



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:06 am BST

PDB ID : 3RC0
Title : Human SETD6 in complex with RelA Lys310 peptide
Authors : Chang, Y.; Levy, D.; Horton, J.R.; Peng, J.; Zhang, X.; Gozani, O.; Cheng, X.
Deposited on : 2011-03-30
Resolution : 2.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

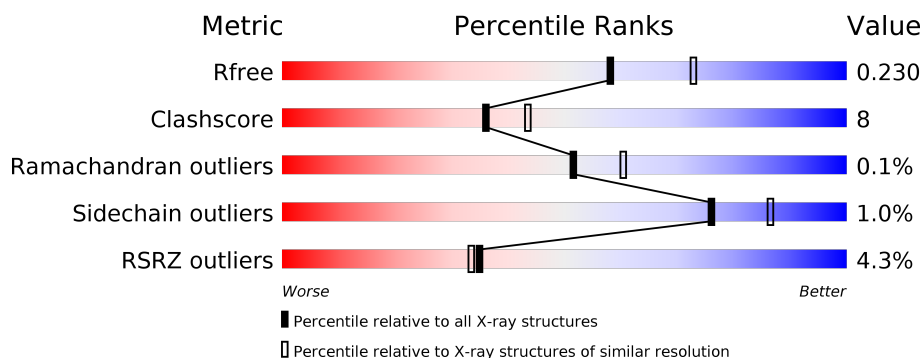
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	449	<div> <div>4%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	B	449	<div> <div>4%</div> <div>80%</div> <div>12%</div> <div>8%</div> </div>
2	P	15	<div> <div>27%</div> <div>27%</div> <div>13%</div> <div>60%</div> </div>
2	Q	15	<div> <div>7%</div> <div>93%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	482	-	-	X	-
3	EDO	B	479	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7181 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.

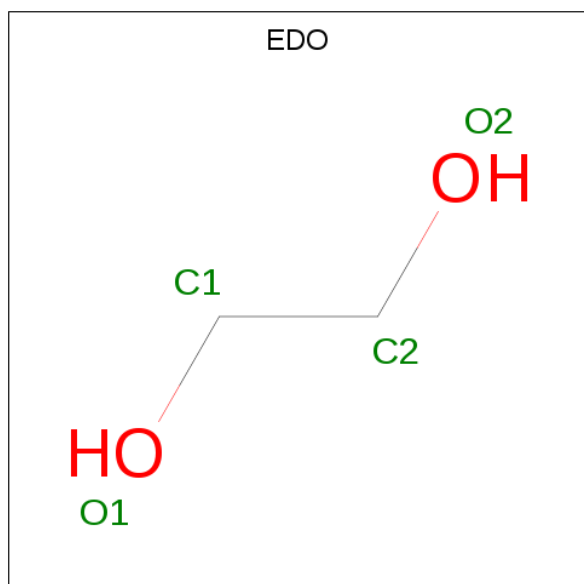
- Molecule 1 is a protein called N-lysine methyltransferase SETD6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	3	0
			3288	2101	567	599	21			
1	B	414	Total	C	N	O	S	0	2	0
			3238	2074	557	586	21			

- Molecule 2 is a protein called Transcription factor p65 peptide.

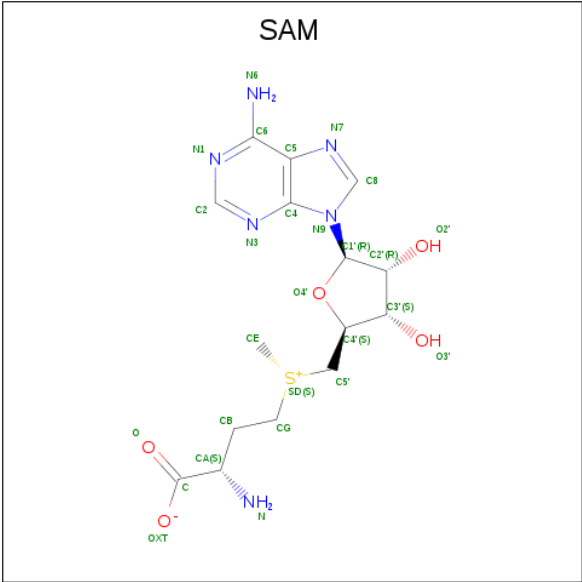
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			43	29	7	7			
2	Q	1	Total	C	N	O	0	0	0
			9	6	2	1			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).

