



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 12:20 PM JST

PDB ID : 6JGR  
Title : Crystal structure of barley exohydrolaseI W434Y in complex with 4'-nitrophenyl thiolaminaribioside  
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Deposited on : 2019-02-14  
Resolution : 2.25 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

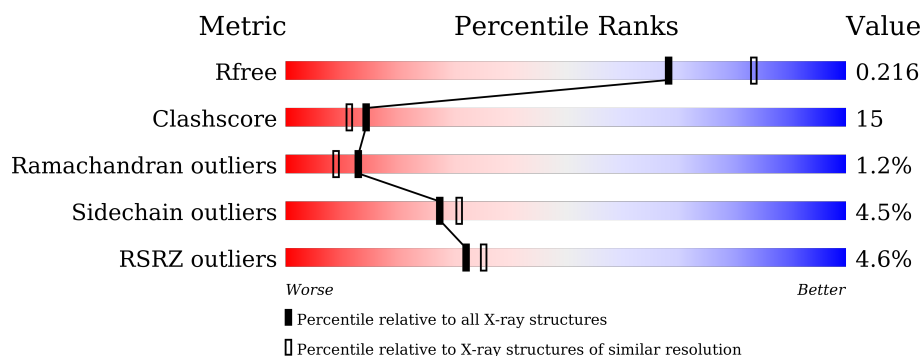
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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>5%</div> <div>82%</div> <div>14%</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	705	-	-	X	-
5	ACT	A	724	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5076 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	4591	2905	790	870	26	0	16	0

There are 6 discrepancies between the modelled and reference sequences:

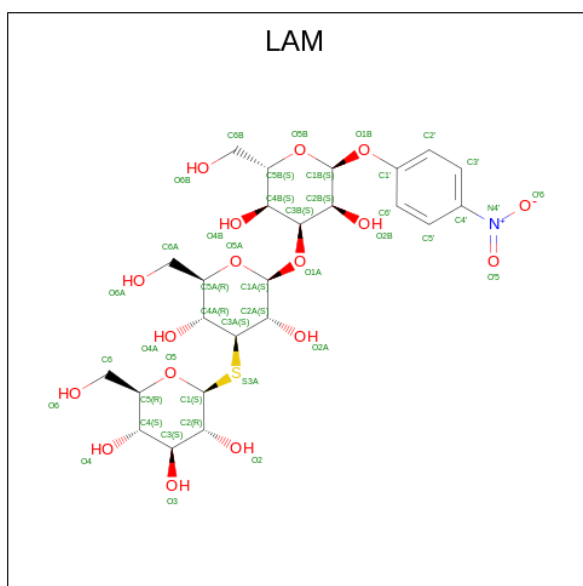
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP A0A287SCR5
A	-2	HIS	-	expression tag	UNP A0A287SCR5
A	-1	ALA	-	expression tag	UNP A0A287SCR5
A	0	ALA	-	expression tag	UNP A0A287SCR5
A	320	LYS	ASN	See sequence details	UNP A0A287SCR5
A	434	TYR	TRP	engineered mutation	UNP A0A287SCR5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



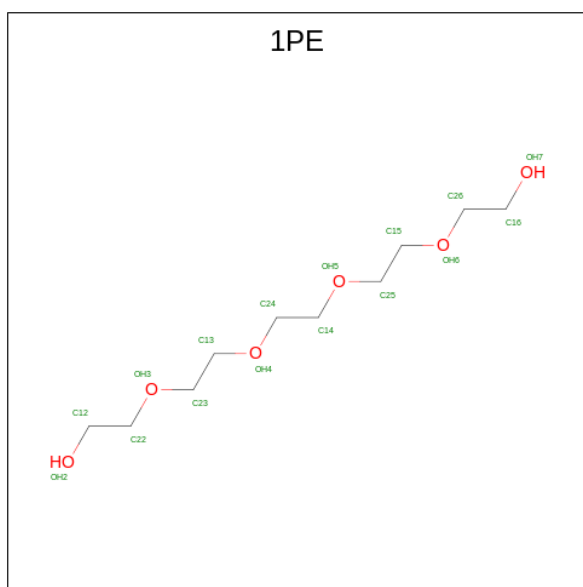
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 4'-NITROPHENYL-S-(BETA-D-GLUCOPYRANOSYL)-(1-3)-(3-THIO-BETA-D-GLUCOPYRANOSYL)-(1-3)-BETA-D-GLUCOPYRANOSIDE (three-letter code: LAM) (formula:  $C_{24}H_{35}NO_{17}S$ ).



