Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 07:15 pm GMT

PDB ID	:	6ZSP
Title	:	Human serine racemase bound to ATP and malonate.
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Deposited on	:	2020-07-16
Resolution	:	1.60 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:

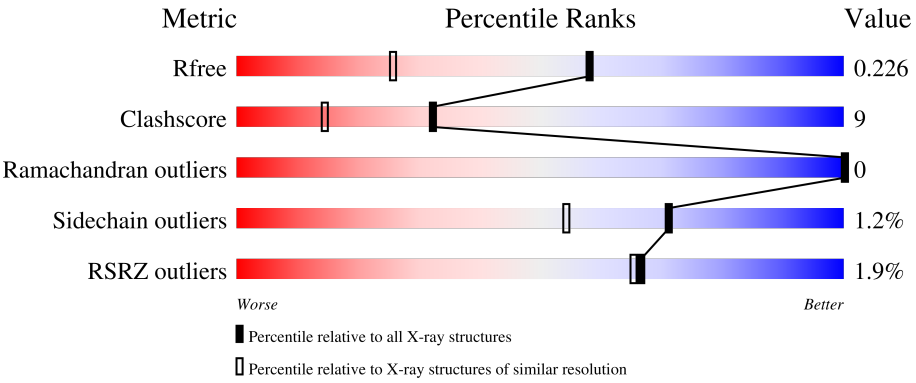
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

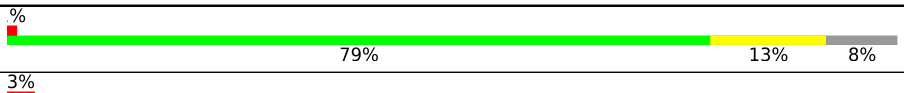
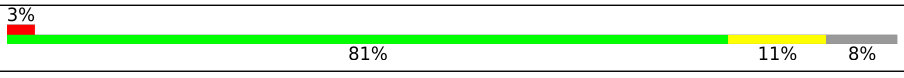
The reported resolution of this entry is 1.60 Å.

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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	347	
1	BBB	347	

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	IMD	AAA	401[B]	-	-	X	-
6	GOL	BBB	502[B]	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5874 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.

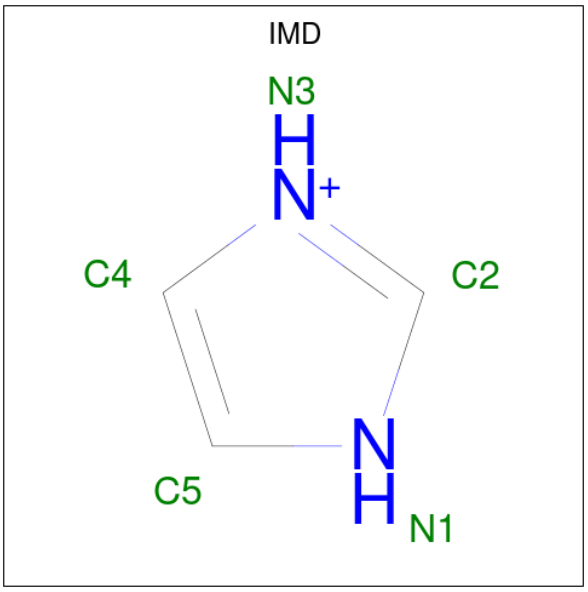
- Molecule 1 is a protein called Serine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	320	Total	C	N	O	P	S	0	34	0
			2680	1715	449	504	1	11			
1	BBB	319	Total	C	N	O	P	S	0	32	0
			2683	1711	450	510	1	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	345	HIS	-	expression tag	UNP Q9GZT4
AAA	346	HIS	-	expression tag	UNP Q9GZT4
AAA	347	GLN	-	expression tag	UNP Q9GZT4
BBB	2	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	6	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	341	HIS	-	expression tag	UNP Q9GZT4
BBB	342	HIS	-	expression tag	UNP Q9GZT4
BBB	343	HIS	-	expression tag	UNP Q9GZT4
BBB	344	HIS	-	expression tag	UNP Q9GZT4
BBB	345	HIS	-	expression tag	UNP Q9GZT4
BBB	346	HIS	-	expression tag	UNP Q9GZT4
BBB	347	GLN	-	expression tag	UNP Q9GZT4

