



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 5ISD / pdb_00005isd
Title : Crystal structure of mouse CARM1 in complex with inhibitor SA0592
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Deposited on : 2016-03-15
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

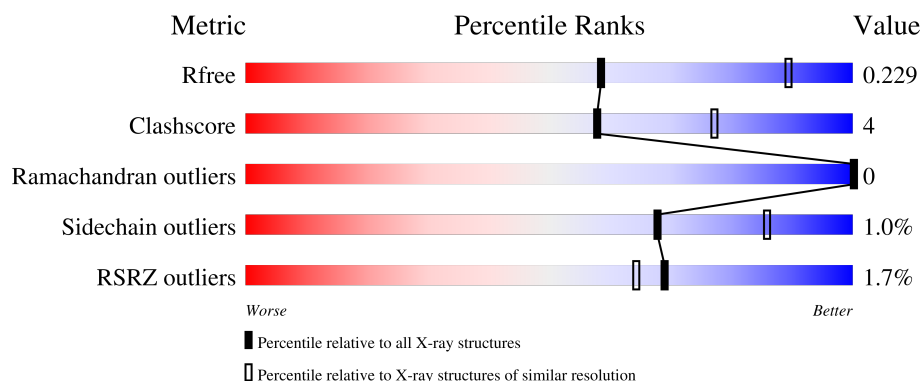
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	361	2% 84% 11% 5%
1	B	361	2% 85% 7% 7%
1	C	361	2% 86% 9% 5%
1	D	361	2% 85% 9% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	501	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22195 atoms, of which 10892 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 Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	1	0
			5468	1785	2706	455	508	14			
1	B	336	Total	C	H	N	O	S	0	0	0
			5340	1741	2646	444	495	14			
1	C	343	Total	C	H	N	O	S	0	0	0
			5450	1776	2699	454	507	14			
1	D	343	Total	C	H	N	O	S	0	0	0
			5450	1776	2699	454	507	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	UNP Q9WVG6
C	128	HIS	-	expression tag	UNP Q9WVG6
C	129	MET	-	expression tag	UNP Q9WVG6
D	127	GLY	-	expression tag	UNP Q9WVG6
D	128	HIS	-	expression tag	UNP Q9WVG6
D	129	MET	-	expression tag	UNP Q9WVG6

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



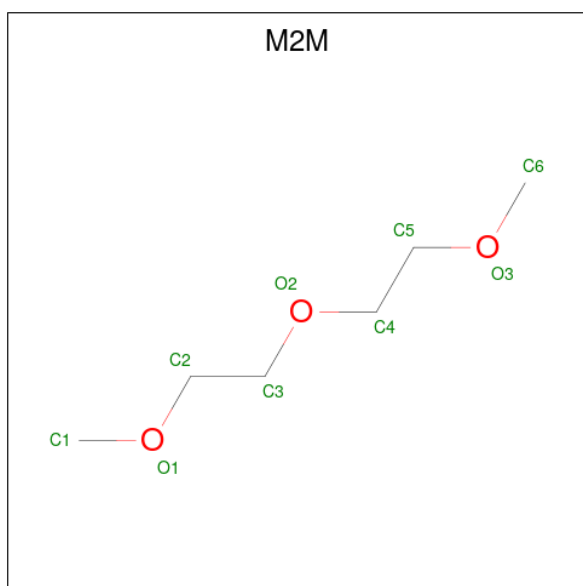
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C H O 10 2 6 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



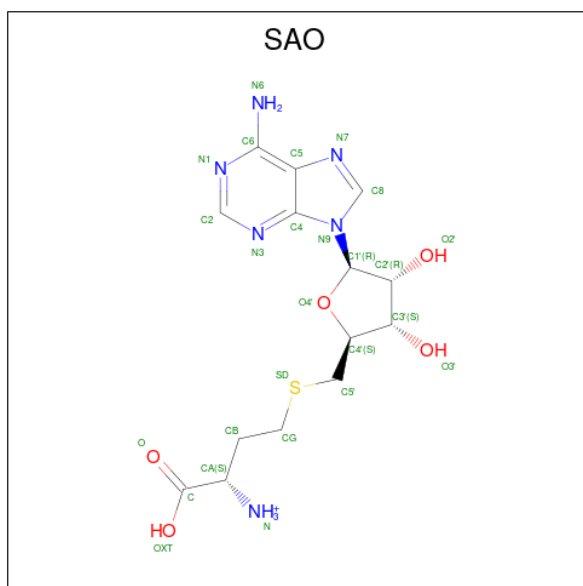
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is 1-METHOXY-2-(2-METHOXYETHOXY)ETHANE (CCD ID: M2M) (formula: C₆H₁₄O₃).



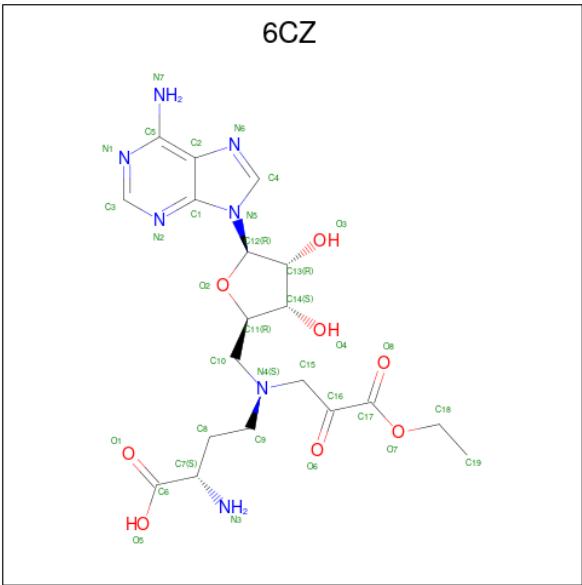
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			23	6	14	3		

- Molecule 5 is 5'-S-[(3S)-3-azaniumyl-3-carboxypropyl]-5'-thioadenosine (CCD ID: SAO) (formula: C₁₄H₂₁N₆O₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 46	C 14	H 20	N 6	O 5	S 1	0	0
5	C	1	Total 46	C 14	H 20	N 6	O 5	S 1	0	0
5	D	1	Total 46	C 14	H 20	N 6	O 5	S 1	0	0

- Molecule 6 is 5'-{[(3S)-3-amino-3-carboxypropyl](3-ethoxy-2,3-dioxopropyl)amino}-5'-deoxy adenosine (CCD ID: 6CZ) (formula: C₁₉H₂₇N₇O₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	0	0
			60	19	26	7	8		

