



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:28 PM UTC

PDB ID : 2VLB / pdb_00002vlb
Title : Structure of unliganded arylmalonate decarboxylase
Authors : Kuettner, E.B.; Keim, A.; Kircher, M.; Rosmus, S.; Strater, N.
Deposited on : 2008-01-11
Resolution : 1.92 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

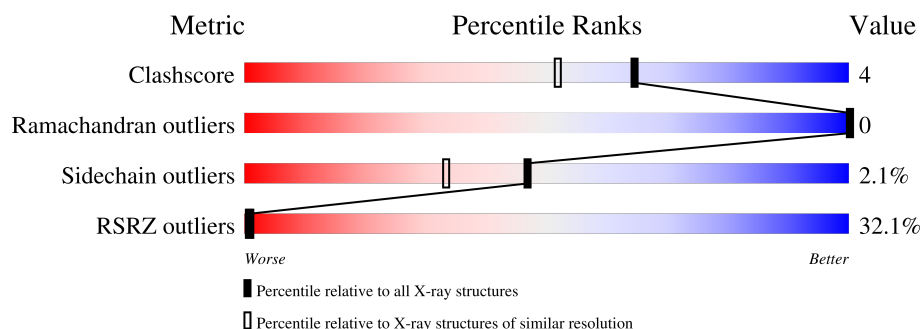
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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))
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	251	16% 88% 5% 6%
1	B	251	45% 72% 13% 14%
1	C	251	28% 85% 9% 6%
1	D	251	27% 82% 9% 8%

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
2	BME	D	1242	-	-	X	-

2 Entry composition [i](#)

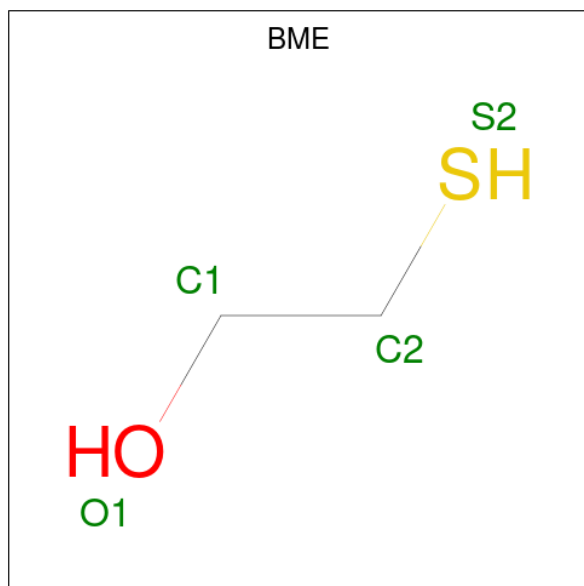
There are 5 unique types of molecules in this entry. The entry contains 7221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ARYLMALONATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	6	0
			1716	1076	302	329	9			
1	B	217	Total	C	N	O	S	0	3	0
			1586	999	281	298	8			
1	C	236	Total	C	N	O	S	0	1	0
			1706	1073	300	324	9			
1	D	230	Total	C	N	O	S	0	3	0
			1680	1055	300	316	9			

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



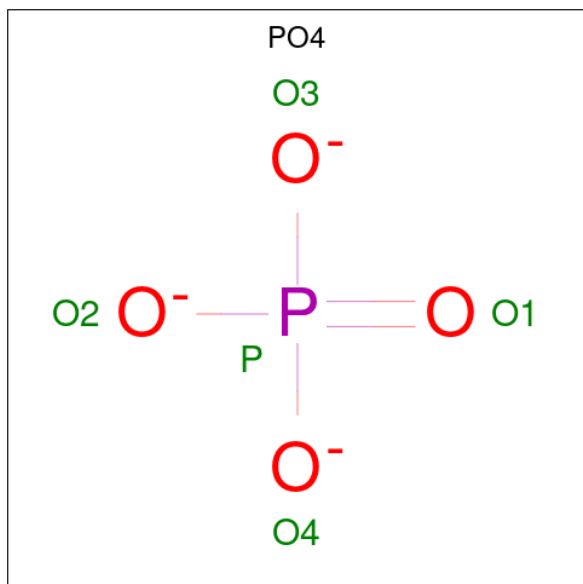
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	1
			8	4	2	2		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	151	Total	O	0	0
			151	151		
5	B	59	Total	O	0	0
			59	59		
5	C	101	Total	O	0	0
			101	101		

