



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:50 am BST

PDB ID : 5Y0M  
Title : Structure of 6-aminohexanoate-oligomer hydrolase from *Arthrobacter* sp. KI72., D36A/D122G/H130Y/E263Q muntant  
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Deposited on : 2017-07-18  
Resolution : 1.03 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

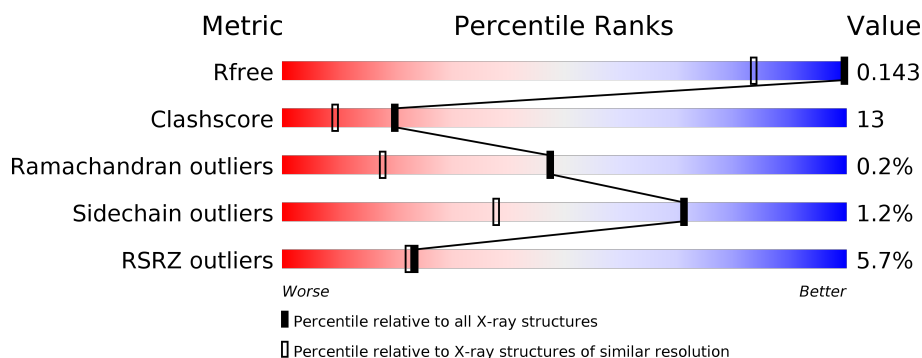
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.03 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	1596 (1.10-0.98)
Clashscore	141614	1677 (1.10-0.98)
Ramachandran outliers	138981	1591 (1.10-0.98)
Sidechain outliers	138945	1589 (1.10-0.98)
RSRZ outliers	127900	1557 (1.10-0.98)

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  $\geq 3$ , 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	355	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• 7%</div> </div> </div>
1	B	355	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>• 6%</div> </div> </div>

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	GOL	A	1003	-	-	X	-
2	GOL	A	1006	-	-	X	-
2	GOL	B	402	-	-	X	-
2	GOL	B	403	-	-	X	-
2	GOL	B	404	-	X	X	-
2	GOL	B	405	-	-	X	-
3	PO4	A	1007	-	-	X	-
3	PO4	B	407	-	-	X	-
4	CL	A	1008	-	-	X	-
4	CL	B	408	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6014 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 Endo-type 6-aminohexanoate oligomer hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	34	0
			2637	1666	474	487	10			
1	B	332	Total	C	N	O	S	0	39	0
			2696	1709	479	496	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ALA	ASP	engineered mutation	UNP Q57326
A	122	GLY	ASP	engineered mutation	UNP Q57326
A	130	TYR	HIS	engineered mutation	UNP Q57326
A	263	GLN	GLU	engineered mutation	UNP Q57326
B	36	ALA	ASP	engineered mutation	UNP Q57326
B	122	GLY	ASP	engineered mutation	UNP Q57326
B	130	TYR	HIS	engineered mutation	UNP Q57326
B	263	GLN	GLU	engineered mutation	UNP Q57326

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	2	Total	Cl	0	0
			2	2		

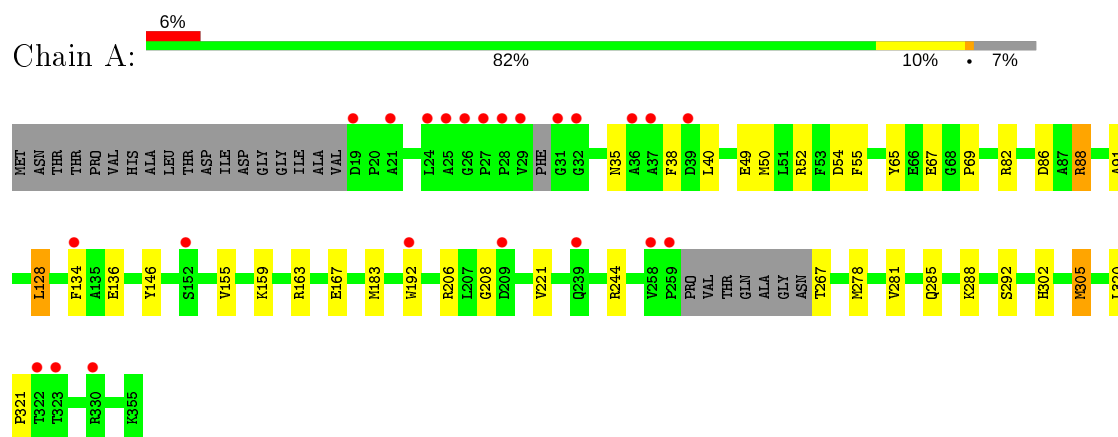
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	291	Total	O	0	0
			291	291		
5	B	304	Total	O	0	0
			304	304		

