



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2019 – 03:28 PM EDT

PDB ID : 6IBR
Title : Crystal structure of human alpha-galactosidase A in complex with alpha-galactose configured cyclophellitol epoxide LWA481
Authors : Rowland, R.J.; Wu, L.; Davies, G.J.
Deposited on : 2018-11-30
Resolution : 2.02 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

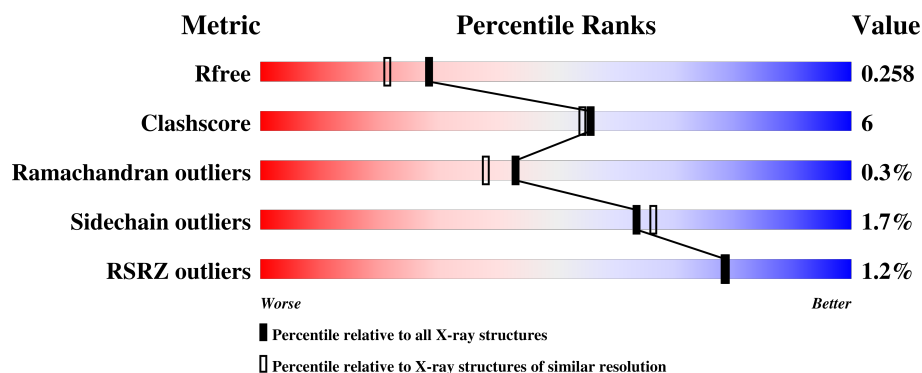
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.02 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}	111664	9172 (2.04-2.00)
Clashscore	122126	10355 (2.04-2.00)
Ramachandran outliers	120053	10237 (2.04-2.00)
Sidechain outliers	120020	10236 (2.04-2.00)
RSRZ outliers	108989	8961 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	398	 87% 11% •
1	B	398	 86% 12% ••

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
6	PEG	A	520	-	-	X	-
6	PEG	B	514	-	-	X	-

2 Entry composition [i](#)

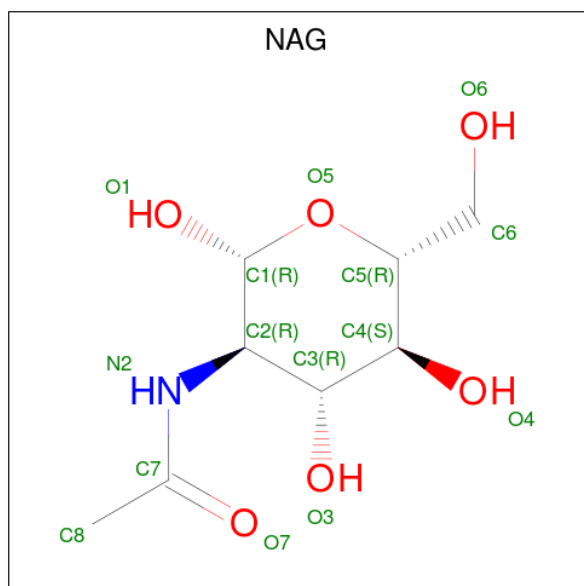
There are 10 unique types of molecules in this entry. The entry contains 6837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	2	0
			3129	1992	537	574	26			
1	B	392	Total	C	N	O	S	0	1	0
			3130	1989	536	578	27			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



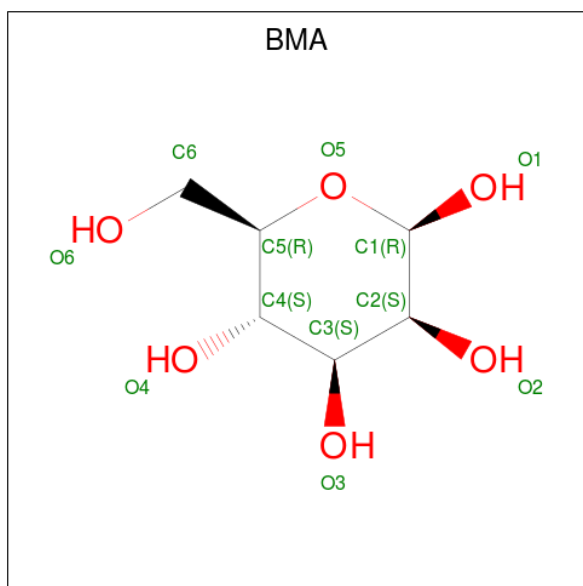
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

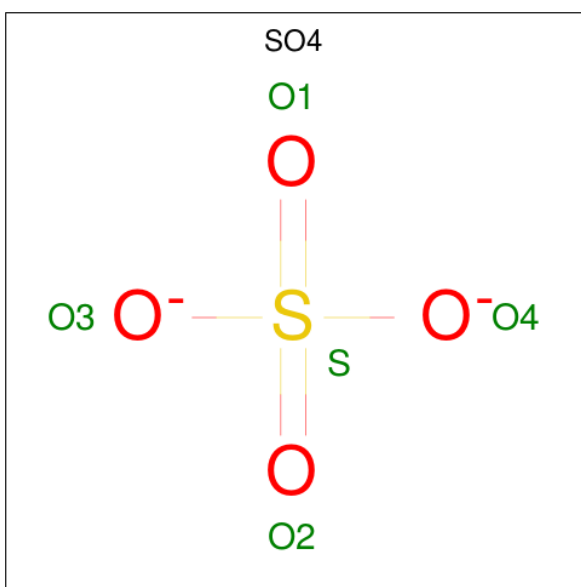
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



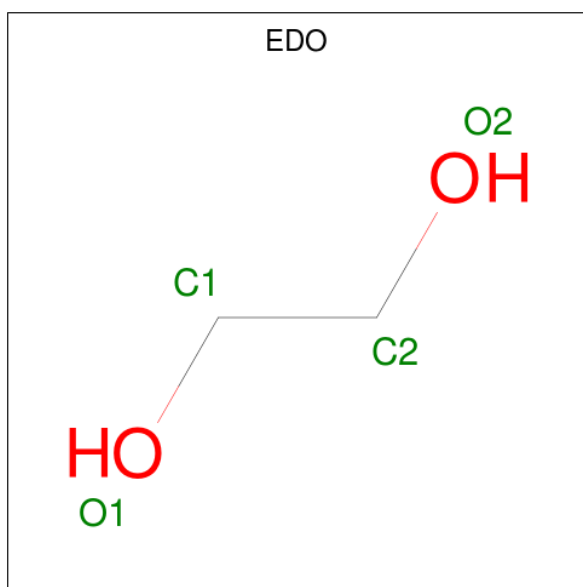
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



