



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 12:12 PM JST

PDB ID : 6JGC
Title : Crystal structure of barley exohydrolaseI W286Y mutant in complex with glucose.
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on : 2019-02-13
Resolution : 2.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-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

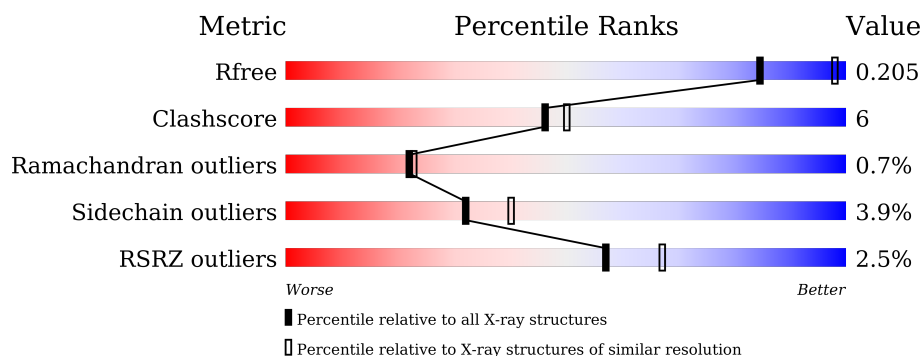
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	609	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5200 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.

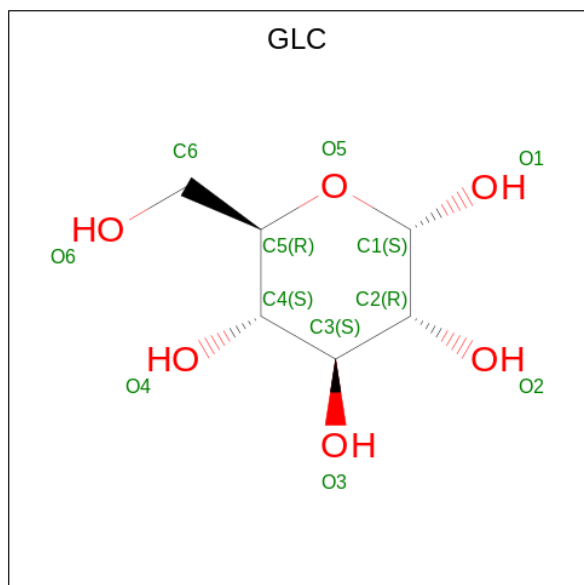
- Molecule 1 is a protein called BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4604	2912	798	868	26	30	3	0

There are 6 discrepancies between the modelled and reference sequences:

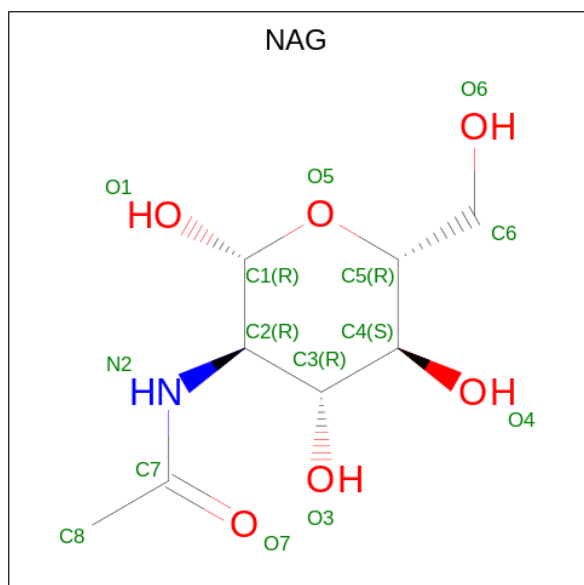
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP A0A287SCR5
A	-2	HIS	-	expression tag	UNP A0A287SCR5
A	-1	ALA	-	expression tag	UNP A0A287SCR5
A	0	ALA	-	expression tag	UNP A0A287SCR5
A	286	TYR	TRP	engineered mutation	UNP A0A287SCR5
A	320	LYS	ASN	conflict	UNP A0A287SCR5

- Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C₆H₁₂O₆).



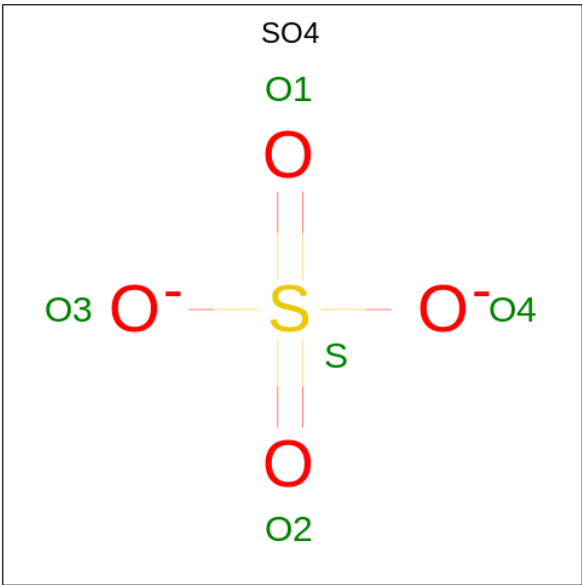
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