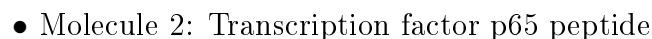
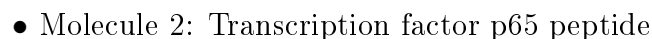


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	228	Total	O	0	0
			228	228		
5	P	2	Total	O	0	0
			2	2		
5	B	255	Total	O	0	0
			255	255		

- Molecule 1: N-lysine methyltransferase SETD6





ARG	LYS	ARG	THR	TYR	GLU	THR	PHE	K310	SER	ILE	MET	LYS	LYS	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.62Å 64.50Å 73.76Å 78.73° 70.60° 64.21°	Depositor
Resolution (Å)	34.72 – 2.19 34.72 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.5 (34.72-2.19) 92.6 (34.72-2.19)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.166 , 0.234 0.164 , 0.230	Depositor DCC
R_{free} test set	2031 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7181	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: EDO, SAM

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	0.32	0/3370	0.48	0/4588
1	B	0.31	0/3317	0.47	0/4518
2	P	0.47	0/43	0.77	0/55
2	Q	0.22	0/8	0.61	0/8
All	All	0.32	0/6738	0.48	0/9169

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain

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	A	3288	0	3235	59	0
1	B	3238	0	3195	39	0
2	P	43	0	40	26	0
2	Q	9	0	12	0	0
3	A	40	0	60	8	0
3	B	24	0	36	7	0
4	A	27	0	22	1	0
4	B	27	0	22	2	0
5	A	228	0	0	2	0
5	B	255	0	0	1	0
5	P	2	0	0	0	0
All	All	7181	0	6622	106	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 8.

