



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:35 PM UTC

PDB ID : 6I6C / pdb_00006i6c
Title : SEPIAPTERIN REDUCTASE IN COMPLEX WITH COMPOUND 2
Authors : Alen, J.; Schade, M.; Wagener, M.; Blaesse, M.
Deposited on : 2018-11-15
Resolution : 1.72 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

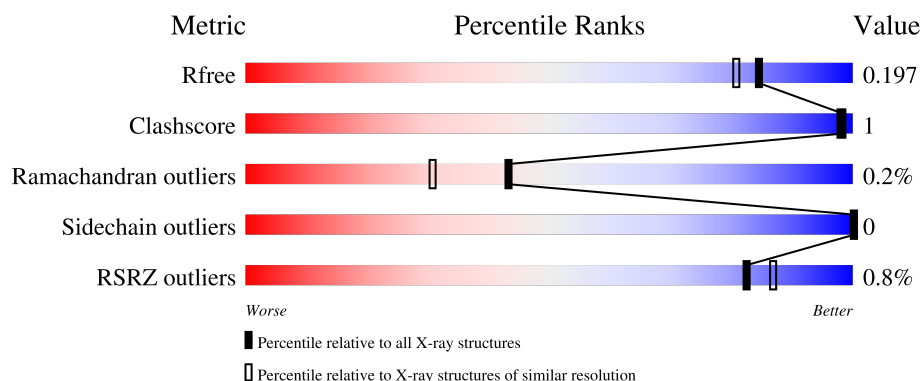
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	276	 95%
1	B	276	 91% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4450 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 Sepiapterin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	21	5	0
			2039	1288	358	382	11			
1	B	257	Total	C	N	O	S	22	8	0
			1993	1256	357	370	10			

There are 30 discrepancies between the modelled and reference sequences:

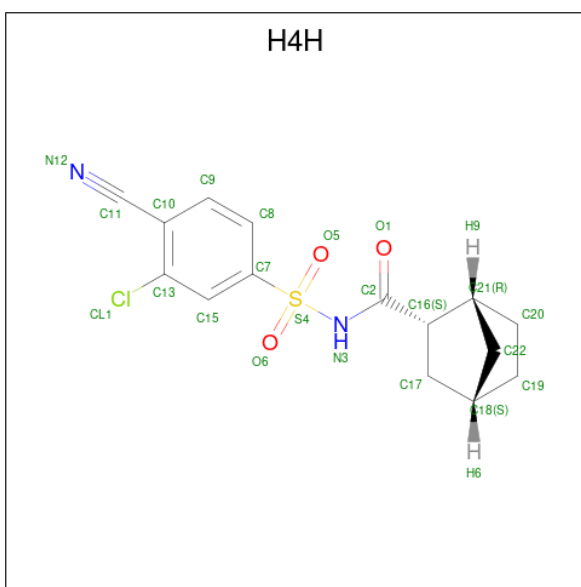
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP P35270
A	-13	GLY	-	expression tag	UNP P35270
A	-12	HIS	-	expression tag	UNP P35270
A	-11	HIS	-	expression tag	UNP P35270
A	-10	HIS	-	expression tag	UNP P35270
A	-9	HIS	-	expression tag	UNP P35270
A	-8	HIS	-	expression tag	UNP P35270
A	-7	HIS	-	expression tag	UNP P35270
A	-6	GLU	-	expression tag	UNP P35270
A	-5	ASN	-	expression tag	UNP P35270
A	-4	LEU	-	expression tag	UNP P35270
A	-3	TYR	-	expression tag	UNP P35270
A	-2	PHE	-	expression tag	UNP P35270
A	-1	GLN	-	expression tag	UNP P35270
A	0	GLY	-	expression tag	UNP P35270
B	-14	MET	-	initiating methionine	UNP P35270
B	-13	GLY	-	expression tag	UNP P35270
B	-12	HIS	-	expression tag	UNP P35270
B	-11	HIS	-	expression tag	UNP P35270
B	-10	HIS	-	expression tag	UNP P35270
B	-9	HIS	-	expression tag	UNP P35270
B	-8	HIS	-	expression tag	UNP P35270
B	-7	HIS	-	expression tag	UNP P35270
B	-6	GLU	-	expression tag	UNP P35270
B	-5	ASN	-	expression tag	UNP P35270

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	LEU	-	expression tag	UNP P35270
B	-3	TYR	-	expression tag	UNP P35270
B	-2	PHE	-	expression tag	UNP P35270
B	-1	GLN	-	expression tag	UNP P35270
B	0	GLY	-	expression tag	UNP P35270

- # NAP

- Molecule 3 is (1 {R},2 {S},4 {S})- {N}-(3-chloranyl-4-cyano-phenyl)sulfonylbicyclo[2.2.1]heptane-2-carboxamide (CCD ID: H4H) (formula: $C_{15}H_{15}ClN_2O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	1
			35	22	2	4	5	2		
3	B	1	Total	C	Cl	N	O	S	0	0
			22	15	1	2	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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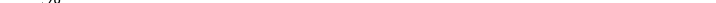
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

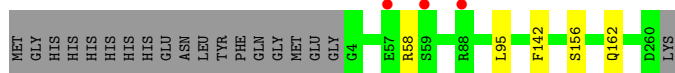
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	120	Total O 120 120	0	0
5	B	115	Total O 117 117	0	2

- Molecule 1: Sepiapterin reductase



- Chain B:  91% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.91Å 77.32Å 59.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.98 – 1.72 63.98 – 1.72	Depositor EDS
% Data completeness (in resolution range)	90.0 (63.98-1.72) 90.0 (63.98-1.72)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.149 , 0.206 (Not available) , 0.197	Depositor DCC
R_{free} test set	2640 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4450	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H4H, NAP, EDO

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	0.71	0/2080	0.95	0/2812
1	B	0.75	0/2035	0.96	0/2752
All	All	0.73	0/4115	0.95	0/5564

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 [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	2039	0	2103	2	0
1	B	1993	0	2075	3	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
3	A	35	0	0	0	0
3	B	22	0	0	0	0
4	A	12	0	18	0	0
4	B	16	0	24	0	0
5	A	120	0	0	0	0
5	B	117	0	0	0	0
All	All	4450	0	4270	5	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 1.