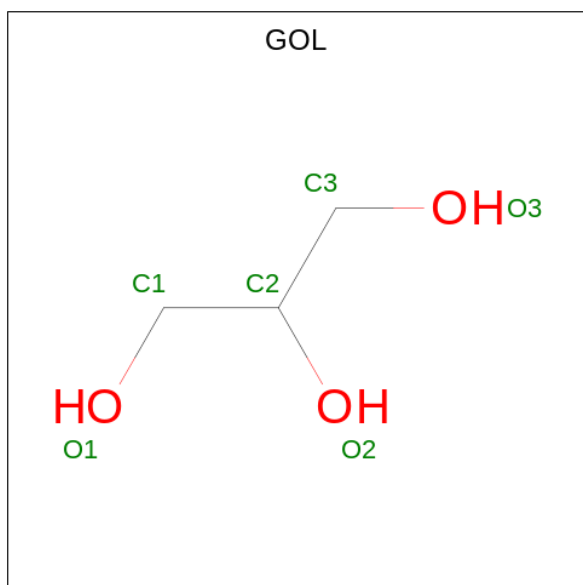
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



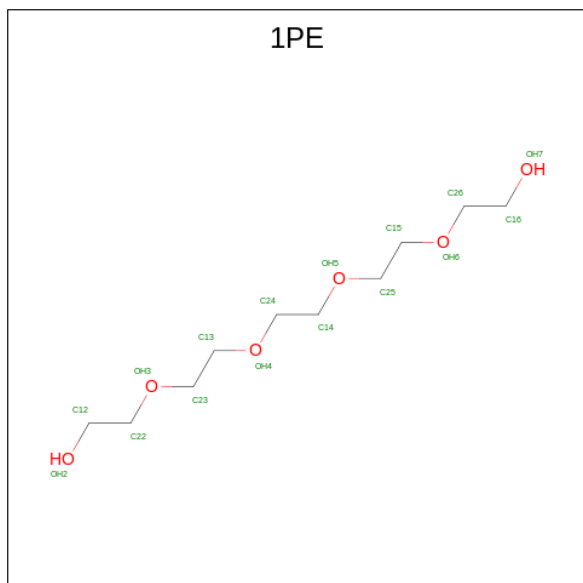
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

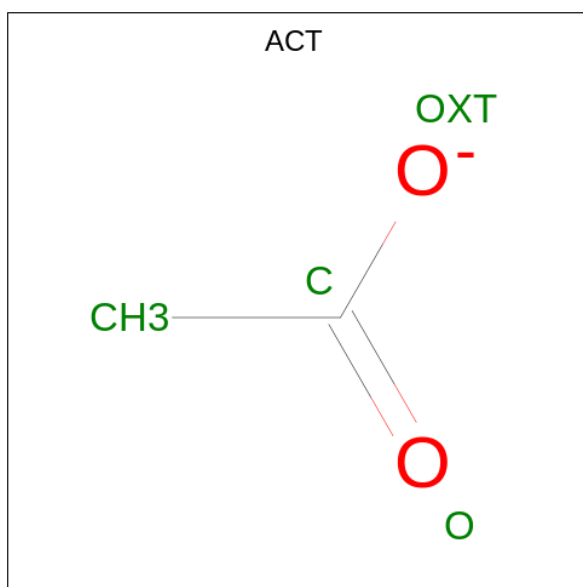
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	7	4		
6	A	1	Total	C	O	0	0
			8	5	3		
6	A	1	Total	C	O	0	0
			8	5	3		
6	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

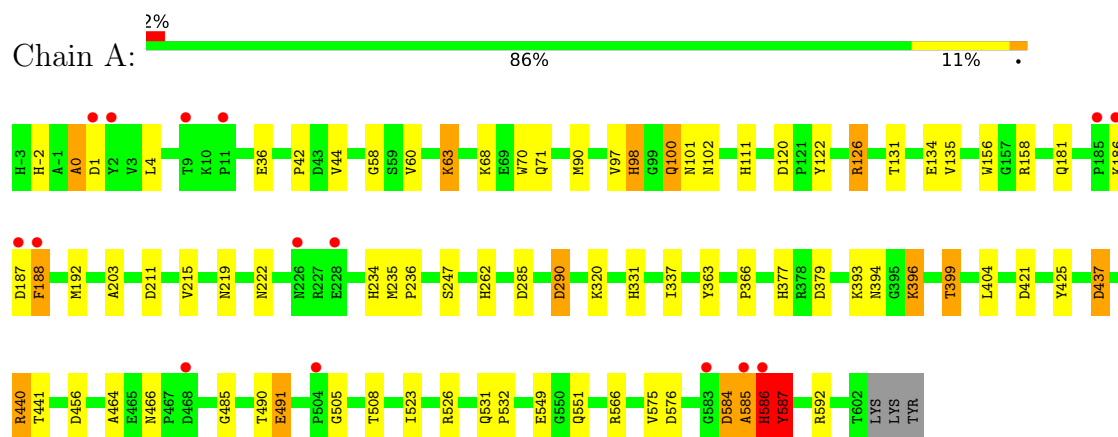
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	347	Total	O	0	0
			347	347		

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, α , β , γ	100.11Å 100.11Å 182.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 2.36 48.27 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.32-2.36) 99.8 (48.27-2.36)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.149 , 0.194 0.161 , 0.205	Depositor DCC
R_{free} test set	1944 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5200	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, GOL, NAG, ACT, SO4, 1PE

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	0.86	3/4711 (0.1%)	1.12	17/6399 (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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	GLU	CD-OE1	-5.63	1.19	1.25
1	A	587	TYR	N-CA	5.31	1.56	1.46
1	A	549	GLU	CD-OE2	5.14	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	ALA	O-C-N	-42.77	54.27	122.70
1	A	0	ALA	CA-C-N	26.01	174.42	117.20
1	A	587	TYR	N-CA-C	8.44	133.80	111.00
1	A	126	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	456	ASP	CB-CG-OD1	6.71	124.33	118.30
1	A	126	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	526	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	456	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	290	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	120	ASP	CB-CG-OD1	5.68	123.41	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	526	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	379	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	421	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	211	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	584	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	440	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	ALA	Peptide,Mainchain
1	A	585	ALA	Peptide

5.2 Too-close contacts [i](#)

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	4604	0	4584	54	0
2	A	24	0	24	0	0
3	A	28	0	26	2	0
4	A	80	0	0	1	0
5	A	66	0	88	8	0
6	A	43	0	53	1	0
7	A	8	0	6	2	0
8	A	347	0	0	14	0
All	All	5200	0	4781	60	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 6.

