



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2024 – 04:19 PM JST

PDB ID : 8HZV
Title : The crystal structure of a Radical SAM Enzyme DesII
Authors : Hou, X.L.; Zhou, J.H.
Deposited on : 2023-01-09
Resolution : 2.33 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 : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

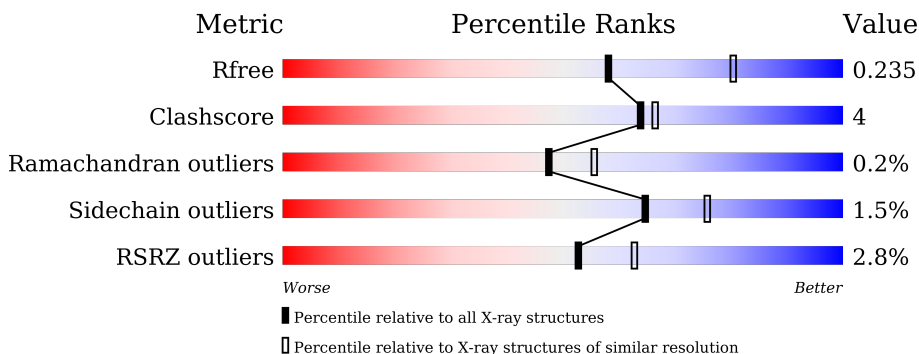
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	493	
1	B	493	
1	C	493	
1	D	493	

2 Entry composition [i](#)

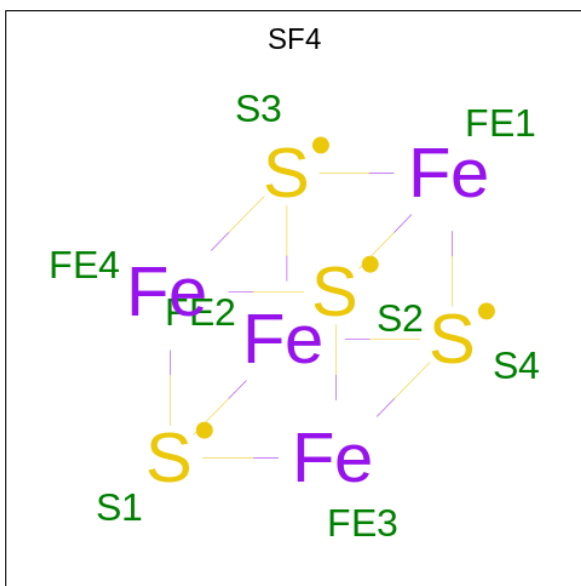
There are 8 unique types of molecules in this entry. The entry contains 15451 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Radical S-Adenosyl-L-methionine Enzyme DesII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	Total 3716	C 2329	N 677	O 701	S 9	0	0	0
1	B	474	Total 3690	C 2313	N 679	O 689	S 9	0	0	0
1	C	477	Total 3704	C 2322	N 675	O 698	S 9	0	0	0
1	D	472	Total 3678	C 2306	N 677	O 686	S 9	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



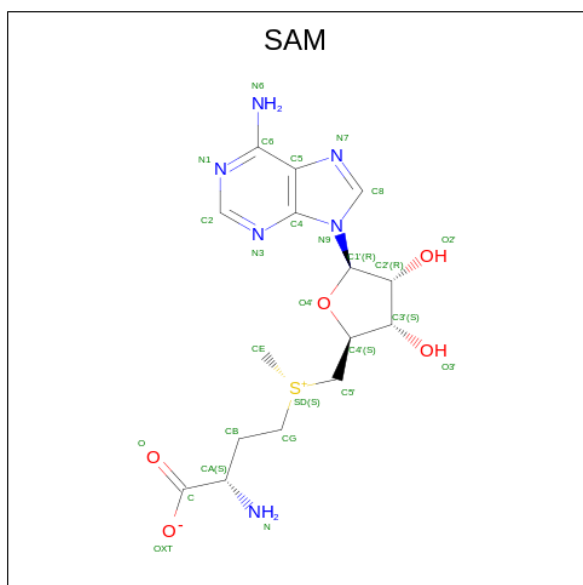
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	Total 8	Fe 4	S 4	0	0
2	B	1	Total 8	Fe 4	S 4	0	0

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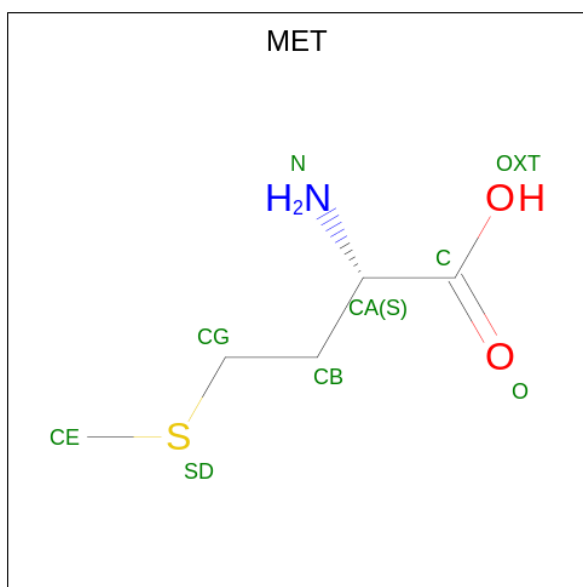
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



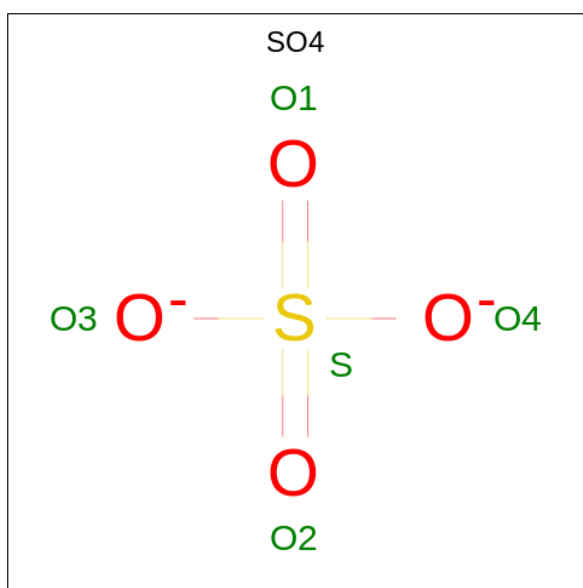
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S) (labeled as "Ligand of Interest" by depositor).



