Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 10:03 AM EDT

PDB ID	:	6CLV
Title	:	Staphylococcus aureus Dihydropteroate Synthase (saDHPS) F17L E208K double mutant structure
Authors	:	Gajewski, S.; Griffith, E.C.; Wu, Y.; White, S.W.
Deposited on	:	2018-03-02
Resolution	:	2.30 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:

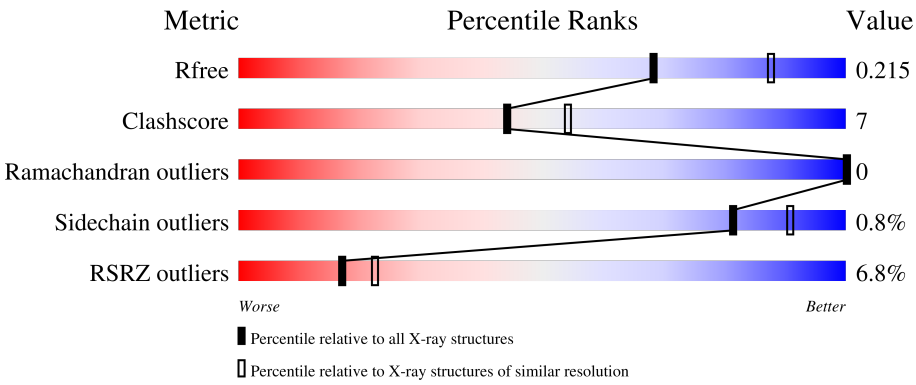
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	A	291	3% 77% 11% 12%
1	B	291	4% 72% 14% 14%
1	C	291	2% 79% 9% 12%
1	D	291	14% 64% 19% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7542 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 Dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	1903	1197	335	359	12	0	0	0
1	B	249	1832	1158	323	340	11	0	0	0
1	C	257	1926	1212	336	366	12	0	0	0
1	D	240	1689	1066	293	319	11	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP O05701
A	-22	GLY	-	expression tag	UNP O05701
A	-21	HIS	-	expression tag	UNP O05701
A	-20	HIS	-	expression tag	UNP O05701
A	-19	HIS	-	expression tag	UNP O05701
A	-18	HIS	-	expression tag	UNP O05701
A	-17	HIS	-	expression tag	UNP O05701
A	-16	HIS	-	expression tag	UNP O05701
A	-15	HIS	-	expression tag	UNP O05701
A	-14	HIS	-	expression tag	UNP O05701
A	-13	HIS	-	expression tag	UNP O05701
A	-12	HIS	-	expression tag	UNP O05701
A	-11	SER	-	expression tag	UNP O05701
A	-10	SER	-	expression tag	UNP O05701
A	-9	GLY	-	expression tag	UNP O05701
A	-8	HIS	-	expression tag	UNP O05701
A	-7	ILE	-	expression tag	UNP O05701
A	-6	GLU	-	expression tag	UNP O05701
A	-5	GLY	-	expression tag	UNP O05701
A	-4	ARG	-	expression tag	UNP O05701
A	-3	HIS	-	expression tag	UNP O05701

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP O05701
A	-1	LEU	-	expression tag	UNP O05701
A	0	GLU	-	expression tag	UNP O05701
A	17	LEU	PHE	engineered mutation	UNP O05701
A	208	LYS	GLU	engineered mutation	UNP O05701
B	-23	MET	-	initiating methionine	UNP O05701
B	-22	GLY	-	expression tag	UNP O05701
B	-21	HIS	-	expression tag	UNP O05701
B	-20	HIS	-	expression tag	UNP O05701
B	-19	HIS	-	expression tag	UNP O05701
B	-18	HIS	-	expression tag	UNP O05701
B	-17	HIS	-	expression tag	UNP O05701
B	-16	HIS	-	expression tag	UNP O05701
B	-15	HIS	-	expression tag	UNP O05701
B	-14	HIS	-	expression tag	UNP O05701
B	-13	HIS	-	expression tag	UNP O05701
B	-12	HIS	-	expression tag	UNP O05701
B	-11	SER	-	expression tag	UNP O05701
B	-10	SER	-	expression tag	UNP O05701
B	-9	GLY	-	expression tag	UNP O05701
B	-8	HIS	-	expression tag	UNP O05701
B	-7	ILE	-	expression tag	UNP O05701
B	-6	GLU	-	expression tag	UNP O05701
B	-5	GLY	-	expression tag	UNP O05701
B	-4	ARG	-	expression tag	UNP O05701
B	-3	HIS	-	expression tag	UNP O05701
B	-2	MET	-	expression tag	UNP O05701
B	-1	LEU	-	expression tag	UNP O05701
B	0	GLU	-	expression tag	UNP O05701
B	17	LEU	PHE	engineered mutation	UNP O05701
B	208	LYS	GLU	engineered mutation	UNP O05701
C	-23	MET	-	initiating methionine	UNP O05701
C	-22	GLY	-	expression tag	UNP O05701
C	-21	HIS	-	expression tag	UNP O05701
C	-20	HIS	-	expression tag	UNP O05701
C	-19	HIS	-	expression tag	UNP O05701
C	-18	HIS	-	expression tag	UNP O05701
C	-17	HIS	-	expression tag	UNP O05701
C	-16	HIS	-	expression tag	UNP O05701
C	-15	HIS	-	expression tag	UNP O05701
C	-14	HIS	-	expression tag	UNP O05701
C	-13	HIS	-	expression tag	UNP O05701