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

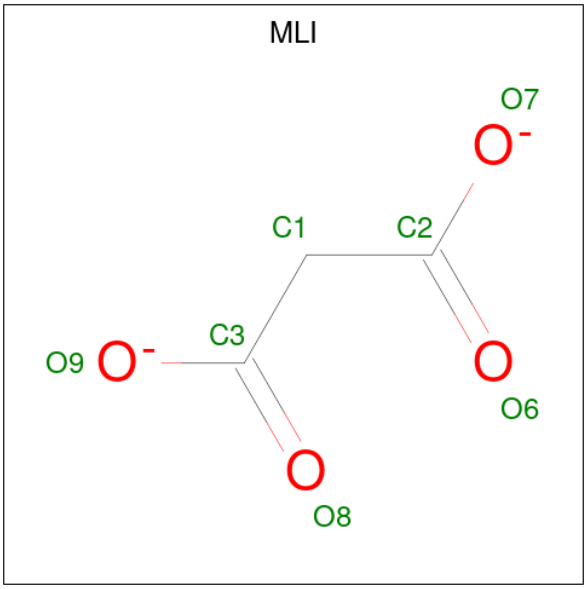


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C N 10 6 4	0	1

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

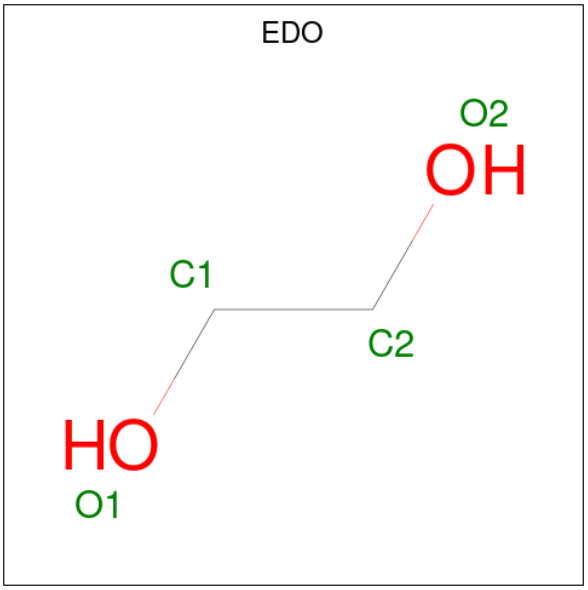
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Mg 1 1	0	0
3	BBB	3	Total Mg 3 3	0	0

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



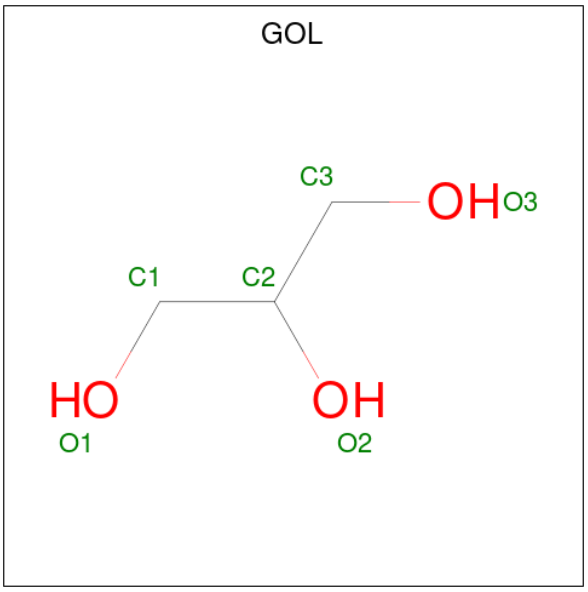
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 7 3 4	0	0
4	BBB	1	Total C O 7 3 4	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



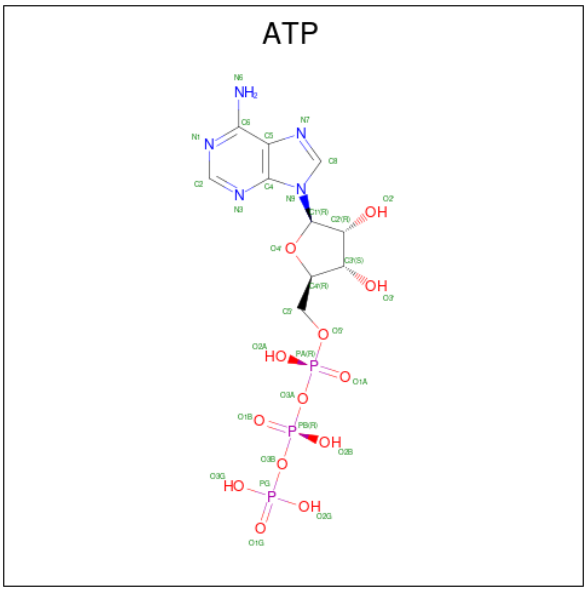
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	1
5	BBB	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	BBB	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	BBB	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is water.

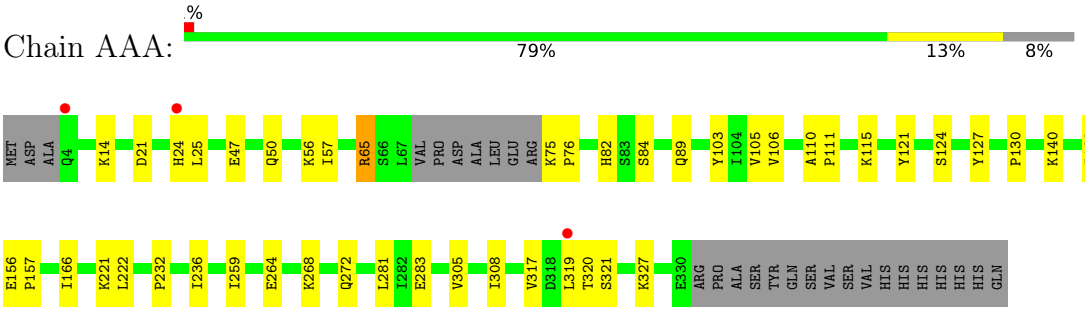
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	186	Total	O	0	11
			197	197		
8	BBB	182	Total	O	0	8
			188	188		

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.