All (106) 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:A:365:GLU:HG2	3:A:482:EDO:H12	1.39	1.01
1:A:296:MET:HG3	2:P:309:PHE:CZ	2.07	0.89
1:A:397:GLU:HG3	1:B:141:ARG:NH2	1.90	0.85
1:A:260:LEU:HB3	2:P:312:ILE:HB	1.56	0.84
3:B:477:EDO:H21	4:B:480:SAM:H2	1.64	0.78
1:A:372:LYS:HD2	1:A:396:GLU:HG3	1.66	0.78
1:A:283:ASN:HD21	2:P:312:ILE:HD12	1.51	0.75
1:A:260:LEU:H	2:P:312:ILE:HG22	1.55	0.72
1:A:260:LEU:HD21	1:A:267:LEU:HD23	1.72	0.71
1:B:260:LEU:HD21	1:B:267:LEU:HD23	1.74	0.70
1:A:225:PHE:CE1	2:P:312:ILE:HG13	2.29	0.68
1:A:20:ASP:N	1:A:21:PRO:HD2	2.09	0.68
1:A:225:PHE:HA	2:P:310:LYS:O	1.94	0.67
2:P:310:LYS:HG2	2:P:312:ILE:HD11	1.77	0.67
1:B:377:PRO:HD2	1:B:380:GLU:OE1	1.96	0.66
1:A:149:GLU:HG2	1:A:152:ARG:HE	1.62	0.65
1:A:225:PHE:HE1	2:P:312:ILE:HG13	1.62	0.64
1:B:449:TRP:HD1	3:B:479:EDO:H22	1.62	0.64
1:B:449:TRP:CD1	3:B:479:EDO:H22	2.31	0.64
1:B:185:ARG:O	1:B:189:GLN:HG2	1.98	0.63
1:B:193:LEU:HB3	1:B:194:PRO:HD3	1.81	0.62
2:P:310:LYS:HB2	2:P:310:LYS:HZ2	1.64	0.62
2:P:310:LYS:HB2	2:P:310:LYS:NZ	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:HG2	3:A:482:EDO:C1	2.24	0.62
1:B:328:THR:O	1:B:332:ARG:HG3	2.01	0.61
2:P:310:LYS:CB	2:P:310:LYS:NZ	2.64	0.61
1:A:260:LEU:H	2:P:312:ILE:CG2	2.14	0.60
1:A:283:ASN:ND2	2:P:312:ILE:HD12	2.16	0.60
1:A:161:GLU:OE2	1:A:165:ARG:HD3	2.02	0.60
1:A:427:TYR:O	3:A:476:EDO:H21	2.03	0.59
1:A:20:ASP:H	1:A:21:PRO:HD2	1.65	0.59
1:A:397:GLU:HG3	1:B:141:ARG:HH22	1.68	0.58
1:A:228:PRO:HG3	2:P:311:SER:OG	2.02	0.58
1:B:97:LEU:HD13	1:B:242:VAL:HG11	1.87	0.57
1:B:188:TYR:HA	1:B:192:VAL:HB	1.87	0.56
1:B:276:PRO:HG2	1:B:279:HIS:CG	2.41	0.56
1:A:288:MET:HE1	2:P:309:PHE:CE2	2.42	0.55
1:B:255:ASN:OD1	3:B:476:EDO:H22	2.07	0.55
1:A:296:MET:HG3	2:P:309:PHE:CE2	2.42	0.54
1:B:323:LEU:HD13	1:B:335:VAL:HG11	1.91	0.53
1:A:162:GLU:O	1:A:166[A]:CYS:HB3	2.10	0.52
2:P:310:LYS:CG	2:P:312:ILE:HD11	2.40	0.51
1:A:141:ARG:HB2	1:A:142:PRO:HD3	1.92	0.51
1:A:332:ARG:O	1:A:335:VAL:HB	2.11	0.50
1:B:409:LYS:HZ2	1:B:411:SER:H	1.59	0.50
1:B:218:ALA:HA	1:B:221:MET:HE2	1.95	0.48
1:A:241:PRO:HB3	2:P:308:THR:CA	2.43	0.48
1:B:161:GLU:HG2	1:B:165:ARG:HD3	1.96	0.48
3:B:477:EDO:C2	4:B:480:SAM:H2	2.38	0.48
1:B:338:ARG:HH12	1:B:376:MET:HG3	1.79	0.48
1:A:147:TRP:CE3	1:A:219:LEU:HD21	2.49	0.48
3:A:483:EDO:H12	5:A:563:HOH:O	2.14	0.48
1:B:328:THR:HG23	1:B:331:GLU:OE2	2.14	0.47
1:B:20:ASP:N	1:B:21:PRO:CD	2.78	0.47
1:A:405:ILE:N	1:A:406:PRO:HD2	2.30	0.47
1:A:425:GLN:HA	3:A:476:EDO:H12	1.96	0.47
1:A:283:ASN:HD21	2:P:312:ILE:CD1	2.25	0.47
1:A:240:SER:OG	1:A:241:PRO:HD2	2.16	0.46
5:A:698:HOH:O	1:B:206:ARG:HD3	2.14	0.46
1:B:450:ARG:HE	3:B:479:EDO:C1	2.28	0.46
1:B:450:ARG:HE	3:B:479:EDO:H12	1.81	0.46
1:A:260:LEU:CB	2:P:312:ILE:HB	2.38	0.46
1:A:347:MET:HE2	1:A:366:GLU:HG3	1.97	0.46
1:A:209:SER:HB3	1:A:212:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:H	3:A:482:EDO:C1	2.29	0.45
1:B:364:GLU:OE2	1:B:399:SER:HB2	2.17	0.45
1:A:20:ASP:N	1:A:21:PRO:CD	2.76	0.45
1:A:226:GLN:CG	2:P:308:THR:H	2.29	0.45
1:A:347:MET:HA	1:A:347:MET:HE2	1.99	0.45
1:A:156:PRO:HA	1:A:159:TRP:CD1	2.52	0.44
1:B:364:GLU:HG3	1:B:400:LEU:HB2	1.98	0.44
1:A:245:PRO:O	1:A:246:ALA:HB3	2.17	0.44
1:A:284:THR:O	2:P:312:ILE:HD13	2.17	0.44
1:A:288:MET:HE1	2:P:309:PHE:HE2	1.81	0.44
1:B:315:MET:HB3	1:B:339:TRP:HH2	1.83	0.44
1:A:135:ALA:HA	1:A:136:PRO:HD3	1.85	0.44
1:B:341:PHE:CE2	1:B:345:LEU:HD11	2.52	0.44
1:A:365:GLU:H	3:A:482:EDO:H11	1.84	0.43
1:A:260:LEU:HD11	1:A:267:LEU:HB3	1.99	0.43
1:B:100:GLN:HG2	5:B:549:HOH:O	2.18	0.43
1:B:316:VAL:HG23	1:B:319:ARG:NH2	2.33	0.43
1:A:37:SER:HA	1:A:38:PRO:HD3	1.88	0.43
1:B:276:PRO:HG2	1:B:279:HIS:CD2	2.54	0.43
1:A:293:LEU:HD22	1:A:299:PHE:CZ	2.53	0.43
1:A:98:LEU:HB3	1:A:243:MET:HB2	2.01	0.43
1:B:402:ILE:HG13	1:B:471:LEU:HD11	2.00	0.43
1:A:199:HIS:N	1:A:200:PRO:HD3	2.34	0.43
1:A:448:SER:O	1:A:452:GLN:HG3	2.19	0.43
1:B:99:SER:HB3	1:B:242:VAL:HG22	2.01	0.43
2:P:311:SER:C	2:P:312:ILE:HG12	2.37	0.43
1:A:147:TRP:CD2	1:A:219:LEU:HD21	2.54	0.42
1:B:20:ASP:N	1:B:21:PRO:HD2	2.35	0.42
1:B:256:HIS:HB2	1:B:282:PHE:O	2.19	0.42
1:B:38:PRO:O	1:B:80:ARG:NH1	2.53	0.42
1:A:193:LEU:N	1:A:194:PRO:HD2	2.35	0.42
1:A:122:TRP:NE1	2:P:307:GLU:O	2.42	0.42
1:A:219:LEU:HD12	1:A:223:TYR:CD2	2.55	0.41
3:A:480:EDO:H11	4:A:484:SAM:N1	2.34	0.41
1:B:367:LEU:HD23	1:B:400:LEU:HD13	2.03	0.41
1:A:110:GLU:OE2	1:A:113:ARG:HD3	2.21	0.41
1:A:123:VAL:HB	1:A:124:PRO:HD3	2.03	0.41
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.89	0.41
1:B:250:LEU:HD12	1:B:250:LEU:N	2.37	0.41
1:B:404:ASN:OD1	1:B:407:LYS:HE3	2.21	0.40
1:A:226:GLN:O	2:P:311:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:TRP:CD1	1:B:142:PRO:HG2	2.56	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	417/449 (93%)	411 (99%)	6 (1%)	0	100	100
1	B	410/449 (91%)	404 (98%)	6 (2%)	0	100	100
2	P	4/15 (27%)	3 (75%)	0	1 (25%)	0	0
All	All	831/913 (91%)	818 (98%)	12 (1%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	309	PHE

