



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:27 PM EDT

PDB ID : 4R34 / pdb_00004r34
Title : X-ray structure of the tryptophan lyase NosL with Tryptophan, 5'-deoxyadenosine and methionine bound
Authors : Nicolet, Y.; Zeppieri, L.; Amara, P.; Fontecilla-Camps, J.-C.
Deposited on : 2014-08-14
Resolution : 1.80 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

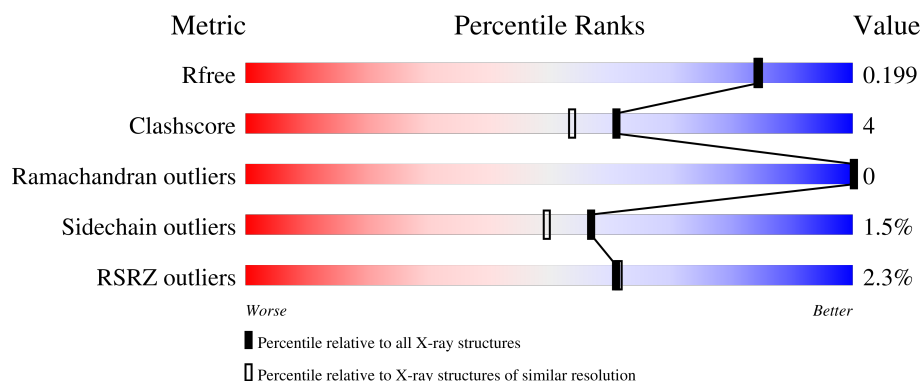
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

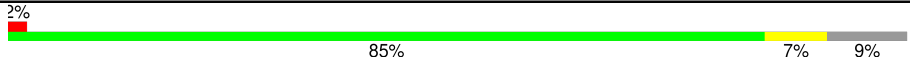
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	420	
1	B	420	

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
8	BR	A	508	-	-	X	-
8	BR	B	510	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6963 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 NosL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	8	0
			3008	1883	535	575	15			
1	B	384	Total	C	N	O	S	0	14	0
			3073	1916	558	581	18			

There are 40 discrepancies between the modelled and reference sequences:

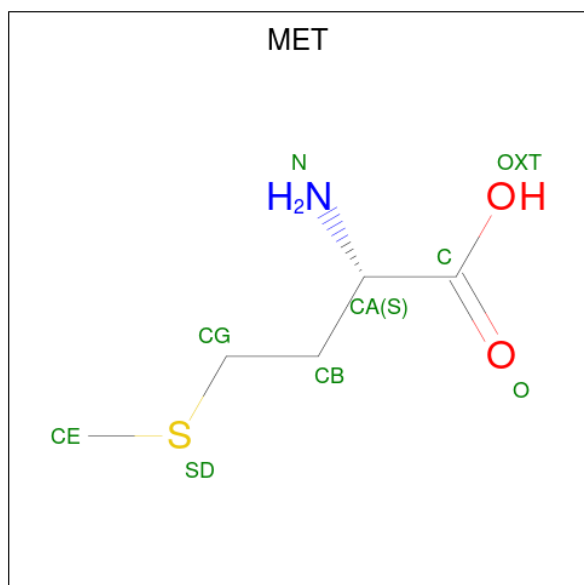
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP C6FX51
A	-18	GLY	-	expression tag	UNP C6FX51
A	-17	SER	-	expression tag	UNP C6FX51
A	-16	SER	-	expression tag	UNP C6FX51
A	-15	HIS	-	expression tag	UNP C6FX51
A	-14	HIS	-	expression tag	UNP C6FX51
A	-13	HIS	-	expression tag	UNP C6FX51
A	-12	HIS	-	expression tag	UNP C6FX51
A	-11	HIS	-	expression tag	UNP C6FX51
A	-10	HIS	-	expression tag	UNP C6FX51
A	-9	SER	-	expression tag	UNP C6FX51
A	-8	SER	-	expression tag	UNP C6FX51
A	-7	GLY	-	expression tag	UNP C6FX51
A	-6	LEU	-	expression tag	UNP C6FX51
A	-5	VAL	-	expression tag	UNP C6FX51
A	-4	PRO	-	expression tag	UNP C6FX51
A	-3	ARG	-	expression tag	UNP C6FX51
A	-2	GLY	-	expression tag	UNP C6FX51
A	-1	SER	-	expression tag	UNP C6FX51
A	0	HIS	-	expression tag	UNP C6FX51
B	-19	MET	-	expression tag	UNP C6FX51
B	-18	GLY	-	expression tag	UNP C6FX51
B	-17	SER	-	expression tag	UNP C6FX51
B	-16	SER	-	expression tag	UNP C6FX51
B	-15	HIS	-	expression tag	UNP C6FX51

Continued on next page...

Continued from previous page...

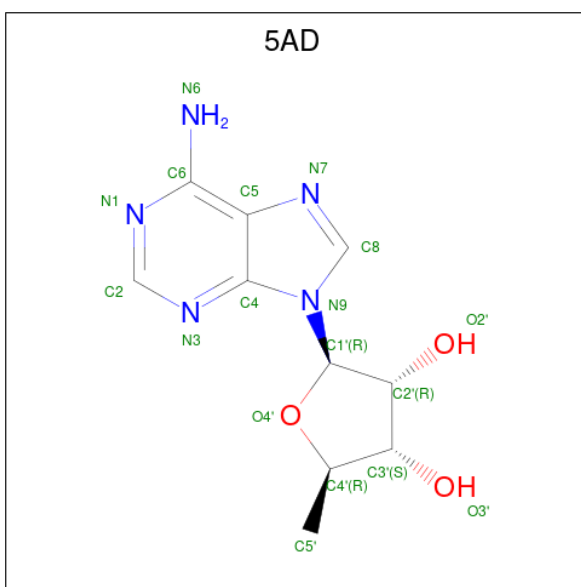
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP C6FX51
B	-13	HIS	-	expression tag	UNP C6FX51
B	-12	HIS	-	expression tag	UNP C6FX51
B	-11	HIS	-	expression tag	UNP C6FX51
B	-10	HIS	-	expression tag	UNP C6FX51
B	-9	SER	-	expression tag	UNP C6FX51
B	-8	SER	-	expression tag	UNP C6FX51
B	-7	GLY	-	expression tag	UNP C6FX51
B	-6	LEU	-	expression tag	UNP C6FX51
B	-5	VAL	-	expression tag	UNP C6FX51
B	-4	PRO	-	expression tag	UNP C6FX51
B	-3	ARG	-	expression tag	UNP C6FX51
B	-2	GLY	-	expression tag	UNP C6FX51
B	-1	SER	-	expression tag	UNP C6FX51
B	0	HIS	-	expression tag	UNP C6FX51