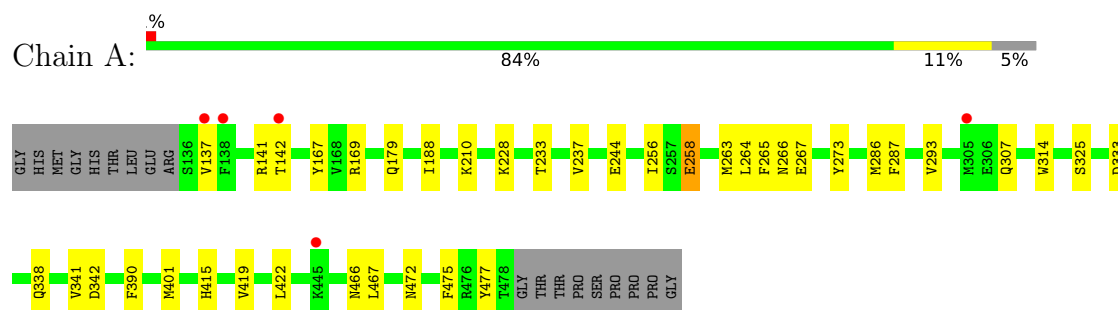
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	1
			61	61		
7	B	30	Total	O	0	1
			31	31		
7	C	43	Total	O	0	0
			43	43		
7	D	32	Total	O	0	0
			32	32		

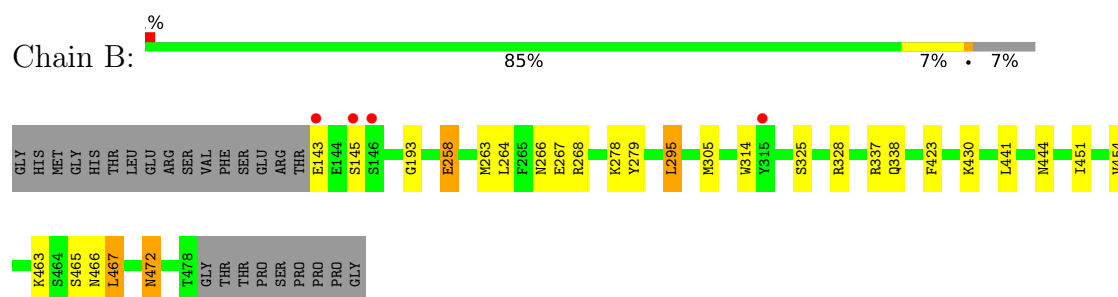
3 Residue-property plots [i](#)

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.

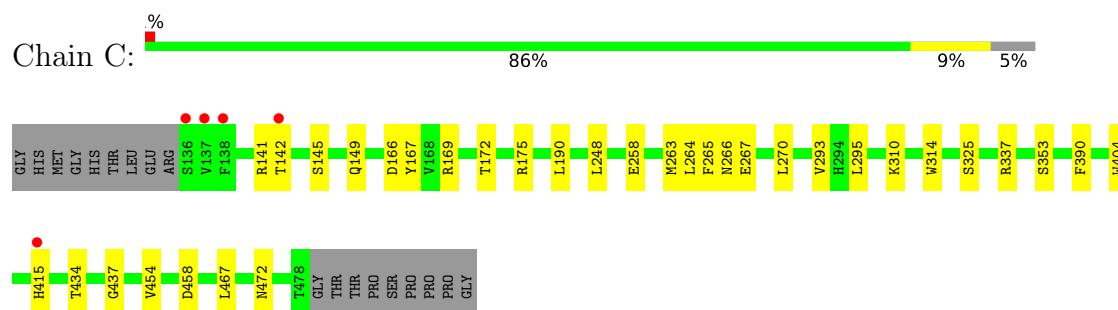
- Molecule 1: Histone-arginine methyltransferase CARM1



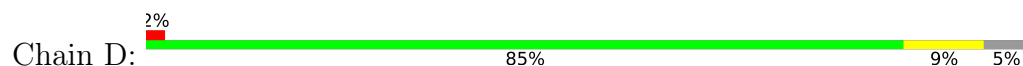
- Molecule 1: Histone-arginine methyltransferase CARM1

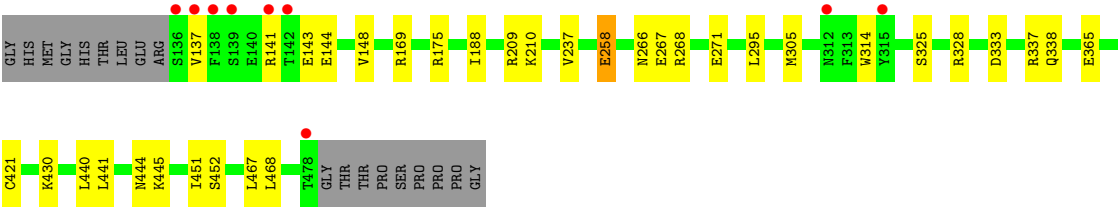


- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.56Å 98.45Å 205.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.60) 99.2 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.59Å)	Xtrriage
Refinement program	PHENIX dev_1951	Depositor
R, R_{free}	0.193 , 0.226 0.194 , 0.229	Depositor DCC
R_{free} test set	2349 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtrriage
Anisotropy	0.389	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22195	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3515e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, M2M, 6CZ, PEG, SAO

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	0.42	0/2833	0.76	2/3839 (0.1%)
1	B	0.39	0/2763	0.72	2/3745 (0.1%)
1	C	0.39	0/2821	0.75	0/3823
1	D	0.40	0/2821	0.73	2/3823 (0.1%)
All	All	0.40	0/11238	0.74	6/15230 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLN	CA-C-N	-6.03	113.73	119.76
1	A	338	GLN	C-N-CA	-6.03	113.73	119.76
1	D	338	GLN	CA-C-N	-5.51	114.25	119.76
1	D	338	GLN	C-N-CA	-5.51	114.25	119.76
1	B	338	GLN	CA-C-N	-5.48	114.28	119.76
1	B	338	GLN	C-N-CA	-5.48	114.28	119.76

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	2762	2706	2707	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2694	2646	2645	22	0
1	C	2751	2699	2699	24	0
1	D	2751	2699	2699	28	0
2	A	12	6	18	0	0
2	B	8	6	12	0	0
2	C	12	0	18	1	0
2	D	4	0	6	0	0
3	A	14	20	20	0	0
3	B	7	10	10	0	0
4	A	9	14	14	2	0
5	A	26	20	0	3	0
5	C	26	20	0	3	0
5	D	26	20	0	1	0
6	B	34	26	0	2	0
7	A	61	0	0	0	0
7	B	31	0	0	0	0
7	C	43	0	0	1	0
7	D	32	0	0	1	0
All	All	11303	10892	10848	99	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 4.