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	347/385 (90%)	343 (99%)	4 (1%)	71	83
1	B	342/385 (89%)	340 (99%)	2 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	4/15 (27%)	3 (75%)	1 (25%)	0	0
2	Q	1/15 (7%)	0	1 (100%)	0	0
All	All	694/800 (87%)	686 (99%)	8 (1%)	76	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166[A]	CYS
1	A	166[B]	CYS
1	A	201	ASP
1	A	396	GLU
2	P	312	ILE
1	B	141	ARG
1	B	323	LEU
2	Q	310	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 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	$\# Z > 2$
3	EDO	A	482	-	3,3,3	0.47	0	2,2,2	0.18	0
3	EDO	A	474	-	3,3,3	0.41	0	2,2,2	0.49	0
3	EDO	A	483	-	3,3,3	0.57	0	2,2,2	0.29	0
3	EDO	A	477	-	3,3,3	0.49	0	2,2,2	0.20	0
3	EDO	B	477	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	A	476	-	3,3,3	0.37	0	2,2,2	0.98	0
4	SAM	B	480	-	21,29,29	1.15	2 (9%)	18,42,42	1.56	2 (11%)
3	EDO	A	480	-	3,3,3	0.53	0	2,2,2	0.26	0
3	EDO	B	474	-	3,3,3	0.50	0	2,2,2	0.40	0
3	EDO	A	479	-	3,3,3	0.50	0	2,2,2	0.26	0
3	EDO	B	475	-	3,3,3	0.57	0	2,2,2	0.21	0
4	SAM	A	484	-	21,29,29	1.14	2 (9%)	18,42,42	1.54	1 (5%)
3	EDO	A	475	-	3,3,3	0.44	0	2,2,2	0.35	0
3	EDO	A	481	-	3,3,3	0.47	0	2,2,2	0.29	0
3	EDO	B	478	-	3,3,3	0.51	0	2,2,2	0.26	0
3	EDO	A	478	-	3,3,3	0.52	0	2,2,2	0.30	0
3	EDO	B	476	-	3,3,3	0.51	0	2,2,2	0.27	0
3	EDO	B	479	-	3,3,3	0.56	0	2,2,2	0.06	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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	482	-	-	0/1/1/1	-
3	EDO	A	474	-	-	1/1/1/1	-
3	EDO	A	483	-	-	0/1/1/1	-
3	EDO	A	477	-	-	0/1/1/1	-
3	EDO	B	477	-	-	0/1/1/1	-
3	EDO	A	476	-	-	1/1/1/1	-
4	SAM	B	480	-	-	2/8/33/33	0/3/3/3
3	EDO	A	480	-	-	1/1/1/1	-
3	EDO	B	474	-	-	1/1/1/1	-
3	EDO	A	479	-	-	0/1/1/1	-
3	EDO	B	475	-	-	0/1/1/1	-
4	SAM	A	484	-	-	3/8/33/33	0/3/3/3
3	EDO	A	475	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	481	-	-	1/1/1/1	-
3	EDO	B	478	-	-	0/1/1/1	-
3	EDO	A	478	-	-	0/1/1/1	-
3	EDO	B	476	-	-	0/1/1/1	-
3	EDO	B	479	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	484	SAM	C2-N3	3.40	1.37	1.32
4	B	480	SAM	C2-N3	3.20	1.37	1.32
4	A	484	SAM	C2-N1	2.33	1.38	1.33
4	B	480	SAM	C2-N1	2.30	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	484	SAM	N3-C2-N1	-5.50	120.08	128.68
4	B	480	SAM	N3-C2-N1	-5.37	120.28	128.68
4	B	480	SAM	C3'-C2'-C1'	2.12	104.17	100.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

