



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:14 PM UTC

PDB ID : 8AGS / pdb_00008ags
Title : Cyclohexane epoxide soak of epoxide hydrolase from metagenomic source ch65 resulting in halogenated compound in the active site
Authors : Isupov, M.N.; De Rose, S.A.; Mitchell, D.; Littlechild, J.A.
Deposited on : 2022-07-20
Resolution : 1.61 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

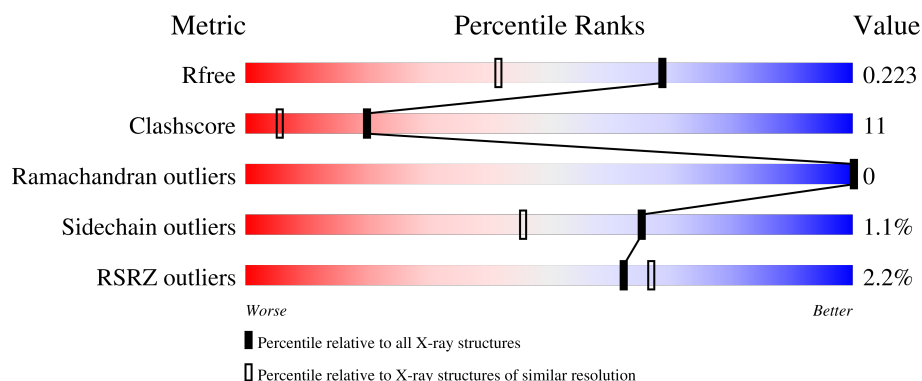
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	AAA	299	 2% 83% 17%
1	BBB	299	 2% 78% 18% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2CH	AAA	301	-	X	-	-
2	2CH	BBB	502	-	X	-	-
3	EDO	AAA	302	-	-	X	-
3	EDO	BBB	503	-	-	X	-
4	PGE	AAA	303	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5661 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.

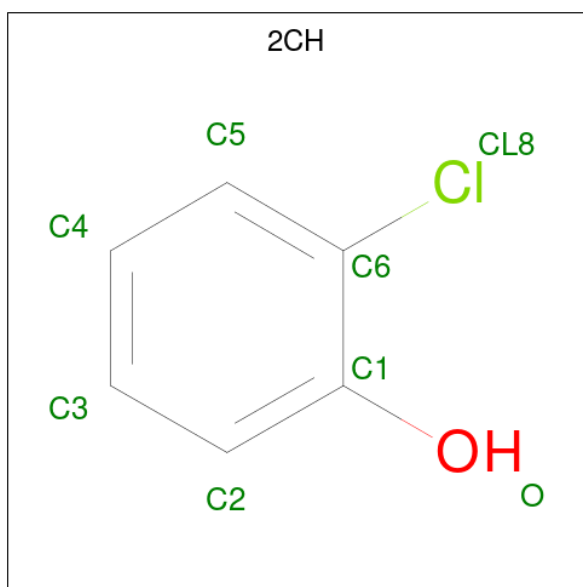
- Molecule 1 is a protein called Alpha/beta epoxide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	298	Total	C	N	O	S	0	46	0
			2720	1819	444	447	10			
1	BBB	288	Total	C	N	O	S	0	32	0
			2558	1705	412	432	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	294	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	295	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	296	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	297	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	298	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	299	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	294	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	295	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	296	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	297	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	298	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	299	HIS	-	expression tag	UNP A0A1U9WZ52

- Molecule 2 is 2-CHLOROPHENOL (CCD ID: 2CH) (formula: C₆H₅ClO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	Cl	O	0	0
			8	6	1	1		
2	BBB	1	Total	C	Cl	O	0	0
			8	6	1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

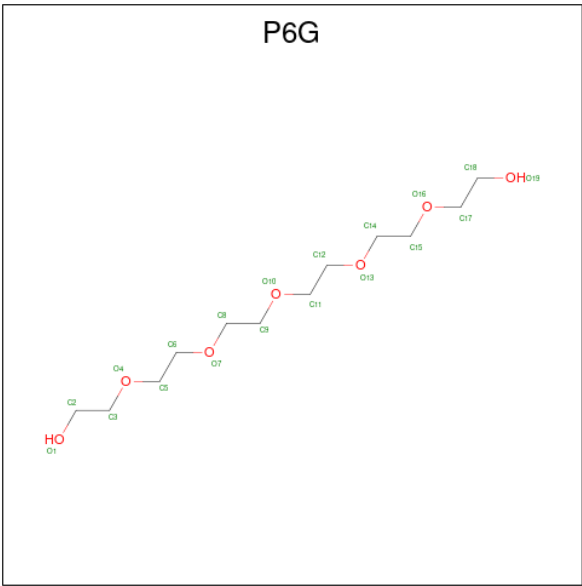


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	2	Total	Cl	0	0
			2	2		

- Molecule 6 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	C	O	0	0
			19	12	7		

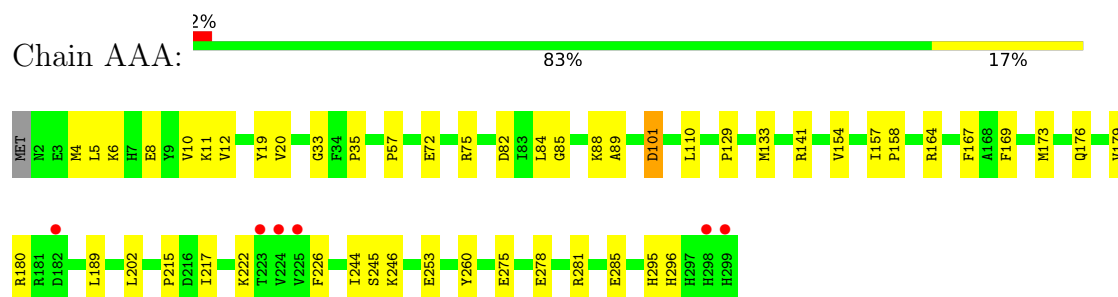
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	198	Total	O	0	0
			198	198		
7	BBB	102	Total	O	0	0
			102	102		

