Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 02:05 PM EDT

PDB ID	:	8EK7
Title	:	Crystal structure of Hepes and Mg bound 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase from Klebsiella aerogenes
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2022-09-20
Resolution	:	1.65 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:

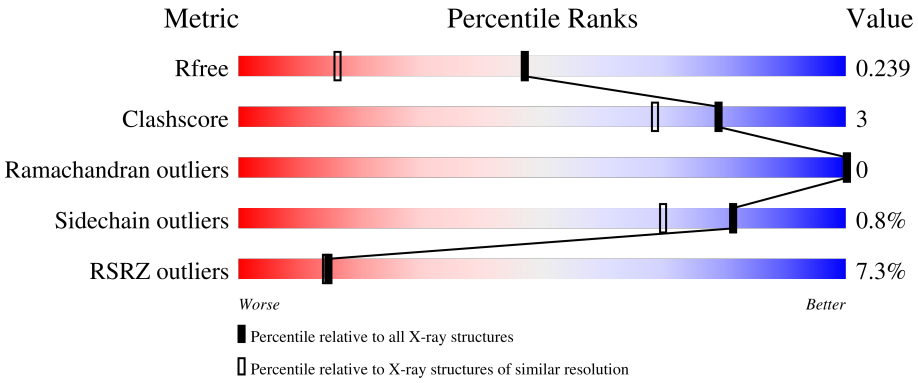
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	253	83% · 14%
1	B	253	13% 79% 6% 14%
1	C	253	81% 5% 13%
1	D	253	11% 82% · 13%
1	E	253	79% 6% 14%

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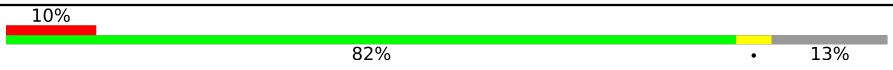
Mol	Chain	Length	Quality of chain
1	F	253	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10637 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	1	0
			1643	1039	286	306	12			
1	B	218	Total	C	N	O	S	0	0	0
			1629	1029	286	303	11			
1	C	219	Total	C	N	O	S	0	1	0
			1654	1046	288	308	12			
1	D	219	Total	C	N	O	S	0	1	0
			1644	1040	287	305	12			
1	E	217	Total	C	N	O	S	0	1	0
			1635	1035	284	304	12			
1	F	220	Total	C	N	O	S	0	1	0
			1652	1046	288	306	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0M3H420
A	2	ALA	-	expression tag	UNP A0A0M3H420
A	3	HIS	-	expression tag	UNP A0A0M3H420
A	4	HIS	-	expression tag	UNP A0A0M3H420
A	5	HIS	-	expression tag	UNP A0A0M3H420
A	6	HIS	-	expression tag	UNP A0A0M3H420
A	7	HIS	-	expression tag	UNP A0A0M3H420
A	8	HIS	-	expression tag	UNP A0A0M3H420
A	42	GLU	ASP	conflict	UNP A0A0M3H420
A	152	MET	THR	conflict	UNP A0A0M3H420
A	182	VAL	ALA	conflict	UNP A0A0M3H420
A	239	VAL	ALA	conflict	UNP A0A0M3H420
A	250	ASN	-	expression tag	UNP A0A0M3H420
A	251	LYS	-	expression tag	UNP A0A0M3H420
A	252	GLY	-	expression tag	UNP A0A0M3H420
A	253	VAL	-	expression tag	UNP A0A0M3H420
B	1	MET	-	initiating methionine	UNP A0A0M3H420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	expression tag	UNP A0A0M3H420
B	3	HIS	-	expression tag	UNP A0A0M3H420
B	4	HIS	-	expression tag	UNP A0A0M3H420
B	5	HIS	-	expression tag	UNP A0A0M3H420
B	6	HIS	-	expression tag	UNP A0A0M3H420
B	7	HIS	-	expression tag	UNP A0A0M3H420
B	8	HIS	-	expression tag	UNP A0A0M3H420
B	42	GLU	ASP	conflict	UNP A0A0M3H420
B	152	MET	THR	conflict	UNP A0A0M3H420
B	182	VAL	ALA	conflict	UNP A0A0M3H420
B	239	VAL	ALA	conflict	UNP A0A0M3H420
B	250	ASN	-	expression tag	UNP A0A0M3H420
B	251	LYS	-	expression tag	UNP A0A0M3H420
B	252	GLY	-	expression tag	UNP A0A0M3H420
B	253	VAL	-	expression tag	UNP A0A0M3H420
C	1	MET	-	initiating methionine	UNP A0A0M3H420
C	2	ALA	-	expression tag	UNP A0A0M3H420
C	3	HIS	-	expression tag	UNP A0A0M3H420
C	4	HIS	-	expression tag	UNP A0A0M3H420
C	5	HIS	-	expression tag	UNP A0A0M3H420
C	6	HIS	-	expression tag	UNP A0A0M3H420
C	7	HIS	-	expression tag	UNP A0A0M3H420
C	8	HIS	-	expression tag	UNP A0A0M3H420
C	42	GLU	ASP	conflict	UNP A0A0M3H420
C	152	MET	THR	conflict	UNP A0A0M3H420
C	182	VAL	ALA	conflict	UNP A0A0M3H420
C	239	VAL	ALA	conflict	UNP A0A0M3H420
C	250	ASN	-	expression tag	UNP A0A0M3H420
C	251	LYS	-	expression tag	UNP A0A0M3H420
C	252	GLY	-	expression tag	UNP A0A0M3H420
C	253	VAL	-	expression tag	UNP A0A0M3H420
D	1	MET	-	initiating methionine	UNP A0A0M3H420
D	2	ALA	-	expression tag	UNP A0A0M3H420
D	3	HIS	-	expression tag	UNP A0A0M3H420
D	4	HIS	-	expression tag	UNP A0A0M3H420
D	5	HIS	-	expression tag	UNP A0A0M3H420
D	6	HIS	-	expression tag	UNP A0A0M3H420
D	7	HIS	-	expression tag	UNP A0A0M3H420
D	8	HIS	-	expression tag	UNP A0A0M3H420
D	42	GLU	ASP	conflict	UNP A0A0M3H420
D	152	MET	THR	conflict	UNP A0A0M3H420
D	182	VAL	ALA	conflict	UNP A0A0M3H420

