



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:33 pm BST

PDB ID : 4FAM
Title : Crystal structure of human 17beta-hydroxysteroid dehydrogenase type 5 in complex with 3-((3,4-dihydroisoquinolin-2(1H)-yl)sulfonyl)benzoic acid (17)
Authors : Turnbull, A.P.; Jamieson, S.M.F.; Brooke, D.G.; Heinrich, D.; Atwell, G.J.; Silva, S.; Hamilton, E.J.; Rigoreau, L.J.M.; Trivier, E.; Soudy, C.; Samlal, S.S.; Owen, P.J.; Schroeder, E.; Raynham, T.; Flanagan, J.U.; Denny, W.A.
Deposited on : 2012-05-22
Resolution : 2.00 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 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 : 2.11
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) : 2.11

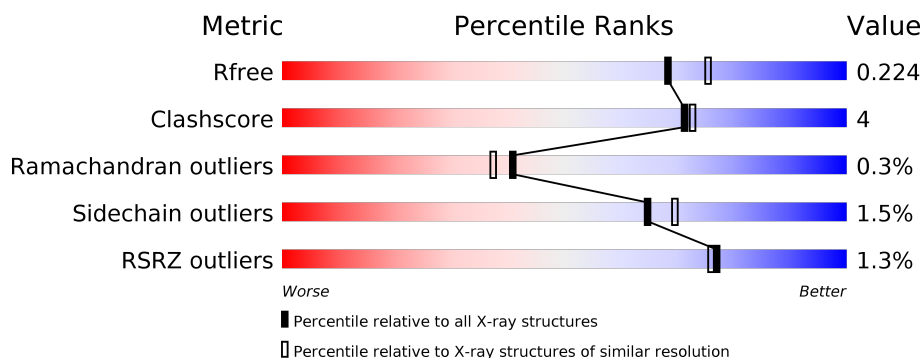
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 84%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 11% 5% </div> </div>
1	B	331	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 8%, green 87%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 87% 8% 5% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5732 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 Aldo-keto reductase family 1 member C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	2	0
			2498	1598	431	456	13			
1	B	314	Total	C	N	O	S	0	1	0
			2487	1589	431	455	12			

There are 16 discrepancies between the modelled and reference sequences:

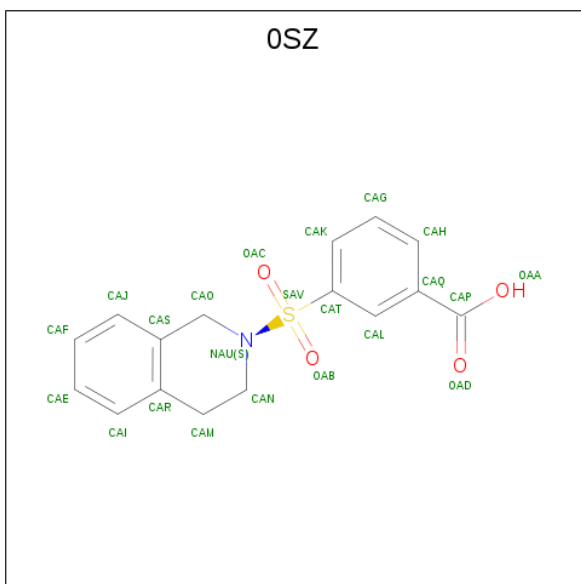
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	LEU	-	EXPRESSION TAG	UNP P42330
A	325	GLU	-	EXPRESSION TAG	UNP P42330
A	326	HIS	-	EXPRESSION TAG	UNP P42330
A	327	HIS	-	EXPRESSION TAG	UNP P42330
A	328	HIS	-	EXPRESSION TAG	UNP P42330
A	329	HIS	-	EXPRESSION TAG	UNP P42330
A	330	HIS	-	EXPRESSION TAG	UNP P42330
A	331	HIS	-	EXPRESSION TAG	UNP P42330
B	324	LEU	-	EXPRESSION TAG	UNP P42330
B	325	GLU	-	EXPRESSION TAG	UNP P42330
B	326	HIS	-	EXPRESSION TAG	UNP P42330
B	327	HIS	-	EXPRESSION TAG	UNP P42330
B	328	HIS	-	EXPRESSION TAG	UNP P42330
B	329	HIS	-	EXPRESSION TAG	UNP P42330
B	330	HIS	-	EXPRESSION TAG	UNP P42330
B	331	HIS	-	EXPRESSION TAG	UNP P42330

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is 3-(3,4-dihydroisoquinolin-2(1H)-ylsulfonyl)benzoic acid (three-letter code: 0SZ) (formula: C₁₆H₁₅NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	16	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			22	16	1	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

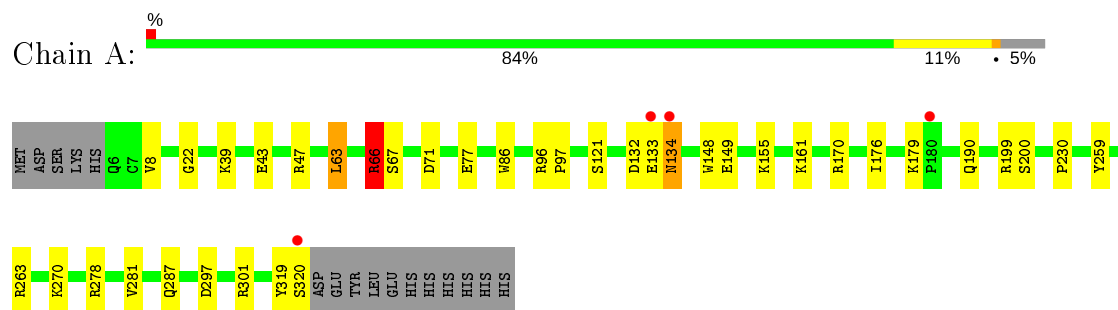
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	288	Total 288	O 288	0	0
5	B	283	Total 283	O 283	0	0

