Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:09 am BST

PDB ID	:	5N6S
Title	:	Thermotoga maritima family 1 Glycoside hydrolase complexed with Carba-Cyclophellitol transition state mimic
Authors	:	Offen, W.; Davies, G.
Deposited on	:	2017-02-16
Resolution	:	2.10 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:

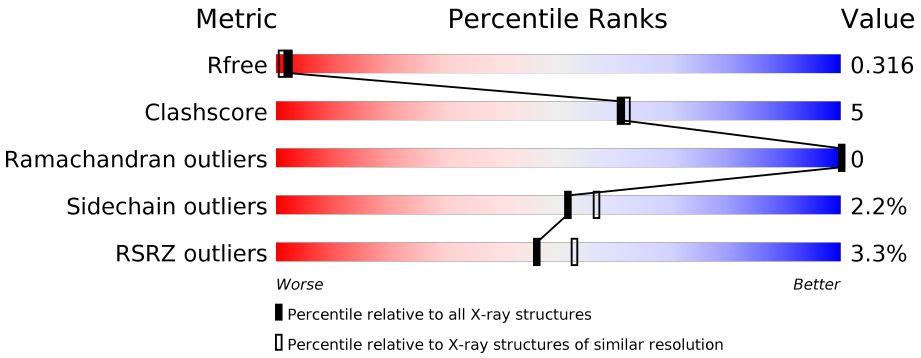
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 <=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	468	86% 8% 5%
1	B	468	82% 13% 5%
1	C	468	6% 80% 10% • 8%
1	D	468	5% 84% 7% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	504	-	-	X	-
8	PGE	B	514	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14780 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-glucosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	2	0
			3608	2353	601	647	7			
1	B	443	Total	C	N	O	S	0	4	0
			3642	2369	612	655	6			
1	C	429	Total	C	N	O	S	0	5	1
			3470	2264	580	619	7			
1	D	431	Total	C	N	O	S	0	2	0
			3435	2252	572	605	6			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q08638
A	-20	GLY	-	expression tag	UNP Q08638
A	-19	SER	-	expression tag	UNP Q08638
A	-18	SER	-	expression tag	UNP Q08638
A	-17	HIS	-	expression tag	UNP Q08638
A	-16	HIS	-	expression tag	UNP Q08638
A	-15	HIS	-	expression tag	UNP Q08638
A	-14	HIS	-	expression tag	UNP Q08638
A	-13	HIS	-	expression tag	UNP Q08638
A	-12	HIS	-	expression tag	UNP Q08638
A	-11	SER	-	expression tag	UNP Q08638
A	-10	SER	-	expression tag	UNP Q08638
A	-9	GLY	-	expression tag	UNP Q08638
A	-8	LEU	-	expression tag	UNP Q08638
A	-7	VAL	-	expression tag	UNP Q08638
A	-6	PRO	-	expression tag	UNP Q08638
A	-5	ARG	-	expression tag	UNP Q08638
A	-4	GLY	-	expression tag	UNP Q08638
A	-3	SER	-	expression tag	UNP Q08638
A	-2	HIS	-	expression tag	UNP Q08638
A	-1	MET	-	expression tag	UNP Q08638

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q08638
A	1	SER	-	expression tag	UNP Q08638
B	-21	MET	-	initiating methionine	UNP Q08638
B	-20	GLY	-	expression tag	UNP Q08638
B	-19	SER	-	expression tag	UNP Q08638
B	-18	SER	-	expression tag	UNP Q08638
B	-17	HIS	-	expression tag	UNP Q08638
B	-16	HIS	-	expression tag	UNP Q08638
B	-15	HIS	-	expression tag	UNP Q08638
B	-14	HIS	-	expression tag	UNP Q08638
B	-13	HIS	-	expression tag	UNP Q08638
B	-12	HIS	-	expression tag	UNP Q08638
B	-11	SER	-	expression tag	UNP Q08638
B	-10	SER	-	expression tag	UNP Q08638
B	-9	GLY	-	expression tag	UNP Q08638
B	-8	LEU	-	expression tag	UNP Q08638
B	-7	VAL	-	expression tag	UNP Q08638
B	-6	PRO	-	expression tag	UNP Q08638
B	-5	ARG	-	expression tag	UNP Q08638
B	-4	GLY	-	expression tag	UNP Q08638
B	-3	SER	-	expression tag	UNP Q08638
B	-2	HIS	-	expression tag	UNP Q08638
B	-1	MET	-	expression tag	UNP Q08638
B	0	ALA	-	expression tag	UNP Q08638
B	1	SER	-	expression tag	UNP Q08638
C	-21	MET	-	initiating methionine	UNP Q08638
C	-20	GLY	-	expression tag	UNP Q08638
C	-19	SER	-	expression tag	UNP Q08638
C	-18	SER	-	expression tag	UNP Q08638
C	-17	HIS	-	expression tag	UNP Q08638
C	-16	HIS	-	expression tag	UNP Q08638
C	-15	HIS	-	expression tag	UNP Q08638
C	-14	HIS	-	expression tag	UNP Q08638
C	-13	HIS	-	expression tag	UNP Q08638
C	-12	HIS	-	expression tag	UNP Q08638
C	-11	SER	-	expression tag	UNP Q08638
C	-10	SER	-	expression tag	UNP Q08638
C	-9	GLY	-	expression tag	UNP Q08638
C	-8	LEU	-	expression tag	UNP Q08638
C	-7	VAL	-	expression tag	UNP Q08638
C	-6	PRO	-	expression tag	UNP Q08638
C	-5	ARG	-	expression tag	UNP Q08638

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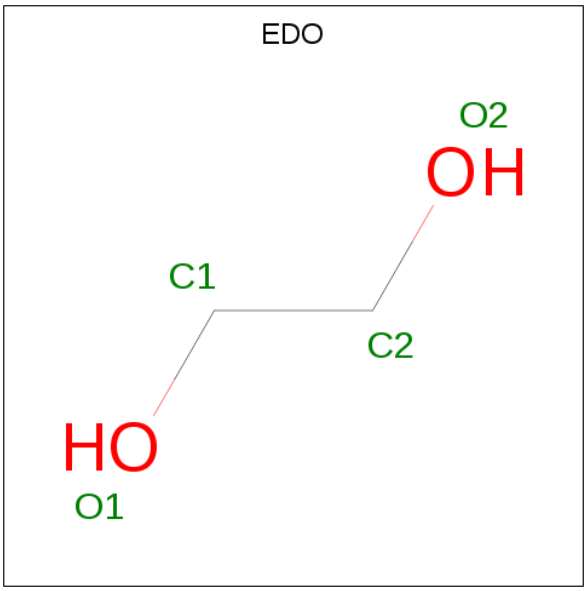
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q08638
C	-3	SER	-	expression tag	UNP Q08638
C	-2	HIS	-	expression tag	UNP Q08638
C	-1	MET	-	expression tag	UNP Q08638
C	0	ALA	-	expression tag	UNP Q08638
C	1	SER	-	expression tag	UNP Q08638
D	-21	MET	-	initiating methionine	UNP Q08638
D	-20	GLY	-	expression tag	UNP Q08638
D	-19	SER	-	expression tag	UNP Q08638
D	-18	SER	-	expression tag	UNP Q08638
D	-17	HIS	-	expression tag	UNP Q08638
D	-16	HIS	-	expression tag	UNP Q08638
D	-15	HIS	-	expression tag	UNP Q08638
D	-14	HIS	-	expression tag	UNP Q08638
D	-13	HIS	-	expression tag	UNP Q08638
D	-12	HIS	-	expression tag	UNP Q08638
D	-11	SER	-	expression tag	UNP Q08638
D	-10	SER	-	expression tag	UNP Q08638
D	-9	GLY	-	expression tag	UNP Q08638
D	-8	LEU	-	expression tag	UNP Q08638
D	-7	VAL	-	expression tag	UNP Q08638
D	-6	PRO	-	expression tag	UNP Q08638
D	-5	ARG	-	expression tag	UNP Q08638
D	-4	GLY	-	expression tag	UNP Q08638
D	-3	SER	-	expression tag	UNP Q08638
D	-2	HIS	-	expression tag	UNP Q08638
D	-1	MET	-	expression tag	UNP Q08638
D	0	ALA	-	expression tag	UNP Q08638
D	1	SER	-	expression tag	UNP Q08638

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	1
			8	4	4		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

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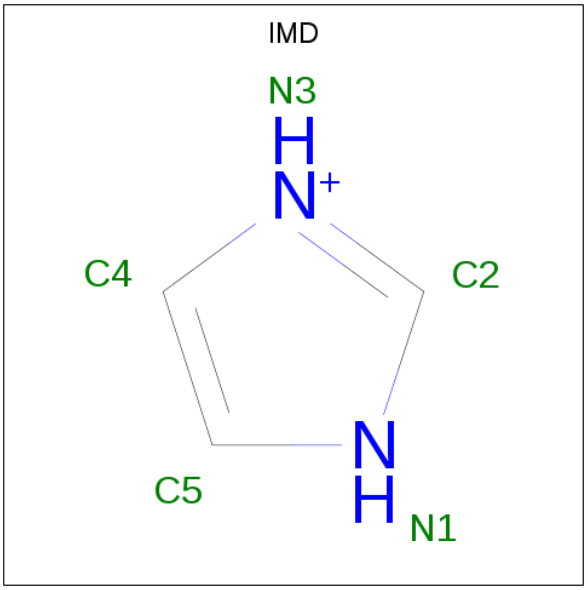
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