All (99) 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:268:ARG:NH2	1:B:444:ASN:O	1.99	0.95
1:C:169:ARG:HD2	1:C:415:HIS:CE1	2.16	0.81
1:C:169:ARG:NH2	5:C:504:SAO:OXT	2.17	0.76
1:B:472:ASN:O	1:B:472:ASN:ND2	2.20	0.74
1:C:295:LEU:HD21	1:C:390:PHE:CE2	2.24	0.73
1:C:166:ASP:OD2	1:C:415:HIS:ND1	2.22	0.72
1:A:188:ILE:HD13	1:A:210:LYS:HB3	1.73	0.69
1:C:404:TRP:CD2	2:C:502:EDO:H12	2.28	0.69
1:D:188:ILE:HD11	1:D:209:ARG:CZ	2.23	0.68
1:B:193:GLY:O	6:B:504:6CZ:N3	2.27	0.68
1:A:188:ILE:CD1	1:A:210:LYS:HB3	2.31	0.61
1:B:430:LYS:HG3	1:C:167:TYR:CE2	2.37	0.60
1:B:465:SER:O	1:B:466:ASN:ND2	2.35	0.60
1:D:325:SER:O	1:D:328:ARG:NH1	2.36	0.59
1:A:169:ARG:NH2	5:A:507:SAO:C	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:SER:O	1:B:328:ARG:NH1	2.36	0.57
1:C:169:ARG:HH22	5:C:504:SAO:C	2.18	0.56
1:D:337:ARG:HG2	1:D:467:LEU:O	2.06	0.56
1:C:265:PHE:CE2	1:C:293:VAL:HG21	2.41	0.56
1:A:169:ARG:NH2	5:A:507:SAO:O	2.40	0.55
1:A:422:LEU:O	1:A:466:ASN:ND2	2.30	0.55
1:B:305:MET:CE	1:D:305:MET:HB3	2.36	0.55
1:B:423:PHE:HD1	1:B:466:ASN:OD1	1.89	0.55
1:D:141:ARG:NH1	1:D:365:GLU:OE2	2.40	0.54
1:C:310:LYS:NZ	7:C:603:HOH:O	2.41	0.54
1:D:169:ARG:NH1	5:D:502:SAO:O	2.36	0.53
1:D:143:GLU:OE2	1:D:445:LYS:NZ	2.36	0.53
1:D:188:ILE:HD11	1:D:209:ARG:NH1	2.24	0.53
1:A:141:ARG:HG3	1:A:142:THR:HG23	1.90	0.52
1:C:295:LEU:HD21	1:C:390:PHE:CD2	2.46	0.51
1:A:210:LYS:HZ1	1:A:237:VAL:HG21	1.77	0.50
1:C:141:ARG:HG3	1:C:142:THR:HG23	1.94	0.50
1:C:169:ARG:HD2	1:C:415:HIS:HE1	1.72	0.50
1:D:141:ARG:HH12	1:D:365:GLU:HG2	1.76	0.50
1:B:454:VAL:CG1	1:B:463:LYS:HE3	2.42	0.50
1:B:314:TRP:O	1:B:325:SER:HA	2.13	0.49
1:D:268:ARG:HD2	1:D:271:GLU:OE2	2.11	0.49
1:B:266:ASN:O	1:B:267:GLU:HB2	2.12	0.49
1:C:172:THR:HG23	1:C:175:ARG:NH2	2.28	0.48
1:B:337:ARG:HG2	1:B:467:LEU:O	2.14	0.48
1:B:423:PHE:CD1	1:B:466:ASN:OD1	2.66	0.48
1:C:337:ARG:HH12	1:C:467:LEU:HD23	1.79	0.48
1:A:258:GLU:OE2	4:A:506:M2M:H63	2.13	0.48
1:A:266:ASN:O	1:A:267:GLU:HB2	2.12	0.47
1:D:141:ARG:HH12	1:D:365:GLU:CG	2.27	0.47
1:A:210:LYS:HZ1	1:A:237:VAL:CG2	2.27	0.47
1:A:228:LYS:HG2	1:A:233:THR:CG2	2.45	0.47
1:C:266:ASN:O	1:C:267:GLU:HB2	2.15	0.46
1:D:188:ILE:HD11	1:D:209:ARG:NE	2.29	0.46
1:C:472:ASN:O	1:C:472:ASN:OD1	2.33	0.46
1:A:137:VAL:HG22	1:A:244:GLU:HG2	1.98	0.46
1:B:143:GLU:HG3	1:B:145:SER:H	1.81	0.46
1:D:137:VAL:O	1:D:141:ARG:HG2	2.16	0.46
1:C:314:TRP:O	1:C:325:SER:HA	2.17	0.45
1:A:265:PHE:CE2	1:A:293:VAL:HG21	2.51	0.45
1:A:263:MET:HE2	1:A:390:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:SER:O	1:C:149:GLN:HG2	2.16	0.45
1:B:466:ASN:C	1:B:467:LEU:HD12	2.42	0.44
1:C:190:LEU:HD13	1:C:248:LEU:HD21	1.99	0.44
1:D:266:ASN:O	1:D:267:GLU:HB2	2.18	0.44
1:A:273:TYR:CZ	1:A:286:MET:HE2	2.52	0.44
1:D:440:LEU:HB3	1:D:452:SER:OG	2.18	0.44
1:D:141:ARG:HH12	1:D:365:GLU:CD	2.26	0.43
1:D:210:LYS:HE2	1:D:237:VAL:HG21	2.00	0.43
1:B:441:LEU:CD2	1:B:451:ILE:HG12	2.47	0.43
1:D:268:ARG:NH2	1:D:444:ASN:O	2.50	0.43
1:A:256:ILE:HG22	1:A:287:PHE:HB2	2.01	0.43
1:D:141:ARG:NH2	1:D:365:GLU:OE2	2.52	0.43
1:D:333:ASP:O	1:D:337:ARG:HG3	2.19	0.43
1:A:341:VAL:O	1:A:342:ASP:HB3	2.18	0.43
1:A:475[B]:PHE:CE1	1:A:477:TYR:HB3	2.54	0.43
1:C:434:THR:OG1	1:C:458:ASP:HB2	2.19	0.43
1:A:267:GLU:OE2	4:A:506:M2M:H13	2.18	0.42
1:A:263:MET:O	1:A:264:LEU:HB3	2.20	0.42
1:A:314:TRP:O	1:A:325:SER:HA	2.19	0.42
1:A:179:GLN:NE2	1:A:401:MET:SD	2.92	0.42
1:D:175:ARG:NH2	7:D:601:HOH:O	2.43	0.42
1:A:169:ARG:HD2	1:A:415:HIS:HE1	1.85	0.42
1:B:465:SER:C	1:B:466:ASN:CG	2.87	0.42
1:A:263:MET:HE3	1:A:419:VAL:HG11	2.02	0.42
1:C:437:GLY:HA3	1:C:454:VAL:O	2.19	0.42
1:C:169:ARG:NH2	5:C:504:SAO:C	2.79	0.41
1:A:169:ARG:NH2	5:A:507:SAO:OXT	2.53	0.41
1:A:472:ASN:OD1	1:A:472:ASN:O	2.38	0.41
1:D:314:TRP:O	1:D:325:SER:HA	2.19	0.41
1:A:167:TYR:CE2	1:D:430:LYS:HG3	2.55	0.41
1:B:258:GLU:OE1	6:B:504:6CZ:O8	2.38	0.41
1:B:295:LEU:HD12	1:B:295:LEU:N	2.35	0.41
1:D:421:CYS:SG	1:D:468:LEU:HD22	2.61	0.41
1:A:137:VAL:CG2	1:A:244:GLU:HG2	2.51	0.41
1:B:466:ASN:O	1:B:467:LEU:HD12	2.21	0.41
1:C:295:LEU:O	1:C:353:SER:HA	2.21	0.41
1:D:144:GLU:O	1:D:148:VAL:HG23	2.21	0.40
1:D:451:ILE:O	1:D:467:LEU:HA	2.21	0.40
1:D:169:ARG:NH1	1:D:258:GLU:OE2	2.50	0.40
1:B:278:LYS:HE3	1:B:279:TYR:CZ	2.56	0.40
1:C:263:MET:O	1:C:264:LEU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:LEU:CD2	1:D:451:ILE:HG12	2.52	0.40
1:B:263:MET:O	1:B:264:LEU:HB3	2.22	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	342/361 (95%)	333 (97%)	9 (3%)	0	100	100
1	B	334/361 (92%)	324 (97%)	10 (3%)	0	100	100
1	C	341/361 (94%)	332 (97%)	9 (3%)	0	100	100
1	D	341/361 (94%)	332 (97%)	9 (3%)	0	100	100
All	All	1358/1444 (94%)	1321 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/313 (96%)	296 (99%)	4 (1%)	61	82
1	B	292/313 (93%)	288 (99%)	4 (1%)	59	81
1	C	299/313 (96%)	297 (99%)	2 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	299/313 (96%)	297 (99%)	2 (1%)	76	89
All	All	1190/1252 (95%)	1178 (99%)	12 (1%)	68	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	A	307	GLN
1	A	333	ASP
1	A	467	LEU
1	B	258	GLU
1	B	295	LEU
1	B	467	LEU
1	B	472	ASN
1	C	258	GLU
1	C	270	LEU
1	D	258	GLU
1	D	295	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	338	GLN
1	A	447	GLN
1	B	165	GLN
1	B	424	GLN
1	C	165	GLN
1	C	251	GLN
1	C	338	GLN
1	C	472	ASN
1	D	447	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	EDO	A	503	-	3,3,3	0.44	0	2,2,2	0.60	0
4	M2M	A	506	-	8,8,8	0.63	0	7,7,7	0.35	0
2	EDO	C	502	-	3,3,3	0.44	0	2,2,2	0.57	0
2	EDO	A	502	-	3,3,3	0.45	0	2,2,2	0.45	0
3	PEG	A	505	-	6,6,6	0.50	0	5,5,5	0.66	0
6	6CZ	B	504	-	35,36,36	1.96	9 (25%)	44,51,51	2.23	12 (27%)
2	EDO	A	501	-	3,3,3	0.44	0	2,2,2	0.55	0
3	PEG	B	503	-	6,6,6	0.49	0	5,5,5	0.47	0
5	SAO	A	507	-	27,28,28	0.40	0	36,40,40	0.79	1 (2%)
2	EDO	C	501	-	3,3,3	0.44	0	2,2,2	0.52	0
3	PEG	A	504	-	6,6,6	0.49	0	5,5,5	0.47	0
5	SAO	C	504	-	27,28,28	0.42	0	36,40,40	0.73	1 (2%)
2	EDO	D	501	-	3,3,3	0.45	0	2,2,2	0.52	0
2	EDO	B	501	-	3,3,3	0.43	0	2,2,2	0.63	0
5	SAO	D	502	-	27,28,28	0.48	0	36,40,40	0.77	1 (2%)
2	EDO	C	503	-	3,3,3	0.44	0	2,2,2	0.60	0
2	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.55	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	EDO	A	503	-	-	1/1/1/1	-
4	M2M	A	506	-	-	3/6/6/6	-
2	EDO	C	502	-	-	1/1/1/1	-
2	EDO	A	502	-	-	1/1/1/1	-
3	PEG	A	505	-	-	4/4/4/4	-
6	6CZ	B	504	-	-	13/28/44/44	0/3/3/3
2	EDO	A	501	-	-	1/1/1/1	-
3	PEG	B	503	-	-	2/4/4/4	-
5	SAO	A	507	-	-	6/15/31/31	0/3/3/3
2	EDO	C	501	-	-	1/1/1/1	-
3	PEG	A	504	-	-	2/4/4/4	-
5	SAO	C	504	-	-	1/15/31/31	0/3/3/3
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
5	SAO	D	502	-	-	2/15/31/31	0/3/3/3
2	EDO	C	503	-	-	1/1/1/1	-
2	EDO	B	502	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	6CZ	O7-C17	6.63	1.46	1.33
6	B	504	6CZ	C5-N7	4.21	1.45	1.34
6	B	504	6CZ	O1-C6	3.46	1.32	1.22
6	B	504	6CZ	C14-C13	-2.76	1.45	1.53
6	B	504	6CZ	C13-C12	-2.59	1.45	1.53
6	B	504	6CZ	C2-C1	2.34	1.43	1.39
6	B	504	6CZ	O8-C17	2.12	1.25	1.21
6	B	504	6CZ	C15-C16	-2.08	1.48	1.52
6	B	504	6CZ	C16-C17	2.07	1.56	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	504	6CZ	O7-C17-C16	7.88	121.90	111.38
6	B	504	6CZ	C2-C1-N2	-5.39	119.29	126.72
6	B	504	6CZ	N2-C1-N5	4.40	134.65	127.17
6	B	504	6CZ	N2-C3-N1	-4.29	122.09	128.58
5	C	504	SAO	CB-CG-SD	-3.83	104.91	113.45
5	A	507	SAO	CB-CG-SD	-3.67	105.26	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	504	6CZ	C3-N2-C1	3.62	120.68	111.83
6	B	504	6CZ	O7-C17-O8	-3.31	117.42	123.37
5	D	502	SAO	CB-CG-SD	-3.29	106.11	113.45
6	B	504	6CZ	C2-N6-C4	3.03	108.21	103.45
6	B	504	6CZ	C1-C2-N6	-2.87	107.30	110.58
6	B	504	6CZ	N5-C4-N6	-2.78	109.99	113.94
6	B	504	6CZ	O8-C17-C16	-2.69	118.96	122.05
6	B	504	6CZ	C1-N5-C4	2.57	108.43	105.74
6	B	504	6CZ	C9-N4-C10	2.41	117.52	111.89