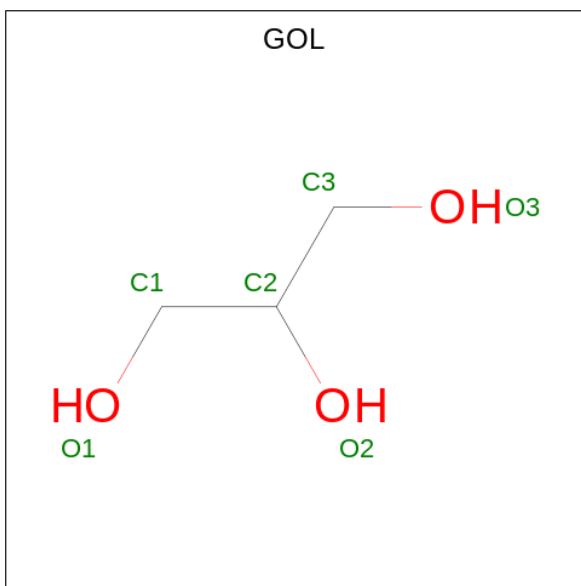
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	9	5	1	2	1	0	0
4	D	1	9	5	1	2	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	B	1	5	4	1	0	0
5	C	1	5	4	1	0	0

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



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Na 1 1	0	0

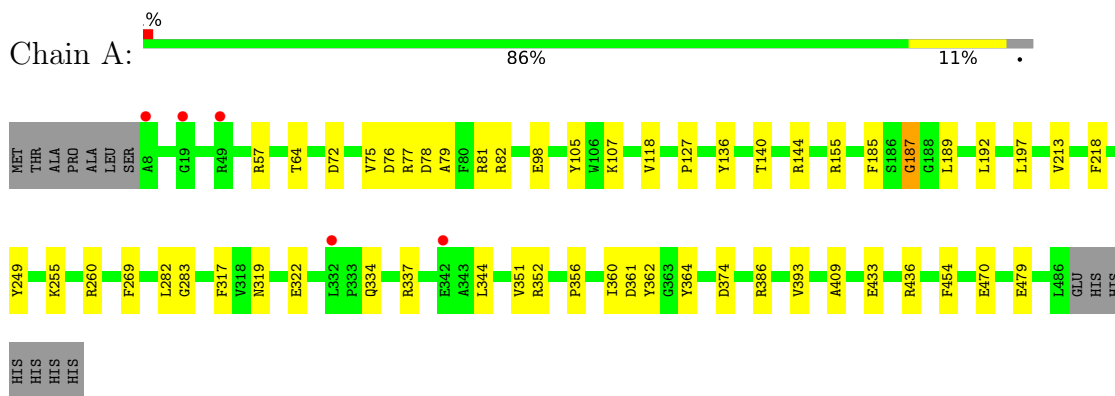
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	112	Total O 112 112	0	0
8	B	141	Total O 141 141	0	0
8	C	122	Total O 122 122	0	0
8	D	149	Total O 149 149	0	0

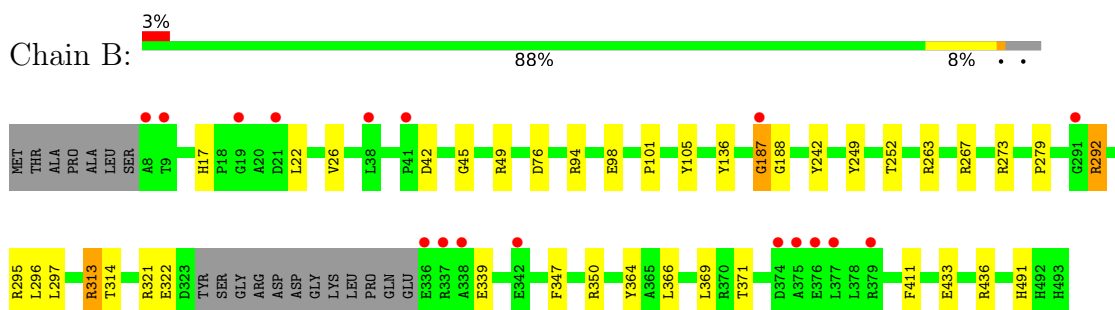
3 Residue-property plots [i](#)

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.

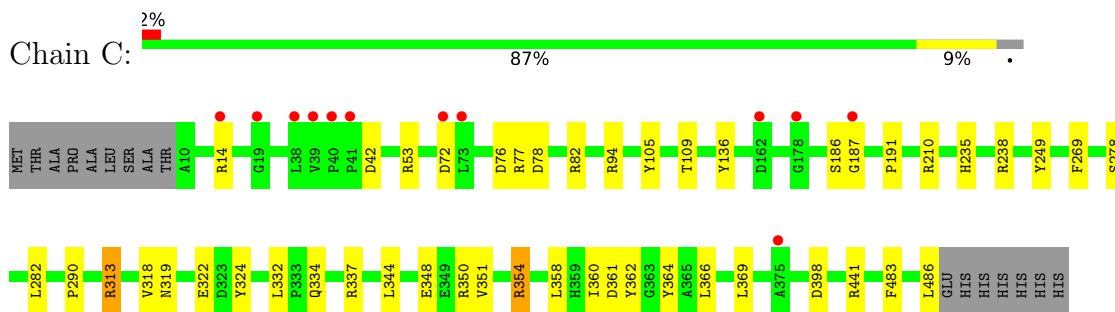
- Molecule 1: Radical S-Adenosyl-L-methionine Enzyme DesII



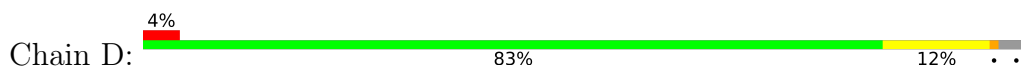
- Molecule 1: Radical S-Adenosyl-L-methionine Enzyme DesII

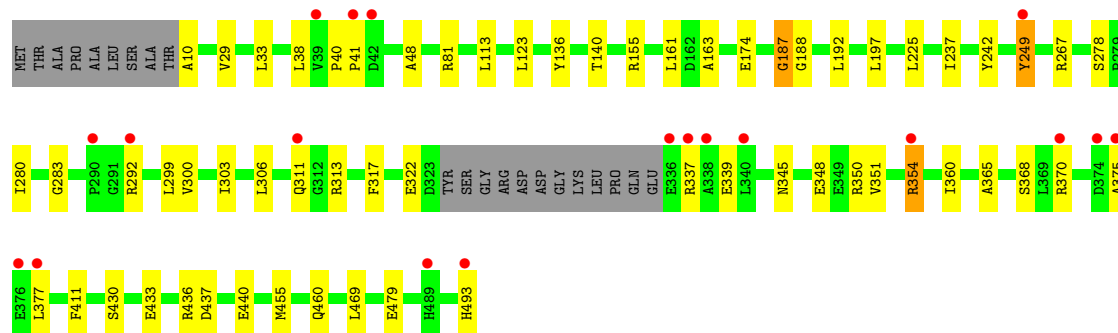


- Molecule 1: Radical S-Adenosyl-L-methionine Enzyme DesII



- Molecule 1: Radical S-Adenosyl-L-methionine Enzyme DesII





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.19Å 140.79Å 116.02Å 90.00° 96.28° 90.00°	Depositor
Resolution (Å)	49.19 – 2.33 49.19 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.19-2.33) 99.9 (49.19-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.235 0.204 , 0.235	Depositor DCC
R_{free} test set	4716 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtrriage
Anisotropy	0.175	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.3	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	0.94	EDS
Total number of atoms	15451	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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: NA, SAM, SO4, GOL, SF4