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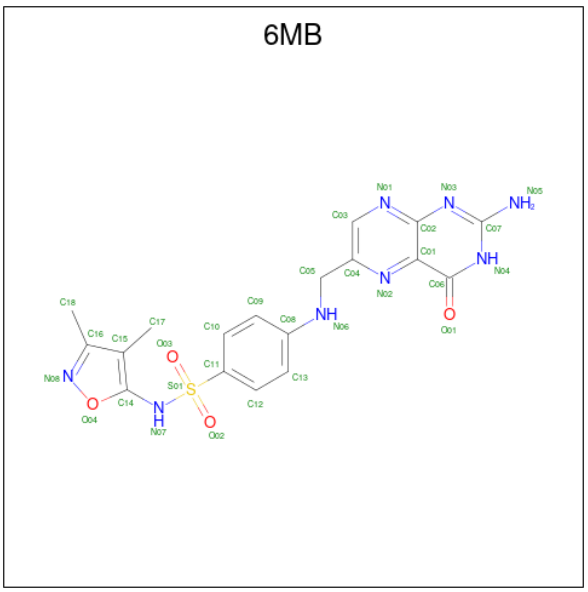
Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP O05701
C	-11	SER	-	expression tag	UNP O05701
C	-10	SER	-	expression tag	UNP O05701
C	-9	GLY	-	expression tag	UNP O05701
C	-8	HIS	-	expression tag	UNP O05701
C	-7	ILE	-	expression tag	UNP O05701
C	-6	GLU	-	expression tag	UNP O05701
C	-5	GLY	-	expression tag	UNP O05701
C	-4	ARG	-	expression tag	UNP O05701
C	-3	HIS	-	expression tag	UNP O05701
C	-2	MET	-	expression tag	UNP O05701
C	-1	LEU	-	expression tag	UNP O05701
C	0	GLU	-	expression tag	UNP O05701
C	17	LEU	PHE	engineered mutation	UNP O05701
C	208	LYS	GLU	engineered mutation	UNP O05701
D	-23	MET	-	initiating methionine	UNP O05701
D	-22	GLY	-	expression tag	UNP O05701
D	-21	HIS	-	expression tag	UNP O05701
D	-20	HIS	-	expression tag	UNP O05701
D	-19	HIS	-	expression tag	UNP O05701
D	-18	HIS	-	expression tag	UNP O05701
D	-17	HIS	-	expression tag	UNP O05701
D	-16	HIS	-	expression tag	UNP O05701
D	-15	HIS	-	expression tag	UNP O05701
D	-14	HIS	-	expression tag	UNP O05701
D	-13	HIS	-	expression tag	UNP O05701
D	-12	HIS	-	expression tag	UNP O05701
D	-11	SER	-	expression tag	UNP O05701
D	-10	SER	-	expression tag	UNP O05701
D	-9	GLY	-	expression tag	UNP O05701
D	-8	HIS	-	expression tag	UNP O05701
D	-7	ILE	-	expression tag	UNP O05701
D	-6	GLU	-	expression tag	UNP O05701
D	-5	GLY	-	expression tag	UNP O05701
D	-4	ARG	-	expression tag	UNP O05701
D	-3	HIS	-	expression tag	UNP O05701
D	-2	MET	-	expression tag	UNP O05701
D	-1	LEU	-	expression tag	UNP O05701
D	0	GLU	-	expression tag	UNP O05701
D	17	LEU	PHE	engineered mutation	UNP O05701
D	208	LYS	GLU	engineered mutation	UNP O05701

- Molecule 2 is 4-{[(2-amino-4-oxo-3,4-dihydropteridin-6-yl)methyl]amino}-N-(3,4-dimethyl-1

,2-oxazol-5-yl)benzene-1-sulfonamide (three-letter code: 6MB) (formula: $C_{18}H_{18}N_8O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	18	8	4	1		
2	B	1	Total	C	N	O	S	0	0
			31	18	8	4	1		
2	C	1	Total	C	N	O	S	0	0
			31	18	8	4	1		

- Molecule 3 is water.

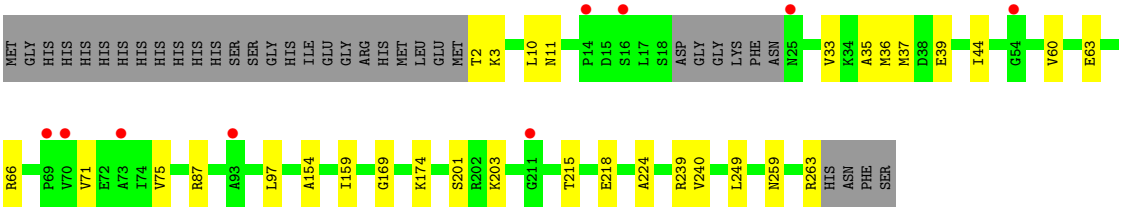
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	34	Total	O	0	0
			34	34		
3	C	28	Total	O	0	0
			28	28		
3	D	7	Total	O	0	0
			7	7		

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.

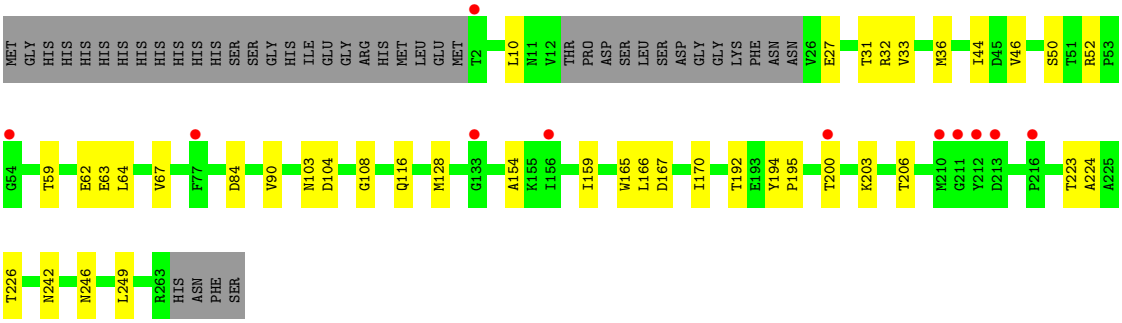
• Molecule 1: Dihydropteroate synthase

Chain A:



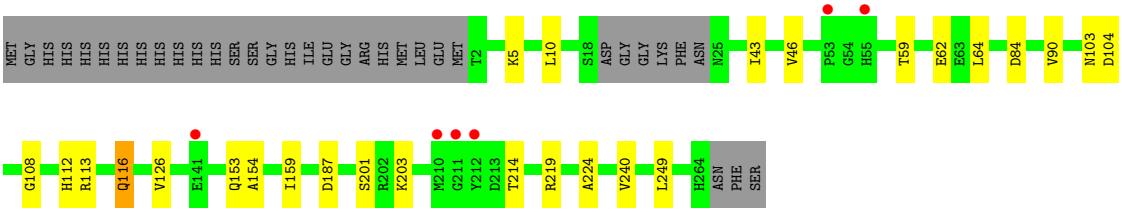
• Molecule 1: Dihydropteroate synthase

Chain B:



• Molecule 1: Dihydropteroate synthase

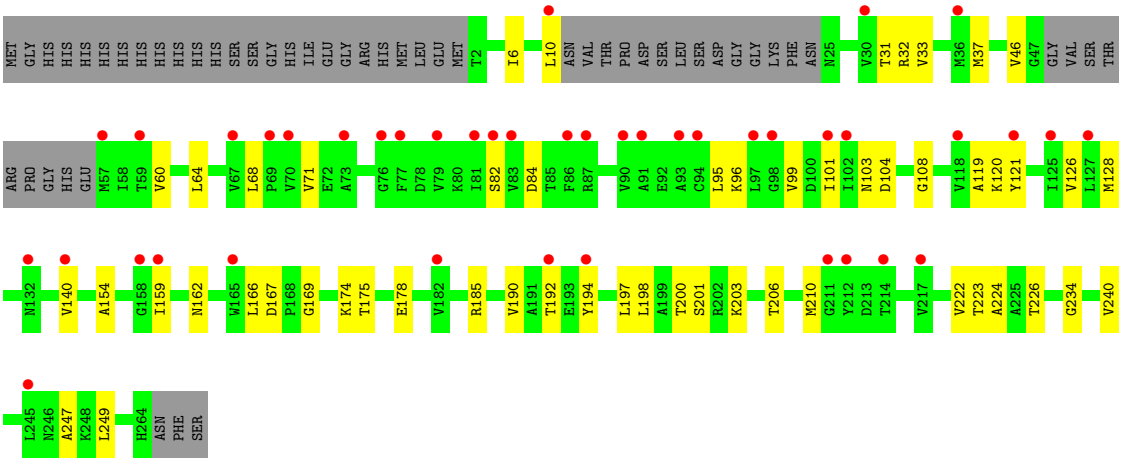
Chain C:



• Molecule 1: Dihydropteroate synthase

Chain D:

14%
64%
19%
18%


MET GLY HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE GLU GLY ARG HIS MET LEU GLU MET T2 I6 L10 ASN VAL THR PRO ASP SER LEU SER ASP GLY GLY LYS PHE ASN N25 V30 T31 R32 V33 M36 M37 V46 G47 GLY VAL SER THR
ARG PRO GLY HIS GLU M57 I58 T59 V60 L64 V67 L68 P69 V70 V71 E72 A73 G76 F77 D78 V79 K80 I81 S82 V83 D84 T85 F86 R87 V90 A91 E92 A93 C94 L95 K96 L97 G98 V99 D100 I101 I102 N103 D104 G108 V118 A119 K120 Y121 I125 V126 L127 M128
N132 V140 A154 G158 I159 N162 W165 L166 D167 P168 G169 K174 T175 E178 V182 R185 V190 A191 T192 E193 Y194 L197 L198 A199 T200 S201 R202 K203 T206 M210 G211 Y212 D213 T214 V217 V222 T223 A224 A225 T226 G234 V240
L245 N246 A247 K248 L249 H264 ASN PHE SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	79.75Å 79.75Å 175.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.43 – 2.30 47.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.43-2.30) 100.0 (47.43-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	56.03 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.191 , 0.210 0.193 , 0.215	Depositor DCC
R_{free} test set	2546 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.320 for h,-k,-l	Xtriage
Reported twinning fraction	0.640 for h,-k,-l	Depositor
Outliers	0 of 48470 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7542	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: 6MB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.39	0/1927	0.48	0/2616
1	B	0.24	0/1855	0.41	0/2517
1	C	0.23	0/1952	0.40	0/2649
1	D	0.35	0/1710	0.51	0/2332
All	All	0.31	0/7444	0.45	0/10114

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 (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	1903	0	1895	20	0
1	B	1832	0	1818	24	0
1	C	1926	0	1909	15	0
1	D	1689	0	1573	37	0
2	A	31	0	0	1	0
2	B	31	0	0	2	0
2	C	31	0	0	1	0
3	A	30	0	0	1	0
3	B	34	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	0	0	0
3	D	7	0	0	0	0
All	All	7542	0	7195	96	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 7.