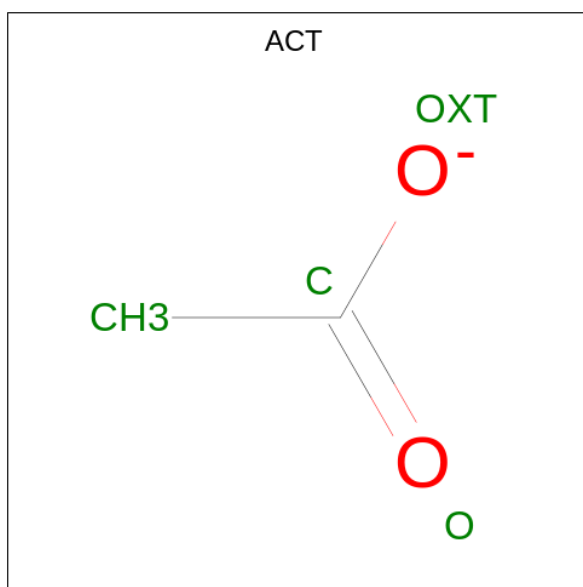
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			23	12	10	1		

- 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 12	C 8	O 4	0	0
4	A	1	Total 9	C 6	O 3	0	0
4	A	1	Total 8	C 5	O 3	0	0
4	A	1	Total 9	C 6	O 3	0	0
4	A	1	Total 16	C 10	O 6	0	0
4	A	1	Total 12	C 7	O 5	0	1
4	A	1	Total 5	C 3	O 2	0	0
4	A	1	Total 12	C 8	O 4	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



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		
5	A	1	Total	C	O	0	0
			4	2	2		

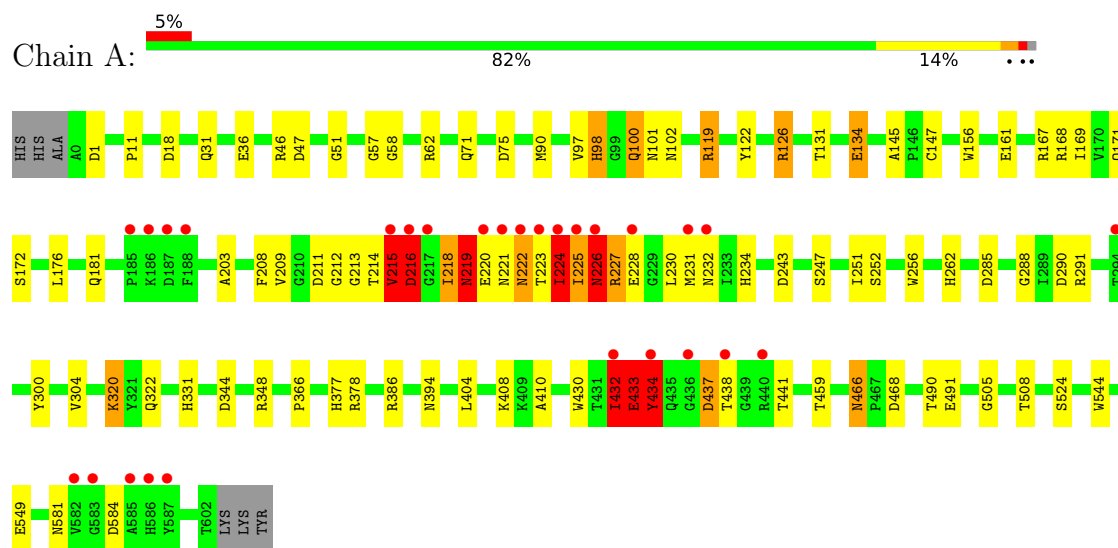
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	309	Total 309	O 309	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: 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, $\alpha$ , $\beta$ , $\gamma$	100.47Å 100.47Å 179.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.85 – 2.25 45.81 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.85-2.25) 99.8 (45.81-2.25)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.163 , 0.208 0.174 , 0.216	Depositor DCC
$R_{free}$ test set	2248 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 59.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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, GOL, 1PE, LAM

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	0.95	2/4736 (0.0%)	0.98	19/6432 (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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	GLU	CD-OE2	6.85	1.33	1.25
1	A	134	GLU	CD-OE1	-5.02	1.20	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ASP	CB-CG-OD1	10.26	127.53	118.30
1	A	75	ASP	CB-CG-OD2	-7.87	111.21	118.30
1	A	126	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	18	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	126	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	433	GLU	N-CA-C	6.28	127.95	111.00
1	A	211	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	A	348	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	216	ASP	N-CA-C	5.87	126.86	111.00
1	A	219	ASN	N-CA-C	5.87	126.85	111.00
1	A	47	ASP	CB-CG-OD1	5.87	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	468	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	434	TYR	CA-CB-CG	5.56	123.96	113.40
1	A	386[A]	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	46	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	47	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	243	ASP	CB-CG-OD1	5.22	122.99	118.30
1	A	18	ASP	CB-CG-OD1	-5.09	113.72	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	VAL	Peptide
1	A	219	ASN	Peptide
1	A	432[A]	ILE	Peptide
1	A	432[B]	ILE	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	4591	0	4545	138	0
2	A	18	0	24	1	0
3	A	23	0	21	3	0
4	A	83	0	102	24	0
5	A	52	0	39	4	0
6	A	309	0	0	15	0
All	All	5076	0	4731	148	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 15.

