



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:11 PM UTC

PDB ID : 3DWF / pdb_00003dwf
Title : Crystal Structure of the Guinea Pig 11beta-Hydroxysteroid Dehydrogenase Type 1 Mutant F278E
Authors : Lawson, A.J.; Ride, J.P.; White, S.A.; Walker, E.A.
Deposited on : 2008-07-22
Resolution : 2.20 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

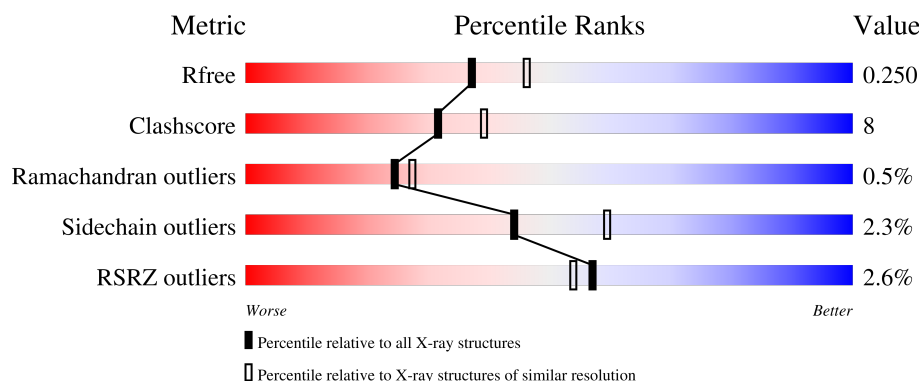
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	2% 84% 12% ..
1	B	276	5% 83% 13% ..
1	C	276	2% 84% 13% ...
1	D	276	% 84% 13% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9153 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 11-beta-hydroxysteroid dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2087	1337	350	385	15			
1	B	275	Total	C	N	O	S	0	0	0
			2117	1359	354	389	15			
1	C	274	Total	C	N	O	S	0	0	0
			2112	1353	355	389	15			
1	D	275	Total	C	N	O	S	0	0	0
			2120	1360	355	390	15			

There are 4 discrepancies between the modelled and reference sequences:

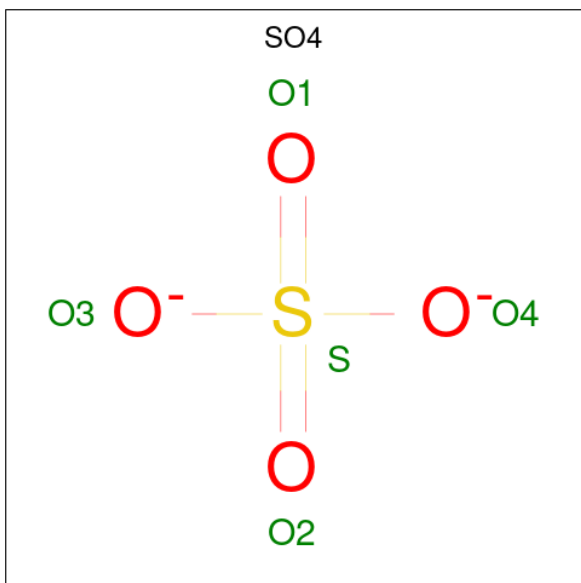
Chain	Residue	Modelled	Actual	Comment	Reference
A	278	GLU	PHE	engineered mutation	UNP Q6QLL4
B	278	GLU	PHE	engineered mutation	UNP Q6QLL4
C	278	GLU	PHE	engineered mutation	UNP Q6QLL4
D	278	GLU	PHE	engineered mutation	UNP Q6QLL4