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	SAO	C4'-C5'-SD-CG
5	A	507	SAO	O4'-C4'-C5'-SD
5	A	507	SAO	C3'-C4'-C5'-SD
6	B	504	6CZ	O1-C6-C7-N3
6	B	504	6CZ	C6-C7-C8-C9
6	B	504	6CZ	N3-C7-C8-C9
6	B	504	6CZ	N4-C15-C16-C17
6	B	504	6CZ	N4-C15-C16-O6
6	B	504	6CZ	C16-C17-O7-C18
6	B	504	6CZ	O8-C17-O7-C18
3	A	504	PEG	O2-C3-C4-O4
6	B	504	6CZ	O5-C6-C7-N3
3	B	503	PEG	O1-C1-C2-O2
6	B	504	6CZ	C11-C10-N4-C9
4	A	506	M2M	O1-C2-C3-O2
3	A	505	PEG	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	A	502	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2
2	C	503	EDO	O1-C1-C2-O2
3	A	505	PEG	O2-C3-C4-O4
3	B	503	PEG	O2-C3-C4-O4
5	A	507	SAO	C-CA-CB-CG
6	B	504	6CZ	C15-C16-C17-O8
6	B	504	6CZ	O6-C16-C17-O8
5	A	507	SAO	N-CA-CB-CG
6	B	504	6CZ	C7-C8-C9-N4
5	D	502	SAO	O4'-C4'-C5'-SD