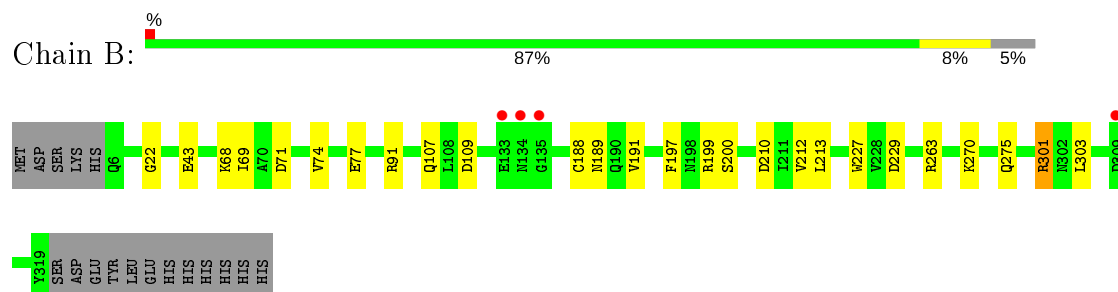
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Aldo-keto reductase family 1 member C3



- Molecule 1: Aldo-keto reductase family 1 member C3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.72Å 106.76Å 74.88Å 90.00° 103.11° 90.00°	Depositor
Resolution (Å)	20.03 – 2.00 19.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.03-2.00) 98.7 (19.87-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.168 , 0.218 0.173 , 0.224	Depositor DCC
R_{free} test set	2524 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5732	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: 0SZ, 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	1.01	3/2562 (0.1%)	0.98	7/3474 (0.2%)
1	B	1.00	1/2545 (0.0%)	0.95	8/3452 (0.2%)
All	All	1.01	4/5107 (0.1%)	0.97	15/6926 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	GLU	CD-OE2	5.54	1.31	1.25
1	B	227	TRP	CD2-CE2	5.50	1.48	1.41
1	A	148	TRP	CD2-CE2	5.09	1.47	1.41
1	A	86	TRP	CD2-CE2	5.09	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	263	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	B	263	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	199	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	63	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	297	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	66	ARG	NE-CZ-NH1	5.74	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	229	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	47	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	301	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	170	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	109	ASP	CB-CG-OD2	-5.21	113.62	118.30
1	B	199	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	91	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	TYR	Peptide

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	2498	0	2479	22	0
1	B	2487	0	2452	13	0
2	A	48	0	25	3	0
2	B	48	0	25	2	0
3	A	22	0	14	0	0
3	B	22	0	14	0	0
4	A	24	0	36	1	0
4	B	12	0	18	1	0
5	A	288	0	0	11	0
5	B	283	0	0	3	3
All	All	5732	0	5063	36	3

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 (36) 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:210:ASP:HB2	5:B:1077:HOH:O	1.67	0.94
1:A:134:ASN:CB	5:A:699:HOH:O	2.13	0.94
1:B:275:GLN:NE2	5:B:1027:HOH:O	1.85	0.91
1:A:230:PRO:HG3	1:B:77:GLU:HB2	1.70	0.73
1:A:8[A]:VAL:HG11	5:A:637:HOH:O	1.88	0.73
1:A:39:LYS:HD2	5:A:749:HOH:O	1.95	0.66
1:A:259:TYR:O	1:A:263:ARG:HG3	2.02	0.60
1:A:320:SER:HB2	5:A:783:HOH:O	2.07	0.54
1:A:320:SER:CA	5:A:783:HOH:O	2.56	0.54
1:B:191:VAL:HG22	1:B:213:LEU:HD11	1.91	0.53
1:A:287:GLN:HG3	5:A:788:HOH:O	2.08	0.53
1:A:149:GLU:OE2	1:A:179:LYS:NZ	2.41	0.52
1:B:189:ASN:O	1:B:213:LEU:HD12	2.09	0.52
1:A:132:ASP:O	1:A:134:ASN:O	2.29	0.51
1:A:43:GLU:HG2	5:A:585:HOH:O	2.09	0.51
1:A:155:LYS:NZ	1:A:161:LYS:O	2.42	0.50
1:A:66:ARG:HG2	1:A:66:ARG:HH11	1.76	0.50
1:A:320:SER:C	5:A:783:HOH:O	2.50	0.50
1:A:278:ARG:O	1:A:281:VAL:HG22	2.12	0.49
1:A:67:SER:HB2	5:A:583:HOH:O	2.12	0.48
1:A:320:SER:CB	5:A:783:HOH:O	2.62	0.47
1:B:69:ILE:HA	1:B:74:VAL:O	2.16	0.46
1:A:270:LYS:O	2:A:401:NAP:H8A	2.15	0.46
1:B:188:CYS:HA	1:B:212:VAL:O	2.17	0.45
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.80	0.44
1:B:191:VAL:CG2	1:B:213:LEU:HD11	2.47	0.44
1:A:71:ASP:C	1:A:71:ASP:OD1	2.57	0.43
1:A:22:GLY:HA3	2:A:401:NAP:H4D	2.00	0.42
1:B:197:PHE:HB2	1:B:303:LEU:O	2.20	0.41
1:B:43:GLU:HG3	1:B:68:LYS:NZ	2.35	0.41
1:B:270:LYS:O	2:B:701:NAP:H8A	2.20	0.41
4:A:405:EDO:C2	5:A:745:HOH:O	2.69	0.41
4:B:704:EDO:H12	5:B:1072:HOH:O	2.19	0.41
1:A:190:GLN:OE1	2:A:401:NAP:H2N	2.21	0.41
1:B:22:GLY:HA3	2:B:701:NAP:H4D	2.03	0.40
1:A:96:ARG:HB3	1:A:97:PRO:HD3	2.03	0.40