All (60) 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:592[B]:ARG:NE	8:A:808:HOH:O	1.88	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592[B]:ARG:NH1	8:A:808:HOH:O	1.99	0.95
1:A:592[B]:ARG:CZ	8:A:808:HOH:O	2.15	0.92
1:A:466[A]:ASN:ND2	1:A:508:THR:OG1	2.13	0.82
1:A:584:ASP:HB3	1:A:586:HIS:CD2	2.15	0.80
5:A:726:GOL:O3	8:A:809:HOH:O	2.01	0.78
1:A:156:TRP:HE1	1:A:219:ASN:HD22	1.35	0.75
1:A:394:ASN:HD21	1:A:404:LEU:H	1.34	0.72
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.63	0.63
1:A:399:THR:HG23	8:A:915:HOH:O	1.98	0.61
1:A:97:VAL:H	1:A:101:ASN:HD21	1.50	0.60
1:A:181:GLN:HE21	1:A:203:ALA:H	1.49	0.60
5:A:724:GOL:H12	8:A:975:HOH:O	2.02	0.60
1:A:71:GLN:HE22	1:A:366:PRO:HA	1.67	0.59
1:A:464:ALA:HB1	5:A:730:GOL:H11	1.85	0.58
4:A:710:SO4:O1	8:A:811:HOH:O	2.17	0.58
1:A:262:HIS:HE1	1:A:285:ASP:H	1.51	0.58
1:A:234:HIS:HE1	8:A:906:HOH:O	1.88	0.57
1:A:592[A]:ARG:NH2	7:A:737:ACT:OXT	2.33	0.57
1:A:58:GLY:H	1:A:102:ASN:ND2	2.02	0.57
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.40	0.57
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.88	0.57
1:A:156:TRP:HE1	1:A:219:ASN:ND2	2.02	0.56
1:A:585:ALA:N	1:A:586:HIS:HD2	2.04	0.56
1:A:4:LEU:HD23	1:A:4:LEU:C	2.29	0.53
3:A:704:NAG:O7	5:A:721:GOL:H2	2.11	0.51
1:A:393:LYS:HE2	1:A:396:LYS:HA	1.93	0.51
1:A:181:GLN:HE22	1:A:247:SER:H	1.58	0.50
1:A:262:HIS:CE1	1:A:285:ASP:H	2.28	0.50
1:A:490:THR:HG22	1:A:491:GLU:HG3	1.95	0.49
1:A:363:TYR:HB2	5:A:725:GOL:H31	1.94	0.49
1:A:156:TRP:CE2	1:A:158:ARG:HB2	2.49	0.47
1:A:235:MET:N	1:A:236:PRO:CD	2.78	0.47
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.28	0.46
1:A:181:GLN:HE22	1:A:247:SER:N	2.14	0.46
1:A:584:ASP:HB3	1:A:586:HIS:CG	2.50	0.45
1:A:566:ARG:NE	8:A:811:HOH:O	2.48	0.45
1:A:97:VAL:H	1:A:101:ASN:ND2	2.15	0.45
1:A:425:TYR:OH	5:A:727:GOL:H31	2.16	0.44
1:A:44:VAL:HG22	5:A:723:GOL:H2	1.99	0.44
1:A:215:VAL:HG23	1:A:222:ASN:O	2.17	0.44
1:A:485:GLY:HA3	1:A:523:ILE:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ASP:HB3	1:A:586:HIS:HD2	1.78	0.44
6:A:732:1PE:H151	8:A:992:HOH:O	2.18	0.44
1:A:63:LYS:HD3	8:A:1139:HOH:O	2.17	0.44
1:A:4:LEU:HD23	1:A:4:LEU:O	2.18	0.43
1:A:437:ASP:HB3	1:A:441:THR:HG21	2.02	0.42
1:A:222:ASN:HB2	3:A:703:NAG:H82	2.02	0.42
1:A:551:GLN:HG2	8:A:903:HOH:O	2.19	0.42
1:A:131:THR:O	1:A:135:VAL:HG23	2.20	0.42
1:A:156:TRP:CZ2	1:A:158:ARG:HB2	2.54	0.41
1:A:575:VAL:HG22	7:A:736:ACT:H3	2.02	0.41
1:A:234:HIS:HD2	8:A:960:HOH:O	2.03	0.41
1:A:98:HIS:CE1	1:A:111:HIS:NE2	2.89	0.41
1:A:60:VAL:HG12	1:A:70:TRP:CZ2	2.56	0.41
1:A:188:PHE:HZ	1:A:192:MET:O	2.03	0.41
1:A:331:HIS:HB3	1:A:337:ILE:HD12	2.03	0.41
5:A:724:GOL:C1	8:A:975:HOH:O	2.62	0.41
1:A:134:GLU:OE2	1:A:377:HIS:CD2	2.71	0.41
1:A:531:GLN:HB2	1:A:532:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	606/609 (100%)	579 (96%)	23 (4%)	4 (1%)	22 23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	PHE
1	A	586	HIS
1	A	587	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	505	GLY

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	489/490 (100%)	470 (96%)	19 (4%)	32	40