- Molecule 2 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



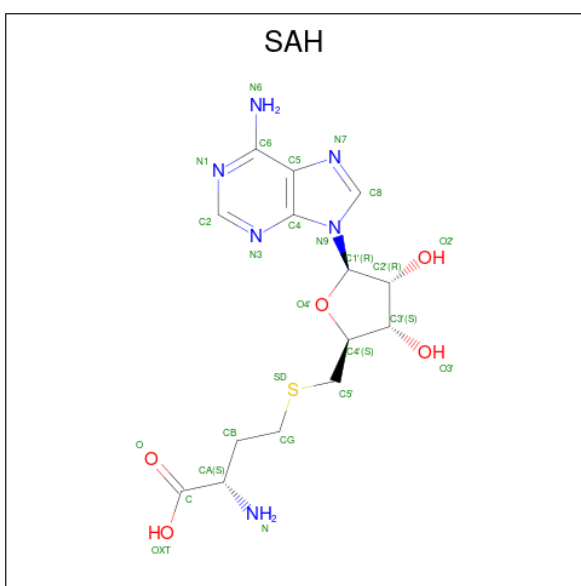
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			9	5	1	2	1		
2	B	1	Total	C	N	O	S	0	1
			9	5	1	2	1		

- Molecule 3 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



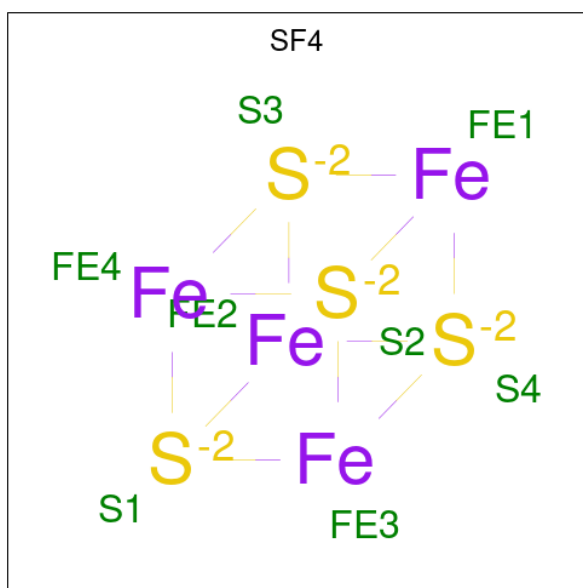
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			18	10	5	3		
3	B	1	Total	C	N	O	0	1
			18	10	5	3		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



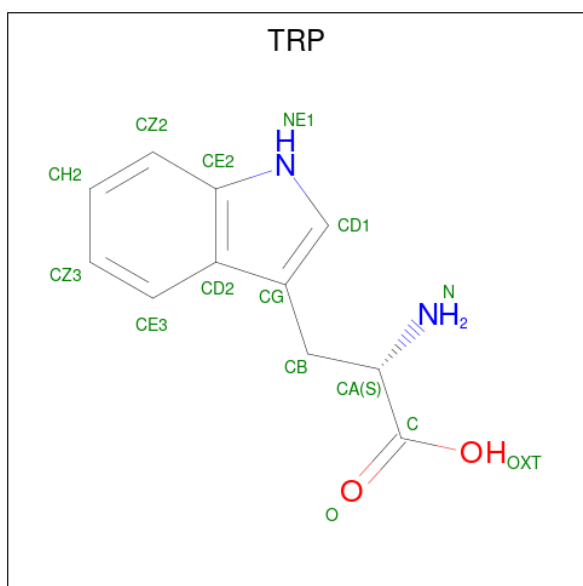
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	1
			26	14	6	5	1		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 6 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



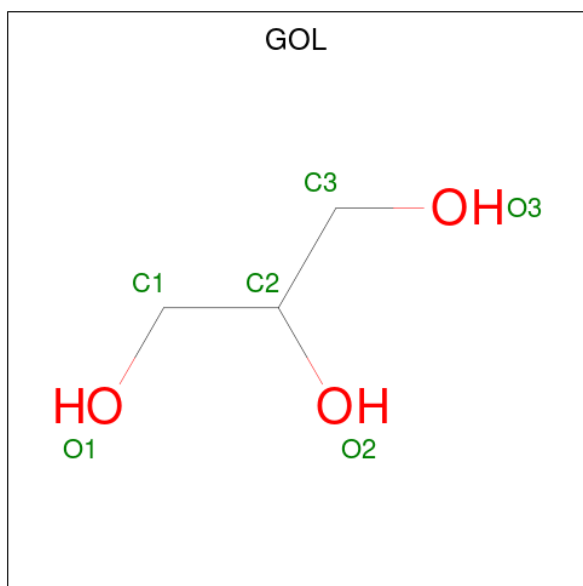
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			15	11	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	Br	0	0
			3	3		
8	B	4	Total	Br	0	0
			4	4		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Na 1	0	0
9	B	1	Total 1	Na 1	0	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total 1	Zn 1	0	0

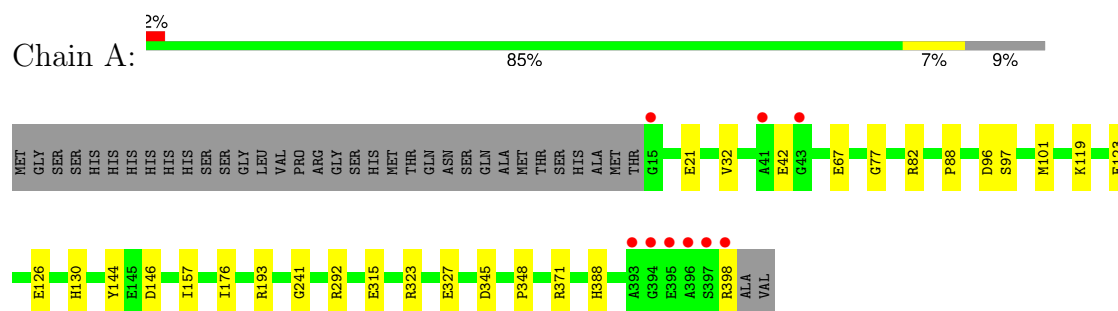
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	298	Total 298	O 298	0	0
11	B	398	Total 398	O 398	0	0