All (96) 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:B:116:GLN:HG3	3:B:412:HOH:O	1.58	1.00
1:D:192:THR:HG23	1:D:194:TYR:H	1.31	0.92
1:B:192:THR:HG23	1:B:194:TYR:H	1.45	0.81
1:D:223:THR:O	1:D:226:THR:HG22	1.82	0.79
1:A:36:MET:HE3	1:A:44:ILE:HD12	1.73	0.70
1:D:120:LYS:HG2	1:D:121:TYR:CD1	2.29	0.67
1:A:71:VAL:O	1:A:75:VAL:HG23	1.94	0.66
1:D:95:LEU:HA	1:D:99:VAL:HG22	1.79	0.65
1:B:224:ALA:HB1	1:B:249:LEU:HD22	1.81	0.63
1:C:5:LYS:HD3	1:C:43:ILE:HD11	1.80	0.63
1:D:6:ILE:HD12	1:D:247:ALA:HA	1.81	0.62
1:C:203:LYS:NZ	2:C:300:6MB:O01	2.32	0.62
1:D:6:ILE:CD1	1:D:247:ALA:HA	2.29	0.62
1:B:59:THR:HG23	1:B:62:GLU:H	1.65	0.61
1:A:224:ALA:HB1	1:A:249:LEU:HD22	1.81	0.61
1:D:120:LYS:HG2	1:D:121:TYR:HD1	1.66	0.60
1:D:140:VAL:HG21	1:D:185:ARG:HD3	1.82	0.60
1:B:203:LYS:NZ	2:B:300:6MB:O01	2.35	0.59
1:D:154:ALA:HB1	1:D:159:ILE:HD12	1.84	0.59
1:A:201:SER:HB2	1:A:240:VAL:HA	1.85	0.58
1:A:259:ASN:HD21	1:A:263:ARG:HE	1.50	0.58
1:A:35:ALA:O	1:A:39:GLU:HG3	2.03	0.58
1:D:33:VAL:HG12	1:D:37:MET:HE2	1.87	0.57
1:D:33:VAL:CG1	1:D:37:MET:HE2	2.36	0.56
1:B:166:LEU:HD12	1:B:192:THR:HG21	1.89	0.55
1:B:84:ASP:HA	1:B:103:ASN:HB3	1.88	0.55
1:C:103:ASN:HA	1:C:126:VAL:HB	1.88	0.54
1:C:10:LEU:HD23	1:C:46:VAL:HG22	1.89	0.54
1:C:214:THR:O	1:C:219:ARG:NH2	2.37	0.54
1:C:224:ALA:HB1	1:C:249:LEU:HD22	1.90	0.54
1:D:224:ALA:HB1	1:D:249:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLU:O	1:B:31:THR:HG23	2.09	0.53
1:D:96:LYS:HG2	1:D:121:TYR:CE2	2.43	0.53
1:C:104:ASP:OD2	1:C:108:GLY:N	2.41	0.53
1:A:10:LEU:HD13	1:A:36:MET:HE2	1.90	0.52
1:B:52:ARG:HE	2:B:300:6MB:C09	2.22	0.52
1:D:68:LEU:HA	1:D:71:VAL:HG12	1.91	0.52
1:B:170:ILE:O	1:B:203:LYS:NZ	2.32	0.52
1:A:239:ARG:NH1	3:A:402:HOH:O	2.37	0.51
1:B:104:ASP:OD2	1:B:108:GLY:N	2.43	0.51
1:C:59:THR:HG23	1:C:62:GLU:H	1.74	0.51
1:D:33:VAL:HG12	1:D:37:MET:CE	2.40	0.51
1:D:185:ARG:HH11	1:D:185:ARG:HB3	1.76	0.51
1:A:154:ALA:HB1	1:A:159:ILE:HD12	1.93	0.51
1:A:203:LYS:NZ	2:A:300:6MB:O01	2.44	0.51
1:D:84:ASP:HA	1:D:103:ASN:HB3	1.92	0.50
1:D:198:LEU:HD21	1:D:226:THR:OG1	2.12	0.50
1:D:96:LYS:HG2	1:D:121:TYR:HE2	1.78	0.49
1:D:210:MET:HG2	1:D:222:VAL:HG11	1.95	0.49
1:B:64:LEU:HD21	1:B:90:VAL:HA	1.95	0.49
1:D:200:THR:OG1	1:D:226:THR:HG21	2.12	0.49
1:A:60:VAL:HG12	1:A:87:ARG:HD2	1.95	0.49
1:C:154:ALA:HB1	1:C:159:ILE:HD12	1.95	0.48
1:B:10:LEU:HD23	1:B:46:VAL:HG22	1.96	0.48
1:A:10:LEU:HD13	1:A:36:MET:CE	2.44	0.48
1:B:154:ALA:HB1	1:B:159:ILE:HD12	1.95	0.47
1:B:50:SER:OG	1:B:52:ARG:NH2	2.47	0.47
1:B:63:GLU:O	1:B:67:VAL:HG22	2.15	0.47
1:B:170:ILE:HG13	1:B:200:THR:HG22	1.97	0.47
1:D:82:SER:HB2	1:D:101:ILE:HB	1.97	0.47
1:D:104:ASP:OD2	1:D:108:GLY:N	2.45	0.47
1:D:175:THR:OG1	1:D:178:GLU:HG3	2.15	0.47
1:C:201:SER:HB2	1:C:240:VAL:HA	1.96	0.46
1:A:259:ASN:ND2	1:A:263:ARG:HE	2.12	0.46
1:D:120:LYS:HG2	1:D:121:TYR:CE1	2.50	0.46
1:D:126:VAL:HG11	1:D:197:LEU:HD23	1.98	0.45
1:C:112:HIS:HE1	1:C:153:GLN:HE21	1.64	0.45
1:D:169:GLY:O	1:D:174:LYS:NZ	2.40	0.45
1:B:203:LYS:O	1:B:206:THR:OG1	2.33	0.45
1:C:64:LEU:HD21	1:C:90:VAL:HA	1.99	0.44
1:D:60:VAL:O	1:D:64:LEU:HD23	2.18	0.44
1:D:190:VAL:HG11	1:D:234:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:O	1:A:37:MET:HG2	2.17	0.44
1:D:119:ALA:HB2	1:D:159:ILE:HG12	2.00	0.43
1:D:185:ARG:HB3	1:D:185:ARG:NH1	2.32	0.43
1:D:166:LEU:HD12	1:D:192:THR:HG21	1.99	0.43
1:A:2:THR:HB	1:A:3:LYS:H	1.66	0.43
1:D:203:LYS:O	1:D:206:THR:OG1	2.32	0.43
1:D:10:LEU:HB3	1:D:46:VAL:HA	2.01	0.43
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.69	0.42
1:B:223:THR:O	1:B:226:THR:OG1	2.27	0.42
1:B:242:ASN:O	1:B:246:ASN:ND2	2.37	0.42
1:D:128:MET:HA	1:D:167:ASP:HB3	2.00	0.42
1:B:165:TRP:CE3	1:B:195:PRO:HB2	2.54	0.42
1:A:75:VAL:HG11	1:A:97:LEU:O	2.20	0.42
1:B:128:MET:HA	1:B:167:ASP:HB3	2.01	0.41
1:A:169:GLY:O	1:A:174:LYS:NZ	2.45	0.41
1:B:32:ARG:O	1:B:36:MET:HG3	2.20	0.41
1:D:192:THR:HG23	1:D:194:TYR:N	2.15	0.41
1:C:113:ARG:HG3	1:C:116:GLN:OE1	2.20	0.41
1:A:215:THR:O	1:A:218:GLU:HG2	2.20	0.41
1:B:33:VAL:HG13	1:B:44:ILE:HD13	2.03	0.41
1:D:201:SER:HB2	1:D:240:VAL:HA	2.02	0.41
1:C:187:ASP:OD1	1:C:187:ASP:N	2.52	0.41
1:C:84:ASP:HA	1:C:103:ASN:HB3	2.02	0.40
1:A:63:GLU:OE1	1:A:87:ARG:NH2	2.51	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	252/291 (87%)	251 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	245/291 (84%)	244 (100%)	1 (0%)	0	100	100
1	C	253/291 (87%)	251 (99%)	2 (1%)	0	100	100
1	D	234/291 (80%)	234 (100%)	0	0	100	100
All	All	984/1164 (84%)	980 (100%)	4 (0%)	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	195/244 (80%)	193 (99%)	2 (1%)	76	87
1	B	183/244 (75%)	183 (100%)	0	100	100
1	C	199/244 (82%)	198 (100%)	1 (0%)	88	95
1	D	154/244 (63%)	151 (98%)	3 (2%)	57	73
All	All	731/976 (75%)	725 (99%)	6 (1%)	81	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	66	ARG
1	C	116	GLN
1	D	31	THR
1	D	32	ARG
1	D	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	B	65	ASN