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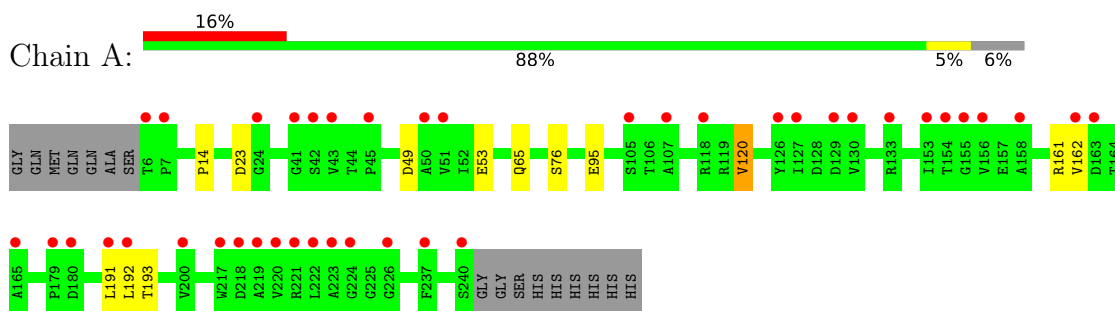
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	135	Total 135	O 135	0	0

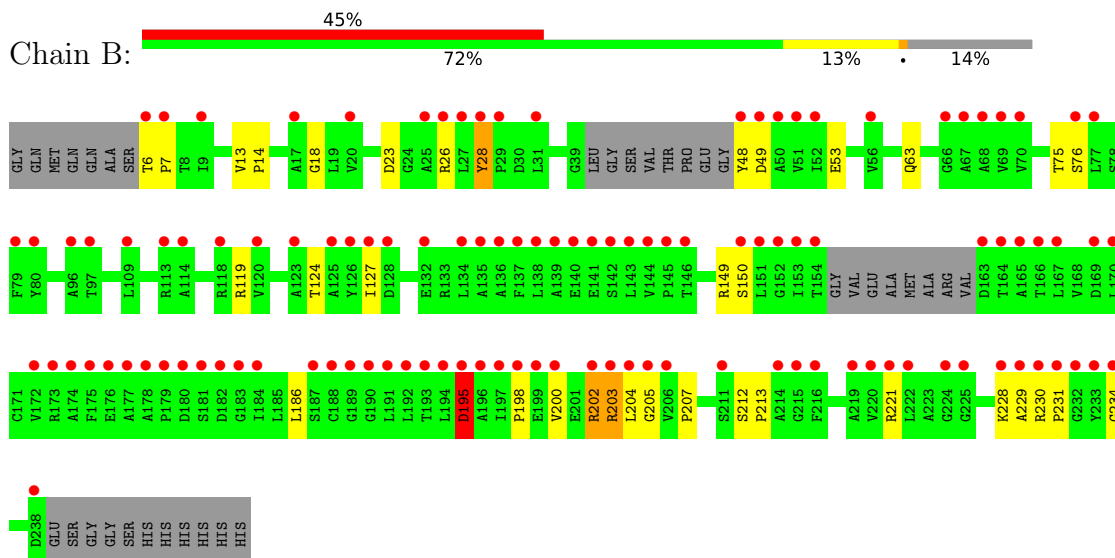
3 Residue-property plots

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.

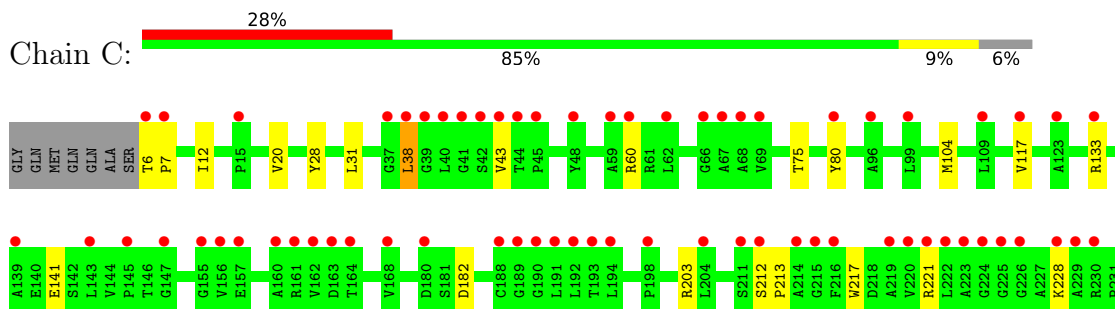
• Molecule 1: ARYLMALONATE DECARBOXYLASE