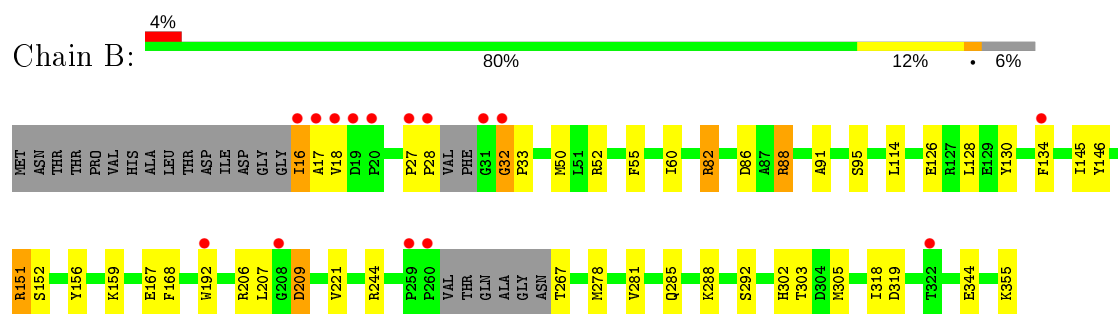
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Endo-type 6-aminohexanoate oligomer hydrolase



- Molecule 1: Endo-type 6-aminohexanoate oligomer hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.42Å 144.42Å 128.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.21 – 1.03 47.95 – 1.03	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.21-1.03) 99.8 (47.95-1.03)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 1.03Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.116 , 0.134 0.126 , 0.143	Depositor DCC
$R_{free}$ test set	16076 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.7	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: GOL, PO4, CL

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	0.83	2/2757 (0.1%)	0.91	3/3739 (0.1%)
1	B	0.94	5/2828 (0.2%)	0.98	12/3834 (0.3%)
All	All	0.89	7/5585 (0.1%)	0.95	15/7573 (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	A	0	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	SER	CA-CB	7.32	1.64	1.52
1	A	49	GLU	CB-CG	-6.62	1.39	1.52
1	B	344	GLU	CD-OE2	-6.61	1.18	1.25
1	A	292	SER	CA-CB	6.47	1.62	1.52
1	B	32	GLY	N-CA	-6.12	1.36	1.46
1	B	156	TYR	CE1-CZ	-5.92	1.30	1.38
1	B	156	TYR	CD2-CE2	5.91	1.48	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	GLY	N-CA-C	8.99	135.58	113.10
1	A	54	ASP	CB-CG-OD1	7.30	124.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86[A]	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	86[B]	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	60[A]	ILE	CG1-CB-CG2	5.71	123.95	111.40
1	B	60[B]	ILE	CG1-CB-CG2	5.71	123.95	111.40
1	B	156	TYR	CG-CD2-CE2	-5.70	116.74	121.30
1	B	168	PHE	CB-CG-CD1	5.66	124.76	120.80
1	B	244	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	207[A]	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	B	207[B]	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	B	82[A]	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	82[B]	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	156	TYR	CG-CD1-CE1	5.21	125.47	121.30
1	B	244	ARG	CD-NE-CZ	5.02	130.63	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88[A]	ARG	Sidechain
1	B	88[A]	ARG	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	2637	0	2651	47	0
1	B	2696	0	2724	79	0
2	A	36	0	48	10	0
2	B	36	0	48	20	0
3	A	5	0	0	7	0
3	B	5	0	0	8	0
4	A	2	0	0	2	0
4	B	2	0	0	3	0
5	A	291	0	0	15	0
5	B	304	0	0	20	1
All	All	6014	0	5471	137	1

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 13.