All (148) 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:227:ARG:CG	1:A:227:ARG:HH11	1.47	1.25
1:A:432[A]:ILE:HG12	6:A:943:HOH:O	1.41	1.16
1:A:227:ARG:HH11	1:A:227:ARG:HG2	0.92	1.07
1:A:220:GLU:OE2	1:A:223:THR:CG2	2.04	1.06
1:A:215:VAL:HG23	1:A:221:ASN:ND2	1.71	1.04
1:A:215:VAL:CG2	1:A:221:ASN:ND2	2.20	1.04
1:A:222:ASN:OD1	1:A:224:ILE:HG22	1.58	1.02
1:A:225:ILE:CG2	1:A:226:ASN:H	1.75	0.99
1:A:227:ARG:HG2	1:A:227:ARG:NH1	1.66	0.98
3:A:704:LAM:O5	6:A:805:HOH:O	1.80	0.98
1:A:97:VAL:HB	4:A:705:1PE:C23	1.94	0.98
1:A:433:GLU:HG2	1:A:434:TYR:HA	1.46	0.97
1:A:225:ILE:HG23	1:A:226:ASN:N	1.80	0.97
3:A:704:LAM:C1	6:A:805:HOH:O	2.12	0.97
1:A:222:ASN:HD22	1:A:222:ASN:N	1.62	0.97
4:A:705:1PE:H261	4:A:705:1PE:OH5	1.62	0.96
1:A:225:ILE:HG23	1:A:226:ASN:H	1.30	0.96
1:A:466[A]:ASN:ND2	1:A:508:THR:OG1	1.98	0.95
1:A:215:VAL:H	1:A:221:ASN:HD21	1.08	0.94
1:A:394:ASN:HD21	1:A:404:LEU:H	1.16	0.93
1:A:433:GLU:CG	1:A:434:TYR:HA	1.99	0.92
1:A:221:ASN:HB2	1:A:222:ASN:ND2	1.85	0.91
1:A:222:ASN:ND2	1:A:222:ASN:H	1.66	0.91
1:A:220:GLU:OE2	1:A:223:THR:HG21	1.70	0.89
1:A:224:ILE:HG12	1:A:225:ILE:N	1.86	0.88
3:A:704:LAM:S3A	6:A:805:HOH:O	2.31	0.88
1:A:222:ASN:HD22	1:A:222:ASN:H	0.88	0.87
1:A:216:ASP:O	1:A:216:ASP:OD1	1.92	0.86
1:A:219:ASN:HB2	1:A:491:GLU:HG3	1.56	0.86
1:A:215:VAL:HG22	1:A:221:ASN:ND2	1.94	0.82
1:A:224:ILE:HG12	1:A:225:ILE:H	1.41	0.82
1:A:227:ARG:CG	1:A:227:ARG:NH1	2.20	0.82
1:A:222:ASN:OD1	1:A:224:ILE:CG2	2.29	0.80
1:A:215:VAL:N	1:A:221:ASN:HD21	1.78	0.79
1:A:432[A]:ILE:CG1	6:A:943:HOH:O	2.13	0.78
1:A:224:ILE:CG1	1:A:225:ILE:H	1.94	0.78
1:A:215:VAL:CG2	1:A:221:ASN:HD22	1.97	0.77
1:A:221:ASN:HB2	1:A:222:ASN:HD22	1.49	0.76
1:A:97:VAL:H	1:A:101:ASN:HD21	1.35	0.74
1:A:215:VAL:CG2	1:A:221:ASN:HD21	1.97	0.74
1:A:226:ASN:ND2	1:A:227:ARG:H	1.85	0.74
1:A:220:GLU:OE2	1:A:223:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:H	1:A:221:ASN:ND2	1.85	0.72
1:A:145:ALA:HB1	4:A:705:1PE:C14	2.21	0.71
1:A:227:ARG:HH11	1:A:227:ARG:HG3	1.49	0.71
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.55	0.70
1:A:225:ILE:CG2	1:A:226:ASN:N	2.37	0.70
1:A:222:ASN:N	1:A:222:ASN:ND2	2.28	0.69
1:A:218:ILE:HG22	1:A:218:ILE:O	1.92	0.68
1:A:224:ILE:O	1:A:225:ILE:HB	1.92	0.68
1:A:408:LYS:H	5:A:717:ACT:H2	1.57	0.68
1:A:216:ASP:O	1:A:216:ASP:CG	2.31	0.67
1:A:145:ALA:HB1	4:A:705:1PE:H142	1.75	0.67
1:A:215:VAL:HG22	1:A:221:ASN:HD21	1.58	0.66
4:A:709:1PE:H141	6:A:1030:HOH:O	1.96	0.65
1:A:156:TRP:HD1	1:A:219:ASN:HB3	1.62	0.64
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.11	0.63
1:A:230:LEU:HB2	1:A:256:TRP:CZ2	2.33	0.63
1:A:225:ILE:HG22	1:A:226:ASN:H	1.61	0.63
4:A:709:1PE:C14	6:A:1030:HOH:O	2.46	0.63
1:A:11:PRO:HB3	4:A:711:1PE:H222	1.81	0.63
1:A:331:HIS:HD2	6:A:1062:HOH:O	1.81	0.62
1:A:212:GLY:O	1:A:218:ILE:HD13	1.99	0.62
4:A:709:1PE:C24	6:A:887:HOH:O	2.48	0.62
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.35	0.62
1:A:57:GLY:HA3	1:A:434:TYR:HB2	1.82	0.61
1:A:225:ILE:O	1:A:226:ASN:HB3	2.01	0.61
1:A:156:TRP:CD1	1:A:219:ASN:HB3	2.37	0.60
1:A:437:ASP:CB	1:A:441:THR:HG21	2.32	0.60
1:A:58:GLY:N	1:A:433:GLU:HB3	2.17	0.59
1:A:156:TRP:CG	1:A:218:ILE:HB	2.37	0.59
1:A:344:ASP:OD1	4:A:712:1PE:H121	2.01	0.59
1:A:214:THR:HB	1:A:215:VAL:HA	1.84	0.59
1:A:224:ILE:HG23	1:A:225:ILE:N	2.18	0.59