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



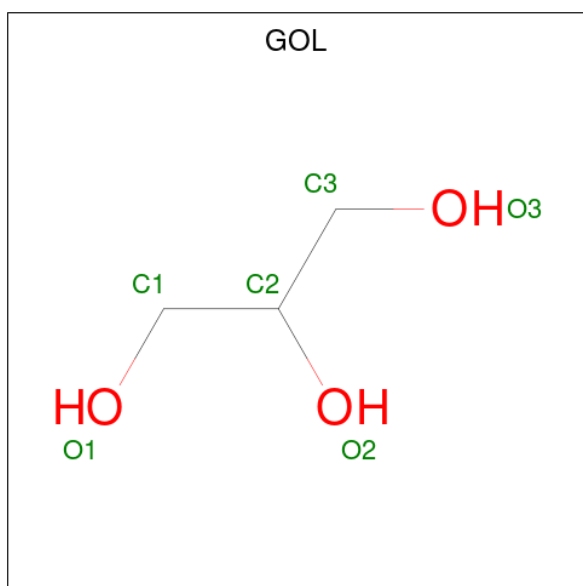
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

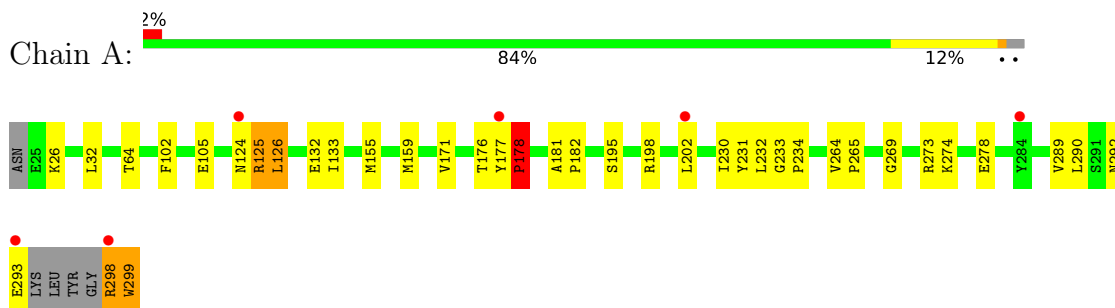
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total	O	0	0
			122	122		
5	B	113	Total	O	0	0
			113	113		
5	C	96	Total	O	0	0
			96	96		
5	D	121	Total	O	0	0
			121	121		

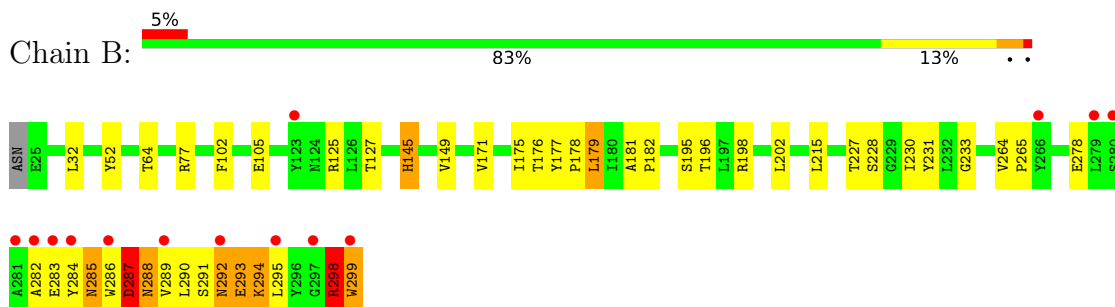
3 Residue-property plots [i](#)

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.

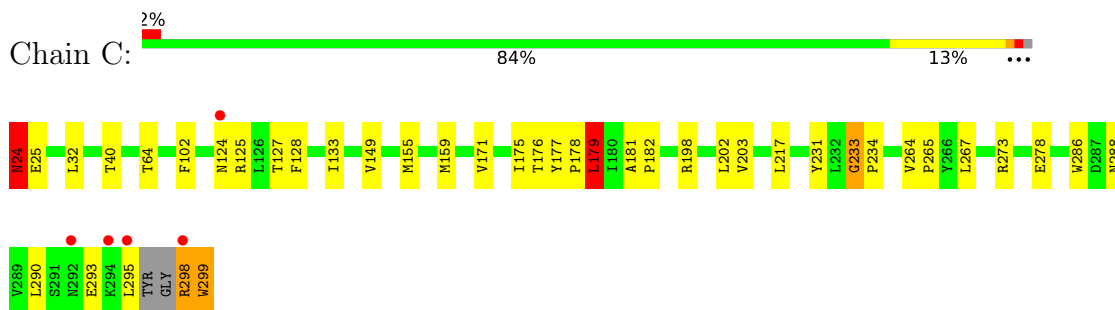
- Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1



