



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:07 PM UTC

PDB ID : 4ATY / pdb_00004aty
Title : Crystal structure of a Terephthalate 1,2-cis-dihydrodioldehydrogenase from Burkholderia xenovorans LB400
Authors : Bains, J.; Boulanger, M.J.
Deposited on : 2012-05-11
Resolution : 1.85 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

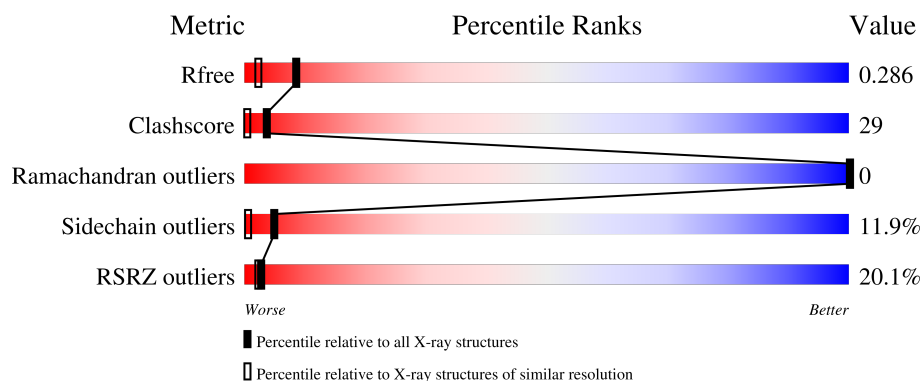
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	349	18% 59% 24% 5% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2447 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.

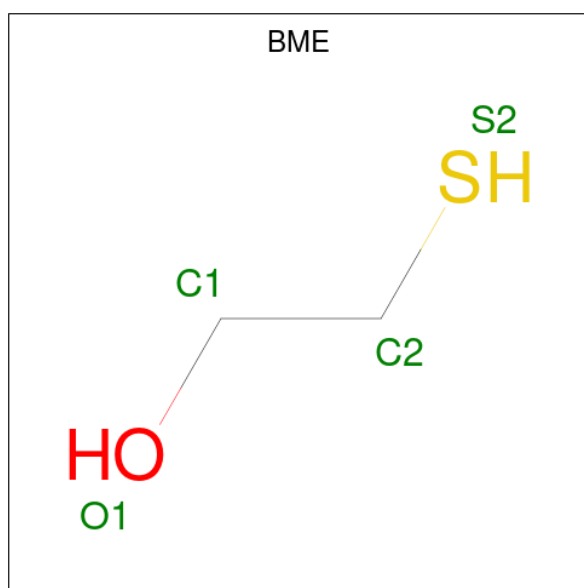
- Molecule 1 is a protein called TEREPHTHALATE 1,2-CIS-DIHYDRODIOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2218	1404	399	402	13			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

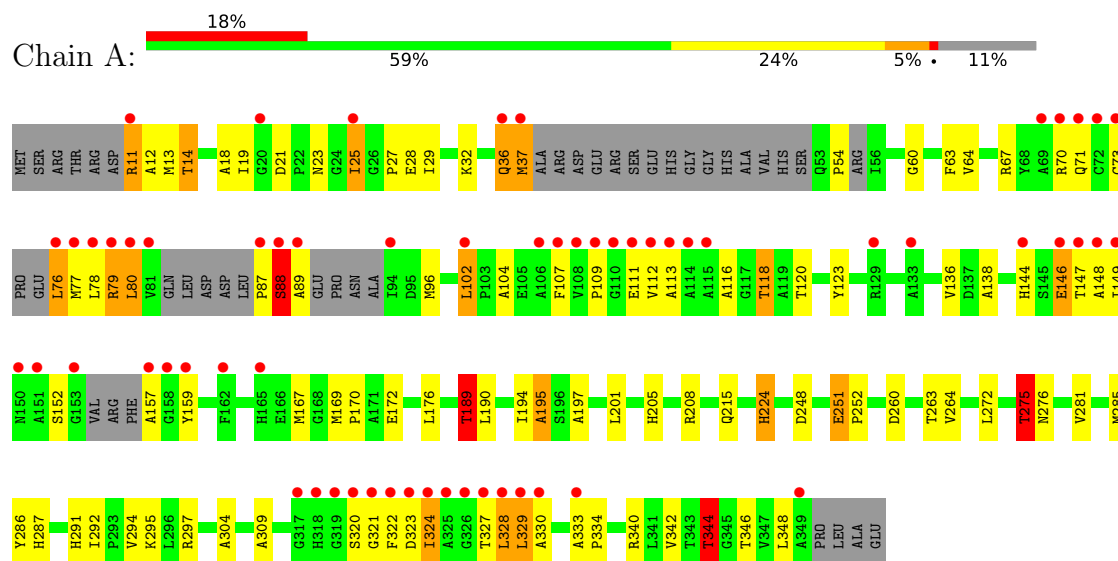
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total 224	O 224	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: TEREPHTHALATE 1,2-CIS-DIHYDRODIOL DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	44.62Å 76.19Å 197.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.79 – 1.85 37.79 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.79-1.85) 99.6 (37.79-1.85)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.210 , 0.266 (Not available) , 0.286	Depositor DCC
R_{free} test set	1486 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.054 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2447	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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: ZN, 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	1.46	16/2252 (0.7%)	1.46	22/3055 (0.7%)

