



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 12:20 PM JST

PDB ID : 6JGN  
Title : Crystal structure of barley exohydrolaseI W434H in complex with 4'-nitrophenyl thiolaminaribioside  
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.  
Deposited on : 2019-02-14  
Resolution : 1.98 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
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)	:	2.31.2

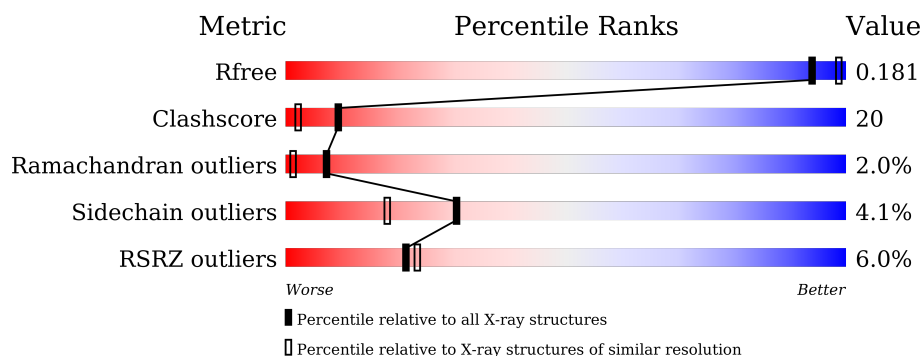
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	609	<div> <div>6%</div> <div>81%</div> <div>15%</div> <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
4	1PE	A	720	-	-	X	-
5	ACT	A	724	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	726	-	-	X	-
5	ACT	A	727	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5350 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.

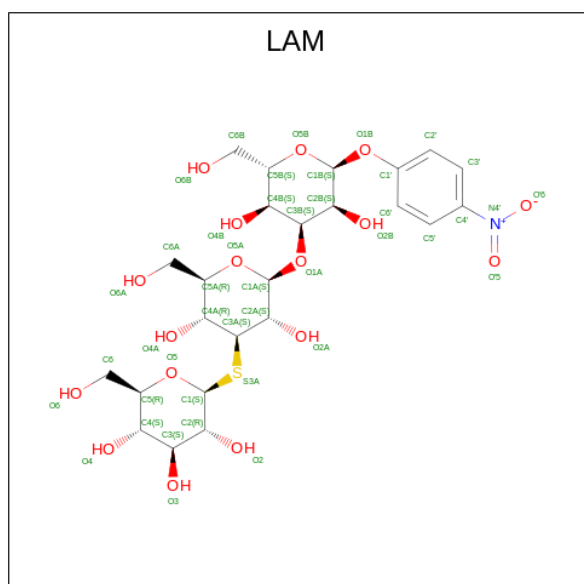
- Molecule 1 is a protein called BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	603	4617	2914	801	874	28	0	28	0

There are 6 discrepancies between the modelled and reference sequences:

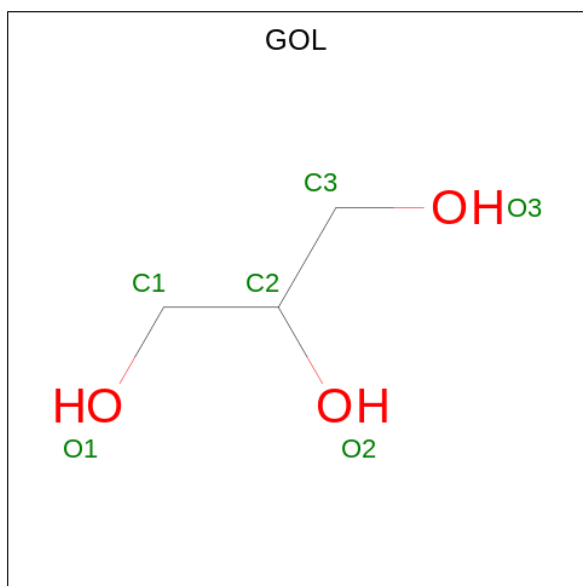
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP A0A287SCR5
A	-2	HIS	-	expression tag	UNP A0A287SCR5
A	-1	ALA	-	expression tag	UNP A0A287SCR5
A	0	ALA	-	expression tag	UNP A0A287SCR5
A	320	LYS	ASN	See sequence details	UNP A0A287SCR5
A	434	HIS	TRP	engineered mutation	UNP A0A287SCR5

- Molecule 2 is 4'-NITROPHENYL-S-(BETA-D-GLUCOPYRANOSYL)-(1-3)-(3-THIO-BETA-D-GLUCOPYRANOSYL)-(1-3)-BETA-D-GLUCOPYRANOSIDE (three-letter code: LAM) (formula: C<sub>24</sub>H<sub>35</sub>NO<sub>17</sub>S).



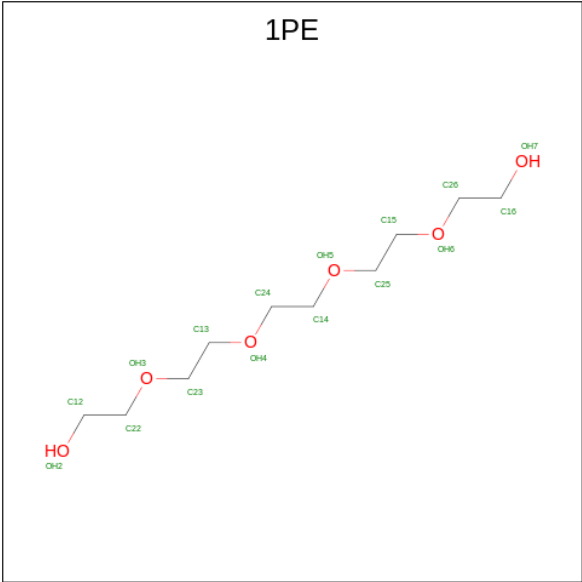
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			23	12	10	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