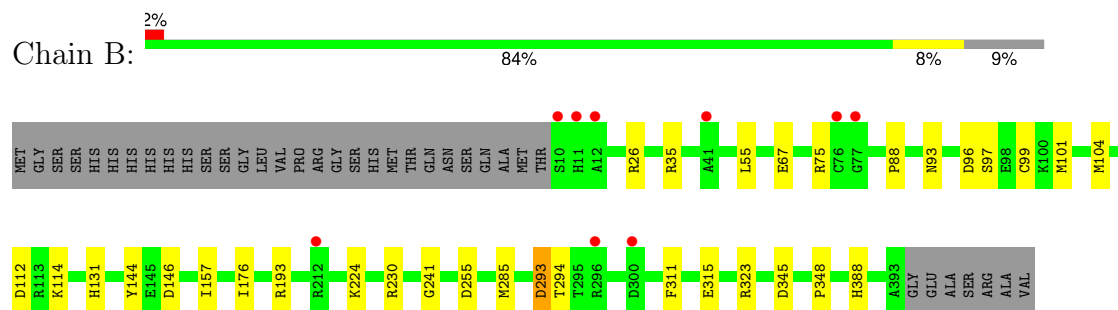
3 Residue-property plots [i](#)

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: NosL



• Molecule 1: NosL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.15Å 47.07Å 113.92Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	40.97 – 1.80 40.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.6 (40.97-1.80) 89.7 (40.97-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.172 , 0.199 0.175 , 0.199	Depositor DCC
R_{free} test set	3947 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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, ZN, SAH, GOL, 5AD, SF4, BR

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	0/3094	0.68	0/4193
1	B	0.36	0/3169	0.70	0/4289
All	All	0.34	0/6263	0.69	0/8482

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3008	0	2909	21	0
1	B	3073	0	3006	24	1
2	A	9	0	8	0	0
2	B	9	0	8	0	0
3	A	18	0	12	1	0
3	B	18	0	12	1	0
4	A	26	0	19	1	0
4	B	26	0	19	1	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
6	A	15	0	9	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	15	0	9	3	0
7	A	6	0	8	0	0
7	B	18	0	24	3	0
8	A	3	0	0	3	0
8	B	4	0	0	2	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	B	1	0	0	0	0
11	A	298	0	0	12	1
11	B	398	0	0	8	2
All	All	6963	0	6043	52	2

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 (52) 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)
3:B:502[A]:5AD:O4'	3:B:502[A]:5AD:C1'	1.63	1.25
3:A:502[A]:5AD:C1'	3:A:502[A]:5AD:O4'	1.63	1.17
1:A:77:GLY:O	11:A:779:HOH:O	1.87	0.91
7:B:508:GOL:O1	11:B:898:HOH:O	2.04	0.76
1:A:146:ASP:OD2	11:A:674:HOH:O	2.04	0.74
1:B:146[A]:ASP:OD1	11:B:743:HOH:O	2.05	0.74
8:A:508:BR:BR	11:A:699:HOH:O	2.63	0.71
1:A:67:GLU:OE1	11:A:686:HOH:O	2.11	0.68
1:A:398:ARG:O	11:A:832:HOH:O	2.13	0.65
1:B:112[B]:ASP:OD2	1:B:114:LYS:NZ	2.30	0.65
1:B:293:ASP:OD1	11:B:687:HOH:O	2.13	0.65
1:B:255[A]:ASP:OD2	11:B:907:HOH:O	2.14	0.64
1:B:255[B]:ASP:OD2	11:B:907:HOH:O	2.15	0.63
1:A:126[A]:GLU:OE1	11:A:723:HOH:O	2.16	0.60
1:B:131:HIS:HA	7:B:507:GOL:H11	1.85	0.59
1:A:193:ARG:HE	1:A:241:GLY:HA3	1.69	0.58
1:A:126[B]:GLU:OE1	11:A:658:HOH:O	2.17	0.57
1:B:388:HIS:HA	8:B:510:BR:BR	2.60	0.57
1:A:327[A]:GLU:OE1	11:A:830:HOH:O	2.16	0.56
1:B:323:ARG:HH22	6:B:505:TRP:N	2.05	0.54
1:B:35:ARG:NH2	1:B:67:GLU:OE2	2.41	0.54
1:A:82:ARG:HG3	8:A:509:BR:BR	2.62	0.54
1:A:327[B]:GLU:OE2	11:A:830:HOH:O	2.18	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:HB3	1:A:348:PRO:HB3	1.90	0.53
1:B:26:ARG:NH2	11:B:955:HOH:O	2.40	0.52
1:A:130:HIS:NE2	11:A:723:HOH:O	1.96	0.52
1:A:96:ASP:HB2	1:A:144:TYR:HA	1.93	0.51
1:A:323:ARG:HH22	6:A:505:TRP:N	2.10	0.49
1:A:371[A]:ARG:HD2	11:B:874:HOH:O	2.12	0.49
1:B:93:ASN:HA	1:B:104:MET:HE3	1.94	0.49
1:B:345:ASP:HB3	1:B:348:PRO:HB3	1.94	0.48
1:B:131:HIS:CE1	7:B:507:GOL:H31	2.48	0.47
1:B:88:PRO:HG3	6:B:505:TRP:CE2	2.50	0.47
1:B:26:ARG:HG2	1:B:55:LEU:HD21	1.97	0.46
1:B:99:CYS:SG	1:B:224:LYS:HD3	2.56	0.45
1:B:75:ARG:HD3	1:B:311:PHE:CE2	2.52	0.45
1:A:292:ARG:NH1	11:A:843:HOH:O	2.45	0.45
1:A:119:LYS:HE3	1:A:123:GLU:OE2	2.16	0.44
1:A:21:GLU:HA	11:A:838:HOH:O	2.16	0.44
8:B:510:BR:BR	11:B:925:HOH:O	2.77	0.44
1:B:157:ILE:HG13	1:B:176:ILE:HG21	2.00	0.44
1:A:388:HIS:HA	8:A:508:BR:BR	2.73	0.44
1:B:193:ARG:HD2	1:B:241:GLY:HA3	1.99	0.43
1:B:96:ASP:HB2	1:B:144:TYR:HA	2.01	0.42
1:B:285[A]:MET:HE2	1:B:285[A]:MET:HB2	1.88	0.42
4:A:503[B]:SAH:H3'	4:A:503[B]:SAH:HG1	2.00	0.42
1:B:88:PRO:HG3	6:B:505:TRP:CD2	2.55	0.41
4:B:503[B]:SAH:HG1	4:B:503[B]:SAH:H3'	2.03	0.41
1:B:285[A]:MET:HE3	1:B:294:THR:HG21	2.03	0.41
1:A:88:PRO:HG3	6:A:505:TRP:CE2	2.56	0.41
1:B:224:LYS:HE3	1:B:230:ARG:CZ	2.50	0.40
1:A:157:ILE:HG13	1:A:176:ILE:HG21	2.01	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:857:HOH:O	11:B:980:HOH:O[2_655]	2.06	0.14
1:B:146[B]:ASP:OD2	11:B:800:HOH:O[2_655]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	390/420 (93%)	379 (97%)	11 (3%)	0	100	100
1	B	396/420 (94%)	383 (97%)	13 (3%)	0	100	100
All	All	786/840 (94%)	762 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	312/346 (90%)	307 (98%)	5 (2%)	55	47
1	B	324/346 (94%)	320 (99%)	4 (1%)	63	57
All	All	636/692 (92%)	627 (99%)	9 (1%)	57	52