All (137) 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:305[C]:MET:SD	1:B:305[C]:MET:CG	2.03	1.47
1:A:288[B]:LYS:HE2	5:A:1193:HOH:O	1.23	1.35
1:B:88[A]:ARG:NH2	3:B:407:PO4:O4	1.61	1.30
1:A:88[A]:ARG:NH2	3:A:1007:PO4:O2	1.65	1.28
1:A:288[B]:LYS:CE	5:A:1193:HOH:O	1.76	1.24
2:B:405:GOL:H12	5:B:696:HOH:O	1.34	1.21
1:B:206:ARG:NH1	1:B:209[B]:ASP:OD1	1.73	1.19
1:B:128[B]:LEU:HD23	5:B:603:HOH:O	1.44	1.15
2:B:405:GOL:C1	5:B:696:HOH:O	1.84	1.12
1:A:128[B]:LEU:HD23	5:A:1211:HOH:O	1.52	1.08
1:B:16:ILE:HD13	1:B:355:LYS:CG	1.83	1.08
2:A:1006:GOL:O1	4:A:1008:CL:CL	2.09	1.05
1:B:16:ILE:CD1	1:B:355:LYS:HG3	1.86	1.04
1:B:305[A]:MET:HE2	5:B:555:HOH:O	1.55	1.04
1:A:88[A]:ARG:CZ	3:A:1007:PO4:P	2.48	1.01
1:B:88[A]:ARG:CZ	3:B:407:PO4:P	2.51	0.98
1:B:146:TYR:H	2:B:404:GOL:H31	1.26	0.98
1:B:128[B]:LEU:CD2	5:B:603:HOH:O	2.05	0.97
1:B:82[A]:ARG:NH2	1:B:278:MET:O	1.98	0.96
1:B:146:TYR:H	2:B:404:GOL:C3	1.79	0.95
1:B:305[A]:MET:CE	5:B:555:HOH:O	2.09	0.93
1:B:16:ILE:HD13	1:B:355:LYS:CB	1.98	0.92
1:A:88[A]:ARG:CZ	3:A:1007:PO4:O1	2.16	0.92
1:B:16:ILE:HD11	1:B:18:VAL:HG22	1.49	0.92
1:B:16:ILE:HD13	1:B:355:LYS:HB2	1.54	0.90
1:B:146:TYR:N	2:B:404:GOL:H31	1.88	0.89
1:B:305[C]:MET:HB3	1:B:305[C]:MET:CE	2.03	0.88
1:A:50[B]:MET:SD	1:A:52:ARG:CZ	2.62	0.87
1:B:16:ILE:CD1	1:B:355:LYS:CG	2.51	0.87
1:A:305[B]:MET:CE	5:A:1122:HOH:O	2.22	0.86
1:B:192[B]:TRP:CD1	5:B:668:HOH:O	2.27	0.86
1:B:221:VAL:HG21	1:B:305[C]:MET:HB2	1.57	0.85
2:A:1003:GOL:H31	5:A:1306:HOH:O	1.78	0.82
1:B:88[A]:ARG:CZ	3:B:407:PO4:O1	2.28	0.82
1:A:192[B]:TRP:CD1	5:A:1274:HOH:O	2.34	0.81
1:B:305[C]:MET:HB3	1:B:305[C]:MET:HE2	1.61	0.81
2:B:402:GOL:H2	5:B:639:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88[A]:ARG:CZ	3:A:1007:PO4:O2	2.29	0.80
1:A:82[B]:ARG:NH2	1:A:278:MET:O	2.13	0.79
1:A:159[B]:LYS:HD3	1:B:159[B]:LYS:HD3	1.63	0.79
1:B:114:LEU:O	2:B:405:GOL:H32	1.82	0.79
1:B:27:PRO:HA	1:B:28:PRO:O	1.83	0.79
1:B:16:ILE:HD11	1:B:18:VAL:CG2	2.13	0.79
1:B:50[B]:MET:SD	1:B:52:ARG:CZ	2.72	0.77
1:A:50[B]:MET:SD	1:A:52:ARG:NH2	2.57	0.77