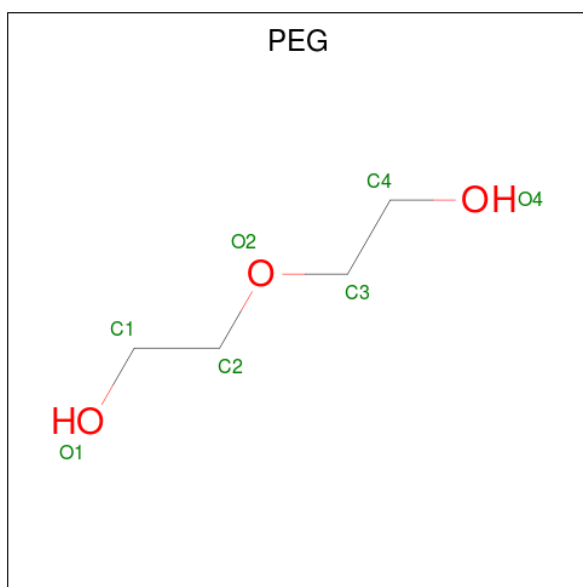
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



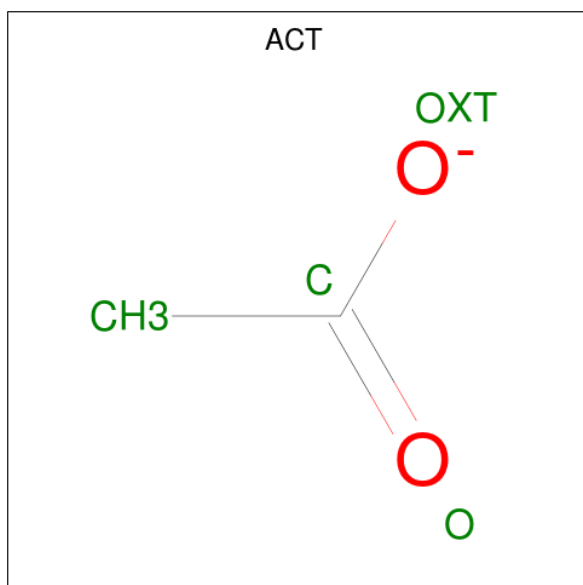
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



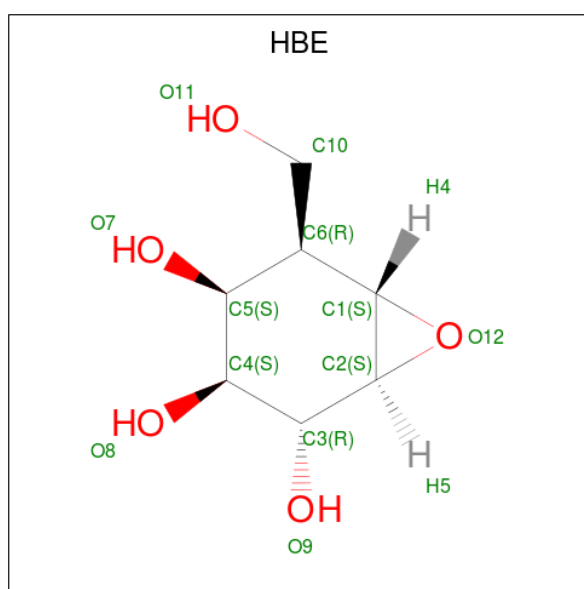
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



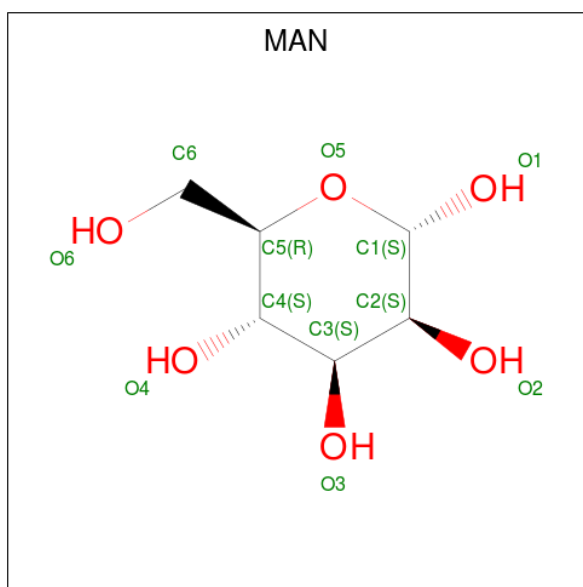
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is (2 {R},3 {S},4 {S},5 {R},6 {S})-5-(hydroxymethyl)-7-oxabicyclo[4.1.0]heptane-2,3,4-triol (three-letter code: HBE) (formula: C₇H₁₂O₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	7	5		
8	B	1	Total	C	O	0	0
			12	7	5		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			11	6	5		

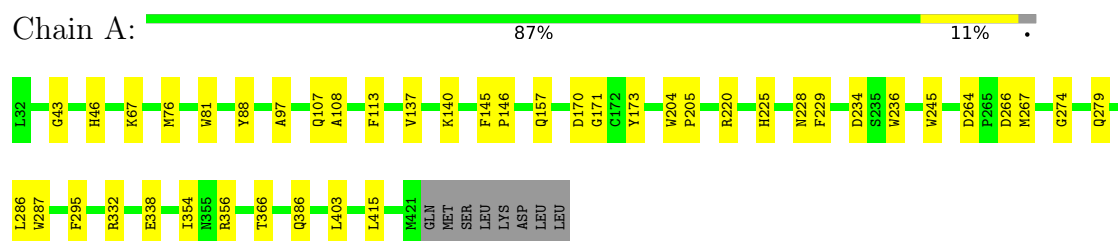
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	131	Total	O	0	0
			131	131		
10	B	102	Total	O	0	0
			102	102		