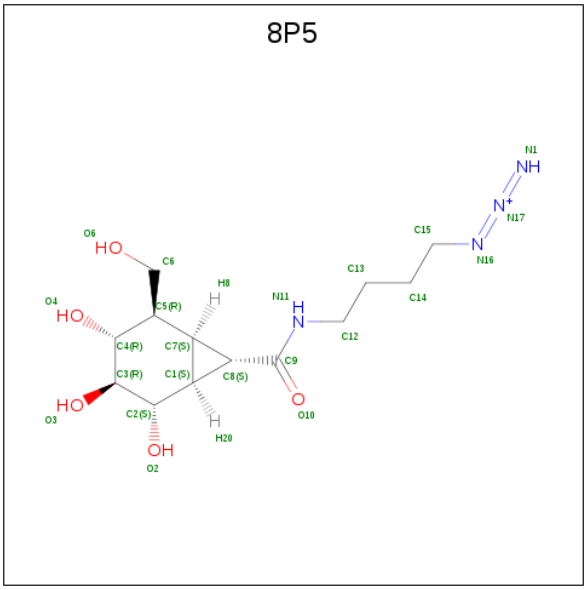
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0
3	D	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



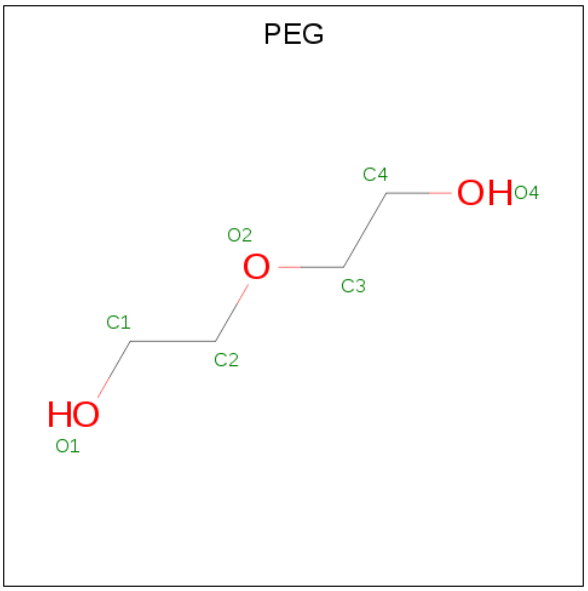
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 5 3 2	0	0

- Molecule 5 is azanylidene-[4-[[(1 {S},2 {R},3 {R},4 {R},5 {S},6 {S},7 {S})-2-(hydroxy methyl)-3,4,5-tris(oxidanyl)-7-bicyclo[4.1.0]heptanyl]carbonylamino]butylimino]azanium (three-letter code: 8P5) (formula: $C_{13}H_{23}N_4O_5$).



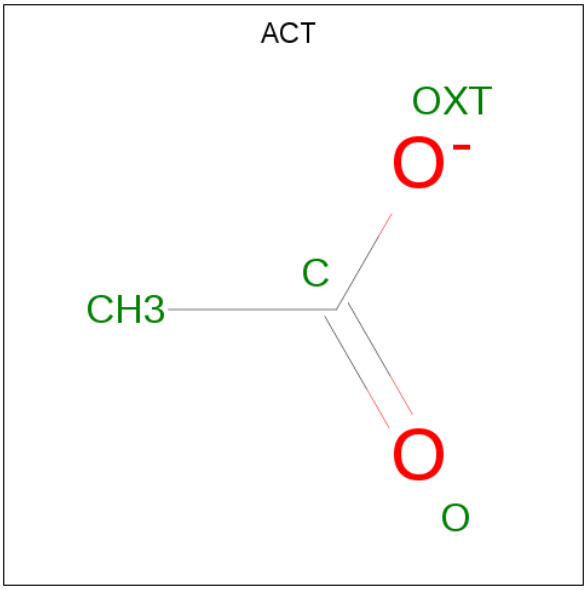
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 44 26 8 10	0	1
5	B	1	Total C N O 22 13 4 5	0	0
5	C	1	Total C N O 22 13 4 5	0	0
5	D	1	Total C N O 15 9 1 5	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



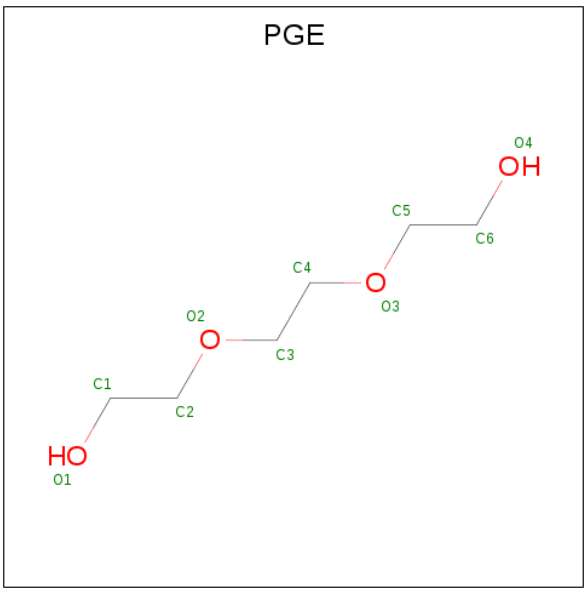
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

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



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 9 is water.

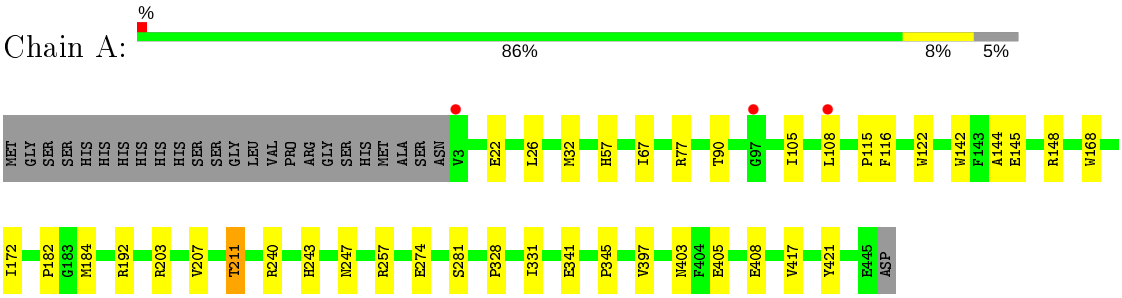
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	154	Total O 154 154	0	0
9	B	131	Total O 131 131	0	0
9	C	64	Total O 64 64	0	0
9	D	54	Total O 54 54	0	0

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.

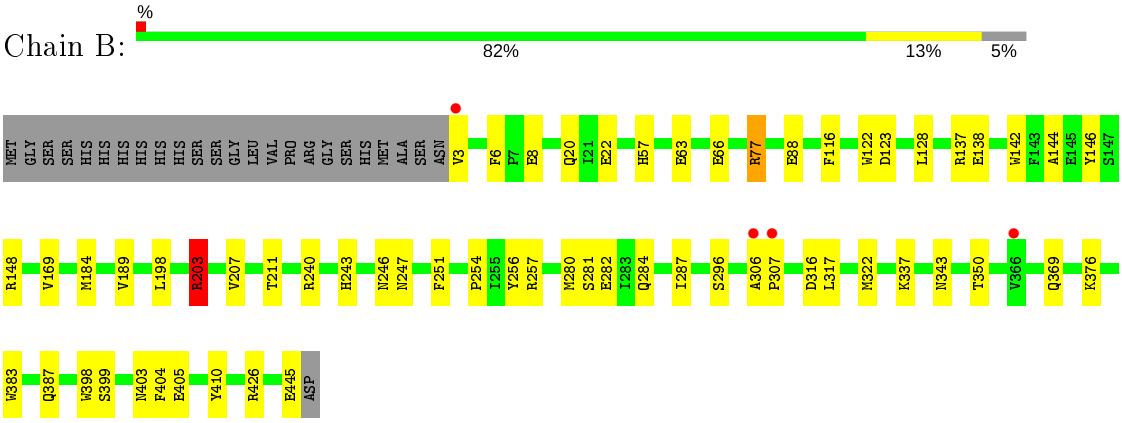
- Molecule 1: Beta-glucosidase A

Chain A:



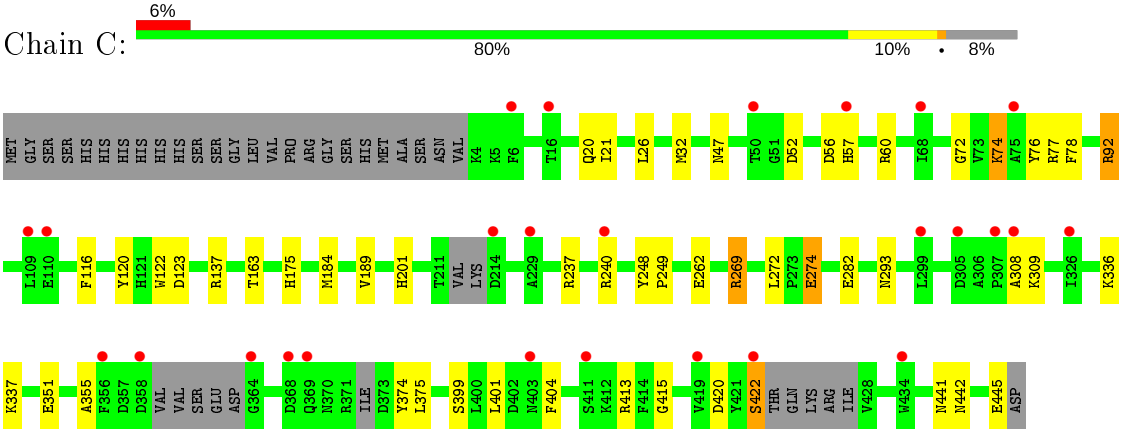
- Molecule 1: Beta-glucosidase A

Chain B:



