



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 07:20 PM EDT

PDB ID : 2PU5  
Title : Crystal Structure of a C-C bond hydrolase, BphD, from Burkholderia xenovorans LB400  
Authors : Bhowmik, S.; Bolin, J.T.  
Deposited on : 2007-05-08  
Resolution : 2.30 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

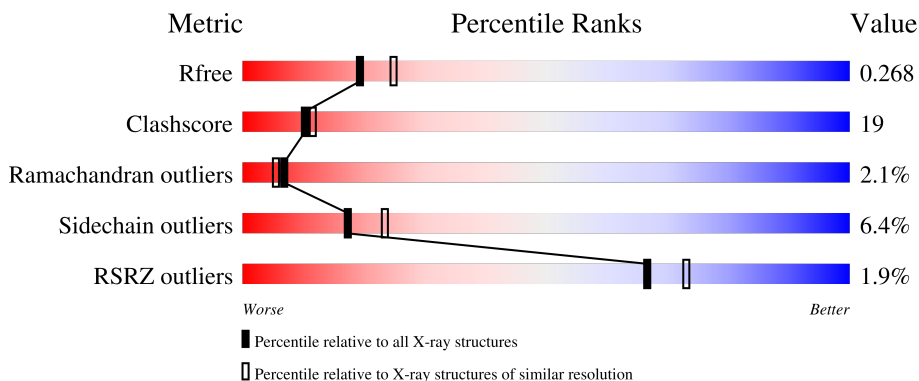
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	286	 80% 17% ..
1	B	286	 4% 48% 44% 7% ..

## 2 Entry composition [i](#)

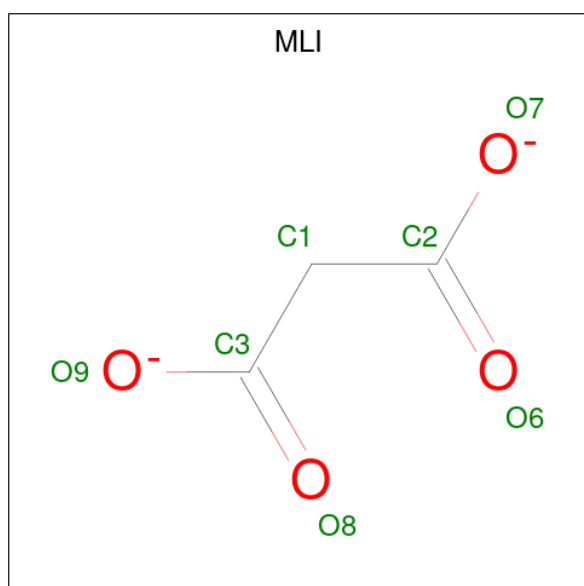
There are 3 unique types of molecules in this entry. The entry contains 4629 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-hydroxy-6-oxo-6-phenylhexa-2,4-dienoate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	2	0
			2265	1451	393	411	10			
1	B	283	Total	C	N	O	S	0	3	0
			2255	1446	388	411	10			

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula:  $C_3H_2O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		

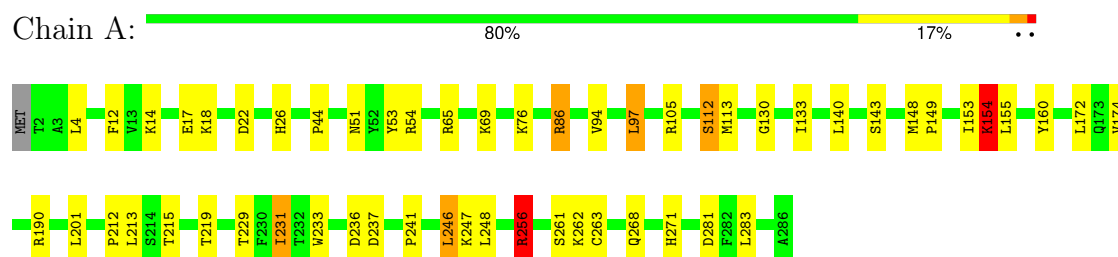
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total 78	O 78	0	0
3	B	17	Total 17	O 17	0	0