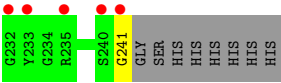


• Molecule 1: ARYLMALONATE DECARBOXYLASE

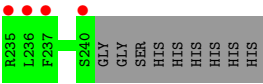
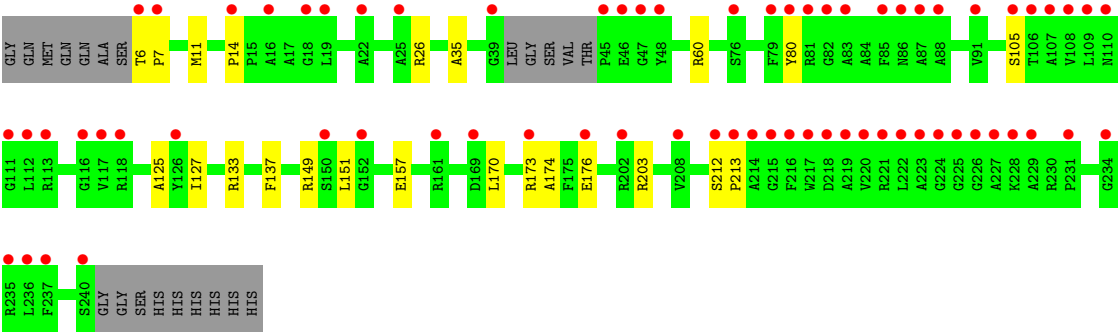
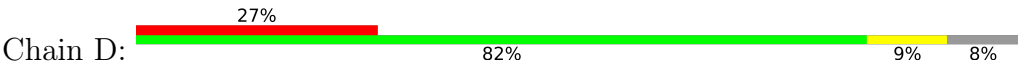


• Molecule 1: ARYLMALONATE DECARBOXYLASE





● Molecule 1: ARYLMALONATE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.21Å 100.99Å 139.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 1.92 29.64 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.64-1.92) 98.8 (29.64-1.92)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.207 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7221	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BME, PO4, 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	1/1778 (0.1%)	0.87	2/2422 (0.1%)
1	B	1.78	22/1628 (1.4%)	1.10	9/2215 (0.4%)
1	C	0.75	1/1739 (0.1%)	0.89	0/2369
1	D	0.85	0/1724	0.89	1/2344 (0.0%)
All	All	1.11	24/6869 (0.3%)	0.94	12/9350 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	VAL	C-O	29.54	1.56	1.24
1	B	195	ASP	CB-CG	22.58	2.08	1.52
1	B	204	LEU	C-N	20.86	1.62	1.33
1	B	195	ASP	CG-OD2	16.65	1.56	1.25
1	B	204	LEU	C-O	16.39	1.47	1.23
1	B	231	PRO	C-N	15.38	1.55	1.33
1	B	119	ARG	CZ-NH1	13.85	1.52	1.32
1	B	200	VAL	C-N	12.16	1.49	1.33
1	B	234	GLY	C-O	11.91	1.34	1.23
1	B	202	ARG	CZ-NH1	10.87	1.48	1.32
1	B	202	ARG	CD-NE	10.32	1.60	1.46
1	B	202	ARG	CZ-NH2	10.29	1.46	1.33
1	B	230	ARG	C-O	-9.13	1.12	1.23
1	B	228	LYS	C-O	7.75	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	TYR	CG-CD1	6.83	1.53	1.39
1	B	205	GLY	N-CA	6.62	1.55	1.45
1	B	228	LYS	C-N	6.34	1.41	1.33
1	B	207	PRO	C-N	6.27	1.41	1.33
1	B	28	TYR	CG-CD2	6.18	1.52	1.39
1	B	28	TYR	CE2-CZ	6.17	1.53	1.38
1	B	119	ARG	CZ-NH2	6.15	1.41	1.33
1	B	195	ASP	CG-OD1	5.52	1.35	1.25
1	C	20	VAL	CA-CB	5.44	1.57	1.54
1	A	14	PRO	CA-C	5.27	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ASP	CB-CG-OD2	-10.60	94.03	118.40
1	B	195	ASP	CA-CB-CG	-9.40	103.20	112.60
1	B	204	LEU	CA-C-N	-7.43	106.89	121.53
1	B	204	LEU	C-N-CA	-7.43	106.89	121.53
1	B	14	PRO	N-CA-C	6.73	118.91	110.70
1	B	200	VAL	O-C-N	6.42	128.55	121.94
1	A	14	PRO	N-CA-C	6.18	118.24	110.70
1	B	195	ASP	OD1-CG-OD2	5.91	137.08	122.90
1	B	119	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	B	204	LEU	O-C-N	5.64	129.01	122.25
1	D	14	PRO	N-CA-C	5.62	117.56	110.70
1	A	120	VAL	CB-CA-C	-5.08	103.12	110.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	195	ASP	Sidechain