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	1	ASP
1	A	36	GLU
1	A	42	PRO
1	A	63	LYS
1	A	68	LYS
1	A	90	MET
1	A	98	HIS
1	A	100	GLN
1	A	186	LYS
1	A	187	ASP
1	A	290	ASP
1	A	320	LYS
1	A	396	LYS
1	A	399	THR
1	A	440	ARG
1	A	576	ASP
1	A	586	HIS
1	A	587	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	219	ASN
1	A	234	HIS
1	A	262	HIS
1	A	331	HIS
1	A	377	HIS
1	A	394	ASN
1	A	586	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

37 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	$\# Z > 2$
6	1PE	A	735	-	15,15,15	1.01	0	14,14,14	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	715	-	4,4,4	0.50	0	6,6,6	1.18	1 (16%)
3	NAG	A	704	1	14,14,15	0.97	0	17,19,21	2.03	6 (35%)
4	SO4	A	709	-	4,4,4	0.45	0	6,6,6	0.50	0
7	ACT	A	736	-	3,3,3	1.22	0	3,3,3	1.73	1 (33%)
5	GOL	A	727	-	5,5,5	0.41	0	5,5,5	0.86	0
5	GOL	A	729	-	5,5,5	0.48	0	5,5,5	0.54	0
5	GOL	A	724	-	5,5,5	0.94	0	5,5,5	1.61	1 (20%)
4	SO4	A	707	-	4,4,4	0.31	0	6,6,6	0.92	0
4	SO4	A	706	-	4,4,4	0.57	0	6,6,6	0.75	0
6	1PE	A	733	-	7,7,15	0.99	0	6,6,14	0.97	0
4	SO4	A	705	-	4,4,4	0.38	0	6,6,6	0.16	0
4	SO4	A	717	-	4,4,4	0.43	0	6,6,6	1.17	0
4	SO4	A	708	-	4,4,4	0.33	0	6,6,6	0.53	0
2	GLC	A	702[A]	-	12,12,12	0.76	0	17,17,17	2.19	5 (29%)
2	GLC	A	701[A]	-	12,12,12	0.87	0	17,17,17	2.41	7 (41%)
5	GOL	A	721	-	5,5,5	0.41	0	5,5,5	0.86	0
5	GOL	A	723	-	5,5,5	0.45	0	5,5,5	1.63	1 (20%)
5	GOL	A	728	-	5,5,5	0.52	0	5,5,5	1.27	0
5	GOL	A	730	-	5,5,5	1.11	0	5,5,5	1.65	2 (40%)
4	SO4	A	720	-	4,4,4	0.34	0	6,6,6	0.32	0
4	SO4	A	714	-	4,4,4	0.48	0	6,6,6	1.72	1 (16%)
5	GOL	A	725	-	5,5,5	0.52	0	5,5,5	0.70	0
4	SO4	A	711	-	4,4,4	0.52	0	6,6,6	1.00	0
4	SO4	A	716	-	4,4,4	0.53	0	6,6,6	0.69	0
5	GOL	A	726	-	5,5,5	0.59	0	5,5,5	0.72	0
4	SO4	A	710	-	4,4,4	0.32	0	6,6,6	1.30	1 (16%)
6	1PE	A	732	-	10,10,15	0.73	0	9,9,14	0.64	0
7	ACT	A	737	-	3,3,3	0.85	0	3,3,3	0.86	0
4	SO4	A	712	-	4,4,4	0.52	0	6,6,6	0.28	0
4	SO4	A	718	-	4,4,4	0.57	0	6,6,6	0.92	0
6	1PE	A	734	-	7,7,15	0.66	0	6,6,14	0.43	0
5	GOL	A	731	-	5,5,5	0.80	0	5,5,5	1.82	1 (20%)
3	NAG	A	703	1	14,14,15	0.79	0	17,19,21	1.73	2 (11%)
4	SO4	A	713	-	4,4,4	0.49	0	6,6,6	1.05	0
4	SO4	A	719	-	4,4,4	0.45	0	6,6,6	0.74	0
5	GOL	A	722	-	5,5,5	0.55	0	5,5,5	1.32	1 (20%)

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
6	1PE	A	735	-	-	10/13/13/13	-
3	NAG	A	704	1	-	2/6/23/26	0/1/1/1
5	GOL	A	729	-	-	3/4/4/4	-
5	GOL	A	727	-	-	2/4/4/4	-
5	GOL	A	724	-	-	2/4/4/4	-
6	1PE	A	733	-	-	2/5/5/13	-
2	GLC	A	702[A]	-	-	0/2/22/22	0/1/1/1
5	GOL	A	721	-	-	2/4/4/4	-
2	GLC	A	701[A]	-	-	1/2/22/22	0/1/1/1
5	GOL	A	723	-	-	4/4/4/4	-
5	GOL	A	730	-	-	2/4/4/4	-
5	GOL	A	728	-	-	1/4/4/4	-
5	GOL	A	725	-	-	4/4/4/4	-
5	GOL	A	726	-	-	2/4/4/4	-
6	1PE	A	732	-	-	6/8/8/13	-
6	1PE	A	734	-	-	4/5/5/13	-
5	GOL	A	731	-	-	2/4/4/4	-
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
5	GOL	A	722	-	-	4/4/4/4	-

