Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 06:48 PM JST

PDB ID	:	5XT6
Title	:	A sulfur-transferring catalytic intermediate of SufS-SufU complex from Bacillus subtilis
Authors	:	Fujishiro, T.; Kunichika, K.; Takahashi, Y.
Deposited on	:	2017-06-17
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

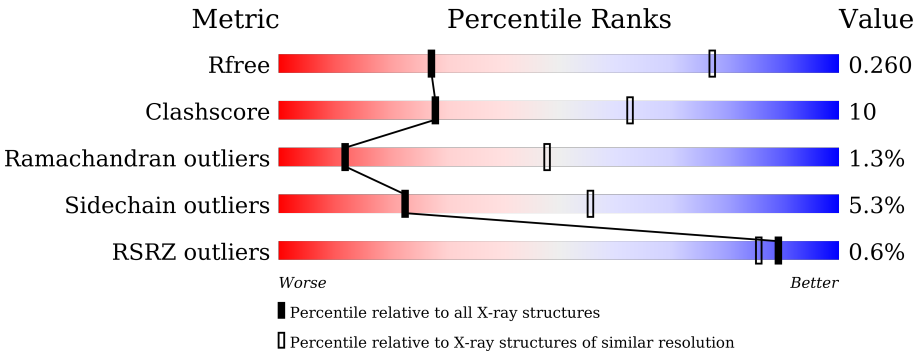
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	D	155	3% 48% 34% 6% 12%
2	A	419	83% 13%
2	B	419	81% 15%
3	C	155	% 55% 29% 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8443 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 Zinc-dependent sulfurtransferase SufU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	137	Total	C	N	O	S	0	0	0
			1050	651	178	209	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	148	LEU	-	expression tag	UNP O32163
D	149	GLU	-	expression tag	UNP O32163
D	150	HIS	-	expression tag	UNP O32163
D	151	HIS	-	expression tag	UNP O32163
D	152	HIS	-	expression tag	UNP O32163
D	153	HIS	-	expression tag	UNP O32163
D	154	HIS	-	expression tag	UNP O32163
D	155	HIS	-	expression tag	UNP O32163

- Molecule 2 is a protein called Cysteine desulfurase SufS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	405	Total	C	N	O	S	0	0	0
			3156	1998	538	606	14			
2	B	405	Total	C	N	O	S	0	0	0
			3153	1997	536	606	14			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP O32164
A	-1	GLY	-	expression tag	UNP O32164
A	0	HIS	-	expression tag	UNP O32164
A	407	VAL	-	expression tag	UNP O32164
A	408	ASP	-	expression tag	UNP O32164
A	409	LEU	-	expression tag	UNP O32164

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Chain	Residue	Modelled	Actual	Comment	Reference
A	410	GLU	-	expression tag	UNP O32164
A	411	HIS	-	expression tag	UNP O32164
A	412	HIS	-	expression tag	UNP O32164
A	413	HIS	-	expression tag	UNP O32164
A	414	HIS	-	expression tag	UNP O32164
A	415	HIS	-	expression tag	UNP O32164
A	416	HIS	-	expression tag	UNP O32164
B	-2	MET	-	expression tag	UNP O32164
B	-1	GLY	-	expression tag	UNP O32164
B	0	HIS	-	expression tag	UNP O32164
B	407	VAL	-	expression tag	UNP O32164
B	408	ASP	-	expression tag	UNP O32164
B	409	LEU	-	expression tag	UNP O32164
B	410	GLU	-	expression tag	UNP O32164
B	411	HIS	-	expression tag	UNP O32164
B	412	HIS	-	expression tag	UNP O32164
B	413	HIS	-	expression tag	UNP O32164
B	414	HIS	-	expression tag	UNP O32164
B	415	HIS	-	expression tag	UNP O32164
B	416	HIS	-	expression tag	UNP O32164

- Molecule 3 is a protein called Zinc-dependent sulfurtransferase SufU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	135	1037	642	175	207	13	0	0	0

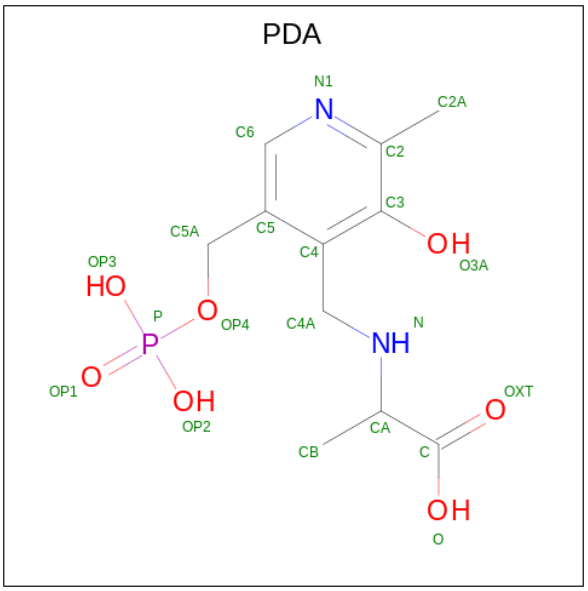
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	148	LEU	-	expression tag	UNP O32163
C	149	GLU	-	expression tag	UNP O32163
C	150	HIS	-	expression tag	UNP O32163
C	151	HIS	-	expression tag	UNP O32163
C	152	HIS	-	expression tag	UNP O32163
C	153	HIS	-	expression tag	UNP O32163
C	154	HIS	-	expression tag	UNP O32163
C	155	HIS	-	expression tag	UNP O32163

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-PROPIONIC ACID (three-letter code: PDA) (formula: $C_{11}H_{17}N_2O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 21 11 2 7 1	0	0
5	B	1	Total C N O P 21 11 2 7 1	0	0