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	42	GLU
1	A	97	SER
1	A	101	MET
1	A	315	GLU
1	B	97	SER
1	B	101	MET
1	B	293	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	315	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	246	ASN
1	B	326	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 10 are 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	$\# Z > 2$
6	TRP	A	505	-	15,16,16	0.72	1 (6%)	18,22,22	0.73	1 (5%)
7	GOL	A	506	-	5,5,5	0.36	0	5,5,5	0.43	0
3	5AD	A	502[A]	-	20,20,20	3.58	11 (55%)	28,30,30	2.40	12 (42%)
5	SF4	A	504	4,1,2	0,12,12	-	-	-	-	-
2	MET	B	501[A]	5	7,8,8	0.86	1 (14%)	5,9,9	1.08	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	506	-	5,5,5	0.27	0	5,5,5	0.46	0
7	GOL	B	508	-	5,5,5	0.36	0	5,5,5	0.33	0
3	5AD	B	502[A]	-	20,20,20	3.59	11 (55%)	28,30,30	2.36	12 (42%)
4	SAH	B	503[B]	5	27,28,28	1.09	4 (14%)	36,40,40	1.98	10 (27%)
4	SAH	A	503[B]	5	27,28,28	1.09	4 (14%)	36,40,40	2.10	11 (30%)
7	GOL	B	507	-	5,5,5	0.40	0	5,5,5	0.29	0
2	MET	A	501[A]	5	7,8,8	0.89	1 (14%)	5,9,9	1.05	1 (20%)
5	SF4	B	504	4,1,2	0,12,12	-	-	-	-	-
6	TRP	B	505	-	15,16,16	0.73	1 (6%)	18,22,22	0.69	1 (5%)

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
6	TRP	A	505	-	-	0/8/8/8	0/2/2/2
7	GOL	A	506	-	-	0/4/4/4	-
3	5AD	A	502[A]	-	-	3/4/20/20	0/3/3/3
5	SF4	A	504	4,1,2	-	-	0/6/5/5
2	MET	B	501[A]	5	-	1/8/8/8	-
7	GOL	B	506	-	-	0/4/4/4	-
7	GOL	B	508	-	-	3/4/4/4	-
3	5AD	B	502[A]	-	-	2/4/20/20	0/3/3/3
5	SF4	B	504	4,1,2	-	-	0/6/5/5
4	SAH	B	503[B]	5	-	0/15/31/31	0/3/3/3
4	SAH	A	503[B]	5	-	2/15/31/31	0/3/3/3
2	MET	A	501[A]	5	-	1/8/8/8	-
7	GOL	B	507	-	-	2/4/4/4	-
6	TRP	B	505	-	-	0/8/8/8	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[A]	5AD	O4'-C1'	9.47	1.63	1.42
3	A	502[A]	5AD	O4'-C1'	9.39	1.63	1.42
3	A	502[A]	5AD	C2'-C1'	-6.85	1.31	1.53
3	B	502[A]	5AD	C2'-C1'	-6.74	1.32	1.53
3	A	502[A]	5AD	C6-N6	5.14	1.47	1.34
3	B	502[A]	5AD	C6-N6	5.11	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	5AD	O4'-C4'	-4.67	1.30	1.44
3	B	502[A]	5AD	O4'-C4'	-4.67	1.30	1.44
3	B	502[A]	5AD	C3'-C4'	3.81	1.58	1.52
3	A	502[A]	5AD	O3'-C3'	-3.73	1.33	1.43
3	B	502[A]	5AD	O3'-C3'	-3.68	1.33	1.43
3	A	502[A]	5AD	C3'-C4'	3.67	1.57	1.52
3	B	502[A]	5AD	O2'-C2'	3.65	1.52	1.43
3	A	502[A]	5AD	O2'-C2'	3.53	1.51	1.43
3	A	502[A]	5AD	C2-N3	2.79	1.38	1.33
3	A	502[A]	5AD	C5-C4	-2.72	1.34	1.39
3	B	502[A]	5AD	C5-C4	-2.70	1.34	1.39
3	B	502[A]	5AD	C2-N3	2.69	1.38	1.33
4	B	503[B]	SAH	C2-N1	2.60	1.38	1.33
4	A	503[B]	SAH	C2-N3	2.59	1.38	1.33
4	A	503[B]	SAH	C2-N1	2.52	1.38	1.33
4	B	503[B]	SAH	C2-N3	2.52	1.38	1.33
3	B	502[A]	5AD	C8-N7	2.43	1.36	1.31
3	B	502[A]	5AD	C4-N3	2.39	1.38	1.34
3	A	502[A]	5AD	C4-N3	2.38	1.38	1.34
3	A	502[A]	5AD	C8-N7	2.29	1.36	1.31
4	A	503[B]	SAH	OXT-C	-2.22	1.23	1.30
4	B	503[B]	SAH	OXT-C	-2.22	1.23	1.30
2	A	501[A]	MET	OXT-C	-2.19	1.23	1.30
2	B	501[A]	MET	OXT-C	-2.18	1.23	1.30
6	A	505	TRP	OXT-C	-2.15	1.23	1.30
4	B	503[B]	SAH	C8-N7	2.09	1.35	1.31
6	B	505	TRP	OXT-C	-2.07	1.24	1.30
4	A	503[B]	SAH	C8-N7	2.04	1.35	1.31