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	A	1	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	HIS	C-O	8.63	1.34	1.24
1	A	195	ALA	C-N	8.08	1.44	1.33
1	A	190	LEU	C-O	-6.50	1.15	1.24
1	A	264	VAL	CA-CB	6.23	1.62	1.54
1	A	295	LYS	C-O	6.03	1.31	1.24
1	A	292	ILE	CA-C	6.00	1.58	1.52
1	A	281	VAL	CA-CB	5.87	1.63	1.55
1	A	79	ARG	CA-C	-5.83	1.45	1.52
1	A	275	THR	CB-CG2	-5.66	1.33	1.52
1	A	294	VAL	CA-CB	-5.65	1.47	1.54
1	A	251	GLU	N-CA	5.60	1.51	1.46
1	A	291	HIS	C-O	5.48	1.30	1.24
1	A	18	ALA	CA-CB	-5.37	1.45	1.53
1	A	189	THR	C-O	-5.11	1.17	1.23
1	A	109	PRO	C-O	-5.11	1.18	1.23
1	A	224	HIS	C-O	-5.02	1.18	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ALA	O-C-N	-18.73	100.31	122.22
1	A	194	ILE	O-C-N	-18.49	103.20	121.87
1	A	194	ILE	CA-C-N	17.54	145.54	120.28
1	A	194	ILE	C-N-CA	17.54	145.54	120.28
1	A	344	THR	N-CA-CB	-7.54	100.97	111.00
1	A	70	ARG	CA-C-N	7.51	130.67	120.38
1	A	70	ARG	C-N-CA	7.51	130.67	120.38
1	A	111	GLU	N-CA-C	-7.01	99.59	109.69
1	A	275	THR	CA-CB-CG2	6.94	122.30	110.50
1	A	189	THR	N-CA-CB	-6.60	100.64	111.66
1	A	248	ASP	N-CA-C	6.59	119.46	111.82
1	A	88	SER	N-CA-C	6.12	116.51	108.07
1	A	276	ASN	CA-C-O	5.78	123.05	119.29
1	A	285	MET	N-CA-C	-5.34	106.93	113.50
1	A	260	ASP	N-CA-C	-5.33	106.37	112.92
1	A	276	ASN	CB-CA-C	5.30	116.18	110.08
1	A	275	THR	OG1-CB-CG2	5.27	119.84	109.30
1	A	111	GLU	CA-C-N	-5.18	115.98	123.03
1	A	111	GLU	C-N-CA	-5.18	115.98	123.03
1	A	189	THR	OG1-CB-CG2	5.09	119.49	109.30
1	A	291	HIS	CA-C-N	-5.02	116.32	120.33
1	A	291	HIS	C-N-CA	-5.02	116.32	120.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	275	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ALA	Mainchain

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	2218	0	2252	130	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	4	0	5	0	0
4	A	224	0	0	12	0
All	All	2447	0	2257	130	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 29.

