



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:22 PM UTC

PDB ID : 7KH7 / pdb_00007kh7
Title : Crystal structure of Staphylococcus aureus ketol-acid reductoisomerase in complex with Mg²⁺, NADPH, and NSC116565
Authors : Kurz, J.L.; Patel, K.P.; Guddat, L.W.
Deposited on : 2020-10-20
Resolution : 2.63 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

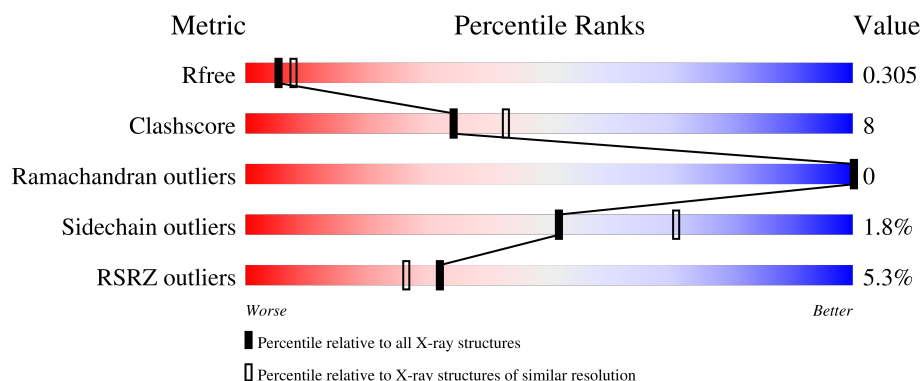
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	340	6% 79% 14% 7%
1	B	340	4% 76% 19% • •

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
5	WBY	B	401	-	X	-	-
5	WBY	B	402	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5158 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 Ketol-acid reductoisomerase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	4	0
			2448	1548	414	478	8			
1	B	325	Total	C	N	O	S	0	1	0
			2522	1600	426	488	8			

There are 12 discrepancies between the modelled and reference sequences:

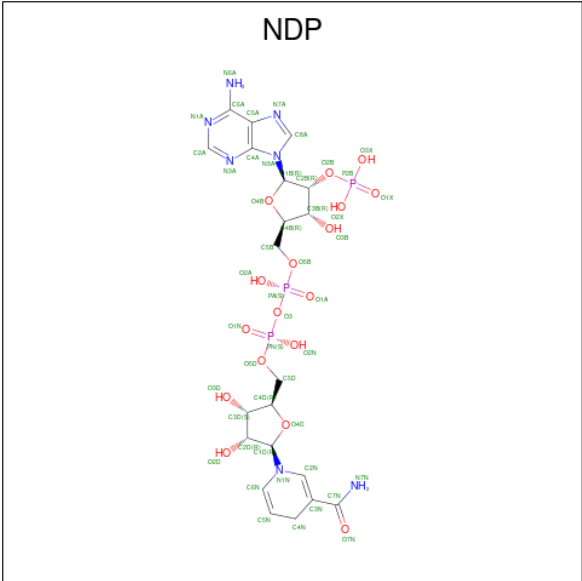
Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP A0A145BYP4
A	336	HIS	-	expression tag	UNP A0A145BYP4
A	337	HIS	-	expression tag	UNP A0A145BYP4
A	338	HIS	-	expression tag	UNP A0A145BYP4
A	339	HIS	-	expression tag	UNP A0A145BYP4
A	340	HIS	-	expression tag	UNP A0A145BYP4
B	335	HIS	-	expression tag	UNP A0A145BYP4
B	336	HIS	-	expression tag	UNP A0A145BYP4
B	337	HIS	-	expression tag	UNP A0A145BYP4
B	338	HIS	-	expression tag	UNP A0A145BYP4
B	339	HIS	-	expression tag	UNP A0A145BYP4
B	340	HIS	-	expression tag	UNP A0A145BYP4

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			48	21	7	17	3		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

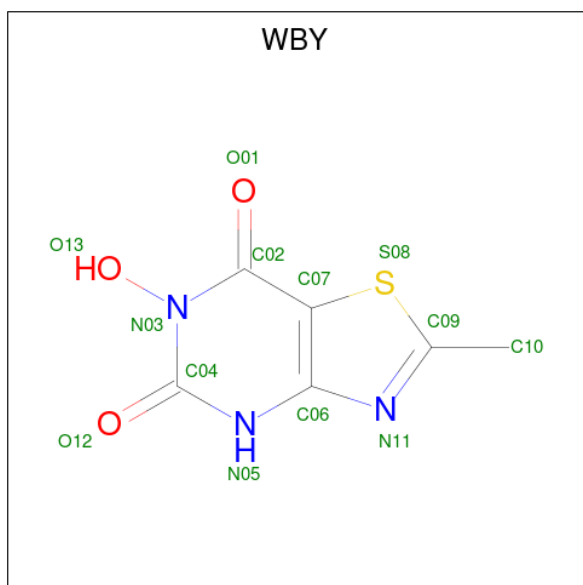


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			48	21	7	17	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	2	Total Mg 2 2	0	0

- Molecule 5 is 6-hydroxy-2-methyl[1,3]thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione (CCD ID: WBY) (formula: C₆H₅N₃O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O S 13 6 3 3 1	0	0
5	B	1	Total C N O S 13 6 3 3 1	0	0

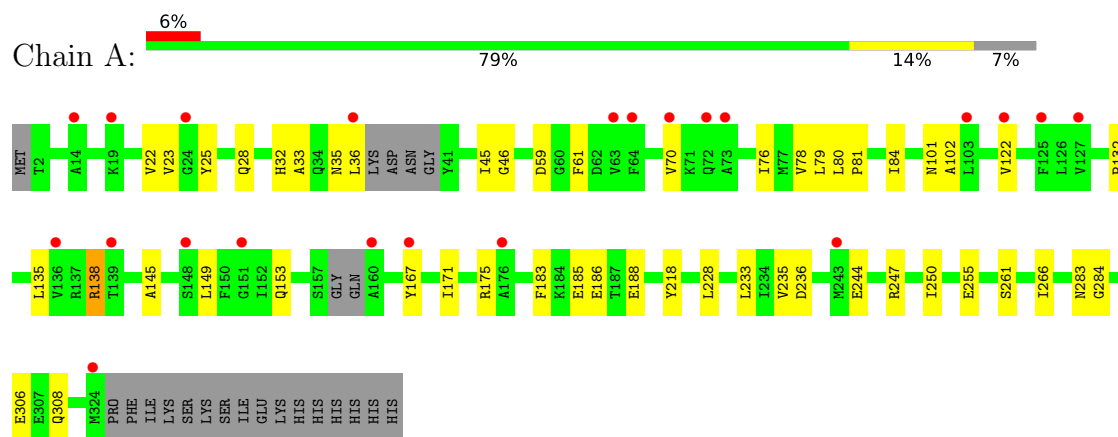
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	29	Total O 29 29	0	0
6	B	32	Total O 32 32	0	0