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	5AD	N3-C2-N1	-5.90	119.65	128.58
3	A	502[A]	5AD	N3-C2-N1	-5.76	119.86	128.58
4	B	503[B]	SAH	N3-C2-N1	-5.54	120.20	128.58
4	A	503[B]	SAH	N3-C2-N1	-5.50	120.26	128.58
4	A	503[B]	SAH	C5-C4-N3	-4.59	120.39	126.72
4	B	503[B]	SAH	C5-C4-N3	-4.56	120.44	126.72
3	A	502[A]	5AD	C5-C4-N3	-4.48	120.54	126.72
3	B	502[A]	5AD	C5-C4-N3	-4.40	120.66	126.72
3	A	502[A]	5AD	N9-C8-N7	-4.25	107.90	113.94
3	A	502[A]	5AD	N6-C6-N1	-4.18	109.07	118.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	5AD	N9-C8-N7	-4.17	108.02	113.94
3	B	502[A]	5AD	N6-C6-N1	-4.12	109.21	118.38
4	A	503[B]	SAH	N9-C8-N7	-3.76	108.60	113.94
4	B	503[B]	SAH	N9-C8-N7	-3.72	108.65	113.94
4	A	503[B]	SAH	C5'-SD-CG	-3.55	91.73	102.26
4	A	503[B]	SAH	C2-N3-C4	3.44	120.22	111.83
4	B	503[B]	SAH	C2-N3-C4	3.41	120.17	111.83
4	A	503[B]	SAH	C5-N7-C8	3.39	108.78	103.45
4	B	503[B]	SAH	C5-N7-C8	3.26	108.57	103.45
3	A	502[A]	5AD	C2-N3-C4	3.24	119.75	111.83
3	B	502[A]	5AD	C2-N3-C4	3.22	119.70	111.83
4	A	503[B]	SAH	O4'-C1'-N9	3.07	113.99	108.09
3	A	502[A]	5AD	C5-C6-N6	3.06	130.85	123.29
3	B	502[A]	5AD	C5-C6-N6	3.05	130.84	123.29
4	B	503[B]	SAH	N3-C4-N9	3.03	132.32	127.17
4	A	503[B]	SAH	N3-C4-N9	2.98	132.23	127.17
3	A	502[A]	5AD	C5-N7-C8	2.92	108.03	103.45
3	B	502[A]	5AD	C5-N7-C8	2.79	107.84	103.45
3	A	502[A]	5AD	C5'-C4'-C3'	-2.71	112.86	115.70
4	B	503[B]	SAH	O4'-C1'-N9	2.70	113.27	108.09
4	A	503[B]	SAH	OXT-C-O	-2.67	118.03	124.08
4	B	503[B]	SAH	OXT-C-O	-2.60	118.19	124.08
6	A	505	TRP	OXT-C-O	-2.57	118.25	124.08
3	B	502[A]	5AD	C5'-C4'-C3'	-2.49	113.08	115.70
6	B	505	TRP	OXT-C-O	-2.46	118.50	124.08
3	A	502[A]	5AD	C4-C5-N7	-2.42	107.81	110.58
4	A	503[B]	SAH	C4-C5-N7	-2.40	107.84	110.58
2	B	501[A]	MET	OXT-C-O	-2.39	118.65	124.08
3	A	502[A]	5AD	N3-C4-N9	2.38	131.21	127.17
4	A	503[B]	SAH	O4'-C4'-C5'	2.36	114.91	108.83
3	B	502[A]	5AD	C4-C5-N7	-2.34	107.90	110.58
3	B	502[A]	5AD	C5-C4-N9	2.34	108.36	105.81
2	A	501[A]	MET	OXT-C-O	-2.33	118.80	124.08
3	B	502[A]	5AD	N3-C4-N9	2.25	130.99	127.17
4	B	503[B]	SAH	C4-C5-N7	-2.25	108.01	110.58
3	A	502[A]	5AD	C5-C4-N9	2.23	108.25	105.81
4	B	503[B]	SAH	O4'-C4'-C5'	2.20	114.51	108.83
3	A	502[A]	5AD	C4-N9-C8	2.16	108.01	105.74
3	B	502[A]	5AD	C4-N9-C8	2.04	107.88	105.74

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[A]	MET	C-CA-CB-CG
4	A	503[B]	SAH	O4'-C4'-C5'-SD
7	B	507	GOL	O1-C1-C2-C3
7	B	508	GOL	O1-C1-C2-C3
7	B	507	GOL	O1-C1-C2-O2
7	B	508	GOL	O1-C1-C2-O2
7	B	508	GOL	O2-C2-C3-O3
3	A	502[A]	5AD	C2'-C1'-N9-C8
3	B	502[A]	5AD	C2'-C1'-N9-C8
2	B	501[A]	MET	C-CA-CB-CG
3	A	502[A]	5AD	O4'-C1'-N9-C8
3	B	502[A]	5AD	O4'-C1'-N9-C8
4	A	503[B]	SAH	C3'-C4'-C5'-SD
3	A	502[A]	5AD	C2'-C1'-N9-C4

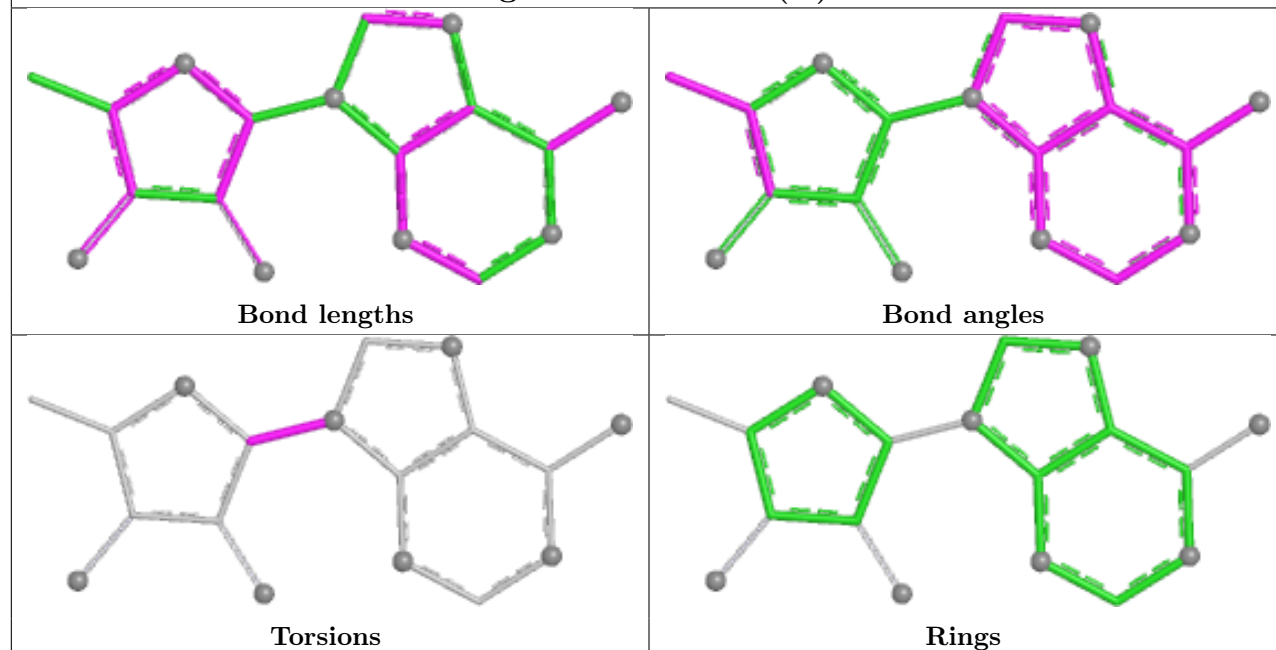
There are no ring outliers.