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	NAG	C1-O5-C5	5.90	120.19	112.19
2	A	702[A]	GLC	O5-C1-C2	5.59	120.26	110.28
2	A	701[A]	GLC	O5-C5-C6	4.21	116.90	106.44
3	A	704	NAG	C1-C2-N2	4.18	117.62	110.49
3	A	704	NAG	C1-O5-C5	3.81	117.36	112.19
2	A	701[A]	GLC	C1-O5-C5	3.71	120.67	113.66
2	A	702[A]	GLC	C1-O5-C5	3.58	120.42	113.66
4	A	714	SO4	O4-S-O3	3.55	124.22	109.06
2	A	701[A]	GLC	O2-C2-C1	3.49	117.25	109.16
2	A	701[A]	GLC	C1-C2-C3	3.40	117.36	110.31
2	A	701[A]	GLC	O5-C1-C2	3.26	116.11	110.28
2	A	702[A]	GLC	O2-C2-C1	3.22	116.63	109.16
2	A	701[A]	GLC	O3-C3-C2	-2.89	103.67	110.35
3	A	704	NAG	C4-C3-C2	-2.85	106.84	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	731	GOL	O1-C1-C2	2.80	123.62	110.20
2	A	701[A]	GLC	C4-C3-C2	-2.76	106.01	110.82
5	A	723	GOL	O1-C1-C2	-2.73	97.09	110.20
5	A	730	GOL	O1-C1-C2	2.63	122.81	110.20
3	A	704	NAG	O5-C5-C6	-2.62	103.10	107.20
2	A	702[A]	GLC	O5-C5-C4	2.56	114.34	109.69
5	A	724	GOL	O1-C1-C2	2.52	122.28	110.20
7	A	736	ACT	OXT-C-CH3	2.33	124.81	115.18
2	A	702[A]	GLC	O3-C3-C2	-2.19	105.29	110.35
4	A	715	SO4	O3-S-O1	2.13	120.41	109.31
5	A	722	GOL	O2-C2-C1	-2.11	99.82	109.12
4	A	710	SO4	O3-S-O2	-2.11	98.28	109.31
3	A	703	NAG	O4-C4-C3	-2.07	105.56	110.35
3	A	704	NAG	O7-C7-C8	2.04	125.85	122.06
5	A	730	GOL	C3-C2-C1	2.01	119.51	111.70
3	A	704	NAG	C3-C4-C5	2.00	113.81	110.24

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	722	GOL	C1-C2-C3-O3
5	A	723	GOL	C1-C2-C3-O3
5	A	724	GOL	O1-C1-C2-O2
5	A	724	GOL	O1-C1-C2-C3
5	A	725	GOL	C1-C2-C3-O3
5	A	725	GOL	O2-C2-C3-O3
5	A	726	GOL	O1-C1-C2-C3
5	A	729	GOL	C1-C2-C3-O3
5	A	730	GOL	C1-C2-C3-O3
5	A	731	GOL	C1-C2-C3-O3
6	A	733	1PE	C25-C15-OH6-C26
6	A	734	1PE	OH6-C15-C25-OH5
6	A	732	1PE	OH6-C15-C25-OH5
6	A	735	1PE	OH5-C14-C24-OH4
6	A	735	1PE	OH4-C13-C23-OH3
5	A	721	GOL	O1-C1-C2-O2
6	A	735	1PE	OH7-C16-C26-OH6
6	A	734	1PE	OH7-C16-C26-OH6
2	A	701[A]	GLC	O5-C5-C6-O6
5	A	721	GOL	O1-C1-C2-C3
5	A	725	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	727	GOL	C1-C2-C3-O3
5	A	729	GOL	O1-C1-C2-C3
6	A	732	1PE	OH7-C16-C26-OH6
6	A	733	1PE	OH7-C16-C26-OH6
6	A	735	1PE	OH6-C15-C25-OH5
5	A	722	GOL	O2-C2-C3-O3
5	A	723	GOL	O2-C2-C3-O3
5	A	725	GOL	O1-C1-C2-O2
5	A	726	GOL	O1-C1-C2-O2
5	A	730	GOL	O2-C2-C3-O3
5	A	731	GOL	O2-C2-C3-O3
6	A	732	1PE	OH5-C14-C24-OH4
5	A	729	GOL	O2-C2-C3-O3
3	A	704	NAG	C4-C5-C6-O6
5	A	723	GOL	O1-C1-C2-O2
5	A	728	GOL	O2-C2-C3-O3
6	A	735	1PE	C23-C13-OH4-C24
6	A	735	1PE	C25-C15-OH6-C26
5	A	722	GOL	O1-C1-C2-O2
6	A	735	1PE	C15-C25-OH5-C14
6	A	732	1PE	C24-C14-OH5-C25
6	A	734	1PE	C16-C26-OH6-C15
3	A	704	NAG	C3-C2-N2-C7
6	A	732	1PE	C16-C26-OH6-C15
6	A	735	1PE	C16-C26-OH6-C15
6	A	735	1PE	C24-C14-OH5-C25
6	A	732	1PE	C15-C25-OH5-C14
5	A	723	GOL	O1-C1-C2-C3
5	A	727	GOL	O2-C2-C3-O3
6	A	735	1PE	C13-C23-OH3-C22
6	A	734	1PE	C25-C15-OH6-C26
5	A	722	GOL	O1-C1-C2-C3

There are no ring outliers.