All (5) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10[B]:CYS:SG	1:A:27:LEU:HD21	2.51	0.50
1:A:156:SER:O	2:A:301:NAP:H6N	2.17	0.44
1:B:156:SER:O	2:B:301:NAP:H6N	2.20	0.42
1:B:95:LEU:HD22	1:B:142:PHE:HB2	2.03	0.40
1:B:162[B]:GLN:HE21	1:B:162[B]:GLN:HB2	1.71	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	267/276 (97%)	263 (98%)	4 (2%)	0	100	100
1	B	263/276 (95%)	260 (99%)	2 (1%)	1 (0%)	30	16
All	All	530/552 (96%)	523 (99%)	6 (1%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	ARG

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	221/225 (98%)	221 (100%)	0	100	100
1	B	217/225 (96%)	217 (100%)	0	100	100
All	All	438/450 (97%)	438 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-7	HIS
1	A	-1	GLN
1	A	182	GLN
1	B	182	GLN
1	B	239	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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
4	EDO	B	304	-	3,3,3	0.55	0	2,2,2	0.32	0
2	NAP	A	301	-	50,52,52	1.09	4 (8%)	71,80,80	1.68	14 (19%)
4	EDO	A	305	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.29	0
2	NAP	B	301	-	50,52,52	1.18	5 (10%)	71,80,80	1.69	16 (22%)
3	H4H	B	302	-	24,24,24	0.99	1 (4%)	32,36,36	2.14	10 (31%)
4	EDO	A	304	-	3,3,3	0.39	0	2,2,2	0.36	0
3	H4H	A	302[B]	-	24,24,24	0.85	0	32,36,36	2.14	8 (25%)
4	EDO	B	305	-	3,3,3	0.51	0	2,2,2	0.14	0
4	EDO	B	306	-	3,3,3	0.50	0	2,2,2	0.22	0
4	EDO	B	303	-	3,3,3	0.40	0	2,2,2	0.39	0
3	H4H	A	302[A]	-	24,24,24	0.90	0	32,36,36	2.94	11 (34%)

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
4	EDO	B	304	-	-	1/1/1/1	-
2	NAP	A	301	-	-	7/35/67/67	0/5/5/5
4	EDO	A	305	-	-	1/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
2	NAP	B	301	-	-	7/35/67/67	0/5/5/5
3	H4H	B	302	-	-	6/17/34/34	0/4/3/3
4	EDO	A	304	-	-	1/1/1/1	-
3	H4H	A	302[B]	-	-	9/17/34/34	0/4/3/3
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
3	H4H	A	302[A]	-	-	6/17/34/34	0/4/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C5A-C4A	4.57	1.47	1.39
2	A	301	NAP	C5A-C4A	4.36	1.46	1.39
2	B	301	NAP	C5A-N7A	-3.03	1.33	1.39
2	A	301	NAP	C5A-C6A	2.43	1.47	1.41
2	B	301	NAP	C4A-N9A	-2.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C8A-N7A	2.39	1.36	1.31
2	A	301	NAP	C4A-N9A	-2.38	1.32	1.37
2	B	301	NAP	C5A-C6A	2.26	1.47	1.41
2	A	301	NAP	C5A-N7A	-2.07	1.35	1.39
3	B	302	H4H	O5-S4	-2.07	1.41	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[A]	H4H	C7-S4-N3	-9.31	91.22	106.06
3	A	302[B]	H4H	C16-C2-N3	6.58	124.23	114.49
3	B	302	H4H	C7-S4-N3	-6.08	96.37	106.06
3	A	302[A]	H4H	C16-C2-N3	5.97	123.33	114.49
3	A	302[A]	H4H	O1-C2-C16	-5.59	114.99	121.67
3	A	302[B]	H4H	O1-C2-C16	-5.59	114.99	121.67
3	B	302	H4H	C16-C2-N3	5.13	122.09	114.49
2	B	301	NAP	C5A-C4A-N3A	-4.96	119.89	126.72
3	A	302[A]	H4H	C15-C7-S4	4.91	124.09	119.06
3	A	302[A]	H4H	O6-S4-O5	4.82	125.37	119.52
2	A	301	NAP	C5A-C4A-N3A	-4.67	120.29	126.72
2	A	301	NAP	N3A-C4A-N9A	4.29	134.47	127.17
2	A	301	NAP	C3N-C7N-N7N	4.18	122.89	117.74
3	A	302[A]	H4H	C8-C7-S4	-4.16	115.19	119.76
2	B	301	NAP	N3A-C4A-N9A	4.08	134.11	127.17
2	A	301	NAP	C4A-N9A-C8A	3.81	109.73	105.74
3	A	302[B]	H4H	O6-S4-C7	-3.76	103.24	107.98
2	B	301	NAP	C3N-C7N-N7N	3.69	122.28	117.74
3	A	302[B]	H4H	O5-S4-C7	-3.51	103.55	107.98
3	B	302	H4H	O1-C2-C16	-3.46	117.53	121.67
3	A	302[A]	H4H	C10-C13-CL1	-3.40	116.56	119.45
2	B	301	NAP	N3A-C2A-N1A	-3.32	123.56	128.58
2	B	301	NAP	C2A-N3A-C4A	3.28	119.84	111.83
2	A	301	NAP	O4B-C1B-N9A	3.16	114.16	108.09
2	B	301	NAP	C4A-N9A-C8A	3.13	109.02	105.74
2	B	301	NAP	C4A-C5A-N7A	-3.11	107.03	110.58
2	B	301	NAP	O4B-C1B-N9A	3.06	113.97	108.09
3	B	302	H4H	C8-C7-S4	3.01	123.07	119.76
2	A	301	NAP	C4A-C5A-N7A	-2.97	107.19	110.58
2	A	301	NAP	O7N-C7N-N7N	-2.94	118.37	122.62
3	B	302	H4H	C2-N3-S4	2.90	129.17	124.18
2	B	301	NAP	O3-PA-O1A	-2.88	102.03	110.70
2	A	301	NAP	C2B-C1B-N9A	-2.78	109.17	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C2B-C1B-N9A	-2.78	109.17	113.75
3	A	302[A]	H4H	C22-C21-C20	-2.72	95.88	101.25
3	A	302[B]	H4H	C22-C21-C20	-2.72	95.88	101.25
2	A	301	NAP	C2A-N3A-C4A	2.70	118.42	111.83
3	A	302[A]	H4H	C13-C10-C11	-2.66	118.42	121.18
2	B	301	NAP	C5A-N7A-C8A	2.65	107.62	103.45
2	A	301	NAP	N3A-C2A-N1A	-2.63	124.60	128.58
3	B	302	H4H	O5-S4-C7	-2.63	104.66	107.98
2	B	301	NAP	N9A-C8A-N7A	-2.53	110.34	113.94
3	B	302	H4H	O6-S4-O5	2.53	122.59	119.52
3	A	302[B]	H4H	C7-S4-N3	2.51	110.06	106.06
3	B	302	H4H	C22-C21-C16	-2.50	97.31	102.70
2	B	301	NAP	O2A-PA-O1A	2.49	124.01	112.44
3	B	302	H4H	C9-C8-C7	2.47	121.84	119.44
2	A	301	NAP	C5A-N7A-C8A	2.36	107.16	103.45
2	B	301	NAP	O7N-C7N-C3N	-2.36	116.71	119.60
2	A	301	NAP	N9A-C8A-N7A	-2.30	110.67	113.94
2	B	301	NAP	O2N-PN-O1N	2.19	122.65	112.44
2	A	301	NAP	O2A-PA-O3	2.19	113.19	107.27
3	A	302[B]	H4H	C13-C15-C7	2.18	120.25	118.80
3	A	302[B]	H4H	O6-S4-O5	2.15	122.13	119.52
3	B	302	H4H	C22-C21-C20	-2.12	97.07	101.25
3	A	302[A]	H4H	C2-N3-S4	2.09	127.78	124.18
2	B	301	NAP	N6A-C6A-N1A	2.08	123.02	118.38
2	A	301	NAP	O2N-PN-O1N	2.05	122.00	112.44
3	A	302[A]	H4H	C9-C8-C7	2.01	121.39	119.44