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	1716	0	1737	10	0
1	B	1586	0	1607	15	0
1	C	1706	0	1732	14	0
1	D	1680	0	1704	16	0
2	A	12	0	15	0	0
2	B	8	0	10	0	0
2	C	8	0	10	0	0
2	D	8	0	10	4	0
3	A	5	0	0	1	0
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	8	0	12	3	0
5	A	151	0	0	1	0
5	B	59	0	0	2	0
5	C	101	0	0	4	0
5	D	135	0	0	2	0
All	All	7221	0	6849	53	0

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

All (53) 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:195:ASP:CB	1:B:195:ASP:CG	2.08	1.26
1:D:151:LEU:HD12	2:D:1242:BME:H11	1.37	1.05
1:D:127:ILE:HB	4:D:1244:EDO:H21	1.43	0.97
1:D:176:GLU:HG3	5:D:2091:HOH:O	1.71	0.87
1:D:125:ALA:HB2	2:D:1242:BME:H12	1.69	0.73
1:D:173:ARG:HD2	4:D:1243:EDO:H12	1.71	0.70
1:A:161:ARG:HE	1:A:192:LEU:HD12	1.55	0.70
1:D:151:LEU:CD1	2:D:1242:BME:H11	2.20	0.68
1:A:161:ARG:NH1	1:A:162:VAL:O	2.32	0.61
1:A:23:ASP:HB2	1:A:191:LEU:O	2.03	0.58
1:B:212:SER:HB3	1:B:213:PRO:HD3	1.87	0.57
1:D:212:SER:HB3	1:D:213:PRO:HD3	1.85	0.57
1:D:149[B]:ARG:HD3	1:D:174:ALA:HA	1.89	0.55
1:B:6:THR:N	1:B:7:PRO:CD	2.70	0.55
1:A:65:GLN:NE2	3:A:1243:PO4:O2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TYR:OH	1:C:141:GLU:OE2	2.24	0.54
1:A:49:ASP:O	1:A:53:GLU:HG2	2.07	0.54
1:D:170:LEU:HA	4:D:1243:EDO:H11	1.90	0.52
1:B:6:THR:N	1:B:7:PRO:HD3	2.25	0.51
1:A:161:ARG:NE	1:A:192:LEU:HD12	2.25	0.51
1:C:104:MET:HE2	5:C:2029:HOH:O	2.10	0.51
1:C:7:PRO:HD2	1:C:31:LEU:HD22	1.93	0.51
1:C:217:TRP:CE2	1:C:221:ARG:HD2	2.47	0.50
1:B:49:ASP:O	1:B:53:GLU:HG2	2.13	0.49
1:A:161:ARG:HD2	5:A:2109:HOH:O	2.12	0.49
1:C:80:TYR:CE1	1:C:133:ARG:HD3	2.48	0.48
1:C:75:THR:HG22	5:C:2026:HOH:O	2.14	0.47
1:D:125:ALA:CB	2:D:1242:BME:H12	2.41	0.46
1:A:95:GLU:OE1	1:D:60[B]:ARG:NH2	2.49	0.46
1:B:28:TYR:CE1	1:B:229:ALA:HA	2.50	0.46
1:C:12:ILE:CG2	1:C:38:LEU:HD13	2.46	0.45
1:D:203:ARG:HD2	5:D:2102:HOH:O	2.16	0.45
1:B:76:SER:HB3	5:B:2058:HOH:O	2.16	0.45
1:C:228:LYS:HB2	1:C:241:GLY:HA3	1.99	0.45
5:B:2033:HOH:O	1:C:60:ARG:HD3	2.16	0.44
1:C:203[B]:ARG:NH2	5:C:2084:HOH:O	2.35	0.44
1:C:212:SER:HB2	1:C:213:PRO:CD	2.48	0.44
1:D:80:TYR:CE1	1:D:133:ARG:HG3	2.53	0.44
1:C:117:VAL:HG13	1:C:182:ASP:HB2	2.01	0.43
1:B:195:ASP:CG	1:B:195:ASP:CA	2.86	0.43
1:C:28:TYR:HB3	1:C:31:LEU:HG	2.01	0.42
1:B:203:ARG:HG2	1:B:203:ARG:NH1	2.35	0.42
1:B:198:PRO:O	1:B:202:ARG:HB2	2.20	0.41
1:D:6:THR:HA	1:D:7:PRO:HD3	1.87	0.41
1:A:23:ASP:CG	1:A:193:THR:H	2.28	0.41
1:B:13:VAL:CG2	1:B:18:GLY:HA2	2.51	0.41
1:C:104:MET:CE	5:C:2029:HOH:O	2.68	0.41
1:B:28:TYR:CE1	1:B:229:ALA:CA	3.04	0.41
1:D:105:SER:HB2	1:D:137:PHE:CZ	2.56	0.41
1:D:11:MET:O	1:D:35:ALA:HA	2.21	0.41
1:B:124:THR:O	1:B:150:SER:HA	2.21	0.40
1:B:75:THR:OG1	3:B:1243:PO4:O1	2.27	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	240/251 (96%)	235 (98%)	5 (2%)	0	100	100
1	B	214/251 (85%)	211 (99%)	3 (1%)	0	100	100
1	C	235/251 (94%)	231 (98%)	4 (2%)	0	100	100
1	D	229/251 (91%)	226 (99%)	3 (1%)	0	100	100
All	All	918/1004 (91%)	903 (98%)	15 (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	181/186 (97%)	180 (99%)	1 (1%)	78	75
1	B	164/186 (88%)	155 (94%)	9 (6%)	19	6
1	C	175/186 (94%)	172 (98%)	3 (2%)	53	41
1	D	173/186 (93%)	171 (99%)	2 (1%)	63	57
All	All	693/744 (93%)	678 (98%)	15 (2%)	47	32