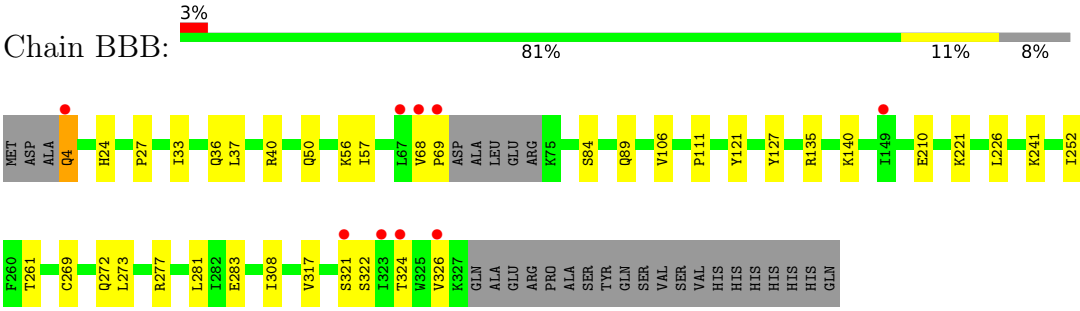
• Molecule 1: Serine racemase

Chain AAA:



• Molecule 1: Serine racemase

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	53.94Å 81.19Å 134.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.65 – 1.60 42.61 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.65-1.60) 96.0 (42.61-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.192 , 0.226 0.192 , 0.226	Depositor DCC
R_{free} test set	3722 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5874	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3463e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, LLP, MLI, IMD, ATP, MG, EDO

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	0.38	0/2713	0.65	0/3691
1	BBB	0.36	0/2711	0.64	0/3687
All	All	0.37	0/5424	0.65	0/7378

There are no bond length outliers.

There are no bond angle outliers.

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	2680	0	2686	53	0
1	BBB	2683	0	2712	42	0
2	AAA	10	0	10	5	0
3	AAA	1	0	0	0	0
3	BBB	3	0	0	0	0
4	AAA	7	0	2	0	0
4	BBB	7	0	2	0	0
5	AAA	12	0	18	0	0
5	BBB	12	0	18	0	0
6	BBB	12	0	16	5	0
7	BBB	62	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AAA	197	0	0	20	0
8	BBB	188	0	0	7	0
All	All	5874	0	5488	98	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 9.

