Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 01:20 pm GMT

PDB ID	:	6Z4N
Title	:	CRYSTAL STRUCTURE OF OASS COMPLEXED WITH UPAR INHIBITOR
Authors	:	Demitri, N.; Storici, P.; Campanini, B.
Deposited on	:	2020-05-25
Resolution	:	1.20 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 (i) 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 (i)) were used in the production of this report:

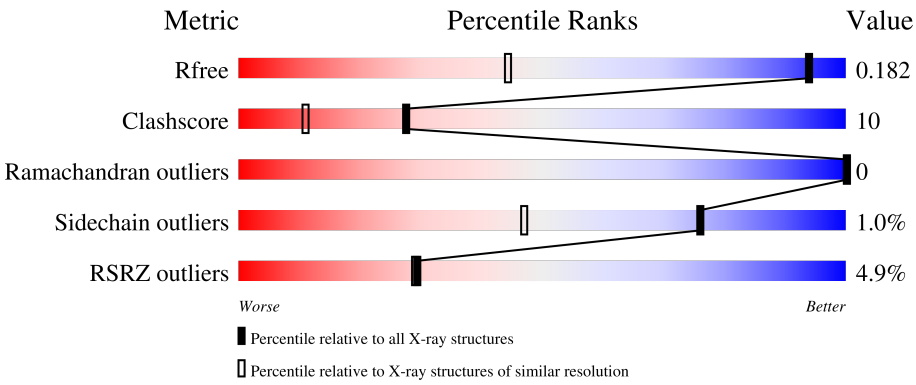
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 <=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	324	5% 88% 10% ••
1	BBB	324	4% 90% 7% •

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
5	GOL	AAA	406	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6208 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.

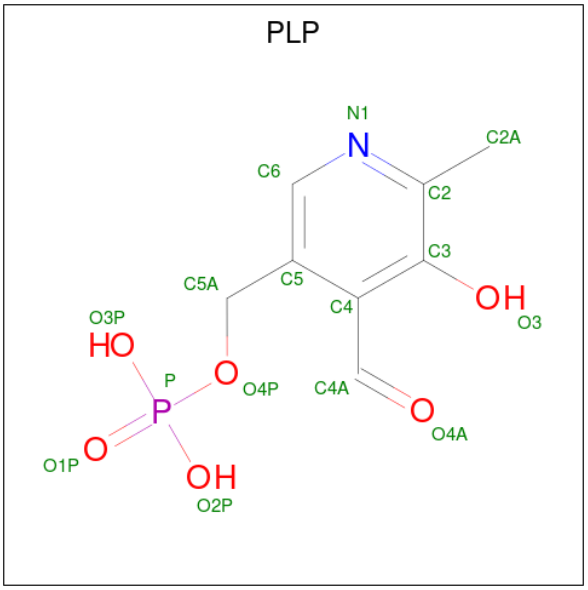
- Molecule 1 is a protein called Cysteine synthase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	321	2580	1635	441	495	9	0	28	0
1	BBB	318	2576	1640	438	489	9	0	29	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-1	HIS	-	expression tag	UNP P0A1E3
BBB	-1	HIS	-	expression tag	UNP P0A1E3

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	AAA	1	15	8	1	5	1	0	0

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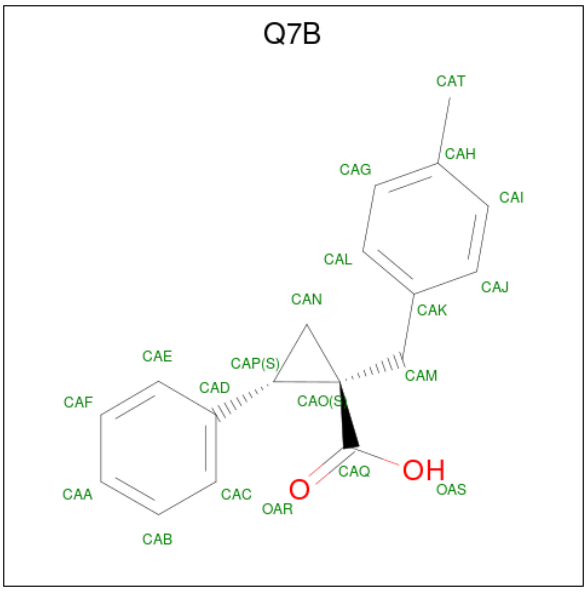
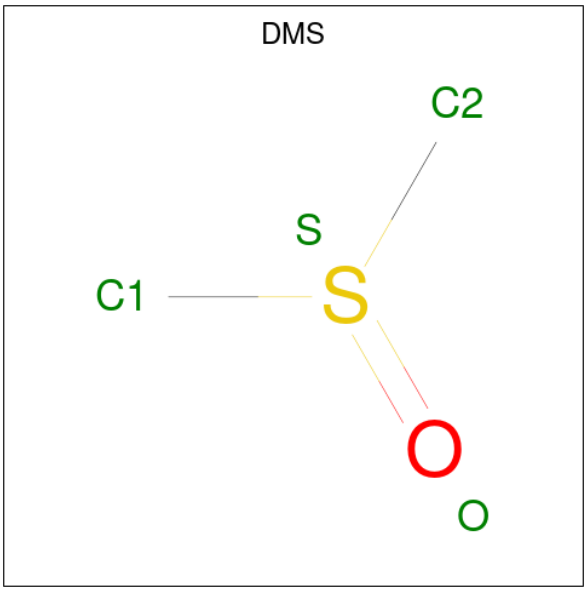
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	BBB	1	15	8	1	5	1	0	0

- Molecule 3 is (1 {S},2 {S})-1-[(4-methylphenyl)methyl]-2-phenyl-cyclopropane-1-carboxylic acid (three-letter code: Q7B) (formula: $C_{18}H_{18}O_2$) (labeled as "Ligand of Interest" by depositor).