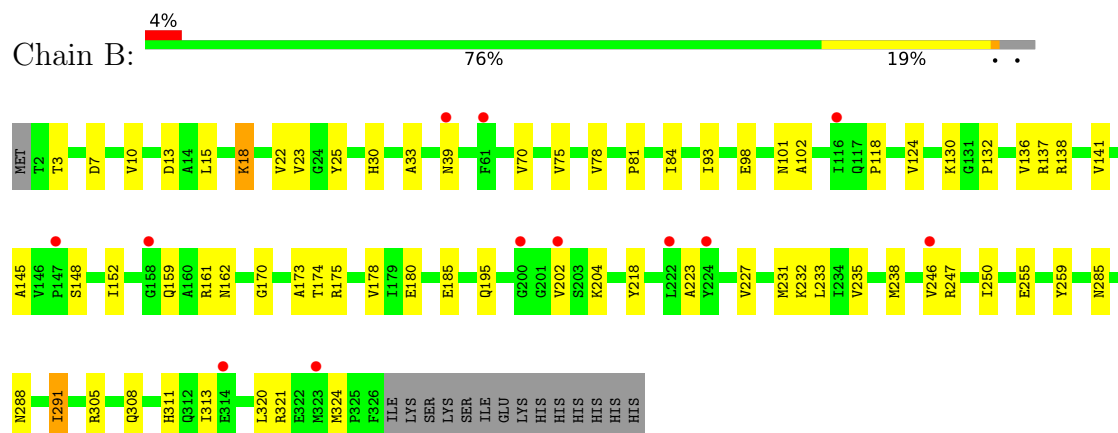
3 Residue-property plots

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: Ketol-acid reductoisomerase (NADP(+))



- Molecule 1: Ketol-acid reductoisomerase (NADP(+))



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.92Å 92.08Å 101.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 – 2.63 48.84 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.84-2.63) 99.6 (48.84-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.246 , 0.303 0.248 , 0.305	Depositor DCC
R_{free} test set	2000 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5158	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: MG, NDP, WBY, NAP

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	0.16	0/2497	0.33	0/3381
1	B	0.14	0/2574	0.32	0/3482
All	All	0.15	0/5071	0.32	0/6863

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	2448	0	2307	43	0
1	B	2522	0	2430	44	0
2	A	48	0	25	2	0
3	A	48	0	25	2	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
5	B	26	0	0	2	0
6	A	29	0	0	2	0
6	B	32	0	0	1	0
All	All	5158	0	4787	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (75) 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:152:ILE:HG13	1:B:161:ARG:HG2	1.69	0.72
2:A:501[A]:NAP:O1N	2:A:501[A]:NAP:N7N	2.25	0.70
3:A:502[B]:NDP:N7N	3:A:502[B]:NDP:O2N	2.33	0.61
1:B:15:LEU:HA	1:B:18:LYS:HD2	1.83	0.59
1:A:81:PRO:HD3	2:A:501[A]:NAP:H52A	1.84	0.58
1:A:228:LEU:HD21	1:B:238:MET:HG2	1.87	0.56
1:A:23:VAL:HG23	1:A:78:VAL:HA	1.89	0.55
1:A:45:ILE:CD1	1:A:61:PHE:CD1	2.90	0.55
1:A:233:LEU:HD22	1:B:132:PRO:HD3	1.90	0.54
1:A:218:TYR:HD1	1:B:185:GLU:HG3	1.72	0.54
1:A:235:VAL:HG11	1:B:235:VAL:HG21	1.90	0.53
1:A:135:LEU:HD12	1:B:233:LEU:HB3	1.90	0.53
1:B:246:VAL:O	1:B:250:ILE:HB	2.10	0.52
1:B:255:GLU:HG2	1:B:259:TYR:CE2	2.45	0.52
1:A:138[A]:ARG:NH2	6:A:605:HOH:O	2.44	0.51
1:A:235:VAL:HG21	1:B:235:VAL:HB	1.93	0.51
1:A:308:GLN:NE2	1:B:247:ARG:HH22	2.08	0.51
1:A:138[A]:ARG:NH1	6:A:604:HOH:O	2.44	0.51
1:A:70:VAL:HG22	1:A:76:ILE:HG21	1.92	0.50
1:B:39:ASN:ND2	1:B:170:GLY:O	2.46	0.49
1:B:7:ASP:OD1	1:B:174:THR:OG1	2.27	0.49
1:B:22:VAL:HG21	1:B:33:ALA:HB2	1.95	0.49
1:A:250:ILE:HA	5:B:402:WBY:N11	2.27	0.48
1:B:288:ASN:HA	1:B:291:ILE:HG22	1.95	0.48
1:A:132:PRO:HG2	1:A:135:LEU:HB2	1.95	0.48
3:A:502[B]:NDP:H41N	5:B:401:WBY:C02	2.44	0.48
1:A:188:GLU:OE1	1:B:218:TYR:OH	2.27	0.48
1:A:185:GLU:HG3	1:B:218:TYR:HD1	1.79	0.47
1:A:22:VAL:HG13	1:A:79:LEU:HD12	1.97	0.47
1:A:261:SER:HB2	1:B:195:GLN:HB3	1.95	0.47
1:A:28:GLN:OE1	1:A:32:HIS:NE2	2.47	0.47
1:A:35:ASN:HB3	1:A:171:ILE:HA	1.97	0.47
1:A:153:GLN:HG3	1:A:183:PHE:CD1	2.50	0.46
1:A:236:ASP:OD1	1:B:232:LYS:NZ	2.37	0.46
1:A:283:ASN:OD1	1:A:284:GLY:N	2.49	0.46
1:A:23:VAL:HG12	1:A:46:GLY:HA3	1.96	0.46
1:A:149:LEU:HD12	1:A:186:GLU:HG2	1.98	0.46
1:B:118:PRO:HG3	1:B:124:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:OH	1:B:30:HIS:ND1	2.39	0.46
1:A:145:ALA:HB2	1:A:175:ARG:HB2	1.96	0.46
1:B:130:LYS:HD3	1:B:130:LYS:HA	1.82	0.45
1:A:266:ILE:HB	1:B:204:LYS:HG2	1.97	0.45
1:A:45:ILE:HD11	1:A:61:PHE:CD1	2.51	0.45
1:B:70:VAL:HG21	1:B:93:ILE:HG12	1.99	0.45
1:B:321:ARG:HA	1:B:324:MET:HE2	1.98	0.45
1:B:159:GLN:HG3	1:B:162:ASN:HD21	1.81	0.45
1:A:247:ARG:NH1	1:B:308:GLN:O	2.50	0.44
1:B:3:THR:HB	1:B:180:GLU:HB3	1.99	0.44
1:A:33:ALA:HB1	1:A:61:PHE:CE1	2.52	0.44
1:B:223:ALA:O	1:B:227:VAL:HG22	2.18	0.43
1:A:36:LEU:HD11	1:A:167:TYR:HE1	1.83	0.43
1:A:45:ILE:HD13	1:A:61:PHE:CD1	2.54	0.43
1:A:36:LEU:HD11	1:A:167:TYR:CE1	2.54	0.43
1:B:81:PRO:HD2	1:B:84:ILE:HD11	2.00	0.42
1:A:81:PRO:HD2	1:A:84:ILE:HD11	2.01	0.42
1:B:13:ASP:N	6:B:504:HOH:O	2.47	0.42
1:A:101:ASN:HB3	1:A:102:ALA:H	1.66	0.42
1:A:25:TYR:OH	1:A:59:ASP:OD2	2.35	0.42
1:A:185:GLU:HG3	1:B:218:TYR:CD1	2.55	0.41
1:B:285:ASN:HA	1:B:288:ASN:ND2	2.35	0.41
1:B:285:ASN:HA	1:B:288:ASN:HD21	1.85	0.41
1:B:101:ASN:HB3	1:B:102:ALA:H	1.69	0.41
1:B:23:VAL:HG22	1:B:78:VAL:HA	2.02	0.41
1:B:145:ALA:HB2	1:B:175:ARG:HB3	2.02	0.41
1:B:320:LEU:HD23	1:B:320:LEU:HA	1.90	0.41
1:A:80:LEU:HB3	1:A:84:ILE:HD11	2.02	0.41
1:A:101:ASN:H	1:A:122:VAL:HG22	1.86	0.41
1:A:255:GLU:OE2	1:B:305:ARG:HD3	2.21	0.41
1:B:98:GLU:HB2	1:B:101:ASN:HD21	1.86	0.41
1:B:311:HIS:ND1	1:B:313:ILE:HG22	2.36	0.41
1:B:137:ARG:O	1:B:141:VAL:HG23	2.21	0.41
1:B:148:SER:OG	1:B:173:ALA:HB1	2.20	0.41
1:B:202:VAL:HG21	1:B:231:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