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Mol	Chain	Res	Type
1	C	112	HIS
1	C	116	GLN
1	D	105	GLN
1	D	152	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	6MB	B	300	-	31,34,34	1.46	3 (9%)	38,50,50	3.16	11 (28%)
2	6MB	A	300	-	31,34,34	1.45	3 (9%)	38,50,50	2.99	11 (28%)
2	6MB	C	300	-	31,34,34	1.44	3 (9%)	38,50,50	2.96	11 (28%)

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	6MB	B	300	-	-	8/14/16/16	0/4/4/4
2	6MB	A	300	-	-	8/14/16/16	0/4/4/4
2	6MB	C	300	-	-	8/14/16/16	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	6MB	C07-N03	4.79	1.44	1.33
2	C	300	6MB	C07-N03	4.73	1.44	1.33
2	A	300	6MB	C07-N03	4.73	1.44	1.33
2	A	300	6MB	C07-N05	3.50	1.42	1.34
2	B	300	6MB	C07-N05	3.48	1.42	1.34
2	C	300	6MB	C07-N05	3.48	1.42	1.34
2	C	300	6MB	C07-N04	2.15	1.42	1.37
2	B	300	6MB	C07-N04	2.15	1.42	1.37
2	A	300	6MB	C07-N04	2.15	1.42	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	300	6MB	O03-S01-O02	-15.84	100.28	119.52
2	A	300	6MB	O03-S01-O02	-15.06	101.23	119.52
2	C	300	6MB	O03-S01-O02	-14.87	101.46	119.52
2	B	300	6MB	C11-S01-N07	4.50	112.46	106.88
2	B	300	6MB	C04-C03-N01	-4.24	119.07	123.14
2	C	300	6MB	C04-C03-N01	-4.08	119.22	123.14
2	A	300	6MB	C04-C03-N01	-3.89	119.40	123.14
2	A	300	6MB	O03-S01-C11	3.56	112.47	107.98
2	B	300	6MB	C17-C15-C14	-3.39	126.81	129.73
2	C	300	6MB	O02-S01-C11	3.24	112.07	107.98
2	A	300	6MB	C01-C06-N04	3.19	120.16	114.07
2	C	300	6MB	C01-C06-N04	3.17	120.12	114.07
2	B	300	6MB	C04-C05-N06	-3.04	106.45	113.13
2	B	300	6MB	C01-C06-N04	3.02	119.84	114.07
2	C	300	6MB	C17-C15-C14	-2.98	127.16	129.73
2	C	300	6MB	C07-N04-C06	-2.93	119.75	125.11
2	B	300	6MB	C07-N04-C06	-2.86	119.87	125.11
2	A	300	6MB	C07-N04-C06	-2.84	119.91	125.11
2	C	300	6MB	O03-S01-C11	2.79	111.49	107.98
2	A	300	6MB	O02-S01-C11	2.66	111.34	107.98
2	B	300	6MB	C01-C02-N03	-2.46	119.74	123.19
2	B	300	6MB	O02-S01-C11	2.43	111.05	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	6MB	O02-S01-N07	2.36	112.50	106.74
2	A	300	6MB	C18-C16-N08	2.35	126.41	119.19
2	A	300	6MB	O03-S01-N07	2.33	112.42	106.74
2	B	300	6MB	C18-C16-N08	2.33	126.35	119.19
2	C	300	6MB	C01-C02-N03	-2.26	120.02	123.19
2	C	300	6MB	C18-C16-N08	2.25	126.11	119.19
2	A	300	6MB	C01-C02-N03	-2.22	120.08	123.19
2	C	300	6MB	O01-C06-C01	-2.20	119.95	124.32
2	A	300	6MB	O01-C06-C01	-2.19	119.97	124.32
2	B	300	6MB	O01-C06-C01	-2.16	120.04	124.32
2	A	300	6MB	C17-C15-C14	-2.15	127.88	129.73

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	6MB	C04-C05-N06-C08
2	A	300	6MB	C14-N07-S01-O02
2	B	300	6MB	C14-N07-S01-C11
2	B	300	6MB	C14-N07-S01-O03
2	C	300	6MB	C14-N07-S01-C11
2	C	300	6MB	C14-N07-S01-O03
2	C	300	6MB	C12-C11-S01-N07
2	C	300	6MB	C10-C11-S01-N07
2	A	300	6MB	C12-C11-S01-N07
2	A	300	6MB	C10-C11-S01-N07
2	B	300	6MB	C12-C11-S01-N07
2	C	300	6MB	C14-N07-S01-O02
2	B	300	6MB	C10-C11-S01-O02
2	B	300	6MB	C12-C11-S01-O02
2	B	300	6MB	C10-C11-S01-N07
2	A	300	6MB	C14-N07-S01-O03
2	B	300	6MB	C04-C05-N06-C08
2	C	300	6MB	C04-C05-N06-C08
2	A	300	6MB	C10-C11-S01-O02
2	A	300	6MB	C14-N07-S01-C11
2	A	300	6MB	C12-C11-S01-O02
2	B	300	6MB	C14-N07-S01-O02
2	C	300	6MB	C10-C11-S01-O02
2	C	300	6MB	C12-C11-S01-O02