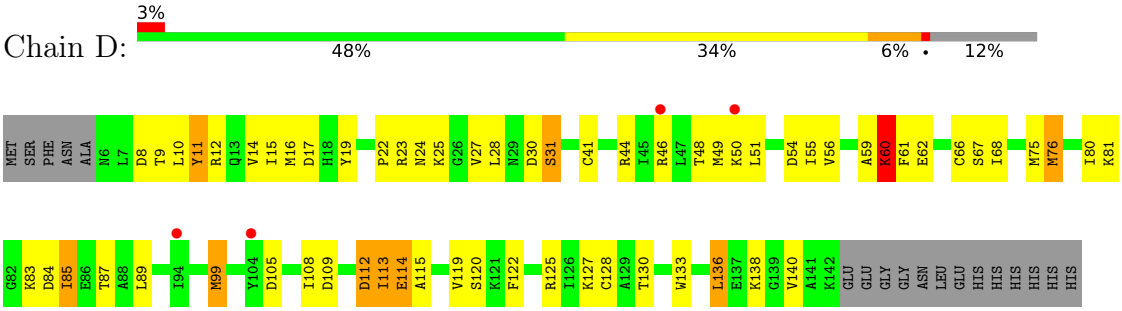
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total O 3 3	0	0

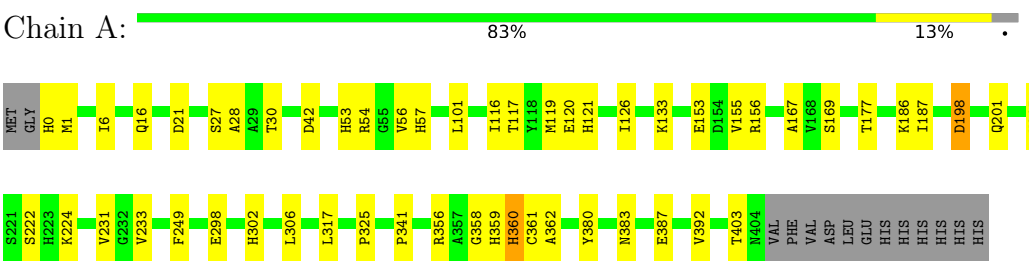
3 Residue-property plots (i)

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.

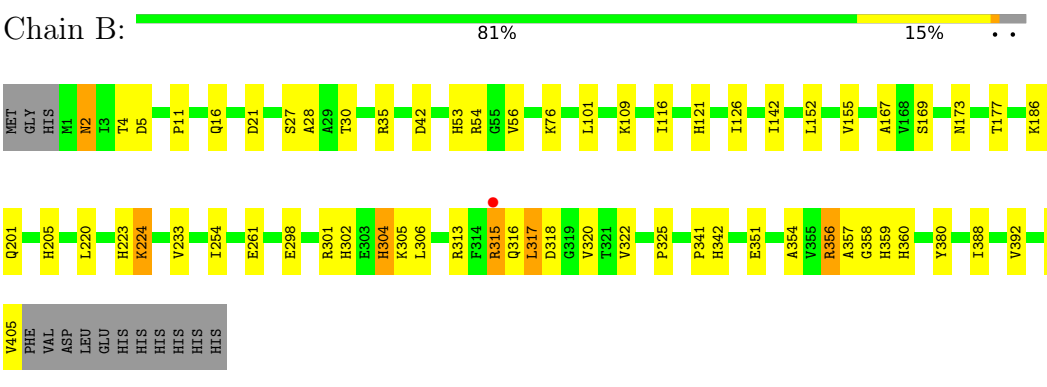
• Molecule 1: Zinc-dependent sulfurtransferase SufU



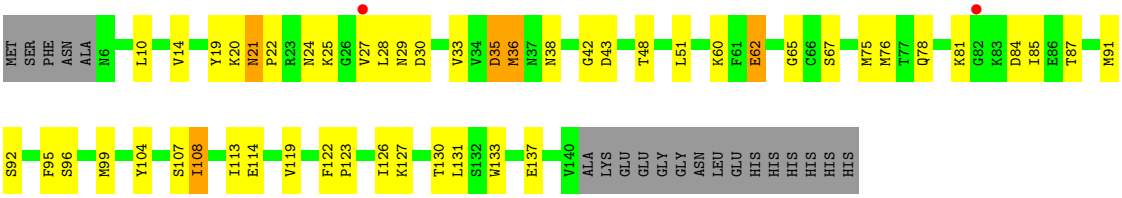
• Molecule 2: Cysteine desulfurase SufS



• Molecule 2: Cysteine desulfurase SufS



• Molecule 3: Zinc-dependent sulfurtransferase SufU


MET SER PHE ASN ALA N6 L10 V14 Y19 K20 N21 P22 R23 N24 K25 G26 V27 L28 N29 D30 V33 V34 D35 M36 N37 N38 G42 D43 T48 L51 K60 F61 E62 G65 C66 S67 M75 M76 T77 Q78 K81 G82 K83 D84 I85 E86 T87 M91
S92 F95 S96 M99 Y104 S107 I108 I113 E114 V119 F122 P123 I126 K127 T130 L131 S132 W133 E137 V140 ALA LYS GLU GLU GLY GLY ASN LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	73.93Å 73.93Å 367.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.29 – 3.50 48.29 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.29-3.50) 99.4 (48.29-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.223 , 0.262 0.218 , 0.260	Depositor DCC
R_{free} test set	709 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	98.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.119 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8443	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PDA, CSS