All (3) 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)
5:B:974:HOH:O	5:B:1062:HOH:O[1_455]	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:931:HOH:O	5:B:1063:HOH:O[1_455]	1.80	0.40
5:B:967:HOH:O	5:B:1058:HOH:O[1_655]	1.84	0.36

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	315/331 (95%)	307 (98%)	6 (2%)	2 (1%)	25	19
1	B	313/331 (95%)	308 (98%)	5 (2%)	0	100	100
All	All	628/662 (95%)	615 (98%)	11 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	133	GLU

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	271/295 (92%)	266 (98%)	5 (2%)	59	63
1	B	267/295 (90%)	263 (98%)	4 (2%)	65	69
All	All	538/590 (91%)	529 (98%)	9 (2%)	65	65

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

Mol	Chain	Res	Type
1	A	63	LEU
1	A	66	ARG
1	A	121	SER
1	A	176	ILE
1	A	200	SER
1	B	107	GLN
1	B	200[A]	SER
1	B	200[B]	SER
1	B	301	ARG

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	107	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	A	404	-	3,3,3	1.28	0	2,2,2	1.25	0
4	EDO	A	405	-	3,3,3	0.57	0	2,2,2	0.36	0
4	EDO	A	408	-	3,3,3	0.95	0	2,2,2	0.30	0
2	NAP	A	401	-	45,52,52	2.22	9 (20%)	56,80,80	1.95	9 (16%)
4	EDO	B	703	-	3,3,3	0.51	0	2,2,2	0.34	0
4	EDO	A	406	-	3,3,3	0.74	0	2,2,2	0.20	0
3	0SZ	A	402	-	22,24,24	2.32	4 (18%)	30,35,35	2.12	6 (20%)
4	EDO	B	704	-	3,3,3	0.37	0	2,2,2	0.78	0
4	EDO	B	705	-	3,3,3	0.59	0	2,2,2	0.27	0
4	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.40	0
2	NAP	B	701	-	45,52,52	2.45	9 (20%)	56,80,80	2.07	11 (19%)
4	EDO	A	403	-	3,3,3	0.58	0	2,2,2	0.16	0
3	0SZ	B	702	-	22,24,24	3.12	8 (36%)	30,35,35	4.59	8 (26%)

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	A	404	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
2	NAP	A	401	-	-	2/31/67/67	0/5/5/5
4	EDO	B	703	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
3	0SZ	A	402	-	-	0/12/25/25	0/3/3/3
4	EDO	B	704	-	-	0/1/1/1	-
4	EDO	B	705	-	-	0/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
2	NAP	B	701	-	-	2/31/67/67	0/5/5/5
4	EDO	A	403	-	-	0/1/1/1	-
3	0SZ	B	702	-	-	0/12/25/25	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	NAP	C2A-N3A	8.53	1.45	1.32
3	B	702	0SZ	SAV-NAU	8.42	1.75	1.63
3	B	702	0SZ	CAT-SAV	-7.94	1.65	1.76
3	A	402	0SZ	CAT-SAV	-7.43	1.66	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	NAP	O4B-C1B	6.62	1.50	1.41
2	A	401	NAP	C2A-N1A	6.50	1.46	1.33
2	A	401	NAP	O4B-C1B	6.31	1.49	1.41
2	B	701	NAP	C2N-N1N	6.23	1.42	1.35
2	A	401	NAP	C2A-N3A	6.04	1.41	1.32
2	B	701	NAP	C2A-N1A	5.94	1.45	1.33
2	A	401	NAP	C2N-N1N	5.14	1.41	1.35
3	B	702	0SZ	CAQ-CAP	-4.42	1.43	1.47
3	A	402	0SZ	CAM-CAR	-4.21	1.44	1.51
3	A	402	0SZ	CAQ-CAP	-4.13	1.43	1.47
3	B	702	0SZ	CAN-CAM	3.74	1.59	1.51
3	B	702	0SZ	OAB-SAV	3.73	1.47	1.43
2	B	701	NAP	C4A-N3A	3.68	1.40	1.35
2	B	701	NAP	P2B-O2B	3.66	1.66	1.59
2	A	401	NAP	C2D-C1D	3.50	1.59	1.53
3	B	702	0SZ	CAM-CAR	-3.09	1.45	1.51
3	A	402	0SZ	CAO-NAU	2.75	1.51	1.47
2	A	401	NAP	P2B-O2B	2.61	1.64	1.59
2	B	701	NAP	O4D-C1D	2.52	1.44	1.41
2	A	401	NAP	C5B-C4B	2.50	1.59	1.51
3	B	702	0SZ	CAO-CAS	-2.36	1.46	1.51
2	A	401	NAP	PA-O2A	-2.34	1.44	1.55
2	B	701	NAP	C3N-C7N	-2.25	1.47	1.50
3	B	702	0SZ	OAC-SAV	2.09	1.45	1.43
2	B	701	NAP	O3D-C3D	2.09	1.47	1.43
2	A	401	NAP	PN-O2N	-2.00	1.45	1.55