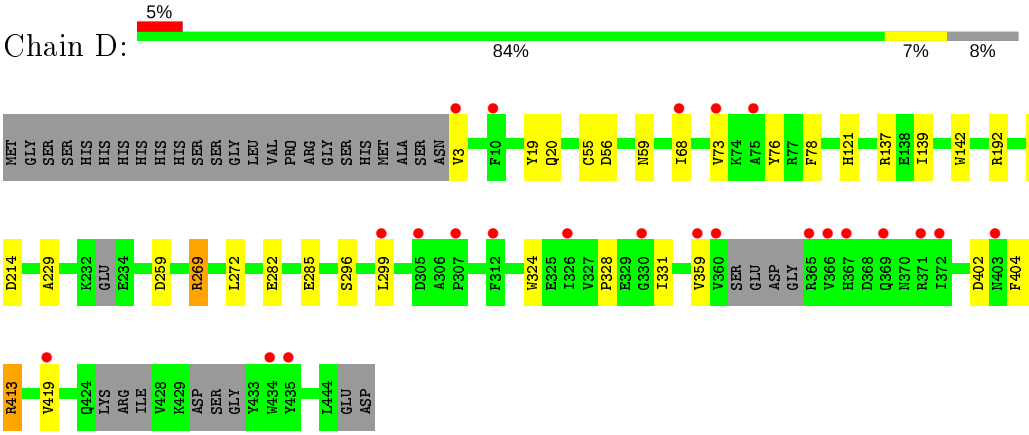
- Molecule 1: Beta-glucosidase A

Chain C:



• Molecule 1: Beta-glucosidase A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.63Å 76.67Å 95.26Å 72.34° 86.39° 85.54°	Depositor
Resolution (Å)	72.91 – 2.10 72.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (72.91-2.10) 97.3 (72.92-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.239 , 0.310 0.244 , 0.316	Depositor DCC
R_{free} test set	5391 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14780	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, IMD, CL, EDO, ACT, PEG, 8P5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.03	2/3724 (0.1%)	0.96	5/5064 (0.1%)
1	B	0.99	1/3758 (0.0%)	0.98	8/5109 (0.2%)
1	C	0.79	0/3578	0.84	3/4865 (0.1%)
1	D	0.78	0/3546	0.87	6/4831 (0.1%)
All	All	0.91	3/14606 (0.0%)	0.92	22/19869 (0.1%)

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	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	VAL	C-O	-5.26	1.13	1.23
1	A	122	TRP	CE3-CZ3	5.22	1.47	1.38
1	B	122	TRP	CG-CD1	-5.21	1.29	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	237	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	C	137	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	192	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	199	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	137	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	123	ASP	CB-CG-OD1	6.16	123.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	77	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	D	259	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	203[A]	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	B	203[B]	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	D	269	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	413	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	257	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	C	240	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	203	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	426	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	240	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	D	199	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	192	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	137	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	257	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	322	MET	CG-SD-CE	5.02	108.24	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	121	HIS	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	3608	0	3443	24	0
1	B	3642	0	3479	40	0
1	C	3470	0	3224	36	0
1	D	3435	0	3202	20	0
2	A	12	0	18	0	0
2	B	36	0	53	8	0
2	C	12	0	18	0	0
2	D	16	0	24	5	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	5	1	0
5	A	44	0	0	0	0
5	B	22	0	0	3	0
5	C	22	0	0	0	0
5	D	15	0	0	1	0
6	A	7	0	10	3	0
6	B	7	0	5	1	0
7	B	4	0	3	1	0
7	C	4	0	3	0	0
8	B	10	0	10	6	0
9	A	154	0	0	4	0
9	B	131	0	0	6	0
9	C	64	0	0	3	0
9	D	54	0	0	1	0
All	All	14780	0	13497	126	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 5.

All (126) 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:C:92:ARG:HH11	1:C:92:ARG:HG2	1.15	1.12
1:B:240[A]:ARG:NH1	9:B:602:HOH:O	1.66	1.02
1:D:19:TYR:HA	2:D:501:EDO:H22	1.48	0.95
1:B:376[A]:LYS:NZ	2:B:504:EDO:H12	1.86	0.90
8:B:514:PGE:H32	8:B:514:PGE:C6	2.03	0.89
1:C:72:GLY:O	1:C:74:LYS:NZ	2.05	0.88
8:B:514:PGE:H32	8:B:514:PGE:O4	1.76	0.85
3:A:504:CL:CL	9:A:727:HOH:O	2.31	0.85
1:B:376[A]:LYS:HZ1	2:B:504:EDO:H12	1.39	0.84
1:C:92:ARG:NH1	1:C:92:ARG:HG2	1.86	0.84
1:D:405:GLU:OE2	5:D:506:8P5:O6	1.98	0.81
1:B:138:GLU:OE1	9:B:604:HOH:O	1.98	0.80
1:A:403:ASN:ND2	9:A:602:HOH:O	2.17	0.77
1:A:105:ILE:HD11	9:A:753:HOH:O	1.86	0.75
1:C:274:GLU:OE2	9:C:601:HOH:O	2.03	0.75
1:B:203[A]:ARG:HG3	1:B:203[A]:ARG:HH11	1.52	0.74
1:B:369:GLN:NE2	7:B:512:ACT:OXT	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.00	0.72
1:B:207:VAL:O	1:B:211:THR:OG1	2.10	0.70
1:B:203[A]:ARG:HG3	1:B:203[A]:ARG:NH1	2.07	0.68
1:A:341:GLU:HA	6:A:508:PEG:H11	1.76	0.67
1:C:269[A]:ARG:O	1:C:269[A]:ARG:HD2	1.94	0.66
1:A:207:VAL:O	1:A:211:THR:OG1	2.14	0.66
8:B:514:PGE:H32	8:B:514:PGE:H62	1.77	0.65
1:B:376[A]:LYS:NZ	2:B:504:EDO:C1	2.61	0.63
1:D:413:ARG:NH1	1:D:419:VAL:O	2.34	0.60
1:C:20:GLN:HA	1:C:404:PHE:HB3	1.84	0.60
1:B:77:ARG:HA	1:B:116:PHE:O	2.01	0.59
1:C:269[A]:ARG:O	1:C:269[A]:ARG:CD	2.51	0.57
1:C:262:GLU:OE1	9:C:602:HOH:O	2.16	0.57
1:B:243:HIS:O	1:B:247:ASN:HB2	2.05	0.56
1:A:22:GLU:HA	1:A:57:HIS:HB3	1.89	0.55
1:B:146:TYR:CG	9:B:676:HOH:O	2.59	0.55
1:A:77:ARG:HA	1:A:116:PHE:O	2.05	0.55
1:C:269[A]:ARG:HD2	1:C:269[A]:ARG:C	2.26	0.54
1:B:203[A]:ARG:CG	1:B:203[A]:ARG:HH11	2.14	0.54
1:C:441:ASN:HD22	1:C:445:GLU:HB3	1.72	0.54
1:B:251:PHE:C	1:B:254:PRO:HD2	2.29	0.53
1:C:355:ALA:HA	1:C:413:ARG:O	2.08	0.53
1:C:442:ASN:O	1:C:442:ASN:ND2	2.42	0.52
1:D:229:ALA:HA	1:D:299:LEU:HD11	1.92	0.52
1:B:128:LEU:HD22	1:B:142:TRP:CE3	2.44	0.52
1:C:163:THR:HG21	1:C:201:HIS:ND1	2.24	0.52
1:A:90:THR:CG2	1:A:142:TRP:CD1	2.93	0.51
1:C:26:LEU:HD21	1:C:32:MET:HG2	1.92	0.51
1:D:76:TYR:CZ	1:D:78:PHE:HB3	2.46	0.50
1:D:269:ARG:HA	1:D:272:LEU:HD12	1.93	0.50
1:B:256:TYR:CE1	2:B:508:EDO:H12	2.47	0.50
6:B:513:PEG:O1	8:B:514:PGE:H42	1.77	0.50
1:C:269[A]:ARG:CD	1:C:269[A]:ARG:C	2.80	0.49
1:D:55:CYS:SG	1:D:402:ASP:O	2.70	0.49
1:B:169:VAL:HG21	5:B:511:8P5:O10	2.12	0.49
1:C:20:GLN:HG2	1:C:404:PHE:O	2.12	0.49
1:C:308:ALA:O	1:C:309:LYS:HB2	2.13	0.48
1:A:341:GLU:HG2	6:A:508:PEG:C2	2.44	0.48
1:C:56:ASP:HB3	1:C:60:ARG:HE	1.78	0.48
1:B:184:MET:CE	1:B:189:VAL:HG21	2.44	0.47
1:D:56:ASP:OD1	1:D:59:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLU:OE1	1:B:343:ASN:ND2	2.37	0.47
1:B:144:ALA:HB2	1:B:203[B]:ARG:HG2	1.96	0.47
1:C:77:ARG:HA	1:C:116:PHE:O	2.14	0.47
1:C:21:ILE:HD12	1:C:57:HIS:CG	2.50	0.47
1:A:243:HIS:O	1:A:247:ASN:HB2	2.15	0.47
1:C:175:HIS:HA	1:C:184[A]:MET:HB3	1.97	0.47
1:B:6:PHE:CZ	1:B:383:TRP:HB2	2.50	0.47
1:B:148[A]:ARG:NH1	1:B:211:THR:CG2	2.78	0.46
1:B:148[A]:ARG:NH1	1:B:211:THR:HG23	2.31	0.46
1:A:328:PRO:O	1:A:331:ILE:HG22	2.15	0.46
1:B:405:GLU:OE1	5:B:511:8P5:O4	2.33	0.46
1:D:406:TRP:HB2	2:D:502:EDO:H11	1.97	0.46
1:A:182:PRO:HB2	1:C:184[B]:MET:CE	2.45	0.46
1:D:406:TRP:HB2	2:D:502:EDO:C1	2.45	0.46
1:C:399:SER:O	1:C:415:GLY:HA2	2.16	0.45
1:B:306:ALA:HB1	1:B:307:PRO:HD2	1.98	0.45
1:B:404:PHE:HB2	1:B:410:TYR:CE1	2.52	0.45
1:D:359:VAL:HG23	1:D:359:VAL:O	2.16	0.45
1:B:146:TYR:CE2	9:B:676:HOH:O	2.68	0.45
8:B:514:PGE:H1	8:B:514:PGE:O4	2.17	0.45
1:B:144:ALA:HB2	1:B:203[A]:ARG:HB3	1.98	0.45
1:D:192:ARG:HG2	2:D:504:EDO:H11	1.98	0.45
1:A:108:LEU:HD13	1:A:115:PRO:HB3	1.99	0.45
1:B:287:ILE:O	2:B:508:EDO:H21	2.17	0.45
1:B:280:MET:O	1:B:284:GLN:HG3	2.17	0.45
1:C:120:TYR:CE2	1:C:122:TRP:HA	2.52	0.45
1:A:184[B]:MET:HB2	1:A:184[B]:MET:HE2	1.88	0.44
1:A:90:THR:HG21	1:A:142:TRP:CD1	2.52	0.44
1:A:67:ILE:HG21	1:A:417:VAL:HG21	1.99	0.44
1:B:376[A]:LYS:HE2	2:B:504:EDO:H11	1.99	0.44
1:C:374:TYR:O	1:C:375:LEU:C	2.56	0.44
1:B:20:GLN:O	1:B:403:ASN:HB2	2.16	0.44
1:C:269[C]:ARG:HA	1:C:272:LEU:HD12	2.00	0.44
1:C:184[B]:MET:SD	1:C:189:VAL:HG11	2.58	0.44
1:A:26:LEU:HD21	1:A:32:MET:HG2	1.98	0.44
1:C:123:ASP:N	1:C:123:ASP:OD1	2.51	0.44
1:B:63:GLU:O	1:B:66:GLU:HB2	2.18	0.43
1:B:376[A]:LYS:HZ3	2:B:504:EDO:H12	1.78	0.43
1:B:376[A]:LYS:HE2	2:B:504:EDO:C1	2.48	0.43
1:A:148:ARG:HD3	1:A:207:VAL:HG13	2.01	0.43
1:A:421:TYR:HB3	4:A:506:IMD:C5	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:CD1	9:B:676:HOH:O	2.72	0.43
1:C:420:ASP:O	1:C:422:SER:N	2.51	0.43
1:D:68:ILE:HG22	1:D:73:VAL:HB	2.00	0.42
1:A:168:TRP:CZ2	1:A:172:ILE:HG21	2.55	0.42
1:C:175:HIS:HA	1:C:184[B]:MET:HB3	2.00	0.42
1:C:72:GLY:O	1:C:74:LYS:CE	2.65	0.42
1:A:341:GLU:HG2	6:A:508:PEG:H22	2.01	0.42
1:C:274:GLU:CD	9:C:601:HOH:O	2.54	0.42
1:C:76:TYR:CZ	1:C:78:PHE:HB3	2.55	0.42
1:D:328:PRO:O	1:D:331:ILE:HG22	2.19	0.42
1:D:296:SER:HB2	1:D:324:TRP:HB3	2.02	0.42
1:D:76:TYR:OH	9:D:602:HOH:O	2.13	0.42
8:B:514:PGE:H32	8:B:514:PGE:H1	1.63	0.42
1:D:410:TYR:CD2	2:D:503:EDO:H11	2.55	0.42
1:D:20:GLN:HG2	1:D:404:PHE:O	2.21	0.41
1:C:248:TYR:CD1	1:C:249:PRO:HD3	2.55	0.41
1:D:206:LYS:HG2	1:D:285:GLU:OE1	2.19	0.41
1:A:405:GLU:O	1:A:408:GLU:HB2	2.19	0.41
1:B:403:ASN:OD1	1:B:403:ASN:C	2.59	0.41
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.85	0.41
5:B:511:8P5:N11	9:B:610:HOH:O	2.37	0.41
1:D:139:ILE:HA	1:D:142:TRP:CE3	2.55	0.41
1:B:398:TRP:HA	1:B:399:SER:HA	1.92	0.41
1:B:22:GLU:HA	1:B:57:HIS:HB3	2.04	0.41
1:C:293:ASN:CG	1:C:351:GLU:HB2	2.41	0.40
1:A:144:ALA:O	1:A:145:GLU:C	2.59	0.40
1:A:345:PRO:O	9:A:603:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/468 (95%)	423 (96%)	20 (4%)	0	100	100
1	B	445/468 (95%)	422 (95%)	23 (5%)	0	100	100
1	C	425/468 (91%)	401 (94%)	24 (6%)	0	100	100
1	D	423/468 (90%)	398 (94%)	25 (6%)	0	100	100
All	All	1736/1872 (93%)	1644 (95%)	92 (5%)	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	A	366/399 (92%)	363 (99%)	3 (1%)	81	86
1	B	372/399 (93%)	357 (96%)	15 (4%)	31	32
1	C	337/399 (84%)	323 (96%)	14 (4%)	30	30
1	D	331/399 (83%)	328 (99%)	3 (1%)	78	84
All	All	1406/1596 (88%)	1371 (98%)	35 (2%)	52	52

