



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:00 AM GMT

PDB ID : 2VLB
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

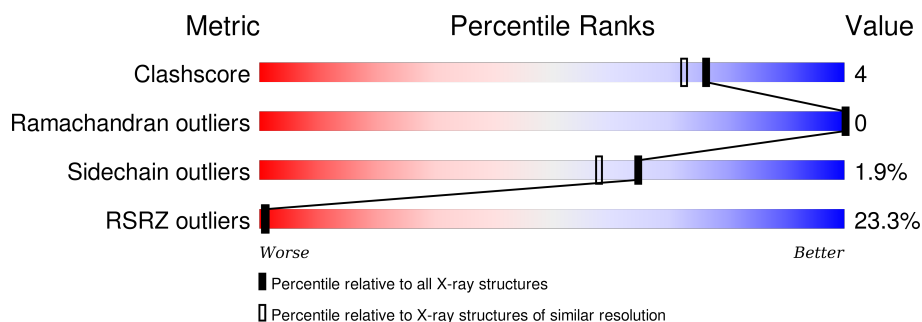
1 Overall quality at a glance

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	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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. 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	
1	B	251	
1	C	251	
1	D	251	

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	A	1241[A]	-	-	-	X
2	BME	B	1239	-	-	-	X
2	BME	D	1242	-	-	X	-
3	PO4	A	1243	-	-	-	X
3	PO4	D	1246	-	-	-	X
4	EDO	D	1243	-	-	-	X
4	EDO	D	1244	-	-	-	X

2 Entry composition [i](#)

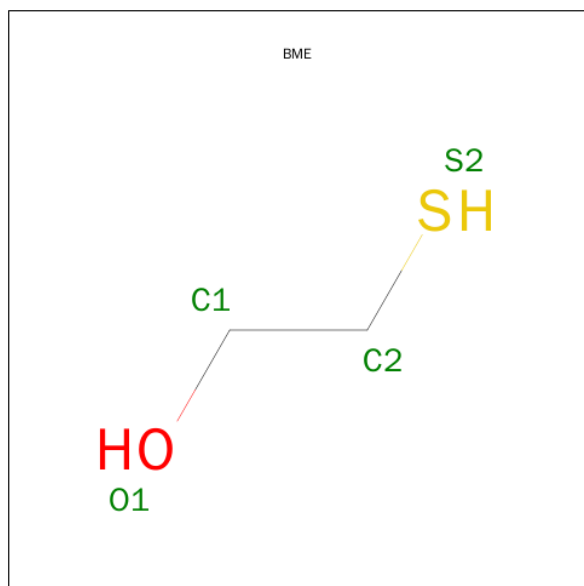
There are 5 unique types of molecules in this entry. The entry contains 7221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: BME) (formula: C₂H₆OS).



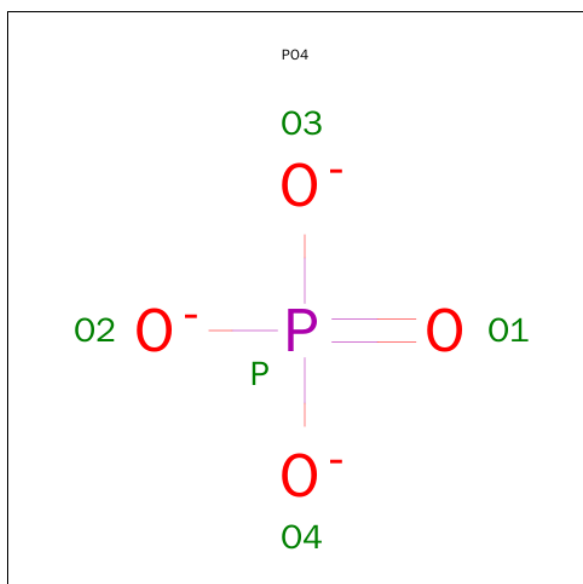
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	1
			8	4	2	2		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

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 (three-letter code: PO4) (formula: O₄P).