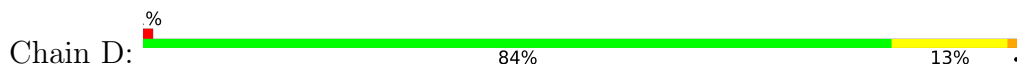
- Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1

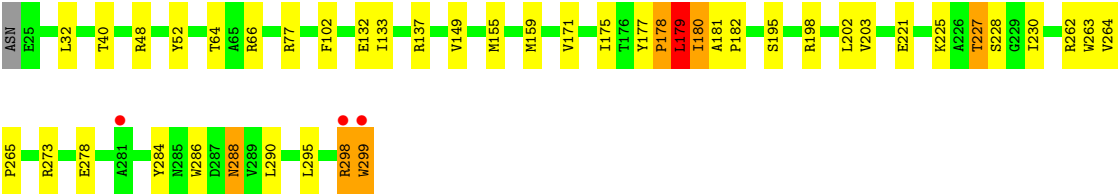


- Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1



- Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.08Å 85.92Å 176.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.68 – 2.20 34.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.68-2.20) 99.7 (34.68-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.255 0.199 , 0.250	Depositor DCC
R_{free} test set	3094 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9153	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: GOL, NAP, SO4

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	0.38	0/2126	0.83	6/2871 (0.2%)
1	B	0.78	6/2158 (0.3%)	1.05	16/2915 (0.5%)
1	C	1.20	3/2151 (0.1%)	0.84	6/2904 (0.2%)
1	D	0.81	2/2161 (0.1%)	0.78	4/2919 (0.1%)
All	All	0.85	11/8596 (0.1%)	0.88	32/11609 (0.3%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	ASN	C-N	-51.93	0.66	1.33
1	D	178	PRO	C-N	-32.24	0.86	1.33
1	B	287	ASP	C-N	-21.54	1.03	1.33
1	B	288	ASN	C-N	15.15	1.54	1.33
1	B	285	ASN	C-N	-11.69	1.18	1.33
1	C	179	LEU	C-N	-6.85	1.24	1.33
1	D	227	THR	C-N	-6.39	1.24	1.33
1	B	284	TYR	C-N	-5.52	1.26	1.33
1	B	145	HIS	ND1-CE1	5.38	1.38	1.32
1	C	288	ASN	CG-OD1	5.16	1.33	1.23
1	B	288	ASN	CG-OD1	5.13	1.33	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ASP	O-C-N	-20.38	95.48	122.59
1	B	287	ASP	CA-C-N	17.41	153.80	122.46
1	B	287	ASP	C-N-CA	17.41	153.80	122.46
1	C	24	ASN	CA-C-N	-14.12	99.33	122.21
1	C	24	ASN	C-N-CA	-14.12	99.33	122.21
1	A	125	ARG	CB-CA-C	12.83	127.54	109.71
1	B	288	ASN	O-C-N	10.78	135.35	122.09
1	A	125	ARG	N-CA-C	-9.86	96.03	110.42
1	A	292	ASN	N-CA-C	9.60	131.24	110.80
1	C	24	ASN	O-C-N	9.56	138.29	123.00
1	B	288	ASN	CA-C-N	-8.91	105.93	121.97
1	B	288	ASN	C-N-CA	-8.91	105.93	121.97
1	B	285	ASN	CA-C-N	-8.07	109.46	120.28
1	B	285	ASN	C-N-CA	-8.07	109.46	120.28
1	D	178	PRO	CA-C-N	7.87	136.06	123.93
1	D	178	PRO	C-N-CA	7.87	136.06	123.93
1	A	178	PRO	CB-CA-C	7.00	123.11	111.56
1	B	285	ASN	O-C-N	6.84	130.60	122.46
1	B	145	HIS	CB-CG-CD2	-6.71	122.47	131.20
1	C	124	ASN	CB-CA-C	6.58	122.74	109.38
1	D	227	THR	O-C-N	-6.21	115.47	122.23
1	B	284	TYR	CA-C-N	6.19	131.44	122.16
1	B	284	TYR	C-N-CA	6.19	131.44	122.16
1	B	298	ARG	N-CA-C	5.95	116.09	108.24
1	A	126	LEU	N-CA-CB	-5.83	100.41	109.34
1	A	292	ASN	CB-CA-C	-5.72	99.04	110.42
1	B	145	HIS	CB-CG-ND1	5.65	131.17	122.70
1	D	179	LEU	O-C-N	-5.63	113.47	121.91
1	B	284	TYR	O-C-N	-5.56	116.84	123.06
1	B	292	ASN	N-CA-C	-5.46	106.65	113.15
1	C	233	GLY	CA-C-N	5.38	125.58	120.31
1	C	233	GLY	C-N-CA	5.38	125.58	120.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	287	ASP	Mainchain
1	C	24	ASN	Mainchain
1	D	179	LEU	Mainchain