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	0SZ	OAB-SAV-NAU	-19.21	89.17	106.69
3	B	702	0SZ	OAC-SAV-NAU	-11.70	96.02	106.69
2	B	701	NAP	N3A-C2A-N1A	-10.72	111.93	128.68
2	A	401	NAP	N3A-C2A-N1A	-9.85	113.28	128.68
3	B	702	0SZ	OAB-SAV-CAT	8.52	118.83	108.05
3	A	402	0SZ	OAC-SAV-NAU	-6.32	100.93	106.69
3	A	402	0SZ	OAB-SAV-NAU	-5.86	101.35	106.69
2	A	401	NAP	O5D-C5D-C4D	4.10	123.11	108.99
2	A	401	NAP	C3N-C7N-N7N	-4.02	112.93	117.75
3	B	702	0SZ	OAC-SAV-CAT	3.90	112.97	108.05
2	B	701	NAP	C2A-N1A-C6A	3.87	125.38	118.75
3	A	402	0SZ	CAQ-CAL-CAT	3.59	122.80	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	0SZ	OAC-SAV-OAB	3.46	125.14	119.52
2	A	401	NAP	C2D-C3D-C4D	-3.43	95.99	102.64
3	A	402	0SZ	CAT-SAV-NAU	3.40	111.35	107.30
2	B	701	NAP	O7N-C7N-N7N	3.35	127.34	122.58
2	B	701	NAP	C5N-C4N-C3N	-3.15	116.61	120.34
2	B	701	NAP	C3N-C7N-N7N	-3.00	114.15	117.75
2	B	701	NAP	C2N-C3N-C4N	2.97	121.62	118.26
2	A	401	NAP	C6N-N1N-C2N	-2.71	119.51	121.97
2	B	701	NAP	C2D-C3D-C4D	-2.67	97.46	102.64
2	A	401	NAP	O4B-C4B-C5B	-2.63	100.73	109.37
2	B	701	NAP	O3X-P2B-O1X	2.58	120.77	110.68
2	A	401	NAP	O7N-C7N-N7N	2.56	126.21	122.58
3	B	702	0SZ	CAG-CAK-CAT	2.37	121.41	118.95
3	A	402	0SZ	CAO-NAU-SAV	2.34	120.68	116.94
2	B	701	NAP	C5B-C4B-C3B	-2.33	106.44	115.18
2	A	401	NAP	C2A-N1A-C6A	2.21	122.54	118.75
2	B	701	NAP	O2X-P2B-O2B	-2.17	96.25	105.99
2	B	701	NAP	C6N-N1N-C2N	-2.12	120.04	121.97
3	B	702	0SZ	CAJ-CAS-CAR	-2.11	116.38	118.98
3	B	702	0SZ	CAK-CAG-CAH	-2.07	117.31	120.25
2	A	401	NAP	C2B-C3B-C4B	2.06	106.47	101.99
3	B	702	0SZ	OAC-SAV-OAB	2.03	122.82	119.52

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C4D-C5D-O5D-PN
2	A	401	NAP	PA-O3-PN-O5D
2	B	701	NAP	PA-O3-PN-O5D
2	B	701	NAP	C4D-C5D-O5D-PN
4	A	404	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

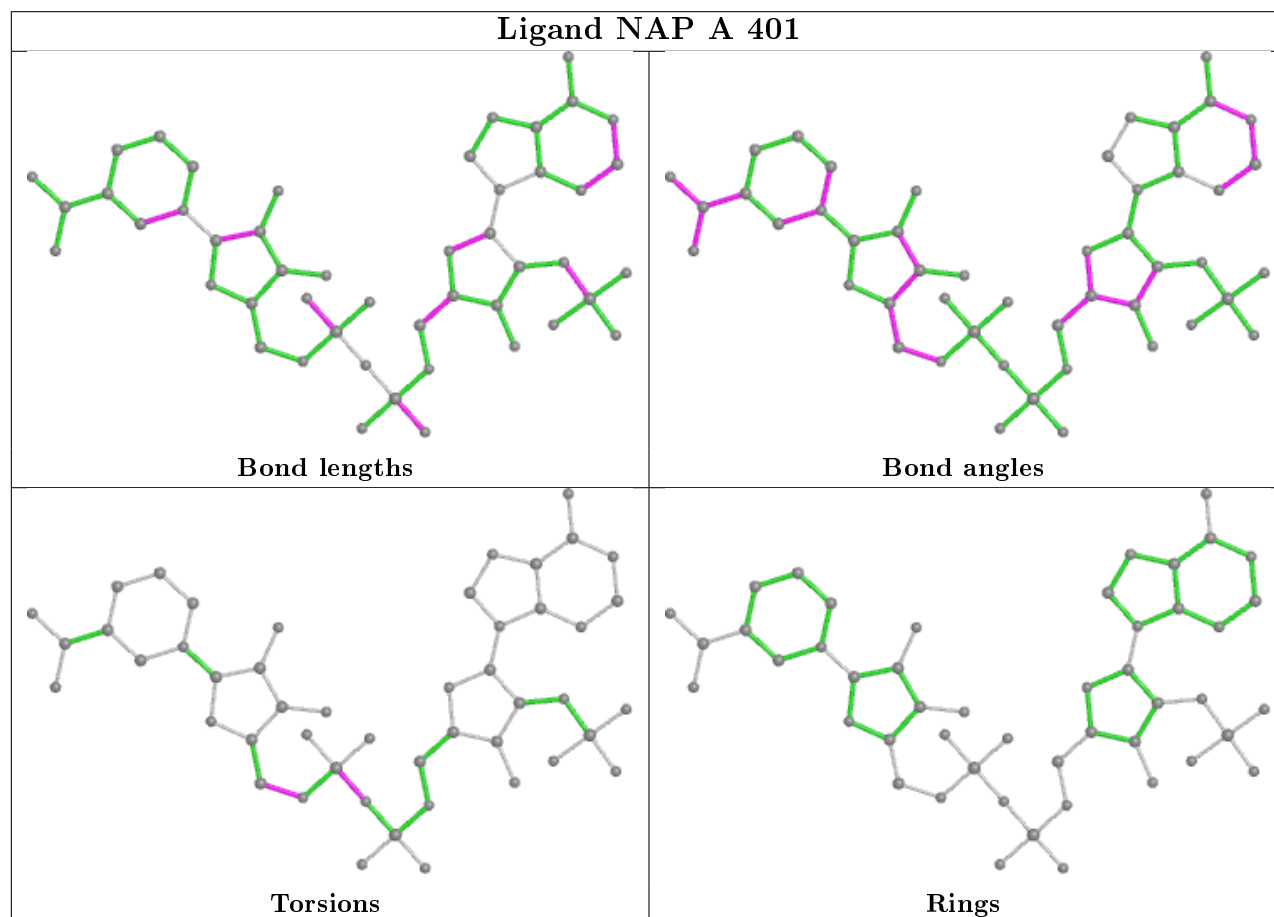
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	EDO	1	0
2	A	401	NAP	3	0
4	B	704	EDO	1	0