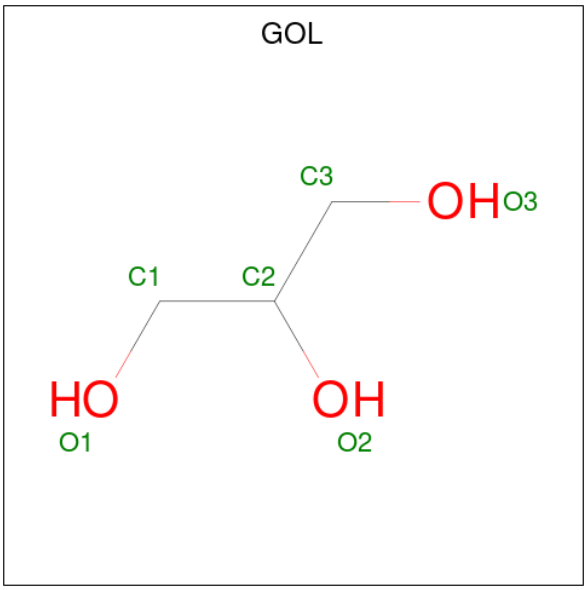
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	AAA	1	20	18	2	0	0
			Total	C	O		
3	BBB	1	20	18	2	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	AAA	1	8	4	2	2	0	1
			Total	C	O	S		
4	AAA	1	4	2	1	1	0	0
			Total	C	O	S		
4	AAA	1	4	2	1	1	0	0
			Total	C	O	S		
4	BBB	1	4	2	1	1	0	0

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



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

- Molecule 6 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Co		
6	AAA	1	1	1	0	0

- Molecule 7 is water.

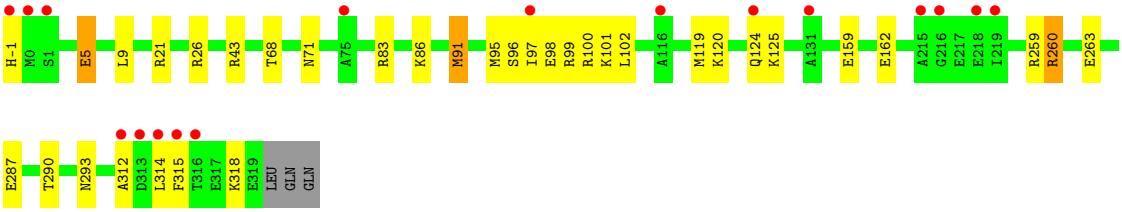
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	AAA	440	467	467	0	23
			Total	O		
7	BBB	429	482	482	0	50

3 Residue-property plots (i)

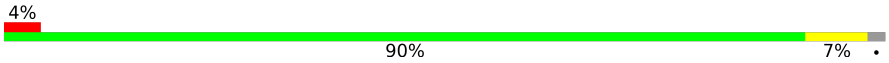
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

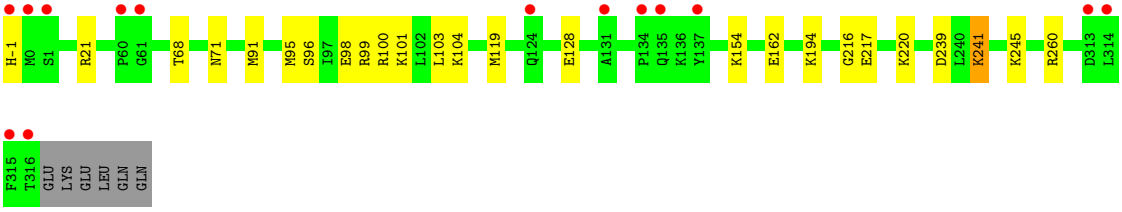
• Molecule 1: Cysteine synthase A

Chain AAA:



• Molecule 1: Cysteine synthase A

Chain BBB: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.26Å 96.28Å 140.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.65 – 1.20 46.60 – 1.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (46.65-1.20) 95.0 (46.60-1.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.154 , 0.179 0.161 , 0.182	Depositor DCC
R_{free} test set	10659 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 99.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6208	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CO, DMS, PLP, GOL, Q7B

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	0.85	6/2671 (0.2%)	0.92	5/3605 (0.1%)
1	BBB	0.77	1/2679 (0.0%)	0.93	3/3615 (0.1%)
All	All	0.81	7/5350 (0.1%)	0.92	8/7220 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	263	GLU	CD-OE1	-7.52	1.17	1.25
1	BBB	260	ARG	NE-CZ	6.83	1.42	1.33
1	AAA	5[A]	GLU	CD-OE1	-5.10	1.20	1.25
1	AAA	5[B]	GLU	CD-OE1	-5.10	1.20	1.25
1	AAA	159	GLU	CD-OE1	-5.06	1.20	1.25
1	AAA	5[A]	GLU	CD-OE2	5.03	1.31	1.25
1	AAA	5[B]	GLU	CD-OE2	5.03	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	260	ARG	NE-CZ-NH2	-16.07	112.27	120.30
1	BBB	260	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	AAA	43	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	AAA	43	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	AAA	260	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	AAA	26	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	AAA	21	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	BBB	21	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2580	0	2700	63	0
1	BBB	2576	0	2735	45	0
2	AAA	15	0	7	1	0
2	BBB	15	0	6	1	0
3	AAA	20	0	0	0	0
3	BBB	20	0	0	0	0
4	AAA	16	0	24	5	0
4	BBB	4	0	6	0	0
5	AAA	6	0	8	8	0
5	BBB	6	0	8	2	0
6	AAA	1	0	0	0	0
7	AAA	467	0	0	25	0
7	BBB	482	0	0	34	0
All	All	6208	0	5494	108	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 10.