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	0.26	0/3798	0.43	0/5162
1	B	0.27	0/3775	0.45	0/5131
1	C	0.26	0/3786	0.42	0/5145
1	D	0.26	0/3763	0.45	0/5114
All	All	0.26	0/15122	0.44	0/20552

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
1	B	0	2
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	GLY	Peptide
1	B	187	GLY	Peptide
1	B	369	LEU	Peptide
1	D	187	GLY	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	A	3716	0	3617	29	0
1	B	3690	0	3578	21	0
1	C	3704	0	3605	30	0
1	D	3678	0	3566	45	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	27	0	22	1	0
3	C	27	0	22	0	0
4	B	9	0	8	0	0
4	D	9	0	8	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	B	12	0	16	0	0
6	D	12	0	16	2	0
7	D	1	0	0	0	0
8	A	112	0	0	1	0
8	B	141	0	0	1	0
8	C	122	0	0	1	0
8	D	149	0	0	3	0
All	All	15451	0	14458	123	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 (123) 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:350:ARG:NH2	1:D:354:ARG:NH1	2.11	0.97
1:D:350:ARG:NH2	1:D:354:ARG:CZ	2.33	0.92
1:D:29:VAL:HG23	1:D:48:ALA:HB1	1.76	0.68
1:C:136:TYR:CD1	1:C:187:GLY:HA2	2.31	0.65
1:D:278:SER:O	1:D:313:ARG:NH2	2.29	0.64
1:B:17:HIS:ND1	1:B:371:THR:HG21	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:SAM:H3'	3:A:502:SAM:HG2	1.80	0.62
1:C:344:LEU:O	1:C:348:GLU:HG3	1.99	0.61
1:A:57:ARG:HD3	1:A:64:THR:HG21	1.83	0.61
1:A:185:PHE:HB2	1:A:213:VAL:HG22	1.82	0.60
1:D:350:ARG:HH22	1:D:354:ARG:NH1	1.99	0.60
1:A:361:ASP:OD2	1:B:491:HIS:HE1	1.83	0.60
1:C:136:TYR:CG	1:C:187:GLY:HA2	2.38	0.59
1:C:319:ASN:ND2	1:C:361:ASP:OD1	2.31	0.59
1:B:322:GLU:HB3	1:B:366:LEU:HD13	1.83	0.59
1:A:155:ARG:NH2	8:A:601:HOH:O	2.36	0.58
1:A:322:GLU:OE1	1:A:337:ARG:NH1	2.32	0.58
1:C:238:ARG:HH12	1:D:493:HIS:CD2	2.22	0.58
1:D:136:TYR:CG	1:D:187:GLY:HA2	2.40	0.57
1:B:42:ASP:OD2	1:B:42:ASP:N	2.38	0.57
1:D:455:MET:HE2	1:D:460:GLN:HG2	1.87	0.56
1:D:113:LEU:HD11	6:D:504:GOL:H32	1.86	0.56
1:D:350:ARG:CZ	1:D:354:ARG:CZ	2.83	0.56
1:B:433:GLU:HG2	1:B:436:ARG:HH22	1.70	0.56
1:C:109:THR:HG1	1:C:364:TYR:HH	1.51	0.56
1:B:273:ARG:NH2	1:B:314:THR:O	2.38	0.55
1:C:318:VAL:HG23	1:C:358:LEU:HD11	1.89	0.55
1:D:113:LEU:CD1	6:D:504:GOL:H32	2.37	0.55
1:D:81:ARG:NH1	8:D:603:HOH:O	2.35	0.54
1:A:78:ASP:OD1	1:A:81:ARG:NH1	2.41	0.54
1:C:76:ASP:OD2	1:C:77:ARG:N	2.40	0.54
1:C:350:ARG:HH11	1:C:354:ARG:CZ	2.21	0.54
1:D:365:ALA:HB2	1:D:377:LEU:HG	1.90	0.54
1:B:136:TYR:CG	1:B:187:GLY:HA2	2.43	0.54
1:C:278:SER:O	1:C:313:ARG:NH1	2.40	0.53
1:C:290:PRO:HA	1:C:332:LEU:HD23	1.89	0.53
1:A:479:GLU:HG3	1:B:279:PRO:HB3	1.90	0.53
1:A:352:ARG:NH1	1:A:356:PRO:O	2.42	0.53
1:D:348:GLU:OE1	1:D:370:ARG:NE	2.42	0.53
1:D:136:TYR:CD1	1:D:187:GLY:HA2	2.44	0.53
1:A:319:ASN:ND2	1:A:361:ASP:OD1	2.40	0.52
1:A:269:PHE:CD1	1:A:282:LEU:HD11	2.45	0.52
1:A:344:LEU:HD22	1:A:362:TYR:CE1	2.45	0.52
1:D:299:LEU:O	1:D:303:ILE:HG12	2.10	0.52
1:C:78:ASP:O	1:C:82:ARG:HG3	2.10	0.51
1:B:188:GLY:HA2	1:B:411:PHE:CZ	2.46	0.51
1:D:33:LEU:HA	1:D:38:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:NH2	1:C:72:ASP:O	2.45	0.50
1:C:269:PHE:CD1	1:C:282:LEU:HD11	2.46	0.50
1:D:10:ALA:N	8:D:608:HOH:O	2.45	0.50
1:B:242:TYR:HB3	1:B:252:THR:HG21	1.94	0.50
1:D:140:THR:HG22	1:D:155:ARG:HB2	1.94	0.49
1:D:433:GLU:OE1	1:D:436:ARG:NH2	2.41	0.49
1:D:354:ARG:HH21	1:D:354:ARG:HG2	1.75	0.49
1:A:351:VAL:HG11	1:A:360:ILE:HD11	1.93	0.49