All (98) 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:65[A]:ARG:HG2	8:AAA:681[A]:HOH:O	1.21	1.36
1:AAA:24[B]:HIS:HB3	8:AAA:621[B]:HOH:O	1.18	1.28
1:BBB:68:VAL:HG13	1:BBB:69:PRO:HD3	1.23	1.20
1:BBB:269[B]:CYS:SG	8:BBB:782[B]:HOH:O	2.14	1.05
1:BBB:135:ARG:HH11	6:BBB:502[B]:GOL:H11	1.29	0.98
1:BBB:68:VAL:CG1	1:BBB:69:PRO:HD3	1.94	0.96
1:BBB:4[A]:GLN:HA	1:BBB:4[A]:GLN:OE1	1.68	0.94
1:BBB:24[A]:HIS:NE2	8:BBB:601:HOH:O	2.01	0.92
1:BBB:4[B]:GLN:HE21	1:BBB:4[B]:GLN:HA	1.31	0.92
2:AAA:401[B]:IMD:N3	8:AAA:504[B]:HOH:O	1.82	0.88
1:BBB:24[A]:HIS:CD2	8:BBB:601:HOH:O	2.28	0.86
1:AAA:24[B]:HIS:O	8:AAA:501:HOH:O	1.99	0.80
1:BBB:4[B]:GLN:HA	1:BBB:4[B]:GLN:NE2	1.92	0.80
1:AAA:50[A]:GLN:HG3	1:AAA:57:ILE:HG21	1.65	0.78
1:AAA:65[A]:ARG:HD3	8:AAA:534:HOH:O	1.84	0.76
1:AAA:281[B]:LEU:HD21	1:BBB:281:LEU:HD13	1.67	0.76
1:AAA:50[A]:GLN:HG3	1:AAA:57:ILE:CG2	2.16	0.75
1:AAA:222[B]:LEU:HD23	1:AAA:222[B]:LEU:O	1.87	0.75
1:AAA:65[A]:ARG:CG	8:AAA:681[A]:HOH:O	1.99	0.74
1:AAA:65[A]:ARG:HG2	8:AAA:654[A]:HOH:O	1.87	0.74
1:AAA:24[C]:HIS:O	8:AAA:501:HOH:O	2.06	0.73
1:AAA:24[A]:HIS:O	8:AAA:501:HOH:O	2.06	0.72
1:AAA:76[B]:PRO:HB3	1:AAA:149[B]:ILE:CD1	2.22	0.70
1:BBB:68:VAL:HG13	1:BBB:69:PRO:CD	2.12	0.69
1:BBB:33:ILE:HD13	1:BBB:277[B]:ARG:HH11	1.56	0.69
1:AAA:236[B]:ILE:HD13	1:AAA:268:LYS:HE3	1.75	0.68
1:BBB:322:SER:O	1:BBB:326[A]:VAL:HG23	1.95	0.66
1:BBB:111:PRO:HD3	8:BBB:726[A]:HOH:O	1.95	0.66
1:AAA:319[B]:LEU:CD1	1:AAA:319[B]:LEU:O	2.44	0.66
1:AAA:236[B]:ILE:CD1	1:AAA:268:LYS:HG3	2.27	0.65
1:BBB:322:SER:O	1:BBB:326[B]:VAL:HG13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:221[B]:LYS:HG3	1:BBB:259[B]:ILE:HD11	1.82	0.62
1:AAA:24[B]:HIS:CB	8:AAA:621[B]:HOH:O	1.99	0.61
1:AAA:76[B]:PRO:HB3	1:AAA:149[B]:ILE:HD11	1.83	0.61
1:AAA:319[B]:LEU:O	1:AAA:319[B]:LEU:HD13	2.03	0.59
1:BBB:68:VAL:HG11	8:BBB:750:HOH:O	2.02	0.59
1:BBB:4[A]:GLN:OE1	1:BBB:4[A]:GLN:CA	2.48	0.58
1:AAA:222[B]:LEU:HD23	1:AAA:222[B]:LEU:C	2.25	0.57
1:BBB:84:SER:HB2	8:BBB:726[B]:HOH:O	2.05	0.56
1:BBB:89[A]:GLN:HE21	1:BBB:121:TYR:HE2	1.54	0.56
1:BBB:40:ARG:HD2	1:BBB:308:ILE:CD1	2.36	0.56
1:AAA:236[B]:ILE:HG21	1:AAA:268:LYS:HE3	1.88	0.55
2:AAA:401[B]:IMD:H5	8:AAA:682:HOH:O	2.07	0.54
2:AAA:401[A]:IMD:N1	8:AAA:504[A]:HOH:O	2.28	0.54
1:BBB:241:LYS:HB2	6:BBB:502[B]:GOL:H2	1.90	0.54
1:AAA:111:PRO:HD2	8:AAA:617[B]:HOH:O	2.07	0.54
1:AAA:21[B]:ASP:HB3	8:AAA:662[B]:HOH:O	2.07	0.53
1:AAA:319[B]:LEU:O	1:AAA:319[B]:LEU:HD12	2.07	0.53
1:AAA:236[B]:ILE:HD13	1:AAA:268:LYS:HG3	1.90	0.53
1:AAA:84:SER:HB2	8:AAA:617[A]:HOH:O	2.09	0.53
1:AAA:110:ALA:O	1:AAA:115:LYS:HE3	2.09	0.52
1:AAA:24[A]:HIS:HB2	8:AAA:537[A]:HOH:O	2.10	0.52
1:AAA:236[B]:ILE:HG12	1:AAA:264:GLU:OE2	2.10	0.52
1:BBB:33:ILE:HD13	1:BBB:277[B]:ARG:NH1	2.25	0.51
1:BBB:135:ARG:NH1	6:BBB:502[B]:GOL:H11	2.12	0.51
1:BBB:40:ARG:HD2	1:BBB:308:ILE:HD11	1.91	0.51
1:AAA:140[B]:LYS:HB2	1:AAA:140[B]:LYS:NZ	2.27	0.50
1:AAA:50[A]:GLN:HG3	1:AAA:57:ILE:HG22	1.93	0.49
1:BBB:241:LYS:CB	6:BBB:502[B]:GOL:H2	2.44	0.48
1:BBB:283:GLU:HA	1:BBB:317:VAL:HB	1.96	0.48
1:AAA:14[B]:LYS:HG3	8:AAA:594:HOH:O	2.14	0.48
1:BBB:50:GLN:HG3	1:BBB:57:ILE:CG2	2.44	0.48
1:BBB:321:SER:O	1:BBB:324:THR:HG22	2.14	0.48
1:BBB:135:ARG:HH11	6:BBB:502[B]:GOL:C1	2.13	0.47
1:BBB:37:LEU:CD1	1:BBB:273:LEU:HD21	2.45	0.47
1:AAA:76[B]:PRO:HB3	1:AAA:149[B]:ILE:HD12	1.98	0.46
1:BBB:33:ILE:HG21	1:BBB:277[B]:ARG:NH1	2.31	0.46
1:BBB:36[A]:GLN:HG3	8:BBB:677:HOH:O	2.14	0.46
1:BBB:140[B]:LYS:NZ	1:BBB:140[B]:LYS:HB2	2.31	0.46
1:AAA:283:GLU:HA	1:AAA:317:VAL:HB	1.98	0.46
2:AAA:401[B]:IMD:C5	1:BBB:27:PRO:HG3	2.46	0.46
1:AAA:50[A]:GLN:CG	1:AAA:57:ILE:CG2	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:47[B]:GLU:OE2	1:AAA:166:ILE:HG12	2.17	0.45
1:AAA:130:PRO:O	1:AAA:232:PRO:HB3	2.17	0.44
1:AAA:140[B]:LYS:HB2	1:AAA:140[B]:LYS:HZ1	1.82	0.44
1:AAA:236[B]:ILE:HG21	1:AAA:268:LYS:CE	2.47	0.44
1:BBB:50:GLN:HG3	1:BBB:57:ILE:HG21	2.00	0.44
1:AAA:140[B]:LYS:NZ	1:AAA:140[B]:LYS:CB	2.81	0.43
1:AAA:75:LYS:N	1:AAA:76[B]:PRO:HD2	2.32	0.43
1:BBB:210:GLU:O	1:BBB:261:THR:HA	2.18	0.43
1:AAA:221[A]:LYS:HD2	1:AAA:259:ILE:HD11	2.00	0.43
1:AAA:89[A]:GLN:HE21	1:AAA:121:TYR:HE2	1.65	0.43
1:AAA:156:GLU:CD	1:AAA:157[B]:PRO:HD2	2.39	0.43
1:BBB:106:VAL:O	1:BBB:127:TYR:HA	2.19	0.43
1:AAA:24[C]:HIS:CD2	8:AAA:651:HOH:O	2.71	0.42
1:AAA:305:VAL:HG12	1:AAA:308[B]:ILE:HD11	2.00	0.42
1:AAA:75:LYS:N	1:AAA:76[A]:PRO:HD2	2.33	0.42
1:AAA:106:VAL:O	1:AAA:127:TYR:HA	2.19	0.42
1:AAA:272:GLN:HE22	1:AAA:327:LYS:H	1.68	0.42
1:AAA:305:VAL:HG12	1:AAA:308[B]:ILE:CD1	2.50	0.42
2:AAA:401[B]:IMD:C2	8:AAA:504[B]:HOH:O	2.49	0.41
1:AAA:272:GLN:NE2	8:AAA:512:HOH:O	2.52	0.41
1:BBB:221[B]:LYS:CE	1:BBB:252:ILE:O	2.69	0.41
1:BBB:221[B]:LYS:HE2	1:BBB:252:ILE:O	2.20	0.40
1:BBB:37:LEU:HD12	1:BBB:273:LEU:HD21	2.03	0.40
1:AAA:82:HIS:HA	1:AAA:105:VAL:O	2.21	0.40
1:AAA:103[B]:TYR:CD2	1:AAA:124[B]:SER:HB3	2.57	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	350/347 (101%)	344 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	BBB	346/347 (100%)	339 (98%)	7 (2%)	0	100 100
All	All	696/694 (100%)	683 (98%)	13 (2%)	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	287/291 (99%)	281 (98%)	6 (2%)	53 29
1	BBB	294/291 (101%)	291 (99%)	3 (1%)	76 61
All	All	581/582 (100%)	572 (98%)	9 (2%)	71 44