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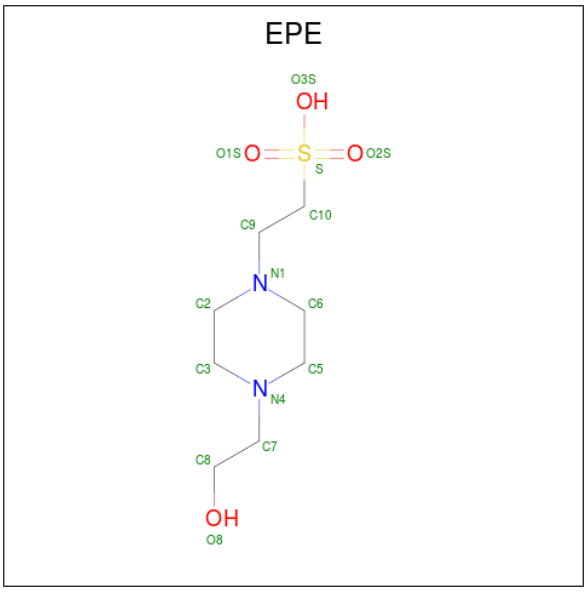
Chain	Residue	Modelled	Actual	Comment	Reference
D	239	VAL	ALA	conflict	UNP A0A0M3H420
D	250	ASN	-	expression tag	UNP A0A0M3H420
D	251	LYS	-	expression tag	UNP A0A0M3H420
D	252	GLY	-	expression tag	UNP A0A0M3H420
D	253	VAL	-	expression tag	UNP A0A0M3H420
E	1	MET	-	initiating methionine	UNP A0A0M3H420
E	2	ALA	-	expression tag	UNP A0A0M3H420
E	3	HIS	-	expression tag	UNP A0A0M3H420
E	4	HIS	-	expression tag	UNP A0A0M3H420
E	5	HIS	-	expression tag	UNP A0A0M3H420
E	6	HIS	-	expression tag	UNP A0A0M3H420
E	7	HIS	-	expression tag	UNP A0A0M3H420
E	8	HIS	-	expression tag	UNP A0A0M3H420
E	42	GLU	ASP	conflict	UNP A0A0M3H420
E	152	MET	THR	conflict	UNP A0A0M3H420
E	182	VAL	ALA	conflict	UNP A0A0M3H420
E	239	VAL	ALA	conflict	UNP A0A0M3H420
E	250	ASN	-	expression tag	UNP A0A0M3H420
E	251	LYS	-	expression tag	UNP A0A0M3H420
E	252	GLY	-	expression tag	UNP A0A0M3H420
E	253	VAL	-	expression tag	UNP A0A0M3H420
F	1	MET	-	initiating methionine	UNP A0A0M3H420
F	2	ALA	-	expression tag	UNP A0A0M3H420
F	3	HIS	-	expression tag	UNP A0A0M3H420
F	4	HIS	-	expression tag	UNP A0A0M3H420
F	5	HIS	-	expression tag	UNP A0A0M3H420
F	6	HIS	-	expression tag	UNP A0A0M3H420
F	7	HIS	-	expression tag	UNP A0A0M3H420
F	8	HIS	-	expression tag	UNP A0A0M3H420
F	42	GLU	ASP	conflict	UNP A0A0M3H420
F	152	MET	THR	conflict	UNP A0A0M3H420
F	182	VAL	ALA	conflict	UNP A0A0M3H420
F	239	VAL	ALA	conflict	UNP A0A0M3H420
F	250	ASN	-	expression tag	UNP A0A0M3H420
F	251	LYS	-	expression tag	UNP A0A0M3H420
F	252	GLY	-	expression tag	UNP A0A0M3H420
F	253	VAL	-	expression tag	UNP A0A0M3H420