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	VAL
1	B	23[A]	ASP

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Mol	Chain	Res	Type
1	B	23[B]	ASP
1	B	26	ARG
1	B	63	GLN
1	B	127	ILE
1	B	149	ARG
1	B	186	LEU
1	B	203	ARG
1	B	221	ARG
1	C	6	THR
1	C	38	LEU
1	C	43	VAL
1	D	26	ARG
1	D	157	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	63	GLN
1	C	58	HIS
1	C	63	GLN
1	C	65	GLN
1	D	131	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands 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
2	BME	D	1242	1	3,3,3	0.40	0	2,2,2	0.31	0
2	BME	C	1242	1	3,3,3	0.24	0	2,2,2	0.41	0
3	PO4	A	1243	-	4,4,4	0.88	0	6,6,6	0.88	0
2	BME	B	1239	1	3,3,3	0.36	0	2,2,2	0.31	0
4	EDO	C	1244	-	3,3,3	0.61	0	2,2,2	0.09	0
3	PO4	D	1245	-	4,4,4	1.16	0	6,6,6	0.88	0
3	PO4	B	1242	-	4,4,4	0.90	0	6,6,6	0.64	0
3	PO4	D	1246	-	4,4,4	1.10	1 (25%)	6,6,6	0.92	0
3	PO4	C	1245	-	4,4,4	0.98	0	6,6,6	0.74	0
4	EDO	B	1241	-	3,3,3	0.47	0	2,2,2	0.20	0
2	BME	A	1241[B]	1	3,3,3	0.25	0	2,2,2	0.38	0
4	EDO	D	1244	-	3,3,3	0.62	0	2,2,2	0.40	0
3	PO4	C	1246	-	4,4,4	0.82	0	6,6,6	0.46	0
4	EDO	D	1243	-	3,3,3	0.48	0	2,2,2	0.23	0
2	BME	A	1242	1	3,3,3	0.29	0	2,2,2	0.11	0
2	BME	A	1241[A]	1	3,3,3	0.24	0	2,2,2	0.25	0
2	BME	C	1243	1	3,3,3	0.46	0	2,2,2	0.57	0
3	PO4	B	1243	-	4,4,4	0.90	0	6,6,6	0.51	0
2	BME	D	1241	1	3,3,3	0.34	0	2,2,2	0.44	0
2	BME	B	1240	1	3,3,3	0.26	0	2,2,2	0.31	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
2	BME	A	1242	1	-	0/1/1/1	-
4	EDO	C	1244	-	-	1/1/1/1	-
4	EDO	B	1241	-	-	1/1/1/1	-
2	BME	A	1241[A]	1	-	1/1/1/1	-
2	BME	C	1243	1	-	0/1/1/1	-
2	BME	D	1242	1	-	1/1/1/1	-
2	BME	A	1241[B]	1	-	1/1/1/1	-
2	BME	C	1242	1	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	1244	-	-	1/1/1/1	-
2	BME	B	1239	1	-	0/1/1/1	-
4	EDO	D	1243	-	-	1/1/1/1	-
2	BME	D	1241	1	-	1/1/1/1	-
2	BME	B	1240	1	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1246	PO4	P-O4	-2.02	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1241[A]	BME	O1-C1-C2-S2
2	A	1241[B]	BME	O1-C1-C2-S2
2	D	1241	BME	O1-C1-C2-S2
2	D	1242	BME	O1-C1-C2-S2
4	C	1244	EDO	O1-C1-C2-O2
4	D	1244	EDO	O1-C1-C2-O2
4	B	1241	EDO	O1-C1-C2-O2
4	D	1243	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
2	D	1242	BME	4	0
3	A	1243	PO4	1	0
4	D	1244	EDO	1	0
4	D	1243	EDO	2	0
3	B	1243	PO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	204:LEU	C	205:GLY	N	1.62