All (108) 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:315:PHE:CZ	1:BBB:104[A]:LYS:HG3	1.48	1.48
1:BBB:104[C]:LYS:NZ	7:BBB:502:HOH:O	1.66	1.28
1:AAA:5[B]:GLU:OE1	5:AAA:406:GOL:H32	1.18	1.25
1:BBB:245[C]:LYS:NZ	7:BBB:501:HOH:O	1.63	1.23
1:BBB:119[B]:MET:HE1	7:BBB:710:HOH:O	1.09	1.21
1:AAA:5[B]:GLU:OE1	5:AAA:406:GOL:C3	1.90	1.19
1:AAA:119[A]:MET:SD	7:AAA:767:HOH:O	2.05	1.09
1:AAA:101[B]:LYS:HE2	7:BBB:554[B]:HOH:O	1.52	1.09
1:BBB:95[B]:MET:SD	7:BBB:750[B]:HOH:O	2.12	1.06
1:BBB:104[C]:LYS:NZ	7:BBB:503:HOH:O	1.88	1.04
1:AAA:101[B]:LYS:CE	7:BBB:554[B]:HOH:O	2.07	1.01
1:AAA:315:PHE:CE2	1:BBB:104[A]:LYS:HG3	1.95	1.00
1:AAA:315:PHE:CZ	1:BBB:104[A]:LYS:CG	2.44	1.00
1:BBB:101[B]:LYS:HE3	7:BBB:508[B]:HOH:O	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:98[B]:GLU:C	7:BBB:510:HOH:O	2.02	0.99
1:AAA:290[B]:THR:HG21	7:AAA:519[B]:HOH:O	1.66	0.94
1:AAA:259[A]:ARG:NH1	7:AAA:501:HOH:O	1.98	0.94
1:AAA:119[A]:MET:HE1	7:AAA:767:HOH:O	1.67	0.93
1:AAA:96[B]:SER:HB2	7:AAA:872[B]:HOH:O	1.70	0.91
1:AAA:315:PHE:CE1	1:BBB:104[A]:LYS:HG3	2.07	0.89
1:BBB:101[B]:LYS:NZ	7:BBB:508[B]:HOH:O	2.05	0.88
1:AAA:119[A]:MET:CE	7:AAA:767:HOH:O	2.14	0.88
1:BBB:101[B]:LYS:CE	7:BBB:508[B]:HOH:O	2.17	0.88
1:AAA:97[B]:ILE:HA	1:AAA:100[B]:ARG:HD2	1.53	0.87
1:AAA:5[B]:GLU:CD	5:AAA:406:GOL:H32	1.94	0.87
1:AAA:91[B]:MET:SD	1:AAA:95[B]:MET:SD	2.73	0.86
1:AAA:314:LEU:HD21	7:AAA:852:HOH:O	1.76	0.85
1:BBB:239:ASP:OD1	1:BBB:241[A]:LYS:HE3	1.78	0.83
1:AAA:97[B]:ILE:HA	1:AAA:100[B]:ARG:CD	2.10	0.81
1:AAA:318:LYS:HG3	7:AAA:758[A]:HOH:O	1.81	0.79
1:AAA:98[A]:GLU:C	7:AAA:507:HOH:O	2.20	0.78
1:BBB:217[A]:GLU:OE2	7:BBB:504:HOH:O	2.00	0.78
5:BBB:403:GOL:H32	7:BBB:748[B]:HOH:O	1.83	0.77
5:AAA:406:GOL:H11	7:AAA:685:HOH:O	1.83	0.77
1:AAA:259[B]:ARG:NH1	1:AAA:314:LEU:HD13	2.01	0.76
1:AAA:162[B]:GLU:OE2	7:AAA:672[B]:HOH:O	2.04	0.74
1:AAA:293:ASN:ND2	7:AAA:502:HOH:O	2.20	0.74
1:BBB:154:LYS:NZ	7:BBB:506[A]:HOH:O	2.03	0.74
1:AAA:96[B]:SER:O	1:AAA:100[B]:ARG:HD2	1.89	0.72
1:AAA:97[B]:ILE:CA	1:AAA:100[B]:ARG:HD2	2.21	0.70
1:BBB:119[B]:MET:CE	7:BBB:710:HOH:O	1.87	0.69
1:BBB:194[A]:LYS:NZ	7:BBB:511:HOH:O	2.26	0.69
1:BBB:162[A]:GLU:OE2	7:BBB:507:HOH:O	2.13	0.67
1:BBB:119[B]:MET:HA	1:BBB:119[B]:MET:HE2	1.77	0.66
1:AAA:5[B]:GLU:CD	7:AAA:529:HOH:O	2.34	0.66
1:AAA:99[A]:ARG:N	7:AAA:507:HOH:O	2.29	0.64
1:AAA:101[B]:LYS:HE3	7:BBB:554[B]:HOH:O	1.85	0.64
1:AAA:5[B]:GLU:HB3	1:AAA:9:LEU:CD1	2.29	0.63
1:BBB:99[B]:ARG:O	1:BBB:103:LEU:HG	1.98	0.62
1:AAA:315:PHE:CE1	1:BBB:104[A]:LYS:CG	2.79	0.62
1:BBB:162[B]:GLU:OE1	7:BBB:774[B]:HOH:O	2.16	0.62
1:BBB:104[C]:LYS:CE	7:BBB:503:HOH:O	2.43	0.61
1:AAA:86[A]:LYS:HE2	7:AAA:599:HOH:O	2.00	0.60
1:BBB:101[A]:LYS:HG3	7:BBB:503:HOH:O	2.00	0.60
1:BBB:98[B]:GLU:HB3	7:BBB:510:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:96[B]:SER:CB	7:AAA:872[B]:HOH:O	2.36	0.60
1:BBB:101[A]:LYS:CG	7:BBB:503:HOH:O	2.50	0.60
1:AAA:290[B]:THR:CG2	7:AAA:519[B]:HOH:O	2.36	0.59
1:AAA:5[B]:GLU:OE1	5:AAA:406:GOL:C2	2.50	0.59
1:AAA:95[B]:MET:O	1:AAA:100[B]:ARG:NE	2.31	0.59
1:BBB:98[B]:GLU:CB	7:BBB:510:HOH:O	2.49	0.59
1:AAA:315:PHE:CE2	1:BBB:104[A]:LYS:CG	2.77	0.58
1:AAA:91[B]:MET:SD	1:AAA:95[B]:MET:CE	2.92	0.57
1:AAA:99[B]:ARG:HD2	7:AAA:517:HOH:O	2.05	0.57
1:BBB:91[B]:MET:HE2	7:BBB:750[B]:HOH:O	2.04	0.57
1:BBB:98[A]:GLU:CG	7:BBB:508[A]:HOH:O	2.53	0.56
1:BBB:239:ASP:OD1	1:BBB:241[A]:LYS:CE	2.51	0.55
1:BBB:98[A]:GLU:OE2	7:BBB:508[A]:HOH:O	2.17	0.54
1:AAA:5[B]:GLU:HB3	1:AAA:9:LEU:HD13	1.88	0.54
1:AAA:259[B]:ARG:HH11	1:AAA:314:LEU:HD13	1.73	0.54
5:BBB:403:GOL:C3	7:BBB:748[B]:HOH:O	2.46	0.53
4:AAA:403[A]:DMS:H22	7:AAA:903:HOH:O	2.09	0.53
1:BBB:98[A]:GLU:HG2	7:BBB:508[A]:HOH:O	2.08	0.53
1:AAA:83:ARG:CZ	5:AAA:406:GOL:H31	2.39	0.52
1:AAA:260:ARG:HH12	4:AAA:405:DMS:C2	2.23	0.51
1:AAA:314:LEU:HG	1:AAA:315:PHE:CD2	2.46	0.51
1:BBB:96[A]:SER:O	1:BBB:100[A]:ARG:HG3	2.12	0.50
4:AAA:404:DMS:C2	7:AAA:913:HOH:O	2.59	0.50
1:AAA:124[B]:GLN:HG3	7:AAA:671:HOH:O	2.12	0.49
1:AAA:314:LEU:HG	1:AAA:315:PHE:CE2	2.46	0.49
1:BBB:104[C]:LYS:HE3	7:BBB:503:HOH:O	2.12	0.48
1:AAA:120:LYS:NZ	1:AAA:124[B]:GLN:OE1	2.44	0.48
1:BBB:119[B]:MET:HG2	7:BBB:851:HOH:O	2.14	0.48
1:BBB:96[B]:SER:HB2	1:BBB:98[B]:GLU:OE2	2.15	0.47
1:AAA:83:ARG:NH1	5:AAA:406:GOL:H31	2.29	0.47
1:BBB:71:ASN:ND2	2:BBB:401:PLP:H2A1	2.30	0.46
1:AAA:259[B]:ARG:NH2	1:AAA:314:LEU:HB2	2.30	0.46
1:BBB:128:GLU:OE1	7:BBB:509:HOH:O	2.20	0.45
1:AAA:287[B]:GLU:HA	1:AAA:290[B]:THR:HG23	1.98	0.45
1:AAA:259[B]:ARG:NH2	1:AAA:312:ALA:O	2.49	0.44
1:AAA:125[A]:LYS:NZ	7:AAA:522:HOH:O	2.51	0.44
1:AAA:260:ARG:HH12	4:AAA:405:DMS:H21	1.83	0.43
1:AAA:259[B]:ARG:CZ	1:AAA:314:LEU:HB2	2.49	0.43
1:AAA:-1:HIS:CE1	7:AAA:802:HOH:O	2.69	0.42
1:AAA:97[B]:ILE:HA	1:AAA:100[B]:ARG:HD3	1.93	0.42
1:BBB:220[B]:LYS:HA	1:BBB:220[B]:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:95[B]:MET:CE	1:BBB:100[B]:ARG:HG2	2.50	0.42
1:AAA:83:ARG:NH2	5:AAA:406:GOL:H31	2.35	0.42
1:AAA:259[B]:ARG:CZ	1:AAA:314:LEU:HD13	2.50	0.42
4:AAA:404:DMS:H23	7:AAA:913:HOH:O	2.18	0.41
1:AAA:95[B]:MET:SD	1:AAA:99[B]:ARG:HG3	2.60	0.41
1:AAA:96[B]:SER:C	1:AAA:100[B]:ARG:HD2	2.41	0.41
1:BBB:95[A]:MET:HE2	7:BBB:605:HOH:O	2.20	0.41
1:AAA:101[B]:LYS:O	1:AAA:102:LEU:C	2.60	0.41
1:AAA:119[A]:MET:HE2	7:AAA:859:HOH:O	2.21	0.41
1:BBB:216:GLY:HA2	7:BBB:639:HOH:O	2.20	0.40
1:AAA:71:ASN:ND2	2:AAA:401:PLP:H2A1	2.37	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	346/324 (107%)	337 (97%)	9 (3%)	0	100	100
1	BBB	347/324 (107%)	335 (96%)	12 (4%)	0	100	100
All	All	693/648 (107%)	672 (97%)	21 (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	284/261 (109%)	281 (99%)	3 (1%)	73	41
1	BBB	285/261 (109%)	281 (99%)	4 (1%)	67	32
All	All	569/522 (109%)	562 (99%)	7 (1%)	76	37