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	25[A]	LEU
1	AAA	25[B]	LEU
1	AAA	65[A]	ARG
1	AAA	65[B]	ARG
1	AAA	320	THR
1	AAA	321	SER
1	BBB	4[A]	GLN
1	BBB	4[B]	GLN
1	BBB	226	LEU

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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	BBB	56	1	23,24,25	0.58	0	25,32,34	0.88	1 (4%)
1	LLP	AAA	56	1	23,24,25	0.58	0	25,32,34	0.94	1 (4%)

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
1	LLP	BBB	56	1	-	2/16/17/19	0/1/1/1
1	LLP	AAA	56	1	-	3/16/17/19	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	56	LLP	OP4-C5'-C5	2.42	113.97	109.35
1	AAA	56	LLP	OP4-C5'-C5	2.25	113.63	109.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	56	LLP	C4-C4'-NZ-CE
1	BBB	56	LLP	C4-C4'-NZ-CE
1	BBB	56	LLP	CG-CD-CE-NZ
1	AAA	56	LLP	C6-C5-C5'-OP4
1	AAA	56	LLP	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	IMD	AAA	401[A]	-	3,5,5	0.31	0	4,5,5	0.72	0
7	ATP	BBB	508	3	26,33,33	0.66	0	31,52,52	0.87	1 (3%)
5	EDO	BBB	509[A]	-	3,3,3	0.03	0	2,2,2	0.16	0
7	ATP	BBB	507	3	26,33,33	0.67	0	31,52,52	0.81	1 (3%)
5	EDO	BBB	510	-	3,3,3	0.11	0	2,2,2	0.22	0
6	GOL	BBB	501	-	5,5,5	0.09	0	5,5,5	0.34	0
6	GOL	BBB	502[B]	-	5,5,5	0.09	0	5,5,5	0.36	0
4	MLI	AAA	403	-	6,6,6	1.43	0	7,7,7	0.94	0
2	IMD	AAA	401[B]	-	3,5,5	0.32	0	4,5,5	0.67	0
4	MLI	BBB	506	-	6,6,6	1.35	0	7,7,7	1.01	0
5	EDO	AAA	405	-	3,3,3	0.03	0	2,2,2	0.16	0
5	EDO	AAA	404	-	3,3,3	0.04	0	2,2,2	0.15	0
5	EDO	AAA	406	-	3,3,3	0.07	0	2,2,2	0.32	0
5	EDO	BBB	511	-	3,3,3	0.06	0	2,2,2	0.11	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
7	ATP	BBB	508	3	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	AAA	401[A]	-	-	-	0/1/1/1
5	EDO	BBB	509[A]	-	-	1/1/1/1	-
7	ATP	BBB	507	3	-	0/18/38/38	0/3/3/3
5	EDO	BBB	510	-	-	0/1/1/1	-
6	GOL	BBB	501	-	-	2/4/4/4	-
6	GOL	BBB	502[B]	-	-	2/4/4/4	-
4	MLI	AAA	403	-	-	0/4/4/4	-
2	IMD	AAA	401[B]	-	-	-	0/1/1/1
4	MLI	BBB	506	-	-	0/4/4/4	-
5	EDO	AAA	405	-	-	0/1/1/1	-
5	EDO	AAA	404	-	-	1/1/1/1	-
5	EDO	AAA	406	-	-	0/1/1/1	-
5	EDO	BBB	511	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	BBB	507	ATP	C5-C6-N6	2.02	123.42	120.35
7	BBB	508	ATP	C5-C6-N6	2.02	123.42	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	BBB	501	GOL	O1-C1-C2-O2
6	BBB	501	GOL	O1-C1-C2-C3
5	AAA	404	EDO	O1-C1-C2-O2
5	BBB	509[A]	EDO	O1-C1-C2-O2
6	BBB	502[B]	GOL	C1-C2-C3-O3
6	BBB	502[B]	GOL	O1-C1-C2-C3

