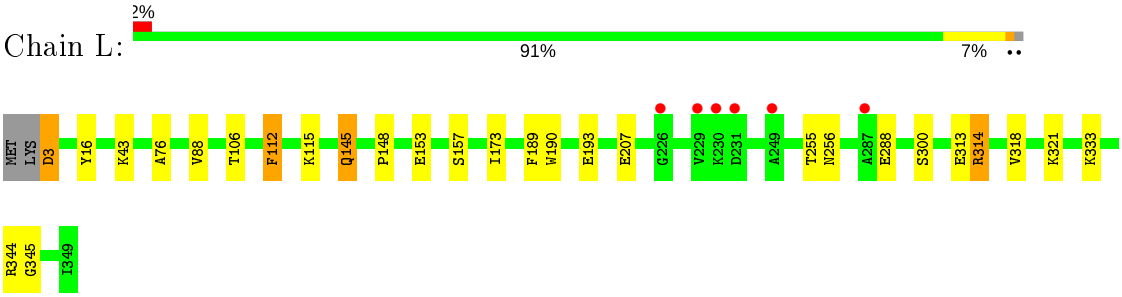
- Molecule 3: HydroxyMethylGlutaryl-CoA synthase

Chain K:



• Molecule 3: HydroxyMethylGlutaryl-CoA synthase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.62Å 144.01Å 230.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 2.75 48.39 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.39-2.75) 100.0 (48.39-2.75)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.190 , 0.225 0.193 , 0.225	Depositor DCC
R_{free} test set	4636 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26928	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CL, NA, K, MG, TRS

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	0.35	0/2981	0.51	0/4032
1	B	0.43	0/2981	0.52	0/4032
1	C	0.38	0/2953	0.50	0/3993
1	D	0.44	0/2981	0.54	0/4032
2	E	0.40	0/1051	0.55	0/1417
2	F	0.47	0/1051	0.56	0/1417
2	G	0.48	0/1051	0.55	0/1417
2	H	0.36	0/1051	0.53	0/1417
3	I	0.47	0/2679	0.54	0/3627
3	J	0.39	0/2688	0.54	1/3638 (0.0%)
3	K	0.46	0/2679	0.55	1/3627 (0.0%)
3	L	0.40	0/2679	0.54	0/3627
All	All	0.42	0/26825	0.53	2/36276 (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
3	J	0	1
3	K	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	301	GLY	N-CA-C	-5.38	99.66	113.10
3	J	301	GLY	N-CA-C	-5.23	100.02	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	301	GLY	Peptide
3	K	301	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2932	0	2884	24	0
1	B	2932	0	2884	16	0
1	C	2905	0	2848	16	0
1	D	2932	0	2884	20	0
2	E	1028	0	1050	4	0
2	F	1028	0	1050	0	0
2	G	1028	0	1050	7	0
2	H	1028	0	1050	3	0
3	I	2623	0	2608	17	0
3	J	2632	0	2621	19	0
3	K	2623	0	2608	15	0
3	L	2623	0	2608	21	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	J	1	0	0	0	0
5	A	24	0	36	0	0
5	B	16	0	24	0	0
5	C	16	0	24	0	0
5	D	8	0	12	0	0
5	F	8	0	12	0	0
5	G	8	0	12	0	0
5	H	8	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	2	0	0	0	0
6	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	1	0	0	0	0
7	C	1	0	0	0	0
7	E	2	0	0	1	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
8	D	1	0	0	0	0
9	D	6	0	8	0	0
9	I	12	0	16	0	0
9	J	6	0	8	0	0
9	K	6	0	8	0	0
9	L	6	0	8	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
11	A	30	0	0	0	0
11	B	66	0	0	0	0
11	C	23	0	0	1	0
11	D	66	0	0	2	0
11	E	28	0	0	3	0
11	F	20	0	0	0	0
11	G	35	0	0	0	0
11	H	8	0	0	0	0
11	I	71	0	0	1	0
11	J	43	0	0	0	0
11	K	47	0	0	0	0
11	L	31	0	0	0	0
All	All	26928	0	26325	145	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 3.