1:A:226:ASN:C	1:A:227:ARG:HG3	2.24	0.58
1:A:97:VAL:H	1:A:101:ASN:ND2	2.02	0.57
1:A:169:ILE:HG12	5:A:724:ACT:H1	1.85	0.57
1:A:262:HIS:HE1	1:A:285:ASP:H	1.51	0.57
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.88	0.56
1:A:145:ALA:HB1	4:A:705:1PE:H141	1.87	0.55
1:A:213:GLY:O	1:A:223:THR:HB	2.06	0.55
1:A:119:ARG:HD2	5:A:724:ACT:H2	1.88	0.54
1:A:97:VAL:HA	4:A:705:1PE:H252	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HE21	1:A:203:ALA:H	1.54	0.53
1:A:226:ASN:CG	1:A:227:ARG:N	2.63	0.52
1:A:58:GLY:H	1:A:102:ASN:ND2	2.08	0.52
1:A:234:HIS:HD2	6:A:972:HOH:O	1.90	0.52
1:A:432[B]:ILE:HD11	1:A:441:THR:HG21	1.91	0.52
1:A:227:ARG:NH1	1:A:227:ARG:HG3	2.12	0.51
1:A:169:ILE:HG12	5:A:724:ACT:CH3	2.41	0.51
1:A:300:TYR:CZ	1:A:320:LYS:HE2	2.46	0.51
1:A:490:THR:OG1	1:A:491:GLU:N	2.43	0.50
1:A:219:ASN:C	1:A:219:ASN:HD22	2.15	0.50
1:A:224:ILE:HG23	1:A:225:ILE:H	1.75	0.50
1:A:430:TRP:HE3	1:A:433:GLU:OE1	1.94	0.49
1:A:218:ILE:O	1:A:218:ILE:CG2	2.61	0.49
1:A:220:GLU:OE2	1:A:220:GLU:HA	2.12	0.49
1:A:167:ARG:HH21	1:A:171:GLN:NE2	2.11	0.48
1:A:344:ASP:OD1	4:A:712:1PE:H222	2.13	0.48
1:A:122:TYR:CZ	1:A:126:ARG:HD2	2.47	0.48
1:A:581:ASN:HD22	4:A:708:1PE:H261	1.79	0.48
1:A:156:TRP:HB2	1:A:218:ILE:HB	1.96	0.47
4:A:707:1PE:C16	6:A:815:HOH:O	2.62	0.47
1:A:219:ASN:HB2	1:A:491:GLU:CG	2.37	0.47
4:A:709:1PE:H142	6:A:1030:HOH:O	2.12	0.47
1:A:100:GLN:HA	1:A:100:GLN:NE2	2.26	0.47
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.68	0.47
1:A:226:ASN:ND2	1:A:227:ARG:N	2.59	0.46
1:A:208:PHE:HA	1:A:209:VAL:HA	1.82	0.46
1:A:230:LEU:HD13	1:A:256:TRP:CE2	2.50	0.46
1:A:262:HIS:CE1	1:A:285:ASP:H	2.32	0.46
1:A:212:GLY:O	1:A:218:ILE:CD1	2.64	0.45
1:A:432[B]:ILE:HG12	1:A:441:THR:HB	1.98	0.45
1:A:71:GLN:HE22	1:A:366:PRO:HA	1.81	0.45
1:A:262:HIS:CE1	1:A:288:GLY:HA3	2.52	0.44
1:A:223:THR:O	1:A:223:THR:OG1	2.36	0.44
1:A:58:GLY:H	1:A:102:ASN:HD21	1.66	0.44
1:A:430:TRP:CZ2	1:A:434:TYR:CE1	3.06	0.44
1:A:98:HIS:HA	4:A:705:1PE:C16	2.48	0.43
1:A:234:HIS:CD2	6:A:972:HOH:O	2.67	0.43
1:A:433:GLU:CB	1:A:434:TYR:HA	2.45	0.43
1:A:145:ALA:CB	4:A:705:1PE:H142	2.44	0.43
1:A:31:GLN:HA	1:A:51:GLY:HA3	2.00	0.43
1:A:230:LEU:C	1:A:232:ASN:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HE22	1:A:247:SER:H	1.67	0.43
1:A:131:THR:HG21	4:A:705:1PE:H152	2.01	0.42
1:A:524:SER:O	1:A:544:TRP:HA	2.20	0.42
1:A:176:LEU:HD21	4:A:705:1PE:H251	2.01	0.42
1:A:466[B]:ASN:OD1	1:A:508:THR:OG1	2.32	0.42
1:A:251:ILE:HG22	1:A:252:SER:N	2.34	0.42
1:A:161:GLU:OE2	4:A:705:1PE:C23	2.67	0.42
1:A:168:ARG:HA	1:A:171:GLN:HE21	1.84	0.42
1:A:394:ASN:HD22	1:A:394:ASN:HA	1.64	0.42
1:A:100:GLN:CA	1:A:100:GLN:NE2	2.81	0.42
1:A:225:ILE:HG22	1:A:256:TRP:CZ2	2.54	0.42
1:A:432[A]:ILE:HD12	1:A:432[A]:ILE:HG23	1.61	0.41
1:A:300:TYR:O	1:A:304:VAL:HG23	2.20	0.41
4:A:705:1PE:OH5	4:A:705:1PE:C26	2.47	0.41
1:A:147:CYS:HB3	4:A:705:1PE:H132	2.03	0.41
1:A:291:ARG:NH1	6:A:816:HOH:O	2.41	0.41
1:A:410:ALA:O	1:A:459:THR:HA	2.21	0.41
1:A:98:HIS:HA	4:A:705:1PE:H162	2.03	0.41
1:A:378:ARG:HD3	2:A:703:GOL:H11	2.02	0.41
1:A:230:LEU:C	1:A:232:ASN:H	2.23	0.40
1:A:230:LEU:HD23	1:A:231:MET:SD	2.61	0.40
1:A:320:LYS:HB2	6:A:1012:HOH:O	2.21	0.40
1:A:322[A]:GLN:OE1	4:A:709:1PE:H241	2.22	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	610/609 (100%)	576 (94%)	26 (4%)	8 (1%)	<b>12</b> <b>8</b>