1:A:305[B]:MET:HE1	5:A:1122:HOH:O	1.82	0.77
1:B:305[C]:MET:SD	1:B:305[C]:MET:CB	2.74	0.76
1:B:88[A]:ARG:CZ	3:B:407:PO4:O4	2.34	0.76
1:A:221:VAL:HG21	1:A:305[A]:MET:HB2	1.67	0.75
1:B:16:ILE:HD11	1:B:18:VAL:HA	1.68	0.75
1:A:88[A]:ARG:NH1	3:A:1007:PO4:P	2.60	0.74
1:B:319[B]:ASP:OD1	5:B:501:HOH:O	2.05	0.74
1:A:88[A]:ARG:NE	3:A:1007:PO4:O1	2.20	0.73
1:B:88[A]:ARG:NH2	3:B:407:PO4:P	2.60	0.72
1:A:305[B]:MET:HE2	5:A:1122:HOH:O	1.87	0.72
1:B:88[A]:ARG:NH1	3:B:407:PO4:P	2.63	0.70
1:B:16:ILE:HD12	1:B:17:ALA:C	2.11	0.70
4:B:409:CL:CL	5:B:739:HOH:O	2.45	0.70
1:B:50[B]:MET:SD	1:B:52:ARG:NH2	2.64	0.70
1:B:88[A]:ARG:NH1	3:B:407:PO4:O2	2.24	0.70
1:A:88[A]:ARG:NH1	3:A:1007:PO4:O4	2.24	0.69
1:A:67[A]:GLU:OE1	5:A:1101:HOH:O	2.11	0.67
1:B:16:ILE:CD1	1:B:18:VAL:HG22	2.24	0.65
1:B:16:ILE:HD13	1:B:355:LYS:CD	2.26	0.65
1:A:167[B]:GLU:OE2	5:A:1103:HOH:O	2.15	0.64
1:B:88[A]:ARG:NE	3:B:407:PO4:O1	2.30	0.64
1:B:145:ILE:HA	2:B:404:GOL:H32	1.80	0.64
1:B:88[B]:ARG:HG2	1:B:302:HIS:CD2	2.33	0.64
1:B:16:ILE:HD12	1:B:355:LYS:HG3	1.78	0.63
1:B:16:ILE:HD11	1:B:18:VAL:CA	2.28	0.63
1:B:126:GLU:HG2	1:B:130[B]:TYR:OH	1.99	0.62
2:A:1006:GOL:H11	5:A:1306:HOH:O	1.99	0.62
1:A:159[B]:LYS:HD3	1:B:159[B]:LYS:CD	2.29	0.62
1:A:267:THR:OG1	2:A:1003:GOL:H32	1.99	0.61
1:A:88[B]:ARG:HG2	1:A:302:HIS:CD2	2.35	0.61
1:A:163[A]:ARG:NH2	5:A:1102:HOH:O	2.12	0.60
1:B:281:VAL:O	1:B:285[B]:GLN:HG2	2.02	0.60
2:B:403:GOL:H2	4:B:408:CL:CL	2.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:THR:N	2:A:1006:GOL:HO3	1.99	0.60
1:B:267:THR:N	2:B:403:GOL:HO3	2.00	0.60
1:B:16:ILE:CD1	1:B:18:VAL:HA	2.32	0.59
1:B:91[A]:ALA:HA	2:B:402:GOL:H31	1.84	0.59
2:B:403:GOL:H11	5:B:686:HOH:O	2.01	0.59
1:B:126:GLU:HG2	1:B:130[B]:TYR:CZ	2.38	0.58
2:B:402:GOL:C3	5:B:505:HOH:O	2.51	0.57
1:B:86:ASP:OD1	1:B:288[B]:LYS:HD2	2.04	0.57
1:B:305[A]:MET:HE1	5:B:555:HOH:O	1.89	0.57
1:B:221:VAL:HG21	1:B:305[A]:MET:HB2	1.87	0.57
1:B:16:ILE:CD1	1:B:355:LYS:CB	2.78	0.56
2:B:402:GOL:H32	5:B:505:HOH:O	2.05	0.56
1:A:128[B]:LEU:CD2	5:A:1211:HOH:O	2.29	0.56