8 monomers are involved in 12 short contacts:

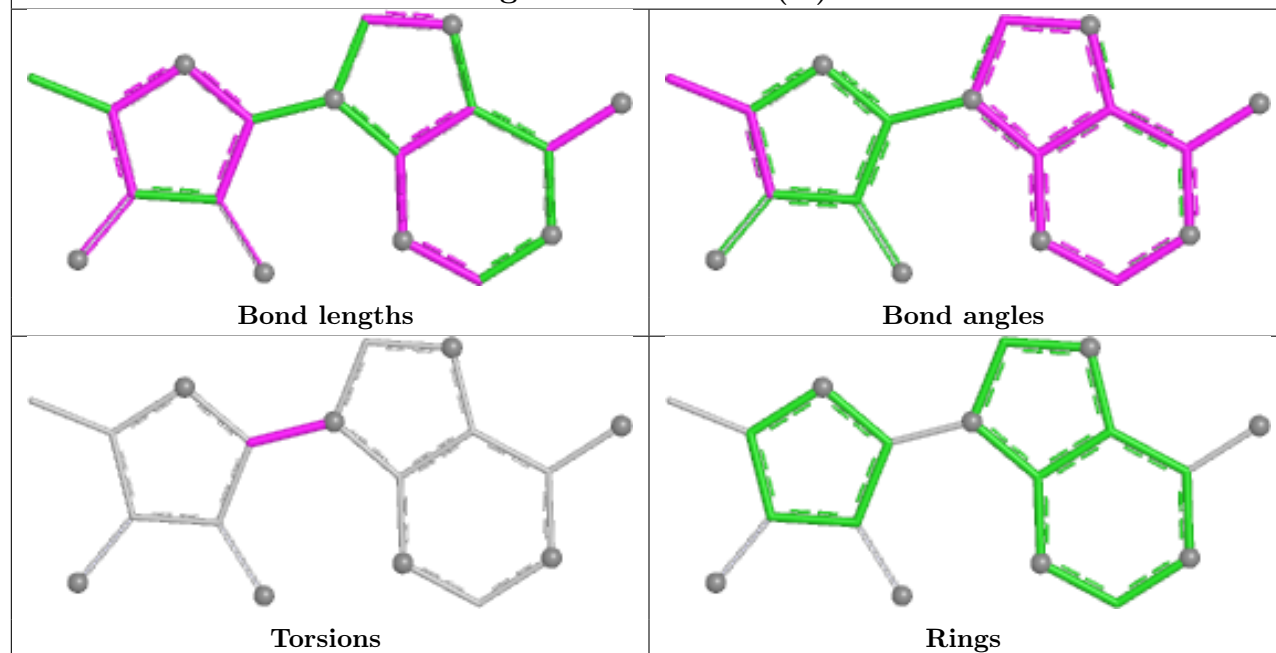
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	505	TRP	2	0
3	A	502[A]	5AD	1	0
7	B	508	GOL	1	0
3	B	502[A]	5AD	1	0
4	B	503[B]	SAH	1	0
4	A	503[B]	SAH	1	0
7	B	507	GOL	2	0
6	B	505	TRP	3	0

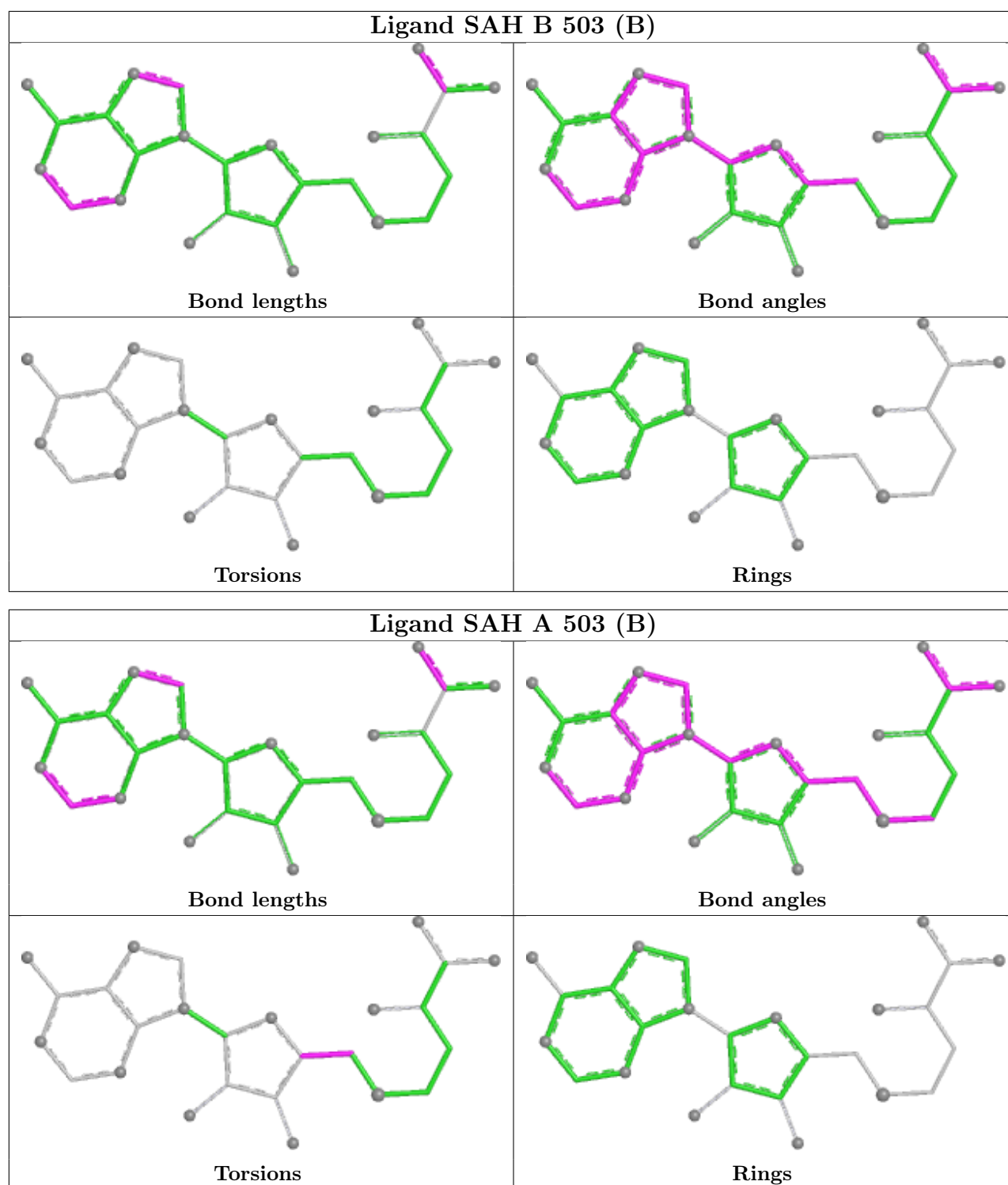
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 5AD A 502 (A)