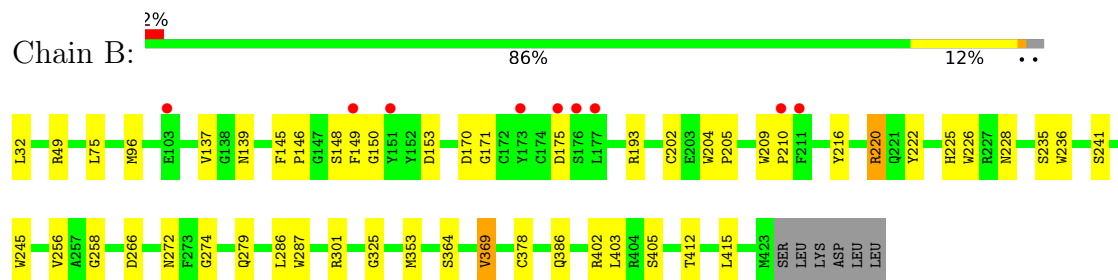
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alpha-galactosidase A



• Molecule 1: Alpha-galactosidase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.38Å 90.38Å 216.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.48 – 2.02 63.40 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.48-2.02) 100.0 (63.40-2.02)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.194 , 0.256 0.200 , 0.258	Depositor DCC
R_{free} test set	3316 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6837	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: BMA, NAG, HBE, EDO, SO4, ACT, PEG, MAN

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	0.67	1/3216 (0.0%)	0.81	1/4368 (0.0%)
1	B	0.69	1/3216 (0.0%)	0.81	1/4370 (0.0%)
All	All	0.68	2/6432 (0.0%)	0.81	2/8738 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	ASP	CG-OD2	8.29	1.44	1.25
1	A	170	ASP	CG-OD2	8.01	1.43	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ARG	CG-CD-NE	-5.65	99.93	111.80
1	B	220	ARG	CG-CD-NE	-5.04	101.22	111.80

There are no chirality outliers.

There are no planarity outliers.