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	235/251 (93%)	1.26	41 (17%) 4 5	27, 42, 53, 64	6 (2%)
1	B	217/251 (86%)	2.34	114 (52%) 0 0	28, 44, 57, 61	3 (1%)
1	C	236/251 (94%)	1.62	71 (30%) 1 1	25, 42, 53, 72	1 (0%)
1	D	230/251 (91%)	1.65	69 (30%) 1 1	27, 42, 53, 77	3 (1%)
All	All	918/1004 (91%)	1.71	295 (32%) 1 1	25, 43, 55, 77	13 (1%)

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	LEU	8.5
1	C	241	GLY	6.8
1	B	152	GLY	6.4
1	C	6	THR	6.1
1	D	217	TRP	5.8
1	D	213	PRO	5.7
1	B	231	PRO	5.7
1	B	137	PHE	5.5
1	B	233	TYR	5.4
1	B	136	ALA	5.3
1	B	191	LEU	5.3
1	B	143	LEU	5.2
1	B	138	LEU	5.2
1	D	218	ASP	5.1
1	B	188	CYS	5.0
1	D	215	GLY	5.0
1	D	222	LEU	4.9
1	D	220	VAL	4.9
1	B	139	ALA	4.9
1	B	197	ILE	4.7
1	B	48	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLU	4.7
1	A	43	VAL	4.6
1	B	142	SER	4.6
1	D	237	PHE	4.5
1	B	172	VAL	4.5
1	C	160	ALA	4.5
1	B	203	ARG	4.5
1	A	222	LEU	4.4
1	D	45	PRO	4.4
1	D	6	THR	4.4
1	B	146	THR	4.3
1	B	165	ALA	4.3
1	C	40	LEU	4.3
1	B	6	THR	4.2
1	D	212	SER	4.2
1	D	214	ALA	4.2
1	D	216	PHE	4.2
1	B	232	GLY	4.1
1	B	153	ILE	4.1
1	B	206	VAL	4.1
1	B	230	ARG	4.1
1	B	192	LEU	4.1
1	B	196	ALA	4.0
1	C	192	LEU	4.0
1	A	219	ALA	4.0
1	B	229	ALA	4.0
1	D	19	LEU	4.0
1	B	28	TYR	3.9
1	D	219	ALA	3.9
1	B	195	ASP	3.9
1	B	17	ALA	3.9
1	C	223	ALA	3.9
1	D	224	GLY	3.9
1	C	216	PHE	3.9
1	B	173	ARG	3.8
1	B	175	PHE	3.8
1	B	216	PHE	3.8
1	B	127	ILE	3.7
1	B	80	TYR	3.7
1	C	42	SER	3.7
1	A	218	ASP	3.7
1	B	151	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	167	LEU	3.6
1	A	154	THR	3.6
1	B	7	PRO	3.6
1	B	154	THR	3.6
1	C	162	VAL	3.6
1	C	228	LYS	3.6
1	C	156	VAL	3.5
1	C	41	GLY	3.5
1	C	240	SER	3.4
1	A	156	VAL	3.4
1	B	204	LEU	3.4
1	B	193	THR	3.4
1	D	228	LYS	3.4
1	A	240	SER	3.4
1	B	134	LEU	3.4
1	B	166	THR	3.4
1	B	189	GLY	3.3
1	B	183	GLY	3.3
1	B	215	GLY	3.3
1	B	177	ALA	3.2
1	B	202	ARG	3.2
1	D	46	GLU	3.2
1	B	126	TYR	3.2
1	B	163	ASP	3.2
1	A	223	ALA	3.2
1	C	219	ALA	3.2
1	B	144	VAL	3.2
1	B	125	ALA	3.2
1	C	80	TYR	3.2
1	A	51	VAL	3.2
1	B	222	LEU	3.2
1	D	236	LEU	3.2
1	D	107	ALA	3.1
1	B	200	VAL	3.1
1	D	82	GLY	3.1
1	B	169	ASP	3.1
1	D	76	SER	3.1
1	B	27	LEU	3.1
1	D	225	GLY	3.1
1	B	109	LEU	3.1
1	C	7	PRO	3.1