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	D	0.63	0/1061	1.00	1/1421 (0.1%)
2	A	0.58	0/3214	0.72	3/4363 (0.1%)
2	B	0.57	0/3210	0.75	4/4358 (0.1%)
3	C	0.62	0/1040	0.94	1/1392 (0.1%)
All	All	0.59	0/8525	0.80	9/11534 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	304	HIS	N-CA-CB	6.73	122.72	110.60
3	C	51	LEU	CA-CB-CG	6.47	130.19	115.30
2	B	317	LEU	CB-CG-CD2	-6.34	100.22	111.00
2	A	198	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	B	315	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	A	198	ASP	CB-CG-OD1	5.80	123.52	118.30
2	A	156	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	B	356	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	D	60	LYS	CA-CB-CG	5.12	124.67	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	316	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1050	0	1056	57	0
2	A	3156	0	3107	43	0
2	B	3153	0	3109	48	0
3	C	1037	0	1038	29	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	21	0	13	5	0
5	B	21	0	14	3	0
6	A	3	0	0	0	0
All	All	8443	0	8337	166	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 (166) 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:D:28:LEU:HD11	1:D:60:LYS:CB	1.56	1.34
1:D:28:LEU:CD1	1:D:60:LYS:CB	2.36	1.04
1:D:27:VAL:HG12	1:D:46:ARG:HH12	0.88	1.03
1:D:27:VAL:HG12	1:D:46:ARG:NH1	1.74	1.00
2:B:223:HIS:CE1	2:B:224:LYS:HD3	1.97	0.99
1:D:28:LEU:CD1	1:D:60:LYS:HB3	1.94	0.97
1:D:28:LEU:HD11	1:D:60:LYS:HB2	1.00	0.97
2:A:117:THR:HG22	2:A:119:MET:H	1.30	0.95
2:B:315:ARG:NH1	2:B:322:VAL:HG11	1.85	0.91
2:A:121:HIS:HE2	5:A:501:PDA:HB2	1.32	0.91
1:D:12:ARG:HG3	1:D:115:ALA:HB1	1.52	0.88
1:D:27:VAL:CG1	1:D:46:ARG:HH12	1.83	0.88
3:C:28:LEU:HD13	3:C:60:LYS:HD2	1.55	0.87
2:A:358:GLY:HA3	2:B:54:ARG:HH12	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:117:THR:HG21	2:A:119:MET:HG2	1.56	0.85
2:A:356:ARG:HH21	2:B:54:ARG:HE	1.25	0.83
2:B:121:HIS:HE2	5:B:501:PDA:HB2	1.41	0.83
1:D:113:ILE:O	1:D:115:ALA:N	2.11	0.82
2:A:1:MET:HG3	2:A:298:GLU:HG3	1.60	0.81
1:D:99:MET:HE1	1:D:119:VAL:HG23	1.62	0.80
3:C:27:VAL:HA	3:C:48:THR:HG21	1.63	0.80
2:A:117:THR:CG2	2:A:119:MET:HG2	2.11	0.80
1:D:113:ILE:HD12	1:D:114:GLU:H	1.48	0.78
2:A:28:ALA:O	2:A:224:LYS:HE3	1.84	0.78
1:D:89:LEU:HD11	1:D:140:VAL:HG21	1.67	0.76
1:D:31:SER:HB3	1:D:50:LYS:HA	1.66	0.76
3:C:78:GLN:HA	3:C:81:LYS:HE3	1.73	0.71
2:A:28:ALA:O	2:A:224:LYS:CE	2.41	0.69
1:D:44:ARG:HH12	1:D:46:ARG:HB2	1.58	0.68
1:D:80:ILE:HA	1:D:83:LYS:HG2	1.73	0.68
1:D:99:MET:CE	1:D:119:VAL:HG23	2.24	0.68
1:D:80:ILE:HA	1:D:83:LYS:CG	2.25	0.67
3:C:123:PRO:HA	3:C:126:ILE:HG13	1.77	0.67
3:C:28:LEU:CD1	3:C:60:LYS:HD2	2.24	0.66
1:D:28:LEU:CD1	1:D:60:LYS:HB2	1.97	0.66
1:D:28:LEU:HD12	1:D:60:LYS:HB3	1.75	0.66
1:D:31:SER:HB2	1:D:49:MET:O	1.98	0.63
2:A:359:HIS:O	2:A:361:CSS:N	2.32	0.63
2:B:142:ILE:HD13	2:B:155:VAL:HG12	1.79	0.63
3:C:87:THR:O	3:C:91:MET:HG3	1.98	0.62
2:B:358:GLY:O	2:B:360:HIS:N	2.30	0.62
1:D:15:ILE:HA	1:D:75:MET:CE	2.30	0.61
2:A:356:ARG:NH2	2:B:54:ARG:HE	1.96	0.61
3:C:99:MET:CE	3:C:119:VAL:HG13	2.30	0.61
2:B:317:LEU:CD2	2:B:320:VAL:HG23	2.31	0.61
1:D:99:MET:CE	1:D:119:VAL:CG2	2.79	0.61
1:D:28:LEU:CD1	1:D:48:THR:OG1	2.49	0.60
2:B:315:ARG:HD3	2:B:322:VAL:HG12	1.84	0.59
2:A:356:ARG:HH12	5:A:501:PDA:C	2.16	0.59
1:D:133:TRP:HA	1:D:136:LEU:HD23	1.85	0.59
1:D:22:PRO:HB2	1:D:25:LYS:HG3	1.84	0.59
3:C:20:LYS:HG2	3:C:21:ASN:OD1	2.02	0.59
3:C:35:ASP:N	3:C:35:ASP:OD1	2.36	0.59
1:D:113:ILE:CD1	1:D:114:GLU:H	2.15	0.58
2:B:2:ASN:OD1	2:B:5:ASP:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:LYS:HE2	5:B:501:PDA:H4A1	1.86	0.58
1:D:99:MET:HE3	1:D:119:VAL:CG2	2.34	0.57
2:B:223:HIS:CE1	2:B:224:LYS:CD	2.81	0.57
2:A:359:HIS:O	2:A:362:ALA:N	2.30	0.56
2:A:1:MET:HE2	2:A:6:ILE:HG13	1.88	0.56
1:D:28:LEU:HD13	1:D:48:THR:OG1	2.06	0.56
1:D:85:ILE:HG13	1:D:87:THR:H	1.70	0.55
2:A:177:THR:HG22	2:A:325:PRO:HG3	1.89	0.55
2:B:2:ASN:OD1	2:B:4:THR:N	2.39	0.55
1:D:15:ILE:HA	1:D:75:MET:HE2	1.87	0.55
1:D:17:ASP:OD2	1:D:23:ARG:NH1	2.40	0.55
3:C:10:LEU:CD1	3:C:119:VAL:HB	2.37	0.55
2:B:169:SER:HA	2:B:198:ASP:HB3	1.89	0.54
3:C:99:MET:HE1	3:C:119:VAL:HG13	1.88	0.54
3:C:107:SER:O	3:C:108:ILE:HB	2.07	0.54
2:B:223:HIS:NE2	2:B:224:LYS:HD3	2.20	0.54
3:C:24:ASN:HB3	3:C:60:LYS:HA	1.90	0.54
1:D:12:ARG:CG	1:D:115:ALA:HB1	2.30	0.54
2:A:358:GLY:HA3	2:B:54:ARG:NH1	2.19	0.53
1:D:99:MET:HE3	1:D:119:VAL:HG22	1.89	0.53
1:D:56:VAL:HG11	1:D:59:ALA:HB2	1.90	0.52