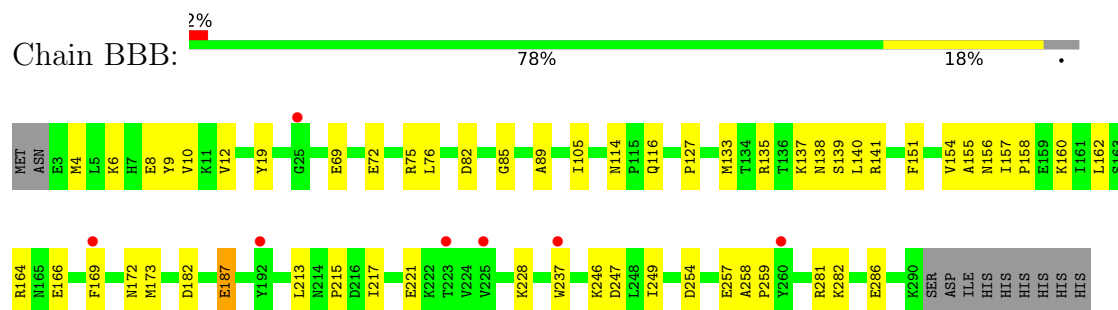
3 Residue-property plots

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: Alpha/beta epoxide hydrolase



- Molecule 1: Alpha/beta epoxide hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.21Å 46.19Å 92.14Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	45.66 – 1.61 45.66 – 1.61	Depositor EDS
% Data completeness (in resolution range)	97.4 (45.66-1.61) 97.4 (45.66-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267, BUSTER	Depositor
R, R_{free}	0.180 , 0.223 0.180 , 0.223	Depositor DCC
R_{free} test set	3603 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5661	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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: 2CH, PGE, CL, EDO, P6G

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	AAA	0.80	1/2928 (0.0%)	1.11	2/3953 (0.1%)
1	BBB	0.66	0/2721	1.00	0/3680
All	All	0.74	1/5649 (0.0%)	1.06	2/7633 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	295	HIS	CE1-NE2	6.82	1.39	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	101	ASP	CA-CB-CG	7.01	119.61	112.60
1	AAA	57	PRO	N-CA-CB	5.21	108.73	102.85

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	AAA	2720	0	2929	69	0
1	BBB	2558	0	2707	62	0
2	AAA	8	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	8	0	5	0	0
3	AAA	24	0	36	11	0
3	BBB	12	0	18	4	0
4	AAA	10	0	14	6	0
5	AAA	2	0	0	0	0
6	BBB	19	0	26	6	0
7	AAA	198	0	0	5	0
7	BBB	102	0	0	4	0
All	All	5661	0	5740	127	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 11.