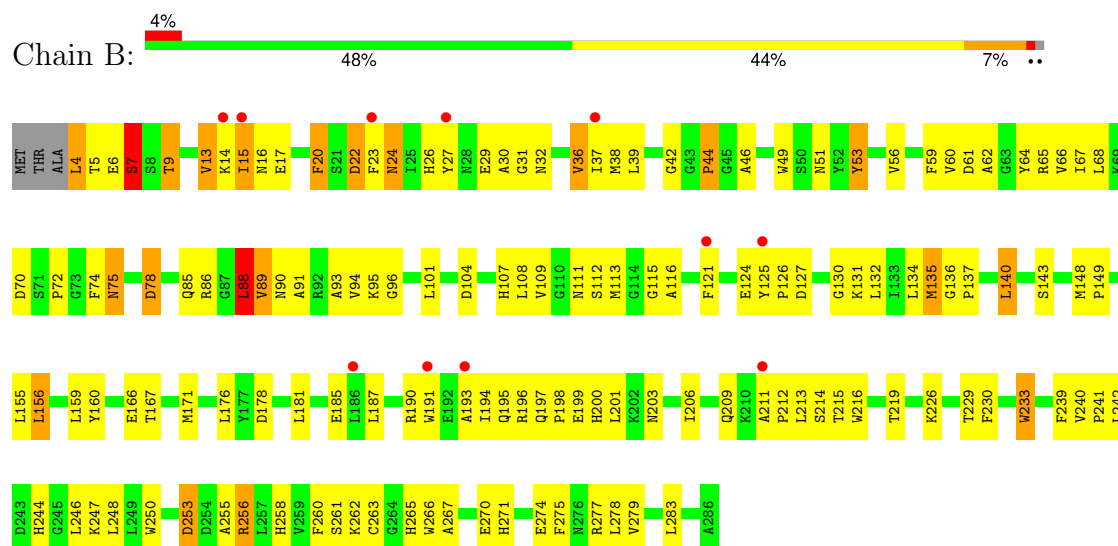
### 3 Residue-property plots

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: 2-hydroxy-6-oxo-6-phenylhexa-2,4-dienoate hydrolase



- Molecule 1: 2-hydroxy-6-oxo-6-phenylhexa-2,4-dienoate hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.18Å 135.18Å 66.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30 47.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 ((Not available)-2.30) 99.6 (47.32-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	12.40	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.270 0.185 , 0.268	Depositor DCC
$R_{free}$ test set	1553 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 40.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MLI

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	1.26	3/2328 (0.1%)	1.22	16/3147 (0.5%)
1	B	0.91	3/2321 (0.1%)	1.01	3/3137 (0.1%)
All	All	1.10	6/4649 (0.1%)	1.12	19/6284 (0.3%)

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	0	2
1	B	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	LYS	N-CA	-27.28	0.91	1.46
1	A	154	LYS	CA-C	10.28	1.79	1.52
1	B	185	GLU	CB-CG	8.01	1.67	1.52
1	B	185	GLU	CG-CD	7.47	1.63	1.51
1	A	53	TYR	CD2-CE2	6.04	1.48	1.39
1	B	270	GLU	CB-CG	5.26	1.62	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	LYS	N-CA-CB	-29.46	57.57	110.60
1	A	153	ILE	C-N-CA	-14.95	84.32	121.70
1	A	256	ARG	NE-CZ-NH1	8.02	124.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	154	LYS	N-CA-C	7.41	131.00	111.00
1	A	256	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	86	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	39	LEU	CB-CG-CD2	-6.27	100.33	111.00
1	B	78	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	253	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	A	65	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	22	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	190	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	237	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	54	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	154	LYS	CA-C-N	-5.06	106.08	117.20
1	A	22	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	246	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	A	231	ILE	N-CA-CB	-5.03	99.22	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	LYS	Mainchain,Peptide
1	B	7	SER	Peptide

## 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	2265	0	2232	34	0
1	B	2255	0	2220	138	0
2	A	7	0	2	0	0
2	B	7	0	2	1	0
3	A	78	0	0	1	0
3	B	17	0	0	1	0
All	All	4629	0	4456	169	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 19.