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	3129	0	2980	33	0
1	B	3130	0	2967	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	84	0	73	0	0
2	B	70	0	62	1	0
3	A	22	0	20	0	0
3	B	11	0	9	0	0
4	A	20	0	0	1	0
4	B	15	0	0	1	0
5	A	24	0	36	0	0
5	B	12	0	18	3	0
6	A	21	0	30	11	0
6	B	7	0	10	13	0
7	A	4	0	3	1	0
7	B	20	0	15	0	0
8	A	12	0	0	0	0
8	B	12	0	0	0	0
9	B	11	0	10	0	0
10	A	131	0	0	2	0
10	B	102	0	0	0	0
All	All	6837	0	6233	71	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 (71) 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:264:ASP:OD2	6:A:520:PEG:H31	1.60	1.02
1:A:295:PHE:H	6:A:520:PEG:H11	1.44	0.80
1:A:274:GLY:O	6:B:514:PEG:H42	1.83	0.79
1:B:148:SER:O	1:B:150:GLY:O	2.02	0.78
1:A:264:ASP:OD2	6:A:520:PEG:C3	2.31	0.77
1:B:274:GLY:O	6:B:514:PEG:H21	1.85	0.77
1:A:264:ASP:CG	6:A:520:PEG:H31	2.06	0.76
1:B:236:TRP:H	6:B:514:PEG:H22	1.52	0.74
1:B:49[A]:ARG:NH1	5:B:512:EDO:O2	2.24	0.70
1:A:295:PHE:H	6:A:520:PEG:C1	2.05	0.70
1:A:274:GLY:O	6:B:514:PEG:C4	2.41	0.69
1:A:267:MET:HA	6:A:520:PEG:H12	1.76	0.66
1:B:369:VAL:HG13	1:B:378:CYS:SG	2.36	0.65
1:A:403:LEU:HD21	1:A:415:LEU:CD1	2.29	0.62
6:A:520:PEG:H42	10:A:635:HOH:O	2.01	0.60
1:B:403:LEU:HD21	1:B:415:LEU:CD1	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASP:HB2	2:B:507:NAG:O7	2.02	0.60
1:B:139:ASN:OD1	1:B:149:PHE:CB	2.51	0.58
1:A:295:PHE:N	6:A:520:PEG:H11	2.18	0.58
1:B:235:SER:HA	6:B:514:PEG:C2	2.34	0.57
1:B:279:GLN:HE22	6:B:514:PEG:H42	1.69	0.56
1:B:236:TRP:H	6:B:514:PEG:C2	2.18	0.55
1:B:236:TRP:N	6:B:514:PEG:H22	2.18	0.55
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.90	0.52
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.46	0.51
1:B:235:SER:HA	6:B:514:PEG:H22	1.92	0.51
1:B:386:GLN:HA	1:B:415:LEU:HD23	1.93	0.51
1:A:264:ASP:OD1	6:A:520:PEG:H31	2.10	0.50
1:B:369:VAL:HG13	1:B:378:CYS:CB	2.42	0.50
1:A:229:PHE:CE2	7:A:522:ACT:H1	2.47	0.49
1:B:49[A]:ARG:HH12	5:B:512:EDO:C2	2.24	0.49
1:B:75:LEU:CD1	1:B:301:ARG:HG2	2.43	0.49
1:A:97:ALA:HB3	1:A:107:GLN:HG3	1.95	0.48
1:A:366:THR:HA	1:A:403:LEU:O	2.14	0.48
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.95	0.48
1:B:75:LEU:HD11	1:B:301:ARG:HG2	1.96	0.47
1:B:209:TRP:N	1:B:210:PRO:HD2	2.29	0.47
1:B:32:LEU:N	1:B:220:ARG:O	2.47	0.47
1:B:96:MET:HE1	1:B:145:PHE:HB2	1.95	0.47
1:B:274:GLY:O	6:B:514:PEG:H31	2.14	0.47
1:A:332:ARG:NH2	4:A:511:SO4:O1	2.48	0.46
1:A:338:GLU:OE2	1:A:356:ARG:NH1	2.48	0.46
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.98	0.46
1:A:137:VAL:HG12	1:A:171:GLY:HA2	1.98	0.46
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.50	0.46
1:B:216:TYR:HB3	1:B:256:VAL:HG11	1.98	0.45
1:B:402:ARG:NH2	4:B:509:SO4:O3	2.50	0.45
1:A:234:ASP:O	1:A:274:GLY:HA3	2.16	0.45
1:B:32:LEU:HD22	1:B:222:TYR:O	2.16	0.45
1:B:49[A]:ARG:NH1	5:B:512:EDO:C2	2.79	0.44
1:B:258:GLY:HA2	1:B:325:GLY:O	2.17	0.44
1:A:140:LYS:HB2	1:A:173:TYR:CD2	2.52	0.44
1:B:353:MET:O	1:B:412:THR:HA	2.18	0.44
1:A:236:TRP:CD1	6:B:514:PEG:H12	2.52	0.44
1:A:386:GLN:HA	1:A:415:LEU:HD23	2.00	0.44
1:A:295:PHE:HB2	6:A:520:PEG:H12	2.00	0.44
1:B:49[A]:ARG:HD3	1:B:272:ASN:OD1	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:OD1	1:B:193:ARG:NH1	2.51	0.43
1:A:108:ALA:HB1	1:A:113:PHE:HB2	2.00	0.43
1:B:145:PHE:HB3	1:B:146:PRO:HD2	2.01	0.43
1:B:204:TRP:HB3	1:B:205:PRO:HD3	2.01	0.42
1:B:235:SER:CA	6:B:514:PEG:H22	2.49	0.42
1:B:148:SER:C	1:B:150:GLY:O	2.56	0.42
1:A:76:MET:HA	1:A:81:TRP:HB2	2.01	0.42
1:B:202:CYS:O	1:B:226:TRP:HA	2.19	0.42
1:A:403:LEU:HD21	1:A:415:LEU:HD11	1.98	0.42
1:A:286:LEU:HD21	1:A:354:ILE:HD11	2.03	0.41
1:A:279:GLN:NE2	6:B:514:PEG:H12	2.36	0.41
1:A:295:PHE:HB2	6:A:520:PEG:C1	2.51	0.41
1:A:43:GLY:HA3	1:A:88:TYR:O	2.21	0.41
1:A:157:GLN:NE2	10:A:609:HOH:O	2.54	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	390/398 (98%)	377 (97%)	12 (3%)	1 (0%)	43	38
1	B	391/398 (98%)	375 (96%)	15 (4%)	1 (0%)	43	38
All	All	781/796 (98%)	752 (96%)	27 (4%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	B	266	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/339 (97%)	326 (99%)	4 (1%)	74	77
1	B	329/339 (97%)	322 (98%)	7 (2%)	56	58
All	All	659/678 (97%)	648 (98%)	11 (2%)	63	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	67	LYS
1	A	225	HIS
1	A	287	TRP
1	B	225	HIS
1	B	241	SER
1	B	286	LEU
1	B	287	TRP
1	B	364	SER
1	B	369	VAL
1	B	405	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	406	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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$
2	NAG	A	501	1,2	14,14,15	0.62	1 (7%)	17,19,21	1.00	1 (5%)
2	NAG	A	502	3,2	14,14,15	0.46	0	17,19,21	1.81	5 (29%)
3	BMA	A	503	2	11,11,12	0.52	0	15,15,17	1.09	1 (6%)
2	NAG	A	504	1,2	14,14,15	0.56	0	17,19,21	1.33	2 (11%)
2	NAG	A	505	3,2	14,14,15	0.44	0	17,19,21	0.88	0
3	BMA	A	506	2	11,11,12	0.49	0	15,15,17	0.87	0
2	NAG	A	507	1,2	14,14,15	0.35	0	17,19,21	1.49	4 (23%)
2	NAG	A	508	2	14,14,15	0.51	0	17,19,21	1.82	5 (29%)
4	SO4	A	509	-	4,4,4	0.23	0	6,6,6	0.15	0
4	SO4	A	510	-	4,4,4	0.27	0	6,6,6	0.06	0
4	SO4	A	511	-	4,4,4	0.41	0	6,6,6	0.15	0
4	SO4	A	512	-	4,4,4	0.25	0	6,6,6	0.12	0
5	EDO	A	513	-	3,3,3	0.12	0	2,2,2	0.18	0
5	EDO	A	514	-	3,3,3	0.08	0	2,2,2	0.20	0
5	EDO	A	515	-	3,3,3	0.19	0	2,2,2	0.20	0
5	EDO	A	516	-	3,3,3	0.18	0	2,2,2	0.43	0
5	EDO	A	517	-	3,3,3	0.15	0	2,2,2	0.39	0
5	EDO	A	518	-	3,3,3	0.33	0	2,2,2	0.40	0
6	PEG	A	519	-	6,6,6	0.14	0	5,5,5	0.08	0
6	PEG	A	520	-	6,6,6	0.23	0	5,5,5	0.47	0
6	PEG	A	521	-	6,6,6	0.29	0	5,5,5	0.20	0
7	ACT	A	522	-	1,3,3	2.12	1 (100%)	0,3,3	0.00	-
8	HBE	A	523	1	12,13,13	0.65	0	14,20,20	1.54	3 (21%)
2	NAG	B	501	1,2	14,14,15	0.28	0	17,19,21	0.91	1 (5%)
2	NAG	B	502	3,2	14,14,15	0.52	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	B	503	9,2	11,11,12	0.55	0	15,15,17	1.39	2 (13%)
9	MAN	B	504	3	11,11,12	0.40	0	15,15,17	1.46	2 (13%)
2	NAG	B	505	1,2	14,14,15	0.44	0	17,19,21	1.07	2 (11%)
2	NAG	B	506	2	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
2	NAG	B	507	1	14,14,15	0.40	0	17,19,21	1.27	2 (11%)
4	SO4	B	508	-	4,4,4	0.33	0	6,6,6	0.06	0
4	SO4	B	509	-	4,4,4	0.40	0	6,6,6	0.17	0
4	SO4	B	510	-	4,4,4	0.28	0	6,6,6	0.06	0
5	EDO	B	511	-	3,3,3	0.16	0	2,2,2	0.29	0
5	EDO	B	512	-	3,3,3	0.26	0	2,2,2	0.58	0
5	EDO	B	513	-	3,3,3	0.08	0	2,2,2	0.37	0
6	PEG	B	514	-	6,6,6	0.73	0	5,5,5	0.61	0
7	ACT	B	515	-	1,3,3	4.14	1 (100%)	0,3,3	0.00	-
7	ACT	B	516	-	1,3,3	3.99	1 (100%)	0,3,3	0.00	-
7	ACT	B	517	-	1,3,3	3.97	1 (100%)	0,3,3	0.00	-
7	ACT	B	518	-	1,3,3	3.77	1 (100%)	0,3,3	0.00	-
7	ACT	B	519	-	1,3,3	5.09	1 (100%)	0,3,3	0.00	-
8	HBE	B	520	1	12,13,13	0.54	0	14,20,20	1.63	3 (21%)