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O2N
2	A	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	O4D-C1D-N1N-C2N
3	A	302[A]	H4H	C17-C16-C2-O1
3	A	302[A]	H4H	C17-C16-C2-N3
3	A	302[B]	H4H	C17-C16-C2-O1
3	A	302[B]	H4H	C17-C16-C2-N3
3	B	302	H4H	C17-C16-C2-O1

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Mol	Chain	Res	Type	Atoms
3	B	302	H4H	C17-C16-C2-N3
3	A	302[A]	H4H	C2-N3-S4-O6
3	A	302[B]	H4H	C2-N3-S4-O6
3	B	302	H4H	C2-N3-S4-O6
3	A	302[A]	H4H	C2-N3-S4-C7
3	A	302[B]	H4H	C2-N3-S4-C7
3	B	302	H4H	C2-N3-S4-C7
3	A	302[B]	H4H	C15-C7-S4-O5
3	A	302[B]	H4H	C8-C7-S4-O5
4	B	306	EDO	O1-C1-C2-O2
3	A	302[B]	H4H	C15-C7-S4-N3
3	A	302[B]	H4H	C8-C7-S4-N3
4	A	305	EDO	O1-C1-C2-O2
2	A	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C2B-O2B-P2B-O3X
2	B	301	NAP	C2B-O2B-P2B-O3X
2	A	301	NAP	O4D-C1D-N1N-C6N
2	B	301	NAP	O4D-C1D-N1N-C6N
3	A	302[A]	H4H	C13-C10-C11-N12
3	B	302	H4H	C13-C10-C11-N12
4	B	304	EDO	O1-C1-C2-O2
2	A	301	NAP	O4B-C4B-C5B-O5B
3	A	302[A]	H4H	C21-C16-C2-O1
3	A	302[B]	H4H	C21-C16-C2-O1
3	B	302	H4H	C21-C16-C2-O1
4	A	304	EDO	O1-C1-C2-O2
2	B	301	NAP	O4B-C4B-C5B-O5B