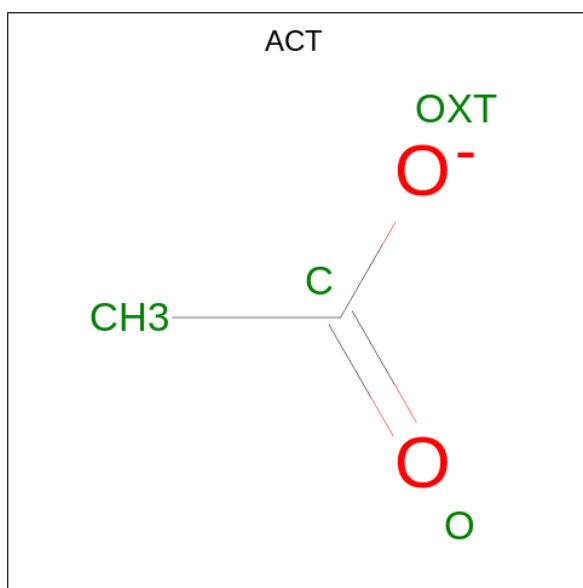
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



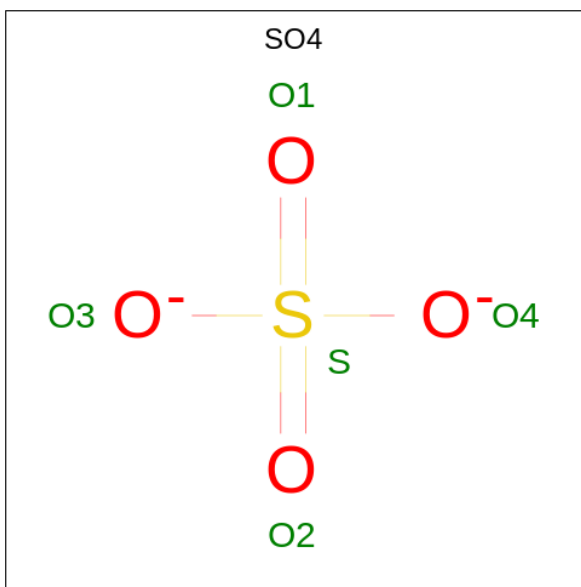
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			14	9	5		
4	A	1	Total	C	O	0	1
			16	10	6		
4	A	1	Total	C	O	0	1
			13	8	5		
4	A	1	Total	C	O	0	1
			15	9	6		
4	A	1	Total	C	O	0	0
			8	5	3		
4	A	1	Total	C	O	0	1
			16	10	6		
4	A	1	Total	C	O	0	1
			7	4	3		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			12	8	4		
4	A	1	Total	C	O	0	1
			9	5	4		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

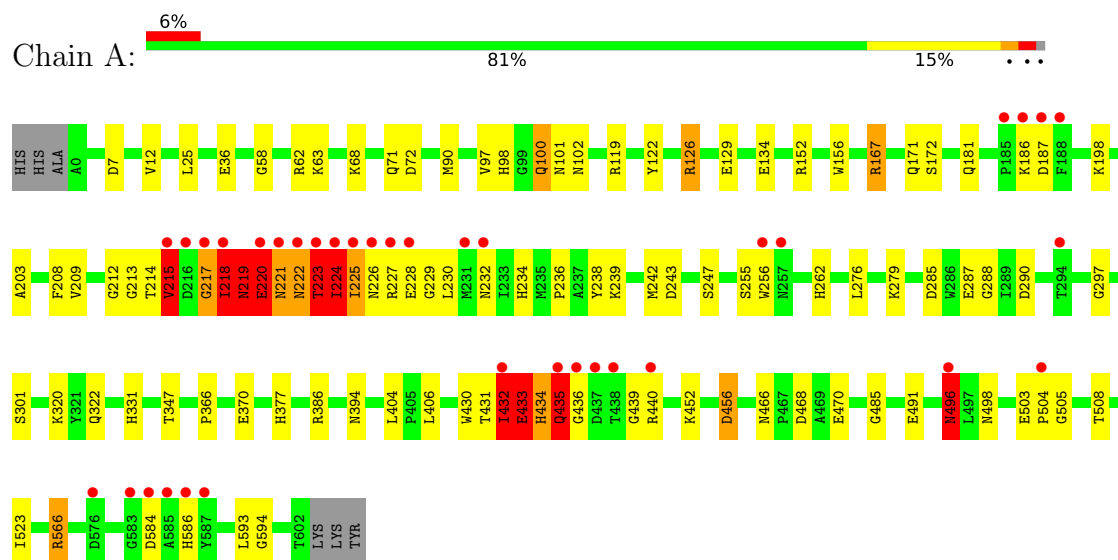
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	467	Total	O	0	0
			467	467		



### 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: BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.39Å 100.39Å 180.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.87 – 1.98 45.83 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.87-1.98) 99.9 (45.83-1.98)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.142 , 0.171 0.156 , 0.181	Depositor DCC
$R_{free}$ test set	3290 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: ACT, 1PE, SO4, LAM, GOL

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	1.02	11/4816 (0.2%)	1.04	21/6532 (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	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439[A]	GLY	C-O	11.24	1.41	1.23
1	A	432[A]	ILE	C-O	8.54	1.39	1.23
1	A	432[B]	ILE	C-O	8.54	1.39	1.23
1	A	503	GLU	CD-OE2	7.17	1.33	1.25
1	A	433	GLU	CD-OE2	-6.94	1.18	1.25
1	A	219	ASN	CG-OD1	6.38	1.38	1.24
1	A	432[A]	ILE	CA-C	5.85	1.68	1.52
1	A	432[B]	ILE	CA-C	5.85	1.68	1.52
1	A	129	GLU	CD-OE2	-5.58	1.19	1.25
1	A	496[B]	ASN	CB-CG	5.06	1.62	1.51
1	A	433	GLU	C-O	5.05	1.32	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	GLU	N-CA-C	12.62	145.07	111.00
1	A	62[A]	ARG	NE-CZ-NH2	-10.38	115.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	126	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	A	62[A]	ARG	CG-CD-NE	-6.82	97.49	111.80
1	A	439[A]	GLY	N-CA-C	6.39	129.07	113.10
1	A	217	GLY	N-CA-C	-6.01	98.08	113.10
1	A	566[A]	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	566[B]	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	468	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	452	LYS	CD-CE-NZ	-5.77	98.43	111.70
1	A	119	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	566[A]	ARG	CG-CD-NE	-5.59	100.06	111.80
1	A	566[B]	ARG	CG-CD-NE	-5.59	100.06	111.80
1	A	218[A]	ILE	CA-CB-CG1	5.50	121.45	111.00
1	A	218[B]	ILE	CA-CB-CG1	5.50	121.45	111.00
1	A	436	GLY	N-CA-C	-5.41	99.57	113.10
1	A	456	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	468	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	243	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	A	7	ASP	CB-CG-OD2	-5.14	113.67	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218[A]	ILE	Peptide
1	A	218[B]	ILE	Peptide
1	A	219	ASN	Peptide
1	A	432[A]	ILE	Peptide
1	A	432[B]	ILE	Peptide
1	A	434	HIS	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	4617	0	4559	147	0
2	A	23	0	21	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	59	4	0
4	A	137	0	132	42	0
5	A	48	0	36	14	0
6	A	10	0	0	1	0
7	A	467	0	0	56	0
All	All	5350	0	4807	188	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 20.