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	2087	0	2112	31	0
1	B	2117	0	2144	47	0
1	C	2112	0	2141	33	0
1	D	2120	0	2148	49	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	D	30	0	40	8	0
5	A	122	0	0	3	0
5	B	113	0	0	6	0
5	C	96	0	0	1	0
5	D	121	0	0	6	0
All	All	9153	0	8709	141	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 (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:PRO:C	1:D:179:LEU:CA	2.17	1.18
1:D:178:PRO:CA	1:D:179:LEU:N	2.09	1.13
1:D:178:PRO:O	1:D:179:LEU:N	1.83	1.09
1:D:178:PRO:C	1:D:179:LEU:N	0.86	0.95
1:D:48:ARG:HH12	4:D:7:GOL:H32	1.34	0.92
1:D:66:ARG:HH11	4:D:8:GOL:H12	1.40	0.86
1:B:52:TYR:OH	1:B:77:ARG:HD2	1.75	0.86
1:D:298:ARG:HD3	5:D:567:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ARG:O	1:C:127:THR:HG22	1.80	0.81
1:B:294:LYS:HE2	1:B:294:LYS:H	1.46	0.80
1:B:285:ASN:ND2	1:B:288:ASN:HB2	1.97	0.80
1:A:231:TYR:HE1	1:B:283:GLU:HB3	1.44	0.79
1:B:288:ASN:O	1:B:292:ASN:CB	2.30	0.78
1:B:178:PRO:O	1:B:179:LEU:HB2	1.82	0.78
1:B:293:GLU:HB2	1:B:294:LYS:HE2	1.63	0.78
1:D:263:TRP:HD1	4:D:2:GOL:H2	1.48	0.78
1:A:231:TYR:CE1	1:B:283:GLU:HB3	2.23	0.74
1:B:288:ASN:O	1:B:292:ASN:CA	2.35	0.73
1:A:124:ASN:O	1:A:125:ARG:C	2.33	0.70
1:B:288:ASN:ND2	1:D:228:SER:HB3	2.08	0.69
1:B:288:ASN:O	1:B:292:ASN:N	2.29	0.65
1:C:178:PRO:O	1:C:179:LEU:HB2	1.97	0.64
1:D:262:ARG:HG2	4:D:2:GOL:H12	1.80	0.63
1:D:48:ARG:NH1	4:D:7:GOL:H32	2.10	0.63
1:A:299:TRP:CD1	1:A:299:TRP:N	2.67	0.62
1:B:299:TRP:CD1	1:B:299:TRP:N	2.67	0.62
1:D:299:TRP:CD1	1:D:299:TRP:N	2.68	0.62
1:B:145:HIS:HD2	5:B:364:HOH:O	1.83	0.62
1:C:299:TRP:N	1:C:299:TRP:CD1	2.67	0.61
1:B:178:PRO:O	1:B:179:LEU:CB	2.47	0.61
1:D:203:VAL:CG1	1:D:290:LEU:HD21	2.35	0.57
1:B:125:ARG:O	1:B:127:THR:HG22	2.05	0.56
1:C:175:ILE:HG22	1:D:273:ARG:HG3	1.87	0.56
1:B:289:VAL:HG13	1:B:295:LEU:HD12	1.88	0.56
1:B:286:TRP:O	1:B:290:LEU:N	2.40	0.55
1:B:231:TYR:CE2	1:B:233:GLY:HA3	2.42	0.54
1:B:291:SER:C	1:B:293:GLU:H	2.17	0.53
1:B:145:HIS:CD2	5:B:364:HOH:O	2.61	0.53
1:C:299:TRP:CD1	1:C:299:TRP:H	2.27	0.53
1:A:232:LEU:HD21	1:D:230:ILE:HD13	1.90	0.53
1:D:288:ASN:OD1	1:D:288:ASN:C	2.52	0.53
1:C:202:LEU:HD11	5:C:603:HOH:O	2.09	0.52
1:D:52:TYR:CE1	1:D:77:ARG:HG2	2.45	0.52
1:B:299:TRP:CD1	1:B:299:TRP:H	2.27	0.52