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ILE
1	A	226	ASN
1	A	433	GLU
1	A	432[A]	ILE
1	A	432[B]	ILE
1	A	505	GLY
1	A	224	ILE
1	A	218	ILE

### 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	494/490 (101%)	470 (95%)	24 (5%)	25	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	36	GLU
1	A	62	ARG
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	172[A]	SER
1	A	172[B]	SER
1	A	215	VAL
1	A	216	ASP
1	A	219	ASN
1	A	222	ASN
1	A	224	ILE
1	A	226	ASN
1	A	227	ARG
1	A	228	GLU
1	A	290	ASP
1	A	320	LYS
1	A	433	GLU

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Mol	Chain	Res	Type
1	A	434	TYR
1	A	437	ASP
1	A	438	THR
1	A	466[A]	ASN
1	A	466[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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	171	GLN
1	A	181	GLN
1	A	221	ASN
1	A	222	ASN
1	A	226	ASN
1	A	232	ASN
1	A	234	HIS
1	A	262	HIS
1	A	331	HIS
1	A	377	HIS
1	A	394	ASN
1	A	581	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

26 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	$\# Z  > 2$
4	1PE	A	707	-	7,7,15	0.97	0	6,6,14	0.83	0
2	GOL	A	703	-	5,5,5	0.77	0	5,5,5	0.94	0
5	ACT	A	718	-	3,3,3	0.98	0	3,3,3	0.37	0
5	ACT	A	725	-	3,3,3	0.82	0	3,3,3	0.82	0
5	ACT	A	722	-	3,3,3	0.87	0	3,3,3	0.72	0
4	1PE	A	708	-	8,8,15	0.62	0	7,7,14	0.42	0
4	1PE	A	709	-	15,15,15	0.52	0	14,14,14	0.94	1 (7%)
3	LAM	A	704	-	23,24,46	1.34	3 (13%)	29,35,67	1.89	6 (20%)
4	1PE	A	712	-	11,11,15	0.76	0	10,10,14	0.72	0
4	1PE	A	711	-	4,4,15	0.86	0	3,3,14	0.55	0
4	1PE	A	710[B]	-	7,7,15	0.63	0	6,6,14	0.50	0
5	ACT	A	723	-	3,3,3	1.03	0	3,3,3	1.14	0
4	1PE	A	706	-	8,8,15	0.72	0	7,7,14	1.06	0
4	1PE	A	710[A]	-	7,7,15	0.61	0	6,6,14	0.62	0
5	ACT	A	724	-	3,3,3	0.77	0	3,3,3	2.66	2 (66%)
4	1PE	A	705	-	11,11,15	0.62	0	10,10,14	1.17	0
5	ACT	A	716	-	3,3,3	0.87	0	3,3,3	1.04	0
2	GOL	A	702	-	5,5,5	0.48	0	5,5,5	1.09	0
5	ACT	A	720	-	3,3,3	0.73	0	3,3,3	1.25	0
5	ACT	A	719	-	3,3,3	0.78	0	3,3,3	0.86	0
5	ACT	A	714	-	3,3,3	0.93	0	3,3,3	0.46	0
2	GOL	A	701	-	5,5,5	0.59	0	5,5,5	1.43	1 (20%)
5	ACT	A	721	-	3,3,3	0.73	0	3,3,3	0.87	0
5	ACT	A	713	-	3,3,3	0.72	0	3,3,3	0.86	0
5	ACT	A	717	-	3,3,3	1.11	0	3,3,3	0.23	0
5	ACT	A	715	-	3,3,3	0.58	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
4	1PE	A	707	-	-	3/5/5/13	-
2	GOL	A	701	-	-	2/4/4/4	-
4	1PE	A	710[B]	-	-	4/5/5/13	-
4	1PE	A	712	-	-	6/9/9/13	-
4	1PE	A	705	-	-	6/9/9/13	-
2	GOL	A	703	-	-	1/4/4/4	-
4	1PE	A	706	-	-	3/6/6/13	-
4	1PE	A	710[A]	-	-	3/5/5/13	-
2	GOL	A	702	-	-	2/4/4/4	-
4	1PE	A	708	-	-	3/6/6/13	-
4	1PE	A	709	-	-	8/13/13/13	-
3	LAM	A	704	-	-	2/8/48/82	0/2/2/4
4	1PE	A	711	-	-	2/2/2/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	LAM	O5-C1	3.94	1.48	1.42
3	A	704	LAM	C4A-C3A	-2.21	1.51	1.53
3	A	704	LAM	C6-C5	2.10	1.58	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	LAM	C1-O5-C5	6.59	124.73	112.58
3	A	704	LAM	C2-C1-S3A	-3.66	105.66	111.30
5	A	724	ACT	O-C-CH3	-3.56	108.48	122.33
5	A	724	ACT	OXT-C-CH3	2.84	126.93	115.18
3	A	704	LAM	O2-C2-C1	-2.75	105.22	110.27
4	A	709	1PE	OH7-C16-C26	-2.68	96.25	111.81
3	A	704	LAM	C4-C3-C2	2.19	114.64	110.82
2	A	701	GOL	O1-C1-C2	2.05	120.01	110.20
3	A	704	LAM	O5-C5-C6	2.04	111.51	106.44
3	A	704	LAM	C1-C2-C3	2.00	114.55	110.59