All (145) 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)
7:E:203:CL:CL	11:E:318:HOH:O	2.24	0.92
3:L:3:ASP:N	3:L:3:ASP:OD1	2.16	0.79
3:K:186:THR:N	3:K:301:GLY:O	2.24	0.70
1:D:117:ASP:OD1	2:G:7:ARG:NH1	2.27	0.67
1:C:17:LEU:O	1:C:114:LYS:NZ	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:O	1:A:114:LYS:NZ	2.28	0.65
1:C:150:ARG:NH2	1:C:199:ASP:OD2	2.30	0.65
3:J:13:ILE:O	3:J:331:ARG:NH2	2.30	0.64
3:I:348:LYS:NZ	3:L:345:GLY:O	2.30	0.63
1:B:17:LEU:O	1:B:114:LYS:NZ	2.32	0.62
1:A:237:LYS:HE2	1:A:392:ARG:O	2.01	0.60
1:D:150:ARG:HD2	11:E:305:HOH:O	2.02	0.59
1:B:286:CYS:SG	1:B:290:ASN:ND2	2.72	0.59
1:D:53:SER:N	1:D:113:GLU:OE2	2.35	0.58
2:G:93:ASP:HB2	2:G:96:LYS:HD2	1.85	0.57
1:A:73:LEU:O	1:A:76:VAL:HG12	2.04	0.57
1:C:51:ASN:O	1:C:80:ARG:NH2	2.37	0.57
3:I:193:GLU:HA	3:K:87:ALA:HB2	1.89	0.54
1:B:150:ARG:NH2	1:B:199:ASP:OD2	2.41	0.54
3:J:186:THR:N	3:J:301:GLY:O	2.37	0.53
1:D:86:ALA:HA	1:D:375:ASN:OD1	2.09	0.53
1:B:37:ALA:O	1:B:39:VAL:N	2.42	0.53
1:A:127:SER:HB3	1:C:61:GLU:HB2	1.90	0.53
2:G:114:GLY:O	3:K:192:ARG:NH2	2.42	0.53
3:L:288:GLU:N	3:L:288:GLU:OE1	2.42	0.53
1:A:171:HIS:NE2	1:A:332:LYS:HE3	2.24	0.53
3:I:189:PHE:HB3	3:I:300:SER:CB	2.39	0.52
3:L:173:ILE:HG22	3:L:314:ARG:HD2	1.91	0.52
1:B:330:GLY:O	1:B:334:ALA:HB3	2.09	0.52
1:A:223:LYS:O	1:A:226:GLU:HG2	2.10	0.51
1:A:61:GLU:HB2	1:C:127:SER:HB3	1.93	0.51
3:J:190:TRP:HA	3:L:88:VAL:O	2.09	0.51
2:H:93:ASP:HB2	2:H:96:LYS:HD2	1.92	0.51
1:A:229:PRO:O	1:A:231:ASP:O	2.29	0.51
1:B:352:GLN:O	1:B:366:ILE:HD11	2.11	0.51
1:D:287:PHE:O	1:D:289:ILE:N	2.44	0.51
3:I:190:TRP:HA	3:K:88:VAL:O	2.10	0.50
3:K:13:ILE:O	3:K:331:ARG:NH2	2.44	0.50
3:J:6:ILE:O	3:J:173:ILE:HG13	2.12	0.50
3:J:170:ASP:N	3:J:170:ASP:OD1	2.45	0.50
1:D:18:TRP:O	2:G:7:ARG:NH2	2.44	0.50
1:D:58:VAL:HG22	2:G:4:ARG:HD3	1.94	0.49
3:I:348:LYS:CE	3:L:345:GLY:O	2.60	0.49
1:D:330:GLY:O	1:D:334:ALA:HB3	2.13	0.49
3:J:88:VAL:O	3:L:190:TRP:HA	2.13	0.48
3:L:76:ALA:HA	3:L:106:THR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:MET:HE2	1:A:188:LEU:HD13	1.95	0.48
1:D:171:HIS:NE2	1:D:332:LYS:HE3	2.28	0.48