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Mol	Chain	Res	Type	Atoms
3	A	505	PEG	C1-C2-O2-C3
3	A	505	PEG	C4-C3-O2-C2
3	A	504	PEG	O1-C1-C2-O2
2	A	503	EDO	O1-C1-C2-O2
2	C	501	EDO	O1-C1-C2-O2
2	C	502	EDO	O1-C1-C2-O2
4	A	506	M2M	C2-C3-O2-C4
4	A	506	M2M	O2-C4-C5-O3
2	B	502	EDO	O1-C1-C2-O2
5	C	504	SAO	OXT-C-CA-N
6	B	504	6CZ	C8-C9-N4-C15
2	D	501	EDO	O1-C1-C2-O2
5	D	502	SAO	C-CA-CB-CG
5	A	507	SAO	OXT-C-CA-N

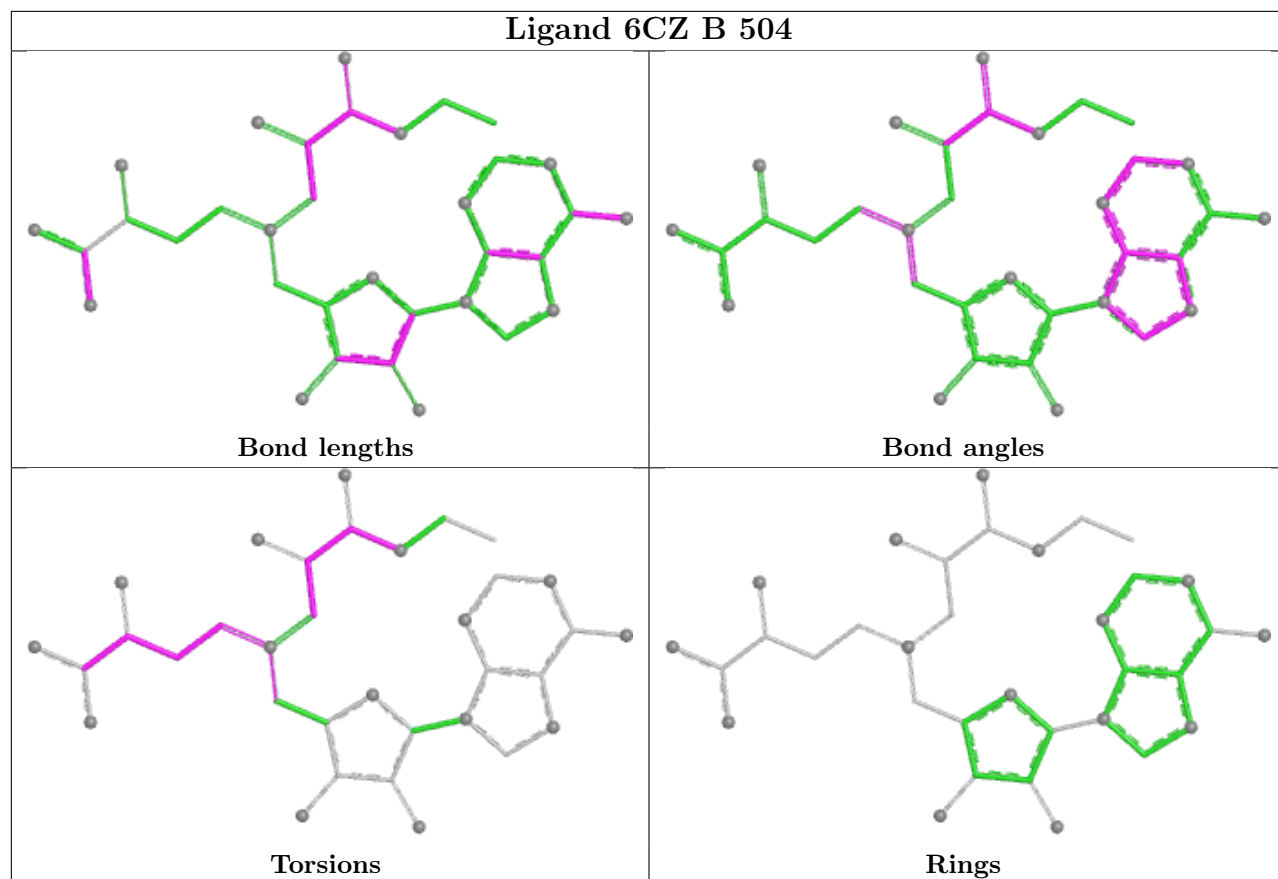
There are no ring outliers.