1:C:350:ARG:HH11	1:C:354:ARG:NH1	2.10	0.49
1:D:123:LEU:HD11	1:D:469:LEU:HD13	1.94	0.49
1:D:350:ARG:CG	1:D:354:ARG:HD3	2.43	0.49
1:D:267:ARG:HG2	1:D:306:LEU:HD23	1.93	0.48
1:A:409:ALA:HB2	1:A:454:PHE:HB3	1.95	0.48
1:B:94:ARG:NH1	1:B:98:GLU:OE2	2.45	0.48
1:D:436:ARG:HG2	1:D:436:ARG:HH11	1.77	0.48
1:D:436:ARG:NH1	1:D:440:GLU:OE1	2.47	0.47
1:B:313:ARG:HG3	1:B:313:ARG:HH21	1.80	0.47
1:B:263:ARG:HD3	1:B:267:ARG:CZ	2.45	0.47
1:A:144:ARG:HG3	1:A:144:ARG:O	2.15	0.47
1:C:76:ASP:CG	1:C:77:ARG:H	2.18	0.47
1:C:351:VAL:HG21	1:C:360:ILE:HD11	1.97	0.47
1:D:350:ARG:HH21	1:D:354:ARG:CZ	2.23	0.47
1:A:433:GLU:HG2	1:A:436:ARG:HH22	1.80	0.46
1:C:94:ARG:NH2	1:C:486:LEU:HB2	2.31	0.46
1:B:17:HIS:CE1	1:B:371:THR:HG21	2.50	0.46
1:A:192:LEU:HD23	1:A:197:LEU:HD23	1.98	0.46
1:D:350:ARG:HG3	1:D:354:ARG:CD	2.45	0.46
1:C:322:GLU:OE2	1:C:337:ARG:NH1	2.34	0.46
1:B:45:GLY:O	1:B:49:ARG:HG3	2.15	0.45
1:C:42:ASP:OD1	1:C:42:ASP:N	2.48	0.45
1:C:105:TYR:CZ	1:C:364:TYR:HB3	2.51	0.45
1:A:269:PHE:CE1	1:A:282:LEU:HD21	2.52	0.45
1:C:136:TYR:HB2	1:C:398:ASP:HA	1.98	0.45
1:C:441:ARG:NH2	8:C:609:HOH:O	2.49	0.45
1:D:188:GLY:HA2	1:D:411:PHE:CZ	2.52	0.45
1:B:105:TYR:CZ	1:B:364:TYR:HB3	2.51	0.45
1:C:334:GLN:H	1:C:334:GLN:CD	2.19	0.45
1:B:22:LEU:O	1:B:26:VAL:HG13	2.16	0.45
1:B:296:LEU:HB3	1:B:347:PHE:CD1	2.52	0.45
1:A:136:TYR:CG	1:A:187:GLY:HA2	2.52	0.44
1:C:186:SER:O	1:C:191:PRO:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:ARG:HH21	1:D:354:ARG:NH1	2.08	0.44
1:C:344:LEU:HD22	1:C:362:TYR:CE1	2.52	0.44
1:D:479:GLU:HG2	8:D:726:HOH:O	2.17	0.44
1:A:105:TYR:CZ	1:A:364:TYR:HB3	2.52	0.44
1:A:127:PRO:HB2	1:A:436:ARG:HG3	1.98	0.44
1:D:283:GLY:HA3	1:D:317:PHE:CZ	2.53	0.44
1:D:300:VAL:HG11	1:D:350:ARG:HG2	2.00	0.43
1:D:237:ILE:HG13	1:D:280:ILE:HD11	1.99	0.43
1:D:242:TYR:HB2	1:D:249:TYR:CE2	2.53	0.43
1:A:75:VAL:HG13	1:A:79:ALA:HB3	2.01	0.43
1:A:98:GLU:HB3	1:A:107:LYS:HE3	2.01	0.43
1:D:174:GLU:CD	1:D:430:SER:HB2	2.39	0.43
1:C:351:VAL:HG11	1:C:360:ILE:HD11	2.01	0.42
1:A:140:THR:HA	1:A:189:LEU:HD13	2.01	0.42
1:D:350:ARG:HG3	1:D:354:ARG:HD3	2.02	0.42
1:D:354:ARG:HG2	1:D:354:ARG:NH2	2.33	0.42
1:A:283:GLY:HA3	1:A:317:PHE:CZ	2.54	0.42
1:D:351:VAL:HG21	1:D:360:ILE:HD11	2.02	0.42
1:D:322:GLU:N	1:D:322:GLU:OE2	2.52	0.42
1:D:40:PRO:HA	1:D:41:PRO:HD3	1.92	0.42
1:B:292:ARG:HG3	1:B:295:ARG:CZ	2.50	0.42
1:A:118:VAL:HG12	1:A:393:VAL:HG22	2.00	0.41
1:A:386:ARG:NH1	1:A:470:GLU:OE1	2.53	0.41
1:C:366:LEU:HD23	1:C:369:LEU:HD12	2.01	0.41
1:D:436:ARG:NH2	1:D:437:ASP:OD2	2.53	0.41
1:D:337:ARG:HA	1:D:339:GLU:OE1	2.19	0.41
1:D:368:SER:OG	1:D:375:ALA:HB3	2.21	0.41
1:A:218:PHE:CE1	1:A:255:LYS:HE3	2.56	0.41
1:B:297:LEU:HD22	1:B:350:ARG:HE	1.85	0.41
1:A:76:ASP:OD1	1:A:77:ARG:N	2.54	0.41
1:A:334:GLN:HA	1:A:337:ARG:HB2	2.03	0.40
1:D:192:LEU:HD23	1:D:197:LEU:HD23	2.02	0.40
1:B:101:PRO:HA	8:B:614:HOH:O	2.21	0.40
1:C:94:ARG:HH22	1:C:486:LEU:HB2	1.86	0.40
1:C:210:ARG:HB3	1:C:235:HIS:HB2	2.02	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	477/493 (97%)	463 (97%)	14 (3%)	0	100	100
1	B	470/493 (95%)	458 (97%)	12 (3%)	0	100	100
1	C	475/493 (96%)	462 (97%)	12 (2%)	1 (0%)	47	55
1	D	468/493 (95%)	454 (97%)	11 (2%)	3 (1%)	25	26
All	All	1890/1972 (96%)	1837 (97%)	49 (3%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	ALA
1	D	161	LEU
1	C	483	PHE
1	D	311	GLN