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

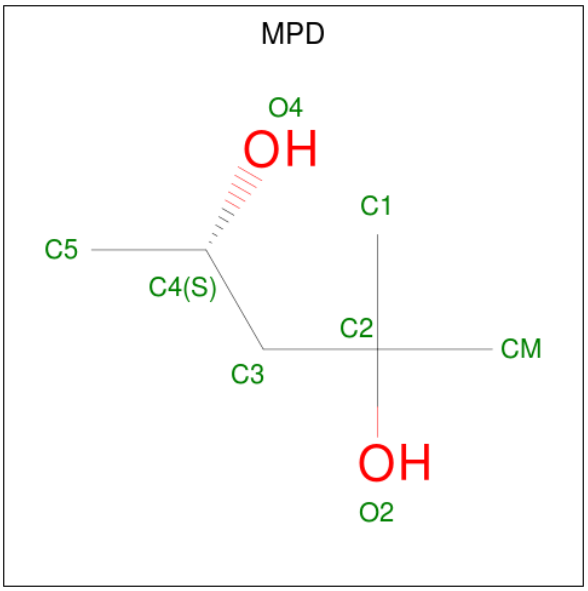


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 15 8 2 4 1	0	0
2	C	1	Total C N O S 15 8 2 4 1	0	0
2	E	1	Total C N O S 15 8 2 4 1	0	0

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

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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	F	1	Total C O 8 6 2	0	0

- Molecule 5 is water.

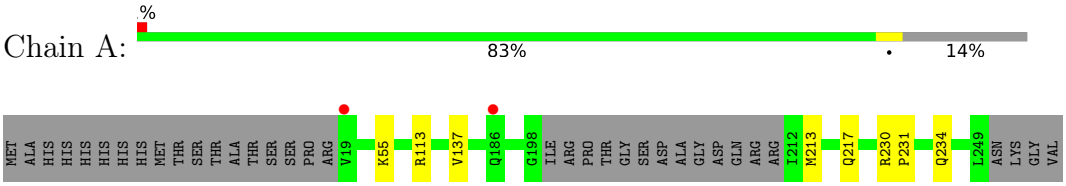
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	118	Total O 118 118	0	0
5	B	97	Total O 97 97	0	0
5	C	158	Total O 158 158	0	0
5	D	93	Total O 93 93	0	0
5	E	131	Total O 131 131	0	0
5	F	88	Total O 88 88	0	0

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.

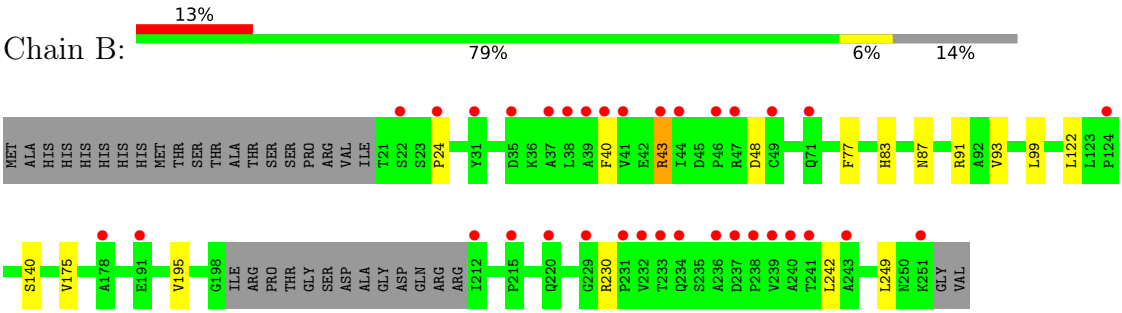
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain A:



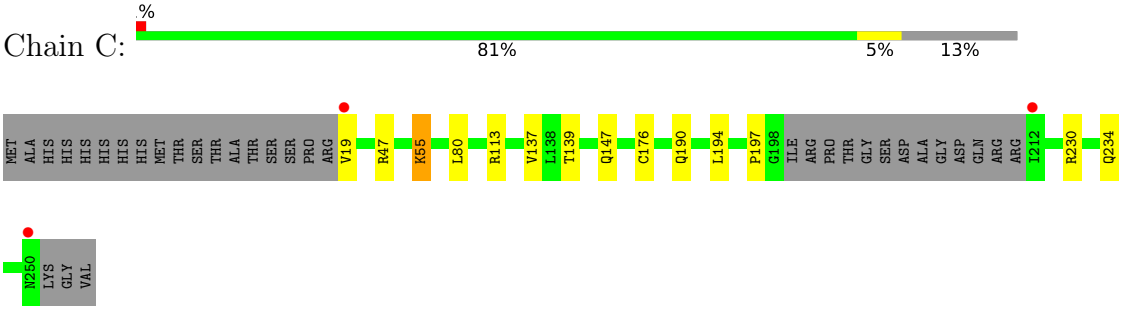
• Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain B:



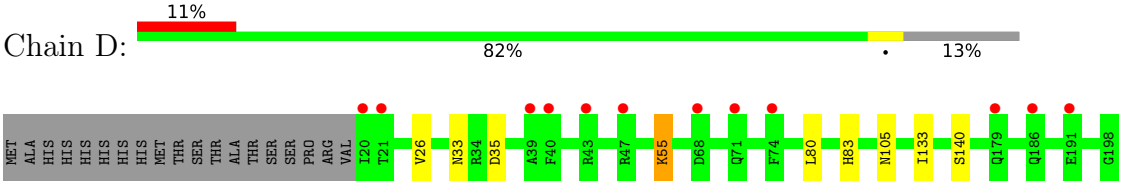
• Molecule 1: Orotidine 5'-phosphate decarboxylase

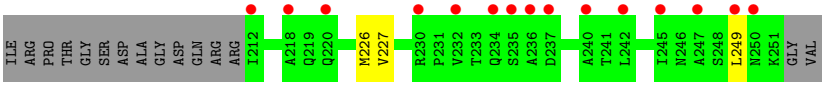
Chain C:



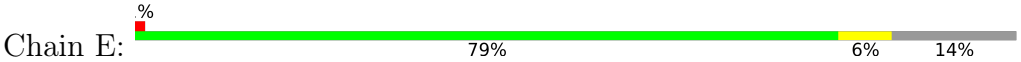
• Molecule 1: Orotidine 5'-phosphate decarboxylase

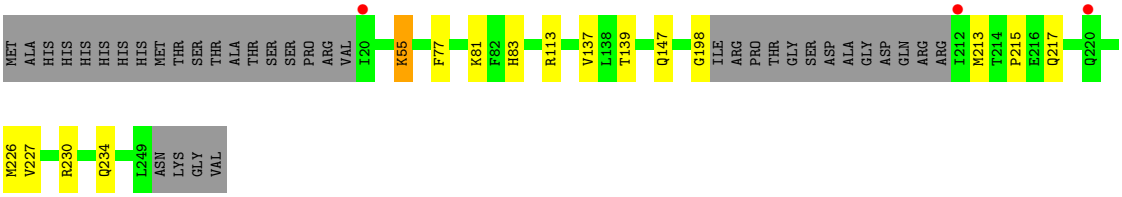
Chain D:



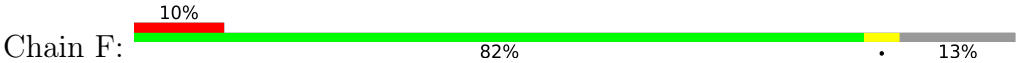


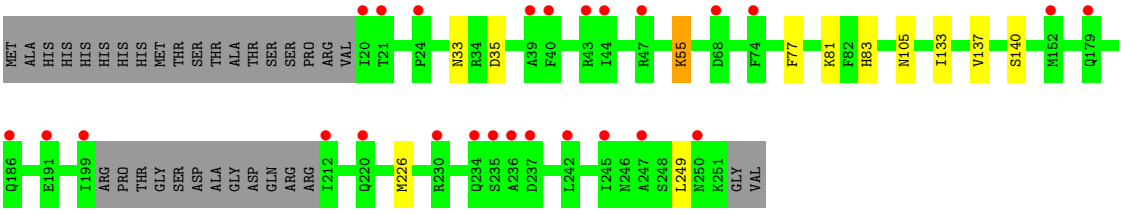
• Molecule 1: Orotidine 5'-phosphate decarboxylase