6 monomers are involved in 12 short contacts:

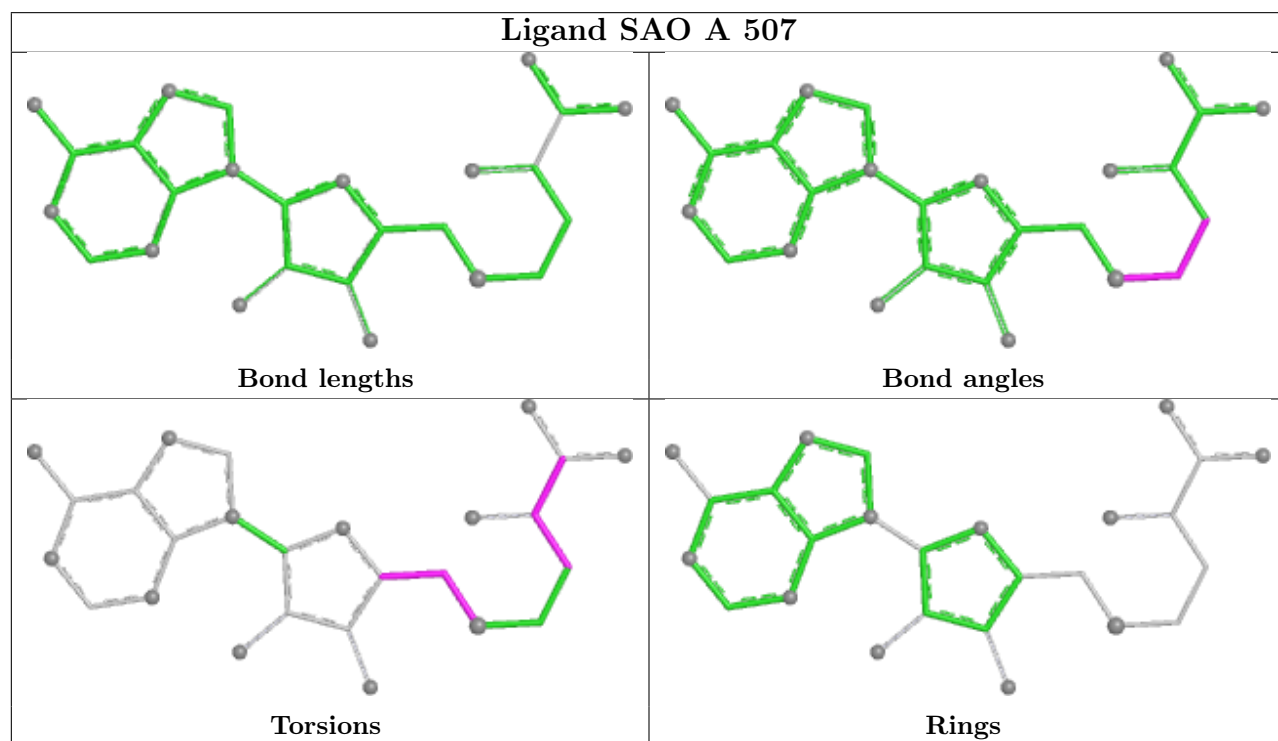
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	M2M	2	0
2	C	502	EDO	1	0
6	B	504	6CZ	2	0
5	A	507	SAO	3	0
5	C	504	SAO	3	0
5	D	502	SAO	1	0

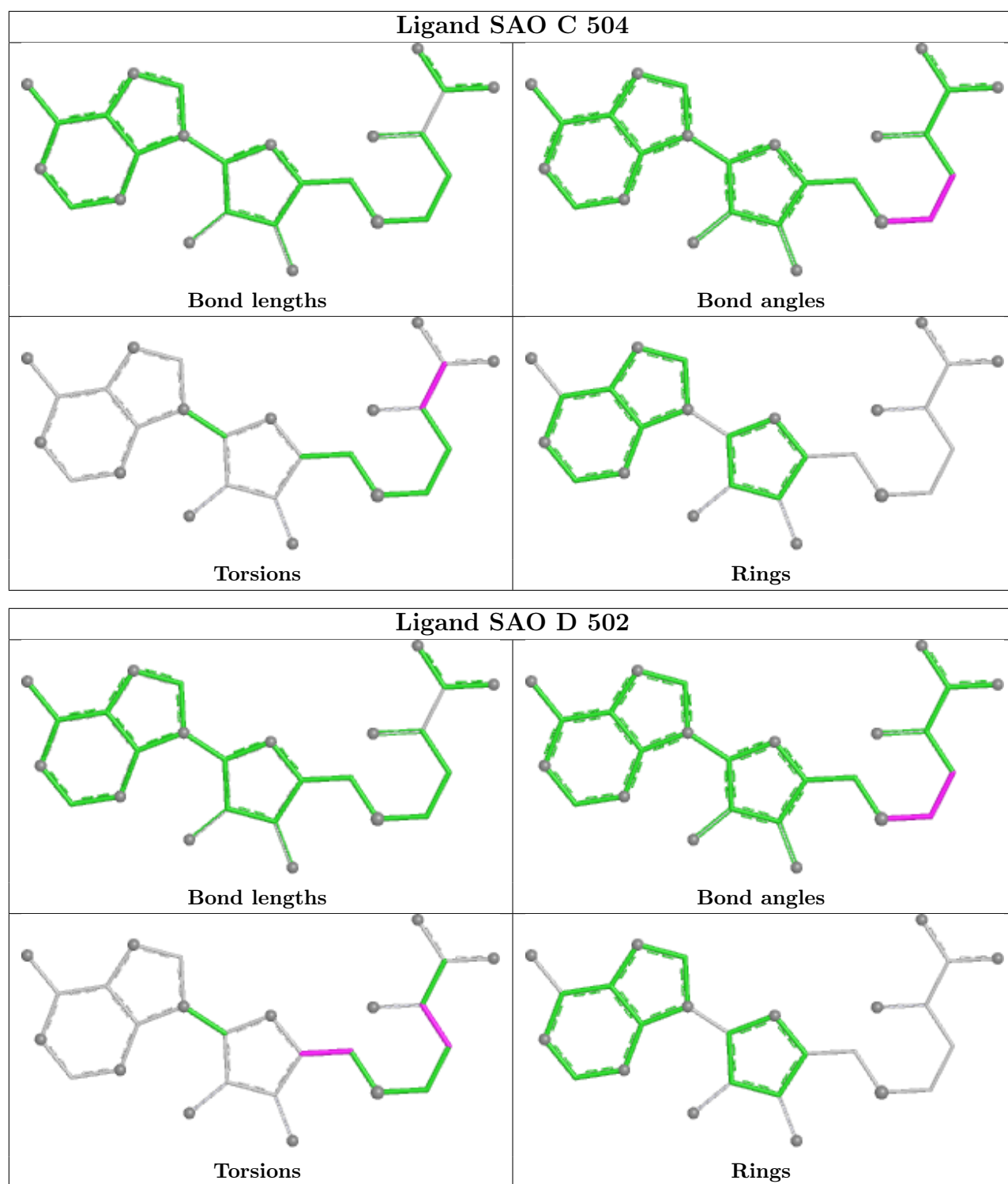
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 6CZ B 504