1:B:287:ASP:O	1:B:291:SER:HB2	2.10	0.52
1:A:299:TRP:CD1	1:A:299:TRP:H	2.27	0.52
1:A:289:VAL:HG12	1:A:290:LEU:N	2.25	0.51
1:D:180:ILE:HG22	5:D:352:HOH:O	2.10	0.51
1:D:137:ARG:HD3	5:D:376:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD21	1:D:230:ILE:CD1	2.40	0.51
1:A:132:GLU:H	1:A:132:GLU:CD	2.18	0.51
1:D:263:TRP:CD1	4:D:2:GOL:H2	2.37	0.51
1:B:181:ALA:HB3	1:B:182:PRO:HD3	1.94	0.50
1:D:178:PRO:C	1:D:179:LEU:CB	2.84	0.50
1:D:299:TRP:CD1	1:D:299:TRP:H	2.28	0.50
1:B:286:TRP:CD1	5:B:336:HOH:O	2.64	0.50
1:C:181:ALA:HB3	1:C:182:PRO:HD3	1.92	0.50
1:B:285:ASN:ND2	1:B:288:ASN:CB	2.72	0.49
1:C:128:PHE:HB2	1:D:295:LEU:O	2.13	0.49
1:D:227:THR:O	1:D:228:SER:C	2.56	0.48
1:B:286:TRP:CZ3	1:B:289:VAL:HG11	2.48	0.48
1:D:298:ARG:HE	1:D:299:TRP:N	2.11	0.48
1:A:234:PRO:HD2	1:C:295:LEU:HD12	1.96	0.48
1:B:289:VAL:HG13	1:B:295:LEU:CD1	2.45	0.47
1:B:298:ARG:HE	1:B:299:TRP:N	2.12	0.47
1:A:155:MET:HG3	1:A:159:MET:HE3	1.96	0.47
1:B:282:ALA:HA	5:B:710:HOH:O	2.14	0.47
1:C:178:PRO:O	1:C:179:LEU:CB	2.63	0.47
1:D:155:MET:HG3	1:D:159:MET:HE3	1.96	0.47
1:A:126:LEU:CD1	1:A:126:LEU:H	2.27	0.47
1:A:231:TYR:CZ	1:A:233:GLY:HA3	2.49	0.47
1:C:155:MET:HG3	1:C:159:MET:HE3	1.95	0.47
1:C:203:VAL:HG12	1:C:290:LEU:HD21	1.97	0.47
1:C:273:ARG:HG3	1:D:175:ILE:HG22	1.96	0.47
1:A:105:GLU:HG3	5:A:733:HOH:O	2.14	0.47
1:A:181:ALA:HB3	1:A:182:PRO:HD3	1.97	0.47
1:B:105:GLU:HG2	5:B:658:HOH:O	2.15	0.47
1:C:24:ASN:CG	1:C:25:GLU:HG3	2.39	0.47
1:A:176:THR:HG21	1:B:195:SER:HB2	1.96	0.46
1:C:298:ARG:HE	1:C:299:TRP:N	2.14	0.46
1:A:298:ARG:HE	1:A:299:TRP:N	2.13	0.46
1:C:24:ASN:OD1	1:C:25:GLU:HB2	2.16	0.46
1:D:203:VAL:HG12	1:D:290:LEU:HD21	1.96	0.46
1:D:264:VAL:N	1:D:265:PRO:CD	2.79	0.46
1:A:232:LEU:HD11	1:D:230:ILE:HD11	1.98	0.46
1:C:176:THR:HG21	1:D:195:SER:HB2	1.98	0.46
1:D:284:TYR:HB2	1:D:286:TRP:CE2	2.51	0.46
1:C:133:ILE:HD13	1:D:149:VAL:HG22	1.98	0.45
1:A:177:TYR:C	1:A:178:PRO:O	2.60	0.45
1:C:64:THR:HB	1:C:102:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ARG:NH1	4:D:8:GOL:H12	2.20	0.45
1:A:273:ARG:HG3	1:B:175:ILE:HG22	1.99	0.45
1:B:292:ASN:CB	1:B:295:LEU:HG	2.46	0.45
1:C:273:ARG:NH1	4:D:1:GOL:O1	2.50	0.45
1:D:221:GLU:HG2	5:D:358:HOH:O	2.16	0.45
1:B:264:VAL:N	1:B:265:PRO:CD	2.80	0.45
1:D:181:ALA:HB3	1:D:182:PRO:HD3	1.97	0.45