All (130) 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:A:102:LEU:HD12	1:A:107:PHE:CD1	1.41	1.55
1:A:102:LEU:HD12	1:A:107:PHE:CE1	1.39	1.53
1:A:64:VAL:CG2	1:A:107:PHE:CE1	2.10	1.33
1:A:102:LEU:HB3	1:A:107:PHE:CZ	1.70	1.24
1:A:102:LEU:CD1	1:A:107:PHE:CD1	2.23	1.20
1:A:102:LEU:CD1	1:A:107:PHE:CE1	2.29	1.15
1:A:224:HIS:CE1	1:A:263:THR:HG23	1.84	1.12
1:A:224:HIS:HE1	1:A:263:THR:HG23	1.11	1.10
1:A:64:VAL:HG21	1:A:107:PHE:CE1	1.78	1.10
1:A:78:LEU:HD23	1:A:96:MET:HE1	1.28	1.10
1:A:25:ILE:HD13	1:A:25:ILE:O	1.52	1.10
1:A:36:GLN:O	1:A:37:MET:HB2	1.52	1.06
1:A:112:VAL:HG23	1:A:322:PHE:CZ	1.89	1.05
1:A:224:HIS:HE1	1:A:263:THR:CG2	1.68	1.05
1:A:25:ILE:HD11	1:A:29:ILE:HG23	1.38	1.02
1:A:64:VAL:HG21	1:A:107:PHE:HE1	1.11	1.01
1:A:64:VAL:HG22	1:A:107:PHE:CD1	2.01	0.95
1:A:64:VAL:HG23	1:A:107:PHE:CE1	2.02	0.95
1:A:189:THR:HG21	1:A:197:ALA:HB1	1.50	0.93
1:A:64:VAL:CG2	1:A:107:PHE:CD1	2.50	0.93
1:A:118:THR:HG22	1:A:152:SER:HB2	1.50	0.92
1:A:25:ILE:HD11	1:A:330:ALA:HB1	1.51	0.92
1:A:25:ILE:CD1	1:A:29:ILE:HG23	1.99	0.91
1:A:21:ASP:HA	1:A:120:THR:HG22	1.54	0.89
1:A:104:ALA:HA	1:A:107:PHE:HD2	1.37	0.88
1:A:112:VAL:HG11	1:A:148:ALA:CB	2.03	0.88
1:A:104:ALA:HA	1:A:107:PHE:CD2	2.09	0.87
1:A:102:LEU:CB	1:A:107:PHE:CZ	2.56	0.86
1:A:146:GLU:H	1:A:146:GLU:CD	1.81	0.86
1:A:112:VAL:CG2	1:A:322:PHE:HZ	1.89	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:SER:O	1:A:89:ALA:CB	2.25	0.84
1:A:112:VAL:CG2	1:A:322:PHE:CZ	2.61	0.83
1:A:102:LEU:CD1	1:A:107:PHE:CG	2.61	0.82
1:A:28:GLU:OE2	1:A:328:LEU:HA	1.80	0.82
1:A:88:SER:O	1:A:89:ALA:HB2	1.81	0.81
1:A:102:LEU:HD12	1:A:107:PHE:CZ	2.15	0.81
1:A:36:GLN:O	1:A:37:MET:CB	2.29	0.80
1:A:112:VAL:HG23	1:A:322:PHE:HZ	1.45	0.79
1:A:112:VAL:HG12	1:A:113:ALA:N	1.99	0.78
1:A:25:ILE:HD11	1:A:330:ALA:CB	2.14	0.77
1:A:112:VAL:HG13	1:A:116:ALA:HB3	1.70	0.74
1:A:112:VAL:CG1	1:A:113:ALA:N	2.52	0.73
1:A:272:LEU:O	1:A:275:THR:HG22	1.88	0.72
1:A:189:THR:HG22	1:A:286:TYR:HA	1.72	0.72
1:A:112:VAL:HG11	1:A:148:ALA:HB1	1.72	0.71
1:A:112:VAL:CG1	1:A:113:ALA:H	2.02	0.71
1:A:73:CYS:HB3	1:A:76:LEU:N	2.06	0.71
1:A:102:LEU:CD1	1:A:107:PHE:CZ	2.71	0.71
1:A:327:THR:OG1	1:A:329:LEU:HB2	1.91	0.70
1:A:324:ILE:HG12	1:A:329:LEU:HB3	1.73	0.70
1:A:189:THR:CG2	1:A:197:ALA:HB1	2.18	0.70
1:A:176:LEU:HD11	1:A:304:ALA:HB1	1.75	0.69
1:A:112:VAL:HG11	1:A:148:ALA:HB2	1.73	0.69
1:A:37:MET:HE2	1:A:54:PRO:HD2	1.75	0.67
1:A:73:CYS:SG	4:A:2020:HOH:O	2.52	0.67
1:A:116:ALA:O	1:A:120:THR:HG23	1.94	0.67
1:A:11:ARG:N	4:A:2001:HOH:O	2.29	0.66
1:A:14:THR:HG23	4:A:2004:HOH:O	1.97	0.65
1:A:112:VAL:CG1	1:A:148:ALA:CB	2.74	0.65
1:A:21:ASP:HA	1:A:120:THR:CG2	2.26	0.64
1:A:78:LEU:HD23	1:A:96:MET:CE	2.16	0.64
1:A:144:HIS:HD2	1:A:159:TYR:OH	1.81	0.64
1:A:25:ILE:CG1	1:A:330:ALA:HB2	2.27	0.64
1:A:112:VAL:CG1	1:A:148:ALA:HB2	2.28	0.64