All (127) 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:AAA:88[B]:LYS:HZ2	1:AAA:88[B]:LYS:HB2	1.14	1.10
1:AAA:88[B]:LYS:HB2	1:AAA:88[B]:LYS:NZ	1.66	1.09
1:AAA:72[B]:GLU:HG3	1:AAA:75[B]:ARG:NH2	1.75	1.01
1:AAA:88[B]:LYS:NZ	1:AAA:88[B]:LYS:CB	2.21	1.01
1:AAA:246:LYS:H	3:AAA:302:EDO:H22	1.26	1.00
1:AAA:88[B]:LYS:CB	1:AAA:88[B]:LYS:HZ3	1.85	0.86
1:AAA:180[A]:ARG:HG3	1:AAA:180[A]:ARG:HH11	1.43	0.84
1:BBB:172:ASN:HD21	6:BBB:501:P6G:H31	1.43	0.81
1:AAA:72[B]:GLU:CG	1:AAA:75[B]:ARG:NH2	2.45	0.80
1:AAA:88[B]:LYS:HZ3	1:AAA:88[B]:LYS:HB3	1.50	0.77
1:BBB:282[A]:LYS:NZ	1:BBB:286[A]:GLU:OE2	2.19	0.74
1:BBB:237:TRP:CZ2	1:BBB:249[A]:ILE:HG21	2.24	0.72
1:AAA:72[B]:GLU:HG3	1:AAA:75[B]:ARG:HH22	1.54	0.72
1:AAA:246:LYS:H	3:AAA:302:EDO:C2	2.01	0.71
1:BBB:157[B]:ILE:HG23	1:BBB:158:PRO:HD3	1.75	0.69
1:AAA:72[B]:GLU:CD	1:AAA:75[B]:ARG:NH2	2.51	0.68
1:AAA:75[A]:ARG:HG2	3:AAA:306:EDO:H12	1.76	0.68
1:BBB:72[B]:GLU:H	1:BBB:72[B]:GLU:CD	1.98	0.68
1:AAA:133[B]:MET:HG3	7:AAA:494:HOH:O	1.92	0.68
1:AAA:245:SER:HA	3:AAA:302:EDO:H21	1.74	0.68
1:BBB:141[B]:ARG:NH2	1:BBB:247:ASP:OD1	2.29	0.65
1:AAA:157[B]:ILE:HD13	1:AAA:158:PRO:HD3	1.78	0.65
1:AAA:75[A]:ARG:HG2	3:AAA:306:EDO:C1	2.28	0.63
1:AAA:244[B]:ILE:HD11	2:AAA:301:2CH:C5	2.28	0.63
1:AAA:246:LYS:HG2	3:AAA:302:EDO:H22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:237:TRP:CZ2	1:BBB:249[A]:ILE:CG2	2.82	0.62
1:BBB:72[A]:GLU:OE1	1:BBB:75[A]:ARG:HD3	2.00	0.62
1:AAA:180[A]:ARG:HG3	1:AAA:180[A]:ARG:NH1	2.15	0.62
1:BBB:114:ASN:HD22	1:BBB:116[A]:GLN:HE22	1.47	0.60
1:BBB:187[B]:GLU:HA	1:BBB:187[B]:GLU:OE1	2.00	0.60
1:BBB:135[A]:ARG:NH1	1:BBB:247:ASP:O	2.35	0.59
1:BBB:154[B]:VAL:HG12	1:BBB:157[B]:ILE:CG2	2.32	0.59
1:AAA:281:ARG:NH1	1:AAA:285:GLU:OE1	2.35	0.59
1:BBB:140:LEU:HB3	3:BBB:503:EDO:H21	1.83	0.59
1:AAA:176:GLN:HG3	4:AAA:303:PGE:H12	1.85	0.58
1:BBB:237:TRP:CE2	1:BBB:249[A]:ILE:HG21	2.39	0.58
1:BBB:254:ASP:HB2	7:BBB:609:HOH:O	2.04	0.57
1:BBB:12:VAL:HG13	1:BBB:85:GLY:HA3	1.86	0.57
1:AAA:72[B]:GLU:HG3	1:AAA:75[B]:ARG:CZ	2.35	0.57
1:AAA:6:LYS:HD3	7:AAA:561:HOH:O	2.05	0.56
1:BBB:72[A]:GLU:HB3	1:BBB:75[A]:ARG:HE	1.70	0.56
1:AAA:141[B]:ARG:NE	3:AAA:302:EDO:O1	2.40	0.54
1:AAA:169:PHE:CD2	4:AAA:303:PGE:H62	2.43	0.54
1:AAA:215:PRO:CB	1:BBB:157[B]:ILE:HD11	2.37	0.54
1:AAA:12[B]:VAL:HG13	1:AAA:85:GLY:HA3	1.90	0.53
1:BBB:12:VAL:HG11	1:BBB:82:ASP:O	2.08	0.53
1:AAA:84[B]:LEU:HG	1:AAA:110:LEU:CD1	2.39	0.53
1:AAA:141[A]:ARG:NH2	1:BBB:141[A]:ARG:NH2	2.57	0.53
1:AAA:180[A]:ARG:NH1	1:AAA:180[A]:ARG:CG	2.70	0.53
1:BBB:173[A]:MET:HE3	6:BBB:501:P6G:C15	2.39	0.53
1:BBB:151:PHE:HE1	1:BBB:157[B]:ILE:HD11	1.74	0.52
1:AAA:12[B]:VAL:HG11	1:AAA:82:ASP:O	2.09	0.52
1:AAA:215:PRO:HB2	1:BBB:157[B]:ILE:HD11	1.92	0.52
1:AAA:167:PHE:HE1	3:AAA:307:EDO:H21	1.75	0.52
1:AAA:133[B]:MET:SD	1:AAA:217:ILE:HG22	2.50	0.51
1:BBB:76[B]:LEU:HD21	1:BBB:105[B]:ILE:HG22	1.92	0.51
1:AAA:244[B]:ILE:HD11	2:AAA:301:2CH:C4	2.41	0.51
1:AAA:154:VAL:HG11	1:AAA:157[B]:ILE:HD12	1.94	0.50
1:AAA:157[B]:ILE:HD11	1:BBB:215:PRO:HG2	1.93	0.50
1:BBB:133[B]:MET:SD	1:BBB:217:ILE:HG22	2.52	0.50
1:BBB:154[B]:VAL:CG1	1:BBB:157[B]:ILE:CG2	2.90	0.50
1:AAA:72[B]:GLU:CD	1:AAA:75[B]:ARG:HH21	2.20	0.49
1:BBB:169:PHE:HE1	1:BBB:173[A]:MET:SD	2.35	0.49
1:BBB:173[A]:MET:HE3	6:BBB:501:P6G:H151	1.95	0.48
1:AAA:169:PHE:HE1	1:AAA:173[B]:MET:SD	2.36	0.48
1:BBB:155:ALA:O	1:BBB:157[B]:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AAA:303:PGE:H1	3:BBB:503:EDO:O2	2.13	0.48
1:BBB:258:ALA:HB1	1:BBB:259:PRO:HD2	1.97	0.47
1:AAA:72[B]:GLU:CG	1:AAA:75[B]:ARG:CZ	2.93	0.47
1:AAA:296:HIS:CD2	1:AAA:296:HIS:O	2.68	0.47
1:AAA:72[B]:GLU:OE1	1:AAA:75[B]:ARG:NH2	2.48	0.47
1:BBB:10[A]:VAL:HG21	1:BBB:89:ALA:HB1	1.97	0.47
1:BBB:156:ASN:ND2	7:BBB:607:HOH:O	2.48	0.47
1:AAA:173[A]:MET:HG3	3:AAA:304:EDO:O2	2.14	0.46
1:AAA:10[A]:VAL:HG21	1:AAA:89:ALA:HB1	1.98	0.46
1:BBB:154[B]:VAL:HG12	1:BBB:157[B]:ILE:HG23	1.96	0.46
1:AAA:253:GLU:HB3	1:AAA:260:TYR:CE2	2.51	0.46
1:BBB:160:LYS:O	1:BBB:164:ARG:HG3	2.16	0.45
4:AAA:303:PGE:C4	3:AAA:304:EDO:O1	2.65	0.45
1:BBB:105[B]:ILE:CD1	1:BBB:127:PRO:O	2.65	0.45
1:BBB:162:LEU:HA	1:BBB:169:PHE:HB3	1.97	0.45
1:BBB:69[B]:GLU:HG3	7:BBB:695:HOH:O	2.17	0.45
1:BBB:173[A]:MET:HA	6:BBB:501:P6G:H92	1.99	0.45
1:AAA:6:LYS:HB2	1:AAA:6:LYS:HE2	1.73	0.45
1:AAA:222[A]:LYS:HB3	7:AAA:422:HOH:O	2.17	0.45
1:AAA:33:GLY:HA3	1:AAA:101:ASP:HB3	1.99	0.45
1:AAA:8:GLU:HB2	1:AAA:19:TYR:CZ	2.51	0.44
1:BBB:228:LYS:HD3	1:BBB:254:ASP:O	2.18	0.44
1:BBB:8:GLU:HG3	1:BBB:9:TYR:H	1.83	0.43
1:BBB:8:GLU:HB3	1:BBB:19:TYR:CZ	2.53	0.43
1:AAA:296:HIS:O	1:AAA:296:HIS:HD2	2.01	0.43
1:BBB:157[B]:ILE:HD13	1:BBB:158:PRO:CD	2.49	0.43
1:BBB:169:PHE:CE1	1:BBB:173[A]:MET:SD	3.11	0.43
1:BBB:172:ASN:HD21	6:BBB:501:P6G:C3	2.22	0.43
1:AAA:141[A]:ARG:NH2	1:BBB:141[A]:ARG:HH22	2.16	0.43
1:AAA:222[B]:LYS:HB3	7:AAA:422:HOH:O	2.18	0.43
1:AAA:246:LYS:N	3:AAA:302:EDO:H22	2.11	0.43
1:BBB:139:SER:HA	3:BBB:503:EDO:H12	2.00	0.43
1:BBB:237:TRP:CH2	1:BBB:249[A]:ILE:HG22	2.54	0.43
1:BBB:137:LYS:HE3	1:BBB:221:GLU:OE2	2.18	0.43
1:AAA:278[A]:GLU:OE2	1:AAA:281:ARG:NH2	2.44	0.42
1:BBB:173[A]:MET:HE3	6:BBB:501:P6G:H152	2.01	0.42
1:AAA:141[A]:ARG:HD2	1:AAA:141[A]:ARG:HA	1.85	0.42
1:AAA:129:PRO:HG2	1:AAA:226:PHE:CZ	2.54	0.42
1:AAA:5[A]:LEU:HD21	1:AAA:20:VAL:HB	2.01	0.41
1:AAA:169:PHE:CE2	4:AAA:303:PGE:H5	2.55	0.41
1:AAA:202[A]:LEU:HD23	1:AAA:202[A]:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:72[B]:GLU:OE1	1:AAA:75[B]:ARG:NE	2.54	0.41
1:BBB:140:LEU:H	3:BBB:503:EDO:C2	2.33	0.41
1:AAA:6:LYS:CG	7:AAA:534:HOH:O	2.69	0.41
1:AAA:141[A]:ARG:HH22	1:BBB:141[A]:ARG:NH2	2.18	0.41
1:AAA:189:LEU:HD23	1:AAA:189:LEU:HA	1.89	0.41
1:BBB:246:LYS:HG3	1:BBB:249[A]:ILE:HD11	2.02	0.41
1:BBB:133[B]:MET:HE1	1:BBB:213:LEU:CD2	2.51	0.41
1:BBB:281:ARG:NH1	7:BBB:608:HOH:O	2.54	0.41
1:AAA:179[A]:VAL:HG22	1:AAA:275:GLU:OE2	2.20	0.40
4:AAA:303:PGE:H22	1:BBB:138:ASN:C	2.46	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	AAA	342/299 (114%)	331 (97%)	11 (3%)	0	100	100
1	BBB	318/299 (106%)	307 (96%)	11 (4%)	0	100	100
All	All	660/598 (110%)	638 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	AAA	312/267 (117%)	310 (99%)	2 (1%)	78	66
1	BBB	288/267 (108%)	283 (98%)	5 (2%)	53	29
All	All	600/534 (112%)	593 (99%)	7 (1%)	65	43