1:C:171:HIS:NE2	1:C:332:LYS:HE3	2.28	0.48
3:K:182:TYR:O	3:K:303:GLY:HA2	2.14	0.48
1:C:308:LYS:H	1:C:308:LYS:HD2	1.77	0.48
1:D:392:ARG:NH2	11:D:502:HOH:O	2.45	0.48
1:A:52:MET:SD	1:A:84:ALA:HA	2.54	0.48
3:I:173:ILE:HG21	3:I:318:VAL:HG21	1.96	0.48
1:A:86:ALA:HA	1:A:375:ASN:OD1	2.14	0.47
1:B:287:PHE:O	1:B:289:ILE:N	2.43	0.47
3:L:148:PRO:HA	3:L:153:GLU:OE2	2.14	0.47
1:C:18:TRP:CG	3:I:208:PRO:HG3	2.49	0.47
1:B:204:MET:O	1:B:332:LYS:HE3	2.15	0.47
3:I:88:VAL:O	3:K:190:TRP:HA	2.15	0.47
3:J:189:PHE:HB3	3:J:300:SER:CB	2.45	0.47
1:A:272:LYS:HG2	1:A:272:LYS:O	2.15	0.47
1:A:196:PRO:HA	1:A:202:THR:HA	1.97	0.46
1:C:279:ASP:OD2	1:C:369:GLY:N	2.48	0.46
1:D:52:MET:HB2	1:D:113:GLU:OE2	2.15	0.46
3:J:189:PHE:HB3	3:J:300:SER:HB3	1.97	0.46
1:A:231:ASP:O	1:A:232:GLU:HB2	2.16	0.46
2:E:2:VAL:N	11:E:301:HOH:O	2.49	0.46
3:I:114:CYS:SG	11:I:525:HOH:O	2.61	0.46
3:L:43:LYS:HB2	3:L:157:SER:HB3	1.98	0.46
1:A:82:GLU:OE2	1:A:84:ALA:N	2.46	0.45
1:B:290:ASN:OD1	1:B:290:ASN:N	2.50	0.45
1:C:86:ALA:HA	1:C:375:ASN:OD1	2.17	0.45
3:J:219:LYS:O	3:J:223:GLU:HG3	2.17	0.45
1:C:330:GLY:O	1:C:334:ALA:HB3	2.17	0.45
3:I:44:SER:OG	3:I:157:SER:HB2	2.17	0.45
3:K:40:VAL:HA	3:K:266:PRO:HA	1.99	0.45
3:K:189:PHE:HB3	3:K:300:SER:CB	2.47	0.44
1:B:189:GLU:N	1:B:189:GLU:OE1	2.47	0.44
1:B:34:ILE:O	1:B:37:ALA:O	2.35	0.44
3:J:326:LEU:HD13	3:J:330:ASN:OD1	2.17	0.44
2:E:21:LYS:O	2:E:21:LYS:HD3	2.17	0.44
3:J:107:ALA:O	3:L:115:LYS:NZ	2.47	0.44
1:D:306:ALA:O	1:D:310:ILE:HG12	2.18	0.44
1:B:2:ARG:NH1	1:B:102:GLY:HA2	2.32	0.44
1:D:20:ASP:O	1:D:114:LYS:HE2	2.17	0.44
3:J:148:PRO:O	3:J:153:GLU:OE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:112:PHE:CD1	3:K:115:LYS:HD3	2.52	0.44
1:A:330:GLY:O	1:A:334:ALA:HB3	2.18	0.43
1:B:169:ILE:HD13	1:B:313:GLY:H	1.82	0.43
3:L:145:GLN:OE1	3:L:344:ARG:HB3	2.18	0.43
3:L:189:PHE:HB3	3:L:300:SER:CB	2.47	0.43
1:D:115:MET:O	1:D:118:VAL:HG12	2.18	0.43
2:E:118:ILE:HG23	3:L:190:TRP:CE2	2.53	0.43
3:J:76:ALA:HA	3:J:106:THR:O	2.17	0.43
3:I:204:PHE:CD1	3:I:208:PRO:HG2	2.54	0.43
1:D:314:LYS:HA	1:D:319:TYR:CG	2.54	0.43