All (188) 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:220:GLU:HA	1:A:223:THR:CG2	1.72	1.18
1:A:224:ILE:HG12	1:A:225:ILE:N	1.53	1.13
4:A:720:1PE:C26	7:A:806:HOH:O	2.01	1.08
1:A:466[A]:ASN:ND2	1:A:508:THR:OG1	1.86	1.07
1:A:224:ILE:CG1	1:A:225:ILE:H	1.67	1.02
4:A:710[A]:1PE:H242	7:A:885:HOH:O	1.55	1.01
2:A:701:LAM:C1	7:A:804:HOH:O	2.09	1.00
2:A:701:LAM:O5	7:A:804:HOH:O	1.78	0.99
1:A:68[B]:LYS:NZ	7:A:805:HOH:O	1.96	0.98
1:A:198:LYS:H	4:A:717:1PE:H222	1.26	0.98
4:A:714:1PE:H231	7:A:1139:HOH:O	1.62	0.97
1:A:220:GLU:HA	1:A:223:THR:HG21	1.45	0.97
1:A:432[B]:ILE:HD11	5:A:724:ACT:CH3	1.95	0.96
1:A:225:ILE:HG23	1:A:226:ASN:N	1.80	0.96
2:A:701:LAM:S3A	7:A:804:HOH:O	2.22	0.95
4:A:720:1PE:H261	7:A:806:HOH:O	1.61	0.94
1:A:224:ILE:HG12	1:A:225:ILE:H	1.16	0.94
4:A:723:1PE:H121	7:A:1114:HOH:O	1.69	0.92
1:A:432[B]:ILE:HD11	5:A:724:ACT:C	2.00	0.92
1:A:394:ASN:HD21	1:A:404:LEU:H	1.19	0.89
1:A:225:ILE:HG23	1:A:226:ASN:H	1.40	0.86
1:A:434:HIS:ND1	7:A:807:HOH:O	2.11	0.84
1:A:224:ILE:O	1:A:225:ILE:HB	1.77	0.84
4:A:714:1PE:C23	7:A:1139:HOH:O	2.19	0.81
4:A:720:1PE:C14	7:A:1168:HOH:O	2.28	0.81
1:A:214:THR:HA	1:A:218[A]:ILE:HD12	1.62	0.80
1:A:220:GLU:OE1	1:A:220:GLU:C	2.20	0.80
4:A:720:1PE:H141	7:A:1168:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172[B]:SER:OG	6:A:736:SO4:O1	1.98	0.78
4:A:710[A]:1PE:C13	7:A:885:HOH:O	2.31	0.77
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.52	0.75
1:A:219:ASN:O	4:A:723:1PE:OH2	2.01	0.74
1:A:432[B]:ILE:CD1	5:A:724:ACT:C	2.65	0.74
1:A:198:LYS:N	4:A:717:1PE:H222	2.03	0.74
4:A:720:1PE:C24	7:A:1168:HOH:O	2.36	0.73
1:A:370[B]:GLU:HG2	7:A:1124:HOH:O	1.87	0.73
1:A:12:VAL:H	4:A:722:1PE:H161	1.54	0.73
4:A:720:1PE:OH5	7:A:806:HOH:O	2.06	0.72
1:A:386[A]:ARG:HH22	4:A:716[A]:1PE:H222	1.55	0.71
4:A:711[A]:1PE:H151	7:A:973:HOH:O	1.91	0.71
1:A:433:GLU:CG	1:A:433:GLU:O	2.38	0.70
1:A:225:ILE:HG22	1:A:256:TRP:CH2	2.27	0.69
4:A:720:1PE:H262	7:A:806:HOH:O	1.82	0.69
1:A:220:GLU:CA	1:A:223:THR:CG2	2.64	0.68
1:A:167:ARG:HH21	1:A:171:GLN:HE22	1.41	0.68
1:A:331:HIS:HD2	7:A:1202:HOH:O	1.77	0.67
1:A:97:VAL:H	1:A:101:ASN:HD21	1.41	0.67
1:A:262:HIS:HE1	1:A:285:ASP:H	1.41	0.67
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.77	0.67
1:A:181:GLN:HE21	1:A:203:ALA:H	1.41	0.66
1:A:68[A]:LYS:HE3	7:A:848:HOH:O	1.94	0.66
1:A:230:LEU:HB2	1:A:256:TRP:CZ2	2.31	0.66
4:A:715[B]:1PE:H152	7:A:916:HOH:O	1.96	0.66
1:A:470[B]:GLU:OE1	7:A:808:HOH:O	2.14	0.65
1:A:221:ASN:O	1:A:222:ASN:HB3	1.96	0.64
1:A:347:THR:HG21	4:A:711[A]:1PE:C15	2.29	0.62
1:A:224:ILE:CD1	1:A:225:ILE:H	2.12	0.62
1:A:504:PRO:HD2	7:A:1021:HOH:O	1.99	0.62
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.13	0.61
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.35	0.61
1:A:586[B]:HIS:HB2	7:A:1217:HOH:O	1.99	0.61
4:A:714:1PE:C24	7:A:838:HOH:O	2.49	0.61
1:A:225:ILE:HG12	1:A:226:ASN:H	1.66	0.60
1:A:347:THR:HG21	4:A:711[A]:1PE:H151	1.84	0.60
1:A:212:GLY:O	1:A:218[A]:ILE:HG13	2.00	0.60
4:A:710[A]:1PE:H131	7:A:885:HOH:O	2.00	0.60
1:A:222:ASN:O	1:A:223:THR:C	2.39	0.60
4:A:711[A]:1PE:C15	7:A:973:HOH:O	2.46	0.60
1:A:12:VAL:H	4:A:722:1PE:C16	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:720:1PE:C13	7:A:821:HOH:O	2.51	0.59
1:A:433:GLU:O	1:A:433:GLU:HG2	2.02	0.59
1:A:167:ARG:HH21	1:A:171:GLN:NE2	2.01	0.59
1:A:370[A]:GLU:HG3	7:A:1124:HOH:O	2.03	0.58
1:A:220:GLU:OE1	1:A:220:GLU:O	2.20	0.58
1:A:432[B]:ILE:CG1	5:A:724:ACT:C	2.81	0.58
1:A:225:ILE:HD13	1:A:229:GLY:HA3	1.85	0.57
4:A:720:1PE:H131	7:A:821:HOH:O	2.04	0.57
1:A:262:HIS:CE1	1:A:285:ASP:H	2.21	0.57
1:A:466[A]:ASN:ND2	1:A:508:THR:HG1	2.02	0.57
1:A:58:GLY:H	1:A:102:ASN:ND2	2.04	0.56
1:A:214:THR:O	1:A:215:VAL:HG22	2.05	0.56
1:A:222:ASN:O	1:A:224:ILE:HB	2.04	0.56
1:A:225:ILE:CG2	1:A:256:TRP:CH2	2.89	0.56
1:A:432[B]:ILE:HD11	5:A:724:ACT:H3	1.82	0.56
1:A:220:GLU:HA	1:A:223:THR:HG22	1.76	0.56
1:A:239[B]:LYS:HD3	1:A:276:LEU:HD22	1.87	0.56