All (169) 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:154:LYS:CA	1:A:154:LYS:C	1.79	1.50
1:B:6:GLU:HA	1:B:7:SER:O	1.43	1.16
1:B:17:GLU:O	1:B:20:PHE:HB2	1.53	1.08
1:B:9:THR:HG22	1:B:29:GLU:O	1.53	1.07
1:B:23:PHE:CE2	1:B:78:ASP:HB2	2.01	0.96
1:B:197:GLN:HG2	1:B:200:HIS:CE1	2.05	0.90
1:B:275:PHE:O	1:B:279:VAL:HG23	1.73	0.89
1:B:49:TRP:O	1:B:53:TYR:HB3	1.73	0.88
1:B:197:GLN:HB3	1:B:200:HIS:ND1	1.91	0.85
1:B:9:THR:CG2	1:B:29:GLU:O	2.28	0.80
1:B:23:PHE:HZ	1:B:78:ASP:O	1.64	0.80
1:B:74:PHE:CZ	1:B:113:MET:HE1	2.19	0.78
1:A:140:LEU:O	1:A:247:LYS:HE2	1.83	0.77
1:B:23:PHE:CZ	1:B:78:ASP:O	2.41	0.74
1:B:124:GLU:C	1:B:126:PRO:HD3	2.09	0.73
1:B:6:GLU:HA	1:B:7:SER:C	2.07	0.72
1:A:154:LYS:CA	1:A:155:LEU:N	2.52	0.71
1:B:260:PHE:HE2	1:B:274[B]:GLU:HG2	1.56	0.71
1:B:159:LEU:HD13	1:B:167:THR:HG22	1.75	0.69
1:B:135:MET:HE1	1:B:266:TRP:HA	1.74	0.69
1:B:156:LEU:HD13	1:B:239:PHE:HE1	1.59	0.68
1:B:199:GLU:O	1:B:203:ASN:ND2	2.26	0.68
1:B:91:ALA:HA	1:B:94:VAL:HG23	1.76	0.68
1:B:197:GLN:HG2	1:B:200:HIS:HE1	1.55	0.67
1:A:231:ILE:HD13	1:A:248:LEU:HB2	1.76	0.66
1:B:88:LEU:O	1:B:89:VAL:C	2.33	0.66
1:B:59:PHE:O	1:B:64:TYR:HB2	1.94	0.66
1:A:154:LYS:C	1:A:154:LYS:HA	2.07	0.66
1:B:60:VAL:C	1:B:62:ALA:H	2.00	0.65
1:B:219:THR:HG21	1:B:247:LYS:HE2	1.79	0.65
1:B:213:LEU:HD22	1:B:216:TRP:CZ2	2.33	0.64
1:B:56:VAL:HG23	1:B:66:VAL:HG11	1.78	0.64
1:B:206:ILE:O	1:B:209:GLN:HB2	1.96	0.64
1:B:155:LEU:HD13	1:B:171:MET:HA	1.82	0.62
1:B:274[A]:GLU:HG3	3:B:302:HOH:O	2.01	0.61
1:B:140:LEU:O	1:B:247:LYS:NZ	2.32	0.60
1:B:86:ARG:O	1:B:90:ASN:HB2	2.01	0.60
1:B:44:PRO:HD3	1:B:160:TYR:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:HIS:CE1	1:B:278:LEU:HD11	2.36	0.60
1:B:37:ILE:HB	1:B:108:LEU:CD2	2.32	0.60
1:B:132:LEU:O	1:B:229:THR:HA	2.00	0.60
1:A:281:ASP:OD1	1:B:277:ARG:HD2	2.02	0.59
1:A:143:SER:HB2	1:A:241:PRO:HG3	1.83	0.59
1:B:90:ASN:O	1:B:93:ALA:HB3	2.03	0.59
1:B:197:GLN:N	1:B:198:PRO:CD	2.65	0.58
1:B:230:PHE:HD1	1:B:256:ARG:HG2	1.68	0.58
1:A:105[B]:ARG:HD3	1:A:130:GLY:N	2.18	0.58
1:B:156:LEU:HD13	1:B:239:PHE:CE1	2.39	0.58
1:B:6:GLU:OE2	1:B:7:SER:HA	2.03	0.58
1:A:154:LYS:C	1:A:154:LYS:CB	2.69	0.58
1:A:17:GLU:HG3	1:A:18:LYS:HB2	1.87	0.57
1:B:14:LYS:HD3	1:B:24:ASN:HB2	1.87	0.57
1:B:258:HIS:NE2	1:B:278:LEU:HD11	2.20	0.56
1:B:263:CYS:HB2	1:B:271:HIS:CD2	2.40	0.56
1:B:260:PHE:CE2	1:B:274[B]:GLU:HG2	2.37	0.55
1:B:26:HIS:O	1:B:70:ASP:HB2	2.06	0.55
1:B:176:LEU:N	1:B:176:LEU:HD23	2.20	0.55
1:B:230:PHE:CD1	1:B:256:ARG:HG2	2.40	0.55