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

Mol	Chain	Res	Type
1	AAA	68	THR
1	AAA	91[A]	MET
1	AAA	91[B]	MET
1	BBB	-1	HIS
1	BBB	68	THR
1	BBB	241[A]	LYS
1	BBB	241[B]	LYS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\#\|Z\| > 2$
4	DMS	AAA	404	-	3,3,3	0.17	0	3,3,3	0.20	0
2	PLP	BBB	401	1	15,15,16	1.26	2 (13%)	20,22,23	1.12	2 (10%)
3	Q7B	BBB	402	-	21,22,22	1.59	4 (19%)	23,32,32	1.13	1 (4%)
4	DMS	AAA	403[B]	-	3,3,3	0.20	0	3,3,3	0.38	0
2	PLP	AAA	401	1	15,15,16	1.40	3 (20%)	20,22,23	1.51	3 (15%)
4	DMS	BBB	404	-	3,3,3	0.42	0	3,3,3	0.24	0
5	GOL	AAA	406	-	5,5,5	0.13	0	5,5,5	0.44	0
5	GOL	BBB	403	-	5,5,5	0.16	0	5,5,5	0.56	0
3	Q7B	AAA	402	-	21,22,22	1.73	5 (23%)	23,32,32	1.17	4 (17%)
4	DMS	AAA	405	-	3,3,3	1.03	0	3,3,3	0.54	0
4	DMS	AAA	403[A]	-	3,3,3	0.21	0	3,3,3	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	BBB	401	1	-	0/6/6/8	0/1/1/1
3	Q7B	BBB	402	-	-	4/15/23/23	0/3/3/3
2	PLP	AAA	401	1	-	0/6/6/8	0/1/1/1
5	GOL	AAA	406	-	-	2/4/4/4	-
5	GOL	BBB	403	-	-	1/4/4/4	-
3	Q7B	AAA	402	-	-	4/15/23/23	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	402	Q7B	CAM-CAK	-4.32	1.44	1.51
3	AAA	402	Q7B	CAD-CAP	-4.29	1.45	1.51
2	BBB	401	PLP	C4A-C4	-3.92	1.43	1.51
3	BBB	402	Q7B	CAD-CAP	-3.90	1.46	1.51
2	AAA	401	PLP	C4A-C4	-2.84	1.45	1.51
3	BBB	402	Q7B	CAT-CAH	-2.77	1.41	1.51
2	AAA	401	PLP	C3-C2	-2.68	1.38	1.40
3	BBB	402	Q7B	CAM-CAK	-2.58	1.47	1.51
2	AAA	401	PLP	P-O1P	2.48	1.58	1.50
3	BBB	402	Q7B	CAN-CAO	-2.44	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	402	Q7B	CAM-CAO	-2.25	1.52	1.55
3	AAA	402	Q7B	CAL-CAK	2.22	1.43	1.38
2	BBB	401	PLP	C3-C2	2.17	1.43	1.40
3	AAA	402	Q7B	CAT-CAH	-2.16	1.43	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	401	PLP	O4P-C5A-C5	3.53	116.07	109.35
2	AAA	401	PLP	C4A-C4-C5	-2.89	117.96	120.94
3	AAA	402	Q7B	CAC-CAD-CAP	-2.74	115.59	121.08
3	AAA	402	Q7B	CAM-CAK-CAJ	-2.54	117.68	121.07
2	BBB	401	PLP	O3-C3-C4	2.43	124.49	118.10
2	AAA	401	PLP	C6-C5-C4	-2.42	116.25	118.16
2	BBB	401	PLP	O4P-C5A-C5	2.32	113.77	109.35
3	AAA	402	Q7B	CAE-CAD-CAP	2.29	125.65	121.08
3	AAA	402	Q7B	CAM-CAK-CAL	2.20	124.01	121.07
3	BBB	402	Q7B	OAR-CAQ-CAO	-2.08	117.19	123.07