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	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	2	-	2/2/19/22	0/1/1/1
2	NAG	A	504	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	505	3,2	-	2/6/23/26	0/1/1/1
3	BMA	A	506	2	-	0/2/19/22	0/1/1/1
2	NAG	A	507	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	508	2	-	3/6/23/26	0/1/1/1
5	EDO	A	513	-	-	0/1/1/1	-
5	EDO	A	514	-	-	0/1/1/1	-
5	EDO	A	515	-	-	0/1/1/1	-
5	EDO	A	516	-	-	0/1/1/1	-
5	EDO	A	517	-	-	1/1/1/1	-
5	EDO	A	518	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	519	-	-	1/4/4/4	-
6	PEG	A	520	-	-	3/4/4/4	-
6	PEG	A	521	-	-	2/4/4/4	-
8	HBE	A	523	1	-	0/2/27/27	0/1/2/2
2	NAG	B	501	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	503	9,2	-	0/2/19/22	0/1/1/1
9	MAN	B	504	3	-	0/2/19/22	0/1/1/1
2	NAG	B	505	1,2	-	1/6/23/26	0/1/1/1
2	NAG	B	506	2	-	1/6/23/26	0/1/1/1
2	NAG	B	507	1	-	0/6/23/26	0/1/1/1
5	EDO	B	511	-	-	0/1/1/1	-
5	EDO	B	512	-	-	1/1/1/1	-
5	EDO	B	513	-	-	0/1/1/1	-
6	PEG	B	514	-	-	3/4/4/4	-
8	HBE	B	520	1	-	0/2/27/27	0/1/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	519	ACT	CH3-C	5.09	1.55	1.48
7	B	515	ACT	CH3-C	4.14	1.54	1.48
7	B	516	ACT	CH3-C	3.99	1.53	1.48
7	B	517	ACT	CH3-C	3.97	1.53	1.48
7	B	518	ACT	CH3-C	3.77	1.53	1.48
7	A	522	ACT	CH3-C	2.12	1.51	1.48
2	A	501	NAG	C2-N2	-2.10	1.42	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	NAG	O4-C4-C5	3.76	118.70	109.29
2	A	508	NAG	O4-C4-C3	-3.71	101.73	110.34
8	A	523	HBE	O12-C1-C2	-3.55	101.13	109.95
9	B	504	MAN	C1-C2-C3	3.43	113.88	109.66
2	A	504	NAG	C1-O5-C5	3.39	116.81	112.20
2	A	507	NAG	O4-C4-C3	-3.24	102.81	110.34
2	A	508	NAG	C2-N2-C7	-3.24	118.28	122.92
8	A	523	HBE	C2-C3-C4	3.15	114.74	110.60
3	A	503	BMA	O5-C5-C6	3.12	112.09	107.15
2	A	508	NAG	O3-C3-C4	-3.10	103.16	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	520	HBE	O12-C1-C2	-3.06	102.35	109.95
2	B	507	NAG	C1-O5-C5	3.03	116.31	112.20
3	B	503	BMA	C3-C4-C5	3.01	115.65	110.23
2	A	507	NAG	O5-C5-C6	3.00	111.89	107.15
8	B	520	HBE	C2-C3-C4	3.00	114.54	110.60
2	A	502	NAG	C3-C4-C5	-2.85	105.10	110.23
9	B	504	MAN	C3-C4-C5	2.84	115.34	110.23
3	B	503	BMA	C1-C2-C3	-2.84	106.17	109.66
2	A	502	NAG	O4-C4-C3	-2.77	103.92	110.34
2	A	504	NAG	O5-C5-C6	2.76	111.52	107.15
2	A	502	NAG	C1-O5-C5	2.68	115.85	112.20
2	A	501	NAG	O5-C5-C6	2.64	111.32	107.15
2	B	501	NAG	C1-C2-N2	2.61	114.94	110.49
2	A	502	NAG	C6-C5-C4	2.43	118.70	113.00
2	A	507	NAG	C3-C4-C5	2.39	114.53	110.23
8	A	523	HBE	C3-C4-C5	-2.33	106.86	110.89
2	A	508	NAG	O5-C5-C6	2.33	110.83	107.15
8	B	520	HBE	O12-C1-C6	2.32	117.28	110.17
2	B	506	NAG	C2-N2-C7	2.31	126.24	122.92
2	A	508	NAG	C4-C3-C2	2.24	114.30	111.02
2	A	507	NAG	O3-C3-C4	-2.20	105.24	110.34
2	B	505	NAG	C4-C3-C2	-2.15	107.87	111.02
2	B	507	NAG	C2-N2-C7	2.14	125.98	122.92
2	B	505	NAG	C1-C2-N2	2.07	114.03	110.49

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	NAG	C4-C5-C6-O6
6	A	520	PEG	O2-C3-C4-O4
2	A	508	NAG	C4-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
6	A	521	PEG	O1-C1-C2-O2
6	A	521	PEG	O2-C3-C4-O4
3	A	503	BMA	C4-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
3	A	503	BMA	O5-C5-C6-O6
2	A	508	NAG	O5-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
5	B	512	EDO	O1-C1-C2-O2
5	A	517	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