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	376/388 (97%)	371 (99%)	5 (1%)	69	79
1	B	373/388 (96%)	367 (98%)	6 (2%)	62	74
1	C	375/388 (97%)	370 (99%)	5 (1%)	69	79
1	D	372/388 (96%)	367 (99%)	5 (1%)	69	79
All	All	1496/1552 (96%)	1475 (99%)	21 (1%)	65	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	82	ARG
1	A	249	TYR
1	A	260	ARG
1	A	374	ASP
1	B	76	ASP
1	B	249	TYR
1	B	292	ARG
1	B	313	ARG
1	B	321	ARG
1	B	339	GLU
1	C	14	ARG
1	C	249	TYR
1	C	313	ARG
1	C	324	TYR
1	C	354	ARG
1	D	225	LEU
1	D	249	TYR
1	D	292	ARG
1	D	345	ASN
1	D	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	489	HIS
1	B	491	HIS
1	D	345	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	D	502	1,4	0,12,12	-	-	-		
4	MET	D	501	2	7,8,8	0.92	1 (14%)	7,9,9	1.50	2 (28%)
6	GOL	B	505	-	5,5,5	0.93	0	5,5,5	0.93	0
2	SF4	C	501	3,1	0,12,12	-	-	-		
6	GOL	D	504	-	5,5,5	0.98	0	5,5,5	0.90	0
2	SF4	A	501	3,1	0,12,12	-	-	-		
3	SAM	C	502	2	24,29,29	1.21	3 (12%)	23,42,42	1.56	3 (13%)
4	MET	B	501	2	7,8,8	0.84	1 (14%)	7,9,9	1.28	2 (28%)
6	GOL	D	505	-	5,5,5	0.93	0	5,5,5	0.95	0
2	SF4	B	502	1,4	0,12,12	-	-	-		
5	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.12	0
6	GOL	B	504	-	5,5,5	0.86	0	5,5,5	0.94	0
5	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SAM	A	502	2	24,29,29	1.23	3 (12%)	23,42,42	1.65	3 (13%)

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	SF4	D	502	1,4	-	-	0/6/5/5
4	MET	D	501	2	-	1/8/8/8	-
6	GOL	B	505	-	-	0/4/4/4	-
6	GOL	D	504	-	-	2/4/4/4	-
2	SF4	C	501	3,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	C	502	2	-	3/12/33/33	0/3/3/3
2	SF4	A	501	3,1	-	-	0/6/5/5
4	MET	B	501	2	-	1/8/8/8	-
6	GOL	D	505	-	-	3/4/4/4	-
2	SF4	B	502	1,4	-	-	0/6/5/5
6	GOL	B	504	-	-	0/4/4/4	-
3	SAM	A	502	2	-	4/12/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	SAM	C2-N3	4.05	1.38	1.32
3	C	502	SAM	C2-N3	3.87	1.38	1.32
3	C	502	SAM	C2-N1	2.53	1.38	1.33
3	A	502	SAM	C2-N1	2.47	1.38	1.33
4	D	501	MET	OXT-C	-2.17	1.23	1.30
3	C	502	SAM	OXT-C	-2.16	1.23	1.30
4	B	501	MET	OXT-C	-2.13	1.23	1.30
3	A	502	SAM	OXT-C	-2.13	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	SAM	N3-C2-N1	-5.66	119.83	128.68
3	A	502	SAM	N3-C2-N1	-5.57	119.98	128.68
3	A	502	SAM	OXT-C-O	-3.45	116.26	124.09
4	D	501	MET	OXT-C-O	-3.02	117.24	124.09
3	C	502	SAM	OXT-C-O	-2.72	117.91	124.09
4	B	501	MET	OXT-C-O	-2.58	118.22	124.09
3	A	502	SAM	OXT-C-CA	2.48	121.83	113.38
4	D	501	MET	OXT-C-CA	2.41	121.60	113.38
3	C	502	SAM	OXT-C-CA	2.19	120.84	113.38
4	B	501	MET	OXT-C-CA	2.13	120.64	113.38

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	SAM	N-CA-CB-CG
3	A	502	SAM	C-CA-CB-CG

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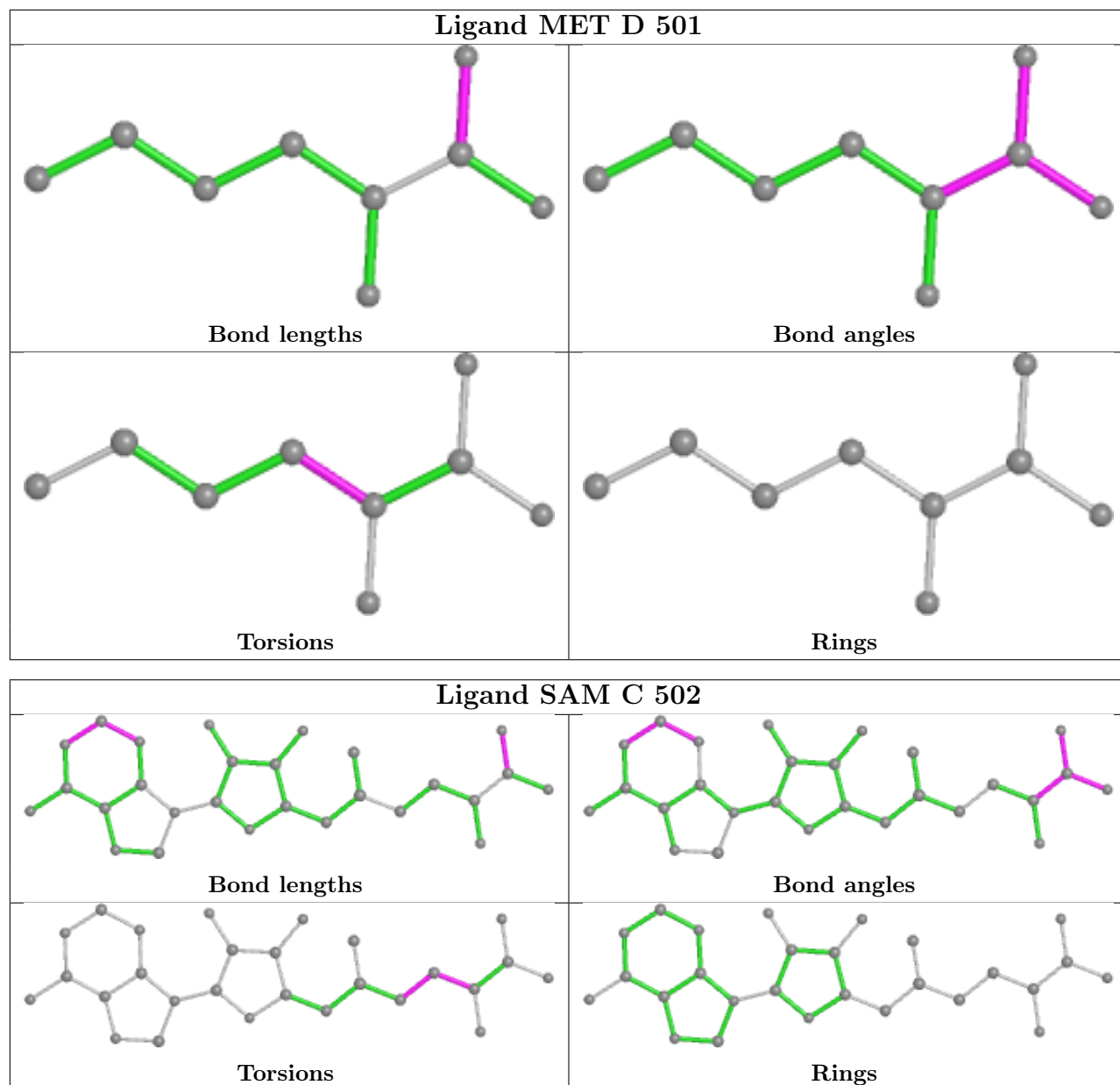
Mol	Chain	Res	Type	Atoms
3	C	502	SAM	C-CA-CB-CG
4	B	501	MET	N-CA-CB-CG
4	D	501	MET	C-CA-CB-CG
6	D	505	GOL	C1-C2-C3-O3
6	D	504	GOL	O1-C1-C2-C3
6	D	504	GOL	O1-C1-C2-O2
6	D	505	GOL	O2-C2-C3-O3
3	C	502	SAM	N-CA-CB-CG
6	D	505	GOL	O1-C1-C2-O2
3	A	502	SAM	O4'-C4'-C5'-SD
3	A	502	SAM	CA-CB-CG-SD
3	C	502	SAM	CA-CB-CG-SD