Ligand SAO A 507





5.7 Other polymers [i](#)

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, 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	343/361 (95%)	-0.27	5 (1%) 72 68	26, 50, 80, 115	1 (0%)
1	B	336/361 (93%)	-0.22	4 (1%) 76 73	35, 56, 83, 132	0
1	C	343/361 (95%)	0.05	5 (1%) 72 68	33, 63, 98, 128	0
1	D	343/361 (95%)	-0.04	9 (2%) 57 51	40, 61, 94, 188	0
All	All	1365/1444 (94%)	-0.12	23 (1%) 69 64	26, 58, 92, 188	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	ARG	4.0
1	A	137	VAL	3.5
1	D	478	THR	3.4
1	A	305	MET	3.4
1	D	139	SER	3.3
1	A	138	PHE	3.3
1	D	138	PHE	3.2
1	C	137	VAL	2.8
1	B	315	TYR	2.8
1	B	143	GLU	2.7
1	D	142	THR	2.7
1	C	415	HIS	2.6
1	D	315	TYR	2.6
1	D	137	VAL	2.6
1	C	138	PHE	2.6
1	A	142	THR	2.5
1	D	136	SER	2.4
1	B	145	SER	2.3
1	C	136	SER	2.3
1	B	146	SER	2.2
1	C	142	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	445	LYS	2.1
1	D	312	ASN	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 oligosaccharides 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.

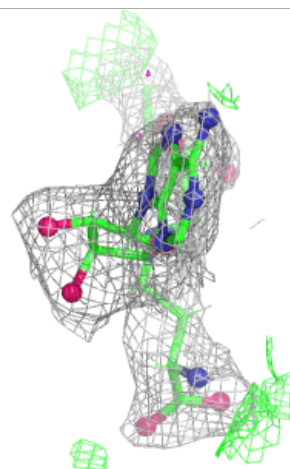
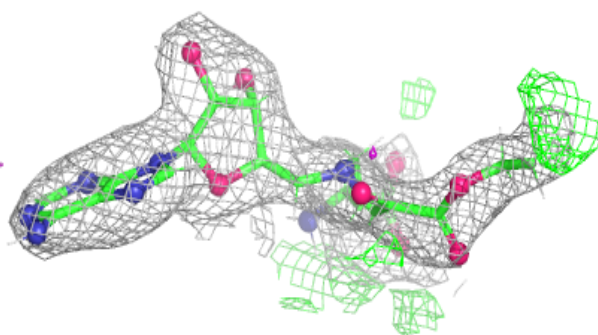
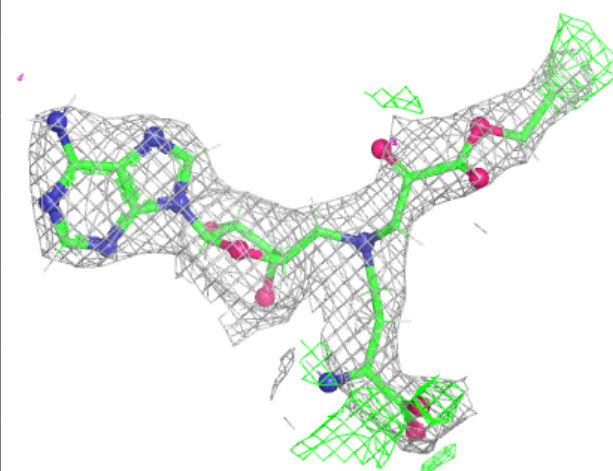
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	A	501	4/4	0.44	0.40	119,143,144,144	0
2	EDO	B	502	4/4	0.68	0.27	75,75,75,77	0
2	EDO	C	502	4/4	0.70	0.23	69,69,71,73	0
2	EDO	C	503	4/4	0.71	0.17	58,58,58,60	0
3	PEG	A	505	7/7	0.71	0.15	70,84,89,89	0
4	M2M	A	506	9/9	0.73	0.17	68,82,87,87	0
3	PEG	B	503	7/7	0.77	0.12	64,77,81,81	0
2	EDO	B	501	4/4	0.78	0.42	142,171,171,171	0
2	EDO	A	502	4/4	0.80	0.15	68,68,68,68	0
6	6CZ	B	504	34/34	0.80	0.12	55,69,84,86	0
5	SAO	C	504	26/26	0.81	0.12	63,73,89,90	0
2	EDO	A	503	4/4	0.82	0.13	51,52,54,54	0
5	SAO	D	502	26/26	0.83	0.12	55,68,80,81	0
3	PEG	A	504	7/7	0.84	0.10	62,75,77,79	0
2	EDO	D	501	4/4	0.86	0.12	47,48,49,50	0
2	EDO	C	501	4/4	0.87	0.14	67,70,72,73	0
5	SAO	A	507	26/26	0.88	0.09	43,59,73,74	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.