1:C:8:GLY:HA3	1:C:37:ALA:HB2	2.00	0.43
1:D:83:ALA:HB2	1:D:90:LEU:HD22	2.01	0.43
1:C:122:THR:HG23	11:C:513:HOH:O	2.19	0.43
1:C:196:PRO:HA	1:C:202:THR:HA	2.00	0.43
1:D:52:MET:N	1:D:113:GLU:OE2	2.51	0.43
3:I:76:ALA:HA	3:I:106:THR:O	2.19	0.43
1:A:229:PRO:HB2	1:A:231:ASP:OD1	2.19	0.42
1:A:8:GLY:HA3	1:A:37:ALA:HB2	2.01	0.42
3:L:16:TYR:HA	3:L:333:LYS:O	2.19	0.42
2:G:59:ILE:HD13	2:G:94:ILE:HG23	2.02	0.42
3:J:215:LEU:O	3:J:219:LYS:HG2	2.20	0.42
3:I:115:LYS:HG2	3:I:115:LYS:O	2.18	0.42
3:J:204:PHE:CD1	3:J:208:PRO:HG2	2.54	0.42
3:L:255:THR:OG1	3:L:256:ASN:N	2.52	0.42
2:H:25:LYS:HD3	2:H:27:TYR:CZ	2.55	0.42
2:H:59:ILE:HD13	2:H:94:ILE:HG23	2.01	0.42
3:K:299:GLY:O	3:K:302:ALA:HA	2.20	0.42
1:D:332:LYS:NZ	11:D:504:HOH:O	2.53	0.42
1:B:245:THR:OG1	1:B:251:ARG:HG3	2.20	0.42
3:I:112:PHE:CD1	3:I:115:LYS:HD3	2.55	0.42
3:L:189:PHE:HB3	3:L:300:SER:HB3	2.02	0.42
1:B:117:ASP:OD2	2:E:7:ARG:NH2	2.52	0.41
3:L:318:VAL:HA	3:L:321:LYS:HG2	2.02	0.41
3:L:148:PRO:O	3:L:153:GLU:OE1	2.38	0.41
1:C:309:VAL:HG22	1:C:310:ILE:HD13	2.02	0.41
1:A:73:LEU:HD12	1:A:73:LEU:N	2.36	0.41
1:D:73:LEU:O	1:D:76:VAL:HG13	2.21	0.41
3:K:6:ILE:O	3:K:173:ILE:HG13	2.20	0.41
1:A:159:THR:HG23	1:A:162:GLU:H	1.86	0.41
3:I:318:VAL:HA	3:I:321:LYS:HD2	2.02	0.41
1:D:83:ALA:CB	1:D:90:LEU:HD22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:299:GLY:O	3:J:302:ALA:HA	2.21	0.41
3:L:112:PHE:CD1	3:L:115:LYS:HD3	2.56	0.41
1:B:309:VAL:CG1	1:B:315:ILE:HG23	2.51	0.41
3:I:189:PHE:HB3	3:I:300:SER:HB3	2.03	0.41
3:J:16:TYR:HA	3:J:333:LYS:O	2.21	0.41
3:K:39:VAL:HB	3:K:242:GLY:HA3	2.02	0.41
2:G:28:PHE:HA	2:G:29:PRO:C	2.42	0.41
3:I:209:ALA:HB1	3:I:298:TYR:OH	2.21	0.41
3:K:228:THR:HG22	3:K:229:VAL:N	2.36	0.41
1:A:2:ARG:NH1	1:A:102:GLY:HA2	2.36	0.40
1:C:2:ARG:HH11	1:C:102:GLY:HA2	1.86	0.40
3:J:115:LYS:HG2	3:J:115:LYS:O	2.20	0.40
1:A:182:PHE:CE2	1:A:208:PRO:HG3	2.56	0.40
3:K:115:LYS:O	3:K:115:LYS:HG2	2.21	0.40
3:J:87:ALA:HB2	3:L:193:GLU:HA	2.03	0.40
1:A:237:LYS:HE2	1:A:392:ARG:C	2.42	0.40
1:A:63:ILE:HD11	1:A:80:ARG:HG3	2.03	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	390/392 (100%)	379 (97%)	10 (3%)	1 (0%)	41 60