2:A:117:THR:HG22	2:A:119:MET:N	2.11	0.52
3:C:75:MET:HE3	3:C:113:ILE:HA	1.92	0.52
1:D:67:SER:OG	1:D:68:ILE:HD12	2.09	0.52
3:C:92:SER:OG	3:C:137:GLU:OE1	2.27	0.52
2:A:359:HIS:O	2:A:360:HIS:C	2.48	0.52
3:C:127:LYS:HA	3:C:130:THR:HB	1.91	0.52
2:A:169:SER:HA	2:A:198:ASP:HB3	1.92	0.51
2:B:317:LEU:CD2	2:B:320:VAL:CG2	2.88	0.51
2:B:11:PRO:HG3	2:B:35:ARG:HH11	1.74	0.51
1:D:51:LEU:HB2	1:D:55:ILE:O	2.10	0.51
3:C:33:VAL:HG12	3:C:48:THR:HG22	1.94	0.50
1:D:19:TYR:CD1	1:D:67:SER:HA	2.46	0.49
2:A:356:ARG:NH1	5:A:501:PDA:C	2.75	0.49
2:B:341:PRO:HB2	2:B:357:ALA:HB1	1.94	0.49
1:D:31:SER:HB3	1:D:50:LYS:CA	2.41	0.49
2:A:121:HIS:NE2	5:A:501:PDA:HB2	2.15	0.49
2:A:317:LEU:HD11	2:A:392:VAL:HG13	1.94	0.49
2:B:152:LEU:HA	2:B:155:VAL:HG22	1.94	0.48
2:B:28:ALA:O	2:B:224:LYS:NZ	2.46	0.48
1:D:133:TRP:O	1:D:136:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:TYR:CD1	3:C:67:SER:HA	2.47	0.48
1:D:15:ILE:HG22	1:D:16:MET:CE	2.44	0.48
2:A:126:ILE:HD13	2:B:254:ILE:HG21	1.95	0.48
3:C:22:PRO:HB2	3:C:25:LYS:HG2	1.96	0.48
2:B:142:ILE:CD1	2:B:155:VAL:HG12	2.44	0.47
2:B:201:GLN:O	2:B:205:HIS:HD2	1.97	0.47
2:A:116:ILE:HG22	2:A:167:ALA:HB3	1.97	0.47
1:D:28:LEU:HD12	1:D:48:THR:OG1	2.14	0.47
2:A:356:ARG:NH1	5:A:501:PDA:O	2.48	0.47
1:D:66:CYS:HB3	2:B:342:HIS:HB2	1.95	0.47
2:B:155:VAL:HG23	2:B:187:ILE:HD13	1.96	0.47
3:C:113:ILE:HD13	3:C:133:TRP:HZ2	1.79	0.47
3:C:24:ASN:HB3	3:C:60:LYS:HG2	1.97	0.46
2:B:177:THR:HG22	2:B:325:PRO:HG3	1.97	0.46
2:A:201:GLN:O	2:A:205:HIS:HD2	1.98	0.46
3:C:10:LEU:HB2	3:C:122:PHE:CE1	2.51	0.46
2:A:117:THR:HG22	2:A:119:MET:HG2	1.92	0.45
1:D:15:ILE:HG22	1:D:16:MET:HE1	1.98	0.45
2:A:249:PHE:HB3	2:B:126:ILE:CG2	2.47	0.45
2:B:16:GLN:NE2	2:B:21:ASP:OD1	2.47	0.45
2:A:356:ARG:HH21	2:B:54:ARG:NE	2.02	0.45
2:B:306:LEU:HB3	2:B:388:ILE:HD11	1.99	0.45
1:D:24:ASN:HB3	1:D:60:LYS:HA	1.98	0.45
1:D:68:ILE:HD13	1:D:125:ARG:NH1	2.31	0.45
3:C:95:PHE:O	3:C:99:MET:HG2	2.17	0.44
2:A:16:GLN:NE2	2:A:21:ASP:OD1	2.50	0.44
3:C:42:GLY:O	3:C:65:GLY:HA2	2.17	0.44
1:D:8:ASP:O	1:D:11:TYR:HD2	2.01	0.44
2:B:313:ARG:NH1	2:B:392:VAL:HG21	2.31	0.44
2:A:27:SER:HA	2:A:30:THR:O	2.18	0.44
2:B:116:ILE:HG22	2:B:167:ALA:HB3	2.00	0.44
2:B:298:GLU:OE1	2:B:301:ARG:NH2	2.45	0.44
2:B:27:SER:HA	2:B:30:THR:O	2.18	0.44
2:B:315:ARG:CZ	2:B:322:VAL:HG11	2.46	0.44
3:C:38:ASN:HB3	3:C:43:ASP:HB2	2.00	0.44
1:D:24:ASN:HD21	1:D:81:LYS:HE2	1.83	0.43
2:A:220:LEU:HG	2:A:233:VAL:HB	2.00	0.43
3:C:36:MET:HB3	3:C:131:LEU:HD11	1.99	0.43
2:A:42:ASP:OD1	2:B:42:ASP:OD1	2.37	0.43
2:A:117:THR:HB	2:A:120:GLU:HG2	2.00	0.43
3:C:99:MET:HE3	3:C:119:VAL:HG13	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:MET:O	1:D:80:ILE:CD1	2.67	0.43
2:B:224:LYS:H	2:B:224:LYS:HG2	1.72	0.43
2:B:302:HIS:NE2	2:B:306:LEU:HD11	2.33	0.43
2:A:153:GLU:OE2	2:A:153:GLU:HA	2.18	0.43
1:D:105:ASP:OD1	1:D:108:ILE:HD11	2.19	0.43
1:D:25:LYS:HA	1:D:61:PHE:O	2.19	0.42
1:D:12:ARG:NH2	1:D:115:ALA:HA	2.33	0.42
1:D:138:LYS:HD2	1:D:138:LYS:HA	1.80	0.42
2:B:304:HIS:O	2:B:305:LYS:C	2.58	0.42
1:D:80:ILE:HA	1:D:83:LYS:HG3	2.01	0.42
2:B:317:LEU:HD23	2:B:320:VAL:HG23	2.02	0.42
3:C:84:ASP:OD2	3:C:85:ILE:N	2.53	0.42
1:D:125:ARG:O	1:D:128:CYS:HB2	2.20	0.41
2:A:57:HIS:CD2	2:B:354:ALA:HB1	2.55	0.41
2:A:155:VAL:HG12	2:A:187:ILE:HG21	2.01	0.41
2:A:222:SER:HB3	2:A:231:VAL:HG13	2.02	0.41
1:D:113:ILE:CG1	1:D:114:GLU:H	2.32	0.41
1:D:112:ASP:HB3	1:D:113:ILE:H	1.70	0.41
1:D:127:LYS:HA	1:D:130:THR:OG1	2.21	0.41
2:A:28:ALA:O	2:A:224:LYS:NZ	2.52	0.41
3:C:27:VAL:HG23	3:C:62:GLU:HB2	2.01	0.41
2:B:315:ARG:NH1	2:B:322:VAL:CG1	2.71	0.41
2:B:220:LEU:HG	2:B:233:VAL:HB	2.02	0.41
2:A:302:HIS:NE2	2:A:306:LEU:HD11	2.35	0.41
2:A:249:PHE:HB3	2:B:126:ILE:HG22	2.03	0.41
2:A:383:ASN:HA	2:A:387:GLU:OE1	2.20	0.41
2:B:2:ASN:CG	2:B:4:THR:H	2.24	0.40
2:B:173:ASN:HB3	5:B:501:PDA:H2A1	2.02	0.40
2:A:1:MET:HG3	2:A:298:GLU:CG	2.41	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	D	135/155 (87%)	116 (86%)	13 (10%)	6 (4%)	2 21
2	A	402/419 (96%)	385 (96%)	15 (4%)	2 (0%)	29 68
2	B	402/419 (96%)	387 (96%)	13 (3%)	2 (0%)	29 68
3	C	132/155 (85%)	117 (89%)	11 (8%)	4 (3%)	4 30
All	All	1071/1148 (93%)	1005 (94%)	52 (5%)	14 (1%)	12 48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	114	GLU
3	C	29	ASN
2	A	360	HIS
2	B	53	HIS
2	B	359	HIS
3	C	30	ASP
3	C	108	ILE
1	D	84	ASP
1	D	112	ASP
1	D	113	ILE
3	C	104	TYR
1	D	85	ILE
1	D	109	ASP
2	A	53	HIS