1:A:152:ARG:H	1:A:218[B]:ILE:HD11	1.71	0.56
1:A:221:ASN:HA	5:A:727:ACT:H1	1.88	0.55
1:A:58:GLY:H	1:A:102:ASN:HD21	1.55	0.55
1:A:220:GLU:HA	1:A:223:THR:HG23	1.79	0.55
1:A:220:GLU:CG	1:A:491:GLU:OE2	2.55	0.55
1:A:217:GLY:O	1:A:219:ASN:N	2.39	0.55
1:A:234:HIS:HD2	7:A:1035:HOH:O	1.89	0.55
1:A:214:THR:HA	1:A:218[A]:ILE:CD1	2.35	0.54
1:A:222:ASN:OD1	1:A:224:ILE:HG22	2.07	0.54
1:A:430:TRP:HE3	1:A:433:GLU:OE1	1.89	0.54
1:A:152:ARG:N	1:A:218[B]:ILE:HD11	2.23	0.54
1:A:433:GLU:C	1:A:435:GLN:N	2.60	0.53
1:A:68[B]:LYS:HE3	1:A:72:ASP:OD1	2.08	0.53
1:A:222:ASN:O	1:A:224:ILE:HG22	2.09	0.53
1:A:432[B]:ILE:HG13	5:A:724:ACT:C	2.39	0.53
4:A:717:1PE:H122	7:A:1010:HOH:O	2.07	0.53
1:A:220:GLU:OE1	1:A:220:GLU:CA	2.55	0.53
1:A:297:GLY:O	1:A:320[C]:LYS:CE	2.57	0.53
1:A:58:GLY:N	1:A:433:GLU:HB3	2.24	0.52
1:A:222:ASN:O	1:A:224:ILE:CB	2.58	0.52
1:A:12:VAL:N	4:A:722:1PE:H161	2.25	0.51
1:A:225:ILE:CG2	1:A:226:ASN:N	2.56	0.51
1:A:225:ILE:HD13	1:A:229:GLY:CA	2.41	0.51
1:A:225:ILE:CG2	1:A:226:ASN:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470[B]:GLU:CG	7:A:808:HOH:O	2.59	0.50
1:A:97:VAL:H	1:A:101:ASN:ND2	2.09	0.50
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.61	0.50
1:A:239[B]:LYS:CD	1:A:276:LEU:HD22	2.42	0.50
3:A:709:GOL:H12	7:A:1003:HOH:O	2.11	0.50
1:A:63[B]:LYS:HE2	7:A:1227:HOH:O	2.12	0.50
4:A:723:1PE:C12	7:A:1114:HOH:O	2.43	0.49
1:A:221:ASN:ND2	1:A:222:ASN:HD22	2.10	0.49
1:A:347:THR:HG21	4:A:711[A]:1PE:H152	1.95	0.48
1:A:221:ASN:CA	5:A:727:ACT:H1	2.43	0.48
1:A:262:HIS:CE1	1:A:288:GLY:HA3	2.48	0.48
1:A:432[B]:ILE:HG13	5:A:724:ACT:O	2.14	0.48
1:A:222:ASN:HA	1:A:255:SER:H	1.78	0.47
1:A:230:LEU:HB2	1:A:256:TRP:HZ2	1.78	0.47
1:A:220:GLU:HG2	1:A:491:GLU:OE2	2.14	0.47
1:A:297:GLY:O	1:A:320[C]:LYS:HE2	2.15	0.47
1:A:301:SER:O	1:A:331:HIS:HE1	1.98	0.47
1:A:470[B]:GLU:HG2	7:A:808:HOH:O	2.14	0.47
1:A:63[B]:LYS:CE	7:A:1227:HOH:O	2.62	0.46
3:A:709:GOL:C1	7:A:1003:HOH:O	2.62	0.46
1:A:181:GLN:HE22	1:A:247:SER:H	1.64	0.46
4:A:717:1PE:C12	7:A:1010:HOH:O	2.64	0.46
1:A:224:ILE:CG1	1:A:225:ILE:N	2.27	0.46
1:A:221:ASN:HD22	1:A:222:ASN:HD22	1.64	0.46
1:A:71:GLN:HE22	1:A:366:PRO:HA	1.81	0.45
1:A:100:GLN:HA	1:A:100:GLN:NE2	2.26	0.45
1:A:297:GLY:CA	1:A:320[C]:LYS:HE2	2.46	0.45
1:A:435:GLN:NE2	7:A:825:HOH:O	2.49	0.45
2:A:701:LAM:H2A1	4:A:715[A]:1PE:H152	1.99	0.45
1:A:287:GLU:OE2	5:A:726:ACT:H3	2.16	0.45
4:A:712[A]:1PE:H151	7:A:1218:HOH:O	2.16	0.45
1:A:58:GLY:H	1:A:433:GLU:HB3	1.81	0.45
1:A:222:ASN:O	1:A:224:ILE:CG2	2.65	0.45
1:A:221:ASN:CB	5:A:727:ACT:H1	2.48	0.44
4:A:712[B]:1PE:H151	7:A:1218:HOH:O	2.16	0.44
4:A:722:1PE:H162	7:A:1144:HOH:O	2.17	0.44
3:A:706:GOL:H32	7:A:1037:HOH:O	2.18	0.44
1:A:224:ILE:O	1:A:225:ILE:CB	2.55	0.44
1:A:287:GLU:OE2	5:A:726:ACT:CH3	2.66	0.44
4:A:720:1PE:C24	7:A:821:HOH:O	2.65	0.43
1:A:322[A]:GLN:OE1	4:A:720:1PE:C23	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:HD22	1:A:221:ASN:C	2.22	0.43
1:A:213:GLY:O	1:A:223:THR:HB	2.19	0.42
1:A:485:GLY:HA3	1:A:523:ILE:O	2.19	0.42
4:A:710[A]:1PE:H132	7:A:885:HOH:O	2.09	0.42
1:A:187:ASP:OD1	1:A:187:ASP:N	2.48	0.42
1:A:208:PHE:HA	1:A:209:VAL:HA	1.90	0.42
1:A:220:GLU:CA	1:A:223:THR:HG21	2.33	0.42
4:A:720:1PE:H242	7:A:821:HOH:O	2.19	0.42
1:A:222:ASN:O	1:A:224:ILE:N	2.53	0.42
3:A:706:GOL:H12	7:A:1111:HOH:O	2.19	0.42
1:A:404:LEU:HD23	1:A:406:LEU:HG	2.02	0.41
1:A:230:LEU:C	1:A:232:ASN:N	2.73	0.41
1:A:225:ILE:CD1	1:A:229:GLY:HA3	2.50	0.41
1:A:238:TYR:O	1:A:242:MET:HG2	2.21	0.41
1:A:167:ARG:NH2	1:A:171:GLN:HE22	2.13	0.41
1:A:219:ASN:O	4:A:723:1PE:C12	2.69	0.41
1:A:279:LYS:HE3	5:A:725:ACT:H1	2.03	0.41
1:A:431:THR:O	1:A:432[B]:ILE:HD13	2.21	0.40
1:A:566[B]:ARG:NE	1:A:594:GLY:O	2.54	0.40
1:A:167:ARG:NE	1:A:232:ASN:O	2.49	0.40
1:A:456:ASP:HB2	7:A:1148:HOH:O	2.22	0.40
4:A:714:1PE:H232	7:A:1139:HOH:O	2.00	0.40
1:A:25:LEU:HB2	5:A:731:ACT:H2	2.03	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	619/609 (102%)	584 (94%)	21 (3%)	14 (2%)	<b>6</b> <b>1</b>