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	GOL	O1-C1-C2-O2
2	A	702	GOL	O1-C1-C2-C3
4	A	709	1PE	OH2-C12-C22-OH3
4	A	708	1PE	OH6-C15-C25-OH5
4	A	710[A]	1PE	OH4-C13-C23-OH3
4	A	710[B]	1PE	OH4-C13-C23-OH3
4	A	705	1PE	OH5-C14-C24-OH4
4	A	709	1PE	OH5-C14-C24-OH4
4	A	712	1PE	OH5-C14-C24-OH4
4	A	707	1PE	C25-C15-OH6-C26
4	A	706	1PE	OH4-C13-C23-OH3
4	A	711	1PE	OH2-C12-C22-OH3
4	A	709	1PE	OH6-C15-C25-OH5
4	A	705	1PE	C25-C15-OH6-C26
4	A	705	1PE	OH7-C16-C26-OH6
2	A	703	GOL	C1-C2-C3-O3
4	A	712	1PE	OH2-C12-C22-OH3
4	A	707	1PE	OH6-C15-C25-OH5
3	A	704	LAM	O5A-C5A-C6A-O6A
4	A	709	1PE	OH4-C13-C23-OH3
4	A	705	1PE	OH6-C15-C25-OH5
4	A	706	1PE	OH2-C12-C22-OH3
4	A	705	1PE	C23-C13-OH4-C24
4	A	710[A]	1PE	C23-C13-OH4-C24
4	A	710[B]	1PE	C23-C13-OH4-C24
4	A	709	1PE	C14-C24-OH4-C13
4	A	710[B]	1PE	C12-C22-OH3-C23
4	A	710[A]	1PE	C12-C22-OH3-C23
4	A	709	1PE	C23-C13-OH4-C24
4	A	712	1PE	C12-C22-OH3-C23
2	A	701	GOL	O2-C2-C3-O3
4	A	708	1PE	C25-C15-OH6-C26
4	A	709	1PE	C24-C14-OH5-C25
4	A	709	1PE	OH7-C16-C26-OH6
4	A	710[B]	1PE	OH2-C12-C22-OH3
4	A	706	1PE	C14-C24-OH4-C13
4	A	711	1PE	C12-C22-OH3-C23
4	A	712	1PE	C15-C25-OH5-C14
4	A	708	1PE	C24-C14-OH5-C25
4	A	712	1PE	C24-C14-OH5-C25
4	A	707	1PE	OH7-C16-C26-OH6
2	A	701	GOL	O1-C1-C2-O2
4	A	705	1PE	C14-C24-OH4-C13