1:A:221:VAL:HG23	2:A:1006:GOL:H31	1.89	0.53
1:B:303:THR:OG1	1:B:305[C]:MET:HG3	2.09	0.53
1:B:16:ILE:HD13	1:B:355:LYS:HD2	1.91	0.53
1:B:28:PRO:HG2	1:B:151[B]:ARG:O	2.09	0.52
2:B:405:GOL:H11	5:B:696:HOH:O	1.69	0.52
1:B:82[B]:ARG:HG3	5:B:645:HOH:O	2.10	0.51
1:B:16:ILE:CD1	1:B:355:LYS:HB2	2.36	0.51
1:B:32:GLY:HA3	1:B:152[A]:SER:O	2.11	0.51
1:B:319[B]:ASP:CG	5:B:501:HOH:O	2.48	0.51
1:B:146:TYR:N	2:B:404:GOL:C3	2.57	0.50
1:B:16:ILE:HG13	1:B:18:VAL:HG23	1.94	0.50
1:A:38:PHE:CD1	1:A:67[B]:GLU:HG2	2.47	0.49
1:A:267:THR:OG1	2:A:1003:GOL:C3	2.60	0.48
1:A:221:VAL:CG2	2:A:1006:GOL:H31	2.44	0.48
1:A:206[A]:ARG:NE	1:A:208:GLY:O	2.33	0.48
1:A:221:VAL:HG21	1:A:305[B]:MET:HB2	1.96	0.47
1:B:16:ILE:CD1	1:B:18:VAL:CG2	2.87	0.47
2:B:403:GOL:C2	4:B:408:CL:CL	2.99	0.47
1:B:32:GLY:HA2	1:B:33[B]:PRO:HD2	1.84	0.47
1:B:16:ILE:HG23	5:B:713:HOH:O	2.15	0.47
1:A:281:VAL:O	1:A:285[B]:GLN:HG2	2.15	0.47
1:A:69:PRO:HB2	1:A:183[B]:MET:CG	2.45	0.47
1:A:320[A]:LEU:HB3	1:A:321:PRO:HD2	1.96	0.47
1:B:305[C]:MET:SD	1:B:305[C]:MET:HB3	2.48	0.46
1:B:16:ILE:CD1	1:B:18:VAL:CA	2.92	0.46
1:A:91[A]:ALA:HB1	2:A:1003:GOL:O3	2.15	0.46
1:A:40:LEU:HB3	1:A:65:TYR:CE1	2.51	0.46
1:A:69:PRO:HB2	1:A:183[B]:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ILE:CG2	5:B:713:HOH:O	2.63	0.46
1:B:267:THR:OG1	2:B:404:GOL:C2	2.64	0.45
1:B:16:ILE:CG1	1:B:18:VAL:HG22	2.46	0.45
1:A:288[B]:LYS:HE3	5:A:1193:HOH:O	1.75	0.44
1:B:16:ILE:CG1	1:B:18:VAL:CG2	2.95	0.44
1:A:244[A]:ARG:HG3	5:A:1305:HOH:O	2.16	0.44
1:A:134[B]:PHE:C	1:A:136:GLU:N	2.72	0.43
1:A:35:ASN:OD1	1:A:155:VAL:HA	2.18	0.43
1:A:159[B]:LYS:HB3	1:A:159[B]:LYS:HE3	1.63	0.43
1:B:167:GLU:OE1	5:B:503:HOH:O	2.20	0.42
1:A:305[A]:MET:HE2	1:A:305[A]:MET:HB3	1.88	0.42
1:B:318[A]:ILE:HG21	1:B:318[A]:ILE:HD13	1.75	0.42
2:A:1006:GOL:C1	4:A:1008:CL:CL	3.01	0.41
1:B:16:ILE:HD12	1:B:17:ALA:O	2.20	0.41
1:A:146:TYR:CE1	1:B:134[B]:PHE:CE1	3.09	0.40
1:B:146:TYR:CB	2:B:404:GOL:H31	2.51	0.40
1:B:95[B]:SER:OG	2:B:405:GOL:H31	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:509:HOH:O	5:B:595:HOH:O[3_455]	1.87	0.33