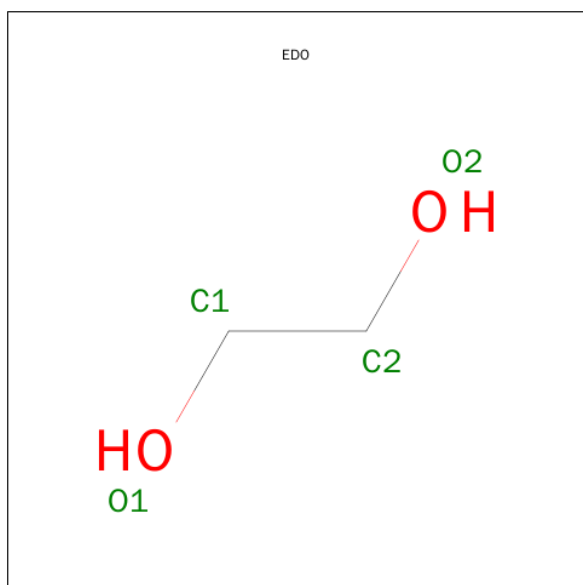
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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 (three-letter code: EDO) (formula: C₂H₆O₂).



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		

Continued on next page...

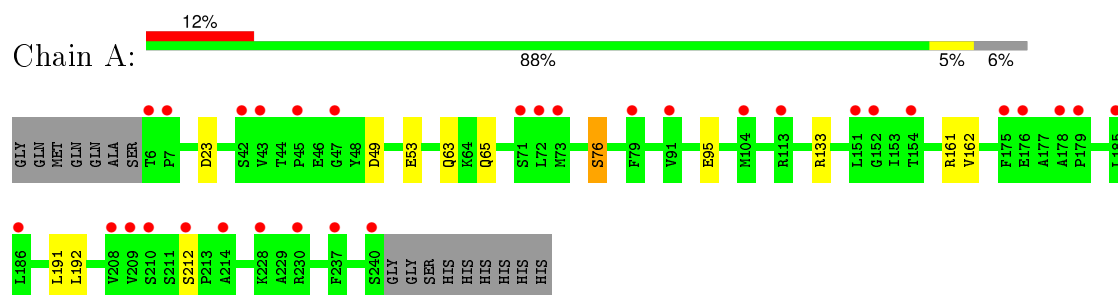
Continued from previous page...

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

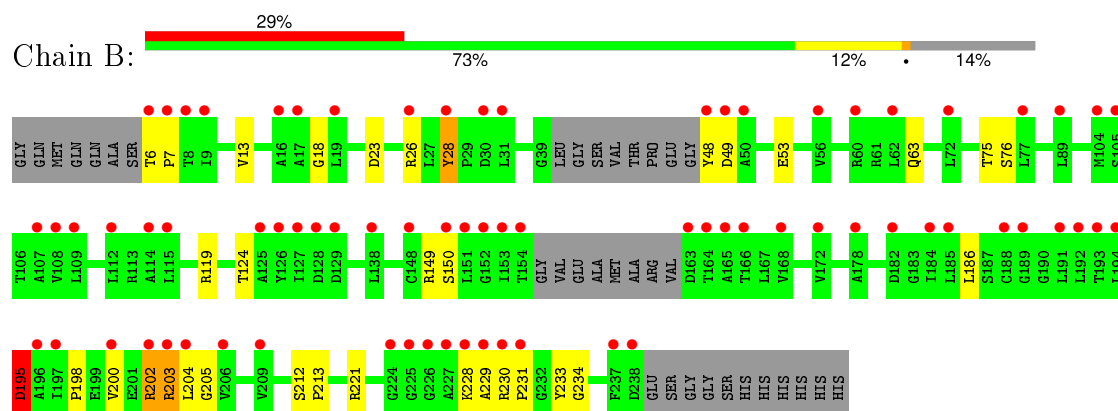
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