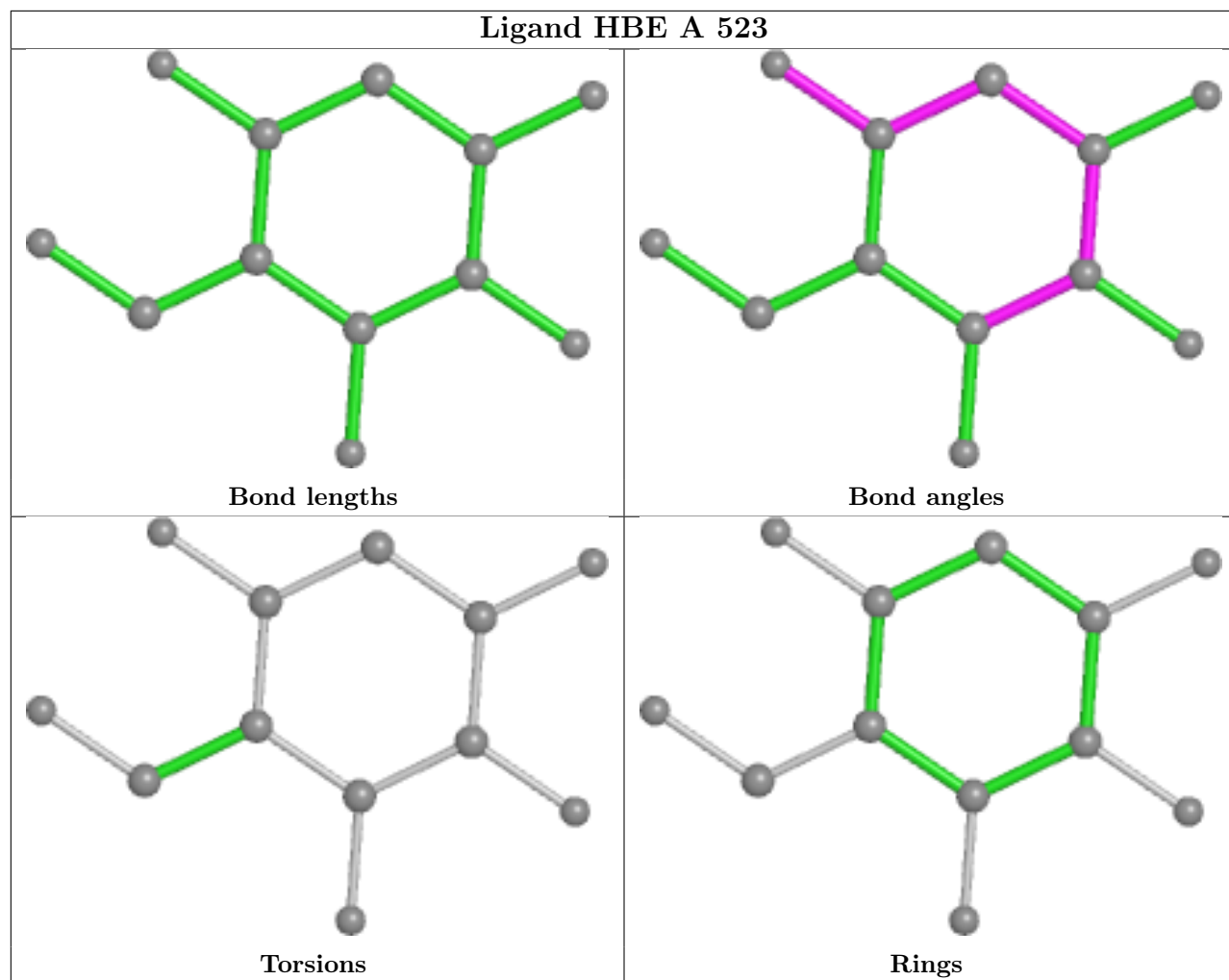
Mol	Chain	Res	Type	Atoms
6	A	520	PEG	O1-C1-C2-O2
2	A	507	NAG	C4-C5-C6-O6
6	B	514	PEG	C1-C2-O2-C3
6	B	514	PEG	O1-C1-C2-O2
6	B	514	PEG	O2-C3-C4-O4
6	A	519	PEG	C4-C3-O2-C2
2	A	507	NAG	O5-C5-C6-O6
2	B	505	NAG	C3-C2-N2-C7
2	B	506	NAG	C3-C2-N2-C7
5	A	518	EDO	O1-C1-C2-O2
6	A	520	PEG	C1-C2-O2-C3
2	A	508	NAG	C8-C7-N2-C2
2	B	501	NAG	C8-C7-N2-C2