13 monomers are involved in 13 short contacts:

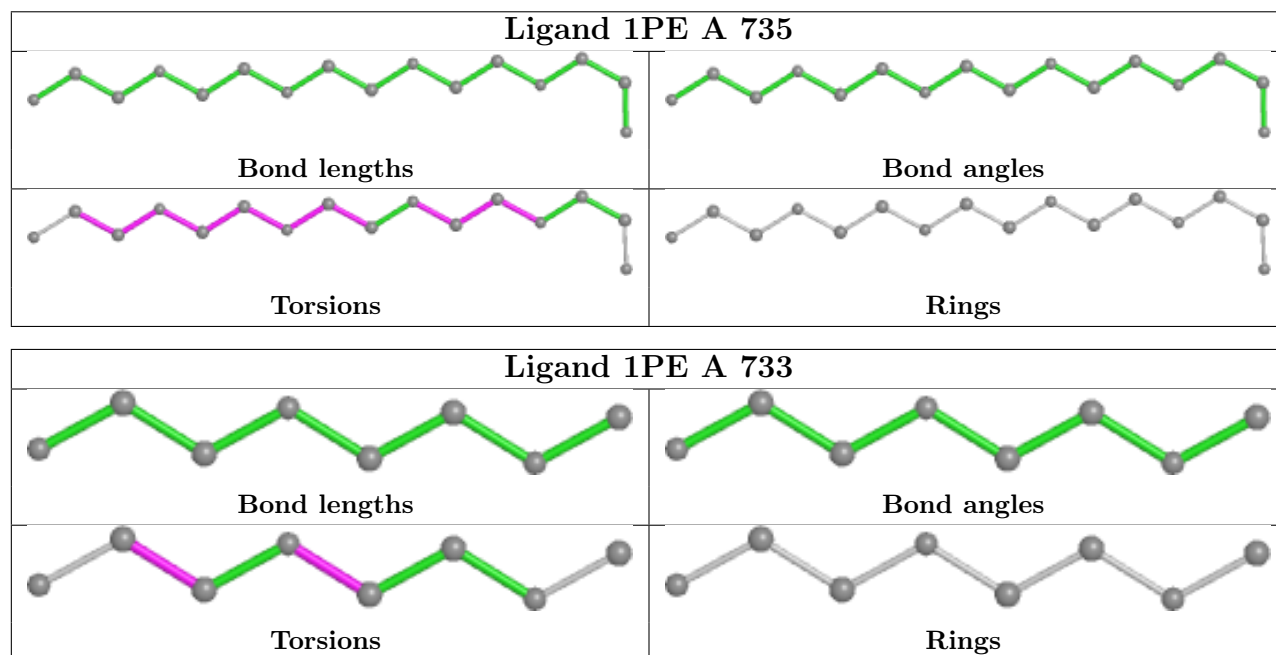
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	NAG	1	0
7	A	736	ACT	1	0
5	A	727	GOL	1	0
5	A	724	GOL	2	0
5	A	721	GOL	1	0

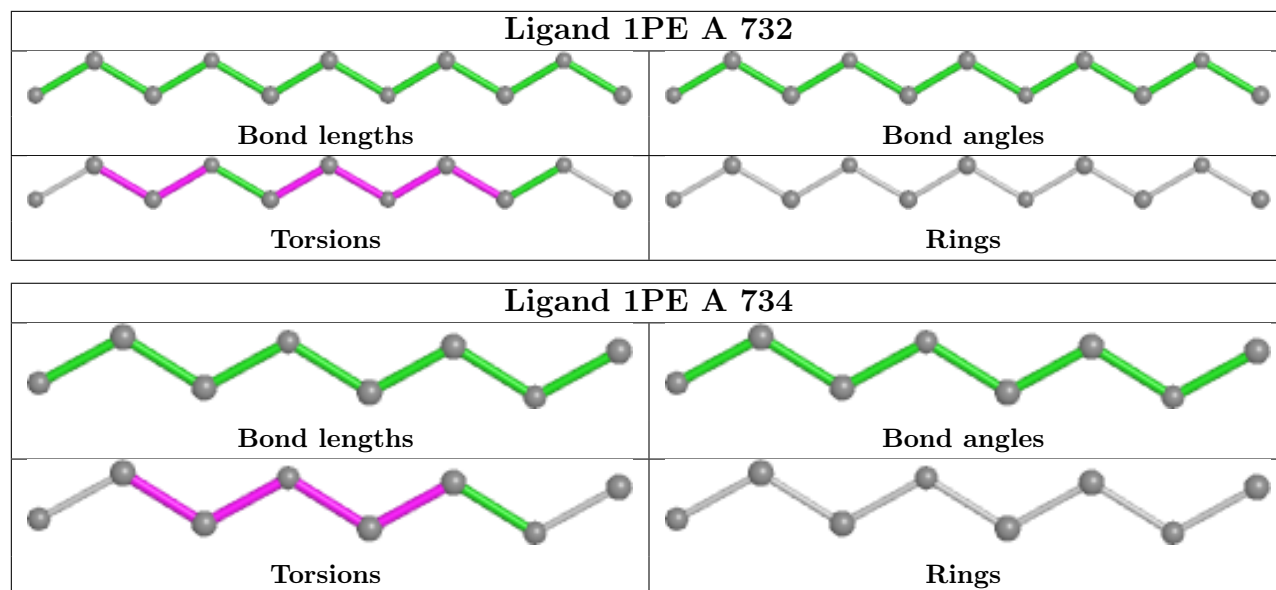
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	723	GOL	1	0
5	A	730	GOL	1	0
5	A	725	GOL	1	0
5	A	726	GOL	1	0
4	A	710	SO4	1	0
6	A	732	1PE	1	0
7	A	737	ACT	1	0
3	A	703	NAG	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	602/609 (98%)	-0.22	15 (2%) 57 67	16, 24, 42, 75	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	ASP	5.1
1	A	1	ASP	4.1
1	A	504	PRO	4.1
1	A	585	ALA	3.9
1	A	188	PHE	3.6
1	A	586	HIS	3.5
1	A	185	PRO	3.3
1	A	9	THR	2.9
1	A	583	GLY	2.8
1	A	2	TYR	2.7
1	A	228	GLU	2.6
1	A	186	LYS	2.4
1	A	226	ASN	2.2
1	A	11	PRO	2.0
1	A	468	ASP	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 monosaccharides in this entry.