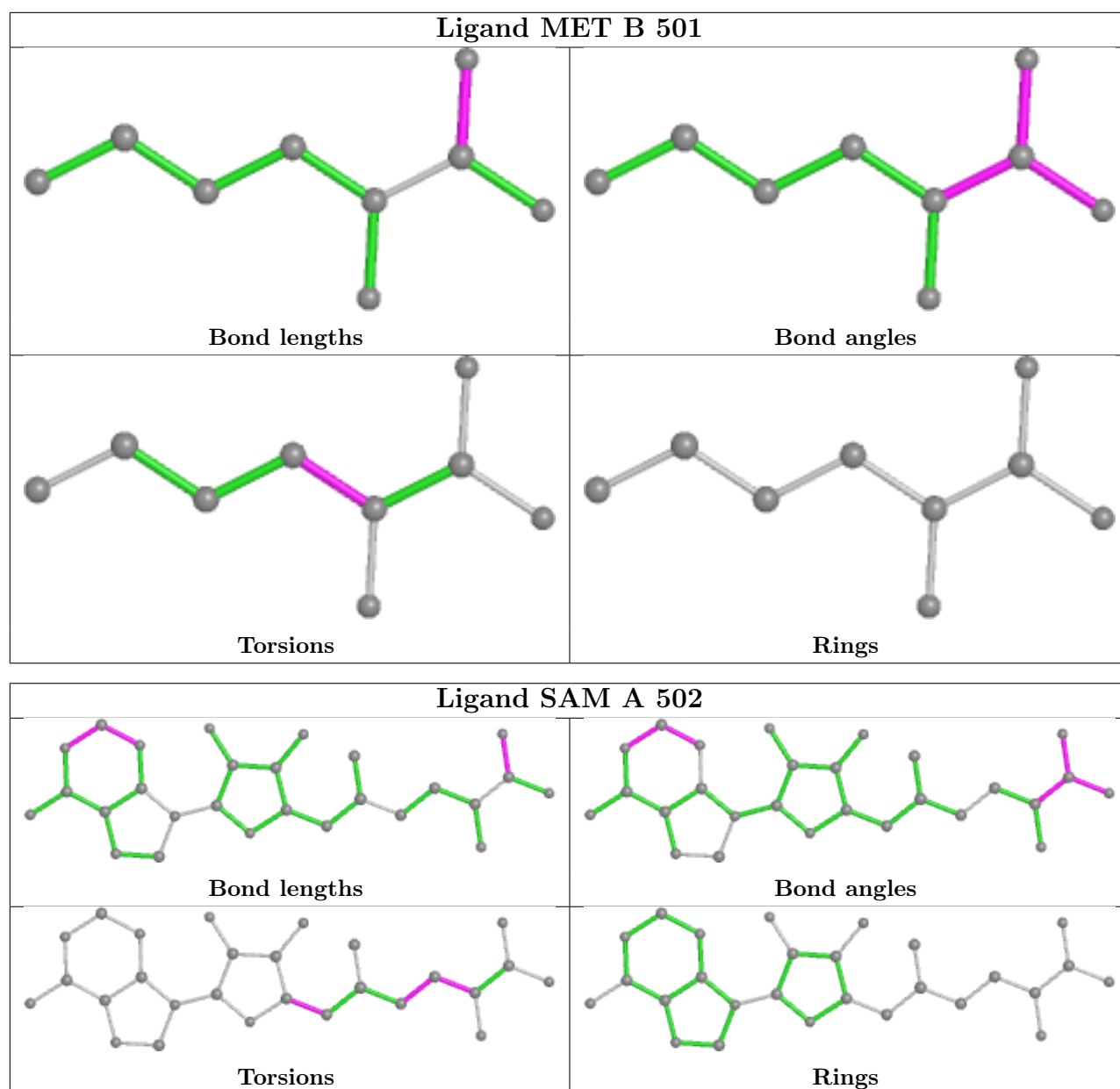
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	504	GOL	2	0
3	A	502	SAM	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.





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	479/493 (97%)	0.12	5 (1%) 82 88	33, 47, 64, 74	0
1	B	474/493 (96%)	0.17	17 (3%) 42 53	28, 43, 68, 86	0
1	C	477/493 (96%)	0.24	12 (2%) 57 66	37, 48, 65, 78	0
1	D	472/493 (95%)	0.09	19 (4%) 38 49	29, 40, 70, 93	0
All	All	1902/1972 (96%)	0.15	53 (2%) 53 63	28, 46, 66, 93	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	ALA	5.0
1	A	8	ALA	4.6
1	D	375	ALA	4.5
1	B	8	ALA	4.3
1	D	377	LEU	4.2
1	D	376	GLU	4.2
1	D	489	HIS	3.9
1	D	41	PRO	3.8
1	C	73	LEU	3.8
1	B	376	GLU	3.6
1	C	39	VAL	3.6
1	B	337	ARG	3.5
1	A	332	LEU	3.4
1	D	340	LEU	3.4
1	C	375	ALA	3.3
1	D	374	ASP	3.3
1	B	377	LEU	3.2
1	B	291	GLY	3.1
1	C	38	LEU	3.0
1	D	338	ALA	3.0
1	A	19	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	19	GLY	2.8
1	B	379	ARG	2.6
1	D	311	GLN	2.5
1	A	49	ARG	2.5
1	B	41	PRO	2.4
1	D	249	TYR	2.4
1	C	41	PRO	2.4
1	D	337	ARG	2.4
1	C	178	GLY	2.3
1	B	19	GLY	2.3
1	C	40	PRO	2.3
1	B	336	GLU	2.3
1	B	374	ASP	2.3
1	B	375	ALA	2.3
1	D	290	PRO	2.3
1	B	9	THR	2.2
1	A	342	GLU	2.2
1	C	187	GLY	2.2
1	C	162	ASP	2.2
1	C	72	ASP	2.2
1	B	21	ASP	2.1
1	D	493	HIS	2.1
1	D	39	VAL	2.1
1	D	354	ARG	2.1
1	B	38	LEU	2.1
1	B	187	GLY	2.1
1	B	342	GLU	2.1
1	D	370	ARG	2.1
1	C	14	ARG	2.0
1	D	292	ARG	2.0
1	D	336	GLU	2.0
1	D	42	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