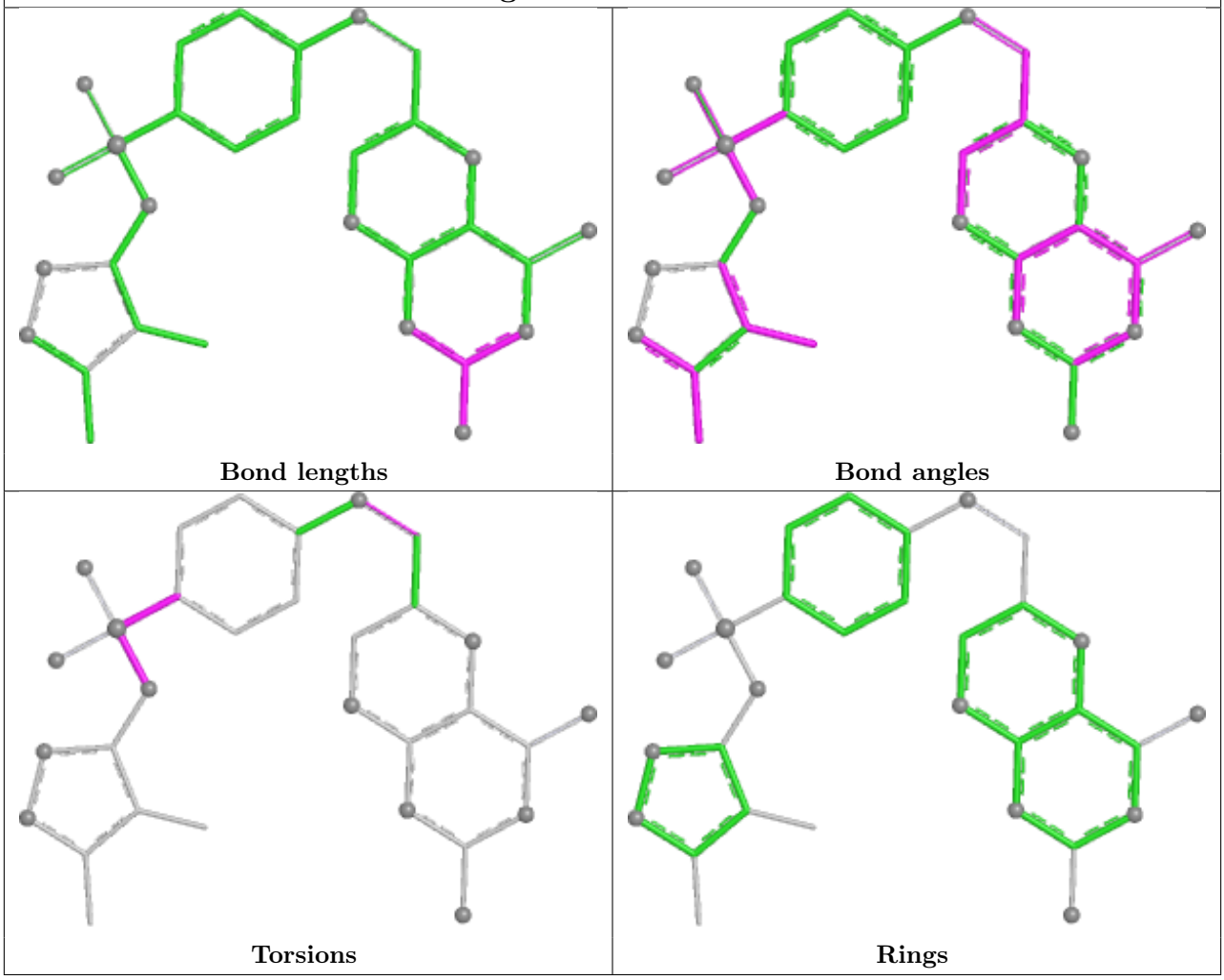
There are no ring outliers.

3 monomers are involved in 4 short contacts:

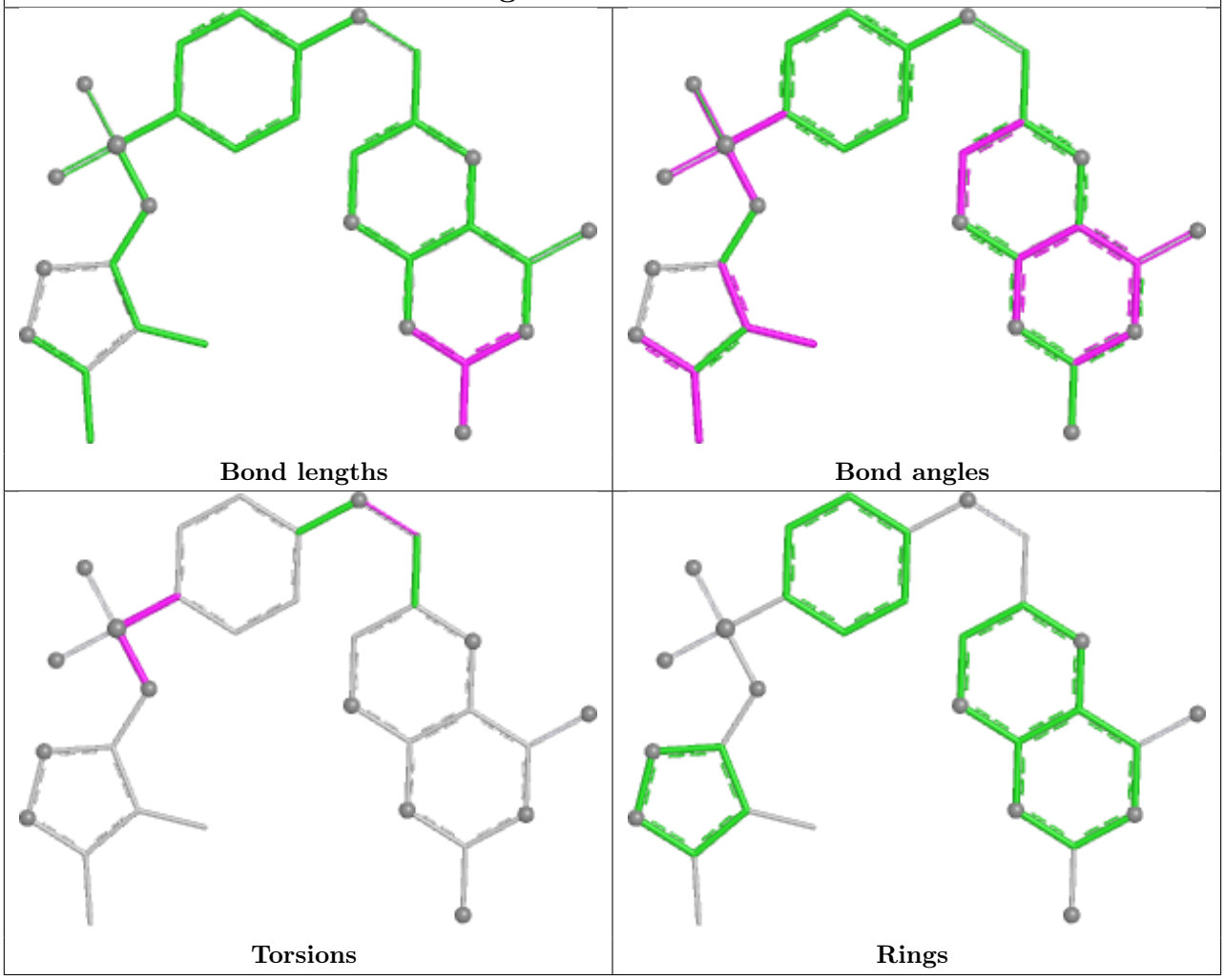
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300	6MB	2	0
2	A	300	6MB	1	0
2	C	300	6MB	1	0