6.4 Ligands ⓘ

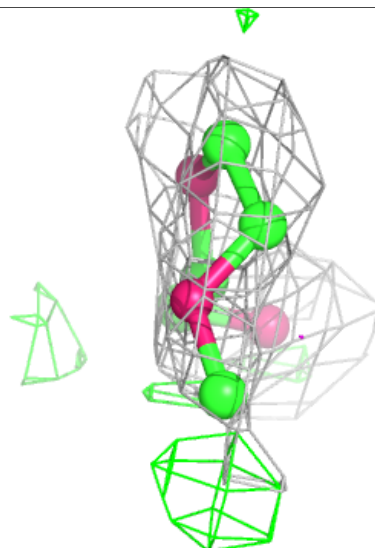
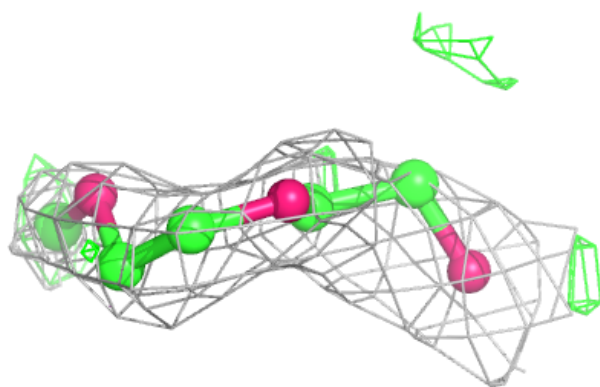
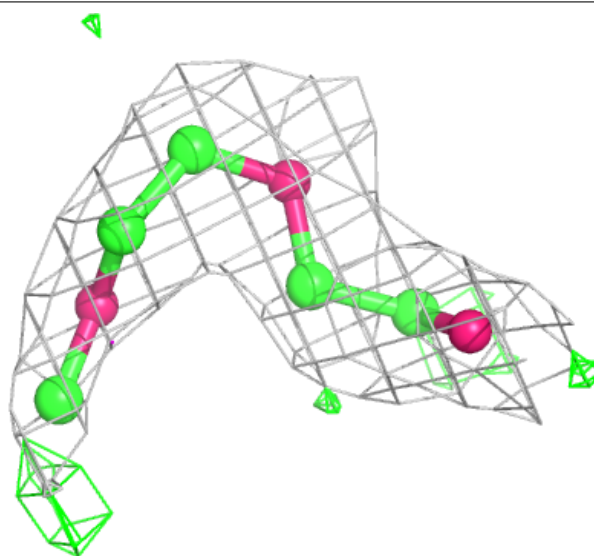
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	1PE	A	733	8/16	0.71	0.27	56,63,67,67	0
7	ACT	A	736	4/4	0.77	0.24	39,42,46,46	0
5	GOL	A	729	6/6	0.81	0.24	36,60,63,75	0
5	GOL	A	730	6/6	0.82	0.18	36,42,53,56	0
6	1PE	A	732	11/16	0.82	0.20	46,59,68,71	0
6	1PE	A	735	16/16	0.84	0.18	31,58,64,67	0
5	GOL	A	724	6/6	0.84	0.15	37,51,56,57	0
5	GOL	A	722	6/6	0.85	0.26	38,42,47,48	0
4	SO4	A	716	5/5	0.86	0.23	31,35,39,41	5
3	NAG	A	704	14/15	0.86	0.18	43,48,50,55	0
4	SO4	A	715	5/5	0.86	0.36	59,67,80,87	0
4	SO4	A	714	5/5	0.87	0.19	47,57,64,73	0
4	SO4	A	711	5/5	0.88	0.27	63,65,77,81	0
5	GOL	A	721	6/6	0.88	0.21	56,62,69,72	0
5	GOL	A	728	6/6	0.88	0.17	44,53,54,56	0
5	GOL	A	727	6/6	0.89	0.29	50,51,58,74	0
4	SO4	A	709	5/5	0.90	0.19	39,44,51,53	5
4	SO4	A	712	5/5	0.90	0.19	63,81,84,93	0
5	GOL	A	726	6/6	0.91	0.20	51,54,55,59	0
4	SO4	A	706	5/5	0.91	0.23	66,66,78,80	0
5	GOL	A	725	6/6	0.91	0.31	53,56,61,63	0
3	NAG	A	703	14/15	0.92	0.18	42,50,56,66	0
5	GOL	A	731	6/6	0.92	0.23	31,49,50,50	0
4	SO4	A	719	5/5	0.92	0.18	60,61,68,77	0
6	1PE	A	734	8/16	0.94	0.09	42,49,50,50	0
4	SO4	A	718	5/5	0.94	0.16	22,26,28,28	5
5	GOL	A	723	6/6	0.94	0.20	46,51,53,56	0
4	SO4	A	713	5/5	0.95	0.27	47,51,63,64	0
4	SO4	A	720	5/5	0.95	0.18	36,39,42,42	5
7	ACT	A	737	4/4	0.95	0.19	38,45,51,55	0
4	SO4	A	705	5/5	0.96	0.26	37,39,40,42	5
4	SO4	A	710	5/5	0.96	0.13	18,19,20,21	5
2	GLC	A	701[A]	12/12	0.96	0.16	24,32,37,38	0
4	SO4	A	708	5/5	0.96	0.10	43,44,45,46	5
4	SO4	A	717	5/5	0.97	0.19	40,52,57,58	0
2	GLC	A	702[A]	12/12	0.98	0.17	18,21,25,28	0
4	SO4	A	707	5/5	0.99	0.18	10,10,10,10	5

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.