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	315/340 (93%)	299 (95%)	16 (5%)	0	100	100
1	B	324/340 (95%)	308 (95%)	16 (5%)	0	100	100
All	All	639/680 (94%)	607 (95%)	32 (5%)	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	249/283 (88%)	246 (99%)	3 (1%)	63	78
1	B	263/283 (93%)	256 (97%)	7 (3%)	39	60
All	All	512/566 (90%)	502 (98%)	10 (2%)	51	68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138[A]	ARG
1	A	138[B]	ARG
1	A	306	GLU
1	B	10	VAL
1	B	18	LYS
1	B	75	VAL
1	B	136	VAL
1	B	138	ARG

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Mol	Chain	Res	Type
1	B	178	VAL
1	B	291	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	72	GLN
1	A	101	ASN
1	B	153	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 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	$\# Z > 2$
5	WBY	B	402	4	14,14,14	4.93	10 (71%)	14,21,21	5.97	9 (64%)
3	NDP	A	502[B]	-	51,52,52	3.89	26 (50%)	71,80,80	1.52	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	501[A]	-	50,52,52	4.05	19 (38%)	71,80,80	1.56	11 (15%)
5	WBY	B	401	4	14,14,14	4.90	11 (78%)	14,21,21	5.92	8 (57%)

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
5	WBY	B	402	4	-	-	0/2/2/2
3	NDP	A	502[B]	-	-	9/34/77/77	0/5/5/5
2	NAP	A	501[A]	-	-	15/35/67/67	0/5/5/5
5	WBY	B	401	4	-	-	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	NAP	O4D-C1D	13.84	1.59	1.40
3	A	502[B]	NDP	C3B-C2B	-12.96	1.24	1.53
2	A	501[A]	NAP	C3B-C2B	-11.09	1.28	1.53
5	B	402	WBY	C06-N11	10.67	1.49	1.36
5	B	401	WBY	C06-N11	10.57	1.49	1.36
5	B	401	WBY	C04-N03	9.35	1.45	1.38
5	B	402	WBY	C04-N03	9.33	1.45	1.38
3	A	502[B]	NDP	C3D-C4D	-9.06	1.30	1.53
2	A	501[A]	NAP	PA-O3	8.90	1.69	1.59
2	A	501[A]	NAP	C3D-C4D	-7.99	1.32	1.53
3	A	502[B]	NDP	O4D-C4D	7.90	1.62	1.45
3	A	502[B]	NDP	C2N-C3N	7.53	1.55	1.35
3	A	502[B]	NDP	O4B-C4B	-7.07	1.29	1.45
2	A	501[A]	NAP	C7N-N7N	6.51	1.45	1.33
2	A	501[A]	NAP	C2B-C1B	6.51	1.69	1.53
3	A	502[B]	NDP	PA-O3	6.50	1.66	1.59
3	A	502[B]	NDP	PN-O3	6.19	1.66	1.59
2	A	501[A]	NAP	C3N-C7N	5.98	1.59	1.50
2	A	501[A]	NAP	O4B-C4B	5.96	1.58	1.45
3	A	502[B]	NDP	C6N-C5N	5.90	1.51	1.33
5	B	402	WBY	C07-S08	-5.85	1.62	1.74
5	B	401	WBY	C07-S08	-5.80	1.62	1.74
3	A	502[B]	NDP	O4D-C1D	-5.61	1.29	1.42
2	A	501[A]	NAP	O4B-C1B	-5.38	1.29	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	NAP	O4D-C4D	5.32	1.56	1.45
5	B	402	WBY	C04-N05	5.01	1.46	1.38
5	B	402	WBY	C06-N05	4.96	1.48	1.37
2	A	501[A]	NAP	C2D-C3D	4.93	1.66	1.53
5	B	401	WBY	C06-N05	4.89	1.48	1.37
5	B	401	WBY	C04-N05	4.82	1.46	1.38
2	A	501[A]	NAP	C5B-C4B	-4.78	1.37	1.51
3	A	502[B]	NDP	C7N-N7N	4.72	1.47	1.33
2	A	501[A]	NAP	PN-O3	4.67	1.64	1.59
3	A	502[B]	NDP	C3B-C4B	4.65	1.64	1.53
2	A	501[A]	NAP	C6A-N6A	4.64	1.46	1.34
3	A	502[B]	NDP	C6A-N6A	4.27	1.45	1.34
3	A	502[B]	NDP	C1B-N9A	-4.11	1.35	1.46
3	A	502[B]	NDP	O4B-C1B	4.05	1.51	1.42
5	B	402	WBY	C02-N03	3.97	1.44	1.39
5	B	401	WBY	C02-N03	3.88	1.44	1.39