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	THR
1	A	274	GLU
1	A	281	SER
1	B	3	VAL
1	B	8	GLU
1	B	88	GLU
1	B	203[A]	ARG
1	B	203[B]	ARG
1	B	246	ASN
1	B	281	SER
1	B	282	GLU
1	B	296	SER
1	B	316	ASP

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Mol	Chain	Res	Type
1	B	317	LEU
1	B	337	LYS
1	B	350	THR
1	B	387	GLN
1	B	445	GLU
1	C	47	ASN
1	C	52	ASP
1	C	74	LYS
1	C	92	ARG
1	C	269[A]	ARG
1	C	269[B]	ARG
1	C	269[C]	ARG
1	C	274	GLU
1	C	282	GLU
1	C	336[A]	LYS
1	C	336[B]	LYS
1	C	337	LYS
1	C	401	LEU
1	C	422	SER
1	D	3	VAL
1	D	214	ASP
1	D	282	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	B	47	ASN
1	C	246	ASN
1	C	442	ASN
1	D	298	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
2	EDO	A	501	-	3,3,3	0.59	0	2,2,2	0.45	0
2	EDO	D	504	-	3,3,3	0.42	0	2,2,2	0.24	0
2	EDO	D	501	-	3,3,3	0.83	0	2,2,2	0.91	0
2	EDO	B	505	-	3,3,3	0.51	0	2,2,2	0.32	0
5	8P5	D	506	-	16,16,23	1.90	3 (18%)	16,25,32	1.49	3 (18%)
8	PGE	B	514	6	9,9,9	0.64	0	8,8,8	0.43	0
6	PEG	B	513	8	6,6,6	0.63	0	5,5,5	0.59	0
5	8P5	A	507[B]	-	22,23,23	1.72	4 (18%)	22,32,32	1.17	3 (13%)
2	EDO	B	504	-	3,3,3	0.32	0	2,2,2	0.78	0
5	8P5	A	507[A]	-	22,23,23	1.54	3 (13%)	22,32,32	1.22	2 (9%)
2	EDO	B	502[A]	-	3,3,3	0.32	0	2,2,2	0.45	0
2	EDO	C	502	-	3,3,3	0.38	0	2,2,2	0.51	0
2	EDO	B	502[B]	-	3,3,3	0.35	0	2,2,2	0.63	0
2	EDO	B	503	-	3,3,3	0.54	0	2,2,2	0.20	0
2	EDO	B	506	-	3,3,3	0.52	0	2,2,2	0.12	0
2	EDO	C	501	-	3,3,3	0.62	0	2,2,2	0.38	0
7	ACT	C	506	-	1,3,3	0.51	0	0,3,3	0.00	-
5	8P5	B	511	-	22,23,23	2.01	6 (27%)	22,32,32	2.45	5 (22%)
6	PEG	A	508	-	6,6,6	0.52	0	5,5,5	0.57	0
7	ACT	B	512	-	1,3,3	1.87	0	0,3,3	0.00	-
2	EDO	C	503	-	3,3,3	0.57	0	2,2,2	0.24	0
2	EDO	A	502	-	3,3,3	0.44	0	2,2,2	0.19	0
2	EDO	D	503	-	3,3,3	0.52	0	2,2,2	0.19	0
4	IMD	A	506	-	3,5,5	0.35	0	4,5,5	0.80	0
5	8P5	C	505	-	22,23,23	1.56	2 (9%)	22,32,32	1.03	1 (4%)
2	EDO	A	503	-	3,3,3	0.61	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	B	501	-	3,3,3	0.59	0	2,2,2	0.49	0
2	EDO	B	508	-	3,3,3	0.48	0	2,2,2	0.87	0
2	EDO	D	502	-	3,3,3	0.65	0	2,2,2	0.46	0
2	EDO	B	507	-	3,3,3	0.52	0	2,2,2	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	D	504	-	-	1/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	B	505	-	-	0/1/1/1	-
5	8P5	D	506	-	-	1/4/35/43	0/2/2/2
8	PGE	B	514	6	-	3/7/7/7	-
6	PEG	B	513	8	-	2/4/4/4	-
5	8P5	A	507[B]	-	-	7/14/43/43	0/2/2/2
2	EDO	B	504	-	-	1/1/1/1	-
5	8P5	A	507[A]	-	-	10/14/43/43	0/2/2/2
2	EDO	B	502[A]	-	-	1/1/1/1	-
2	EDO	C	502	-	-	1/1/1/1	-
2	EDO	B	502[B]	-	-	0/1/1/1	-
2	EDO	B	503	-	-	1/1/1/1	-
2	EDO	B	506	-	-	1/1/1/1	-
2	EDO	C	501	-	-	1/1/1/1	-
5	8P5	B	511	-	-	8/14/43/43	0/2/2/2
6	PEG	A	508	-	-	3/4/4/4	-
2	EDO	C	503	-	-	0/1/1/1	-
2	EDO	A	502	-	-	1/1/1/1	-
4	IMD	A	506	-	-	-	0/1/1/1
2	EDO	D	503	-	-	1/1/1/1	-
5	8P5	C	505	-	-	2/14/43/43	0/2/2/2
2	EDO	A	503	-	-	1/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	B	508	-	-	1/1/1/1	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	B	507	-	-	1/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	511	8P5	N17-N16	6.63	1.40	1.23
5	D	506	8P5	C8-C9	-6.02	1.47	1.51
5	C	505	8P5	N17-N16	5.96	1.39	1.23
5	A	507[B]	8P5	N17-N16	5.83	1.38	1.23
5	A	507[A]	8P5	N17-N16	5.39	1.37	1.23
5	A	507[B]	8P5	C5-C4	-3.21	1.49	1.53
5	B	511	8P5	C5-C4	-3.14	1.50	1.53
5	B	511	8P5	C8-C7	2.69	1.56	1.52
5	D	506	8P5	C5-C4	-2.63	1.50	1.53
5	A	507[A]	8P5	C5-C4	-2.33	1.50	1.53
5	A	507[A]	8P5	C8-C7	2.32	1.55	1.52
5	B	511	8P5	C8-C1	2.28	1.55	1.52
5	C	505	8P5	C5-C4	-2.28	1.50	1.53
5	A	507[B]	8P5	C5-C7	-2.24	1.50	1.54
5	B	511	8P5	C5-C7	-2.21	1.50	1.54
5	B	511	8P5	C8-C9	2.12	1.55	1.51
5	D	506	8P5	C8-C1	2.12	1.55	1.52
5	A	507[B]	8P5	C8-C1	2.04	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	511	8P5	C8-C9-N11	8.97	128.48	115.64
5	D	506	8P5	O2-C2-C3	-3.97	101.17	110.35
5	B	511	8P5	O10-C9-C8	-3.60	114.56	122.37
5	B	511	8P5	O10-C9-N11	-2.86	116.86	122.99
5	A	507[B]	8P5	C8-C9-N11	2.81	119.65	115.64
5	B	511	8P5	O4-C4-C3	2.77	116.76	110.35
5	A	507[A]	8P5	C2-C3-C4	2.68	115.50	110.82
5	A	507[B]	8P5	C13-C12-N11	-2.65	104.62	112.21
5	A	507[A]	8P5	C12-N11-C9	-2.65	117.87	122.59
5	A	507[B]	8P5	O10-C9-N11	-2.52	117.58	122.99
5	C	505	8P5	C5-C4-C3	-2.51	106.45	110.74
5	D	506	8P5	O3-C3-C2	-2.38	104.84	110.35
5	B	511	8P5	O3-C3-C2	-2.27	105.10	110.35
5	D	506	8P5	C5-C4-C3	-2.25	106.89	110.74