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	402	Q7B	CAN-CAO-CAQ-OAS
3	AAA	402	Q7B	CAN-CAO-CAQ-OAR
3	AAA	402	Q7B	CAL-CAK-CAM-CAO
3	BBB	402	Q7B	CAJ-CAK-CAM-CAO
3	BBB	402	Q7B	CAL-CAK-CAM-CAO
3	AAA	402	Q7B	CAJ-CAK-CAM-CAO
5	AAA	406	GOL	C1-C2-C3-O3
3	BBB	402	Q7B	CAN-CAO-CAQ-OAS
3	BBB	402	Q7B	CAN-CAO-CAQ-OAR
5	AAA	406	GOL	O2-C2-C3-O3
5	BBB	403	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	404	DMS	2	0
2	BBB	401	PLP	1	0

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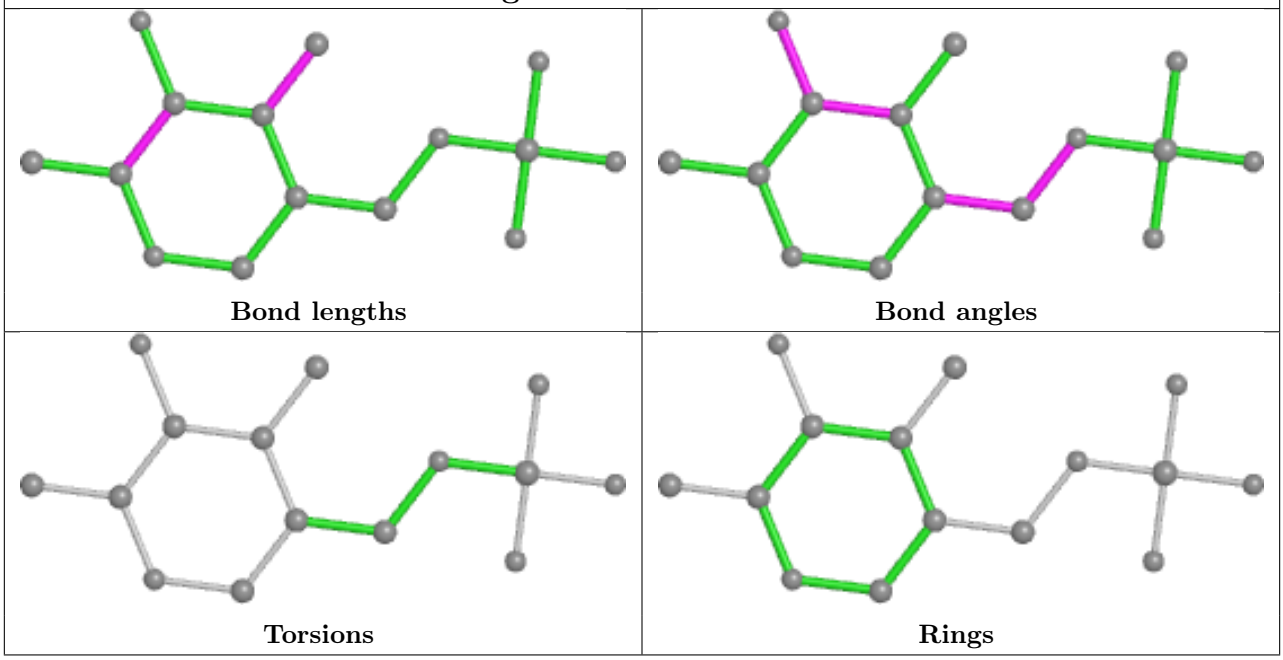
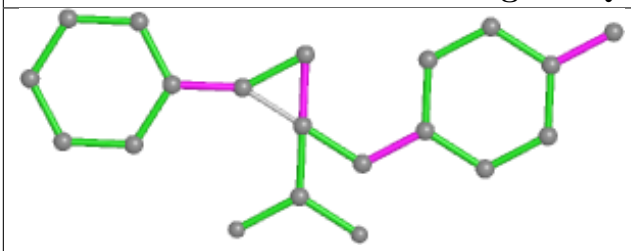
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	PLP	1	0
5	AAA	406	GOL	8	0
5	BBB	403	GOL	2	0
4	AAA	405	DMS	2	0
4	AAA	403[A]	DMS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