3	A	502[B]	NDP	P2B-O2B	3.82	1.66	1.59
5	B	402	WBY	C09-S08	-3.59	1.64	1.73
5	B	401	WBY	C09-S08	-3.48	1.64	1.73
3	A	502[B]	NDP	C7N-C3N	3.34	1.55	1.48
3	A	502[B]	NDP	O3D-C3D	3.15	1.50	1.43
3	A	502[B]	NDP	C8A-N9A	-2.99	1.32	1.37
3	A	502[B]	NDP	C6N-N1N	2.90	1.44	1.37
5	B	402	WBY	C09-N11	2.76	1.39	1.31
5	B	401	WBY	C09-N11	2.76	1.39	1.31
2	A	501[A]	NAP	O7N-C7N	-2.62	1.19	1.24
3	A	502[B]	NDP	O2D-C2D	-2.60	1.36	1.43
5	B	401	WBY	C02-C07	2.56	1.52	1.43
3	A	502[B]	NDP	C4N-C3N	2.50	1.54	1.50
2	A	501[A]	NAP	O3B-C3B	2.49	1.49	1.43
5	B	402	WBY	C02-C07	2.42	1.52	1.43
5	B	401	WBY	O12-C04	-2.39	1.18	1.23
3	A	502[B]	NDP	O2B-C2B	2.36	1.52	1.44
3	A	502[B]	NDP	C5A-N7A	-2.35	1.34	1.39
5	B	402	WBY	O12-C04	-2.33	1.18	1.23
3	A	502[B]	NDP	O7N-C7N	-2.32	1.19	1.24
3	A	502[B]	NDP	O3B-C3B	2.28	1.48	1.43
2	A	501[A]	NAP	C3B-C4B	2.21	1.58	1.53
2	A	501[A]	NAP	C4A-N9A	-2.14	1.33	1.37
5	B	401	WBY	O01-C02	-2.03	1.18	1.23
2	A	501[A]	NAP	C5A-N7A	-2.03	1.35	1.39
3	A	502[B]	NDP	PN-O5D	2.01	1.67	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	WBY	C09-S08-C07	17.89	99.03	89.55
5	B	402	WBY	C09-S08-C07	17.87	99.02	89.55
5	B	402	WBY	C07-C06-N11	-8.35	110.47	117.89
5	B	401	WBY	C07-C06-N11	-7.84	110.93	117.89
5	B	402	WBY	S08-C09-N11	-7.33	109.58	114.64
5	B	401	WBY	S08-C09-N11	-7.03	109.80	114.64
2	A	501[A]	NAP	C5A-C4A-N3A	-4.90	119.97	126.72
3	A	502[B]	NDP	C5A-C4A-N3A	-4.77	120.14	126.72
5	B	401	WBY	O13-N03-C04	4.76	119.83	116.38
2	A	501[A]	NAP	C4D-O4D-C1D	-4.29	105.99	109.92
3	A	502[B]	NDP	N3A-C2A-N1A	-4.26	122.14	128.58
2	A	501[A]	NAP	N3A-C2A-N1A	-4.25	122.15	128.58
5	B	402	WBY	O13-N03-C04	4.14	119.39	116.38
3	A	502[B]	NDP	C4A-C5A-N7A	-3.59	106.48	110.58
2	A	501[A]	NAP	C4A-C5A-N7A	-3.38	106.71	110.58
2	A	501[A]	NAP	C5A-N7A-C8A	3.34	108.71	103.45
5	B	401	WBY	N05-C04-N03	3.34	120.07	115.65
5	B	402	WBY	N05-C04-N03	3.32	120.05	115.65
3	A	502[B]	NDP	C5A-N7A-C8A	3.28	108.61	103.45
3	A	502[B]	NDP	C2A-N3A-C4A	3.22	119.69	111.83
2	A	501[A]	NAP	N3A-C4A-N9A	3.22	132.64	127.17
2	A	501[A]	NAP	C2A-N3A-C4A	3.17	119.58	111.83
2	A	501[A]	NAP	N9A-C8A-N7A	-3.12	109.51	113.94
3	A	502[B]	NDP	N3A-C4A-N9A	3.05	132.36	127.17
3	A	502[B]	NDP	N9A-C8A-N7A	-3.05	109.61	113.94
5	B	402	WBY	O13-N03-C02	2.83	120.38	116.67
5	B	402	WBY	O12-C04-N03	-2.59	120.41	123.45
5	B	401	WBY	O12-C04-N03	-2.59	120.41	123.45
5	B	401	WBY	O13-N03-C02	2.51	119.97	116.67
3	A	502[B]	NDP	C3N-C2N-N1N	-2.39	119.69	123.20
2	A	501[A]	NAP	C2D-C3D-C4D	2.30	107.04	102.61
5	B	402	WBY	O01-C02-C07	-2.28	120.04	125.33
2	A	501[A]	NAP	C2B-C1B-N9A	-2.28	110.00	113.75
3	A	502[B]	NDP	C2B-C3B-C4B	2.20	106.73	101.99
5	B	401	WBY	C07-C02-N03	2.08	119.79	114.27
2	A	501[A]	NAP	C3N-C7N-N7N	2.08	120.30	117.74
3	A	502[B]	NDP	C2B-C1B-N9A	-2.07	110.34	113.75
5	B	402	WBY	C07-C02-N03	2.04	119.68	114.27
3	A	502[B]	NDP	P2B-O2B-C2B	-2.02	118.03	123.43
3	A	502[B]	NDP	C2D-C3D-C4D	2.02	106.51	102.61