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	VAL
1	A	218[A]	ILE
1	A	218[B]	ILE
1	A	220	GLU
1	A	222	ASN
1	A	225	ILE
1	A	433	GLU
1	A	224	ILE
1	A	435	GLN
1	A	505	GLY
1	A	432[A]	ILE
1	A	432[B]	ILE
1	A	223	THR
1	A	496[B]	ASN

### 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	503/490 (103%)	483 (96%)	20 (4%)	31 19

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	167	ARG
1	A	186	LYS
1	A	215	VAL
1	A	220	GLU
1	A	221	ASN
1	A	223	THR
1	A	224	ILE
1	A	227	ARG
1	A	228	GLU

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Mol	Chain	Res	Type
1	A	236	PRO
1	A	290	ASP
1	A	435	GLN
1	A	440	ARG
1	A	496[B]	ASN
1	A	498	ASN
1	A	593	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	100	GLN
1	A	101	ASN
1	A	102	ASN
1	A	112	ASN
1	A	171	GLN
1	A	181	GLN
1	A	199	ASN
1	A	221	ASN
1	A	234	HIS
1	A	262	HIS
1	A	331	HIS
1	A	361	ASN
1	A	377	HIS
1	A	394	ASN
1	A	496[B]	ASN
1	A	498	ASN