1:A:138:ALA:HB1	1:A:342:VAL:HG11	1.78	0.64
1:A:102:LEU:HB3	1:A:107:PHE:CE2	2.30	0.63
1:A:102:LEU:HD13	1:A:107:PHE:CG	2.34	0.62
1:A:102:LEU:HB3	1:A:107:PHE:HZ	1.58	0.62
1:A:118:THR:HG22	1:A:152:SER:CB	2.27	0.61
1:A:333:ALA:HB3	1:A:334:PRO:HD3	1.82	0.61
1:A:224:HIS:CE1	1:A:263:THR:CG2	2.58	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:HG21	1:A:322:PHE:HZ	1.64	0.61
1:A:149:ILE:HG21	1:A:157:ALA:HB2	1.82	0.61
1:A:102:LEU:HD13	1:A:107:PHE:CD2	2.36	0.60
1:A:138:ALA:CB	1:A:342:VAL:HG11	2.32	0.60
1:A:28:GLU:OE2	1:A:32:LYS:NZ	2.34	0.60
1:A:21:ASP:CA	1:A:120:THR:HG22	2.31	0.58
1:A:28:GLU:CD	1:A:328:LEU:HA	2.30	0.57
1:A:224:HIS:HE1	1:A:263:THR:HG21	1.63	0.57
1:A:77:MET:HG2	4:A:2022:HOH:O	2.06	0.55
1:A:172:GLU:OE2	4:A:2092:HOH:O	2.18	0.55
1:A:67:ARG:O	1:A:71:GLN:HG3	2.07	0.55
1:A:118:THR:HG21	4:A:2041:HOH:O	2.06	0.55
1:A:344:THR:CG2	1:A:346:THR:OG1	2.54	0.55
1:A:14:THR:CG2	4:A:2004:HOH:O	2.53	0.55
1:A:25:ILE:CD1	1:A:29:ILE:CG2	2.81	0.54
1:A:25:ILE:CD1	1:A:330:ALA:HB1	2.33	0.54
1:A:25:ILE:HD13	1:A:25:ILE:C	2.29	0.54
1:A:63:PHE:CE1	1:A:107:PHE:CG	2.68	0.53
1:A:25:ILE:HD11	1:A:29:ILE:CG2	2.26	0.53
1:A:208:ARG:NH1	4:A:2124:HOH:O	2.32	0.52
1:A:340:ARG:O	1:A:344:THR:HB	2.09	0.51
1:A:112:VAL:CG1	1:A:148:ALA:HB1	2.38	0.51
1:A:172:GLU:HG2	1:A:205:HIS:CE1	2.46	0.51
1:A:19:ILE:HD12	1:A:27:PRO:HG3	1.92	0.51
1:A:112:VAL:HG13	1:A:113:ALA:H	1.75	0.51
1:A:13:MET:HE1	1:A:342:VAL:HG12	1.94	0.49
1:A:25:ILE:O	1:A:25:ILE:CD1	2.42	0.49
1:A:344:THR:HG22	1:A:346:THR:H	1.77	0.49
1:A:25:ILE:CG1	1:A:330:ALA:CB	2.91	0.48
1:A:25:ILE:HG12	1:A:330:ALA:HB2	1.94	0.48
1:A:113:ALA:HB1	4:A:2040:HOH:O	2.13	0.48
1:A:25:ILE:CD1	1:A:330:ALA:CB	2.88	0.47
1:A:112:VAL:HG12	1:A:113:ALA:H	1.70	0.47
1:A:169:MET:HB2	1:A:170:PRO:HD2	1.96	0.46
1:A:11:ARG:HG3	1:A:12:ALA:H	1.81	0.46
1:A:251:GLU:HB2	1:A:252:PRO:HD3	1.97	0.46
1:A:60:GLY:HA2	1:A:123:TYR:CD1	2.50	0.46
1:A:63:PHE:CE1	1:A:107:PHE:CD1	3.03	0.46
1:A:63:PHE:CE1	1:A:107:PHE:CE1	2.90	0.46
1:A:104:ALA:HA	1:A:107:PHE:CE2	2.51	0.45
1:A:37:MET:CE	1:A:54:PRO:HD2	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:CG2	4:A:2041:HOH:O	2.63	0.45
1:A:102:LEU:CG	1:A:107:PHE:CE1	2.97	0.44
1:A:80:LEU:N	1:A:80:LEU:HD23	2.32	0.44
1:A:25:ILE:HG13	1:A:330:ALA:HB2	1.99	0.44
1:A:102:LEU:CD1	1:A:107:PHE:CD2	2.97	0.43
1:A:63:PHE:HE1	1:A:107:PHE:CG	1.80	0.43
1:A:102:LEU:CD1	1:A:107:PHE:CE2	3.02	0.43
1:A:25:ILE:HG22	1:A:321:GLY:H	1.84	0.42
1:A:11:ARG:N	4:A:2002:HOH:O	2.52	0.42
1:A:102:LEU:HD13	1:A:107:PHE:CE2	2.55	0.42
1:A:88:SER:O	1:A:89:ALA:HB3	2.17	0.42
1:A:215:GLN:NE2	4:A:2129:HOH:O	2.37	0.42
1:A:324:ILE:HG12	1:A:329:LEU:CB	2.46	0.41
1:A:167:MET:HG3	1:A:309:ALA:HB1	2.01	0.41
1:A:104:ALA:CA	1:A:107:PHE:HD2	2.19	0.41
1:A:272:LEU:O	1:A:275:THR:HB	2.21	0.41
1:A:102:LEU:CB	1:A:107:PHE:CE1	3.03	0.41
1:A:23:ASN:HD21	1:A:107:PHE:HA	1.86	0.41