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[A]	NAP	C5D-O5D-PN-O3
2	A	501[A]	NAP	C5D-O5D-PN-O1N
2	A	501[A]	NAP	C5D-O5D-PN-O2N
2	A	501[A]	NAP	O4D-C1D-N1N-C2N
2	A	501[A]	NAP	O4D-C1D-N1N-C6N
2	A	501[A]	NAP	C2D-C1D-N1N-C2N
2	A	501[A]	NAP	C2D-C1D-N1N-C6N
3	A	502[B]	NDP	C5D-O5D-PN-O3
3	A	502[B]	NDP	C5D-O5D-PN-O1N
3	A	502[B]	NDP	C5D-O5D-PN-O2N
2	A	501[A]	NAP	C3D-C4D-C5D-O5D
2	A	501[A]	NAP	O4B-C4B-C5B-O5B
2	A	501[A]	NAP	O4D-C4D-C5D-O5D
2	A	501[A]	NAP	C3B-C4B-C5B-O5B
3	A	502[B]	NDP	O4D-C4D-C5D-O5D
3	A	502[B]	NDP	C3D-C4D-C5D-O5D
3	A	502[B]	NDP	O4B-C4B-C5B-O5B
2	A	501[A]	NAP	C5B-O5B-PA-O2A
2	A	501[A]	NAP	C5B-O5B-PA-O3
3	A	502[B]	NDP	O4D-C1D-N1N-C6N
3	A	502[B]	NDP	C3B-C4B-C5B-O5B
3	A	502[B]	NDP	C2D-C1D-N1N-C6N
2	A	501[A]	NAP	PA-O3-PN-O2N
2	A	501[A]	NAP	C2B-O2B-P2B-O1X

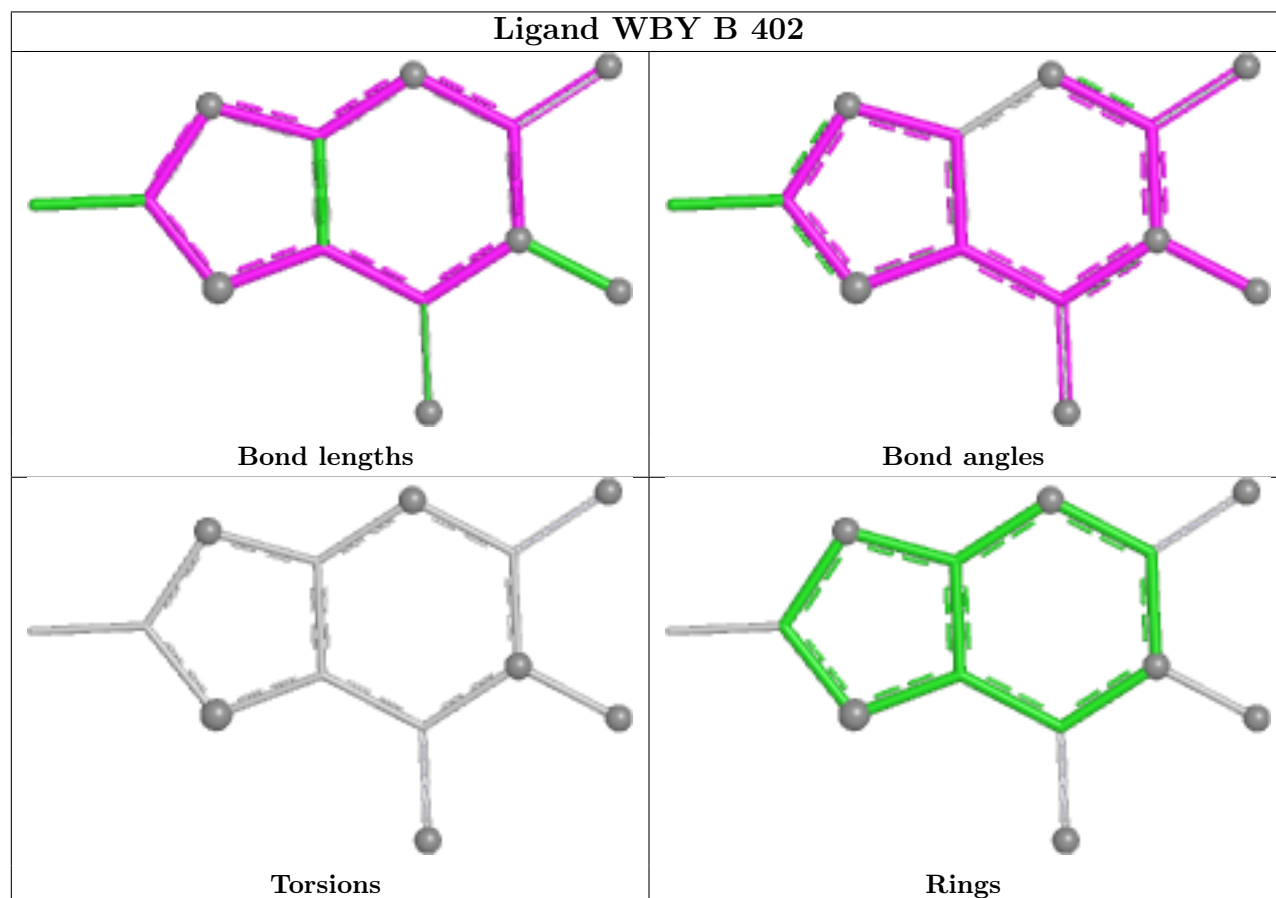
There are no ring outliers.