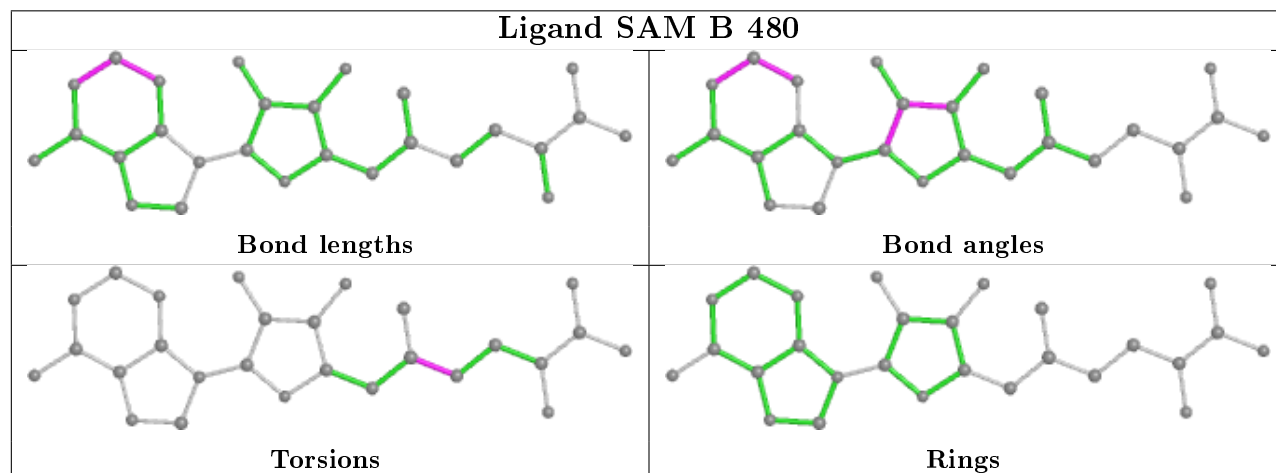
Mol	Chain	Res	Type	Atoms
4	B	480	SAM	CB-CG-SD-CE
4	B	480	SAM	CB-CG-SD-C5'
4	A	484	SAM	CB-CG-SD-CE
4	A	484	SAM	CB-CG-SD-C5'
3	A	475	EDO	O1-C1-C2-O2
3	A	480	EDO	O1-C1-C2-O2
3	A	481	EDO	O1-C1-C2-O2
4	A	484	SAM	C-CA-CB-CG
3	A	474	EDO	O1-C1-C2-O2
3	A	476	EDO	O1-C1-C2-O2
3	B	474	EDO	O1-C1-C2-O2