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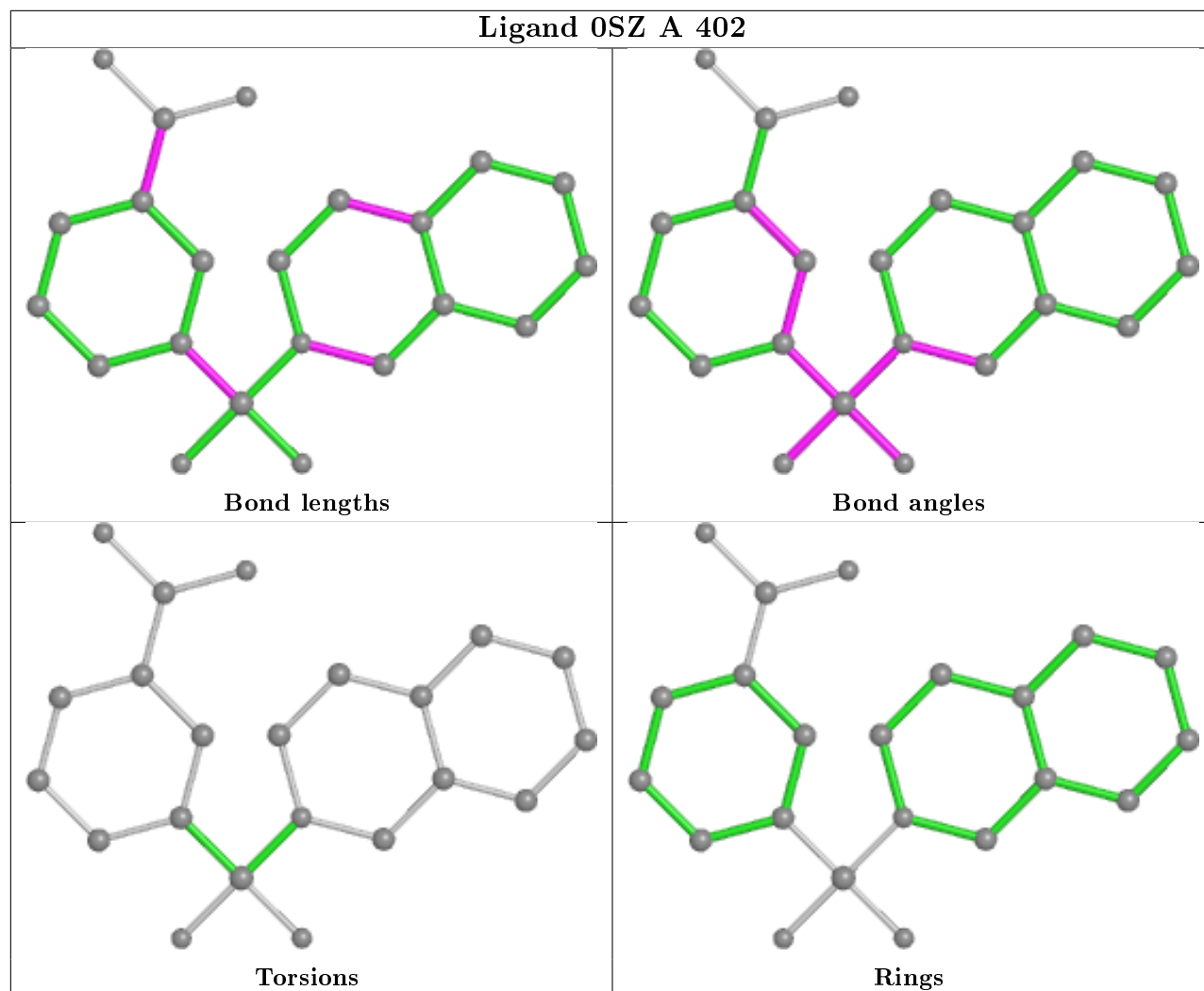
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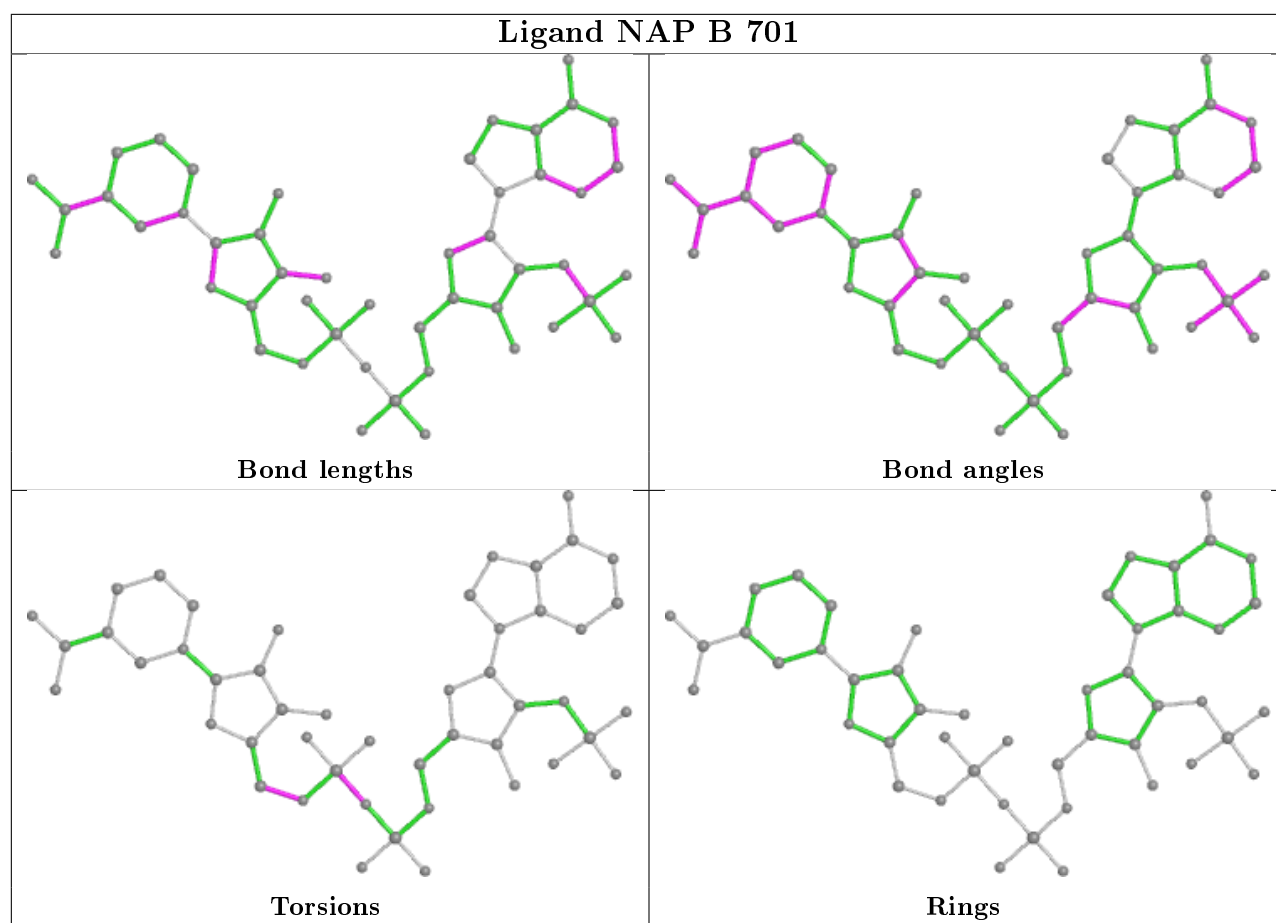
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	NAP	2	0