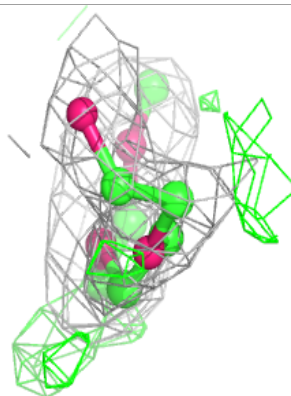
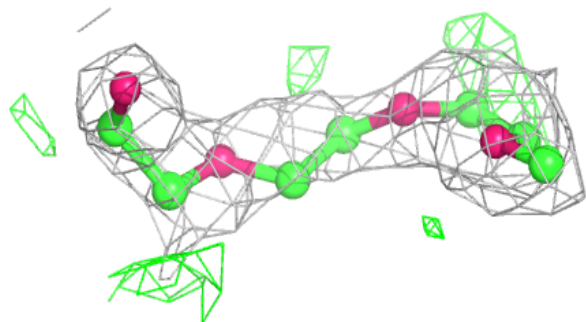
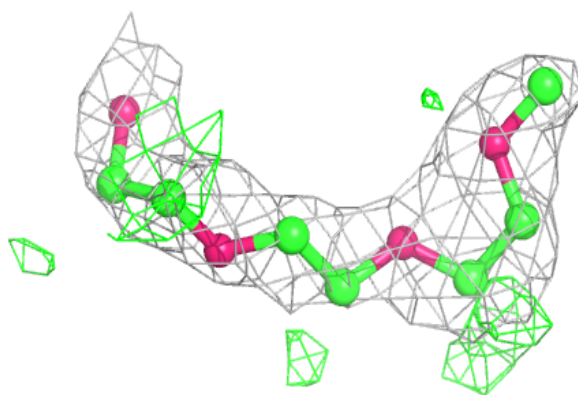
Electron density around 1PE A 733:

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

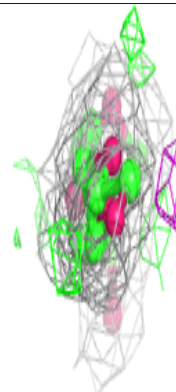
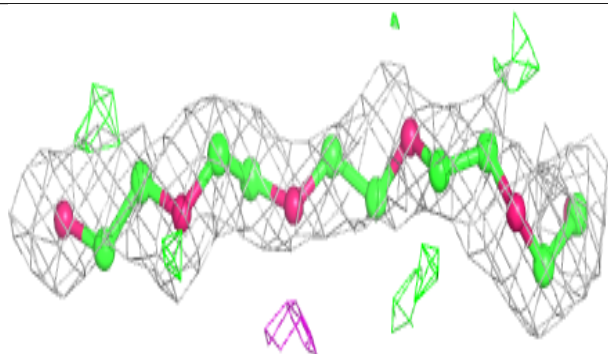
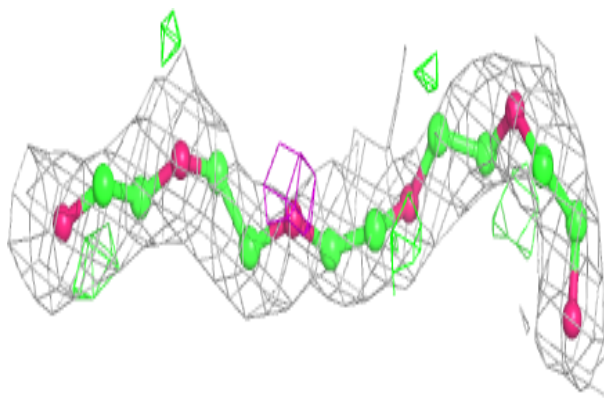


Electron density around 1PE A 732:

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

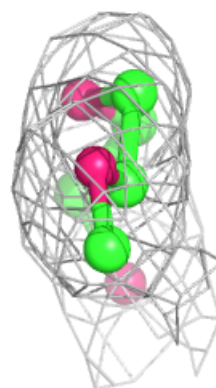
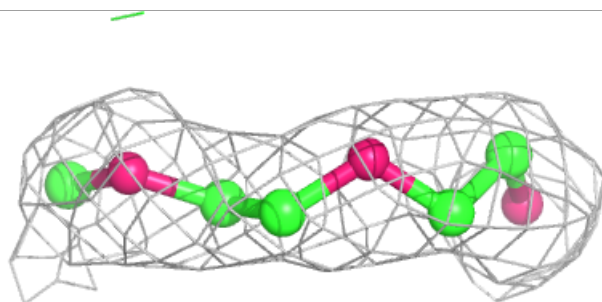
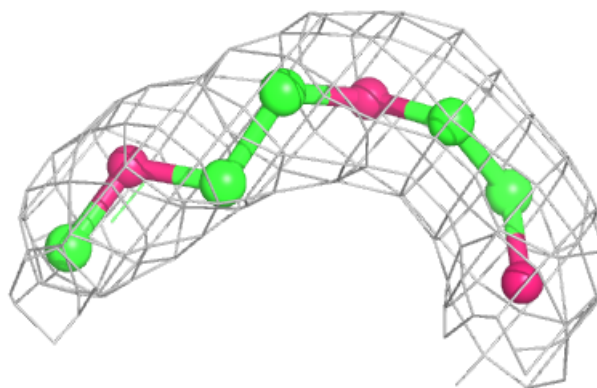
**Electron density around 1PE A 735:**

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



Electron density around 1PE A 734:

$2mF_o-DF_c$ (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.