Ligand 5AD B 502 (A)





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/420 (91%)	0.03	9 (2%) 61 61	16, 35, 62, 86	8 (2%)
1	B	384/420 (91%)	-0.27	9 (2%) 61 61	11, 24, 48, 72	14 (3%)
All	All	768/840 (91%)	-0.12	18 (2%) 61 61	11, 29, 58, 86	22 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	HIS	4.5
1	A	393	ALA	3.5
1	A	398	ARG	3.4
1	B	12	ALA	3.2
1	B	10	SER	3.2
1	A	43	GLY	3.1
1	A	396	ALA	2.9
1	B	41	ALA	2.9
1	B	300	ASP	2.8
1	A	394	GLY	2.4
1	A	41	ALA	2.4
1	B	76[A]	CYS	2.4
1	A	397	SER	2.3
1	B	77[A]	GLY	2.2
1	B	296	ARG	2.2
1	A	15	GLY	2.1
1	A	395	GLU	2.1
1	B	212	ARG	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

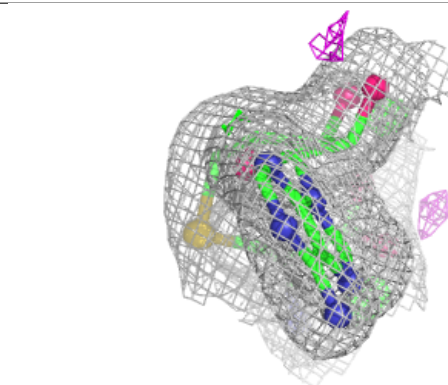
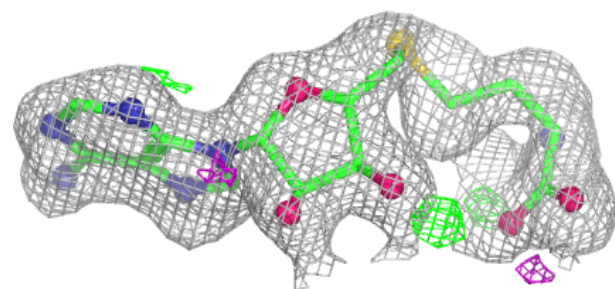
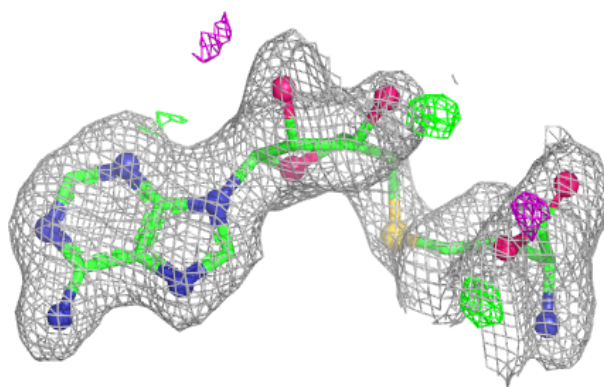
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	BR	B	511	1/1	0.86	0.14	80,80,80,80	1
7	GOL	B	507	6/6	0.89	0.12	51,58,62,62	0
7	GOL	B	508	6/6	0.91	0.11	31,36,43,51	0
8	BR	A	507	1/1	0.93	0.13	80,80,80,80	1
4	SAH	A	503[B]	26/26	0.94	0.08	24,29,32,33	26
4	SAH	B	503[B]	26/26	0.94	0.07	16,21,24,25	26
7	GOL	A	506	6/6	0.95	0.07	29,33,40,42	0
7	GOL	B	506	6/6	0.95	0.08	23,26,31,33	0
3	5AD	A	502[A]	18/18	0.95	0.06	23,28,31,31	18
2	MET	B	501[A]	9/9	0.96	0.09	16,20,22,23	9
3	5AD	B	502[A]	18/18	0.96	0.06	18,21,23,27	18
8	BR	A	508	1/1	0.96	0.11	55,55,55,55	1
6	TRP	A	505	15/15	0.96	0.06	21,24,32,32	0
8	BR	B	514	1/1	0.96	0.07	39,39,39,39	1
8	BR	B	510	1/1	0.97	0.08	50,50,50,50	1
2	MET	A	501[A]	9/9	0.97	0.09	28,30,33,41	9
6	TRP	B	505	15/15	0.97	0.05	16,20,23,26	0
9	NA	B	512	1/1	0.97	0.05	37,37,37,37	0
8	BR	A	509	1/1	0.98	0.08	58,58,58,58	1
9	NA	A	510	1/1	0.98	0.07	37,37,37,37	0
8	BR	B	509	1/1	0.98	0.06	45,45,45,45	1
10	ZN	B	513	1/1	0.98	0.04	40,40,40,40	1
5	SF4	A	504	8/8	0.99	0.03	29,30,32,32	0
5	SF4	B	504	8/8	0.99	0.05	15,20,23,25	0