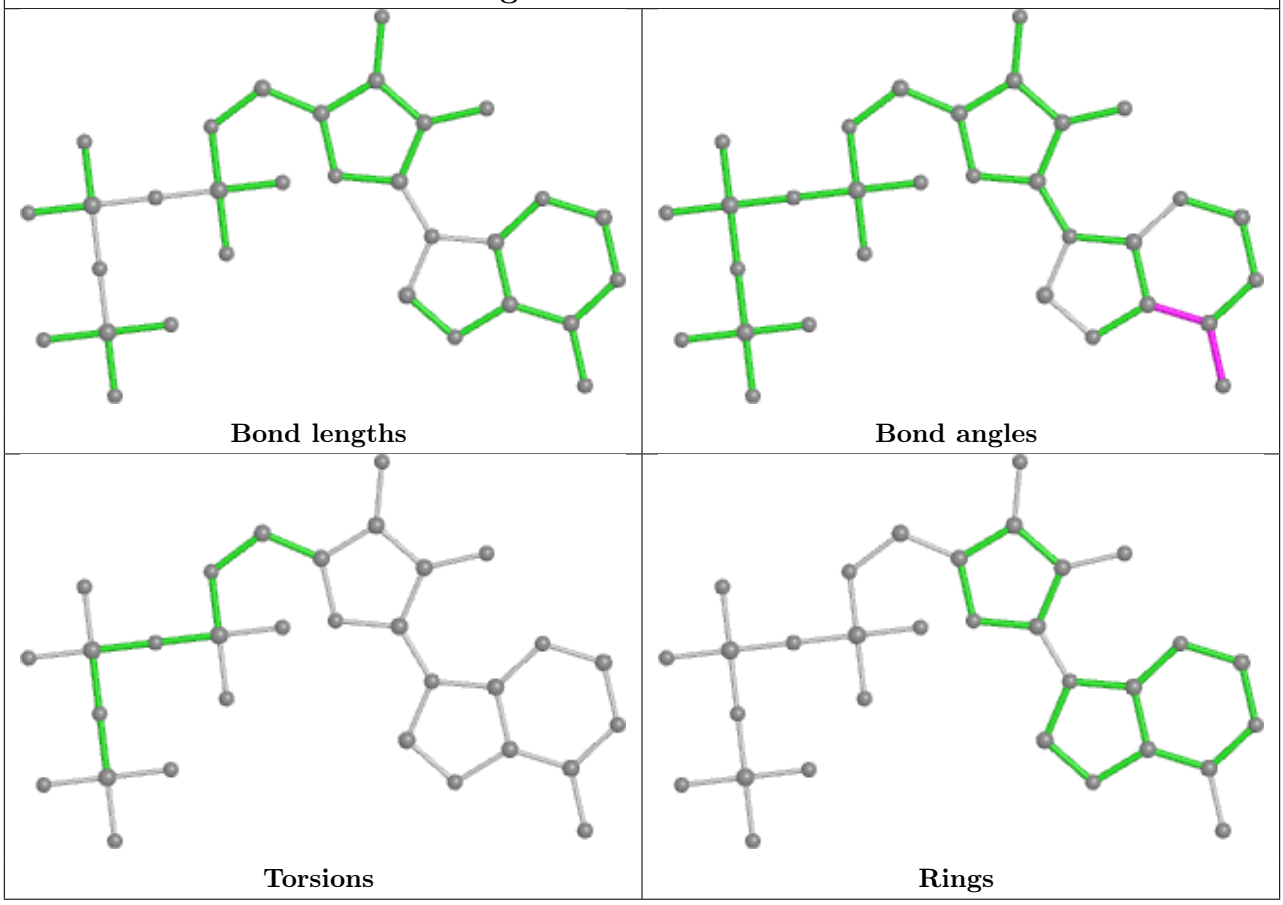
There are no ring outliers.

3 monomers are involved in 10 short contacts:

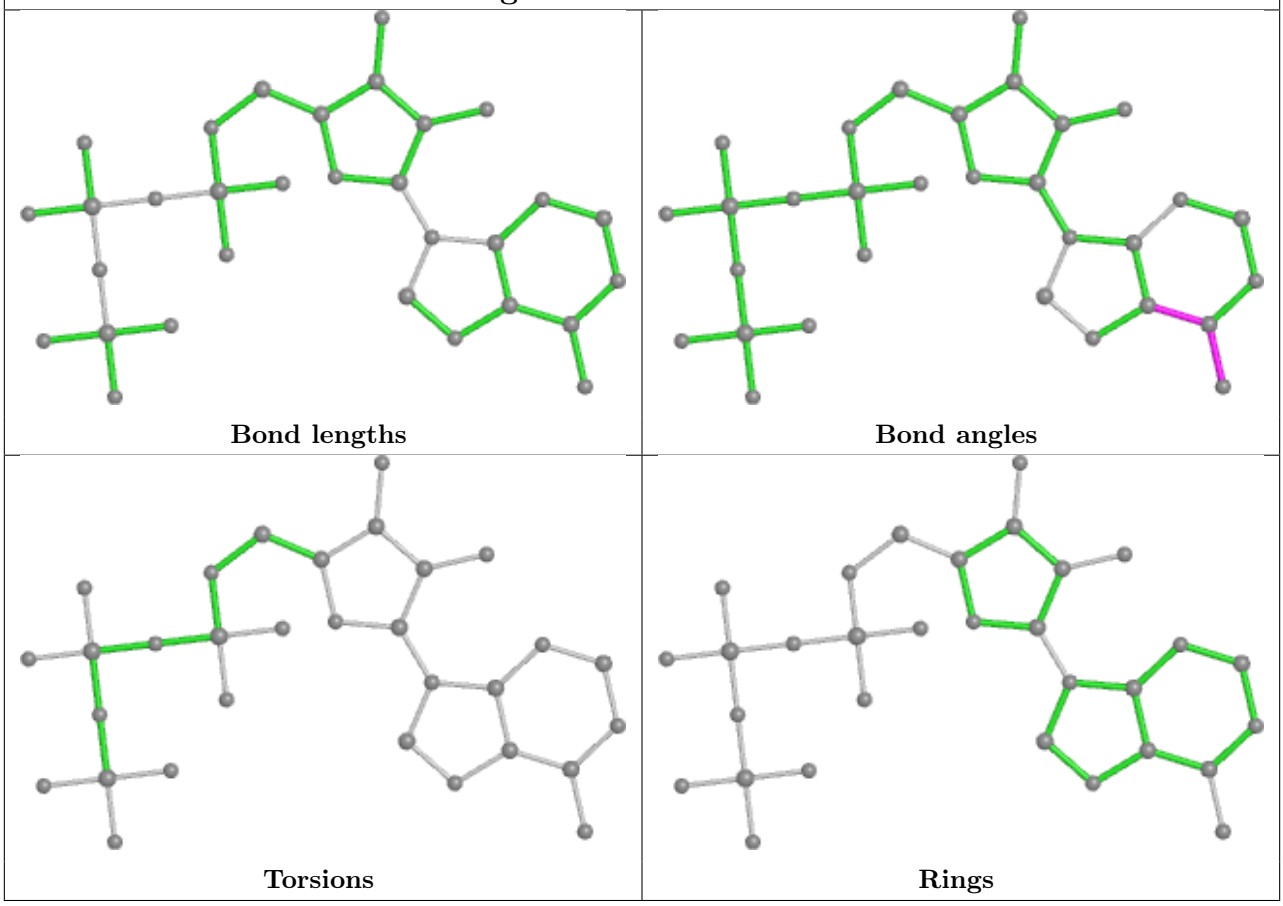
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401[A]	IMD	1	0
6	BBB	502[B]	GOL	5	0
2	AAA	401[B]	IMD	4	0