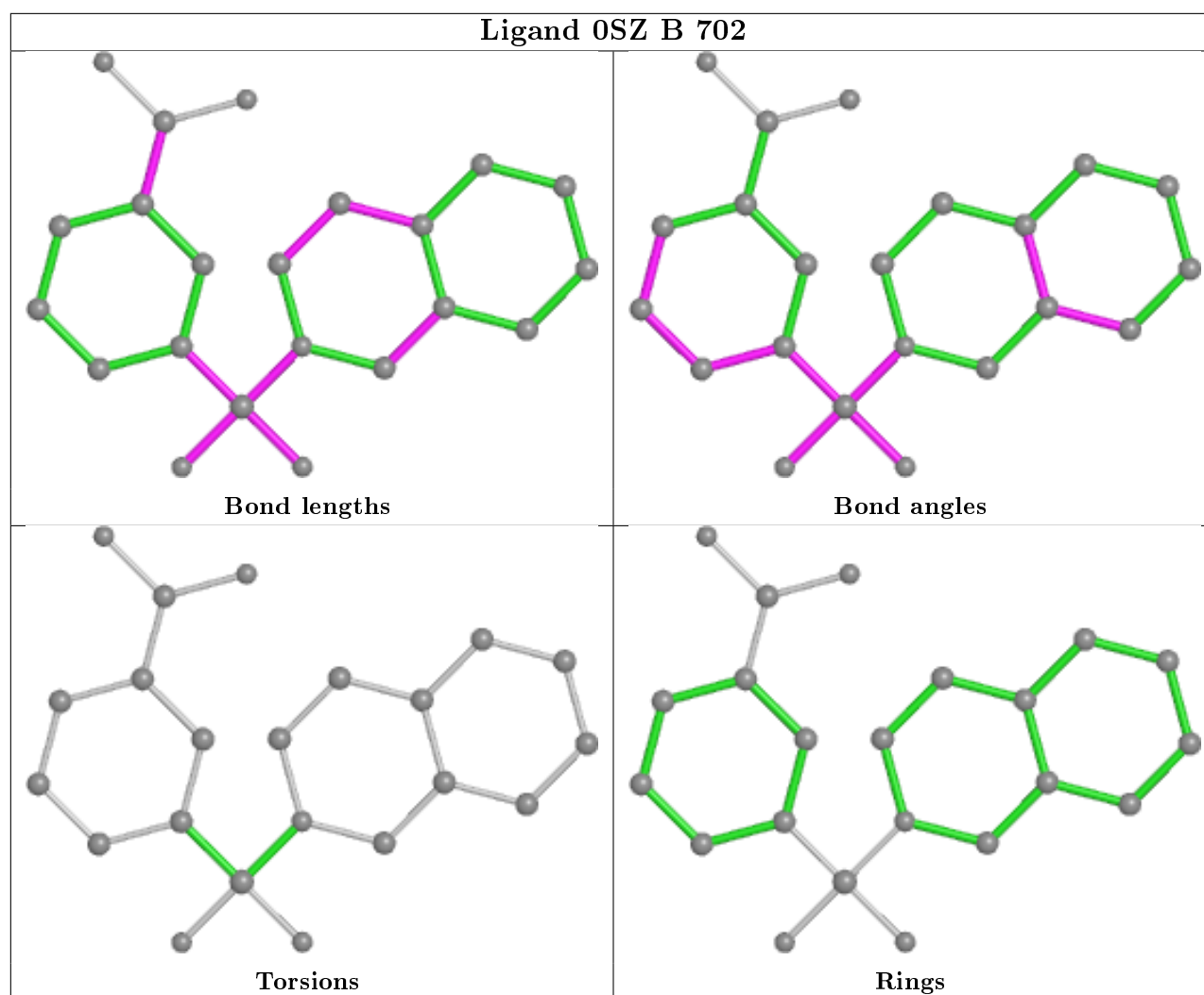
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 0SZ A 402