### 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

43 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	$\# Z  > 2$
5	ACT	A	727	-	3,3,3	0.70	0	3,3,3	1.02	0
2	LAM	A	701	-	23,24,46	0.88	1 (4%)	29,35,67	1.82	5 (17%)
3	GOL	A	704	-	5,5,5	0.27	0	5,5,5	0.89	0
4	1PE	A	718	-	5,5,15	0.61	0	4,4,14	0.44	0
5	ACT	A	729	-	3,3,3	1.23	0	3,3,3	0.79	0
5	ACT	A	731	-	3,3,3	1.35	0	3,3,3	0.45	0
5	ACT	A	734	-	3,3,3	0.61	0	3,3,3	1.55	0
6	SO4	A	736	-	4,4,4	0.22	0	6,6,6	1.22	0
4	1PE	A	711[B]	-	9,9,15	0.51	0	8,8,14	0.61	0
4	1PE	A	711[A]	-	9,8,15	0.60	0	8,7,14	1.41	1 (12%)
4	1PE	A	717	-	4,4,15	0.94	0	3,3,14	0.75	0
5	ACT	A	732	-	3,3,3	0.81	0	3,3,3	0.49	0
5	ACT	A	733	-	3,3,3	0.93	0	3,3,3	0.52	0
4	1PE	A	715[B]	-	9,9,15	0.57	0	8,8,14	0.47	0
4	1PE	A	714	-	7,7,15	0.50	0	6,6,14	0.69	0
3	GOL	A	706	-	5,5,5	0.44	0	5,5,5	1.14	0
4	1PE	A	720	-	11,11,15	0.55	0	10,10,14	1.51	2 (20%)
4	1PE	A	715[A]	-	9,9,15	0.48	0	8,8,14	0.31	0
3	GOL	A	707	-	5,5,5	0.54	0	5,5,5	0.28	0
5	ACT	A	725	-	3,3,3	0.91	0	3,3,3	0.39	0
5	ACT	A	730	-	3,3,3	0.87	0	3,3,3	0.56	0
4	1PE	A	721[A]	-	6,6,15	0.57	0	5,5,14	0.51	0
5	ACT	A	726	-	3,3,3	1.04	0	3,3,3	0.77	0
3	GOL	A	708	-	5,5,5	0.40	0	5,5,5	0.47	0
5	ACT	A	728	-	3,3,3	0.97	0	3,3,3	0.41	0
4	1PE	A	716[B]	-	4,4,15	0.72	0	3,3,14	0.70	0
4	1PE	A	716[A]	-	4,4,15	0.72	0	3,3,14	0.43	0
5	ACT	A	735	-	3,3,3	0.79	0	3,3,3	1.43	0
4	1PE	A	722	-	4,4,15	0.84	0	3,3,14	0.87	0
3	GOL	A	705	-	5,5,5	0.59	0	5,5,5	1.37	0
4	1PE	A	723	-	5,5,15	0.55	0	4,4,14	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	A	737	-	4,4,4	0.32	0	6,6,6	0.36	0
3	GOL	A	709	-	5,5,5	0.78	0	5,5,5	1.10	0
4	1PE	A	721[B]	-	6,6,15	0.42	0	5,5,14	0.81	0
4	1PE	A	719	-	4,4,15	0.90	0	3,3,14	0.30	0
4	1PE	A	713[B]	-	13,13,15	0.80	0	12,12,14	0.85	0
4	1PE	A	712[B]	-	11,11,15	0.68	0	10,10,14	0.80	0
4	1PE	A	712[A]	-	11,11,15	0.68	0	10,10,14	0.80	0
3	GOL	A	702	-	5,5,5	0.30	0	5,5,5	0.83	0
4	1PE	A	713[A]	-	13,13,15	0.80	0	12,12,14	0.85	0
5	ACT	A	724	-	3,3,3	0.93	0	3,3,3	1.25	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	LAM	A	701	-	-	1/8/48/82	0/2/2/4
3	GOL	A	704	-	-	3/4/4/4	-
4	1PE	A	718	-	-	2/3/3/13	-
4	1PE	A	711[B]	-	-	5/7/7/13	-
4	1PE	A	711[A]	-	-	5/7/6/13	-
4	1PE	A	717	-	-	2/2/2/13	-
4	1PE	A	715[B]	-	-	3/7/7/13	-
4	1PE	A	714	-	-	3/5/5/13	-
3	GOL	A	706	-	-	2/4/4/4	-
4	1PE	A	720	-	-	4/9/9/13	-
4	1PE	A	715[A]	-	-	2/7/7/13	-
3	GOL	A	707	-	-	0/4/4/4	-
4	1PE	A	721[A]	-	-	0/4/4/13	-
3	GOL	A	708	-	-	2/4/4/4	-
4	1PE	A	716[B]	-	-	1/2/2/13	-
4	1PE	A	716[A]	-	-	1/2/2/13	-
4	1PE	A	722	-	-	2/2/2/13	-
3	GOL	A	705	-	-	0/4/4/4	-
4	1PE	A	723	-	-	1/3/3/13	-
3	GOL	A	709	-	-	2/4/4/4	-
4	1PE	A	721[B]	-	-	0/4/4/13	-
4	1PE	A	719	-	-	1/2/2/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	A	713[B]	-	-	6/11/11/13	-
4	1PE	A	712[B]	-	-	5/9/9/13	-
4	1PE	A	712[A]	-	-	5/9/9/13	-
3	GOL	A	702	-	-	2/4/4/4	-
4	1PE	A	713[A]	-	-	6/11/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	LAM	C4A-C3A	-2.22	1.51	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	LAM	C1-O5-C5	5.52	122.77	112.58
2	A	701	LAM	C2-C1-S3A	-3.66	105.66	111.30
2	A	701	LAM	C1-C2-C3	3.33	117.16	110.59
4	A	720	1PE	OH7-C16-C26	-2.78	95.72	111.81
2	A	701	LAM	O2-C2-C1	-2.67	105.37	110.27
2	A	701	LAM	O5-C5-C6	2.38	112.36	106.44
4	A	720	1PE	OH6-C26-C16	-2.31	99.90	110.07
4	A	711[A]	1PE	OH6-C15-C25	2.25	120.53	110.39

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GOL	O1-C1-C2-C3
3	A	704	GOL	C1-C2-C3-O3
3	A	706	GOL	O1-C1-C2-C3
4	A	711[A]	1PE	C16-C26-OH6-C15
4	A	715[B]	1PE	C25-C15-OH6-C26
4	A	711[B]	1PE	C16-C26-OH6-C15
4	A	711[B]	1PE	OH6-C15-C25-OH5
4	A	711[A]	1PE	OH6-C15-C25-OH5
4	A	715[A]	1PE	OH6-C15-C25-OH5
4	A	715[B]	1PE	OH6-C15-C25-OH5
4	A	711[A]	1PE	C24-C14-OH5-C25
4	A	712[A]	1PE	OH5-C14-C24-OH4
4	A	712[B]	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
4	A	711[B]	1PE	OH7-C16-C26-OH6
4	A	711[A]	1PE	OH7-C16-C26-OH6
4	A	716[A]	1PE	OH2-C12-C22-OH3
4	A	720	1PE	OH7-C16-C26-OH6
4	A	719	1PE	OH7-C16-C26-OH6
4	A	713[A]	1PE	C13-C23-OH3-C22
4	A	713[B]	1PE	C13-C23-OH3-C22
3	A	704	GOL	O1-C1-C2-C3
3	A	708	GOL	O1-C1-C2-C3
3	A	709	GOL	C1-C2-C3-O3
4	A	712[A]	1PE	OH6-C15-C25-OH5
4	A	712[B]	1PE	OH6-C15-C25-OH5
4	A	713[A]	1PE	OH5-C14-C24-OH4
4	A	713[B]	1PE	OH5-C14-C24-OH4
3	A	702	GOL	O1-C1-C2-O2
3	A	704	GOL	O2-C2-C3-O3
3	A	706	GOL	O1-C1-C2-O2
3	A	708	GOL	O1-C1-C2-O2
3	A	709	GOL	O2-C2-C3-O3
4	A	718	1PE	OH2-C12-C22-OH3
4	A	717	1PE	OH2-C12-C22-OH3
4	A	713[A]	1PE	C25-C15-OH6-C26
4	A	713[B]	1PE	C25-C15-OH6-C26
4	A	716[B]	1PE	OH2-C12-C22-OH3
4	A	722	1PE	OH7-C16-C26-OH6
4	A	712[A]	1PE	OH4-C13-C23-OH3
4	A	712[B]	1PE	OH4-C13-C23-OH3
2	A	701	LAM	O5A-C5A-C6A-O6A
4	A	720	1PE	OH5-C14-C24-OH4
4	A	717	1PE	C12-C22-OH3-C23
4	A	718	1PE	C13-C23-OH3-C22
4	A	720	1PE	C15-C25-OH5-C14
4	A	711[B]	1PE	C24-C14-OH5-C25
4	A	711[B]	1PE	C25-C15-OH6-C26
4	A	722	1PE	C16-C26-OH6-C15
4	A	715[A]	1PE	C15-C25-OH5-C14
4	A	713[A]	1PE	OH4-C13-C23-OH3
4	A	713[B]	1PE	OH4-C13-C23-OH3
4	A	714	1PE	C23-C13-OH4-C24
4	A	711[A]	1PE	C15-C25-OH5-C14
4	A	720	1PE	C16-C26-OH6-C15
4	A	715[B]	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
4	A	712[A]	1PE	C14-C24-OH4-C13
4	A	712[B]	1PE	C14-C24-OH4-C13
4	A	713[A]	1PE	C14-C24-OH4-C13
4	A	713[B]	1PE	C14-C24-OH4-C13
4	A	723	1PE	C13-C23-OH3-C22
4	A	713[A]	1PE	OH6-C15-C25-OH5
4	A	713[B]	1PE	OH6-C15-C25-OH5
4	A	712[A]	1PE	C13-C23-OH3-C22
4	A	712[B]	1PE	C13-C23-OH3-C22
4	A	714	1PE	OH2-C12-C22-OH3
4	A	714	1PE	OH4-C13-C23-OH3