4 monomers are involved in 5 short contacts:

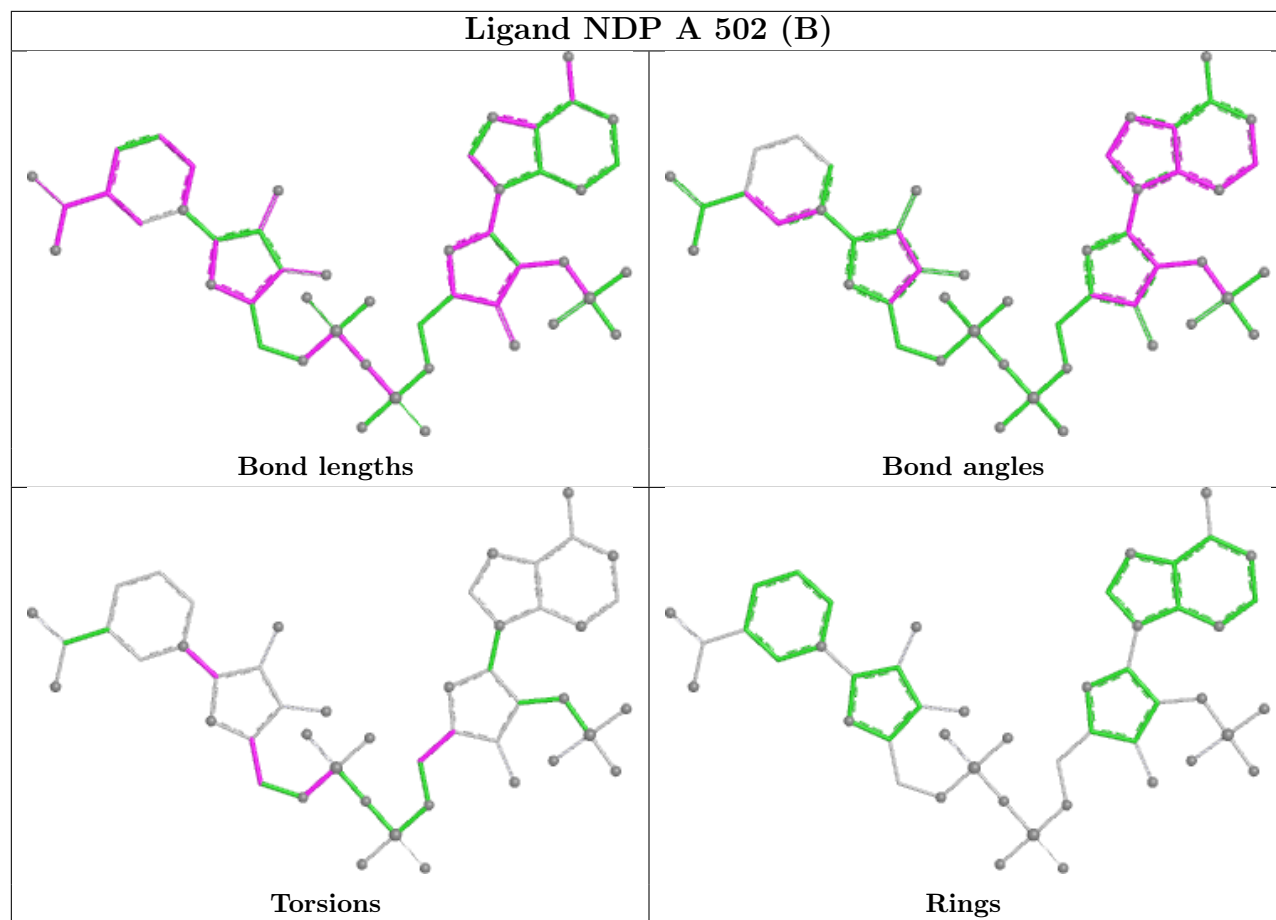
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	WBY	1	0
3	A	502[B]	NDP	2	0
2	A	501[A]	NAP	2	0
5	B	401	WBY	1	0

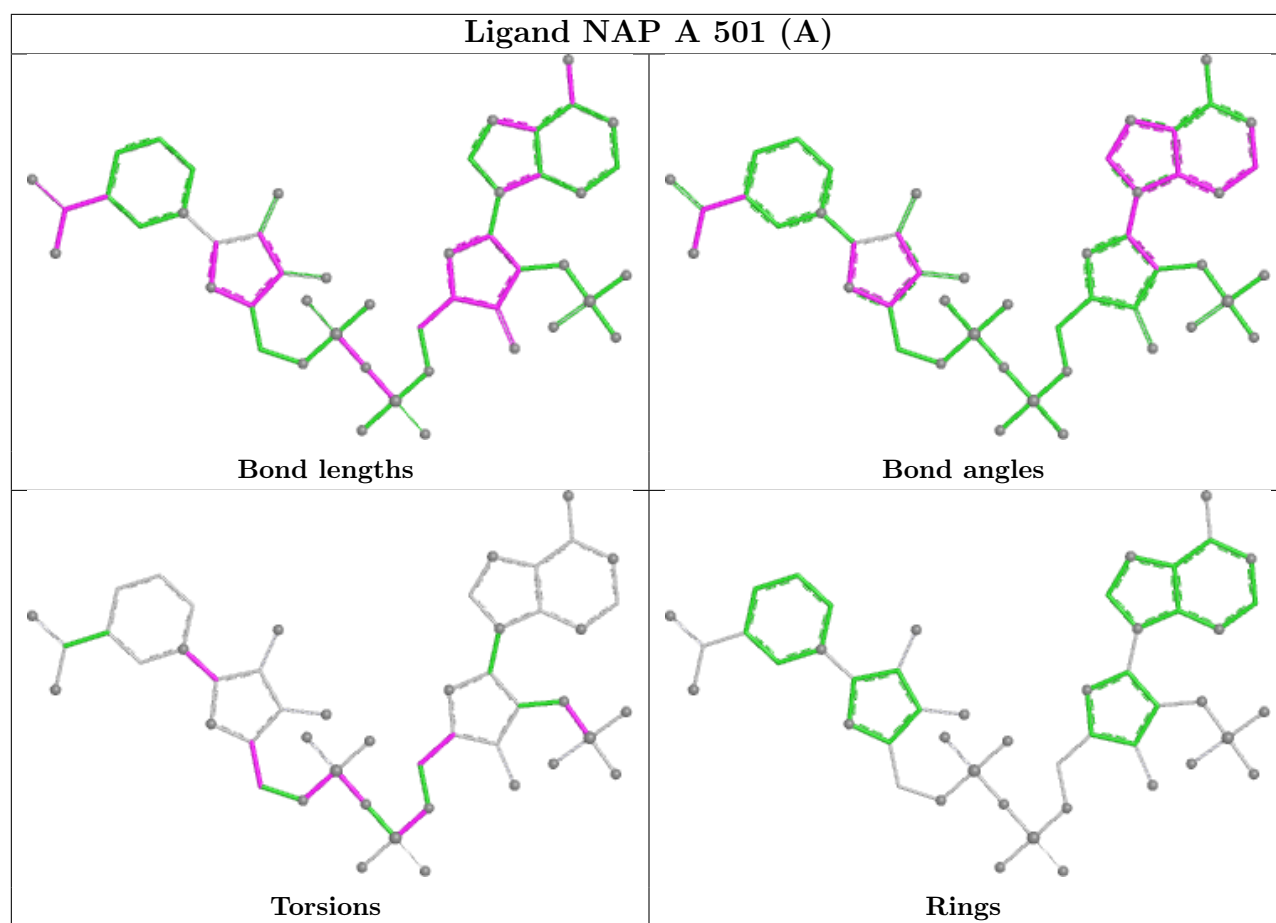
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