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507[B]	8P5	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	507[B]	8P5	C7-C5-C6-O6
5	A	507[B]	8P5	C8-C9-N11-C12
5	A	507[B]	8P5	O10-C9-N11-C12
5	A	507[B]	8P5	C13-C14-C15-N16
5	A	507[A]	8P5	C4-C5-C6-O6
5	A	507[A]	8P5	C7-C5-C6-O6
5	A	507[A]	8P5	C1-C8-C9-O10
5	A	507[A]	8P5	C1-C8-C9-N11
5	B	511	8P5	C7-C8-C9-O10
5	B	511	8P5	C7-C8-C9-N11
8	B	514	PGE	C1-C2-O2-C3
6	B	513	PEG	C1-C2-O2-C3
5	A	507[B]	8P5	N11-C12-C13-C14
5	A	507[A]	8P5	N11-C12-C13-C14
5	C	505	8P5	N11-C12-C13-C14
6	B	513	PEG	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
8	B	514	PGE	C6-C5-O3-C4
5	B	511	8P5	C7-C5-C6-O6
2	D	501	EDO	O1-C1-C2-O2
2	B	506	EDO	O1-C1-C2-O2
2	A	503	EDO	O1-C1-C2-O2
5	A	507[A]	8P5	O10-C9-N11-C12
6	A	508	PEG	C4-C3-O2-C2
5	A	507[A]	8P5	C8-C9-N11-C12
5	A	507[A]	8P5	C15-N16-N17-N1
5	A	507[B]	8P5	C12-C13-C14-C15
5	C	505	8P5	C12-C13-C14-C15
2	D	504	EDO	O1-C1-C2-O2
2	C	502	EDO	O1-C1-C2-O2
2	C	501	EDO	O1-C1-C2-O2
5	B	511	8P5	N11-C12-C13-C14
5	B	511	8P5	C4-C5-C6-O6
2	B	503	EDO	O1-C1-C2-O2
5	B	511	8P5	C1-C8-C9-O10
5	A	507[A]	8P5	C7-C8-C9-N11
2	B	502[A]	EDO	O1-C1-C2-O2
2	B	508	EDO	O1-C1-C2-O2
5	B	511	8P5	C12-C13-C14-C15
2	B	504	EDO	O1-C1-C2-O2
2	A	502	EDO	O1-C1-C2-O2
8	B	514	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
5	A	507[A]	8P5	C7-C8-C9-O10
6	A	508	PEG	O2-C3-C4-O4
5	B	511	8P5	C1-C8-C9-N11
2	D	503	EDO	O1-C1-C2-O2
2	B	507	EDO	O1-C1-C2-O2
5	D	506	8P5	C7-C5-C6-O6
6	A	508	PEG	C1-C2-O2-C3

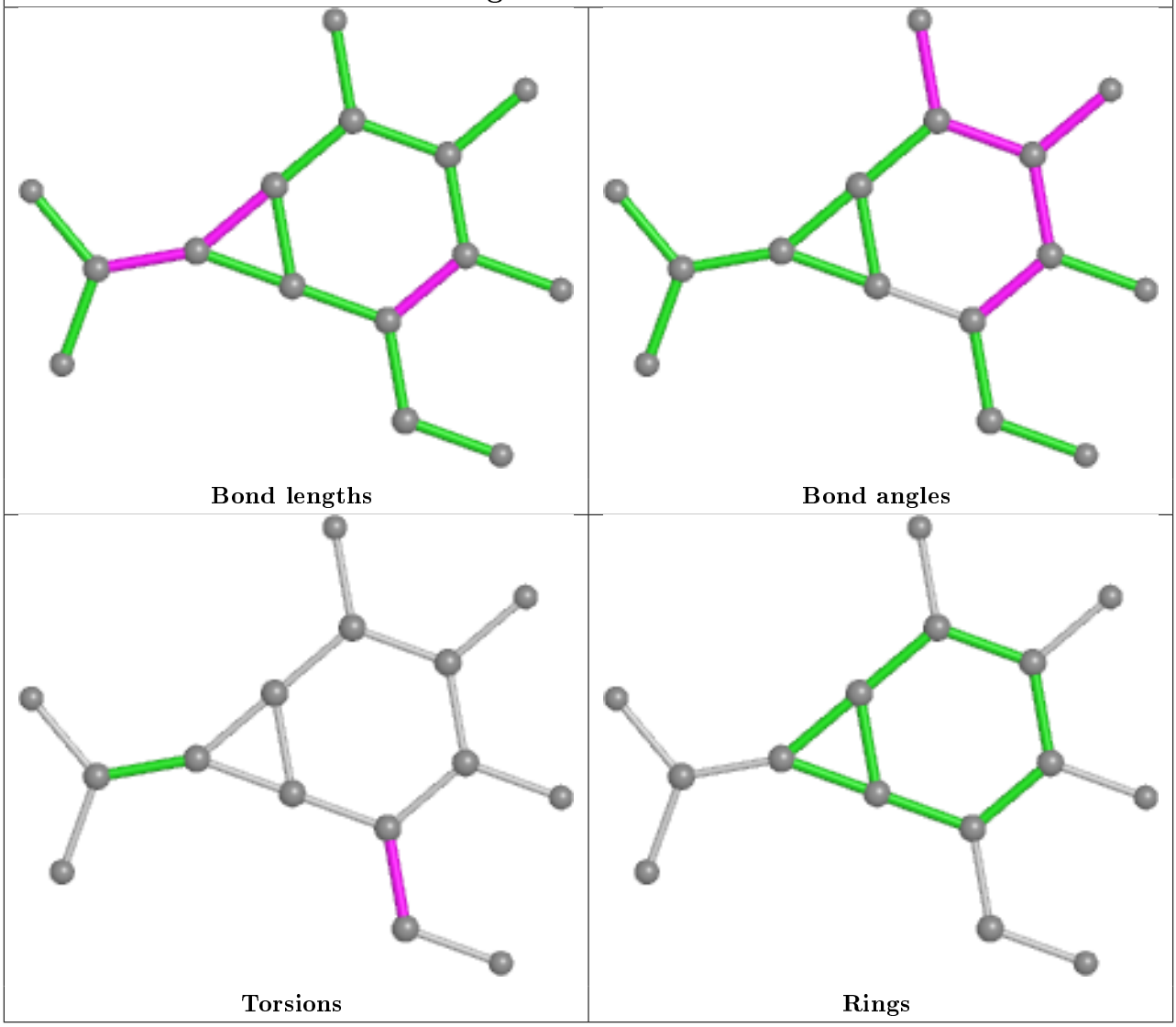
There are no ring outliers.