• Molecule 1: Orotidine 5'-phosphate decarboxylase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.52Å 70.14Å 115.98Å 90.00° 93.34° 90.00°	Depositor
Resolution (Å)	41.69 – 1.65 49.41 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.69-1.65) 99.6 (49.41-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.230 0.219 , 0.239	Depositor DCC
R_{free} test set	8037 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10637	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8608e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, MPD, MLZ, EPE

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	0.46	0/1661	0.65	0/2252
1	B	0.44	0/1645	0.63	0/2232
1	C	0.48	0/1672	0.65	0/2267
1	D	0.41	0/1662	0.64	0/2254
1	E	0.47	0/1653	0.66	0/2241
1	F	0.43	0/1670	0.64	0/2265
All	All	0.45	0/9963	0.64	0/13511

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1643	0	1671	7	0
1	B	1629	0	1642	10	0
1	C	1654	0	1686	9	0
1	D	1644	0	1669	8	0
1	E	1635	0	1665	14	0
1	F	1652	0	1680	12	0
2	A	15	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	17	0	0
2	E	15	0	17	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
4	A	8	0	14	3	0
4	B	8	0	14	0	0
4	C	8	0	14	3	0
4	E	8	0	14	3	0
4	F	8	0	14	2	0
5	A	118	0	0	0	0
5	B	97	0	0	2	0
5	C	158	0	0	1	0
5	D	93	0	0	0	0
5	E	131	0	0	1	0
5	F	88	0	0	0	0
All	All	10637	0	10134	56	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 (56) 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:D:226:MET:HE1	1:D:249:LEU:HD11	1.68	0.75
1:E:113:ARG:NH2	1:F:140:SER:O	2.20	0.75
1:B:87:ASN:OD1	1:B:91:ARG:NH1	2.23	0.72
1:F:226:MET:HE1	1:F:249:LEU:HD11	1.74	0.68
1:E:230:ARG:NH1	1:E:234:GLN:OE1	2.28	0.67
1:F:137:VAL:O	4:F:301:MPD:HM3	1.95	0.66
4:E:305:MPD:HM1	4:E:305:MPD:H52	1.77	0.65
1:E:147:GLN:NE2	5:E:402:HOH:O	2.27	0.63
1:C:230:ARG:NH1	1:C:234:GLN:OE1	2.31	0.63
4:C:305:MPD:HM1	4:C:305:MPD:H52	1.81	0.61
1:C:113:ARG:NH2	1:D:140:SER:O	2.36	0.59
1:E:55:MLZ:HCM1	1:F:55:MLZ:HCM1	1.84	0.58
4:A:305:MPD:HM1	4:A:305:MPD:H52	1.87	0.56
1:C:147:GLN:NE2	5:C:403:HOH:O	2.32	0.55
1:E:55:MLZ:HCM2	1:F:83:HIS:H	1.70	0.55
1:B:24:PRO:HG2	1:B:249:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:O	4:A:305:MPD:HM3	2.09	0.53
4:C:305:MPD:HM1	4:C:305:MPD:C5	2.38	0.53
1:E:55:MLZ:HCM2	1:F:83:HIS:N	2.23	0.53
1:B:93:VAL:HG12	1:B:122:LEU:HD21	1.91	0.53
1:E:55:MLZ:HCM3	1:E:81:LYS:O	2.09	0.52
4:A:305:MPD:HM1	4:A:305:MPD:C5	2.40	0.51
1:E:215:PRO:HB3	1:E:226:MET:HE1	1.92	0.51
1:A:113:ARG:NH2	1:B:140:SER:O	2.44	0.51
4:E:305:MPD:HM1	4:E:305:MPD:C5	2.42	0.50
1:E:83:HIS:H	1:F:55:MLZ:HCM2	1.77	0.49
1:B:48:ASP:HB3	1:B:242:LEU:HD23	1.94	0.48
1:E:137:VAL:O	4:E:305:MPD:HM3	2.14	0.48
1:C:55:MLZ:CM	1:D:83:HIS:H	2.27	0.47
4:F:301:MPD:HM1	4:F:301:MPD:H52	1.97	0.46
1:A:230:ARG:NH1	1:A:234:GLN:OE1	2.48	0.46
1:B:40:PHE:HA	1:B:43:ARG:HD2	1.98	0.45
1:A:55:MLZ:HE3	5:B:438:HOH:O	2.16	0.45
1:C:137:VAL:O	4:C:305:MPD:HM3	2.17	0.45
1:F:55:MLZ:HCM3	1:F:81:LYS:O	2.16	0.45
1:E:83:HIS:N	1:F:55:MLZ:HCM2	2.32	0.45
1:C:176[A]:CYS:SG	1:C:194:LEU:HB3	2.58	0.44
1:B:48:ASP:CB	1:B:242:LEU:HD23	2.47	0.44
1:D:226:MET:HE1	1:D:249:LEU:CD1	2.43	0.44
1:A:213:MET:HG2	1:A:217:GLN:HB2	2.00	0.44
1:E:213:MET:HG2	1:E:217:GLN:HB2	2.00	0.44
1:B:91:ARG:NH2	5:B:401:HOH:O	2.25	0.43
1:C:19:VAL:HG11	1:C:47:ARG:CG	2.48	0.43
1:C:139:THR:CG2	1:C:197:PRO:HG3	2.48	0.43
1:F:105:ASN:HA	1:F:133:ILE:O	2.18	0.43
1:A:55:MLZ:CM	1:B:83:HIS:H	2.31	0.43
1:E:55:MLZ:CM	1:F:83:HIS:H	2.32	0.43
1:E:198:GLY:HA2	1:E:227:VAL:O	2.19	0.43
1:C:55:MLZ:HE2	1:C:80:LEU:O	2.18	0.42
1:D:105:ASN:HA	1:D:133:ILE:O	2.19	0.42
1:A:230:ARG:N	1:A:231:PRO:CD	2.83	0.42
1:D:26:VAL:O	1:D:227:VAL:HA	2.20	0.41
1:B:175:VAL:HA	1:B:195:VAL:O	2.20	0.41
1:D:55:MLZ:HCM3	1:D:80:LEU:O	2.21	0.41
1:F:33:ASN:OD1	1:F:35:ASP:N	2.54	0.41
1:D:33:ASN:OD1	1:D:35:ASP:N	2.54	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	214/253 (85%)	210 (98%)	4 (2%)	0	100	100
1	B	213/253 (84%)	209 (98%)	4 (2%)	0	100	100
1	C	215/253 (85%)	211 (98%)	4 (2%)	0	100	100
1	D	215/253 (85%)	209 (97%)	6 (3%)	0	100	100
1	E	213/253 (84%)	208 (98%)	5 (2%)	0	100	100
1	F	216/253 (85%)	211 (98%)	5 (2%)	0	100	100
All	All	1286/1518 (85%)	1258 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	173/202 (86%)	173 (100%)	0	100	100
1	B	169/202 (84%)	165 (98%)	4 (2%)	49	23
1	C	175/202 (87%)	174 (99%)	1 (1%)	86	76
1	D	172/202 (85%)	172 (100%)	0	100	100
1	E	172/202 (85%)	170 (99%)	2 (1%)	71	53
1	F	173/202 (86%)	172 (99%)	1 (1%)	86	76
All	All	1034/1212 (85%)	1026 (99%)	8 (1%)	81	70