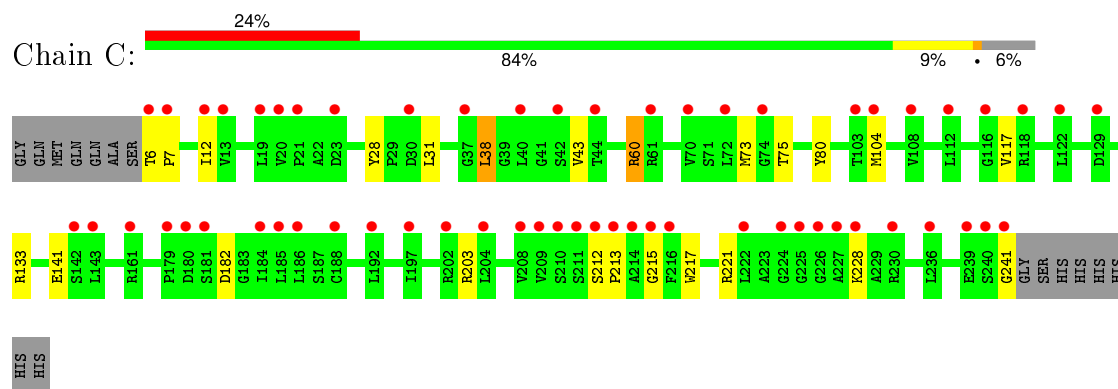
• Molecule 1: ARYLMALONATE DECARBOXYLASE



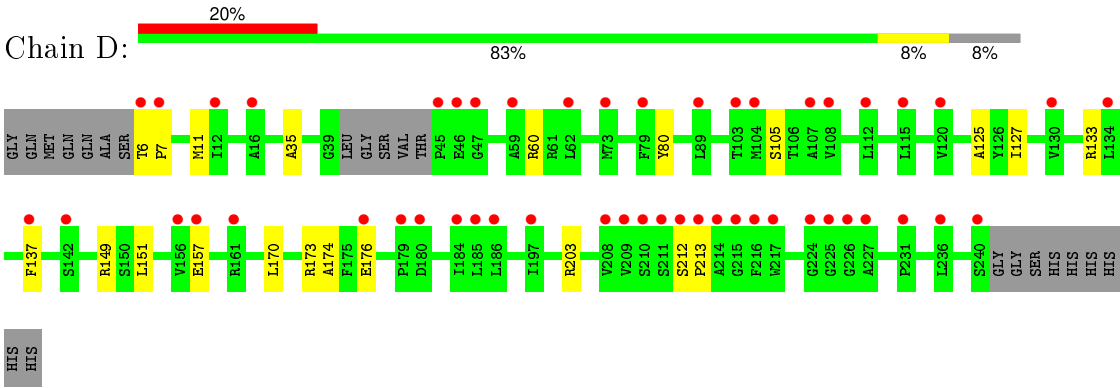
• Molecule 1: ARYLMALONATE DECARBOXYLASE



• 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 29.17 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.64-1.92) 98.8 (29.17-1.92)	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.	DCC
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 89246 reflections	Xtriage
F_o, F_c correlation	0.95	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, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, EDO, BME

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	0.84	3/1778 (0.2%)	0.72	4/2422 (0.2%)
1	B	1.56	22/1628 (1.4%)	1.05	11/2215 (0.5%)
1	C	0.56	0/1739	0.64	2/2369 (0.1%)
1	D	0.67	0/1724	0.66	0/2344
All	All	0.98	25/6869 (0.4%)	0.78	17/9350 (0.2%)