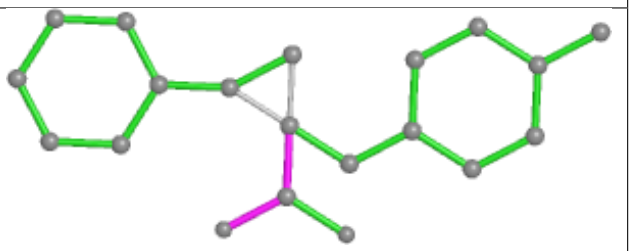
Ligand PLP BBB 401



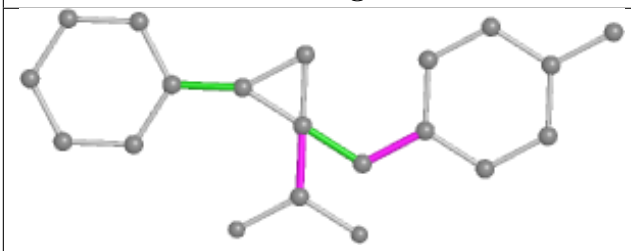
Ligand Q7B BBB 402



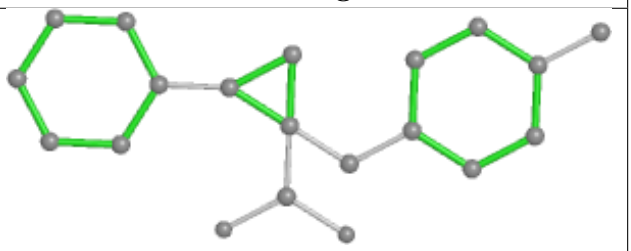
Bond lengths



Bond angles

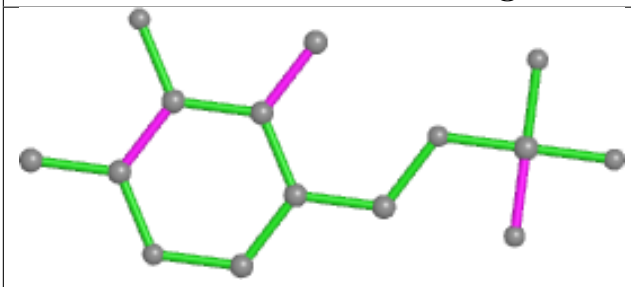


Torsions

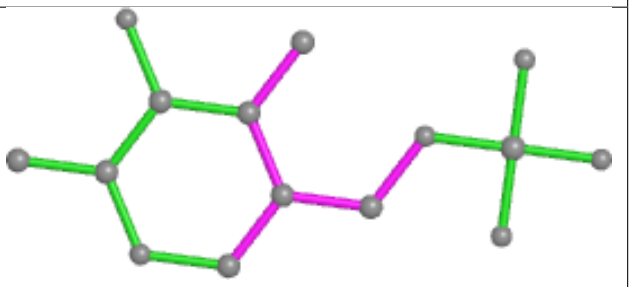


Rings

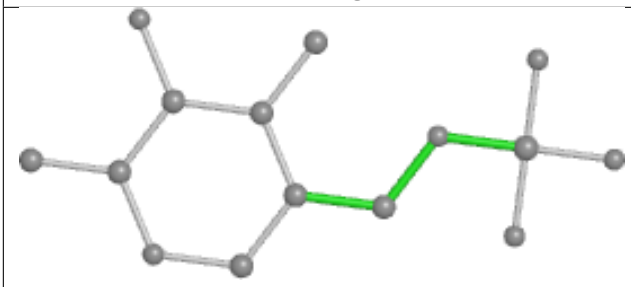
Ligand PLP AAA 401



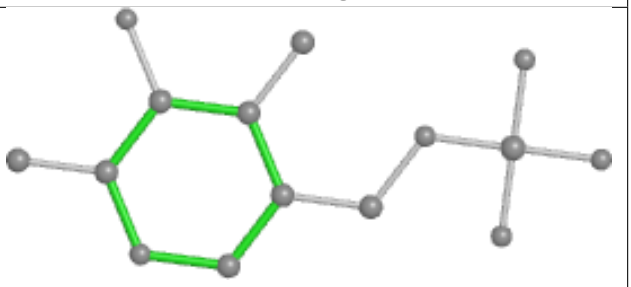
Bond lengths



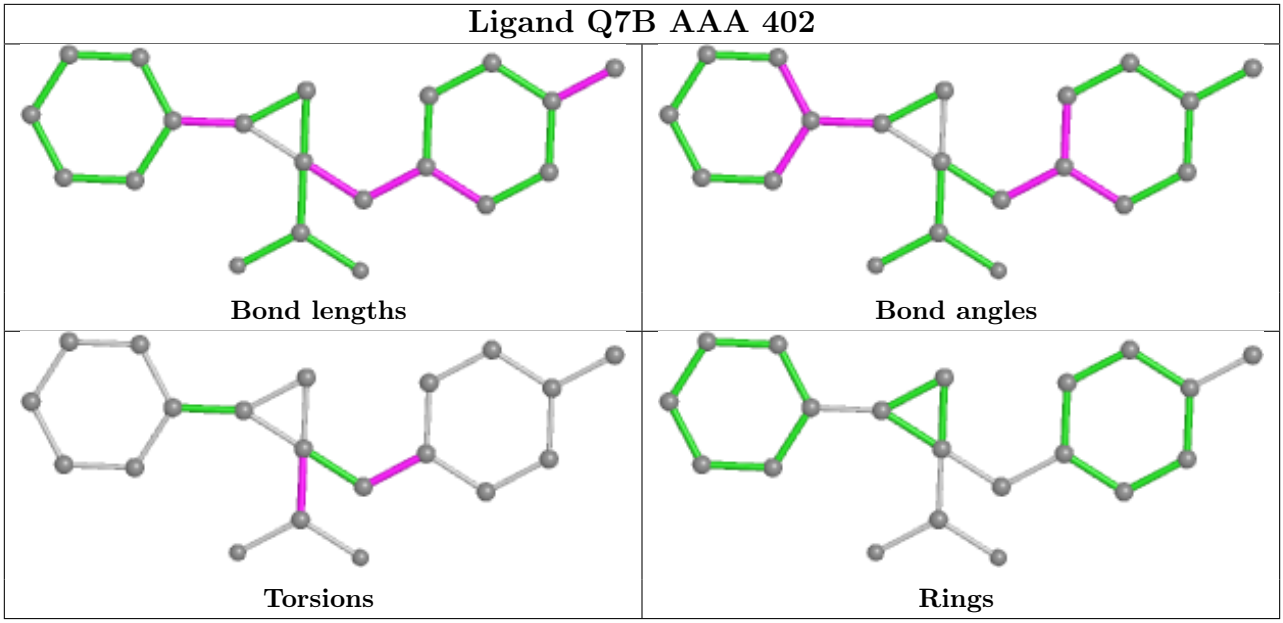
Bond angles



Torsions



Rings



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	321/324 (99%)	0.25	17 (5%)	26	26	11, 15, 28, 43	13 (4%)
1	BBB	318/324 (98%)	0.13	14 (4%)	34	34	10, 14, 28, 42	10 (3%)
All	All	639/648 (98%)	0.19	31 (4%)	29	29	10, 14, 28, 43	23 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	0	MET	6.4
1	BBB	315	PHE	5.4
1	BBB	0	MET	4.7
1	BBB	313	ASP	4.0
1	BBB	-1	HIS	3.7
1	BBB	60	PRO	3.5
1	AAA	216	GLY	3.4
1	AAA	313	ASP	3.3
1	BBB	131	ALA	3.2
1	AAA	116	ALA	3.2
1	AAA	312	ALA	3.1
1	BBB	135	GLN	3.0
1	AAA	-1	HIS	3.0
1	AAA	97[A]	ILE	3.0
1	AAA	131	ALA	2.9
1	AAA	218	GLU	2.9
1	AAA	314	LEU	2.9
1	BBB	1	SER	2.7
1	BBB	61	GLY	2.7
1	AAA	316	THR	2.7
1	BBB	314	LEU	2.6
1	BBB	316	THR	2.5
1	AAA	1	SER	2.5
1	BBB	124[A]	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	AAA	315	PHE	2.4
1	AAA	219	ILE	2.4
1	BBB	134	PRO	2.3
1	AAA	75	ALA	2.3
1	AAA	215	ALA	2.1
1	AAA	124[A]	GLN	2.1
1	BBB	137	TYR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