There are no ring outliers.

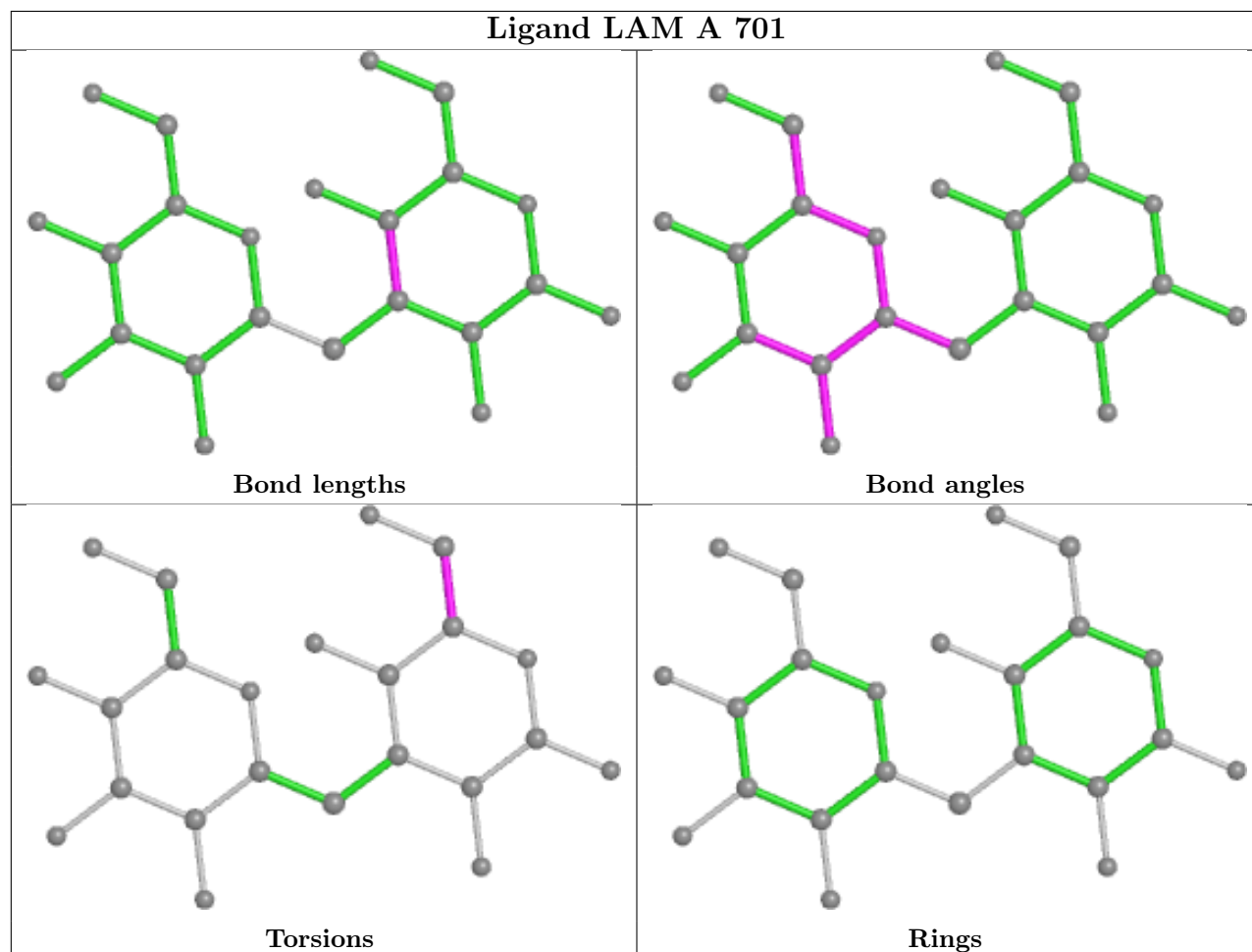
20 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	727	ACT	3	0
2	A	701	LAM	4	0
5	A	731	ACT	1	0
6	A	736	SO4	1	0
4	A	711[A]	1PE	5	0
4	A	717	1PE	4	0
4	A	715[B]	1PE	1	0
4	A	714	1PE	4	0
3	A	706	GOL	2	0
4	A	720	1PE	12	0
4	A	715[A]	1PE	1	0
5	A	725	ACT	1	0
5	A	726	ACT	2	0
4	A	716[A]	1PE	1	0
4	A	722	1PE	4	0
4	A	723	1PE	4	0
3	A	709	GOL	2	0
4	A	712[B]	1PE	1	0
4	A	712[A]	1PE	1	0
5	A	724	ACT	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	603/609 (99%)	0.06	36 (5%) 21 23	14, 21, 47, 82	8 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ILE	17.1
1	A	224	ILE	15.2
1	A	215	VAL	11.8
1	A	223	THR	9.2
1	A	222	ASN	7.9
1	A	586[B]	HIS	7.2
1	A	231	MET	6.7
1	A	432[A]	ILE	6.4
1	A	221	ASN	6.4
1	A	216	ASP	5.5
1	A	217	GLY	5.4
1	A	220	GLU	5.2
1	A	226	ASN	4.6
1	A	187	ASP	4.4
1	A	585	ALA	4.4
1	A	437	ASP	4.1
1	A	504	PRO	3.8
1	A	435	GLN	3.7
1	A	440	ARG	3.6
1	A	232	ASN	3.5
1	A	228	GLU	3.2
1	A	583	GLY	3.1
1	A	294	THR	3.1
1	A	256	TRP	3.0
1	A	188	PHE	3.0
1	A	438	THR	2.9
1	A	584[A]	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	576[A]	ASP	2.7
1	A	587	TYR	2.7
1	A	257	ASN	2.6
1	A	227	ARG	2.5
1	A	185	PRO	2.5
1	A	496[B]	ASN	2.5
1	A	218[A]	ILE	2.4
1	A	436	GLY	2.4
1	A	186	LYS	2.3