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 ATP BBB 508



Ligand ATP BBB 507



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

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	AAA	319/347 (91%)	-0.41	3 (0%)	84	84	10, 18, 38, 65	0
1	BBB	318/347 (91%)	-0.30	9 (2%)	53	50	11, 18, 38, 79	0
All	All	637/694 (91%)	-0.35	12 (1%)	66	65	10, 18, 38, 79	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	68	VAL	6.4
1	BBB	69	PRO	5.4
1	BBB	67	LEU	4.6
1	AAA	319[A]	LEU	3.4
1	BBB	4[A]	GLN	3.3
1	BBB	326[A]	VAL	2.7
1	AAA	4	GLN	2.5
1	BBB	324	THR	2.5
1	BBB	323	ILE	2.5
1	BBB	321	SER	2.4
1	AAA	24[A]	HIS	2.2
1	BBB	149	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	LLP	AAA	56	24/25	0.98	0.05	8,10,12,12	0
1	LLP	BBB	56	24/25	0.98	0.06	10,12,13,14	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

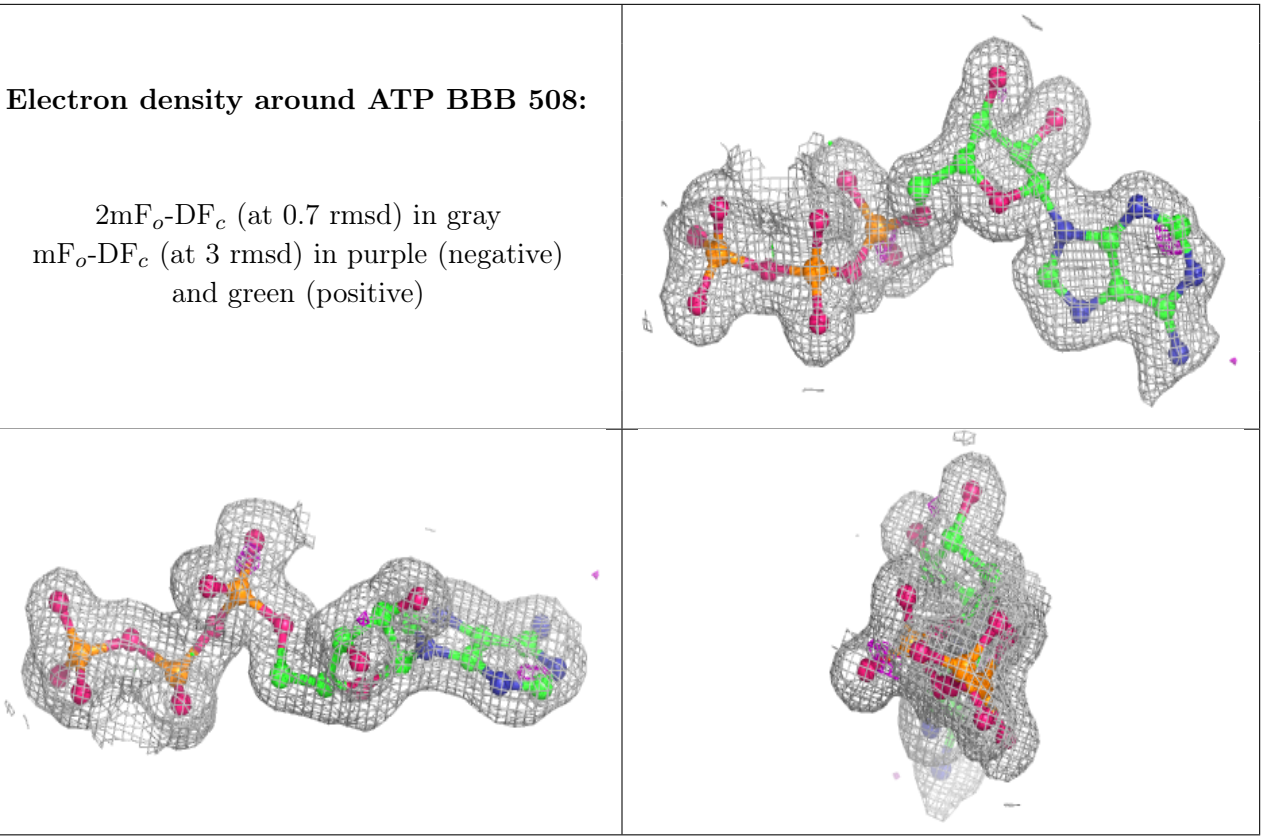
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	EDO	AAA	406	4/4	0.64	0.23	45,46,47,49	0
6	GOL	BBB	501	6/6	0.76	0.29	49,51,53,59	0
5	EDO	AAA	405	4/4	0.77	0.14	41,42,44,46	0
5	EDO	BBB	511	4/4	0.80	0.16	46,50,50,55	0
5	EDO	BBB	510	4/4	0.82	0.18	34,36,37,39	0
2	IMD	AAA	401[A]	5/5	0.82	0.22	39,40,41,41	5
2	IMD	AAA	401[B]	5/5	0.82	0.22	42,42,43,43	5
5	EDO	BBB	509[A]	4/4	0.90	0.12	29,29,29,32	4
6	GOL	BBB	502[B]	6/6	0.91	0.21	25,27,28,29	6
5	EDO	AAA	404	4/4	0.93	0.08	29,29,30,33	0
4	MLI	AAA	403	7/7	0.97	0.07	14,15,17,17	0
7	ATP	BBB	508	31/31	0.97	0.07	14,18,30,31	0
7	ATP	BBB	507	31/31	0.98	0.06	13,15,28,29	0
4	MLI	BBB	506	7/7	0.98	0.05	16,17,17,17	0
3	MG	AAA	402	1/1	0.99	0.03	15,15,15,15	0
3	MG	BBB	504	1/1	0.99	0.04	17,17,17,17	0
3	MG	BBB	505	1/1	0.99	0.04	13,13,13,13	0
3	MG	BBB	503	1/1	1.00	0.09	13,13,13,13	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.