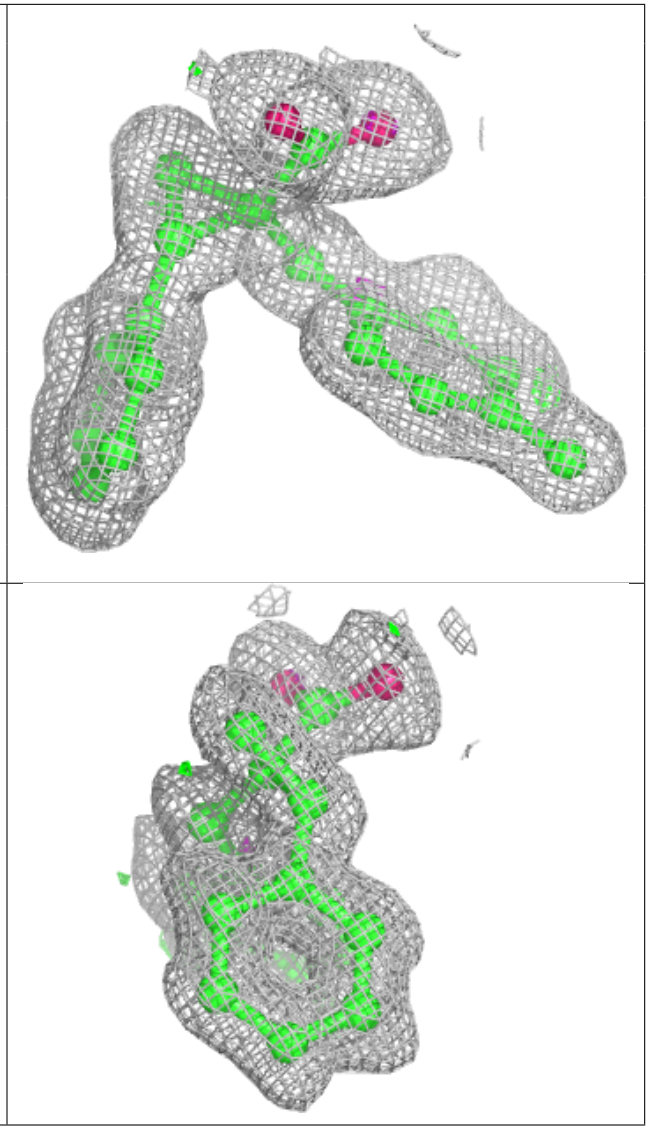
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	AAA	406	6/6	0.83	0.21	19,23,28,28	6
5	GOL	BBB	403	6/6	0.83	0.23	25,30,32,37	6
4	DMS	AAA	405	4/4	0.92	0.14	21,24,31,32	4
4	DMS	BBB	404	4/4	0.96	0.12	24,27,32,33	4
3	Q7B	AAA	402	20/20	0.97	0.07	12,13,14,15	0
4	DMS	AAA	403[A]	4/4	0.97	0.09	29,40,44,45	4
4	DMS	AAA	403[B]	4/4	0.97	0.09	20,20,21,24	4
4	DMS	AAA	404	4/4	0.97	0.15	36,38,38,39	4
3	Q7B	BBB	402	20/20	0.98	0.08	10,12,14,18	0
2	PLP	AAA	401	15/16	0.98	0.08	10,11,18,21	0
6	CO	AAA	407	1/1	0.98	0.04	27,27,27,27	1
2	PLP	BBB	401	15/16	0.99	0.06	9,10,12,12	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.

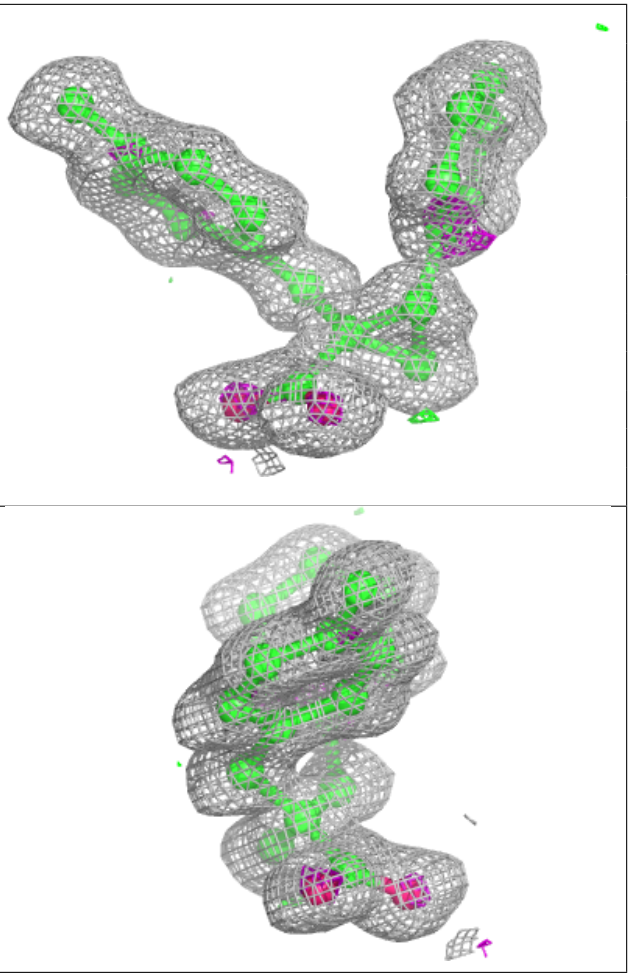
Electron density around Q7B AAA 402:

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



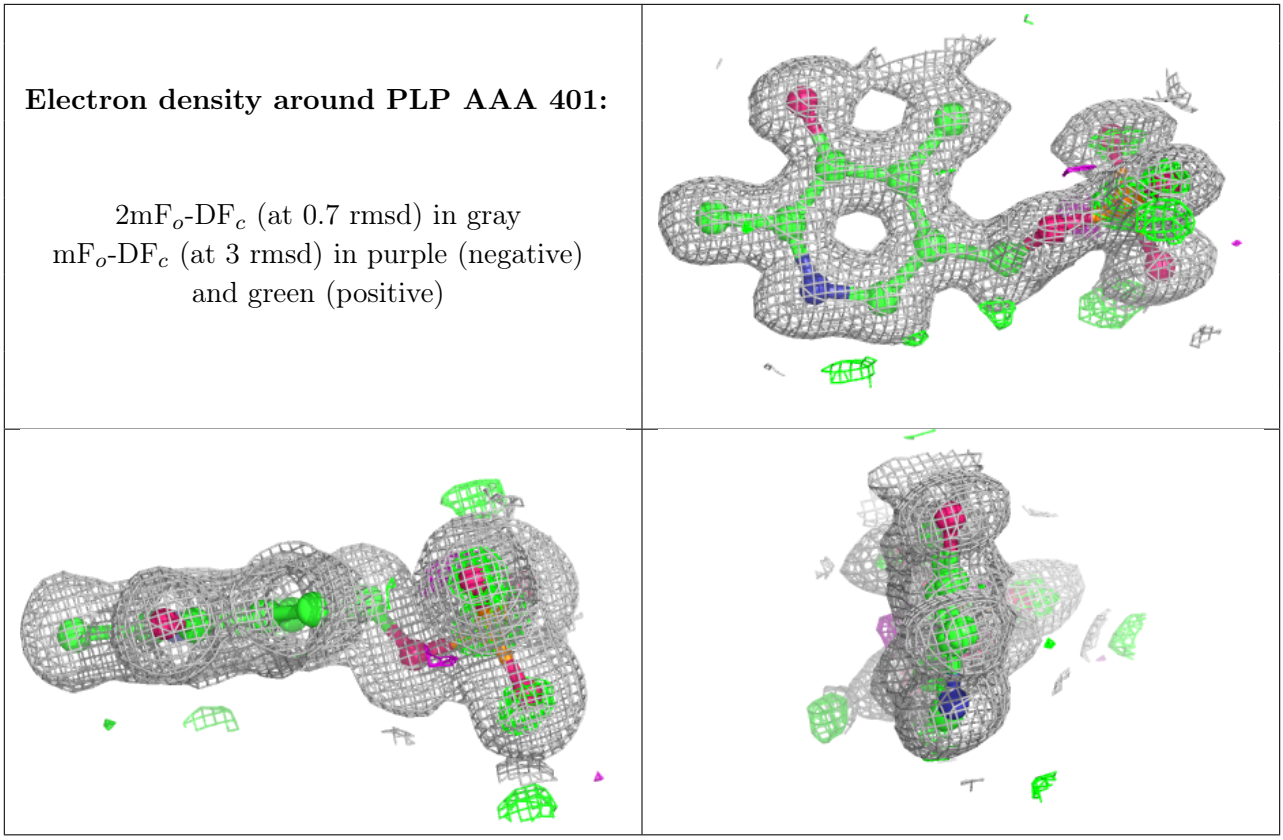
Electron density around Q7B BBB 402:

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



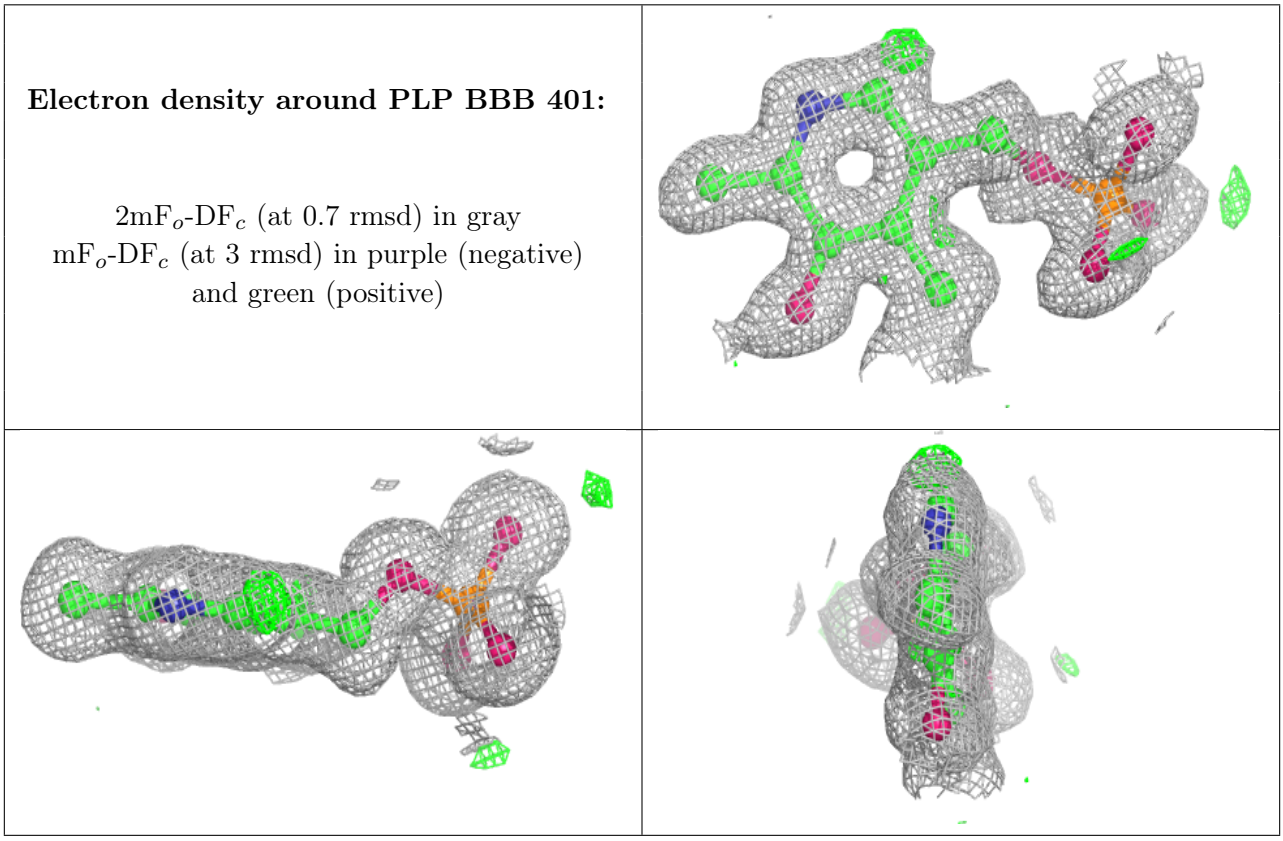
Electron density around PLP AAA 401:

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



Electron density around PLP BBB 401:

$2mF_o$-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.