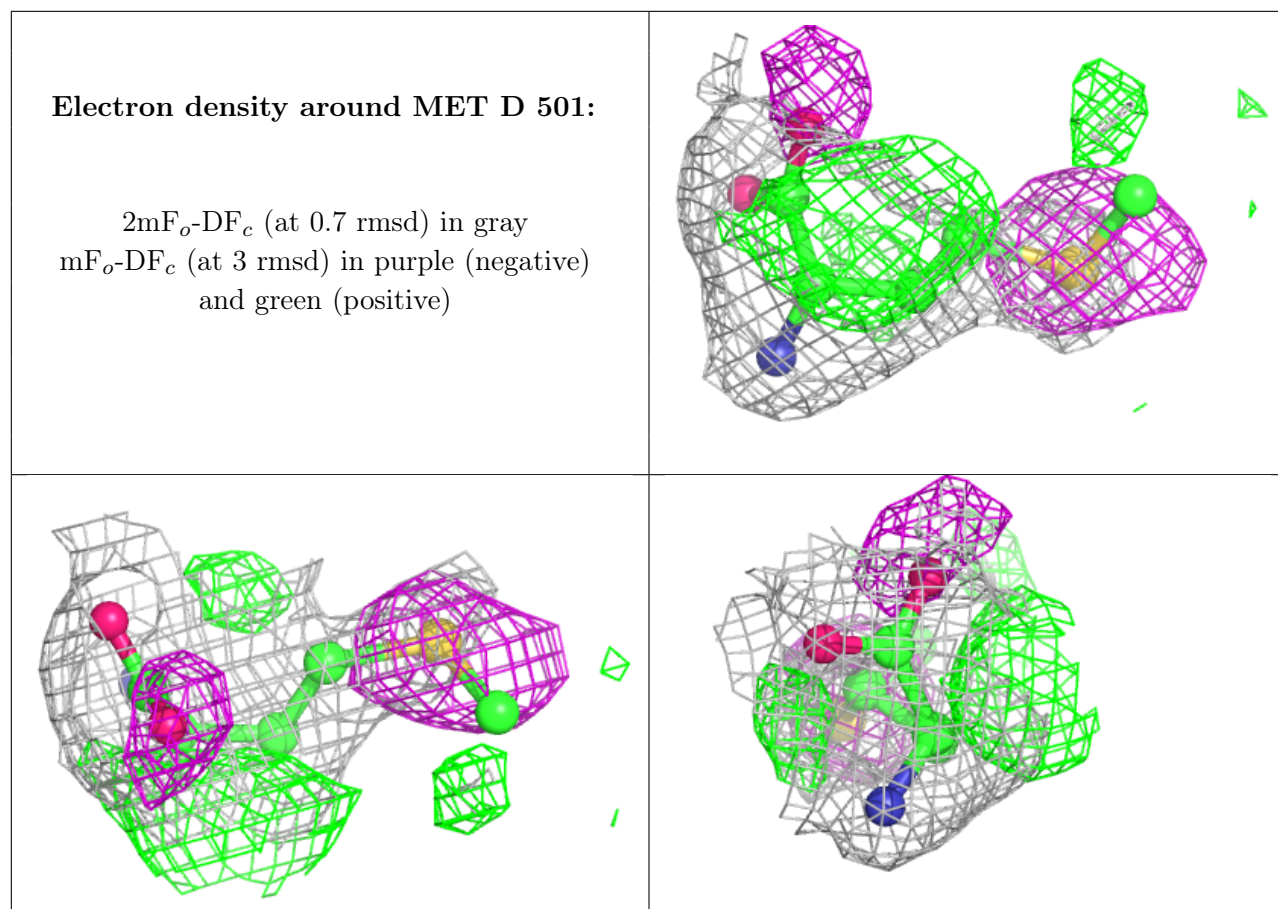
There are no monosaccharides in this entry.

6.4 Ligands

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.

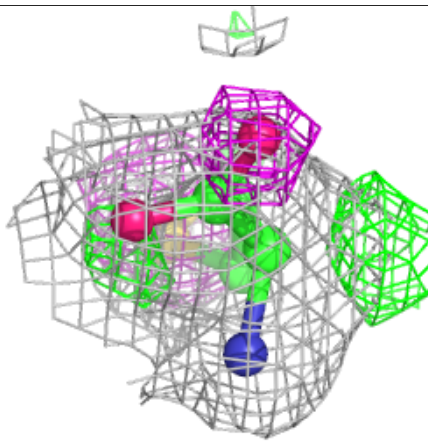
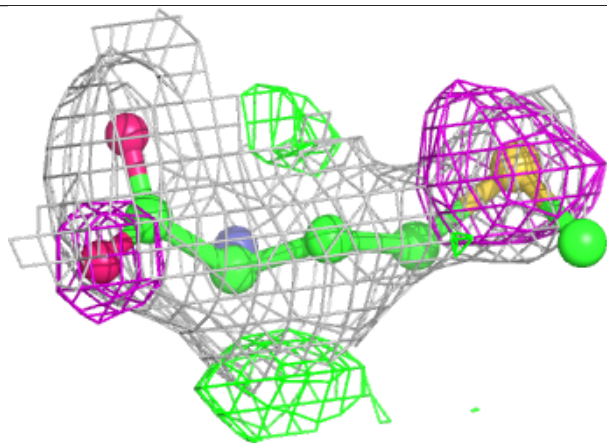
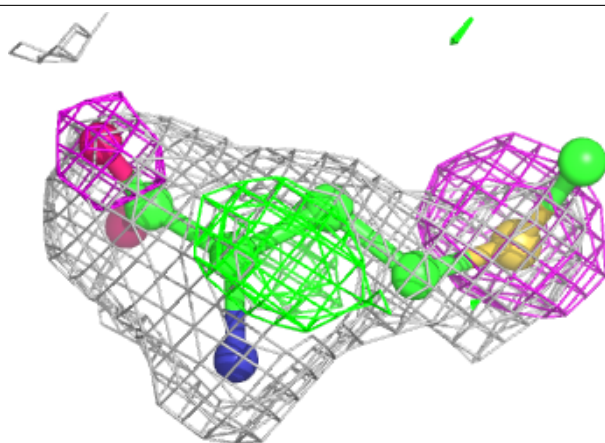
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MET	D	501	9/9	0.69	0.33	42,45,60,64	0
6	GOL	B	505	6/6	0.78	0.22	52,54,55,56	0
4	MET	B	501	9/9	0.79	0.23	40,41,63,67	0
6	GOL	B	504	6/6	0.84	0.16	46,47,48,50	0
7	NA	D	503	1/1	0.86	0.16	54,54,54,54	0
3	SAM	A	502	27/27	0.88	0.19	36,41,49,52	0
6	GOL	D	504	6/6	0.89	0.21	49,51,51,53	0
6	GOL	D	505	6/6	0.90	0.15	48,49,49,50	0
5	SO4	B	503	5/5	0.92	0.11	55,58,59,60	0
3	SAM	C	502	27/27	0.93	0.19	38,42,44,45	0
2	SF4	C	501	8/8	0.97	0.16	34,37,40,44	0
2	SF4	A	501	8/8	0.98	0.16	31,32,34,35	0
2	SF4	D	502	8/8	0.98	0.12	29,35,37,41	0
2	SF4	B	502	8/8	0.98	0.13	32,34,37,37	0
5	SO4	C	503	5/5	0.99	0.11	41,44,45,47	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.