1	B	390/392 (100%)	376 (96%)	14 (4%)	0	100 100
1	C	385/392 (98%)	374 (97%)	10 (3%)	1 (0%)	41 60
1	D	390/392 (100%)	381 (98%)	9 (2%)	0	100 100
2	E	126/130 (97%)	122 (97%)	4 (3%)	0	100 100
2	F	126/130 (97%)	124 (98%)	2 (2%)	0	100 100
2	G	126/130 (97%)	123 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
3	I	345/349 (99%)	333 (96%)	11 (3%)	1 (0%)	41	60
3	J	346/349 (99%)	335 (97%)	9 (3%)	2 (1%)	25	42
3	K	345/349 (99%)	333 (96%)	10 (3%)	2 (1%)	25	42
3	L	345/349 (99%)	334 (97%)	10 (3%)	1 (0%)	41	60
All	All	3440/3484 (99%)	3337 (97%)	95 (3%)	8 (0%)	47	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLY
3	K	302	ALA
3	I	112	PHE
3	J	112	PHE
3	J	302	ALA
3	L	112	PHE
3	K	112	PHE
1	C	54	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	302/303 (100%)	298 (99%)	4 (1%)	69	81
1	B	302/303 (100%)	297 (98%)	5 (2%)	60	76
1	C	299/303 (99%)	293 (98%)	6 (2%)	55	72
1	D	302/303 (100%)	301 (100%)	1 (0%)	92	95
2	E	113/115 (98%)	112 (99%)	1 (1%)	78	87
2	F	113/115 (98%)	110 (97%)	3 (3%)	44	65
2	G	113/115 (98%)	112 (99%)	1 (1%)	78	87
2	H	113/115 (98%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	265/267 (99%)	265 (100%)	0	100	100
3	J	266/267 (100%)	262 (98%)	4 (2%)	65	78
3	K	265/267 (99%)	261 (98%)	4 (2%)	65	78
3	L	265/267 (99%)	260 (98%)	5 (2%)	57	73
All	All	2718/2740 (99%)	2684 (99%)	34 (1%)	69	81

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	187	THR
1	A	254	MET
1	A	303	LYS
1	B	81	VAL
1	B	85	CYS
1	B	90	LEU
1	B	252	GLU
1	B	322	PHE
1	C	63	ILE
1	C	90	LEU
1	C	308	LYS
1	C	309	VAL
1	C	310	ILE
1	C	312	GLU
1	D	56	LEU
2	E	39	ARG
2	F	15	LEU
2	F	44	GLU
2	F	108	ARG
2	G	129	THR
3	J	169	LYS
3	J	170	ASP
3	J	326	LEU
3	J	331	ARG
3	K	110	LEU
3	K	170	ASP
3	K	192	ARG
3	K	313	GLU
3	L	3	ASP
3	L	145	GLN
3	L	207	GLU

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Mol	Chain	Res	Type
3	L	313	GLU
3	L	314	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 22 are monoatomic - leaving 17 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	TRS	H	202	-	7,7,7	0.29	0	9,9,9	0.87	1 (11%)