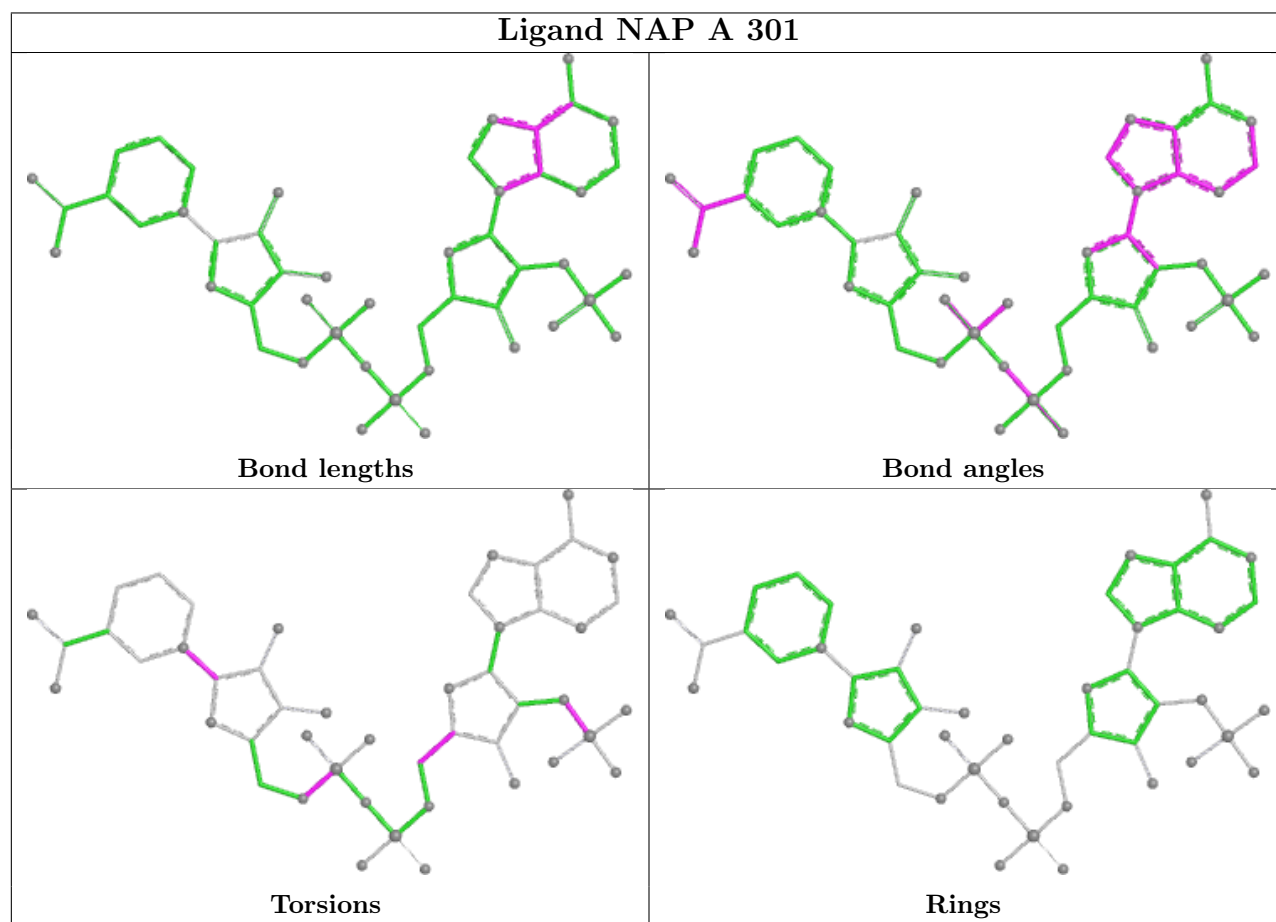
There are no ring outliers.

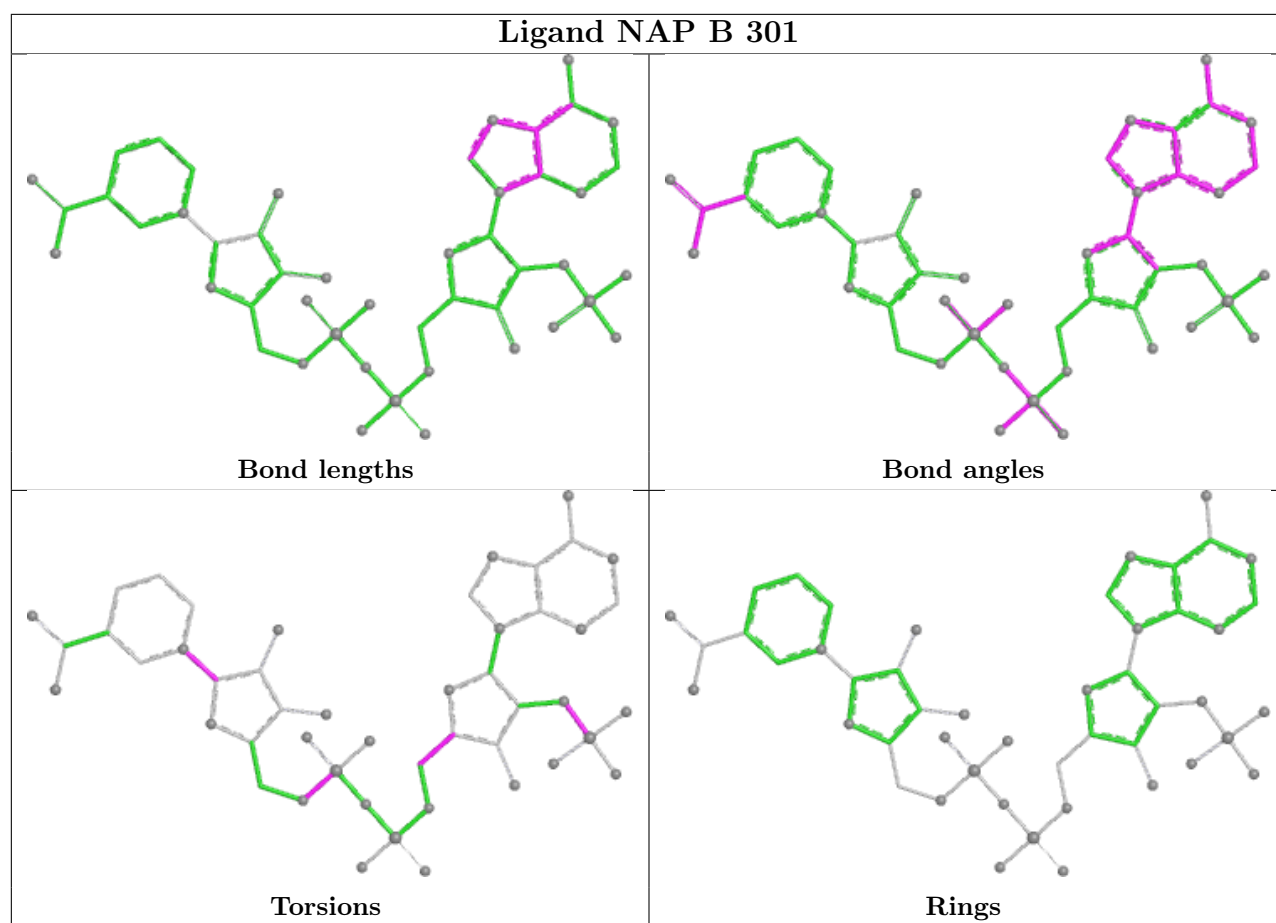
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	1	0
2	B	301	NAP	1	0