## 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
5	ACT	A	733	4/4	0.61	0.20	54,56,56,62	0
5	ACT	A	735	4/4	0.68	0.33	49,52,54,57	0
4	1PE	A	716[A]	5/16	0.75	0.24	39,40,51,55	2
4	1PE	A	716[B]	5/16	0.75	0.24	39,40,51,55	2
4	1PE	A	713[B]	14/16	0.77	0.22	54,59,66,67	1
4	1PE	A	719	5/16	0.77	0.28	44,55,58,62	0
4	1PE	A	721[A]	7/16	0.77	0.35	42,49,57,60	2
4	1PE	A	721[B]	7/16	0.77	0.35	38,49,57,60	2
4	1PE	A	714	8/16	0.77	0.22	52,56,58,61	0
4	1PE	A	713[A]	14/16	0.77	0.22	54,59,67,67	1
5	ACT	A	725	4/4	0.78	0.22	55,60,62,68	0
5	ACT	A	732	4/4	0.78	0.17	54,57,58,61	0
3	GOL	A	707	6/6	0.82	0.19	48,53,57,62	0
5	ACT	A	734	4/4	0.83	0.16	47,52,59,64	0

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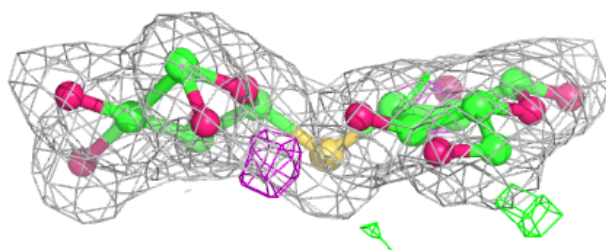
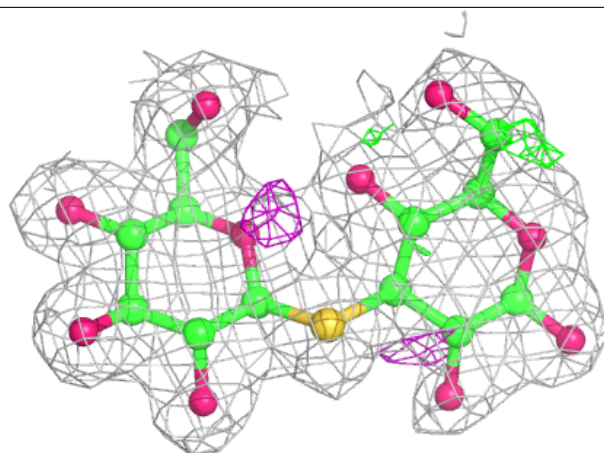
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	1PE	A	710[A]	14/16	0.83	0.17	29,52,63,66	0
4	1PE	A	723	6/16	0.84	0.21	32,46,58,58	0
4	1PE	A	722	5/16	0.84	0.30	35,41,48,57	0
4	1PE	A	715[B]	10/16	0.86	0.34	26,37,68,75	6
3	GOL	A	704	6/6	0.86	0.28	31,43,54,56	0
3	GOL	A	708	6/6	0.86	0.19	44,54,55,60	0
4	1PE	A	715[A]	10/16	0.86	0.34	39,45,68,75	6
5	ACT	A	724	4/4	0.86	0.23	52,56,65,67	0
4	1PE	A	711[A]	9/16	0.87	0.20	15,27,47,54	6
5	ACT	A	731	4/4	0.87	0.21	33,49,51,57	0
4	1PE	A	711[B]	10/16	0.87	0.20	36,41,54,57	6
4	1PE	A	718	6/16	0.88	0.35	45,62,69,71	0
4	1PE	A	712[B]	12/16	0.89	0.20	38,52,63,64	1
3	GOL	A	705	6/6	0.89	0.15	29,41,47,56	0
3	GOL	A	702	6/6	0.89	0.15	50,51,55,69	0
4	1PE	A	712[A]	12/16	0.89	0.20	38,52,63,64	1
5	ACT	A	728	4/4	0.89	0.17	63,66,68,70	0
4	1PE	A	717	5/16	0.90	0.23	33,35,45,46	0
4	1PE	A	720	12/16	0.91	0.14	20,39,47,47	0
6	SO4	A	736	5/5	0.92	0.19	32,34,35,36	5
3	GOL	A	706	6/6	0.93	0.18	20,42,46,50	0
5	ACT	A	729	4/4	0.93	0.21	45,51,55,56	0
5	ACT	A	730	4/4	0.93	0.17	56,57,57,63	0
3	GOL	A	709	6/6	0.95	0.22	25,39,40,47	0
3	GOL	A	703[B]	6/6	0.95	0.12	31,33,38,39	0
5	ACT	A	727	4/4	0.95	0.14	59,59,62,67	0
2	LAM	A	701	23/43	0.95	0.13	15,22,44,46	0
6	SO4	A	737	5/5	0.95	0.27	40,45,48,52	5
5	ACT	A	726	4/4	0.97	0.09	39,44,44,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around LAM A 701:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.