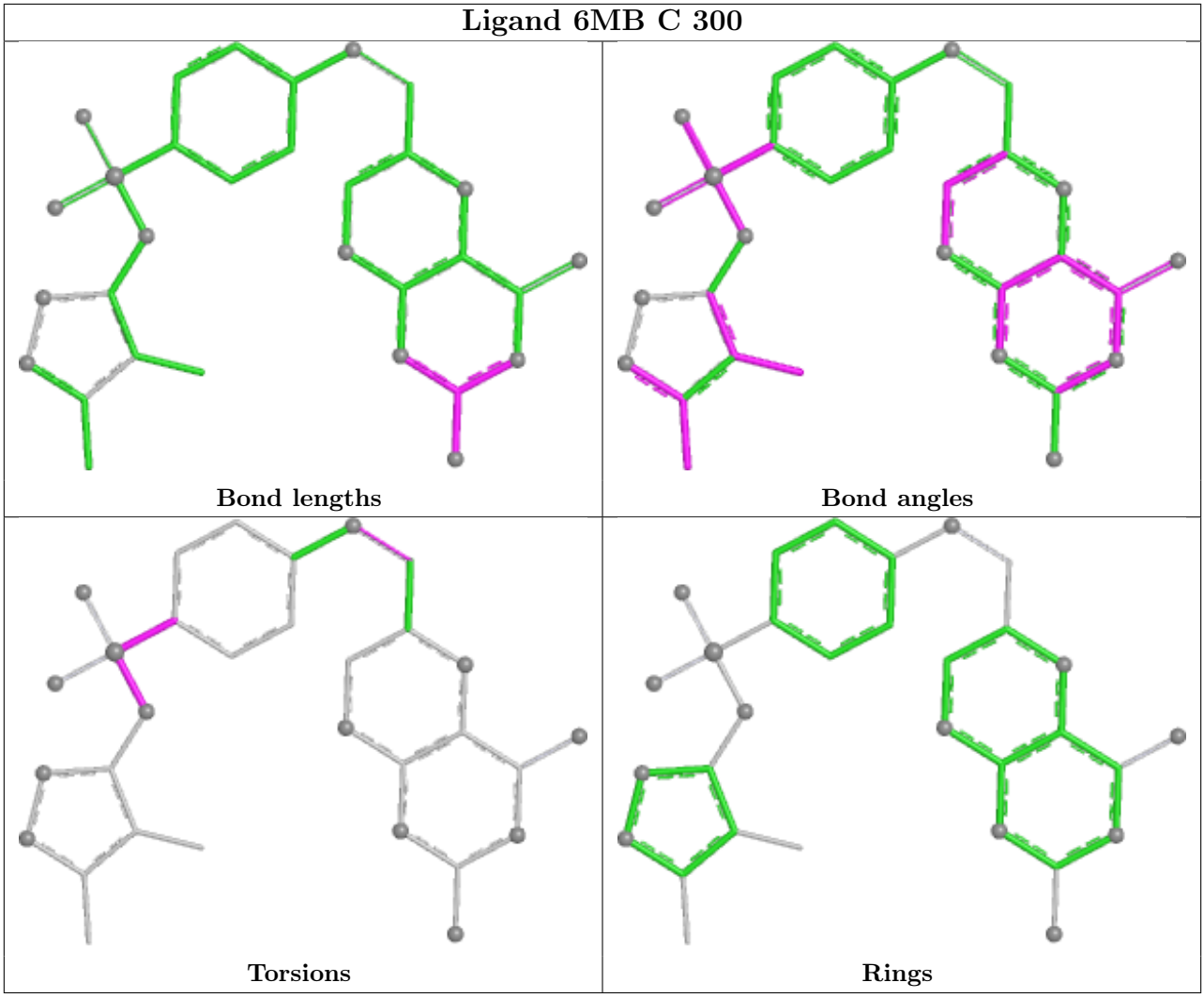
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 6MB B 300



Ligand 6MB A 300





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	256/291 (87%)	0.48	9 (3%) 44 51	32, 47, 73, 92	0
1	B	249/291 (85%)	0.54	11 (4%) 34 41	30, 46, 74, 115	0
1	C	257/291 (88%)	0.49	6 (2%) 60 67	31, 45, 69, 168	0
1	D	240/291 (82%)	1.14	42 (17%) 1 1	41, 66, 96, 124	0
All	All	1002/1164 (86%)	0.66	68 (6%) 17 22	30, 50, 83, 168	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	GLY	7.7
1	C	55	HIS	7.4
1	D	76	GLY	6.8
1	D	158	GLY	6.7
1	C	211	GLY	5.1
1	D	70	VAL	4.7
1	D	211	GLY	4.7
1	D	94	CYS	4.6
1	D	194	TYR	4.5
1	D	217	VAL	4.5
1	D	101	ILE	4.3
1	D	159	ILE	4.2
1	D	59	THR	4.2
1	A	54	GLY	3.8
1	D	93	ALA	3.8
1	C	212	TYR	3.6
1	D	125	ILE	3.6
1	D	73	ALA	3.6
1	B	54	GLY	3.6
1	D	91	ALA	3.3
1	D	69	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	118	VAL	3.1
1	D	165	TRP	3.1
1	B	200	THR	3.1
1	D	97	LEU	3.0
1	B	211	GLY	3.0
1	D	77	PHE	3.0
1	D	83	VAL	2.9
1	A	211	GLY	2.9
1	D	10	LEU	2.7
1	D	67	VAL	2.7
1	C	53	PRO	2.7
1	A	14	PRO	2.6
1	D	132	ASN	2.6
1	B	216	PRO	2.6
1	A	93	ALA	2.6
1	D	102	ILE	2.6
1	B	77	PHE	2.6
1	D	121	TYR	2.5
1	B	2	THR	2.5
1	D	87	ARG	2.4
1	B	213	ASP	2.4
1	B	156	ILE	2.4
1	D	245	LEU	2.4
1	B	133	GLY	2.4
1	D	30	VAL	2.4
1	D	57	MET	2.4
1	D	36	MET	2.3
1	D	212	TYR	2.3
1	B	210	MET	2.3
1	D	79	VAL	2.3
1	D	182	VAL	2.3
1	C	141	GLU	2.3
1	A	25	ASN	2.2
1	B	212	TYR	2.2
1	A	70	VAL	2.2
1	D	81	ILE	2.2
1	D	214	THR	2.1
1	D	90	VAL	2.1
1	A	73	ALA	2.1
1	A	69	PRO	2.1
1	C	210	MET	2.1
1	D	127	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	16	SER	2.1
1	D	192	THR	2.0
1	D	82	SER	2.0
1	D	140	VAL	2.0
1	D	86	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