13 monomers are involved in 28 short contacts:

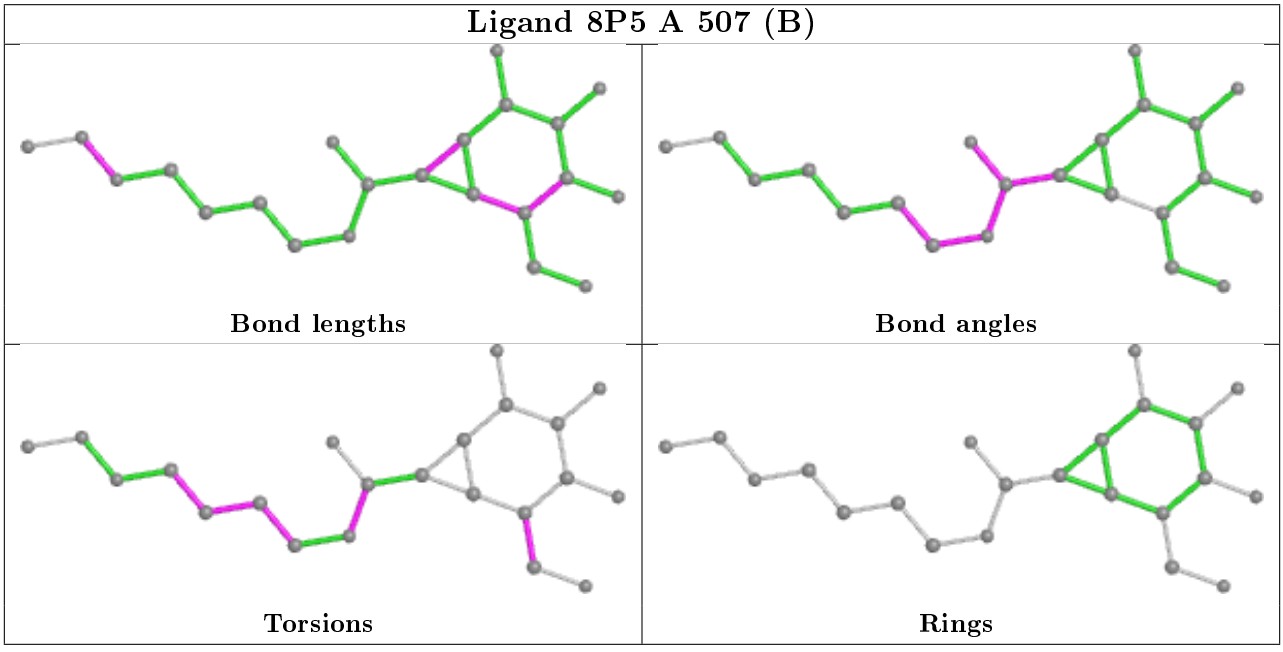
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	504	EDO	1	0
2	D	501	EDO	1	0
5	D	506	8P5	1	0
8	B	514	PGE	6	0
6	B	513	PEG	1	0
2	B	504	EDO	6	0
5	B	511	8P5	3	0
6	A	508	PEG	3	0
7	B	512	ACT	1	0
2	D	503	EDO	1	0
4	A	506	IMD	1	0
2	B	508	EDO	2	0
2	D	502	EDO	2	0

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 then 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.

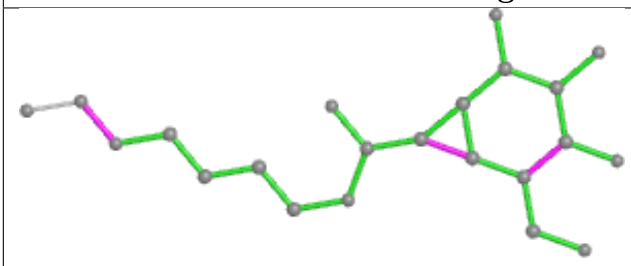
Ligand 8P5 D 506



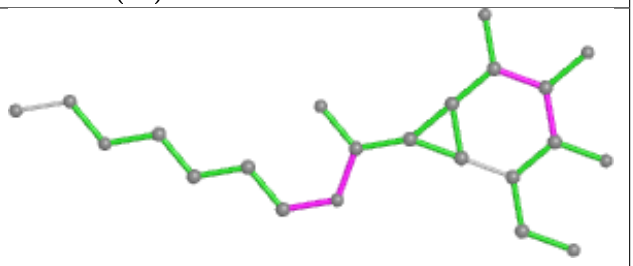
Ligand 8P5 A 507 (B)



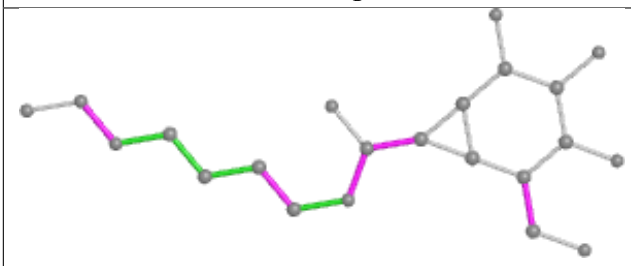
Ligand 8P5 A 507 (A)