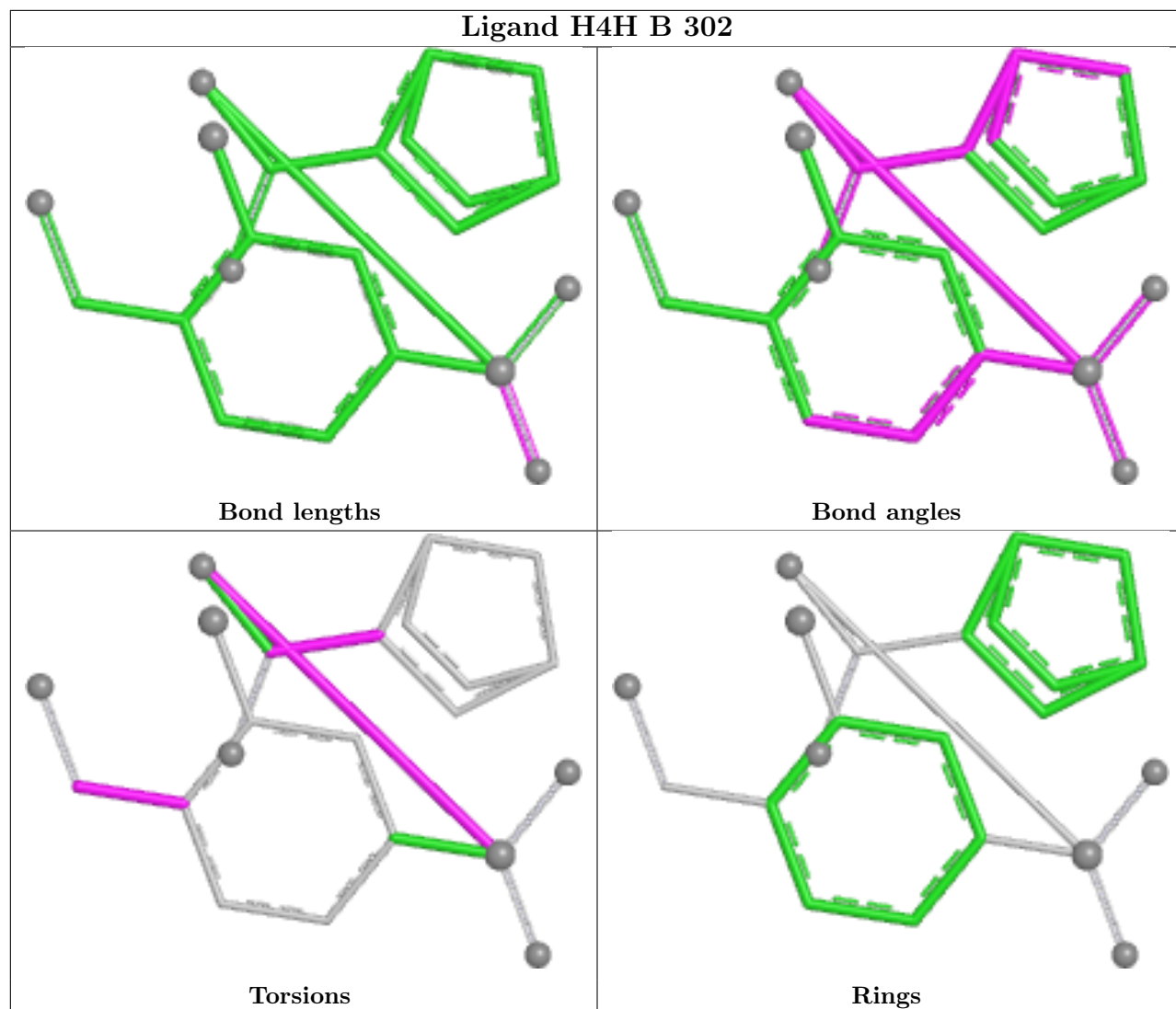
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