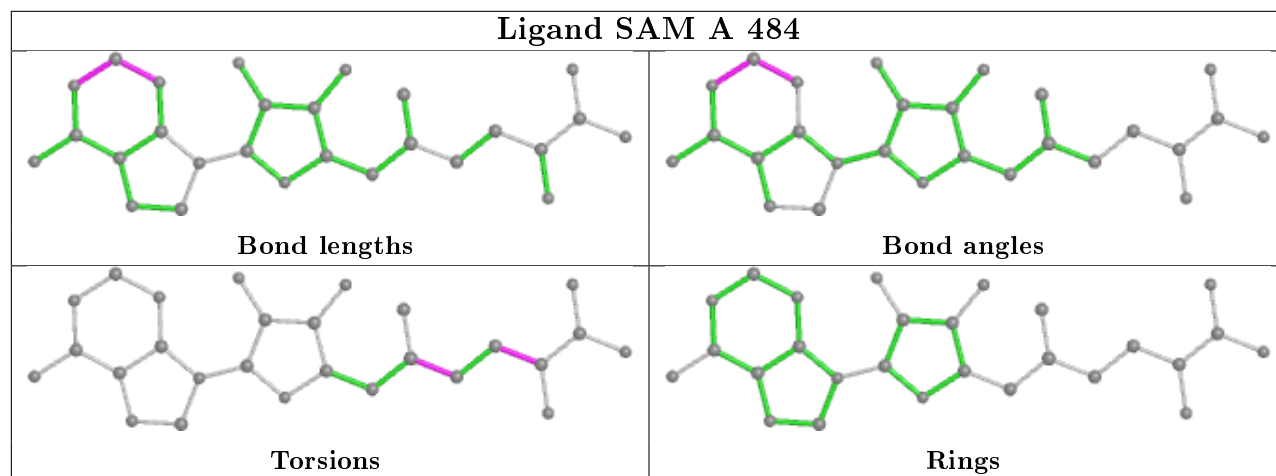
There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	482	EDO	4	0
3	A	483	EDO	1	0
3	B	477	EDO	2	0
3	A	476	EDO	2	0
4	B	480	SAM	2	0
3	A	480	EDO	1	0
4	A	484	SAM	1	0
3	B	476	EDO	1	0
3	B	479	EDO	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 than 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.





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, 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	420/449 (93%)	-0.06	16 (3%) 40 38	14, 27, 59, 87	0
1	B	414/449 (92%)	-0.16	16 (3%) 39 37	13, 26, 57, 85	0
2	P	6/15 (40%)	7.28	4 (66%) 0 0	45, 57, 63, 64	0
2	Q	1/15 (6%)	1.84	0 100 100	34, 34, 34, 34	0
All	All	841/928 (90%)	-0.06	36 (4%) 35 33	13, 26, 58, 87	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	309	PHE	16.9
2	P	311	SER	10.7
2	P	308	THR	7.6
1	A	384	LEU	5.2
1	B	333	HIS	5.1
2	P	312	ILE	4.6
1	A	387	GLN	4.5
1	B	328	THR	4.4
1	A	382	ARG	4.2
1	B	19	LEU	3.8
1	B	229	LEU	3.7
1	A	378	ALA	3.6
1	A	381	PHE	3.6
1	B	381	PHE	3.6
1	B	378	ALA	3.4
1	A	328	THR	3.4
1	A	19	LEU	3.3
1	A	333	HIS	3.2
1	A	386	ASP	3.1
1	B	231	GLU	3.0
1	B	399	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	384	LEU	2.8
1	A	341	PHE	2.7
1	A	236	LYS	2.6
1	A	330	ALA	2.6
1	B	330	ALA	2.6
1	A	385	LYS	2.6
1	B	332	ARG	2.5
1	A	377	PRO	2.5
1	A	340	ASP	2.3
1	B	329	GLU	2.2
1	B	377	PRO	2.2
1	B	386	ASP	2.1
1	B	340	ASP	2.1
1	A	334	LEU	2.0
1	B	331	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