1:B:258:HIS:NE2	1:B:274[B]:GLU:OE2	2.33	0.55
1:B:216:TRP:N	1:B:216:TRP:CD1	2.74	0.55
1:B:125:TYR:N	1:B:126:PRO:HD3	2.22	0.55
1:B:191:TRP:O	1:B:195:GLN:HG3	2.06	0.54
1:B:23:PHE:CZ	1:B:78:ASP:HB2	2.42	0.54
1:B:74:PHE:CE1	1:B:113:MET:HE1	2.43	0.54
1:B:74:PHE:CE1	1:B:113:MET:CE	2.91	0.54
1:B:135:MET:HE2	1:B:267:ALA:N	2.24	0.53
1:B:115:GLY:HA3	1:B:137:PRO:HB3	1.90	0.53
1:B:4:LEU:CD2	1:B:5:THR:N	2.72	0.53
1:B:124:GLU:O	1:B:126:PRO:HD3	2.08	0.53
1:B:29:GLU:HG2	1:B:30:ALA:N	2.23	0.53
1:A:219:THR:OG1	1:A:247:LYS:HE3	2.09	0.52
1:B:4:LEU:HD23	1:B:5:THR:H	1.75	0.52
1:A:155:LEU:CD1	1:A:174:VAL:HG21	2.39	0.51
1:A:261:SER:HB2	1:B:255:ALA:O	2.10	0.51
1:B:219:THR:CG2	1:B:247:LYS:HE2	2.40	0.51
1:B:166[A]:GLU:HA	1:B:166[A]:GLU:OE2	2.10	0.51
1:B:27:TYR:CZ	1:B:101:LEU:HD11	2.45	0.51
1:A:97:LEU:C	1:A:97:LEU:HD23	2.31	0.51
1:B:131:LYS:NZ	1:B:283:LEU:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:TRP:HA	1:B:191:TRP:CE3	2.46	0.50
1:B:195:GLN:O	1:B:198:PRO:HD3	2.11	0.50
1:B:36:VAL:HG13	1:B:107:HIS:HB2	1.92	0.50
1:A:12:PHE:CE2	1:A:26:HIS:HB2	2.46	0.50
1:A:105[B]:ARG:HD3	1:A:130:GLY:CA	2.41	0.50
1:B:38:MET:HG2	1:B:109:VAL:HB	1.94	0.49
1:B:261:SER:O	1:B:262:LYS:HB2	2.11	0.49
1:B:70:ASP:OD2	1:B:75:ASN:HB3	2.12	0.49
1:B:136:GLY:O	1:B:240:VAL:HG21	2.12	0.49
1:B:31:GLY:O	1:B:65:ARG:HG3	2.13	0.49
1:A:112:SER:OG	1:A:113:MET:N	2.43	0.49
1:B:212:PRO:O	1:B:215:THR:N	2.30	0.49
1:B:111:ASN:OD1	1:B:111:ASN:C	2.49	0.49
1:B:94:VAL:C	1:B:96:GLY:N	2.65	0.48
1:B:136:GLY:N	1:B:137:PRO:HD3	2.28	0.48
1:B:4:LEU:HD22	1:B:5:THR:N	2.28	0.48
1:B:16:ASN:HA	1:B:20:PHE:O	2.14	0.48
1:B:27:TYR:OH	1:B:101:LEU:HD11	2.13	0.48
1:B:44:PRO:HG2	1:B:159:LEU:HB3	1.95	0.48
1:B:49:TRP:HA	1:B:68:LEU:HD13	1.96	0.48
1:B:211:ALA:O	1:B:212:PRO:C	2.51	0.47
1:B:42:GLY:HA2	1:B:113:MET:CE	2.44	0.47
1:B:134:LEU:HB3	1:B:137:PRO:HG3	1.96	0.47
1:B:60:VAL:C	1:B:62:ALA:N	2.68	0.46
1:B:143:SER:HB2	1:B:241:PRO:HG3	1.96	0.46
1:B:15:ILE:O	1:B:15:ILE:HG12	2.11	0.46
1:B:88:LEU:O	1:B:90:ASN:N	2.47	0.46
1:B:46:ALA:HA	1:B:190:ARG:NH1	2.30	0.46
1:B:42:GLY:HA2	1:B:113:MET:HE1	1.96	0.45
1:B:241:PRO:O	1:B:244:HIS:HB2	2.16	0.45
1:B:178:ASP:OD1	1:B:178:ASP:C	2.54	0.45
1:B:239:PHE:CD2	1:B:240:VAL:HG13	2.52	0.45
1:B:258:HIS:CE1	1:B:278:LEU:CD1	2.99	0.45
1:B:258:HIS:NE2	1:B:278:LEU:CD1	2.79	0.45
1:A:262:LYS:HE3	1:B:253:ASP:O	2.16	0.45
1:B:36:VAL:HG13	1:B:107:HIS:CB	2.47	0.45
1:B:212:PRO:O	1:B:214:SER:N	2.50	0.45
1:A:14:LYS:HD3	1:A:14:LYS:HA	1.69	0.45
1:B:113:MET:O	1:B:116:ALA:HB3	2.17	0.44