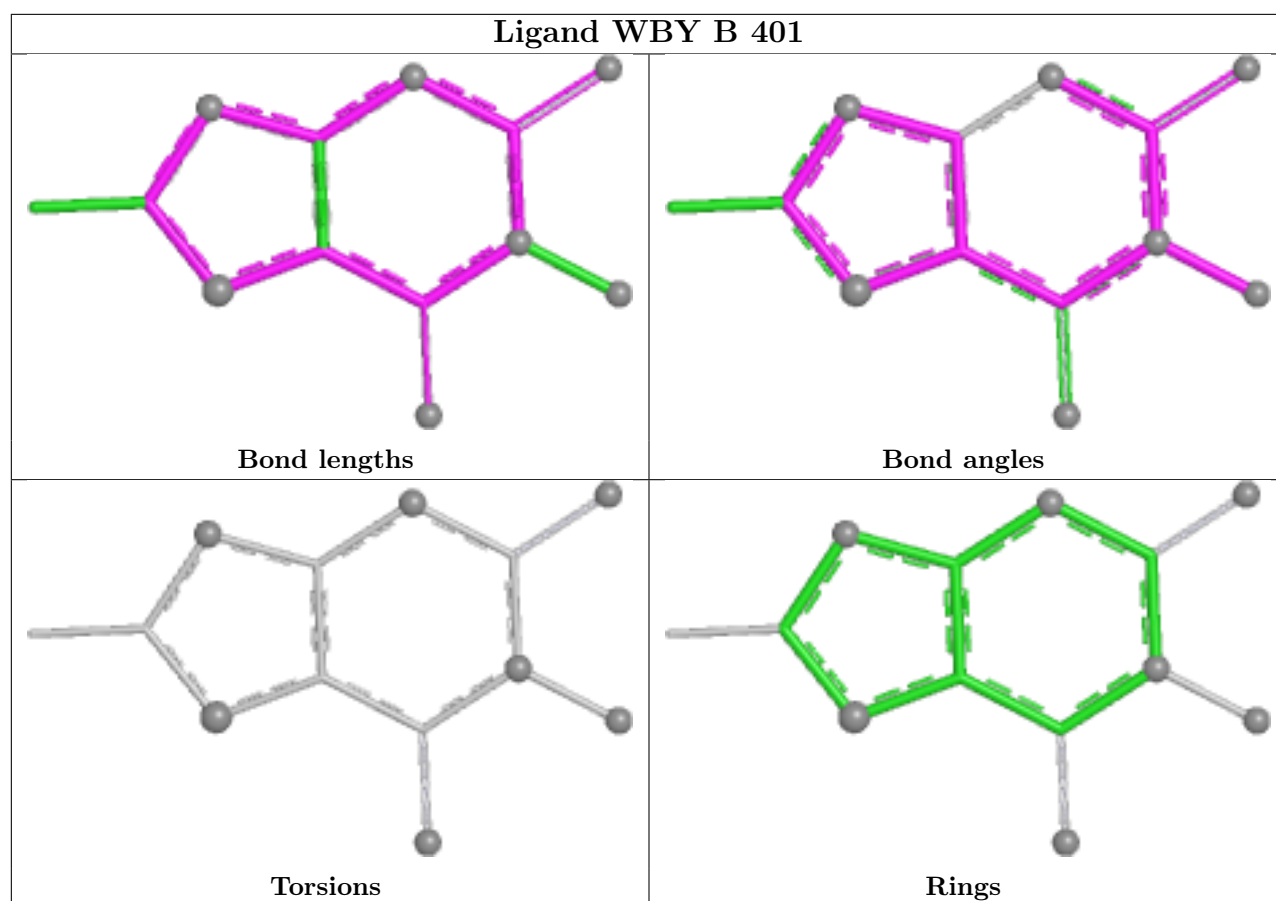
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand NDP A 502 (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

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	317/340 (93%)	0.79	22 (6%)	23 19	26, 66, 92, 97	4 (1%)
1	B	325/340 (95%)	0.64	12 (3%)	45 39	28, 59, 80, 100	1 (0%)
All	All	642/680 (94%)	0.71	34 (5%)	32 26	26, 61, 88, 100	5 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	ALA	3.6
1	A	176	ALA	3.0
1	A	125	PHE	3.0
1	A	167	TYR	2.9
1	A	127	VAL	2.9
1	A	36	LEU	2.8
1	B	246	VAL	2.7
1	B	39	ASN	2.6
1	B	314[A]	GLU	2.6
1	B	222	LEU	2.5
1	B	224	TYR	2.5
1	B	200	GLY	2.4
1	A	160	ALA	2.4
1	A	24	GLY	2.4
1	A	64	PHE	2.4
1	A	72	GLN	2.4
1	A	139	THR	2.3
1	B	61	PHE	2.3
1	B	116	ILE	2.3
1	A	324	MET	2.3
1	A	151	GLY	2.3
1	A	63	VAL	2.3
1	B	202	VAL	2.3
1	A	19	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	243[A]	MET	2.2
1	A	14	ALA	2.2
1	B	158	GLY	2.1
1	A	122	VAL	2.1
1	A	70	VAL	2.1
1	B	323	MET	2.1
1	A	136	VAL	2.1
1	A	148	SER	2.0
1	B	147	PRO	2.0
1	A	103	LEU	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](#)