1	D	7	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	77	LEU	3.0
1	D	173	ARG	3.0
1	A	179	PRO	3.0
1	B	225	GLY	3.0
1	C	43	VAL	3.0
1	A	6	THR	3.0
1	B	145	PRO	3.0
1	D	18	GLY	3.0
1	D	116	GLY	3.0
1	B	50	ALA	3.0
1	A	127	ILE	3.0
1	B	141	GLU	3.0
1	C	194	LEU	3.0
1	C	212	SER	3.0
1	B	49	ASP	3.0
1	B	228	LYS	3.0
1	B	180	ASP	2.9
1	B	238	ASP	2.9
1	C	37	GLY	2.9
1	D	223	ALA	2.9
1	C	180	ASP	2.9
1	A	220	VAL	2.9
1	B	190	GLY	2.9
1	C	214	ALA	2.9
1	C	38	LEU	2.9
1	C	222	LEU	2.9
1	C	147	GLY	2.9
1	C	189	GLY	2.9
1	D	117	VAL	2.8
1	B	182	ASP	2.8
1	C	225	GLY	2.8
1	C	39	GLY	2.8
1	C	226	GLY	2.8
1	A	153	ILE	2.8
1	C	221	ARG	2.8
1	B	198	PRO	2.8
1	C	69	VAL	2.8
1	B	178	ALA	2.8
1	D	113	ARG	2.8
1	D	47	GLY	2.8
1	D	111	GLY	2.8
1	B	199	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	221	ARG	2.7
1	D	109	LEU	2.7
1	B	221	ARG	2.7
1	D	87	ALA	2.7
1	D	152	GLY	2.7
1	B	184	ILE	2.7
1	C	60	ARG	2.7
1	B	56	VAL	2.7
1	D	16	ALA	2.7
1	D	169	ASP	2.7
1	D	105	SER	2.7
1	B	219	ALA	2.6
1	D	83	ALA	2.6
1	B	187	SER	2.6
1	D	86	ASN	2.6
1	A	155	GLY	2.6
1	C	155	GLY	2.6
1	D	39	GLY	2.6
1	C	139	ALA	2.6
1	B	31	LEU	2.6
1	D	161	ARG	2.6
1	B	114	ALA	2.6
1	B	211	SER	2.6
1	A	221	ARG	2.6
1	A	41	GLY	2.6
1	B	224	GLY	2.6
1	B	135	ALA	2.6
1	B	220	VAL	2.6
1	B	29	PRO	2.5
1	D	126	TYR	2.5
1	B	67	ALA	2.5
1	D	88	ALA	2.5
1	B	150	SER	2.5
1	B	51	VAL	2.5
1	C	164	THR	2.5
1	D	118	ARG	2.5
1	C	198	PRO	2.5
1	C	233	TYR	2.5
1	D	80	TYR	2.5
1	A	237	PHE	2.5
1	C	62	LEU	2.5
1	C	191	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	190	GLY	2.5
1	C	215	GLY	2.5
1	C	96	ALA	2.5
1	C	188	CYS	2.5
1	C	48	TYR	2.5
1	A	191	LEU	2.5
1	C	161	ARG	2.5
1	C	224	GLY	2.4
1	C	230	ARG	2.4
1	B	9	ILE	2.4
1	D	108	VAL	2.4
1	A	224	GLY	2.4
1	A	192	LEU	2.4
1	C	99	LEU	2.4
1	D	150	SER	2.4
1	C	67	ALA	2.4
1	C	68	ALA	2.4
1	D	202	ARG	2.4
1	B	69	VAL	2.4
1	D	110	ASN	2.4
1	C	232	GLY	2.4
1	A	118	ARG	2.4
1	A	158	ALA	2.4
1	C	59	ALA	2.4
1	A	42	SER	2.4
1	D	240	SER	2.4
1	B	118	ARG	2.3
1	D	48	TYR	2.3
1	D	79	PHE	2.3
1	D	176	GLU	2.3
1	C	66	GLY	2.3
1	A	129	ASP	2.3
1	C	44	THR	2.3
1	D	85	PHE	2.3
1	D	227	ALA	2.3
1	D	22	ALA	2.3
1	D	25	ALA	2.3
1	B	234	GLY	2.3
1	B	120	VAL	2.3
1	C	168	VAL	2.3
1	C	220	VAL	2.3