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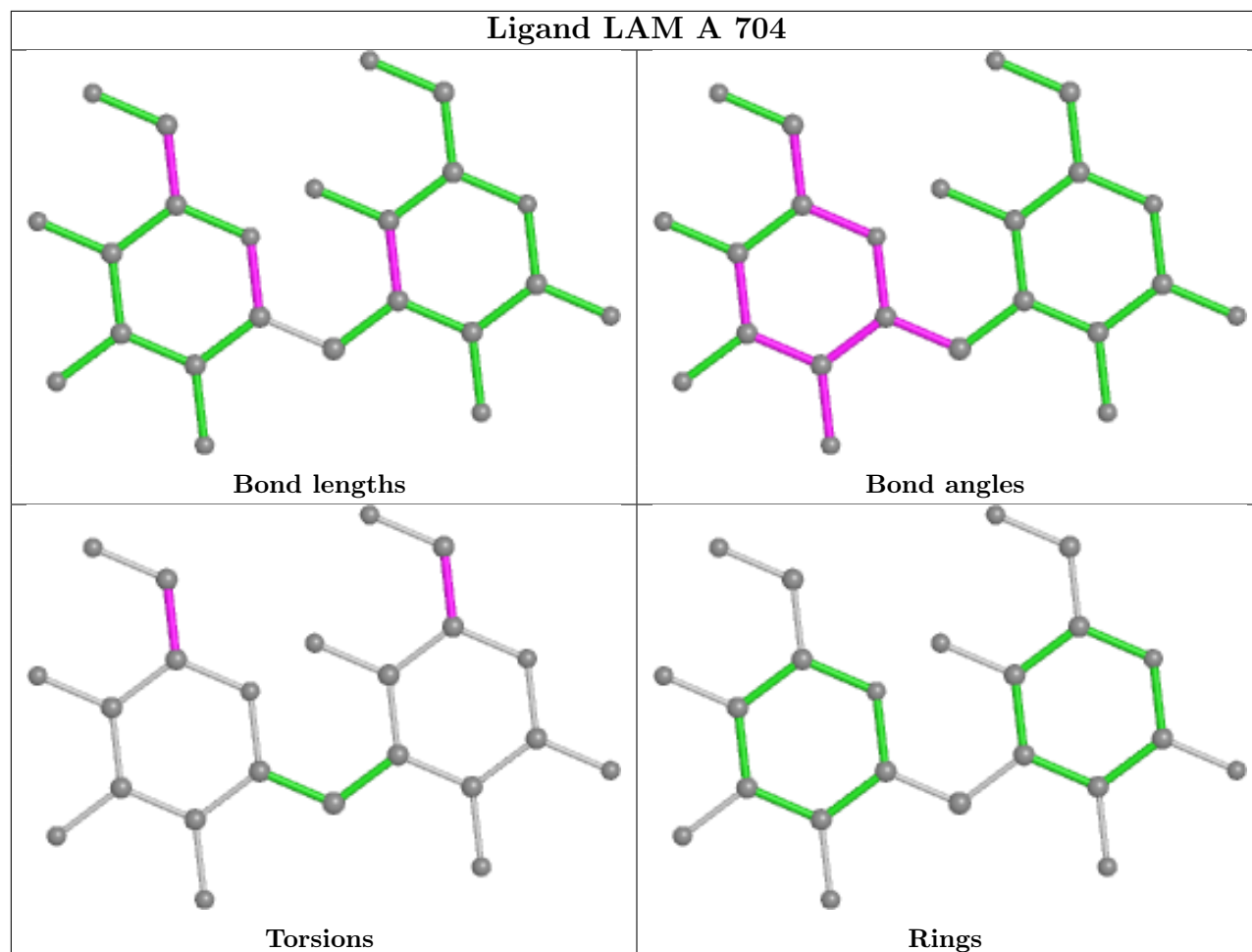
Mol	Chain	Res	Type	Atoms
3	A	704	LAM	O5-C5-C6-O6
4	A	712	1PE	C14-C24-OH4-C13

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	707	1PE	1	0
2	A	703	GOL	1	0
4	A	708	1PE	1	0
4	A	709	1PE	5	0
3	A	704	LAM	3	0
4	A	712	1PE	2	0
4	A	711	1PE	1	0
5	A	724	ACT	3	0
4	A	705	1PE	14	0
5	A	717	ACT	1	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%)	-0.15	28 (4%)	32 35	19, 29, 57, 85	12 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ILE	11.8
1	A	221	ASN	11.3
1	A	224	ILE	11.2
1	A	223	THR	10.2
1	A	215	VAL	8.8
1	A	222	ASN	8.1
1	A	220	GLU	6.8
1	A	231	MET	6.4
1	A	217	GLY	5.5
1	A	216	ASP	5.1
1	A	586	HIS	4.8
1	A	226	ASN	4.3
1	A	187	ASP	4.2
1	A	583	GLY	3.7
1	A	434	TYR	3.5
1	A	228	GLU	3.5
1	A	294	THR	3.5
1	A	585	ALA	3.4
1	A	440	ARG	3.3
1	A	232	ASN	3.0
1	A	432[A]	ILE	2.6
1	A	587	TYR	2.5
1	A	438	THR	2.5
1	A	186	LYS	2.4
1	A	188	PHE	2.4
1	A	436	GLY	2.1
1	A	185	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	582	VAL	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
5	ACT	A	721	4/4	0.50	0.30	65,70,71,78	0
5	ACT	A	716	4/4	0.74	0.25	57,63,63,64	0
5	ACT	A	717	4/4	0.74	0.20	35,39,47,56	0
4	1PE	A	706	9/16	0.74	0.24	58,62,69,70	0
5	ACT	A	719	4/4	0.78	0.23	74,74,74,75	0
4	1PE	A	708	9/16	0.80	0.21	64,71,78,81	0
4	1PE	A	711	5/16	0.82	0.34	50,51,60,61	0
4	1PE	A	707	8/16	0.83	0.13	47,60,62,64	0
5	ACT	A	725	4/4	0.83	0.26	56,58,66,70	0
4	1PE	A	712	12/16	0.84	0.25	46,62,66,67	0
2	GOL	A	701	6/6	0.84	0.19	31,46,48,57	0
5	ACT	A	718	4/4	0.85	0.17	55,65,68,69	0
5	ACT	A	713	4/4	0.85	0.16	57,58,66,66	0
5	ACT	A	722	4/4	0.86	0.24	47,55,57,57	0
5	ACT	A	715	4/4	0.87	0.13	57,59,64,64	0
4	1PE	A	709	16/16	0.88	0.15	29,56,67,68	0
5	ACT	A	723	4/4	0.89	0.21	51,53,54,68	0
2	GOL	A	703	6/6	0.89	0.19	34,48,53,56	0
4	1PE	A	710[A]	8/16	0.90	0.15	53,63,67,68	4
4	1PE	A	710[B]	8/16	0.90	0.15	39,57,67,68	4
5	ACT	A	714	4/4	0.91	0.20	57,61,64,65	0
5	ACT	A	724	4/4	0.93	0.18	39,40,43,52	0