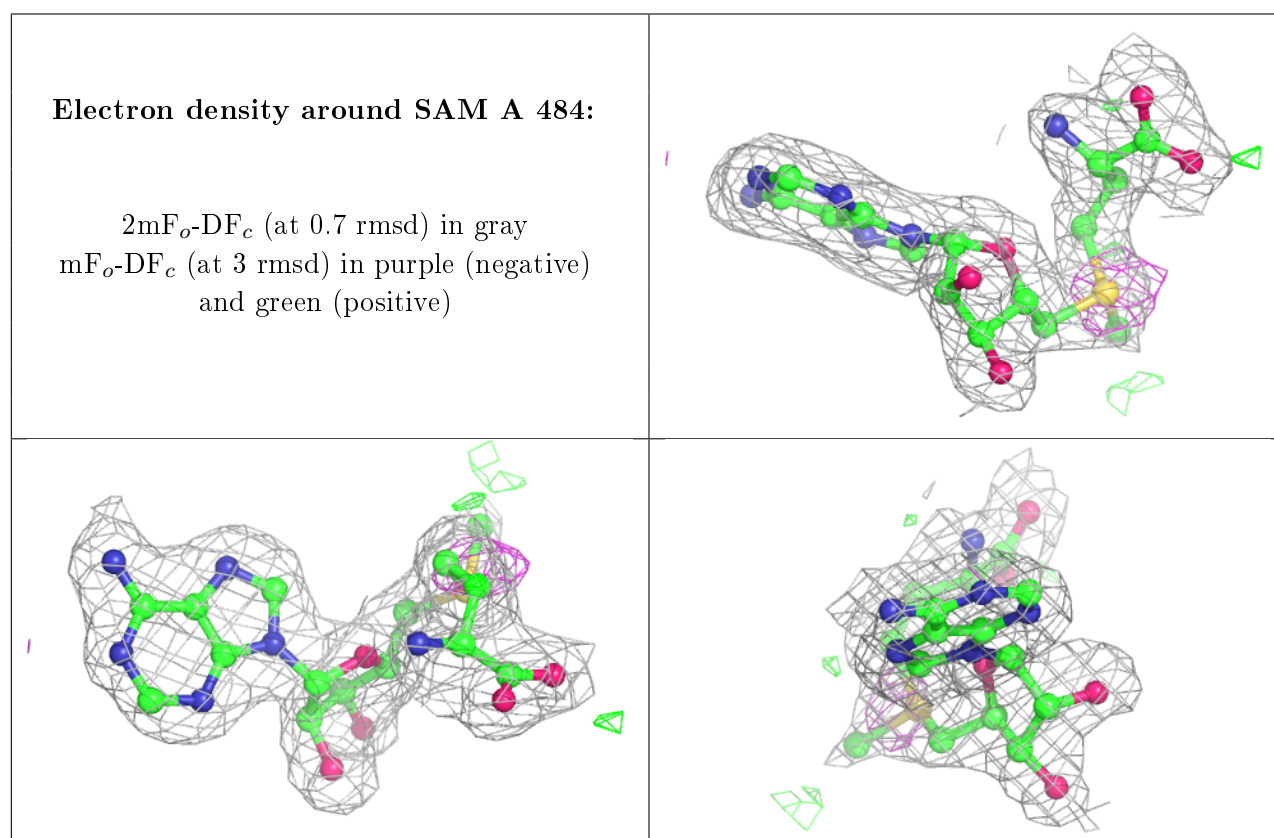
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	475	4/4	0.84	0.18	31,35,36,42	0
3	EDO	A	477	4/4	0.86	0.17	39,41,44,44	0
3	EDO	A	483	4/4	0.86	0.18	34,39,40,44	0
3	EDO	B	479	4/4	0.87	0.37	24,28,32,42	0
3	EDO	B	477	4/4	0.89	0.25	28,32,39,41	0
3	EDO	A	480	4/4	0.90	0.15	20,29,31,39	0
3	EDO	A	482	4/4	0.91	0.15	39,39,43,46	0
3	EDO	A	481	4/4	0.92	0.13	36,39,41,43	0