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	11	LYS
1	AAA	35	PRO
1	BBB	4	MET
1	BBB	6	LYS
1	BBB	182	ASP
1	BBB	187[A]	GLU
1	BBB	187[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	BBB	505	-	3,3,3	0.08	0	2,2,2	0.10	0
3	EDO	AAA	306	-	3,3,3	0.15	0	2,2,2	0.27	0
3	EDO	BBB	503	-	3,3,3	0.31	0	2,2,2	0.38	0
3	EDO	BBB	504	-	3,3,3	0.06	0	2,2,2	0.35	0
3	EDO	AAA	307	-	3,3,3	0.17	0	2,2,2	0.82	0
2	2CH	BBB	502	-	8,8,8	9.19	8 (100%)	10,10,10	7.75	9 (90%)
4	PGE	AAA	303	-	9,9,9	0.22	0	8,8,8	0.16	0
3	EDO	AAA	304	-	3,3,3	0.21	0	2,2,2	0.15	0
3	EDO	AAA	305	-	3,3,3	0.16	0	2,2,2	0.37	0
6	P6G	BBB	501	-	18,18,18	0.21	0	17,17,17	0.29	0
2	2CH	AAA	301	-	8,8,8	8.53	8 (100%)	10,10,10	8.50	10 (100%)
3	EDO	AAA	302	-	3,3,3	0.35	0	2,2,2	0.56	0
3	EDO	AAA	308	-	3,3,3	0.09	0	2,2,2	0.13	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
3	EDO	BBB	505	-	-	1/1/1/1	-
3	EDO	AAA	306	-	-	1/1/1/1	-
3	EDO	BBB	503	-	-	1/1/1/1	-
3	EDO	BBB	504	-	-	1/1/1/1	-
3	EDO	AAA	307	-	-	1/1/1/1	-
4	PGE	AAA	303	-	-	7/7/7/7	-
2	2CH	BBB	502	-	-	-	0/1/1/1
3	EDO	AAA	304	-	-	1/1/1/1	-
3	EDO	AAA	305	-	-	0/1/1/1	-
6	P6G	BBB	501	-	-	7/16/16/16	-
2	2CH	AAA	301	-	-	-	0/1/1/1
3	EDO	AAA	302	-	-	0/1/1/1	-
3	EDO	AAA	308	-	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	502	2CH	C1-C6	15.70	1.54	1.39
2	AAA	301	2CH	C1-C6	13.05	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	502	2CH	C3-C2	10.91	1.57	1.38
2	AAA	301	2CH	C3-C2	9.31	1.54	1.38
2	AAA	301	2CH	C2-C1	8.86	1.54	1.39
2	AAA	301	2CH	C4-C3	8.46	1.56	1.38
2	AAA	301	2CH	C4-C5	8.45	1.53	1.38
2	BBB	502	2CH	C2-C1	8.20	1.53	1.39
2	BBB	502	2CH	C4-C5	8.15	1.52	1.38
2	BBB	502	2CH	C4-C3	7.73	1.55	1.38
2	AAA	301	2CH	C5-C6	7.23	1.53	1.38
2	BBB	502	2CH	C5-C6	7.20	1.53	1.38
2	BBB	502	2CH	O-C1	7.19	1.50	1.36
2	AAA	301	2CH	O-C1	6.58	1.49	1.36
2	BBB	502	2CH	C6-CL8	3.65	1.82	1.73
2	AAA	301	2CH	C6-CL8	2.92	1.80	1.73