1:A:133:ILE:HD11	1:A:283:LEU:HD21	1.98	0.44
1:B:75:ASN:OD1	1:B:193:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HA	1:B:248:LEU:HD23	1.73	0.44
1:B:274[A]:GLU:HG3	1:B:274[A]:GLU:H	1.23	0.44
1:A:160:TYR:CD2	1:A:201:LEU:HA	2.53	0.44
1:B:29:GLU:HG2	1:B:30:ALA:H	1.81	0.44
1:B:191:TRP:HA	1:B:191:TRP:HE3	1.82	0.44
1:A:86:ARG:HD2	3:A:329:HOH:O	2.17	0.44
1:B:37:ILE:HB	1:B:108:LEU:HD23	2.00	0.43
1:B:112:SER:HA	1:B:137:PRO:HA	1.99	0.43
1:B:135:MET:HE2	1:B:267:ALA:H	1.83	0.43
1:B:239:PHE:CD2	1:B:265:HIS:CE1	3.06	0.43
1:A:219:THR:OG1	1:A:247:LYS:CE	2.67	0.43
1:B:148:MET:HA	1:B:149:PRO:C	2.38	0.43
1:B:23:PHE:CD2	1:B:23:PHE:C	2.92	0.43
1:B:137:PRO:HD2	1:B:233:TRP:CZ3	2.54	0.43
1:B:86:ARG:O	1:B:90:ASN:CB	2.67	0.43
1:B:197:GLN:N	1:B:198:PRO:HD2	2.32	0.43
1:B:181:LEU:HD23	1:B:181:LEU:HA	1.88	0.43
1:A:4:LEU:HD23	1:A:4:LEU:C	2.39	0.43
1:B:67:ILE:O	1:B:67:ILE:HG22	2.19	0.43
1:B:136:GLY:N	1:B:137:PRO:CD	2.82	0.43
1:B:190:ARG:NH2	2:B:287:MLI:O6	2.36	0.43
1:B:23:PHE:CZ	1:B:78:ASP:CB	3.02	0.42
1:B:191:TRP:CZ3	1:B:194:ILE:HG21	2.54	0.42
1:A:69:LYS:HE3	1:A:94:VAL:HA	2.01	0.42
1:A:236:ASP:HB2	1:A:263:CYS:O	2.19	0.42
1:A:268:GLN:OE1	1:A:268:GLN:N	2.50	0.42
1:B:74:PHE:CE1	1:B:113:MET:HE3	2.55	0.42
1:B:212:PRO:O	1:B:215:THR:HG23	2.19	0.42
1:B:246:LEU:O	1:B:250:TRP:HD1	2.03	0.42
1:B:111:ASN:OD1	1:B:112:SER:N	2.52	0.42
1:A:148:MET:HA	1:A:149:PRO:C	2.40	0.41
1:B:112:SER:HB2	1:B:265:HIS:CE1	2.55	0.41
1:B:135:MET:CE	1:B:266:TRP:HA	2.47	0.41
1:A:26:HIS:CG	1:A:76:LYS:HB2	2.56	0.41
1:B:4:LEU:HD23	1:B:5:THR:N	2.34	0.41
1:B:132:LEU:HD11	1:B:134:LEU:HD21	2.02	0.41
1:A:229:THR:O	1:A:256:ARG:HD2	2.21	0.41
1:A:263:CYS:SG	1:A:271:HIS:CD2	3.13	0.41
1:A:44:PRO:HG3	1:A:160:TYR:CD1	2.55	0.41
1:B:44:PRO:HB2	1:B:159:LEU:HD23	2.02	0.41
1:B:60:VAL:O	1:B:62:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:O	1:A:215:THR:OG1	2.34	0.41
1:A:246:LEU:HA	1:A:246:LEU:HD23	1.90	0.41
1:B:121:PHE:CE2	1:B:125:TYR:HB2	2.56	0.41
1:B:132:LEU:HG	1:B:229:THR:HG23	2.02	0.41
1:B:197:GLN:CG	1:B:200:HIS:CE1	2.92	0.41
1:B:159:LEU:HD12	1:B:159:LEU:HA	1.89	0.40
1:B:72:PRO:HD2	1:B:90:ASN:OD1	2.21	0.40
1:B:121:PHE:O	1:B:121:PHE:CD2	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	285/286 (100%)	275 (96%)	10 (4%)	0	100	100
1	B	284/286 (99%)	243 (86%)	29 (10%)	12 (4%)	3	1
All	All	569/572 (100%)	518 (91%)	39 (7%)	12 (2%)	7	5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	SER
1	B	61	ASP
1	B	88	LEU
1	B	89	VAL
1	B	140	LEU
1	B	22	ASP
1	B	75	ASN
1	B	95	LYS
1	B	242	LEU
1	B	130	GLY