5	TRS	D	403	-	7,7,7	0.46	0	9,9,9	0.50	0
5	TRS	A	403	-	7,7,7	0.63	0	9,9,9	0.54	0
9	GOL	J	403	-	5,5,5	0.40	0	5,5,5	0.23	0
5	TRS	A	402	-	7,7,7	0.47	0	9,9,9	1.02	1 (11%)
9	GOL	I	405	-	5,5,5	0.34	0	5,5,5	0.22	0
5	TRS	G	202	-	7,7,7	0.41	0	9,9,9	0.60	0
5	TRS	B	401	-	7,7,7	0.38	0	9,9,9	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	GOL	I	404	-	5,5,5	0.36	0	5,5,5	0.26	0
5	TRS	C	401	-	7,7,7	0.51	0	9,9,9	0.49	0
9	GOL	D	405	-	5,5,5	0.36	0	5,5,5	0.42	0
5	TRS	B	402	-	7,7,7	0.65	0	9,9,9	1.38	1 (11%)
9	GOL	L	401	-	5,5,5	0.39	0	5,5,5	0.29	0
5	TRS	C	404	-	7,7,7	0.40	0	9,9,9	0.75	0
5	TRS	F	202	-	7,7,7	0.32	0	9,9,9	1.02	1 (11%)
5	TRS	A	404	-	7,7,7	0.54	0	9,9,9	0.43	0
9	GOL	K	402	-	5,5,5	0.39	0	5,5,5	0.24	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	TRS	H	202	-	-	1/9/9/9	-
5	TRS	D	403	-	-	0/9/9/9	-
5	TRS	A	403	-	-	0/9/9/9	-
9	GOL	J	403	-	-	0/4/4/4	-
5	TRS	A	402	-	-	6/9/9/9	-
9	GOL	I	405	-	-	2/4/4/4	-
5	TRS	G	202	-	-	9/9/9/9	-
5	TRS	B	401	-	-	4/9/9/9	-
9	GOL	I	404	-	-	1/4/4/4	-
5	TRS	C	401	-	-	5/9/9/9	-
9	GOL	D	405	-	-	4/4/4/4	-
5	TRS	B	402	-	-	1/9/9/9	-
9	GOL	L	401	-	-	4/4/4/4	-
5	TRS	C	404	-	-	3/9/9/9	-
5	TRS	F	202	-	-	3/9/9/9	-
5	TRS	A	404	-	-	4/9/9/9	-
9	GOL	K	402	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	402	TRS	O1-C1-C	-2.75	102.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	402	TRS	O2-C2-C	-2.66	102.56	111.00
5	H	202	TRS	O1-C1-C	-2.24	103.89	111.00
5	F	202	TRS	O3-C3-C	-2.07	104.43	111.00

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	TRS	C2-C-C1-O1
5	G	202	TRS	N-C-C2-O2
9	I	405	GOL	O2-C2-C3-O3
9	L	401	GOL	O1-C1-C2-C3
5	C	404	TRS	C2-C-C1-O1
9	I	405	GOL	C1-C2-C3-O3
9	D	405	GOL	O1-C1-C2-C3
9	D	405	GOL	C1-C2-C3-O3
9	L	401	GOL	C1-C2-C3-O3
9	K	402	GOL	O1-C1-C2-C3
9	D	405	GOL	O1-C1-C2-O2
9	L	401	GOL	O2-C2-C3-O3
9	K	402	GOL	O1-C1-C2-O2
5	G	202	TRS	C2-C-C1-O1
5	G	202	TRS	C1-C-C2-O2
5	G	202	TRS	C1-C-C3-O3
5	C	404	TRS	C3-C-C1-O1
5	A	402	TRS	C3-C-C1-O1
5	A	402	TRS	C3-C-C2-O2
9	D	405	GOL	O2-C2-C3-O3
5	B	401	TRS	N-C-C1-O1
5	F	202	TRS	N-C-C3-O3
5	G	202	TRS	N-C-C1-O1