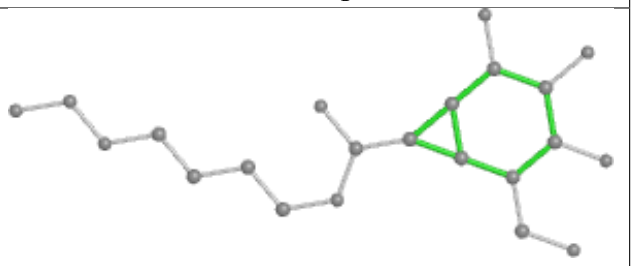
Bond lengths



Bond angles

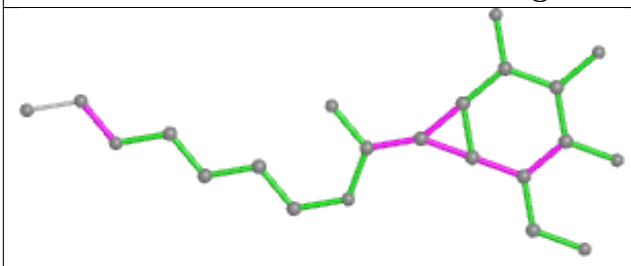


Torsions

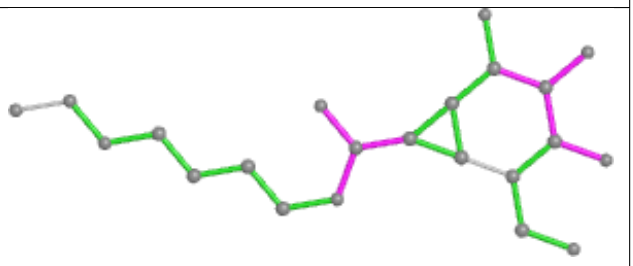


Rings

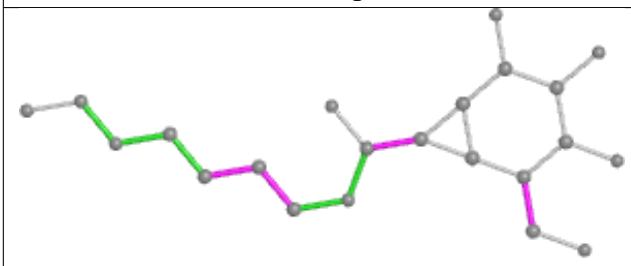
Ligand 8P5 B 511



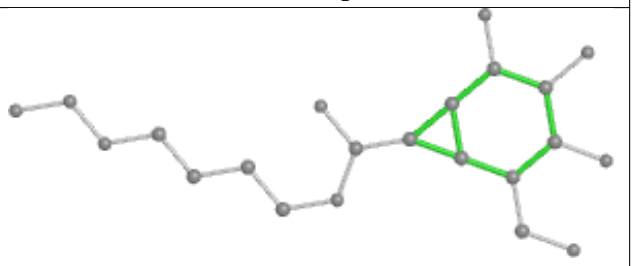
Bond lengths



Bond angles

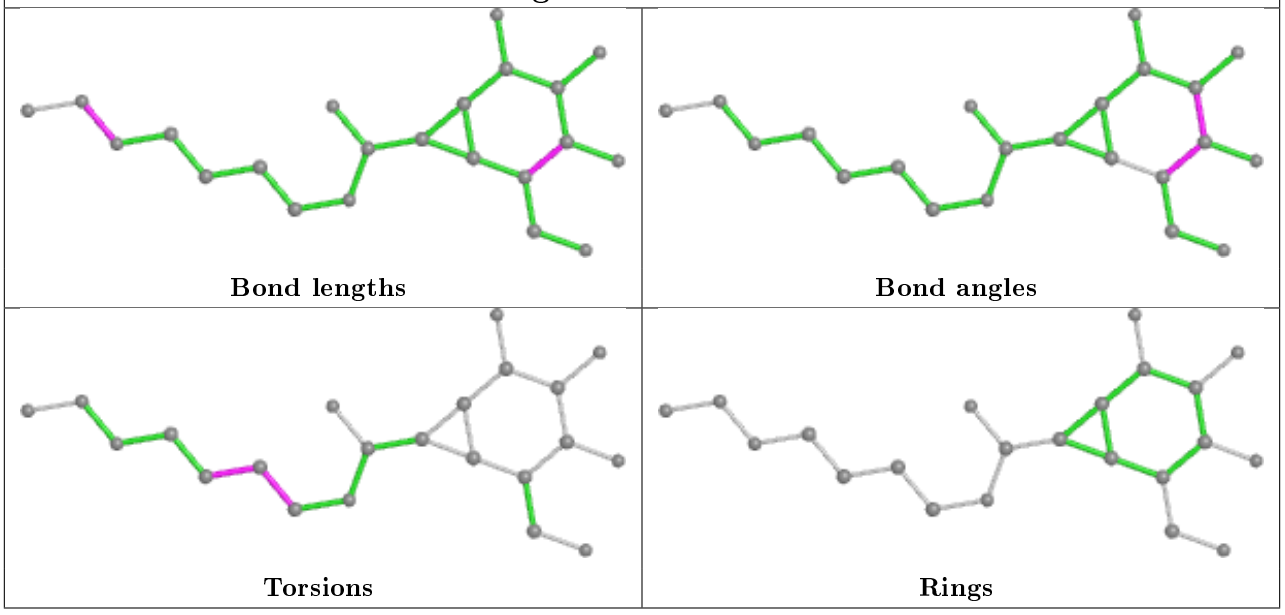


Torsions



Rings

Ligand 8P5 C 505



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	443/468 (94%)	0.14	3 (0%)	87	89	13, 26, 40, 56	11 (2%)
1	B	443/468 (94%)	0.14	4 (0%)	84	86	14, 26, 40, 62	16 (3%)
1	C	429/468 (91%)	0.53	26 (6%)	21	26	15, 37, 57, 65	49 (11%)
1	D	431/468 (92%)	0.51	24 (5%)	24	29	16, 37, 56, 63	45 (10%)
All	All	1746/1872 (93%)	0.33	57 (3%)	46	53	13, 30, 54, 65	121 (6%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	360	VAL	5.2
1	D	359	VAL	4.7
1	C	419	VAL	4.6
1	D	366	VAL	4.6
1	D	419	VAL	4.6
1	C	356	PHE	4.4
1	C	308	ALA	4.2
1	C	326	ILE	4.2
1	D	326	ILE	4.0
1	D	367	HIS	3.9
1	B	306	ALA	3.9
1	B	307	PRO	3.8
1	D	3	VAL	3.8
1	C	109	LEU	3.6
1	D	68	ILE	3.5
1	D	307	PRO	3.3
1	C	411	SER	3.3
1	D	435	TYR	3.3
1	C	75	ALA	3.0
1	D	305	ASP	3.0
1	D	365	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	73	VAL	3.0
1	C	299	LEU	2.9
1	C	434	TRP	2.9
1	C	364	GLY	2.8
1	A	3	VAL	2.8
1	C	358	ASP	2.8
1	D	372	ILE	2.8
1	C	403	ASN	2.7
1	C	50	THR	2.7
1	B	3	VAL	2.7
1	B	366	VAL	2.6
1	C	110	GLU	2.6
1	C	229	ALA	2.5
1	D	403	ASN	2.5
1	C	369	GLN	2.5
1	D	369	GLN	2.5
1	C	240	ARG	2.4
1	C	305	ASP	2.3
1	D	75	ALA	2.3
1	C	68	ILE	2.3
1	C	214	ASP	2.2
1	D	205	VAL	2.2
1	C	6	PHE	2.2
1	D	10	PHE	2.2
1	D	312	PHE	2.2
1	C	57	HIS	2.1
1	C	307	PRO	2.1
1	C	16	THR	2.1
1	A	108	LEU	2.0
1	D	330	GLY	2.0
1	C	422	SER	2.0
1	D	371	ARG	2.0
1	A	97	GLY	2.0
1	D	434	TRP	2.0
1	D	299	LEU	2.0
1	C	368	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 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, 95^{th} 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
5	8P5	A	507[B]	22/22	0.70	0.25	23,29,30,35	22
5	8P5	A	507[A]	22/22	0.70	0.25	30,41,47,52	22
5	8P5	B	511	22/22	0.75	0.22	21,39,44,49	0
6	PEG	A	508	7/7	0.76	0.30	21,23,25,29	7
8	PGE	B	514	10/10	0.79	0.27	31,37,46,47	10
2	EDO	B	504	4/4	0.82	0.32	21,22,22,24	4
6	PEG	B	513	7/7	0.82	0.20	31,39,47,49	7
2	EDO	D	502	4/4	0.82	0.11	30,32,33,36	0
2	EDO	C	503	4/4	0.84	0.12	49,51,53,54	0
2	EDO	B	503	4/4	0.86	0.19	19,19,19,19	4
2	EDO	C	502	4/4	0.86	0.28	20,20,21,22	4
2	EDO	B	507	4/4	0.86	0.16	41,42,44,46	0
3	CL	C	504	1/1	0.87	0.10	58,58,58,58	0
5	8P5	C	505	22/22	0.87	0.15	27,33,37,39	7
2	EDO	B	505	4/4	0.88	0.27	12,13,14,15	4
2	EDO	A	503	4/4	0.88	0.23	16,16,16,17	4
5	8P5	D	506	15/22	0.88	0.16	28,32,35,41	0
7	ACT	C	506	4/4	0.88	0.24	25,26,27,27	4
2	EDO	D	504	4/4	0.89	0.24	20,20,20,21	4
7	ACT	B	512	4/4	0.89	0.12	39,46,46,46	0
2	EDO	A	501	4/4	0.90	0.14	21,22,23,25	0
2	EDO	B	508	4/4	0.91	0.21	13,14,14,16	4
2	EDO	C	501	4/4	0.91	0.12	28,32,33,33	0
2	EDO	D	501	4/4	0.91	0.15	34,35,37,37	0
3	CL	B	509	1/1	0.92	0.06	58,58,58,58	0
2	EDO	B	506	4/4	0.92	0.25	23,23,25,25	4
2	EDO	D	503	4/4	0.92	0.11	44,45,47,48	0
3	CL	D	505	1/1	0.92	0.15	60,60,60,60	0
2	EDO	A	502	4/4	0.93	0.11	31,35,35,36	0
3	CL	B	510	1/1	0.94	0.07	44,44,44,44	0
3	CL	A	505	1/1	0.94	0.16	46,46,46,46	0
2	EDO	B	502[B]	4/4	0.94	0.22	31,33,33,34	4

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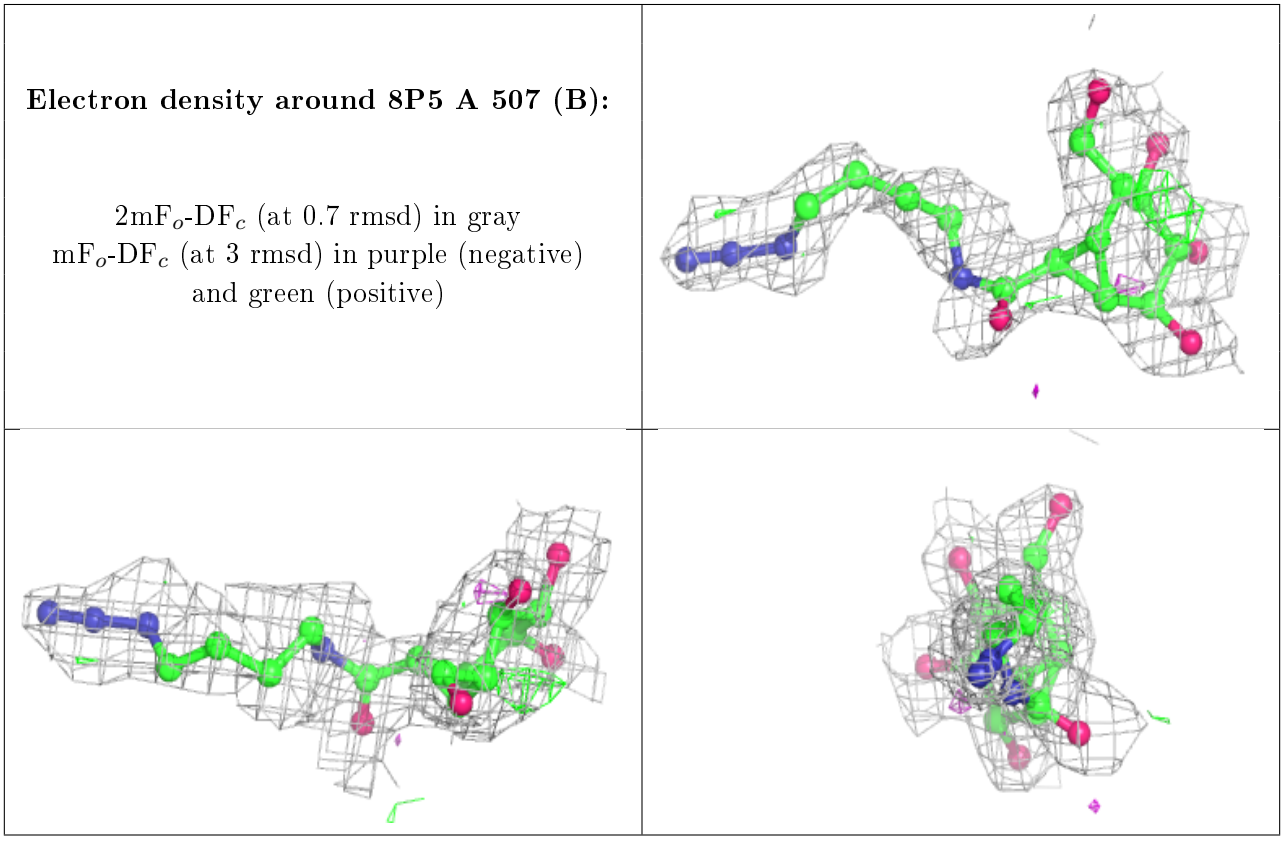
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	B	502[A]	4/4	0.94	0.22	25,25,26,28	4
2	EDO	B	501	4/4	0.95	0.09	29,31,32,33	0
4	IMD	A	506	5/5	0.96	0.16	42,43,46,49	0
3	CL	A	504	1/1	0.96	0.05	49,49,49,49	0

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.