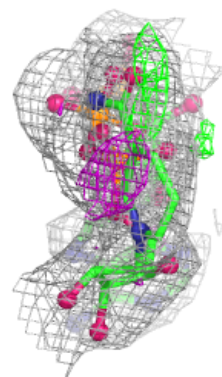
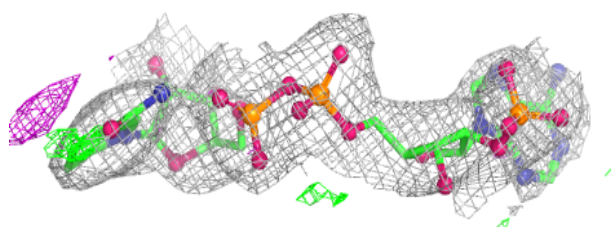
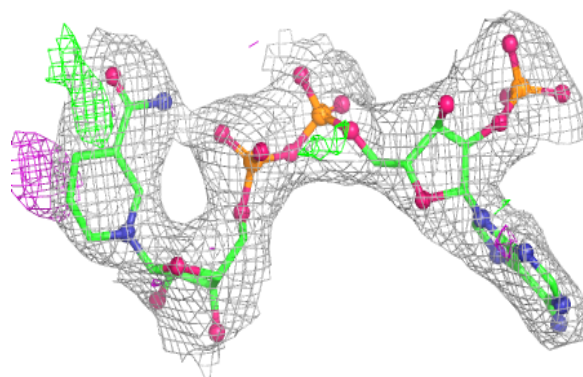
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	505	1/1	0.70	0.10	85,85,85,85	0
3	NDP	A	502[B]	48/48	0.79	0.12	56,65,76,76	48
2	NAP	A	501[A]	48/48	0.84	0.11	56,66,76,76	48
5	WBY	B	401	13/13	0.93	0.13	46,54,63,63	0
5	WBY	B	402	13/13	0.94	0.09	38,43,53,57	0
4	MG	A	504	1/1	0.97	0.05	46,46,46,46	0
4	MG	B	403	1/1	0.97	0.05	52,52,52,52	0
4	MG	A	503	1/1	0.98	0.04	45,45,45,45	0
4	MG	B	404	1/1	0.99	0.02	45,45,45,45	0

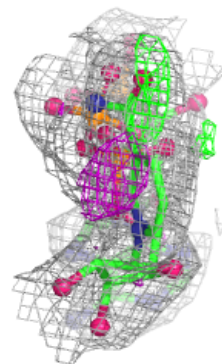
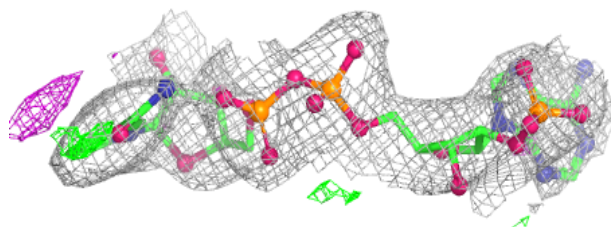
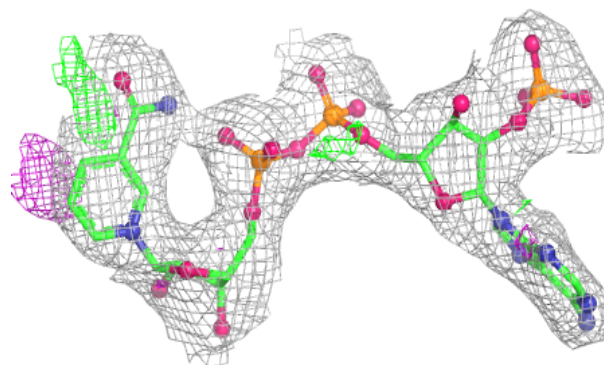
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP A 502 (B):

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

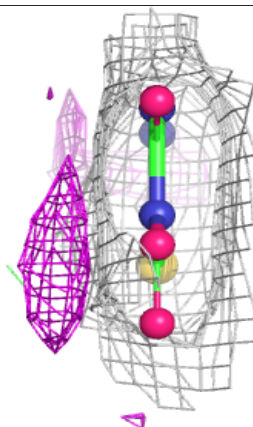
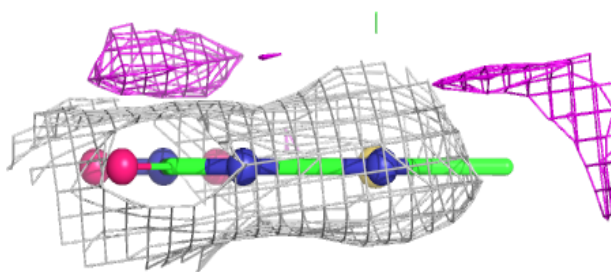
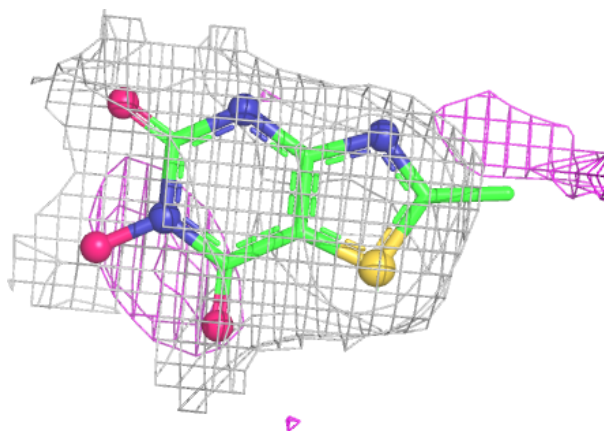
**Electron density around NAP A 501 (A):**

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

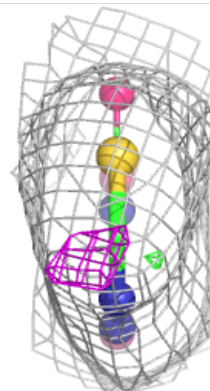
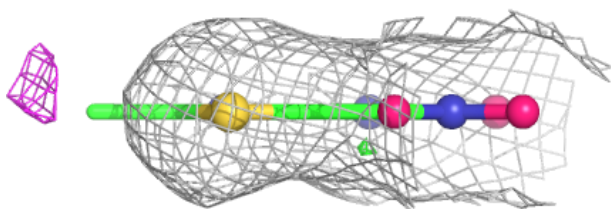
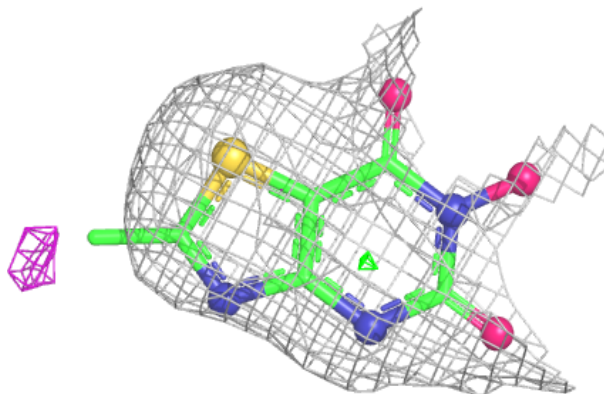


Electron density around WBY B 401:

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

**Electron density around WBY B 402:**

$2mF_o-DF_c$ (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.