5	G	202	TRS	N-C-C3-O3
5	C	404	TRS	N-C-C1-O1
5	A	402	TRS	N-C-C1-O1
5	A	402	TRS	C1-C-C2-O2
5	A	402	TRS	N-C-C2-O2
5	C	401	TRS	N-C-C1-O1
5	C	401	TRS	N-C-C3-O3
5	A	404	TRS	C2-C-C1-O1
9	L	401	GOL	O1-C1-C2-O2
5	B	401	TRS	C3-C-C1-O1
5	B	401	TRS	C1-C-C2-O2

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Mol	Chain	Res	Type	Atoms
5	F	202	TRS	C1-C-C3-O3
5	F	202	TRS	C2-C-C3-O3
5	G	202	TRS	C3-C-C1-O1
5	G	202	TRS	C3-C-C2-O2
5	A	402	TRS	C2-C-C1-O1
5	C	401	TRS	C3-C-C1-O1
5	C	401	TRS	C1-C-C3-O3
5	C	401	TRS	C2-C-C3-O3
5	A	404	TRS	C3-C-C1-O1
5	H	202	TRS	C3-C-C1-O1
5	G	202	TRS	C2-C-C3-O3
5	B	402	TRS	C3-C-C1-O1
5	A	404	TRS	N-C-C1-O1
5	A	404	TRS	C2-C-C3-O3
9	I	404	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	392/392 (100%)	0.11	11 (2%) 53 62	37, 61, 95, 120	0
1	B	392/392 (100%)	-0.30	5 (1%) 77 84	28, 41, 78, 124	0
1	C	389/392 (99%)	0.08	8 (2%) 63 72	38, 58, 90, 125	0
1	D	392/392 (100%)	-0.40	1 (0%) 94 96	24, 39, 67, 117	0
2	E	128/130 (98%)	0.12	2 (1%) 72 79	39, 59, 98, 124	0
2	F	128/130 (98%)	-0.37	1 (0%) 86 90	30, 47, 96, 126	0
2	G	128/130 (98%)	-0.23	3 (2%) 60 69	27, 48, 85, 107	0
2	H	128/130 (98%)	0.56	17 (13%) 3 4	47, 69, 117, 137	0
3	I	347/349 (99%)	-0.51	0 100 100	26, 38, 62, 83	0
3	J	348/349 (99%)	-0.27	0 100 100	37, 53, 75, 106	0
3	K	347/349 (99%)	-0.54	0 100 100	25, 38, 64, 80	0
3	L	347/349 (99%)	-0.12	6 (1%) 70 78	34, 54, 86, 123	0
All	All	3466/3484 (99%)	-0.20	54 (1%) 72 79	24, 49, 86, 137	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	PHE	4.3
2	H	42	GLU	4.1
2	H	43	LEU	4.1
1	C	230	LYS	3.9
2	H	20	CYS	3.7
3	L	229	VAL	3.7
2	H	22	THR	3.4
2	H	23	CYS	3.4
2	E	50	GLY	3.3
3	L	230	LYS	3.3
2	H	37	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	36	ASP	3.1
1	C	224	ALA	3.1
2	H	25	LYS	3.1
2	H	41	GLY	3.1
1	C	233	ILE	3.0
3	L	226	GLY	3.0
2	H	21	LYS	3.0
1	C	228	ALA	2.9
3	L	249	ALA	2.8
1	A	51	ASN	2.8
3	L	287	ALA	2.8
1	C	221	ALA	2.7
2	H	19	ARG	2.7
1	A	190	GLN	2.7
2	E	28	PHE	2.7
1	A	318	ASP	2.7
1	A	185	LYS	2.6
1	B	320	ASP	2.5
2	H	27	TYR	2.5
1	A	53	SER	2.5
2	H	129	THR	2.4
1	A	186	THR	2.4
2	H	40	LYS	2.4