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	D	117/132 (89%)	102 (87%)	15 (13%)	4 22
2	A	335/348 (96%)	325 (97%)	10 (3%)	41 71
2	B	335/348 (96%)	320 (96%)	15 (4%)	27 61
3	C	115/131 (88%)	107 (93%)	8 (7%)	15 46
All	All	902/959 (94%)	854 (95%)	48 (5%)	22 55

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	9	THR
1	D	10	LEU
1	D	11	TYR
1	D	14	VAL
1	D	30	ASP
1	D	31	SER
1	D	41	CYS
1	D	54	ASP
1	D	60	LYS
1	D	62	GLU
1	D	76	MET
1	D	99	MET
1	D	120	SER
1	D	122	PHE
1	D	136	LEU
2	A	0	HIS
2	A	54	ARG
2	A	56	VAL
2	A	101	LEU
2	A	133	LYS
2	A	186	LYS
2	A	207	LYS
2	A	341	PRO
2	A	380	TYR
2	A	403	THR
2	B	2	ASN
2	B	56	VAL
2	B	76	LYS
2	B	101	LEU
2	B	109	LYS
2	B	186	LYS
2	B	224	LYS
2	B	261	GLU
2	B	318	ASP
2	B	351	GLU
2	B	356	ARG
2	B	380	TYR
2	B	396	GLN
2	B	399	LYS
2	B	405	VAL
3	C	14	VAL
3	C	21	ASN

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Mol	Chain	Res	Type
3	C	35	ASP
3	C	36	MET
3	C	62	GLU
3	C	76	MET
3	C	96	SER
3	C	114	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	6	ASN
1	D	21	ASN
2	A	359	HIS
3	C	38	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
2	CSS	A	361	2	4,6,7	1.12	0	1,6,8	0.49	0
3	CSS	C	41	3	4,6,7	0.54	0	1,6,8	1.16	0
2	CSS	B	361	2	4,6,7	0.86	0	1,6,8	0.08	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	CSS	A	361	2	-	0/1/5/7	-
3	CSS	C	41	3	-	1/1/5/7	-
2	CSS	B	361	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	41	CSS	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	CSS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	PDA	A	501	-	20,21,21	2.96	3 (15%)	26,30,30	1.63	7 (26%)
5	PDA	B	501	-	20,21,21	3.09	3 (15%)	26,30,30	1.31	5 (19%)