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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	ASP	CB-CG	27.02	2.08	1.51
1	B	200	VAL	C-O	17.65	1.56	1.23
1	B	204	LEU	C-N	16.49	1.62	1.33
1	B	119	ARG	CZ-NH1	14.68	1.52	1.33
1	A	76[B]	SER	CB-OG	-14.43	1.23	1.42
1	A	76[C]	SER	CB-OG	-14.43	1.23	1.42
1	A	76[A]	SER	CB-OG	-14.43	1.23	1.42
1	B	195	ASP	CG-OD2	13.75	1.56	1.25
1	B	204	LEU	C-O	12.80	1.47	1.23
1	B	231	PRO	C-N	12.35	1.55	1.33
1	B	202	ARG	CZ-NH1	11.47	1.48	1.33
1	B	28	TYR	CG-CD1	11.19	1.53	1.39
1	B	28	TYR	CE2-CZ	11.17	1.53	1.38
1	B	202	ARG	CZ-NH2	10.60	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	TYR	CG-CD2	10.14	1.52	1.39
1	B	28	TYR	CE1-CZ	8.87	1.50	1.38
1	B	202	ARG	CD-NE	8.38	1.60	1.46
1	B	233	TYR	CG-CD1	7.46	1.48	1.39
1	B	233	TYR	CE2-CZ	7.32	1.48	1.38
1	B	234	GLY	C-O	6.86	1.34	1.23
1	B	200	VAL	C-N	6.83	1.49	1.34
1	B	119	ARG	CZ-NH2	6.46	1.41	1.33
1	B	205	GLY	N-CA	6.10	1.55	1.46
1	B	230	ARG	C-O	-5.84	1.12	1.23
1	B	228	LYS	C-O	5.35	1.33	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	ASP	CB-CG-OD2	-26.96	94.03	118.30
1	B	119	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	A	76[B]	SER	CA-CB-OG	8.46	134.04	111.20
1	A	76[C]	SER	CA-CB-OG	8.46	134.04	111.20
1	A	76[A]	SER	CA-CB-OG	8.46	134.04	111.20
1	B	204	LEU	C-N-CA	-7.34	106.89	122.30
1	B	195	ASP	OD1-CG-OD2	7.25	137.08	123.30
1	B	202	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	28	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	B	204	LEU	CA-C-N	-5.94	104.32	116.20
1	B	195	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	60	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	133	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	230	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	119	ARG	NH1-CZ-NH2	5.07	124.97	119.40
1	B	28	TYR	CG-CD2-CE2	-5.04	117.27	121.30
1	C	60	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	9	0
1	B	1586	0	1607	14	0
1	C	1706	0	1732	15	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	52	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 (52) 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	1.21
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:104:MET:HE2	5:C:2029:HOH:O	2.18	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: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:C:73:MET:HE1	1:C:215:GLY:HA3	2.03	0.41
1:D:6:THR:HA	1:D:7:PRO:HD3	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	178 (98%)	3 (2%)	68	63
1	B	164/186 (88%)	156 (95%)	8 (5%)	31	18
1	C	175/186 (94%)	172 (98%)	3 (2%)	68	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	173/186 (93%)	172 (99%)	1 (1%)	90	90
All	All	693/744 (93%)	678 (98%)	15 (2%)	65	52

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

Mol	Chain	Res	Type
1	A	63	GLN
1	A	212[A]	SER
1	A	212[B]	SER
1	B	23[A]	ASP
1	B	23[B]	ASP
1	B	26	ARG
1	B	63	GLN
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	157	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	C	63	GLN
1	C	65	GLN