## 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	357/355 (101%)	345 (97%)	12 (3%)	0	100	100
1	B	367/355 (103%)	347 (95%)	18 (5%)	2 (0%)	29	7
All	All	724/710 (102%)	692 (96%)	30 (4%)	2 (0%)	47	14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209[A]	ASP
1	B	209[B]	ASP

### 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	268/260 (103%)	263 (98%)	5 (2%)	57	21
1	B	278/260 (107%)	274 (99%)	4 (1%)	67	32
All	All	546/520 (105%)	537 (98%)	9 (2%)	71	27

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	128[A]	LEU
1	A	128[B]	LEU
1	A	305[A]	MET
1	A	305[B]	MET
1	B	16	ILE
1	B	55	PHE
1	B	151[A]	ARG
1	B	151[B]	ARG

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

Mol	Chain	Res	Type
1	A	284	ASN
1	A	302	HIS
1	B	239	GLN
1	B	302	HIS

### 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 ⓘ

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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$
2	GOL	B	404	-	5,5,5	0.57	0	5,5,5	2.60	2 (40%)
2	GOL	A	1001	-	5,5,5	0.61	0	5,5,5	0.26	0
3	PO4	B	407	-	4,4,4	0.93	0	6,6,6	1.39	1 (16%)
2	GOL	A	1004	-	5,5,5	0.42	0	5,5,5	0.52	0
2	GOL	B	405	-	5,5,5	0.59	0	5,5,5	1.07	0
2	GOL	B	406	-	5,5,5	0.89	0	5,5,5	1.49	1 (20%)
3	PO4	A	1007	-	4,4,4	1.08	1 (25%)	6,6,6	1.59	1 (16%)
2	GOL	B	402	-	5,5,5	0.60	0	5,5,5	1.08	0
2	GOL	A	1003	-	5,5,5	0.81	0	5,5,5	1.18	1 (20%)
2	GOL	B	401	-	5,5,5	0.94	0	5,5,5	0.36	0
2	GOL	A	1006	-	5,5,5	0.77	0	5,5,5	1.58	1 (20%)
2	GOL	B	403	-	5,5,5	0.43	0	5,5,5	1.79	2 (40%)
2	GOL	A	1005	-	5,5,5	1.03	0	5,5,5	0.46	0
2	GOL	A	1002	-	5,5,5	0.68	0	5,5,5	0.90	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	GOL	B	404	-	-	4/4/4/4	-
2	GOL	A	1001	-	-	1/4/4/4	-
2	GOL	A	1004	-	-	0/4/4/4	-
2	GOL	B	405	-	-	1/4/4/4	-
2	GOL	B	406	-	-	2/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	B	402	-	-	4/4/4/4	-
2	GOL	A	1003	-	-	2/4/4/4	-
2	GOL	A	1006	-	-	0/4/4/4	-
2	GOL	B	403	-	-	2/4/4/4	-
2	GOL	A	1005	-	-	0/4/4/4	-
2	GOL	A	1002	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	PO4	P-O3	-2.03	1.48	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	404	GOL	C3-C2-C1	-4.67	93.55	111.70
2	B	403	GOL	O2-C2-C3	2.66	120.85	109.12
2	A	1006	GOL	O1-C1-C2	-2.62	97.64	110.20
3	A	1007	PO4	O3-P-O1	-2.62	101.31	110.89
3	B	407	PO4	O3-P-O1	-2.61	101.35	110.89
2	B	403	GOL	O3-C3-C2	2.55	122.44	110.20
2	B	404	GOL	O3-C3-C2	2.34	121.42	110.20
2	B	406	GOL	O2-C2-C3	2.25	119.02	109.12
2	A	1003	GOL	C3-C2-C1	2.08	119.80	111.70