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	43	ARG
1	B	77	PHE
1	B	99	LEU
1	B	230	ARG
1	C	190	GLN
1	E	77	PHE
1	E	139	THR
1	F	77	PHE

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

Mol	Chain	Res	Type
1	A	179	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MLZ	A	55	1	8,9,10	0.73	0	4,9,11	0.98	0
1	MLZ	D	55	1	8,9,10	0.79	0	4,9,11	1.92	1 (25%)
1	MLZ	E	55	1	8,9,10	0.95	0	4,9,11	1.92	1 (25%)
1	MLZ	C	55	1	8,9,10	0.70	0	4,9,11	1.33	1 (25%)
1	MLZ	B	55	1	7,8,10	0.68	0	3,8,11	0.22	0
1	MLZ	F	55	1	8,9,10	0.73	0	4,9,11	1.40	1 (25%)

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
1	MLZ	A	55	1	-	2/7/8/10	-
1	MLZ	D	55	1	-	4/7/8/10	-
1	MLZ	E	55	1	-	1/7/8/10	-
1	MLZ	C	55	1	-	1/7/8/10	-
1	MLZ	B	55	1	-	2/6/7/10	-
1	MLZ	F	55	1	-	1/7/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	55	MLZ	CM-NZ-CE	3.76	122.81	111.95
1	E	55	MLZ	CM-NZ-CE	3.68	122.57	111.95
1	F	55	MLZ	CM-NZ-CE	2.56	119.36	111.95
1	C	55	MLZ	CG-CD-CE	-2.06	103.79	113.56

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	55	MLZ	C-CA-CB-CG
1	D	55	MLZ	O-C-CA-CB
1	A	55	MLZ	CG-CD-CE-NZ
1	D	55	MLZ	CG-CD-CE-NZ
1	F	55	MLZ	CG-CD-CE-NZ
1	B	55	MLZ	CA-CB-CG-CD
1	E	55	MLZ	CG-CD-CE-NZ
1	B	55	MLZ	N-CA-CB-CG
1	A	55	MLZ	CE-CD-CG-CB
1	C	55	MLZ	CD-CE-NZ-CM
1	D	55	MLZ	CE-CD-CG-CB