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
5	PDA	A	501	-	-	9/15/15/15	0/1/1/1
5	PDA	B	501	-	-	6/15/15/15	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	PDA	C3-C2	9.52	1.50	1.40
5	A	501	PDA	C3-C2	9.01	1.49	1.40
5	B	501	PDA	C5-C4	6.83	1.50	1.40
5	B	501	PDA	C3-C4	6.76	1.50	1.40
5	A	501	PDA	C3-C4	6.62	1.50	1.40
5	A	501	PDA	C5-C4	5.96	1.48	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	501	PDA	OP3-P-OP2	2.84	118.49	107.64
5	A	501	PDA	C6-N1-C2	2.80	124.36	119.17
5	A	501	PDA	C4A-C4-C3	2.78	123.02	120.04
5	A	501	PDA	CB-CA-C	2.71	116.33	110.20
5	A	501	PDA	OP3-P-OP4	-2.63	99.72	106.73
5	B	501	PDA	C6-N1-C2	2.59	123.97	119.17
5	A	501	PDA	C4-C4A-N	-2.55	104.75	111.78
5	B	501	PDA	O3A-C3-C2	2.19	122.27	117.49
5	B	501	PDA	C4-C3-C2	-2.14	116.78	120.06
5	B	501	PDA	C2A-C2-C3	2.14	123.53	120.89
5	A	501	PDA	C-CA-N	-2.11	105.19	112.77
5	A	501	PDA	C4-C3-C2	-2.05	116.92	120.06

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	PDA	CB-CA-N-C4A
5	A	501	PDA	C-CA-N-C4A
5	B	501	PDA	CB-CA-N-C4A
5	B	501	PDA	C-CA-N-C4A
5	B	501	PDA	C3-C4-C4A-N

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Mol	Chain	Res	Type	Atoms
5	B	501	PDA	C5-C4-C4A-N
5	A	501	PDA	C5-C4-C4A-N
5	A	501	PDA	C4-C4A-N-CA
5	B	501	PDA	C4-C4A-N-CA
5	A	501	PDA	O-C-CA-CB
5	A	501	PDA	O-C-CA-N
5	A	501	PDA	OXT-C-CA-CB
5	A	501	PDA	OXT-C-CA-N
5	A	501	PDA	C3-C4-C4A-N
5	B	501	PDA	C5A-OP4-P-OP1

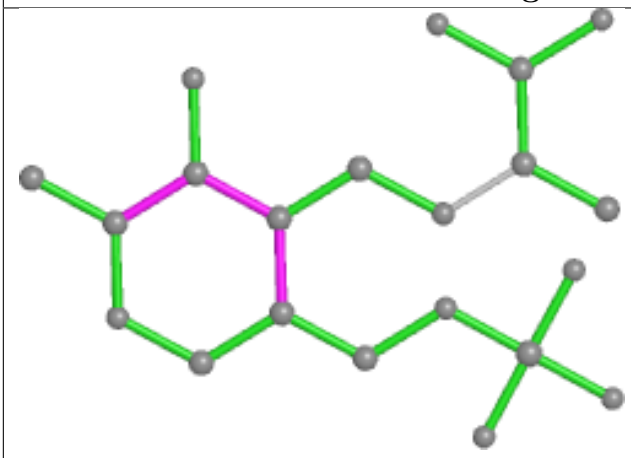
There are no ring outliers.

2 monomers are involved in 8 short contacts:

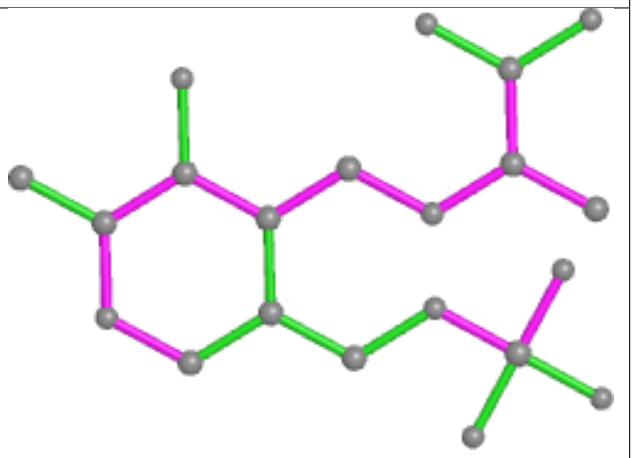
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	PDA	5	0
5	B	501	PDA	3	0

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.