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	315/331 (95%)	-0.43	4 (1%) 77 76	11, 18, 31, 51	4 (1%)
1	B	314/331 (94%)	-0.37	4 (1%) 77 76	11, 18, 30, 68	5 (1%)
All	All	629/662 (95%)	-0.40	8 (1%) 77 76	11, 18, 31, 68	9 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	5.1
1	B	134	ASN	5.1
1	B	133	GLU	3.7
1	B	309	ASP	3.0
1	A	133	GLU	2.7
1	A	134	ASN	2.5
1	A	320	SER	2.4
1	A	180	PRO	2.2

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 carbohydrates 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,

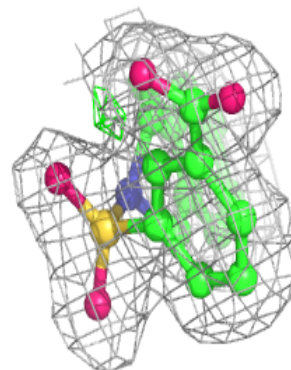
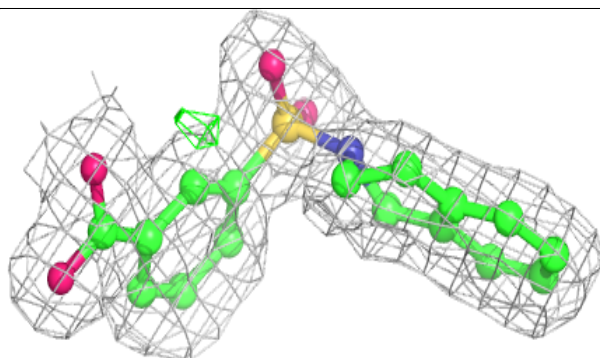
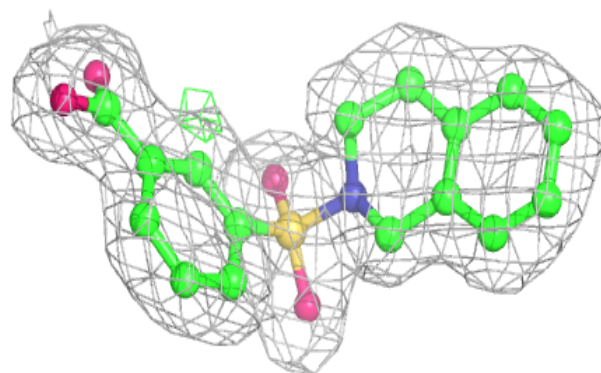
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	404	4/4	0.70	0.22	34,36,37,38	0
4	EDO	B	704	4/4	0.82	0.31	41,46,46,47	0
4	EDO	A	405	4/4	0.88	0.23	26,32,34,37	0
4	EDO	B	705	4/4	0.89	0.12	31,32,32,33	0
4	EDO	A	406	4/4	0.93	0.10	26,28,29,32	0
4	EDO	A	407	4/4	0.93	0.12	28,30,32,32	0
4	EDO	B	703	4/4	0.95	0.12	16,17,17,19	0
3	0SZ	A	402	22/22	0.97	0.08	13,15,17,18	0
2	NAP	B	701	48/48	0.97	0.07	11,13,16,18	0
4	EDO	A	403	4/4	0.97	0.10	15,16,17,18	0
3	0SZ	B	702	22/22	0.97	0.07	14,17,19,20	0
2	NAP	A	401	48/48	0.98	0.07	10,13,18,20	0
4	EDO	A	408	4/4	0.98	0.07	16,19,19,20	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.

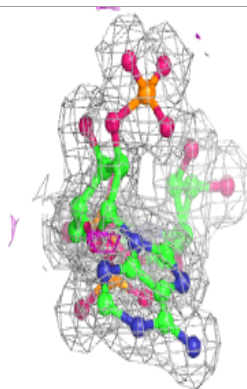
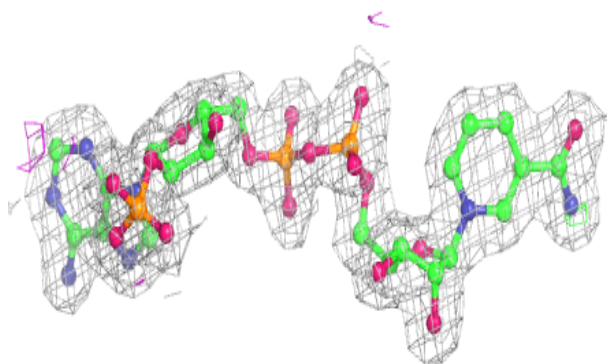
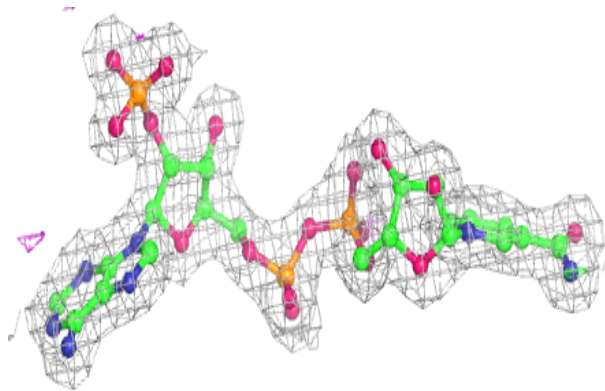
Electron density around 0SZ A 402:

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

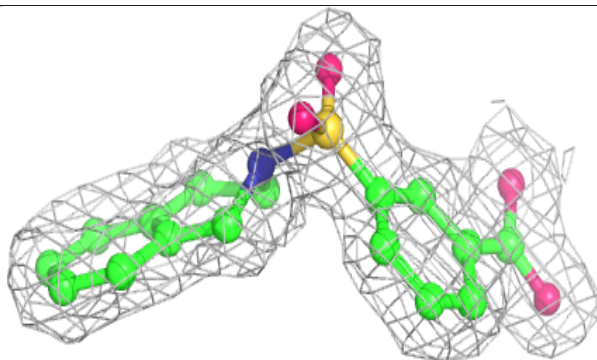
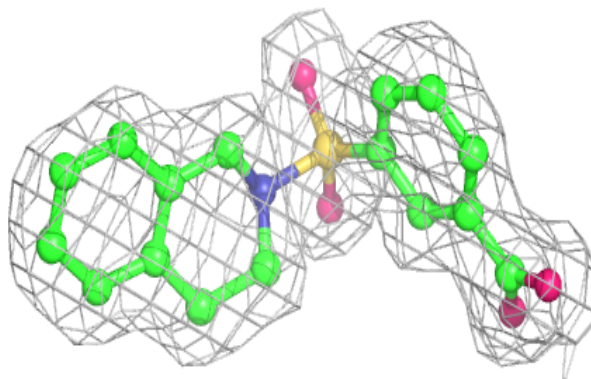


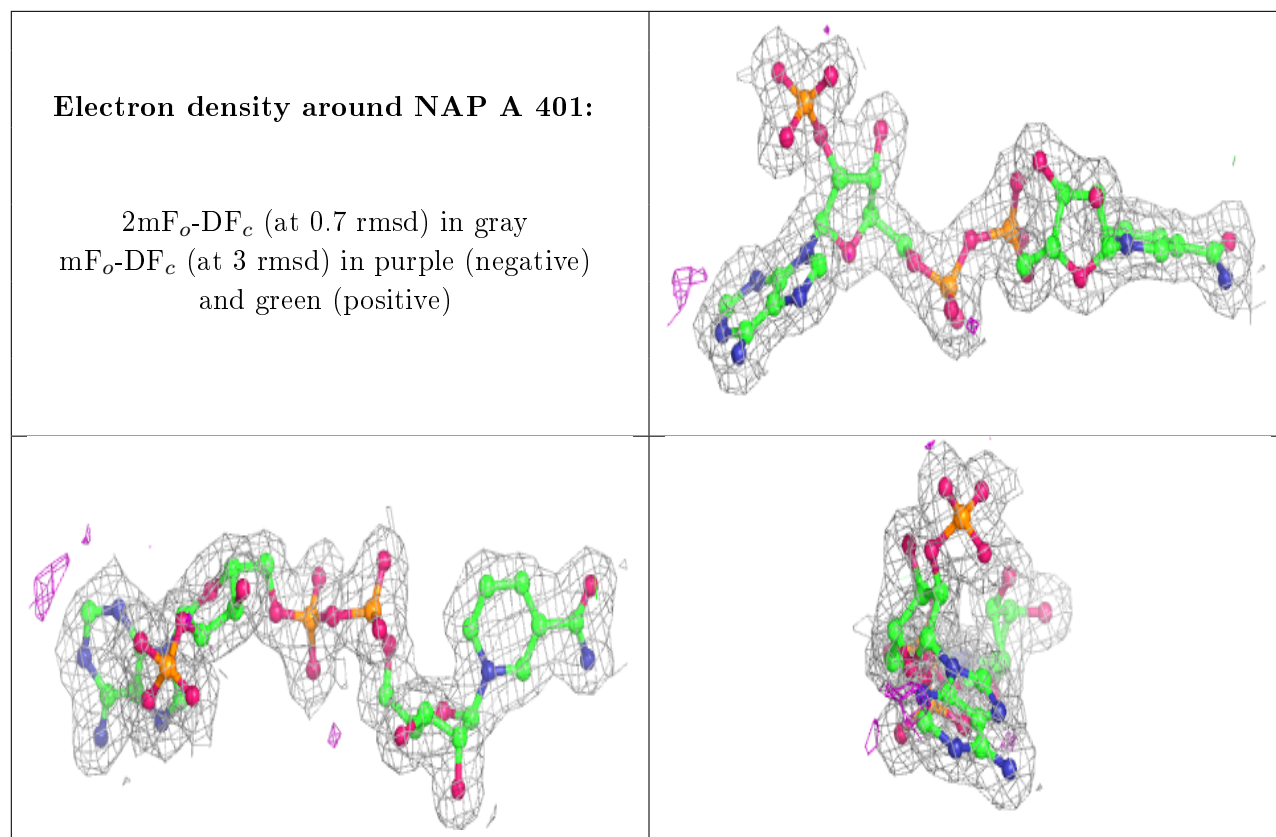
Electron density around NAP B 701:

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

**Electron density around OSZ B 702:**

$2mF_o-DF_c$ (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.