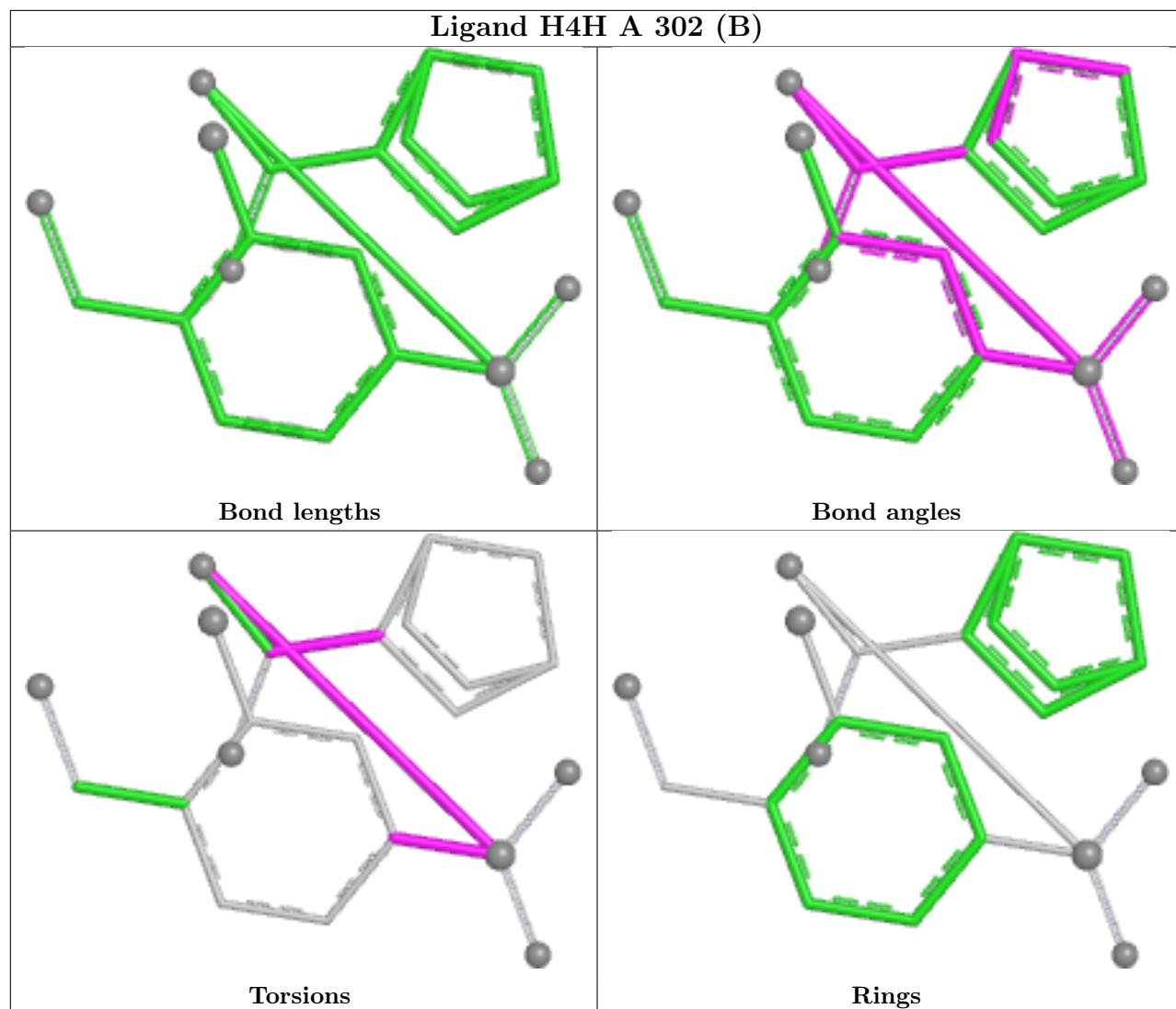


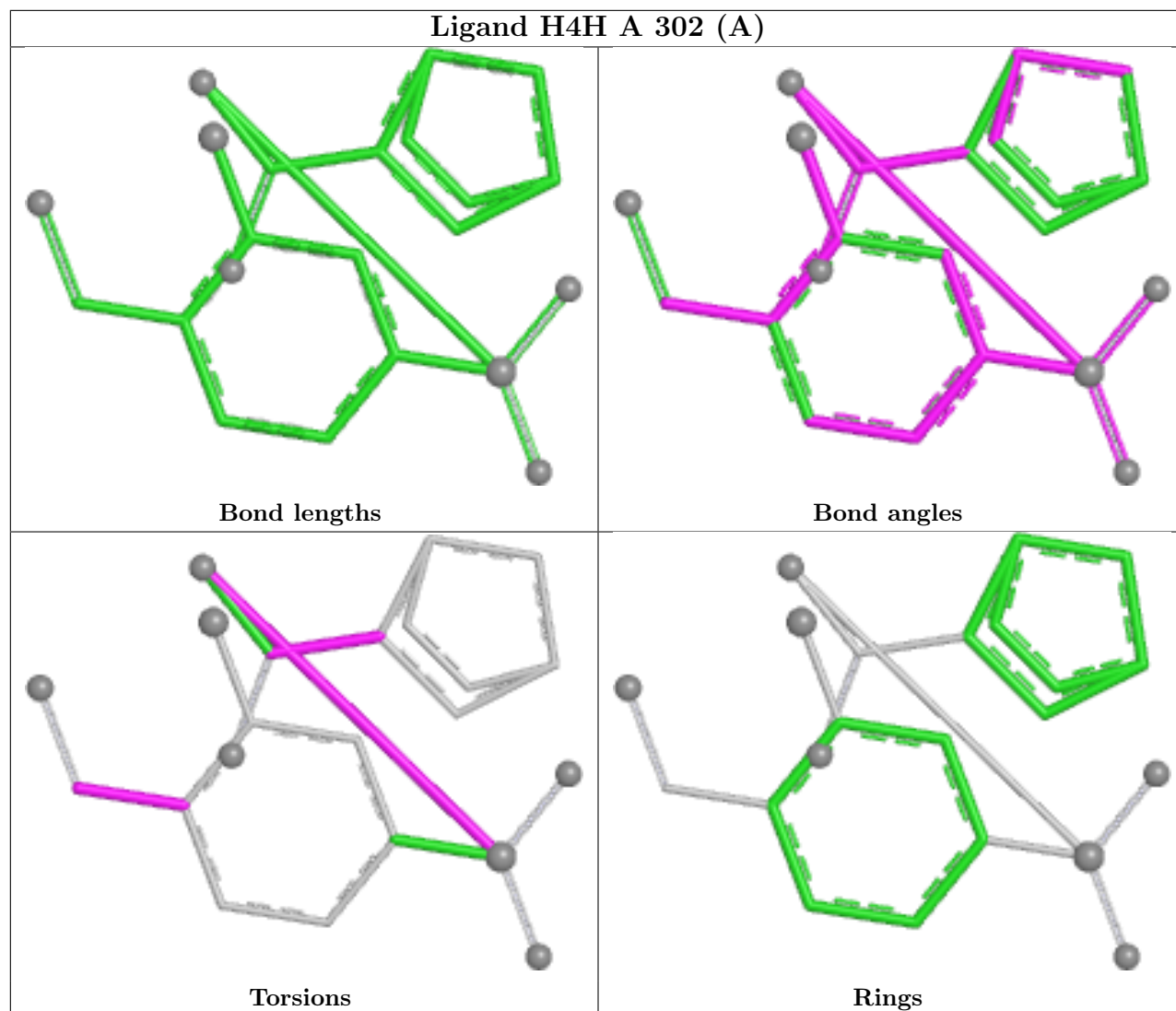


Ligand H4H B 302



Ligand H4H A 302 (B)





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 [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	266/276 (96%)	-0.23	1 (0%) 88 91	10, 23, 40, 69	11 (4%)
1	B	257/276 (93%)	-0.09	3 (1%) 76 81	10, 25, 42, 80	16 (6%)
All	All	523/552 (94%)	-0.16	4 (0%) 82 87	10, 24, 42, 80	27 (5%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	GLU	3.2
1	B	59	SER	2.4
1	A	83	LEU	2.2
1	B	88[A]	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 [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
4	EDO	B	305	4/4	0.88	0.14	48,54,54,56	0

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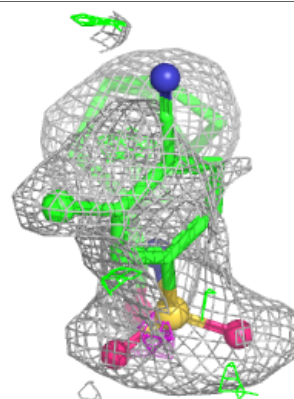