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	301	2CH	C3-C4-C5	-13.38	103.74	120.24
2	BBB	502	2CH	C3-C4-C5	-12.08	105.34	120.24
2	AAA	301	2CH	C4-C3-C2	-11.70	105.81	120.24
2	BBB	502	2CH	C5-C6-C1	-11.32	112.01	120.38
2	AAA	301	2CH	C3-C2-C1	-10.01	107.69	120.05
2	AAA	301	2CH	C2-C1-C6	-9.36	109.69	118.49
2	AAA	301	2CH	C5-C6-C1	-9.12	113.63	120.38
2	BBB	502	2CH	C2-C1-C6	-8.60	110.40	118.49
2	BBB	502	2CH	C4-C3-C2	-8.51	109.73	120.24
2	BBB	502	2CH	C3-C2-C1	-7.81	110.41	120.05
2	BBB	502	2CH	C1-C6-CL8	-7.22	106.58	119.43
2	AAA	301	2CH	C4-C5-C6	-6.91	109.05	119.42
2	BBB	502	2CH	O-C1-C6	-6.68	103.17	119.25
2	AAA	301	2CH	C1-C6-CL8	-5.97	108.80	119.43
2	AAA	301	2CH	C5-C6-CL8	-4.62	109.31	118.42
2	AAA	301	2CH	O-C1-C2	-4.21	108.07	119.36
2	AAA	301	2CH	O-C1-C6	-3.53	110.76	119.25
2	BBB	502	2CH	C5-C6-CL8	-3.51	111.52	118.42
2	BBB	502	2CH	C4-C5-C6	-3.18	114.65	119.42

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	BBB	501	P6G	C9-C8-O7-C6
4	AAA	303	PGE	C3-C4-O3-C5
6	BBB	501	P6G	O7-C8-C9-O10
3	BBB	503	EDO	O1-C1-C2-O2
6	BBB	501	P6G	O1-C2-C3-O4
3	AAA	307	EDO	O1-C1-C2-O2
4	AAA	303	PGE	O2-C3-C4-O3
4	AAA	303	PGE	O3-C5-C6-O4
4	AAA	303	PGE	C6-C5-O3-C4
6	BBB	501	P6G	C6-C5-O4-C3
4	AAA	303	PGE	C1-C2-O2-C3
6	BBB	501	P6G	C14-C15-O16-C17
3	AAA	306	EDO	O1-C1-C2-O2
6	BBB	501	P6G	C11-C12-O13-C14
4	AAA	303	PGE	C4-C3-O2-C2
4	AAA	303	PGE	O1-C1-C2-O2
3	BBB	505	EDO	O1-C1-C2-O2
6	BBB	501	P6G	O16-C17-C18-O19
3	AAA	304	EDO	O1-C1-C2-O2
3	BBB	504	EDO	O1-C1-C2-O2