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	55	MLZ	2	0
1	D	55	MLZ	1	0
1	E	55	MLZ	5	0
1	C	55	MLZ	2	0
1	F	55	MLZ	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	MPD	A	305	-	7,7,7	0.33	0	9,10,10	0.75	0
4	MPD	E	305	-	7,7,7	0.37	0	9,10,10	0.62	0
4	MPD	B	302	-	7,7,7	0.34	0	9,10,10	0.68	0
4	MPD	C	305	-	7,7,7	0.41	0	9,10,10	0.73	0
4	MPD	F	301	-	7,7,7	0.31	0	9,10,10	0.47	0
2	EPE	C	301	-	15,15,15	0.70	0	18,20,20	1.73	4 (22%)
2	EPE	A	301	-	15,15,15	0.76	1 (6%)	18,20,20	1.72	4 (22%)
2	EPE	E	301	-	15,15,15	0.89	1 (6%)	18,20,20	1.40	4 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	A	305	-	-	2/5/5/5	-
4	MPD	E	305	-	-	1/5/5/5	-
4	MPD	B	302	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	C	305	-	-	1/5/5/5	-
4	MPD	F	301	-	-	2/5/5/5	-
2	EPE	C	301	-	-	1/9/19/19	0/1/1/1
2	EPE	A	301	-	-	4/9/19/19	0/1/1/1
2	EPE	E	301	-	-	1/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	EPE	C10-S	2.98	1.81	1.77
2	A	301	EPE	C10-S	2.44	1.81	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	EPE	O2S-S-C10	4.05	111.79	106.92
2	C	301	EPE	O1S-S-C10	3.95	111.67	106.92
2	A	301	EPE	C5-N4-C3	3.51	116.74	108.83
2	C	301	EPE	C5-N4-C3	3.39	116.47	108.83
2	E	301	EPE	C5-N4-C3	3.13	115.88	108.83
2	E	301	EPE	O2S-S-C10	2.93	110.45	106.92
2	C	301	EPE	C7-N4-C5	2.92	118.69	111.23
2	C	301	EPE	C9-N1-C6	-2.33	105.28	111.23
2	A	301	EPE	C7-N4-C5	2.22	116.90	111.23
2	E	301	EPE	O3S-S-C10	2.14	109.22	105.77
2	E	301	EPE	C9-N1-C2	-2.04	106.02	111.23
2	A	301	EPE	O3S-S-C10	2.04	109.06	105.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	EPE	C8-C7-N4-C5
2	C	301	EPE	C8-C7-N4-C5
2	E	301	EPE	C8-C7-N4-C3
4	A	305	MPD	C2-C3-C4-O4
2	A	301	EPE	C10-C9-N1-C2
4	A	305	MPD	C2-C3-C4-C5
4	F	301	MPD	O2-C2-C3-C4
4	C	305	MPD	C2-C3-C4-C5
4	E	305	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	F	301	MPD	C2-C3-C4-C5
2	A	301	EPE	C9-C10-S-O1S
2	A	301	EPE	C10-C9-N1-C6