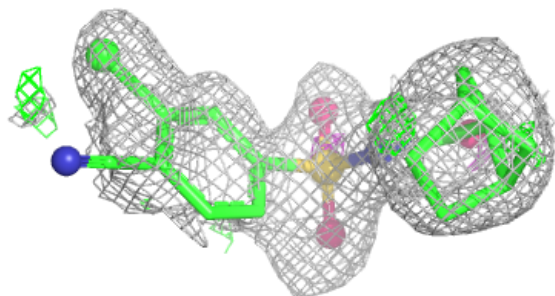
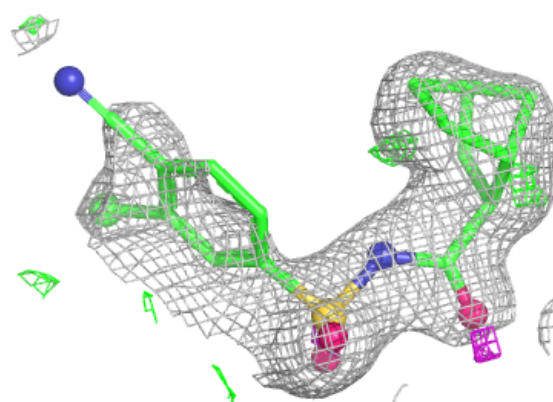
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	303	4/4	0.90	0.12	33,37,38,49	0
4	EDO	B	306	4/4	0.90	0.12	49,50,53,54	0
4	EDO	A	305	4/4	0.93	0.09	51,52,53,53	0
3	H4H	A	302[A]	22/22	0.94	0.12	25,36,59,64	13
3	H4H	A	302[B]	22/22	0.94	0.12	25,35,46,57	13
4	EDO	A	303	4/4	0.95	0.07	28,31,34,44	0
3	H4H	B	302	22/22	0.96	0.08	25,31,50,70	0
4	EDO	A	304	4/4	0.96	0.08	22,24,34,34	0
4	EDO	B	304	4/4	0.97	0.07	24,25,28,29	0
2	NAP	A	301	48/48	0.99	0.03	14,17,19,22	0
2	NAP	B	301	48/48	0.99	0.04	17,20,25,27	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.

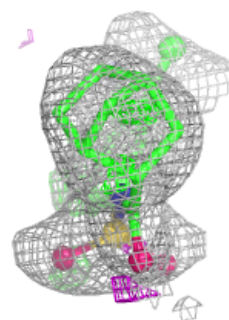
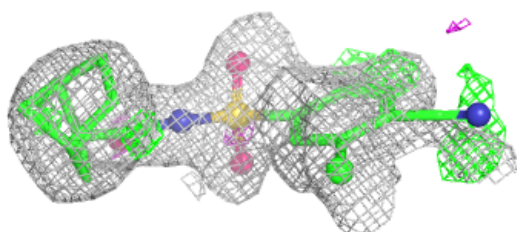
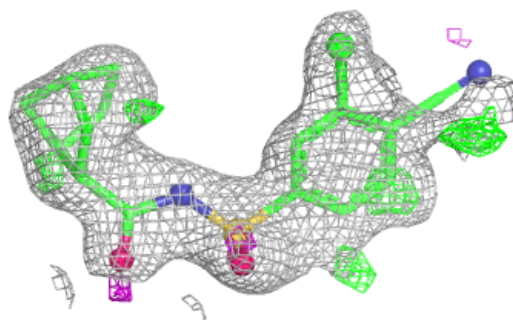
Electron density around H4H A 302 (A):