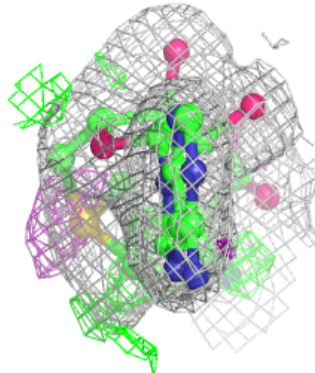
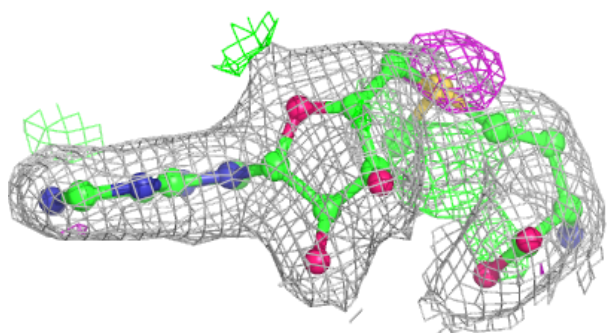
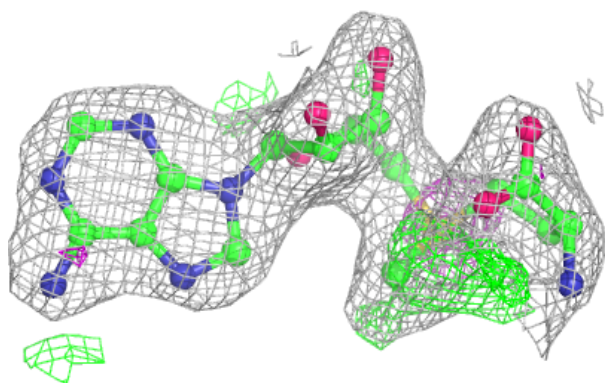


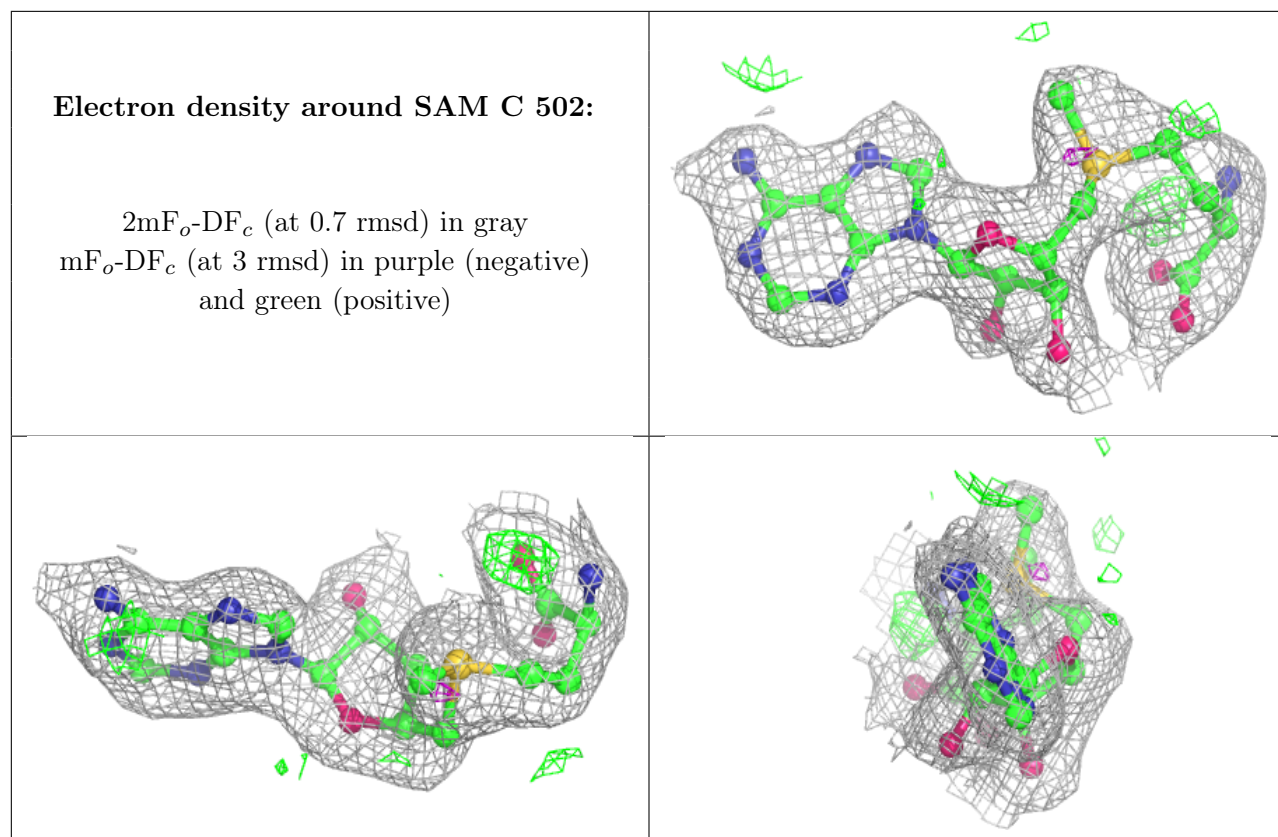
Electron density around MET B 501:

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

**Electron density around SAM A 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.