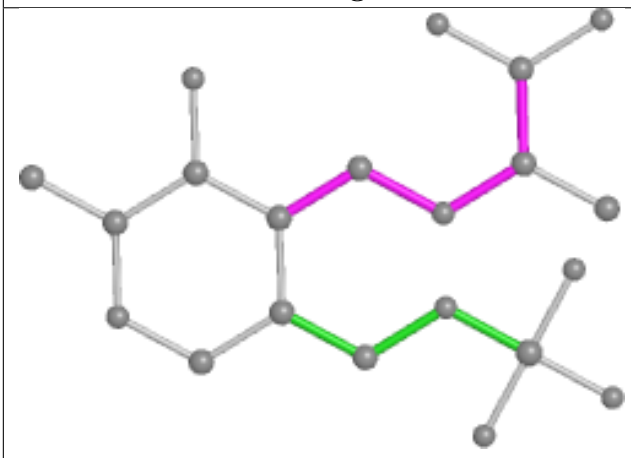
Ligand PDA A 501



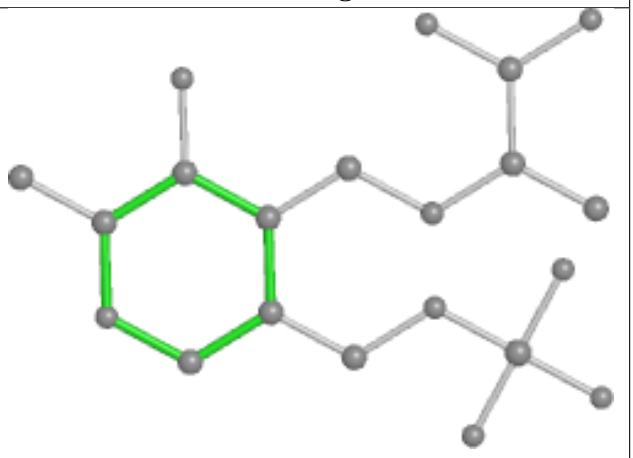
Bond lengths



Bond angles

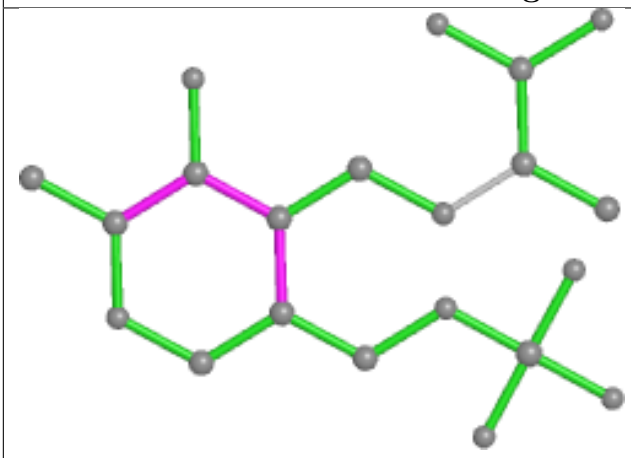


Torsions

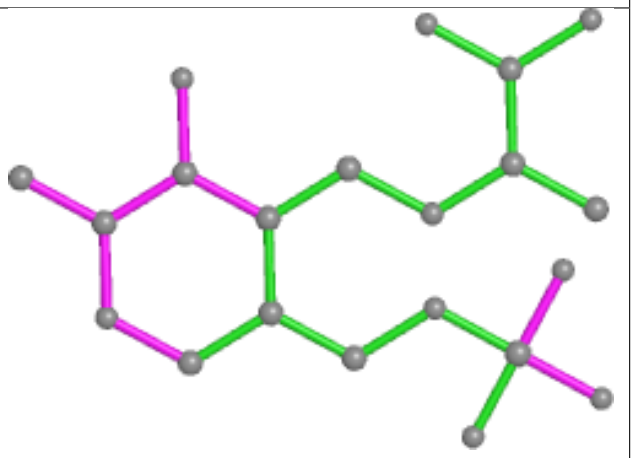


Rings

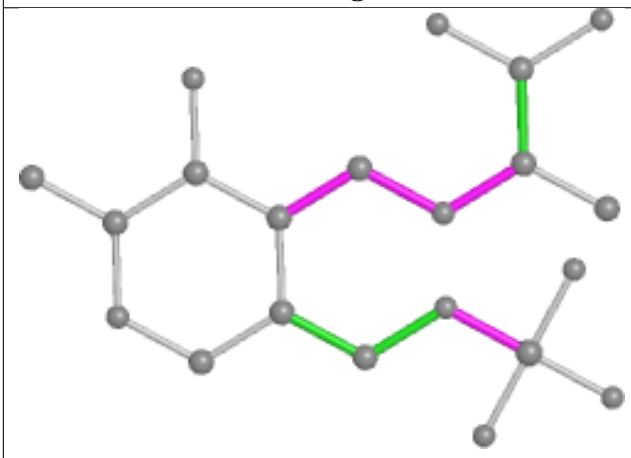
Ligand PDA B 501



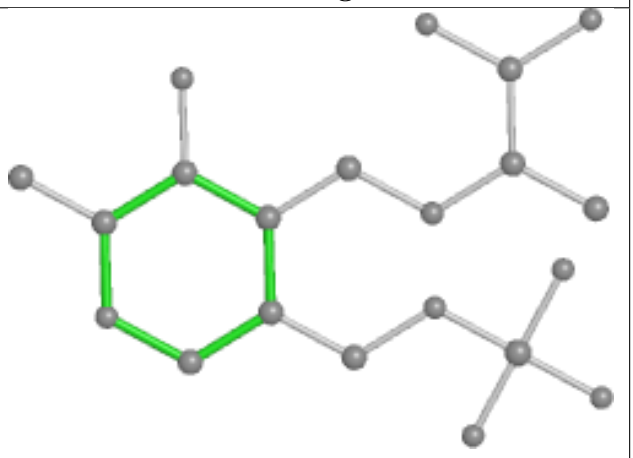
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	D	137/155 (88%)	0.31	4 (2%) 51 45	114, 158, 196, 300	0
2	A	404/419 (96%)	-0.31	0 100 100	73, 101, 130, 161	0
2	B	404/419 (96%)	-0.32	1 (0%) 95 93	73, 110, 144, 190	0
3	C	134/155 (86%)	0.07	2 (1%) 73 68	109, 127, 162, 173	0
All	All	1079/1148 (93%)	-0.19	7 (0%) 89 86	73, 113, 165, 300	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	27	VAL	2.4
1	D	46	ARG	2.2
1	D	104	TYR	2.1
1	D	50	LYS	2.1
2	B	315	ARG	2.0
3	C	82	GLY	2.0
1	D	94	ILE	2.0

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
3	CSS	C	41	7/8	0.67	0.34	156,161,165,169	0
2	CSS	B	361	7/8	0.85	0.19	112,119,123,127	0
2	CSS	A	361	7/8	0.94	0.20	96,97,98,99	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

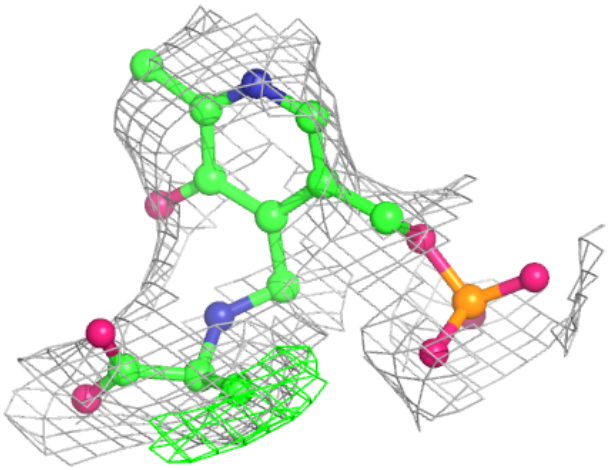
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