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

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	A	1241[A]	1	3,3,3	0.24	0	2,2,2	0.24	0
2	BME	A	1241[B]	1	3,3,3	0.24	0	2,2,2	0.43	0
2	BME	A	1242	1	3,3,3	0.29	0	2,2,2	0.15	0
3	PO4	A	1243	-	4,4,4	0.41	0	6,6,6	0.29	0
2	BME	B	1239	1	3,3,3	0.34	0	2,2,2	0.25	0
2	BME	B	1240	1	3,3,3	0.25	0	2,2,2	0.26	0
4	EDO	B	1241	-	3,3,3	0.50	0	2,2,2	0.23	0
3	PO4	B	1242	-	4,4,4	0.45	0	6,6,6	0.28	0
3	PO4	B	1243	-	4,4,4	0.44	0	6,6,6	0.27	0
2	BME	C	1242	1	3,3,3	0.23	0	2,2,2	0.43	0
2	BME	C	1243	1	3,3,3	0.45	0	2,2,2	0.56	0
4	EDO	C	1244	-	3,3,3	0.64	0	2,2,2	0.12	0
3	PO4	C	1245	-	4,4,4	0.50	0	6,6,6	0.28	0
3	PO4	C	1246	-	4,4,4	0.36	0	6,6,6	0.27	0
2	BME	D	1241	1	3,3,3	0.32	0	2,2,2	0.38	0
2	BME	D	1242	1	3,3,3	0.39	0	2,2,2	0.26	0
4	EDO	D	1243	-	3,3,3	0.52	0	2,2,2	0.26	0
4	EDO	D	1244	-	3,3,3	0.65	0	2,2,2	0.42	0
3	PO4	D	1245	-	4,4,4	0.59	0	6,6,6	0.29	0
3	PO4	D	1246	-	4,4,4	0.67	0	6,6,6	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	A	1241[A]	1	-	0/1/1/1	0/0/0/0
2	BME	A	1241[B]	1	-	0/1/1/1	0/0/0/0
2	BME	A	1242	1	-	0/1/1/1	0/0/0/0
3	PO4	A	1243	-	-	0/0/0/0	0/0/0/0
2	BME	B	1239	1	-	0/1/1/1	0/0/0/0
2	BME	B	1240	1	-	0/1/1/1	0/0/0/0
4	EDO	B	1241	-	-	0/1/1/1	0/0/0/0
3	PO4	B	1242	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1243	-	-	0/0/0/0	0/0/0/0
2	BME	C	1242	1	-	0/1/1/1	0/0/0/0
2	BME	C	1243	1	-	0/1/1/1	0/0/0/0
4	EDO	C	1244	-	-	0/1/1/1	0/0/0/0
3	PO4	C	1245	-	-	0/0/0/0	0/0/0/0
3	PO4	C	1246	-	-	0/0/0/0	0/0/0/0
2	BME	D	1241	1	-	0/1/1/1	0/0/0/0
2	BME	D	1242	1	-	0/1/1/1	0/0/0/0
4	EDO	D	1243	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1244	-	-	0/1/1/1	0/0/0/0
3	PO4	D	1245	-	-	0/0/0/0	0/0/0/0
3	PO4	D	1246	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1243	PO4	1	0
3	B	1243	PO4	1	0
2	D	1242	BME	4	0
4	D	1243	EDO	2	0
4	D	1244	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	235/251 (93%)	1.05	31 (13%)	4 5	36, 42, 53, 64	0
1	B	217/251 (86%)	2.01	74 (34%)	0 0	37, 44, 57, 61	0
1	C	236/251 (94%)	1.41	59 (25%)	1 1	35, 42, 53, 72	0
1	D	230/251 (91%)	1.32	50 (21%)	1 1	36, 42, 53, 77	0
All	All	918/1004 (91%)	1.44	214 (23%)	1 1	35, 43, 55, 77	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	10.0
1	B	126	TYR	9.7
1	B	192	LEU	9.1
1	C	241	GLY	9.0
1	B	153	ILE	8.7
1	C	225	GLY	7.5