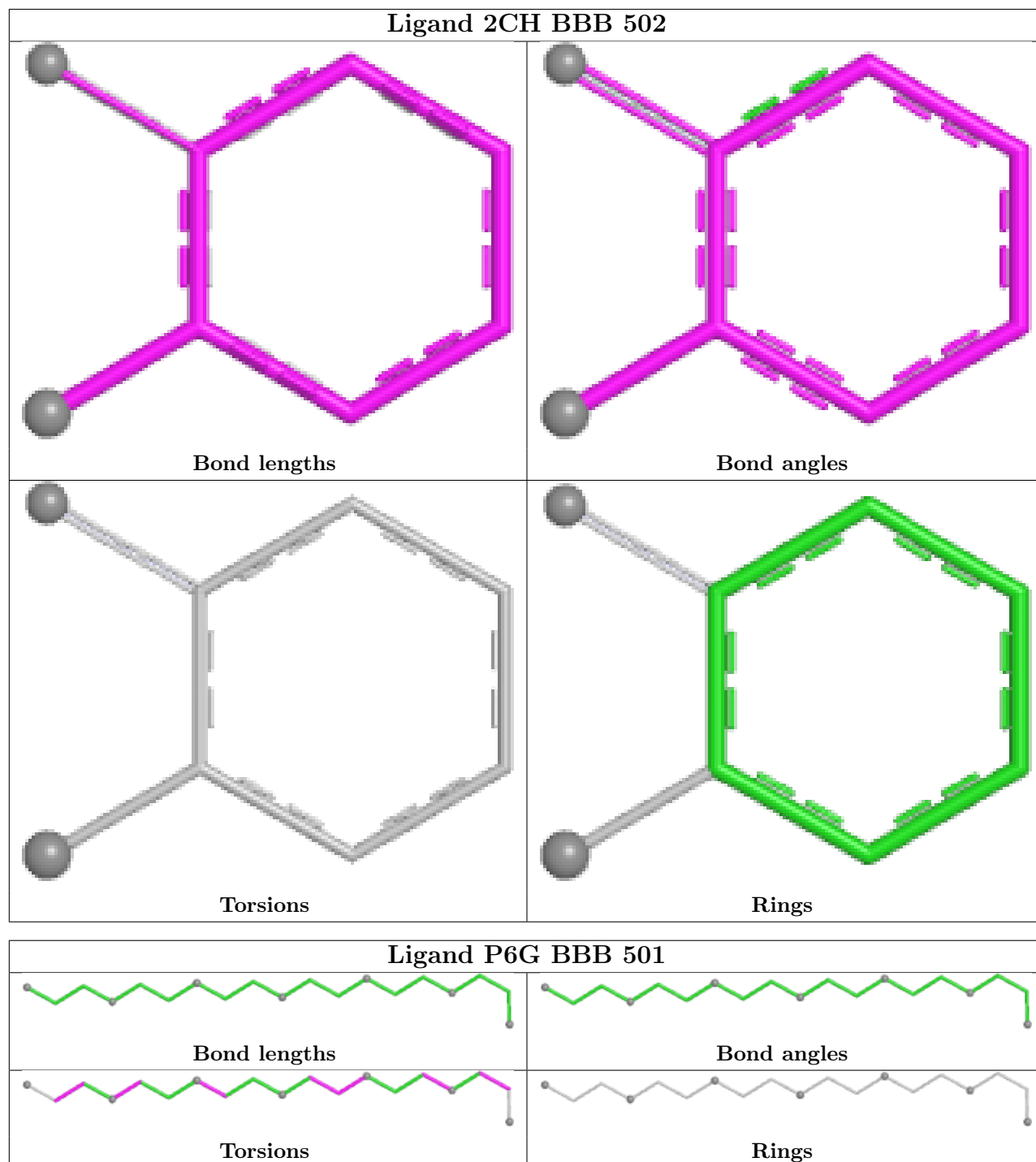
There are no ring outliers.