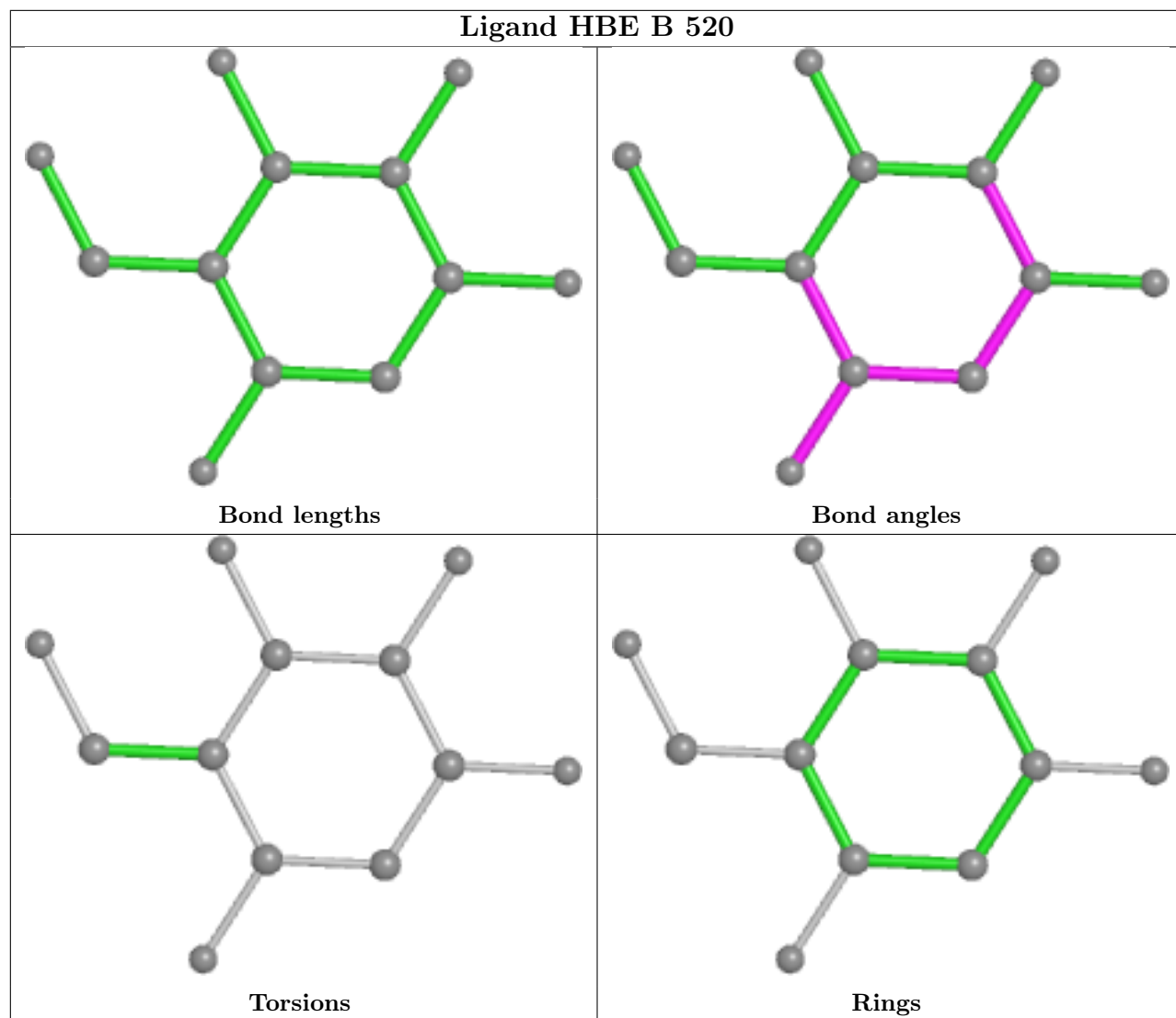
There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	520	PEG	11	0
2	B	507	NAG	1	0
5	B	512	EDO	3	0
6	B	514	PEG	13	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	390/398 (97%)	-0.45	0	100 100	37, 49, 66, 99	4 (1%)
1	B	392/398 (98%)	-0.20	9 (2%)	60 60	38, 56, 81, 109	3 (0%)
All	All	782/796 (98%)	-0.33	9 (1%)	79 78	37, 52, 76, 109	7 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ASP	4.9
1	B	149	PHE	4.8
1	B	211	PHE	4.0
1	B	151	TYR	3.0
1	B	210	PRO	2.7
1	B	176	SER	2.6
1	B	177	LEU	2.4
1	B	173	TYR	2.3
1	B	103	GLU	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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.