1:C:203:VAL:CG1	1:C:290:LEU:HD21	2.47	0.44
1:A:198:ARG:O	1:A:202:LEU:HG	2.18	0.44
1:A:264:VAL:N	1:A:265:PRO:CD	2.80	0.44
1:C:171:VAL:HG12	1:C:177:TYR:HE2	1.82	0.44
1:C:231:TYR:CE2	1:C:233:GLY:HA3	2.52	0.44
1:A:133:ILE:HD13	1:B:149:VAL:HG22	2.00	0.44
1:A:230:ILE:HG23	1:B:289:VAL:CG2	2.47	0.44
1:B:171:VAL:HG12	1:B:177:TYR:HE2	1.83	0.44
1:B:286:TRP:HD1	5:B:336:HOH:O	2.00	0.44
1:B:289:VAL:C	1:B:291:SER:N	2.76	0.44
1:C:264:VAL:N	1:C:265:PRO:CD	2.81	0.44
1:B:52:TYR:CZ	1:B:77:ARG:HD2	2.53	0.44
1:D:64:THR:HB	1:D:102:PHE:CE1	2.53	0.43
1:A:64:THR:HB	1:A:102:PHE:CE1	2.53	0.43
5:A:1107:HOH:O	1:C:295:LEU:HD21	2.19	0.43
1:B:230:ILE:HD12	1:B:230:ILE:N	2.34	0.43
1:D:198:ARG:O	1:D:202:LEU:HG	2.19	0.43
1:A:177:TYR:O	1:A:178:PRO:C	2.62	0.43
1:B:64:THR:HB	1:B:102:PHE:CE1	2.54	0.43
1:D:52:TYR:CZ	1:D:77:ARG:HG2	2.54	0.43
1:D:66:ARG:HB2	2:D:301:NAP:O3X	2.19	0.43
1:A:177:TYR:O	1:B:196:THR:HG23	2.19	0.42
1:C:290:LEU:O	1:C:293:GLU:HB2	2.19	0.42
1:A:171:VAL:HG12	1:A:177:TYR:HE2	1.85	0.42
1:B:198:ARG:O	1:B:202:LEU:HG	2.19	0.41
1:C:40:THR:HA	1:C:64:THR:HG22	2.02	0.41
1:D:40:THR:HA	1:D:64:THR:HG22	2.02	0.41
1:A:195:SER:HB2	1:B:176:THR:HG21	2.02	0.41
1:A:26:LYS:HA	5:A:888:HOH:O	2.19	0.41
1:C:203:VAL:HG11	1:C:286:TRP:CZ3	2.56	0.41
1:D:171:VAL:HG12	1:D:177:TYR:HE2	1.85	0.41
1:B:227:THR:O	1:B:228:SER:C	2.63	0.41
1:C:217:LEU:HB3	1:C:234:PRO:O	2.20	0.41
1:C:267:LEU:HD12	1:C:267:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASN:N	1:C:25:GLU:N	2.29	0.41
1:C:149:VAL:HG22	1:D:133:ILE:HD13	2.02	0.41
1:D:225:LYS:HD2	5:D:358:HOH:O	2.20	0.41
1:A:269:GLY:O	1:A:274:LYS:HE2	2.21	0.40
1:B:286:TRP:HA	1:B:289:VAL:HB	2.02	0.40
1:D:298:ARG:NE	1:D:299:TRP:N	2.69	0.40
1:C:198:ARG:O	1:C:202:LEU:HG	2.21	0.40
1:D:137:ARG:HG2	5:D:328:HOH:O	2.22	0.40
1:D:178:PRO:HA	1:D:179:LEU:N	2.24	0.40
1:D:263:TRP:C	1:D:265:PRO:HD2	2.47	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	267/276 (97%)	252 (94%)	14 (5%)	1 (0%)	30	34
1	B	273/276 (99%)	257 (94%)	14 (5%)	2 (1%)	18	19
1	C	270/276 (98%)	260 (96%)	9 (3%)	1 (0%)	30	34
1	D	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	30	34
All	All	1083/1104 (98%)	1032 (95%)	46 (4%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	LEU
1	A	178	PRO
1	B	293	GLU
1	C	179	LEU
1	D	180	ILE