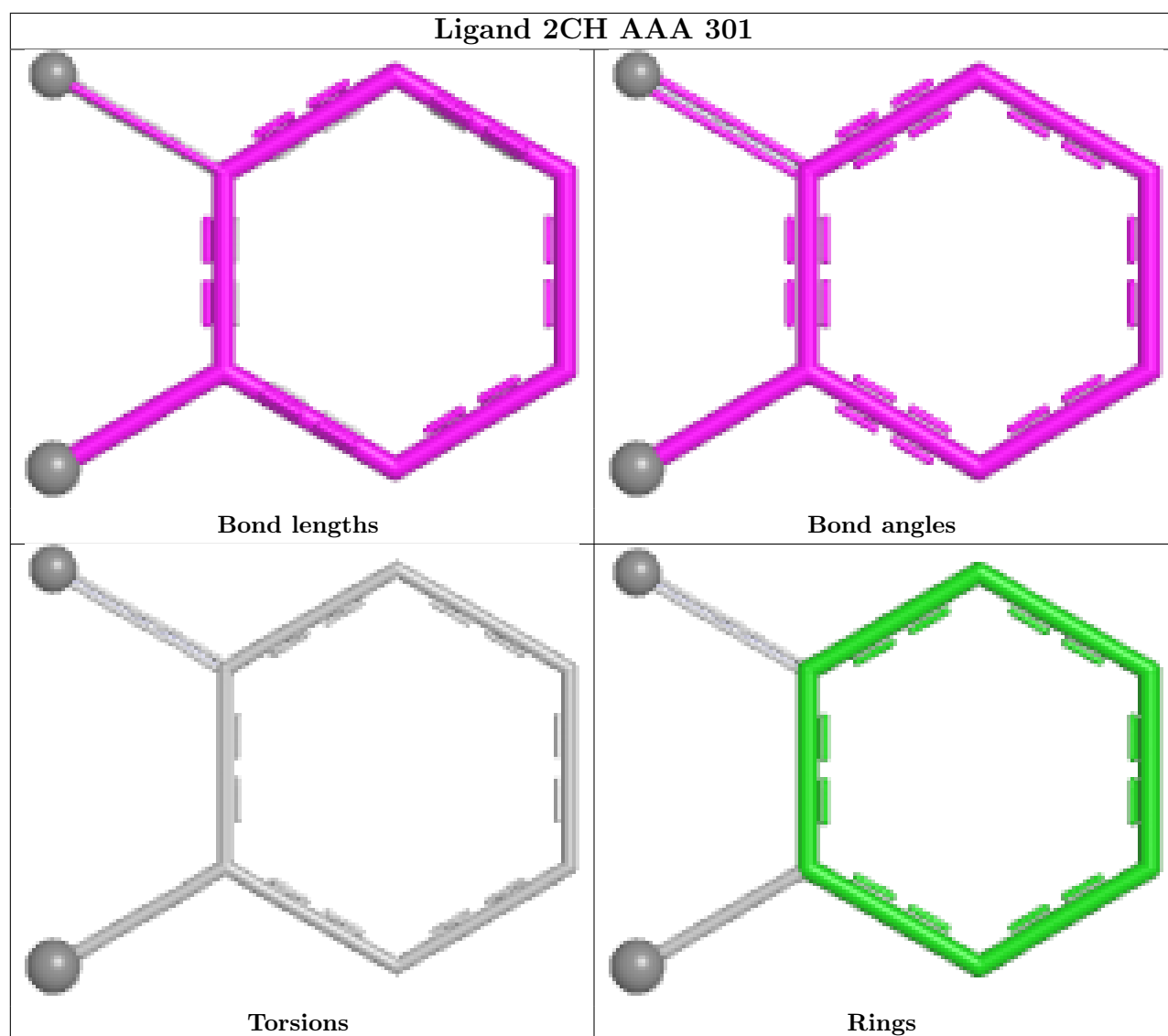
8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	306	EDO	2	0
3	BBB	503	EDO	4	0
3	AAA	307	EDO	1	0
4	AAA	303	PGE	6	0
3	AAA	304	EDO	2	0
6	BBB	501	P6G	6	0
2	AAA	301	2CH	2	0
3	AAA	302	EDO	6	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	AAA	298/299 (99%)	-0.14	6 (2%) 65 70	9, 22, 45, 86	46 (15%)
1	BBB	288/299 (96%)	0.44	7 (2%) 59 64	14, 33, 60, 117	32 (11%)
All	All	586/598 (97%)	0.15	13 (2%) 62 67	9, 27, 56, 117	78 (13%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	223	THR	3.5
1	BBB	169	PHE	2.9
1	BBB	223	THR	2.8
1	BBB	25	GLY	2.6
1	AAA	225	VAL	2.5
1	AAA	299	HIS	2.5
1	BBB	225	VAL	2.5
1	BBB	237	TRP	2.4
1	BBB	260[A]	TYR	2.3
1	AAA	298	HIS	2.3
1	BBB	192	TYR	2.3
1	AAA	182	ASP	2.1
1	AAA	224	VAL	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 oligosaccharides in this entry.

6.4 Ligands

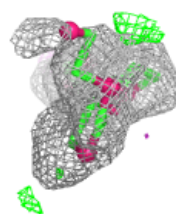
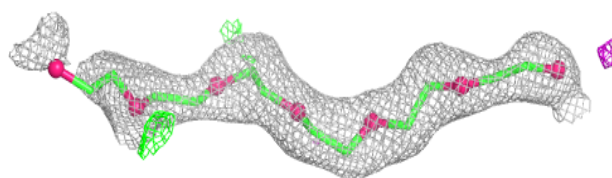
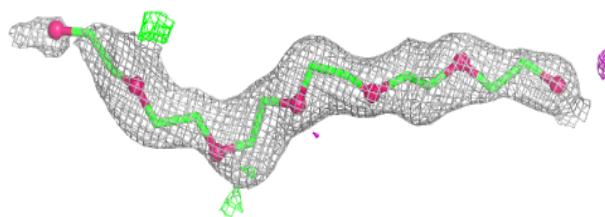
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	BBB	503	4/4	0.79	0.16	46,47,53,61	0
3	EDO	BBB	504	4/4	0.80	0.11	48,55,56,69	0
3	EDO	AAA	306	4/4	0.86	0.11	50,54,62,64	0
4	PGE	AAA	303	10/10	0.86	0.12	41,58,67,74	0
3	EDO	AAA	307	4/4	0.87	0.11	31,39,44,49	0
3	EDO	AAA	308	4/4	0.88	0.11	49,50,58,60	0
6	P6G	BBB	501	19/19	0.88	0.12	37,53,75,81	0
3	EDO	AAA	302	4/4	0.89	0.09	31,34,42,54	0
3	EDO	BBB	505	4/4	0.89	0.09	44,60,64,65	0
3	EDO	AAA	304	4/4	0.91	0.12	38,39,47,49	0
2	2CH	BBB	502	8/8	0.93	0.09	26,34,40,41	0
3	EDO	AAA	305	4/4	0.93	0.10	28,42,42,58	0
5	CL	AAA	310	1/1	0.94	0.13	34,34,34,34	0
2	2CH	AAA	301	8/8	0.95	0.09	23,29,30,33	0
5	CL	AAA	309	1/1	0.95	0.09	41,41,41,41	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.