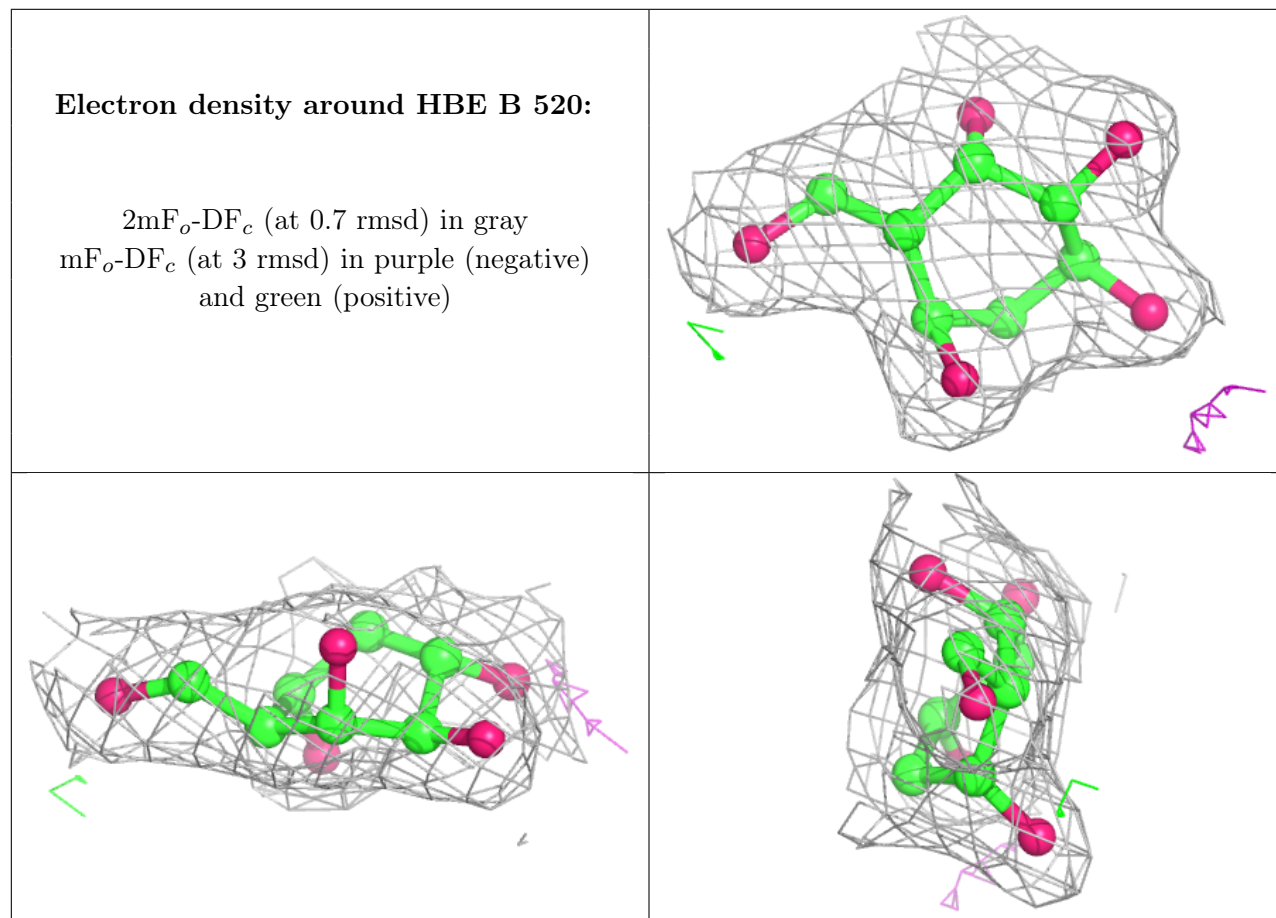
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	A	521	7/7	0.56	0.23	78,84,91,93	0
3	BMA	A	503	11/12	0.64	0.21	106,115,127,128	0
3	BMA	A	506	11/12	0.66	0.33	103,118,131,133	0
6	PEG	B	514	7/7	0.73	0.32	24,26,31,31	7
5	EDO	A	516	4/4	0.75	0.34	73,82,83,87	0
7	ACT	B	519	4/4	0.77	0.13	83,86,90,91	0
4	SO4	A	512	5/5	0.78	0.17	109,120,130,133	0
2	NAG	B	507	14/15	0.78	0.29	86,103,108,108	0
2	NAG	B	506	14/15	0.79	0.31	102,120,127,134	0
2	NAG	A	504	14/15	0.83	0.15	67,76,85,98	0
3	BMA	B	503	11/12	0.83	0.13	78,88,104,106	0
4	SO4	B	510	5/5	0.84	0.28	118,123,126,129	0
2	NAG	A	505	14/15	0.84	0.29	84,104,117,123	0
5	EDO	A	517	4/4	0.84	0.32	57,58,68,70	0
9	MAN	B	504	11/12	0.85	0.11	85,90,93,97	0
5	EDO	A	518	4/4	0.85	0.23	66,76,79,82	0
5	EDO	B	512	4/4	0.86	0.15	68,70,73,75	0
2	NAG	A	508	14/15	0.87	0.35	70,77,82,86	0
6	PEG	A	520	7/7	0.87	0.21	26,28,30,39	7
4	SO4	B	508	5/5	0.90	0.20	96,96,106,119	0
4	SO4	A	510	5/5	0.90	0.14	87,102,107,109	0
2	NAG	B	505	14/15	0.90	0.19	90,99,105,114	0
8	HBE	B	520	12/12	0.90	0.08	48,52,54,56	0
2	NAG	B	502	14/15	0.91	0.17	79,85,87,89	0
5	EDO	A	515	4/4	0.91	0.17	64,64,67,68	0
2	NAG	B	501	14/15	0.91	0.13	61,69,74,78	0
2	NAG	A	507	14/15	0.92	0.17	63,70,85,87	0
7	ACT	A	522	4/4	0.92	0.14	69,71,71,74	0
5	EDO	B	511	4/4	0.92	0.14	66,69,75,75	0
5	EDO	A	513	4/4	0.92	0.16	58,67,70,74	0
6	PEG	A	519	7/7	0.93	0.11	71,73,76,76	0
2	NAG	A	502	14/15	0.93	0.10	63,72,82,89	0
7	ACT	B	517	4/4	0.94	0.09	77,79,80,91	0
5	EDO	B	513	4/4	0.94	0.10	71,75,77,78	0
5	EDO	A	514	4/4	0.94	0.20	70,72,73,80	0
8	HBE	A	523	12/12	0.96	0.06	42,44,48,48	0
7	ACT	B	516	4/4	0.96	0.08	75,76,78,82	0
7	ACT	B	518	4/4	0.96	0.07	64,72,72,81	0
4	SO4	A	509	5/5	0.96	0.07	71,72,78,88	0
7	ACT	B	515	4/4	0.96	0.07	71,74,76,78	0
2	NAG	A	501	14/15	0.97	0.08	52,56,64,64	0

Continued on next page...

Continued from previous page...

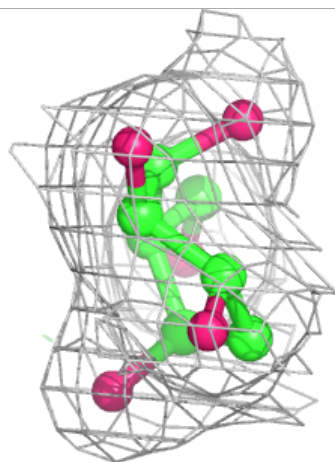
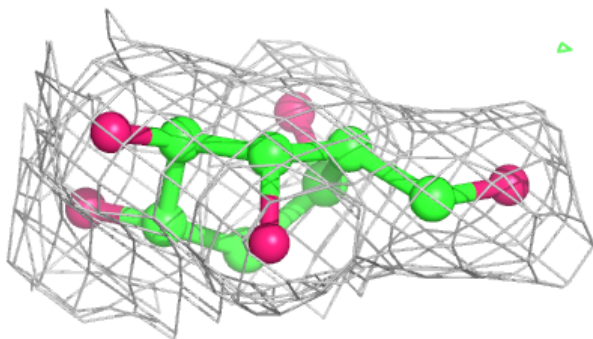
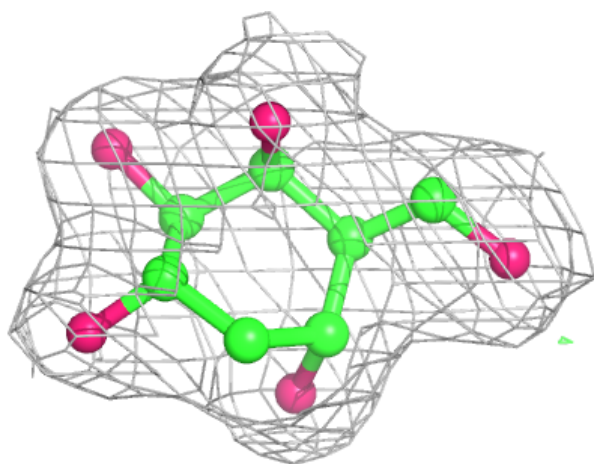
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	511	5/5	0.99	0.10	61,64,70,81	0
4	SO4	B	509	5/5	0.99	0.09	66,67,80,84	0

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 HBE A 523:

$2mF_o-DF_c$ (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.