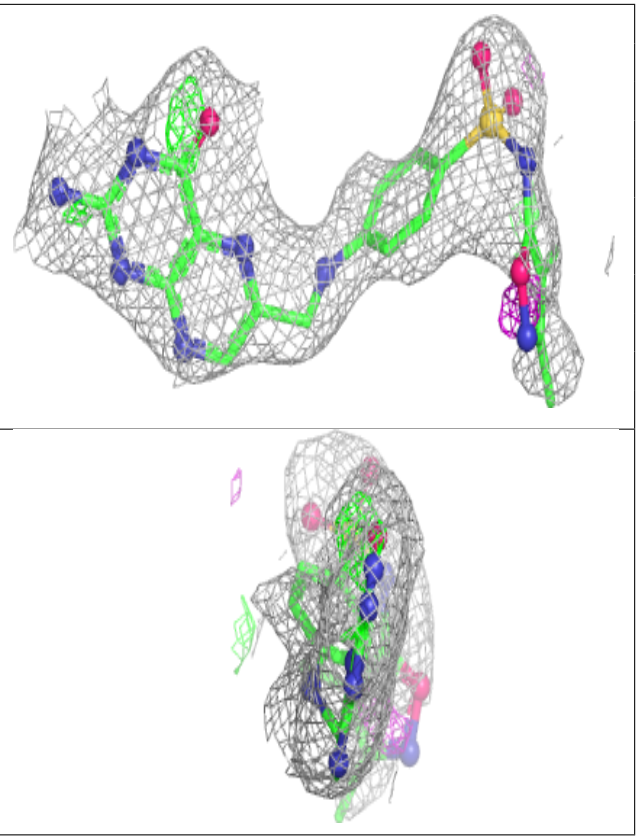
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6MB	B	300	31/31	0.80	0.24	58,70,82,84	0
2	6MB	C	300	31/31	0.83	0.29	59,66,78,78	0
2	6MB	A	300	31/31	0.87	0.21	55,60,67,69	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.

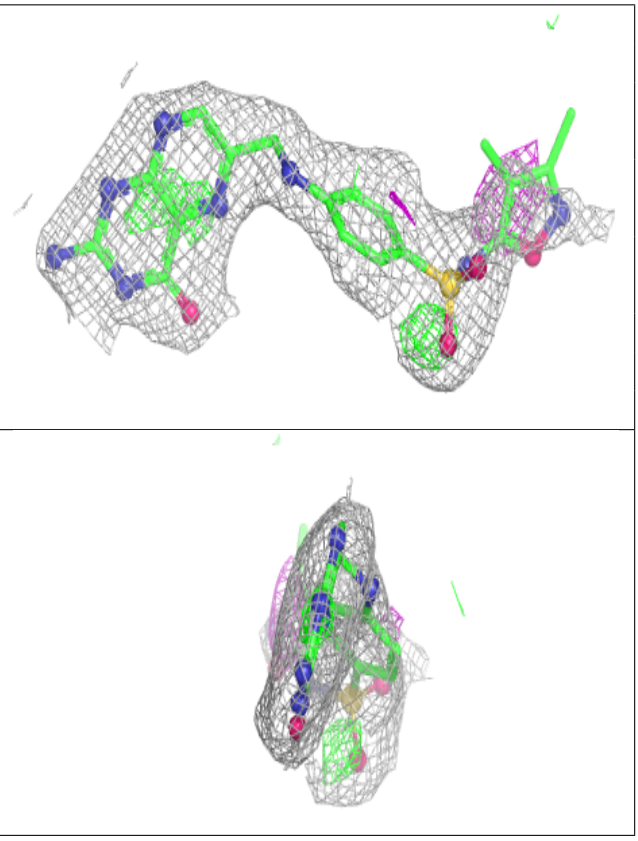
Electron density around 6MB B 300:

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



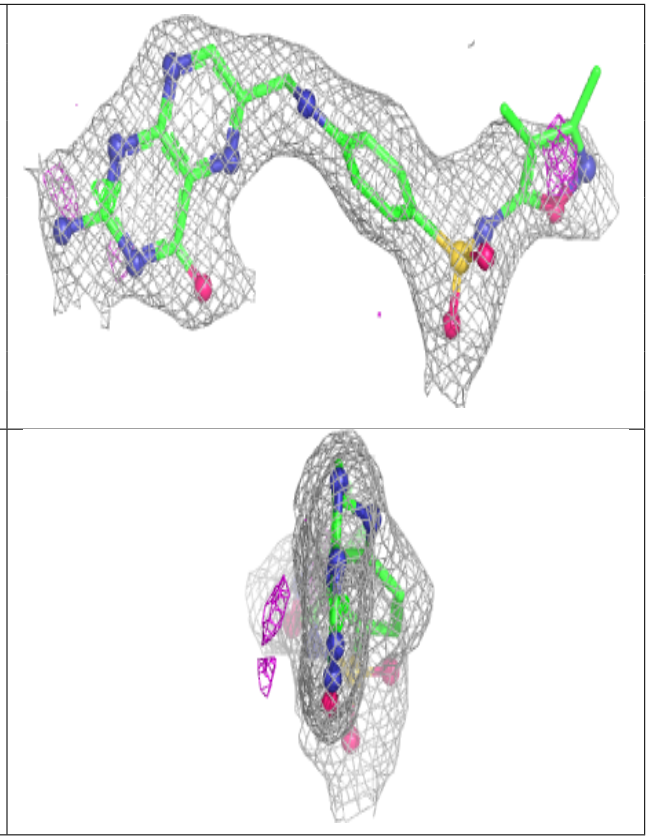
Electron density around 6MB C 300:

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



Electron density around 6MB A 300:

$2mF_o$-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.