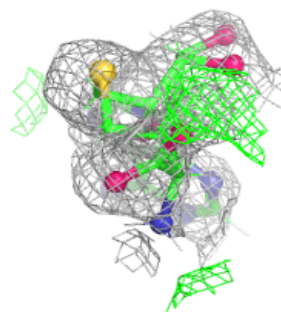
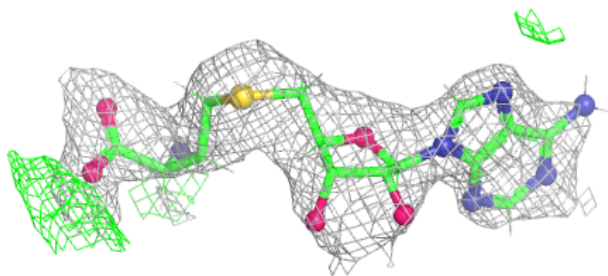
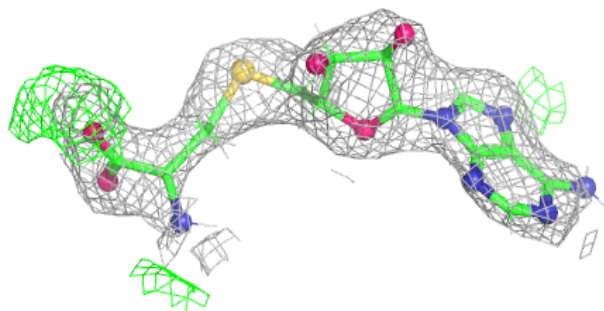
Electron density around 6CZ B 504:

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

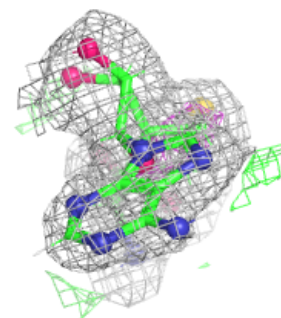
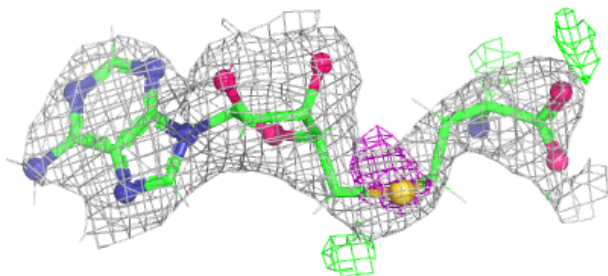
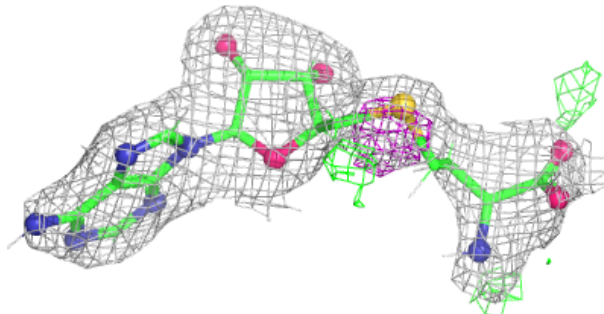


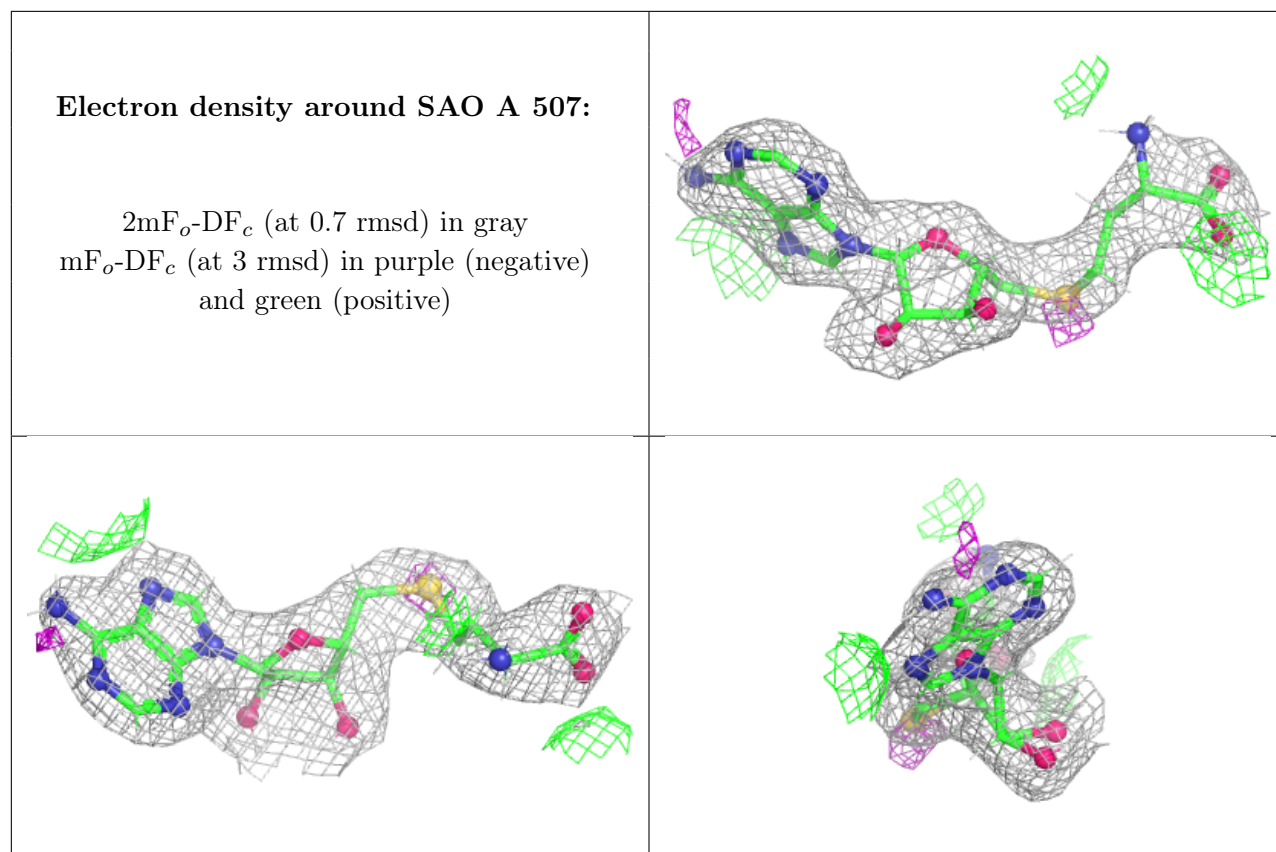
Electron density around SAO C 504:

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

**Electron density around SAO D 502:**

$2mF_o-DF_c$ (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.