1	D	6	THR	7.3
1	B	127	ILE	6.9
1	B	6	THR	6.7
1	B	31	LEU	6.4
1	B	152	GLY	6.4
1	D	225	GLY	6.4
1	B	154	THR	6.3
1	C	226	GLY	6.2
1	B	165	ALA	6.1
1	B	48	TYR	6.0
1	B	226	GLY	6.0
1	D	45	PRO	5.9
1	B	172	VAL	5.9
1	B	114	ALA	5.5
1	B	30	ASP	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	194	LEU	5.4
1	D	226	GLY	5.4
1	C	6	THR	5.3
1	B	50	ALA	5.1
1	D	16	ALA	4.8
1	C	240	SER	4.8
1	C	185	LEU	4.7
1	B	49	ASP	4.7
1	A	43	VAL	4.6
1	D	240	SER	4.6
1	D	185	LEU	4.5
1	D	47	GLY	4.5
1	C	180	ASP	4.4
1	B	148	CYS	4.4
1	B	188	CYS	4.4
1	A	154	THR	4.3
1	A	208	VAL	4.3
1	A	6	THR	4.3
1	C	209	VAL	4.3
1	D	7	PRO	4.3
1	D	214	ALA	4.2
1	B	202	ARG	4.2
1	B	200	VAL	4.1
1	C	224	GLY	4.1
1	C	228	LYS	4.1
1	C	30	ASP	4.1
1	C	227	ALA	4.1
1	B	224	GLY	4.0
1	B	163	ASP	4.0
1	C	20	VAL	4.0
1	D	134	LEU	3.9
1	C	186	LEU	3.9
1	B	225	GLY	3.9
1	B	228	LYS	3.8
1	D	46	GLU	3.8
1	B	184	ILE	3.8
1	B	16	ALA	3.7
1	B	209	VAL	3.7
1	A	72	LEU	3.7
1	B	193	THR	3.7
1	D	209	VAL	3.7
1	B	164	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	115	LEU	3.7
1	D	186	LEU	3.6
1	C	108	VAL	3.6
1	B	128	ASP	3.5
1	B	227	ALA	3.5
1	C	179	PRO	3.5
1	D	224	GLY	3.5
1	D	108	VAL	3.5
1	D	157	GLU	3.4
1	D	179	PRO	3.4
1	A	185	LEU	3.3
1	C	202	ARG	3.3
1	B	166	THR	3.3
1	D	217	TRP	3.3
1	B	112	LEU	3.3
1	C	211	SER	3.3
1	C	40	LEU	3.2
1	D	208	VAL	3.2
1	B	151	LEU	3.2
1	B	229	ALA	3.2
1	B	104	MET	3.2
1	C	72	LEU	3.2
1	B	28	TYR	3.2
1	B	72	LEU	3.2
1	C	42	SER	3.2
1	B	185	LEU	3.1
1	C	212	SER	3.1
1	B	204	LEU	3.1
1	B	17	ALA	3.1
1	A	42	SER	3.1
1	C	222	LEU	3.1
1	C	104	MET	3.1
1	C	216	PHE	3.0
1	B	108	VAL	3.0
1	D	104	MET	3.0
1	D	107	ALA	3.0
1	A	209	VAL	2.9
1	C	116	GLY	2.9
1	B	230	ARG	2.9
1	C	161	ARG	2.9
1	B	203	ARG	2.8
1	C	208	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	79	PHE	2.8
1	B	238	ASP	2.8
1	C	143	LEU	2.8
1	D	180	ASP	2.8
1	B	178	ALA	2.8
1	C	103	THR	2.8
1	B	196	ALA	2.8
1	C	70	VAL	2.8
1	A	45	PRO	2.8
1	D	12	ILE	2.7
1	A	212[A]	SER	2.7
1	B	129	ASP	2.7
1	C	74	GLY	2.7
1	D	215	GLY	2.7
1	D	236	LEU	2.7
1	C	12	ILE	2.7
1	B	26	ARG	2.7
1	B	107	ALA	2.7
1	B	231	PRO	2.7
1	C	210	SER	2.7
1	D	212	SER	2.7
1	C	239	GLU	2.7
1	D	176	GLU	2.7
1	A	228	LYS	2.6
1	A	71	SER	2.6
1	D	59	ALA	2.6
1	C	230	ARG	2.6
1	D	156	VAL	2.6
1	A	7	PRO	2.6
1	B	206	VAL	2.6
1	C	118	ARG	2.6
1	B	7	PRO	2.6
1	B	125	ALA	2.5
1	C	214	ALA	2.5
1	B	105	SER	2.5
1	C	129	ASP	2.5