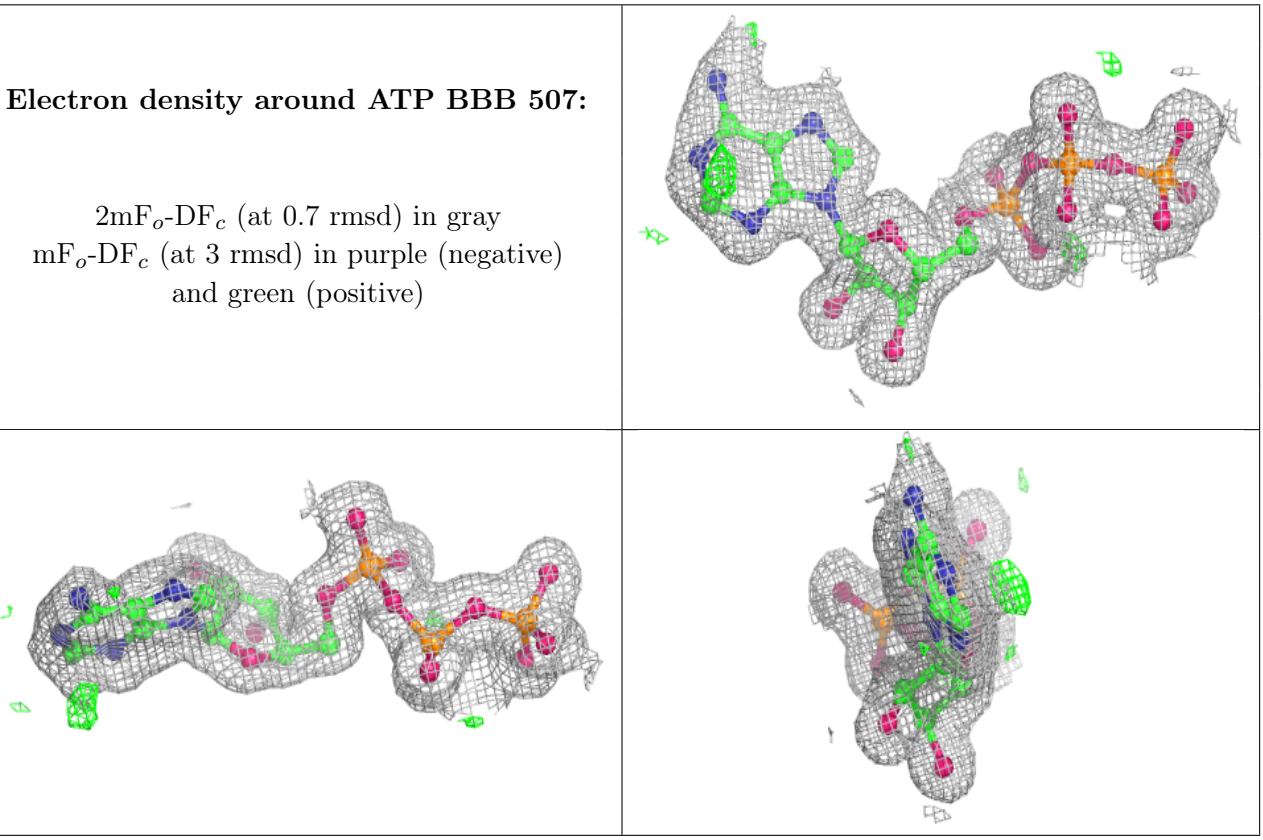
Electron density around ATP BBB 508:

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



Electron density around ATP BBB 507:

$2mF_o$-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.