2	H	44	GLU	2.4
1	A	353	LEU	2.4
1	B	183	GLY	2.4
2	H	24	GLY	2.4
1	A	168	VAL	2.4
1	B	119	GLU	2.3
2	G	21	LYS	2.3
1	B	319	TYR	2.3
1	A	58	VAL	2.3
1	A	110	GLY	2.3
1	B	188	LEU	2.2
2	F	129	THR	2.2
1	A	319	TYR	2.2
2	G	129	THR	2.2
3	L	231	ASP	2.1
2	H	46	PHE	2.1
2	G	46	PHE	2.1
1	D	56	LEU	2.0
1	C	53	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	307	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	GOL	I	404	6/6	0.70	0.32	51,54,55,55	0
9	GOL	I	405	6/6	0.74	0.44	57,61,64,66	0
8	MG	D	401	1/1	0.75	0.29	53,53,53,53	0
6	K	C	402	1/1	0.76	0.12	113,113,113,113	0
6	K	K	401	1/1	0.79	0.14	82,82,82,82	0
6	K	A	405	1/1	0.81	0.45	110,110,110,110	0
9	GOL	D	405	6/6	0.81	0.30	51,53,60,60	0
7	CL	E	202	1/1	0.83	0.20	73,73,73,73	0
5	TRS	A	403	8/8	0.85	0.19	40,43,46,47	0
5	TRS	B	401	8/8	0.85	0.17	42,44,50,51	0
9	GOL	L	401	6/6	0.88	0.30	54,59,59,60	0
5	TRS	D	403	8/8	0.89	0.13	34,41,45,47	0
5	TRS	F	202	8/8	0.89	0.19	37,40,47,51	0
5	TRS	B	402	8/8	0.89	0.17	36,42,46,47	0
9	GOL	J	403	6/6	0.89	0.25	47,50,52,52	0
5	TRS	A	404	8/8	0.89	0.24	45,48,51,52	0
9	GOL	K	402	6/6	0.89	0.21	52,54,55,56	0
5	TRS	C	404	8/8	0.90	0.14	36,42,48,48	0
6	K	I	402	1/1	0.91	0.12	92,92,92,92	0
4	NA	A	401	1/1	0.91	0.12	58,58,58,58	0
5	TRS	A	402	8/8	0.91	0.20	31,32,35,36	0
5	TRS	H	202	8/8	0.92	0.16	47,50,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CL	H	203	1/1	0.92	0.12	87,87,87,87	0
4	NA	J	401	1/1	0.92	0.13	58,58,58,58	0
5	TRS	C	401	8/8	0.92	0.21	39,40,45,45	0
6	K	B	403	1/1	0.93	0.21	64,64,64,64	0
5	TRS	G	202	8/8	0.93	0.13	35,39,40,44	0
10	ZN	H	201	1/1	0.94	0.16	108,108,108,108	0
6	K	J	402	1/1	0.94	0.25	60,60,60,60	0
6	K	I	401	1/1	0.94	0.18	55,55,55,55	0
10	ZN	F	201	1/1	0.95	0.04	81,81,81,81	0
6	K	D	404	1/1	0.95	0.15	61,61,61,61	0
7	CL	E	203	1/1	0.96	0.16	30,30,30,30	0
10	ZN	G	201	1/1	0.97	0.05	61,61,61,61	0
10	ZN	E	201	1/1	0.97	0.03	93,93,93,93	0
7	CL	I	403	1/1	0.97	0.11	47,47,47,47	0
7	CL	G	203	1/1	0.98	0.12	33,33,33,33	0
7	CL	C	403	1/1	0.98	0.14	53,53,53,53	0
4	NA	D	402	1/1	0.98	0.10	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.