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

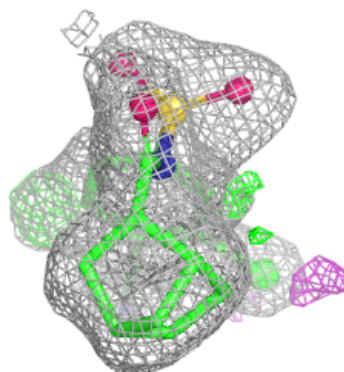
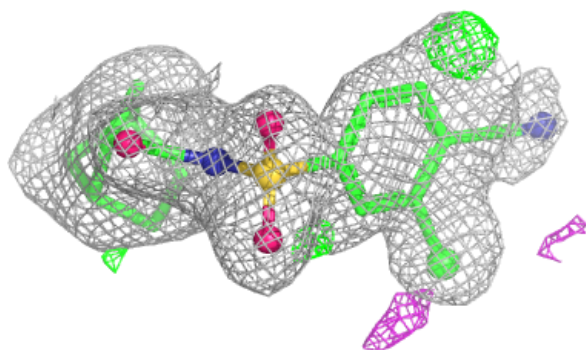
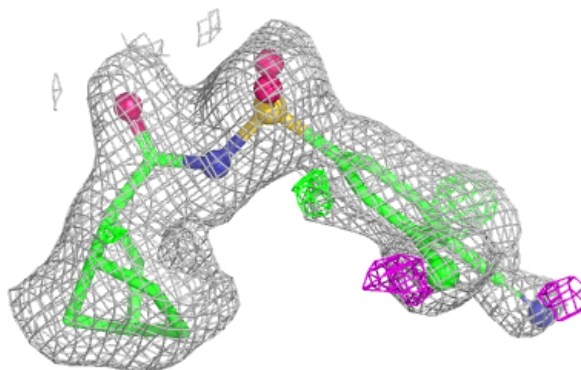


Electron density around H4H A 302 (B):

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

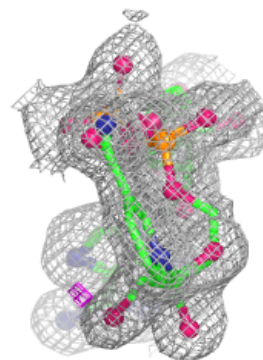
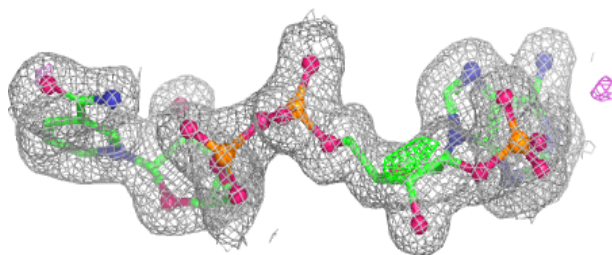
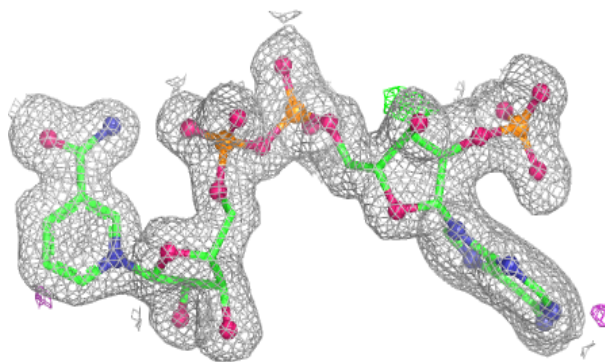
**Electron density around H4H B 302:**

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

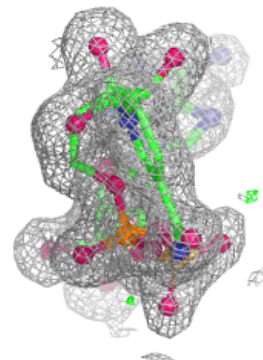
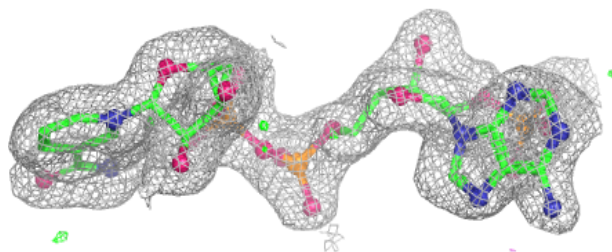
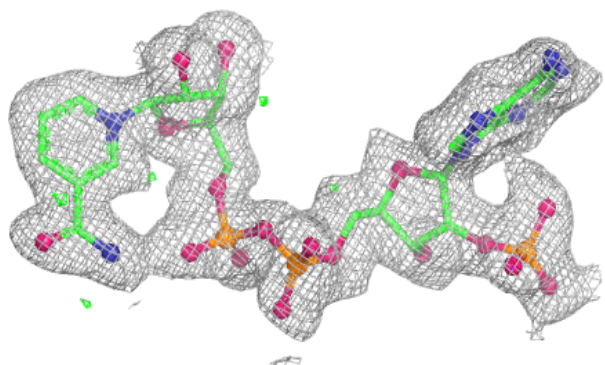


Electron density around NAP A 301:

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

**Electron density around NAP B 301:**

$2mF_o-DF_c$ (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.