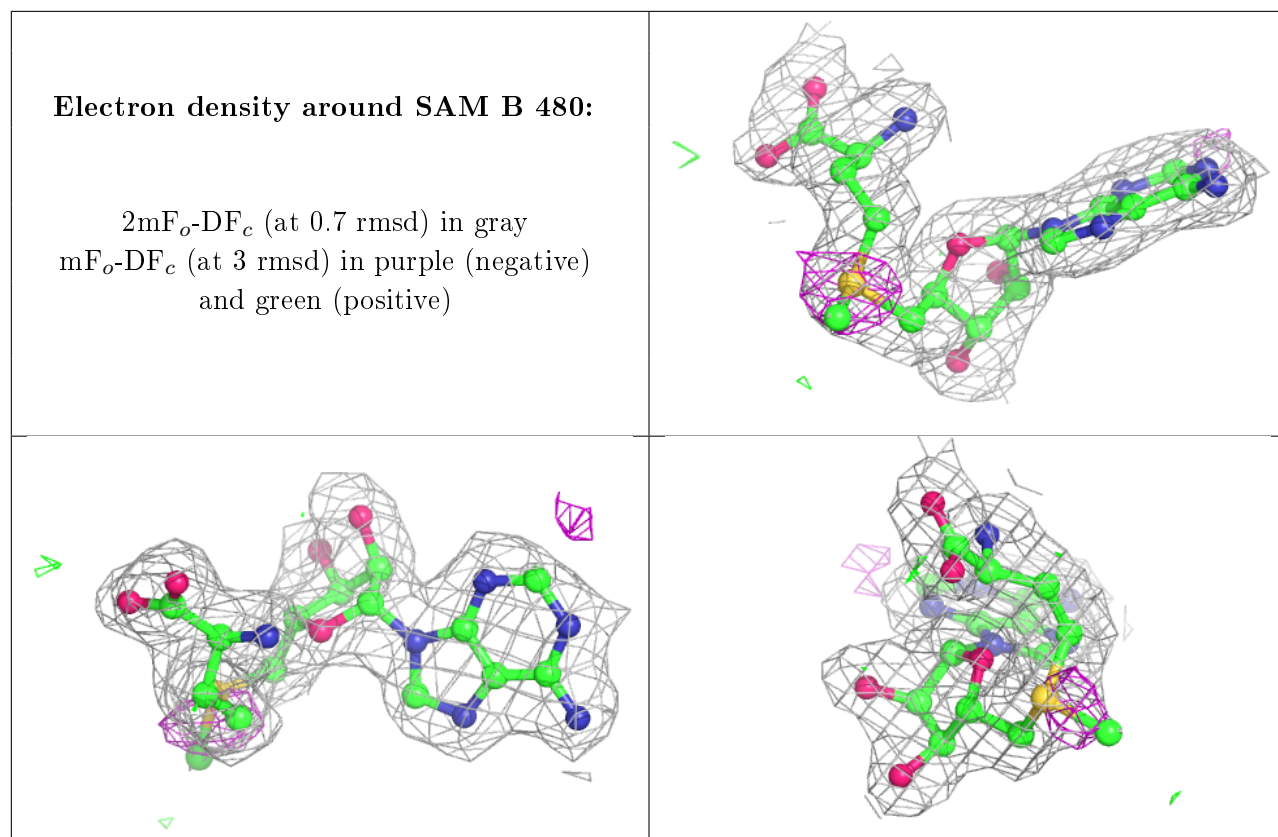
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	476	4/4	0.92	0.13	39,41,42,44	0
3	EDO	A	476	4/4	0.92	0.18	23,34,34,34	0
3	EDO	A	478	4/4	0.94	0.11	21,22,25,32	0
3	EDO	B	474	4/4	0.94	0.10	28,29,29,35	0
3	EDO	B	478	4/4	0.94	0.14	31,33,34,42	0
4	SAM	A	484	27/27	0.96	0.11	11,18,29,33	0
4	SAM	B	480	27/27	0.96	0.10	12,18,29,33	0
3	EDO	A	475	4/4	0.97	0.11	27,27,28,40	0
3	EDO	A	474	4/4	0.97	0.11	29,30,33,34	0
3	EDO	A	479	4/4	0.97	0.08	26,27,32,36	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.