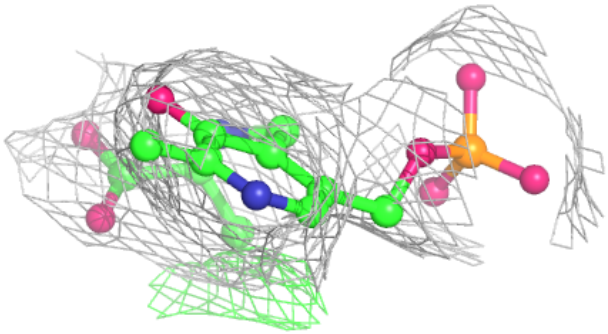
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PDA	A	501	21/21	0.92	0.25	76,94,104,127	0
5	PDA	B	501	21/21	0.93	0.25	83,123,142,144	0
4	ZN	D	201	1/1	0.97	0.06	81,81,81,81	0
4	ZN	C	201	1/1	0.98	0.11	95,95,95,95	0

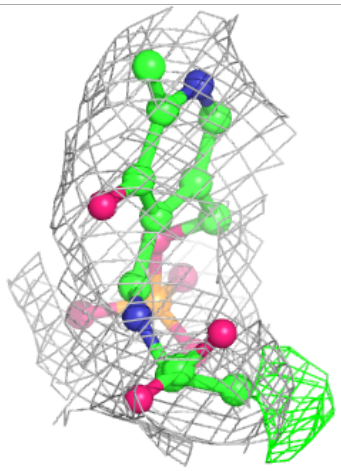
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PDA A 501:

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

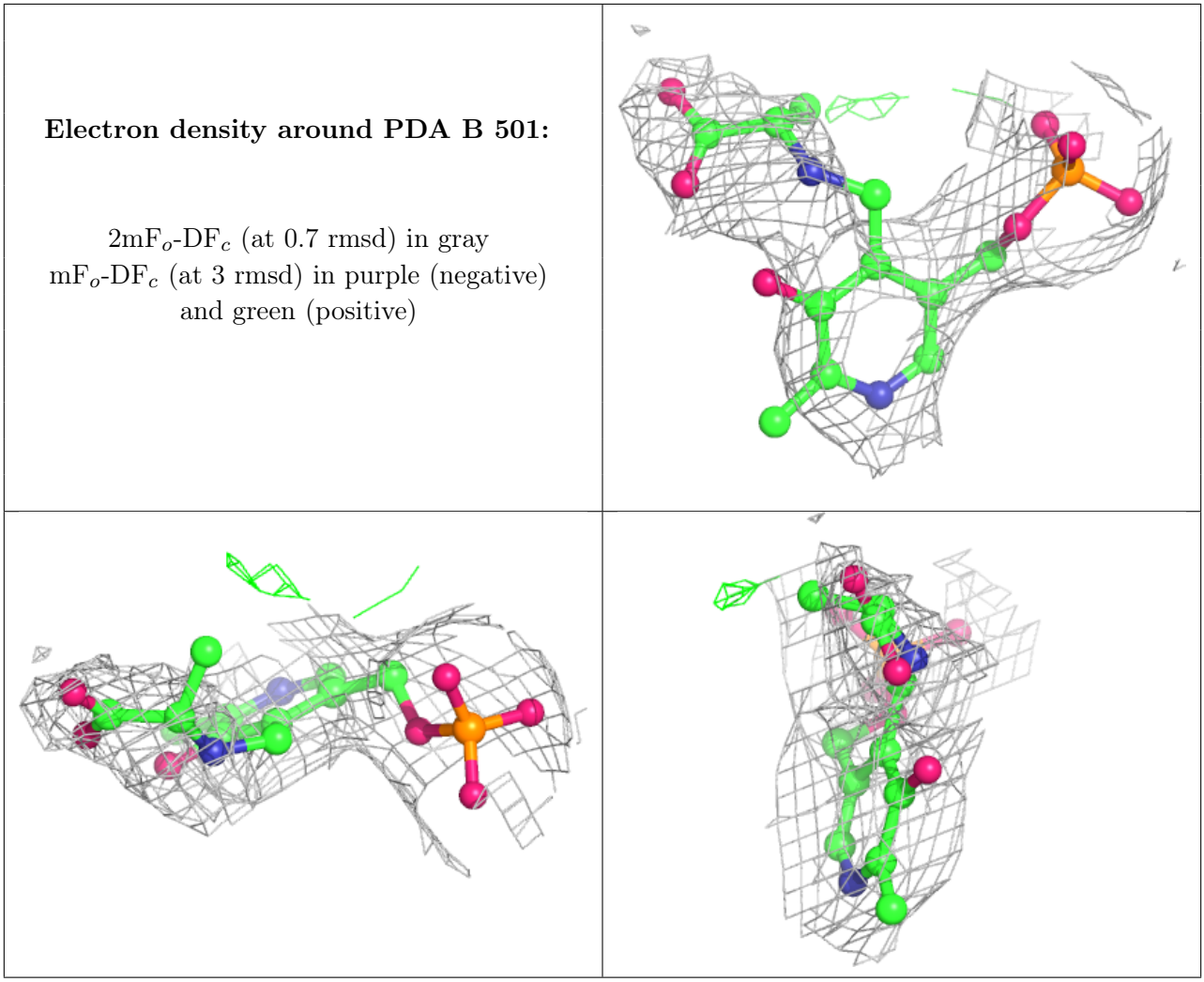






Electron density around PDA B 501:

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



6.5 Other polymers

There are no such residues in this entry.