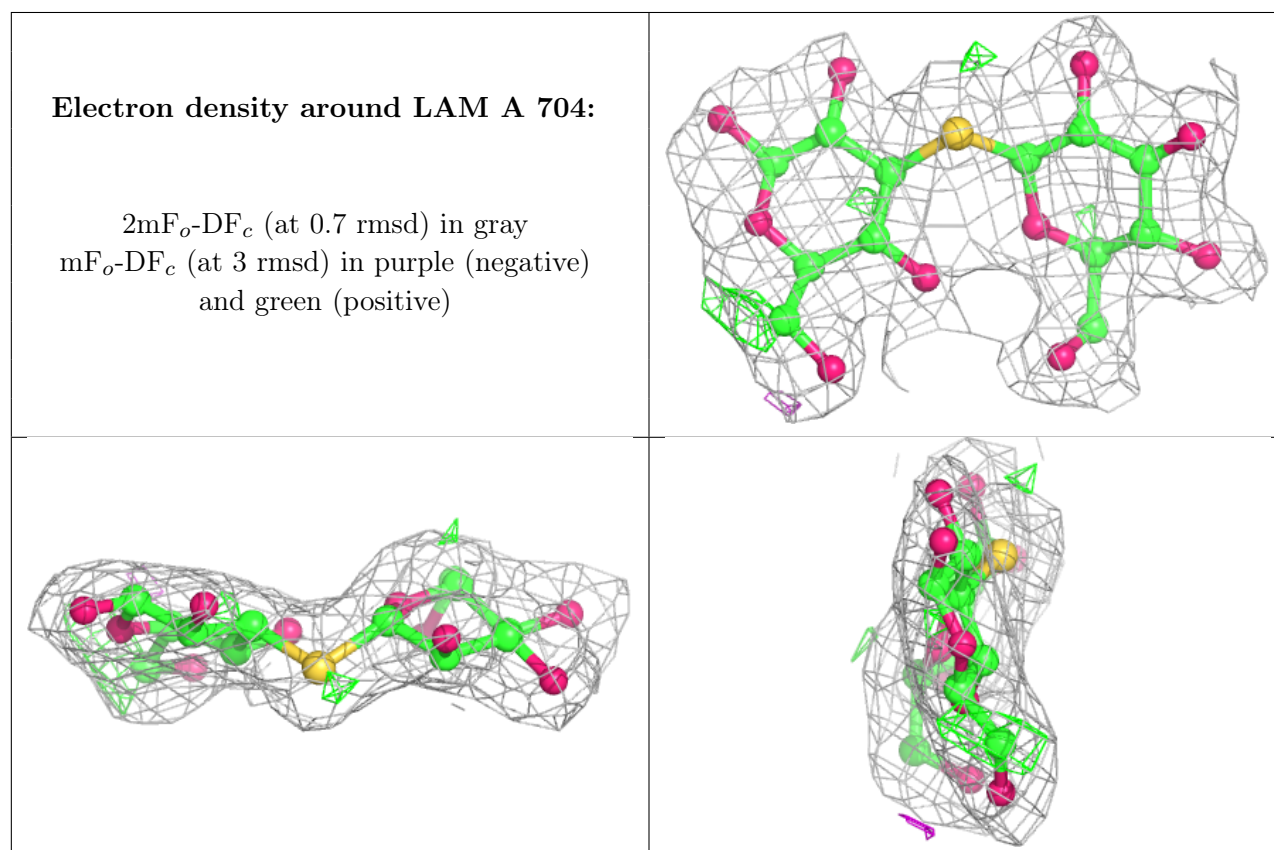
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	A	720	4/4	0.94	0.14	44,57,61,61	0
3	LAM	A	704	23/43	0.94	0.15	21,30,56,58	0
4	1PE	A	705	12/16	0.96	0.18	25,30,32,33	12
2	GOL	A	702	6/6	0.96	0.14	42,45,46,46	0

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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.