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	MPD	3	0
4	E	305	MPD	3	0
4	C	305	MPD	3	0
4	F	301	MPD	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	217/253 (85%)	0.17	2 (0%) 84 86	14, 22, 40, 53	0
1	B	217/253 (85%)	1.04	34 (15%) 2 1	14, 25, 46, 53	0
1	C	218/253 (86%)	0.16	3 (1%) 75 79	12, 20, 34, 53	0
1	D	218/253 (86%)	0.76	27 (12%) 4 3	15, 29, 48, 59	0
1	E	216/253 (85%)	0.13	3 (1%) 75 79	12, 20, 38, 56	0
1	F	219/253 (86%)	0.64	26 (11%) 4 3	14, 28, 45, 52	0
All	All	1305/1518 (85%)	0.48	95 (7%) 15 14	12, 24, 44, 59	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	VAL	8.1
1	B	236	ALA	6.1
1	B	240	ALA	6.0
1	B	39	ALA	5.7
1	A	19	VAL	5.3
1	B	31	TYR	5.3
1	D	242	LEU	5.1
1	B	41	VAL	5.0
1	F	199	ILE	5.0
1	F	242	LEU	4.9
1	B	46	PRO	4.8
1	C	19	VAL	4.8
1	F	39	ALA	4.4
1	D	186	GLN	4.4
1	B	38	LEU	4.2
1	B	212	ILE	4.1
1	B	231	PRO	4.1
1	D	43	ARG	3.9
1	D	235	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	39	ALA	3.8
1	D	245	ILE	3.7
1	B	178	ALA	3.7
1	C	212	ILE	3.6
1	B	239	VAL	3.6
1	B	237	ASP	3.6
1	D	236	ALA	3.6
1	B	35	ASP	3.6
1	B	215	PRO	3.5
1	B	40	PHE	3.5
1	D	40	PHE	3.5
1	D	220	GLN	3.4
1	C	250	ASN	3.3
1	F	245	ILE	3.3
1	D	230	ARG	3.2
1	F	235	SER	3.2
1	B	44	ILE	3.2
1	F	24	PRO	3.2
1	D	68	ASP	3.2
1	B	191	GLU	3.2
1	E	212	ILE	3.1
1	B	229	GLY	3.0
1	F	236	ALA	3.0
1	F	186	GLN	2.9
1	D	21	THR	2.9
1	F	212	ILE	2.9
1	F	21	THR	2.9
1	D	212	ILE	2.8
1	F	43	ARG	2.8
1	B	43	ARG	2.8
1	F	250	ASN	2.8
1	F	191	GLU	2.7
1	B	251	LYS	2.7
1	B	24	PRO	2.7
1	B	243	ALA	2.7
1	F	247	ALA	2.6
1	F	220	GLN	2.6
1	D	250	ASN	2.6
1	D	20	ILE	2.6
1	D	47	ARG	2.6
1	B	71	GLN	2.6
1	B	22	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	237	ASP	2.5
1	B	37	ALA	2.5
1	D	234	GLN	2.5
1	B	124	PRO	2.5
1	A	186	GLN	2.5
1	F	20	ILE	2.5
1	F	237	ASP	2.5
1	D	232	VAL	2.5
1	B	233	THR	2.4
1	D	71	GLN	2.4
1	D	218	ALA	2.4
1	B	49	CYS	2.4
1	F	68	ASP	2.4
1	D	191	GLU	2.4
1	B	238	PRO	2.3
1	F	74	PHE	2.3
1	D	247	ALA	2.3
1	F	152	MET	2.3
1	E	220	GLN	2.2
1	D	249	LEU	2.2
1	F	44	ILE	2.2
1	F	40	PHE	2.2
1	B	234	GLN	2.2
1	E	20	ILE	2.2
1	F	234	GLN	2.2
1	D	240	ALA	2.2
1	B	220	GLN	2.1
1	D	179	GLN	2.1
1	B	47	ARG	2.1
1	F	47	ARG	2.1
1	F	179	GLN	2.1
1	F	230	ARG	2.1
1	D	74	PHE	2.0
1	B	241	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	MLZ	B	55	9/11	0.84	0.16	24,28,42,42	0
1	MLZ	D	55	10/11	0.84	0.14	23,28,35,36	0
1	MLZ	F	55	10/11	0.89	0.14	20,24,33,36	0
1	MLZ	A	55	10/11	0.90	0.14	17,23,29,30	0
1	MLZ	E	55	10/11	0.93	0.10	16,23,31,31	0
1	MLZ	C	55	10/11	0.93	0.12	17,24,31,32	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
4	MPD	F	301	8/8	0.80	0.26	58,58,59,59	0
4	MPD	B	302	8/8	0.82	0.20	34,39,42,43	0
3	MG	C	304	1/1	0.84	0.09	35,35,35,35	0
3	MG	A	304	1/1	0.85	0.14	54,54,54,54	0
3	MG	A	303	1/1	0.88	0.07	32,32,32,32	0
3	MG	E	303	1/1	0.90	0.10	36,36,36,36	0
4	MPD	A	305	8/8	0.91	0.09	33,34,36,37	0
4	MPD	C	305	8/8	0.92	0.12	31,31,32,33	0
4	MPD	E	305	8/8	0.93	0.11	33,35,35,36	0
3	MG	C	303	1/1	0.93	0.10	43,43,43,43	0
2	EPE	C	301	15/15	0.94	0.11	27,29,33,34	0
2	EPE	E	301	15/15	0.94	0.09	27,29,34,36	0
2	EPE	A	301	15/15	0.95	0.09	33,33,37,37	0
3	MG	B	301	1/1	0.95	0.29	34,34,34,34	0
3	MG	A	302	1/1	0.96	0.06	25,25,25,25	0
3	MG	E	302	1/1	0.96	0.07	22,22,22,22	0
3	MG	E	304	1/1	0.98	0.15	30,30,30,30	0
3	MG	C	302	1/1	0.98	0.06	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.