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	404	GOL	O1-C1-C2-O2
2	B	404	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	404	GOL	C1-C2-C3-O3
2	B	404	GOL	O2-C2-C3-O3
2	B	402	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	A	1003	GOL	C1-C2-C3-O3
2	B	403	GOL	C1-C2-C3-O3
2	A	1002	GOL	C1-C2-C3-O3
2	B	406	GOL	O2-C2-C3-O3
2	A	1003	GOL	O2-C2-C3-O3
2	B	406	GOL	C1-C2-C3-O3
2	B	402	GOL	O2-C2-C3-O3
2	B	403	GOL	O2-C2-C3-O3
2	B	402	GOL	O1-C1-C2-O2
2	A	1001	GOL	C1-C2-C3-O3
2	B	405	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	404	GOL	7	0
3	B	407	PO4	8	0
2	B	405	GOL	5	0
3	A	1007	PO4	7	0
2	B	402	GOL	4	0
2	A	1003	GOL	4	0
2	A	1006	GOL	6	0
2	B	403	GOL	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	329/355 (92%)	-0.02	23 (6%)	16 17	6, 11, 24, 42	1 (0%)
1	B	332/355 (93%)	-0.11	15 (4%)	33 29	6, 10, 24, 38	0
All	All	661/710 (93%)	-0.06	38 (5%)	23 22	6, 10, 24, 42	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ILE	13.9
1	B	31	GLY	9.1
1	B	28	PRO	6.8
1	B	17	ALA	6.7
1	B	18	VAL	6.3
1	A	29	VAL	6.2
1	A	19	ASP	6.0
1	A	27	PRO	5.9
1	A	31	GLY	5.3
1	A	28	PRO	4.6
1	A	259	PRO	4.6
1	B	19	ASP	4.0
1	A	322	THR	3.9
1	B	27	PRO	3.8
1	A	39	ASP	3.5
1	B	20	PRO	3.3
1	B	260	PRO	3.0
1	B	259	PRO	3.0
1	A	239	GLN	3.0
1	A	21	ALA	2.9
1	B	192[A]	TRP	2.6
1	A	25	ALA	2.6
1	A	258	VAL	2.6
1	A	32	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	209	ASP	2.4
1	A	36	ALA	2.4
1	B	134[A]	PHE	2.4
1	A	26	GLY	2.4
1	A	134[A]	PHE	2.4
1	A	323	THR	2.3
1	A	24	LEU	2.1
1	A	192[A]	TRP	2.1
1	B	322	THR	2.1
1	B	32	GLY	2.1
1	B	208[A]	GLY	2.1
1	A	152	SER	2.0
1	A	37	ALA	2.0
1	A	330	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. 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( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	1007	5/5	0.83	0.36	21,21,28,29	0
2	GOL	B	402	6/6	0.83	0.26	33,41,45,45	0
4	CL	A	1009	1/1	0.83	0.12	28,28,28,28	0
2	GOL	B	405	6/6	0.84	0.30	17,32,39,44	0
3	PO4	B	407	5/5	0.84	0.34	21,23,26,31	0
2	GOL	A	1004	6/6	0.86	0.12	31,33,38,40	0
2	GOL	B	406	6/6	0.90	0.21	19,23,34,38	0
2	GOL	A	1003	6/6	0.92	0.16	23,34,36,60	0
4	CL	B	409	1/1	0.92	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	401	6/6	0.94	0.15	13,15,17,20	0
2	GOL	B	404	6/6	0.94	0.19	10,25,30,50	0
2	GOL	A	1006	6/6	0.96	0.18	13,22,34,40	0
2	GOL	A	1005	6/6	0.96	0.11	15,22,25,35	0
2	GOL	B	403	6/6	0.97	0.12	12,29,44,49	0
2	GOL	A	1001	6/6	0.97	0.10	12,13,13,16	0
2	GOL	A	1002	6/6	0.97	0.08	15,22,30,42	0
4	CL	A	1008	1/1	0.99	0.07	19,19,19,19	0
4	CL	B	408	1/1	1.00	0.07	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.