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Mol	Chain	Res	Type
1	B	13	VAL
1	B	44	PRO

### 5.3.2 Protein sidechains ⓘ

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	236/235 (100%)	229 (97%)	7 (3%)	41	57
1	B	236/235 (100%)	213 (90%)	23 (10%)	8	9
All	All	472/470 (100%)	442 (94%)	30 (6%)	17	23

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	97	LEU
1	A	112	SER
1	A	172	LEU
1	A	213	LEU
1	A	233	TRP
1	A	256	ARG
1	B	4	LEU
1	B	9	THR
1	B	13	VAL
1	B	15	ILE
1	B	20	PHE
1	B	22	ASP
1	B	24	ASN
1	B	32	ASN
1	B	36	VAL
1	B	51	ASN
1	B	53	TYR
1	B	85	GLN
1	B	88	LEU
1	B	104	ASP

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Mol	Chain	Res	Type
1	B	127	ASP
1	B	135	MET
1	B	156	LEU
1	B	187	LEU
1	B	196	ARG
1	B	201	LEU
1	B	226	LYS
1	B	233	TRP
1	B	256	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	MLI	A	287	-	6,6,6	1.39	1 (16%)	7,7,7	2.24	4 (57%)
2	MLI	B	287	-	6,6,6	1.01	0	7,7,7	1.54	2 (28%)

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	MLI	A	287	-	-	1/4/4/4	-
2	MLI	B	287	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	287	MLI	C1-C2	-2.42	1.47	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	287	MLI	O8-C3-C1	-3.67	111.66	122.11
2	A	287	MLI	O6-C2-C1	-2.89	113.89	122.11
2	B	287	MLI	O8-C3-C1	-2.25	115.69	122.11
2	A	287	MLI	O9-C3-O8	2.18	128.93	123.33
2	B	287	MLI	O7-C2-C1	2.12	121.09	114.51
2	A	287	MLI	O7-C2-O6	2.07	128.67	123.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	287	MLI	C2-C1-C3-O8
2	B	287	MLI	C2-C1-C3-O8
2	B	287	MLI	C2-C1-C3-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	287	MLI	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	285/286 (99%)	-0.33	0 100 100	21, 33, 53, 77	0
1	B	283/286 (98%)	0.20	11 (3%) 39 46	33, 62, 93, 118	0
All	All	568/572 (99%)	-0.07	11 (1%) 66 73	21, 44, 86, 118	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	PHE	5.7
1	B	191	TRP	3.7
1	B	27	TYR	3.2
1	B	121	PHE	3.0
1	B	125	TYR	2.7
1	B	186	LEU	2.7
1	B	211	ALA	2.4
1	B	14	LYS	2.3
1	B	193	ALA	2.3
1	B	15	ILE	2.3
1	B	37	ILE	2.1

### 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MLI	B	287	7/7	0.98	0.17	47,66,98,104	0
2	MLI	A	287	7/7	0.99	0.12	25,29,39,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.