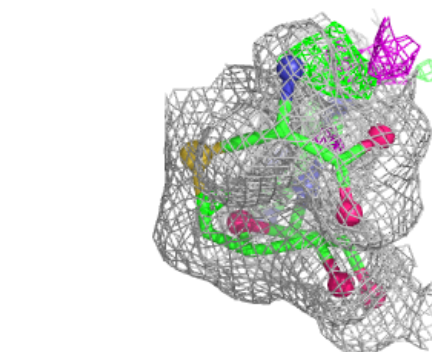
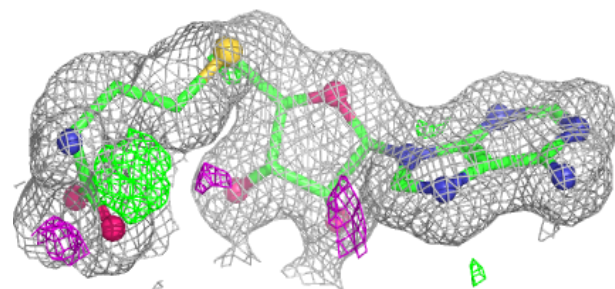
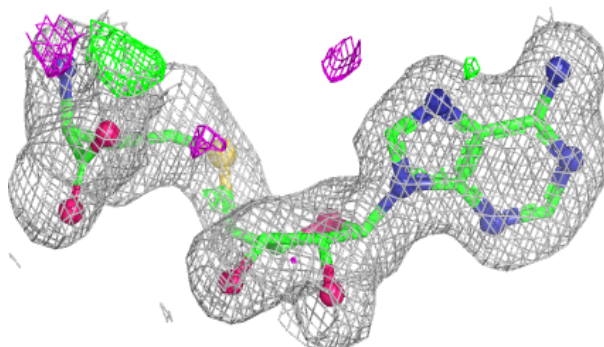
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH A 503 (B):

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

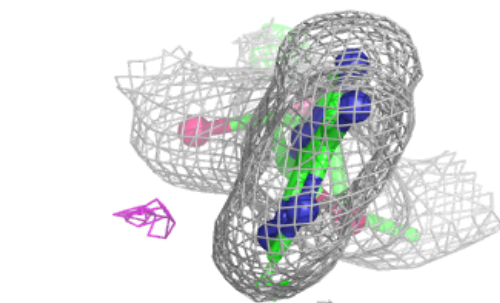
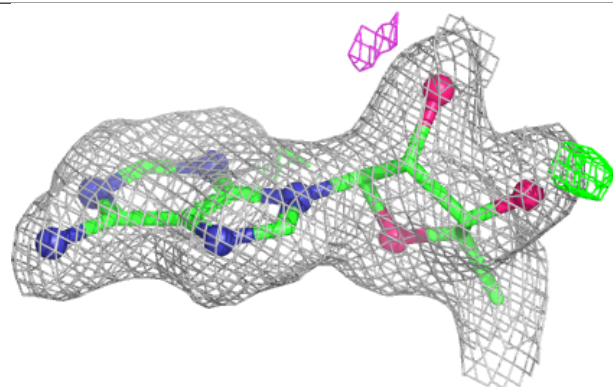
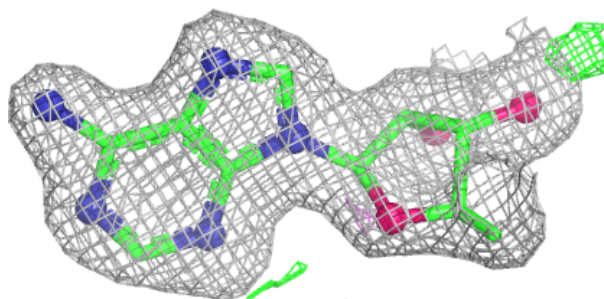
**Electron density around SAH B 503 (B):**

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

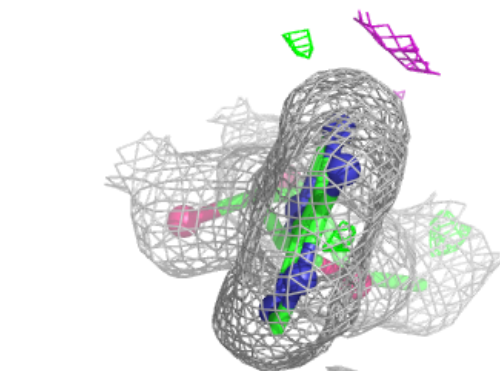
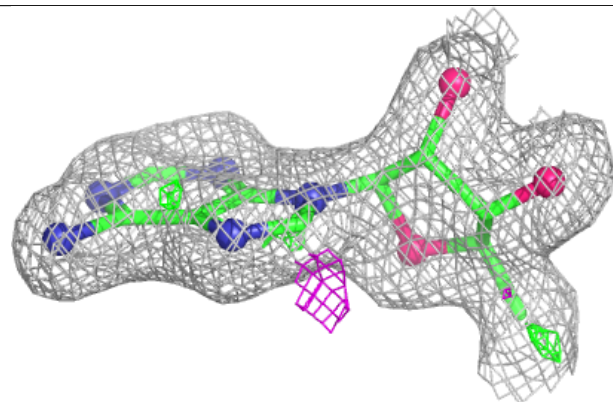
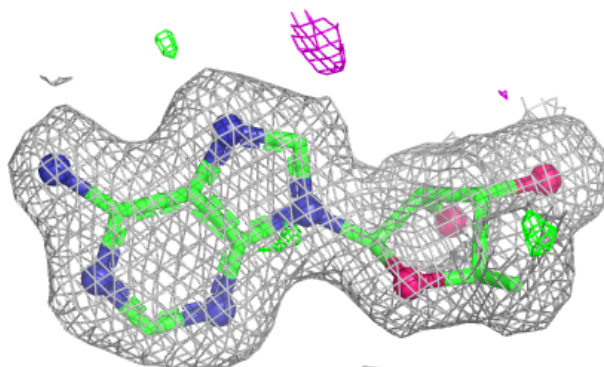


Electron density around 5AD A 502 (A):

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

**Electron density around 5AD B 502 (A):**

$2mF_o-DF_c$ (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.