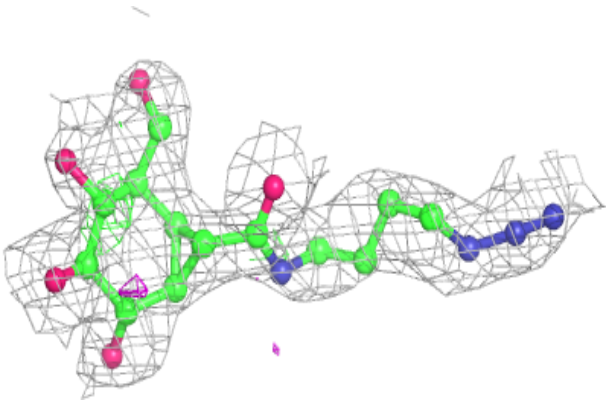
Electron density around 8P5 A 507 (B):

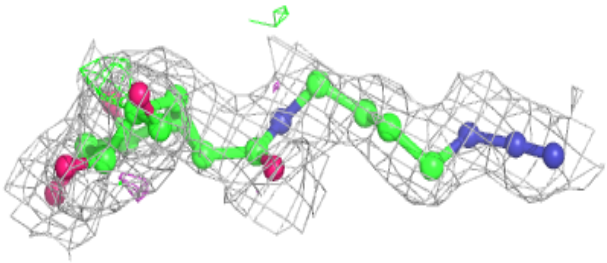
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

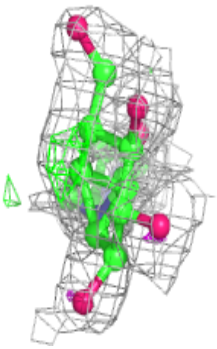


Electron density around 8P5 A 507 (A):

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

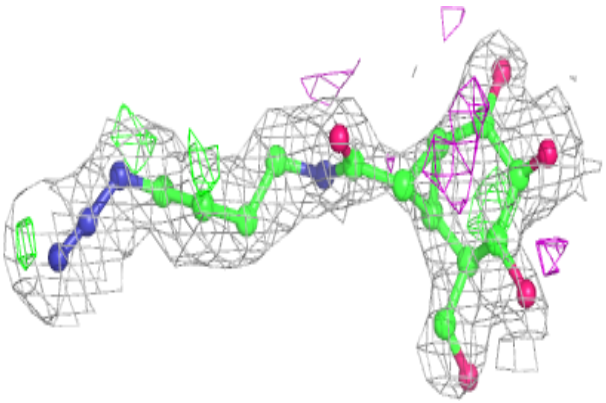


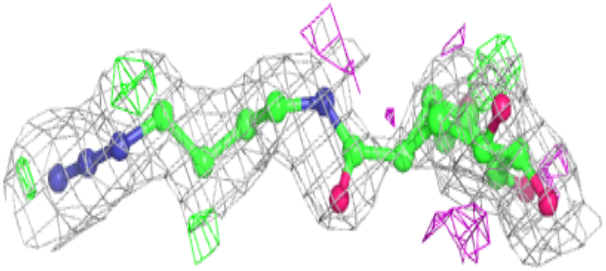


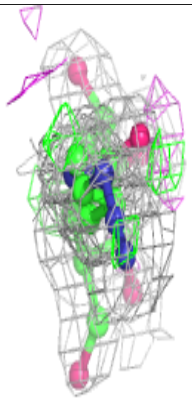


Electron density around 8P5 B 511:

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

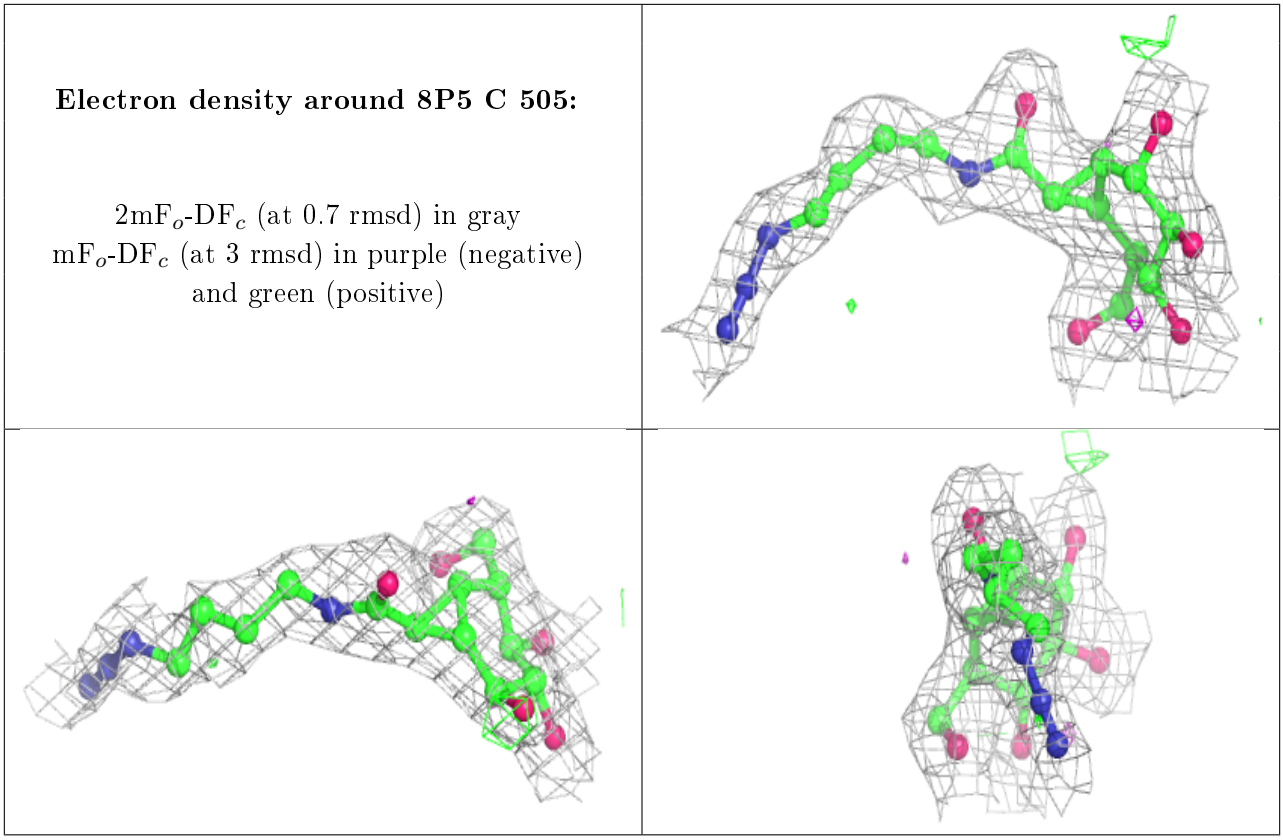






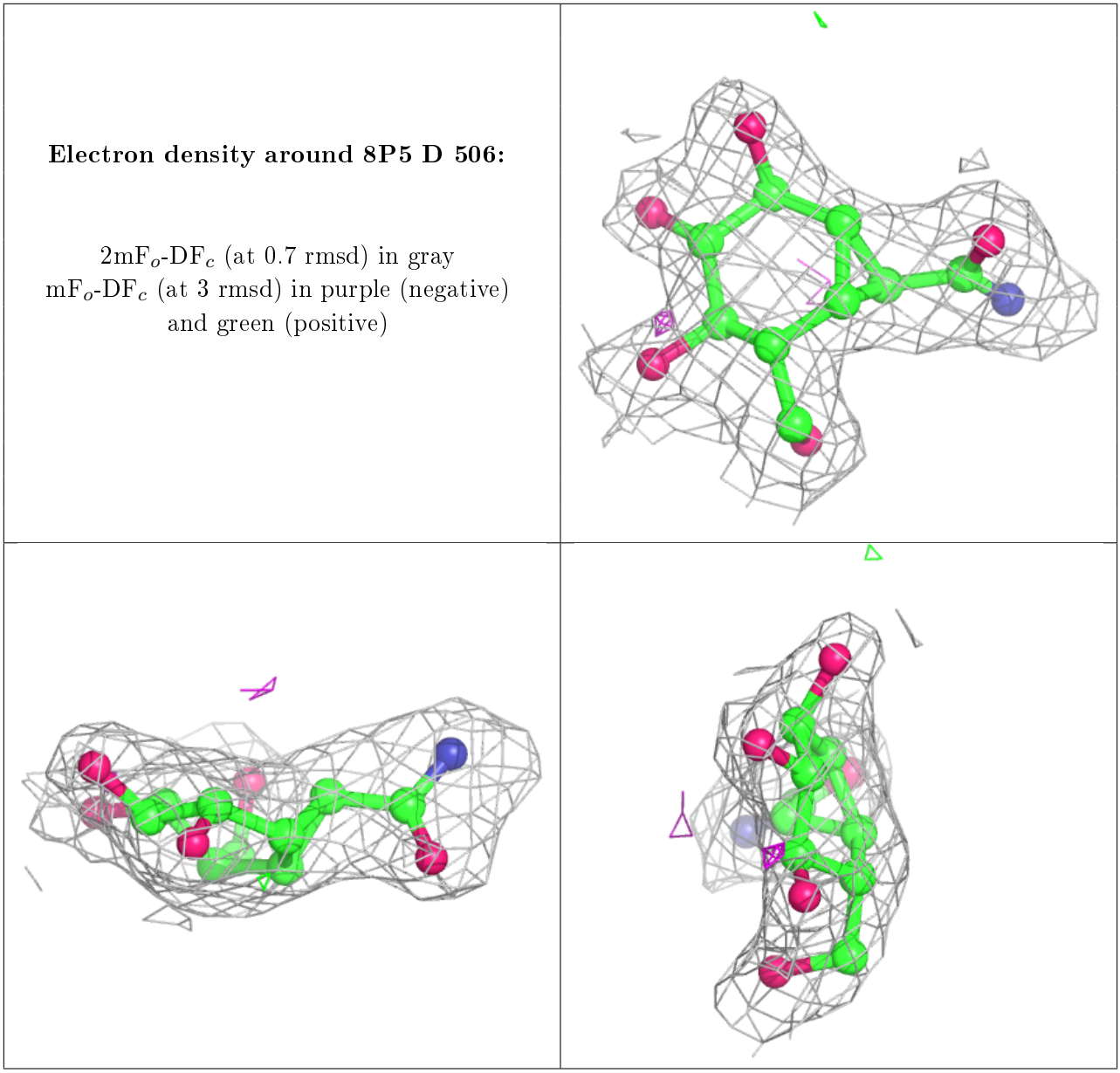
Electron density around 8P5 C 505:

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



Electron density around 8P5 D 506:

$2mF_o$-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

There are no such residues in this entry.