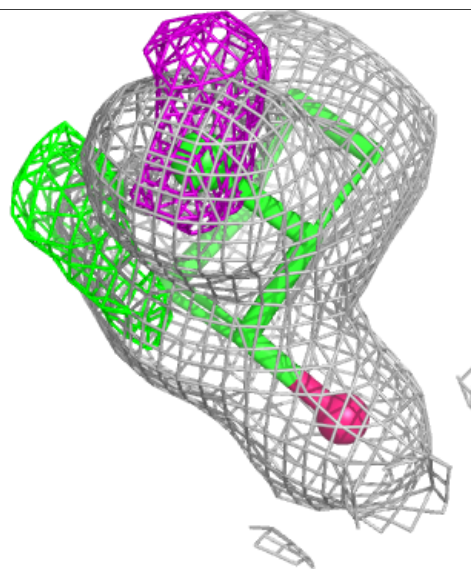
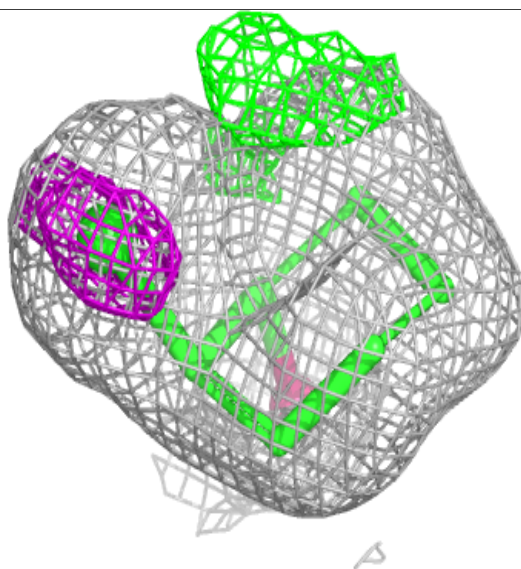
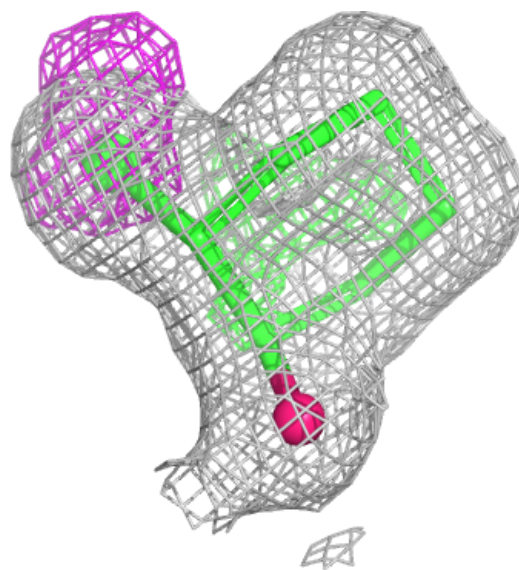
Electron density around P6G BBB 501:

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



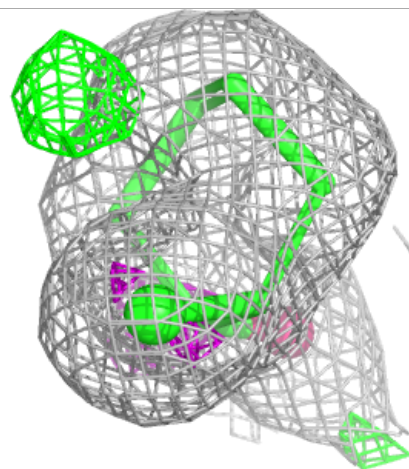
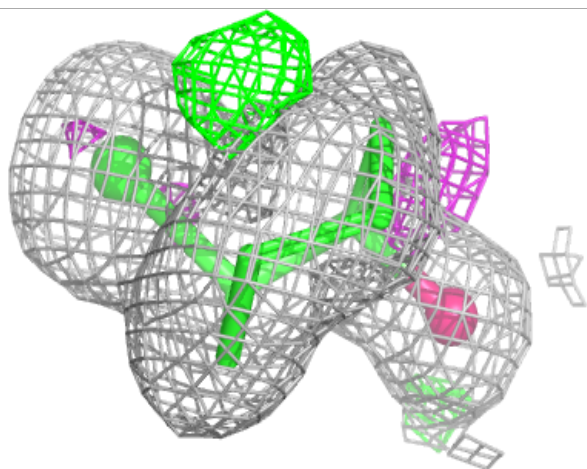
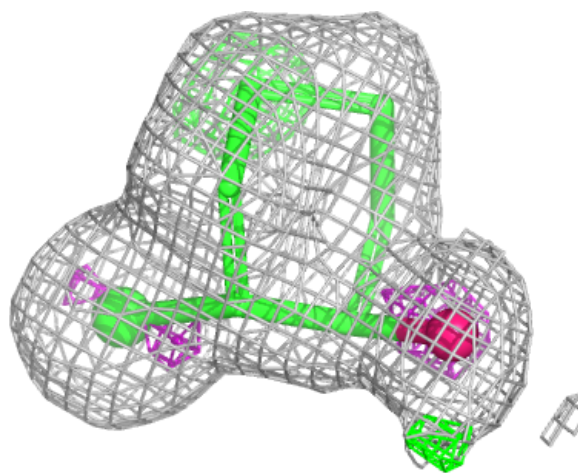
Electron density around 2CH BBB 502:

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



Electron density around 2CH AAA 301:

$2mF_o-DF_c$ (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.