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	295/349 (84%)	283 (96%)	12 (4%)	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	218/254 (86%)	192 (88%)	26 (12%)	5 0

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	14	THR
1	A	25	ILE
1	A	36	GLN
1	A	37	MET
1	A	76	LEU
1	A	79	ARG
1	A	80	LEU
1	A	87	PRO
1	A	88	SER
1	A	102	LEU
1	A	118	THR
1	A	136	VAL
1	A	146	GLU
1	A	147	THR
1	A	189	THR
1	A	201	LEU
1	A	275	THR
1	A	297	ARG
1	A	320	SER
1	A	323	ASP
1	A	324	ILE
1	A	328	LEU
1	A	329	LEU
1	A	344	THR
1	A	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	144	HIS
1	A	224	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	233	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	BME	A	1351	2	3,3,3	0.44	0	2,2,2	0.95	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
3	BME	A	1351	2	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1351	BME	O1-C1-C2-S2

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, 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	309/349 (88%)	0.84	62 (20%) 3 2	12, 26, 61, 73	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	PHE	11.4
1	A	89	ALA	6.7
1	A	87	PRO	6.2
1	A	112	VAL	5.9
1	A	329	LEU	5.6
1	A	76	LEU	5.1
1	A	158	GLY	5.0
1	A	157	ALA	4.9
1	A	327	THR	4.5
1	A	324	ILE	4.4
1	A	106	ALA	4.0
1	A	73	CYS	3.9
1	A	78	LEU	3.6
1	A	318	HIS	3.5
1	A	151	ALA	3.5
1	A	328	LEU	3.5
1	A	322	PHE	3.4
1	A	320	SER	3.4
1	A	323	ASP	3.3
1	A	319	GLY	3.3
1	A	80	LEU	3.3
1	A	147	THR	3.3
1	A	109	PRO	3.2
1	A	94	ILE	3.1
1	A	79	ARG	3.1
1	A	77	MET	3.1
1	A	114	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	11	ARG	3.1
1	A	20	GLY	3.1
1	A	88	SER	3.0
1	A	113	ALA	3.0
1	A	330	ALA	2.9
1	A	317	GLY	2.9
1	A	72	CYS	2.9
1	A	146	GLU	2.7
1	A	321	GLY	2.7
1	A	108	VAL	2.7
1	A	162	PHE	2.6
1	A	349	ALA	2.6
1	A	165	HIS	2.6
1	A	37	MET	2.6
1	A	71	GLN	2.6
1	A	144	HIS	2.5
1	A	115	ALA	2.5
1	A	81	VAL	2.5
1	A	36	GLN	2.5
1	A	133	ALA	2.5
1	A	153	GLY	2.4
1	A	325	ALA	2.4
1	A	69	ALA	2.4
1	A	150	ASN	2.3
1	A	111	GLU	2.3
1	A	159	TYR	2.2
1	A	149	ILE	2.2
1	A	102	LEU	2.2
1	A	148	ALA	2.2
1	A	25	ILE	2.1
1	A	70	ARG	2.1
1	A	110	GLY	2.1
1	A	326	GLY	2.1
1	A	333	ALA	2.1
1	A	129	ARG	2.0

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

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($\text{\AA}^2$)	Q<0.9
3	BME	A	1351	4/4	0.89	0.14	42,42,47,51	0
2	ZN	A	1350	1/1	0.99	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.