1	C	193	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	133	ARG	2.2
1	A	50	ALA	2.2
1	A	126	TYR	2.2
1	B	79	PHE	2.2
1	B	176	GLU	2.2
1	C	229	ALA	2.2
1	D	14	PRO	2.2
1	B	97	THR	2.2
1	D	106	THR	2.2
1	C	204	LEU	2.2
1	D	112	LEU	2.2
1	A	226	GLY	2.2
1	B	179	PRO	2.2
1	B	181	SER	2.2
1	C	45	PRO	2.2
1	D	231	PRO	2.2
1	A	165	ALA	2.2
1	B	96	ALA	2.2
1	A	133	ARG	2.2
1	D	235	ARG	2.2
1	A	200	VAL	2.2
1	D	208	VAL	2.2
1	B	164	THR	2.2
1	B	205	GLY	2.2
1	C	163	ASP	2.2
1	D	226	GLY	2.2
1	B	68	ALA	2.2
1	B	174	ALA	2.2
1	B	52	ILE	2.2
1	C	235	ARG	2.2
1	B	20	VAL	2.2
1	B	70	VAL	2.2
1	A	163	ASP	2.2
1	A	105	SER	2.2
1	C	143	LEU	2.2
1	C	15	PRO	2.2
1	C	123	ALA	2.2
1	D	229	ALA	2.2
1	B	76	SER	2.1
1	A	24	GLY	2.1
1	D	234	GLY	2.1
1	C	145	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	81[A]	ARG	2.1
1	A	130	VAL	2.1
1	B	113	ARG	2.1
1	C	211	SER	2.1
1	B	132	GLU	2.1
1	A	45	PRO	2.1
1	C	109	LEU	2.1
1	A	107	ALA	2.1
1	B	25	ALA	2.1
1	B	123	ALA	2.1
1	B	214	ALA	2.1
1	A	180	ASP	2.1
1	B	66	GLY	2.0
1	A	162	VAL	2.0
1	A	217	TRP	2.0
1	B	170	LEU	2.0
1	B	128	ASP	2.0
1	C	157	GLU	2.0
1	A	7	PRO	2.0
1	B	26	ARG	2.0
1	C	117	VAL	2.0
1	D	91	VAL	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 oligosaccharides 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
4	EDO	D	1243	4/4	0.72	0.25	65,69,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	1242	5/5	0.76	0.24	52,54,55,56	5
3	PO4	B	1243	5/5	0.77	0.19	66,67,70,71	5
2	BME	B	1240	4/4	0.79	0.34	60,61,62,62	4
3	PO4	C	1245	5/5	0.80	0.17	57,58,61,61	5
3	PO4	C	1246	5/5	0.81	0.12	81,81,84,85	0
4	EDO	C	1244	4/4	0.82	0.28	43,56,59,63	0
2	BME	C	1242	4/4	0.82	0.23	42,43,45,48	4
3	PO4	D	1246	5/5	0.84	0.21	32,49,54,56	5
4	EDO	B	1241	4/4	0.86	0.16	54,58,60,62	0
4	EDO	D	1244	4/4	0.86	0.27	40,57,58,61	0
2	BME	A	1241[B]	4/4	0.87	0.20	44,44,45,48	4
2	BME	A	1241[A]	4/4	0.87	0.20	42,43,45,47	4
2	BME	B	1239	4/4	0.88	0.22	77,82,83,85	0
3	PO4	D	1245	5/5	0.91	0.14	47,53,57,59	0
2	BME	D	1242	4/4	0.92	0.25	40,45,54,69	0
2	BME	A	1242	4/4	0.94	0.18	44,45,48,56	0
3	PO4	A	1243	5/5	0.94	0.17	34,40,43,44	5
2	BME	D	1241	4/4	0.96	0.17	36,42,42,46	0
2	BME	C	1243	4/4	0.97	0.16	39,39,41,42	0

6.5 Other polymers

There are no such residues in this entry.