1	B	109	LEU	2.5
1	D	211	SER	2.5
1	A	179	PRO	2.5
1	B	138	LEU	2.5
1	B	8	THR	2.5
1	D	213	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	13	VAL	2.4
1	C	23	ASP	2.4
1	C	37	GLY	2.4
1	D	197	ILE	2.4
1	B	77	LEU	2.4
1	D	142	SER	2.4
1	A	230	ARG	2.4
1	C	142	SER	2.4
1	A	178	ALA	2.4
1	D	130	VAL	2.4
1	D	216	PHE	2.3
1	C	188	CYS	2.3
1	A	186	LEU	2.3
1	D	112	LEU	2.3
1	B	197	ILE	2.3
1	D	161	ARG	2.3
1	B	237	PHE	2.3
1	C	181	SER	2.2
1	A	104	MET	2.2
1	D	115	LEU	2.2
1	C	213	PRO	2.2
1	D	231	PRO	2.2
1	C	197	ILE	2.2
1	D	227	ALA	2.2
1	A	240	SER	2.2
1	B	150	SER	2.2
1	C	112	LEU	2.2
1	C	236	LEU	2.2
1	B	56	VAL	2.2
1	C	21	PRO	2.2
1	A	237	PHE	2.2
1	D	137	PHE	2.2
1	A	151	LEU	2.2
1	B	62	LEU	2.2
1	D	103	THR	2.2
1	B	182	ASP	2.1
1	B	9	ILE	2.1
1	A	73	MET	2.1
1	A	214	ALA	2.1
1	A	210	SER	2.1
1	B	60[A]	ARG	2.1
1	A	79	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	168	VAL	2.1
1	C	215	GLY	2.1
1	D	73	MET	2.1
1	C	19	LEU	2.1
1	C	192	LEU	2.1
1	D	89	LEU	2.1
1	A	91	VAL	2.1
1	A	47	GLY	2.1
1	B	189	GLY	2.1
1	A	175	PHE	2.0
1	B	19	LEU	2.0
1	B	89	LEU	2.0
1	C	204	LEU	2.0
1	D	62	LEU	2.0
1	D	210	SER	2.0
1	C	44	THR	2.0
1	D	120	VAL	2.0
1	A	176	GLU	2.0
1	A	113	ARG	2.0
1	C	184	ILE	2.0
1	D	184	ILE	2.0
1	A	152	GLY	2.0
1	C	122	LEU	2.0
1	C	7	PRO	2.0
1	C	61	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PO4	D	1246	5/5	0.84	0.28	5.59	32,49,54,56	5
4	EDO	D	1244	4/4	0.81	0.28	4.62	40,57,58,61	0
3	PO4	A	1243	5/5	0.95	0.23	3.70	34,40,43,44	5
2	BME	B	1239	4/4	0.92	0.33	3.01	77,82,83,85	0
4	EDO	D	1243	4/4	0.78	0.25	2.27	65,69,71,72	0
2	BME	A	1241[A]	4/4	0.85	0.22	2.07	42,43,45,47	4
3	PO4	C	1245	5/5	0.88	0.27	1.91	57,58,61,61	5
3	PO4	B	1243	5/5	0.89	0.27	1.89	66,67,70,71	5
2	BME	A	1241[B]	4/4	0.85	0.22	1.84	44,44,45,48	4
2	BME	D	1242	4/4	0.97	0.21	1.36	40,45,54,69	0
2	BME	D	1241	4/4	0.95	0.16	1.22	36,42,42,46	0
3	PO4	B	1242	5/5	0.90	0.21	1.20	52,54,55,56	5
4	EDO	B	1241	4/4	0.80	0.18	1.09	54,58,60,62	0
4	EDO	C	1244	4/4	0.89	0.22	0.89	43,56,59,63	0
2	BME	C	1242	4/4	0.83	0.18	0.87	42,43,45,48	4
2	BME	C	1243	4/4	0.97	0.14	-0.73	39,39,41,42	0
2	BME	A	1242	4/4	0.95	0.11	-0.75	44,45,48,56	0
3	PO4	D	1245	5/5	0.96	0.12	-1.43	47,53,57,59	0
2	BME	B	1240	4/4	0.89	0.21	-	60,61,62,62	4
3	PO4	C	1246	5/5	0.90	0.43	-	81,81,84,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.