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	222/226 (98%)	217 (98%)	5 (2%)	44	59
1	B	224/226 (99%)	218 (97%)	6 (3%)	39	53
1	C	225/226 (100%)	221 (98%)	4 (2%)	51	68
1	D	225/226 (100%)	219 (97%)	6 (3%)	39	53
All	All	896/904 (99%)	875 (98%)	21 (2%)	44	59

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

Mol	Chain	Res	Type
1	A	32	LEU
1	A	278	GLU
1	A	293	GLU
1	A	298	ARG
1	A	299	TRP
1	B	32	LEU
1	B	215	LEU
1	B	278	GLU
1	B	294	LYS
1	B	298	ARG
1	B	299	TRP
1	C	32	LEU
1	C	278	GLU
1	C	298	ARG
1	C	299	TRP
1	D	32	LEU
1	D	132	GLU
1	D	278	GLU
1	D	288	ASN
1	D	298	ARG
1	D	299	TRP

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	87	HIS
1	A	292	ASN
1	C	162	GLN
1	C	207	ASN
1	D	124	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
2	NAP	C	301	-	50,52,52	1.61	4 (8%)	71,80,80	1.56	11 (15%)
4	GOL	A	9	-	5,5,5	0.38	0	5,5,5	0.19	0
4	GOL	D	2	-	5,5,5	0.47	0	5,5,5	0.26	0
4	GOL	D	5	-	5,5,5	0.36	0	5,5,5	0.48	0
3	SO4	A	1	-	4,4,4	0.24	0	6,6,6	0.24	0
4	GOL	D	1	-	5,5,5	0.30	0	5,5,5	0.56	0
3	SO4	D	4	-	4,4,4	0.22	0	6,6,6	0.15	0
2	NAP	D	301	-	50,52,52	1.60	3 (6%)	71,80,80	1.53	9 (12%)
4	GOL	D	8	-	5,5,5	0.41	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	3	-	4,4,4	0.21	0	6,6,6	0.11	0
4	GOL	D	7	-	5,5,5	0.36	0	5,5,5	0.27	0
4	GOL	B	6	-	5,5,5	0.38	0	5,5,5	0.23	0
2	NAP	A	301	-	50,52,52	1.59	4 (8%)	71,80,80	1.54	9 (12%)
4	GOL	B	4	-	5,5,5	0.40	0	5,5,5	0.33	0
3	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.14	0
2	NAP	B	301	-	50,52,52	1.63	5 (10%)	71,80,80	1.48	9 (12%)
3	SO4	C	5	-	4,4,4	0.23	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	301	-	-	8/35/67/67	0/5/5/5
4	GOL	A	9	-	-	2/4/4/4	-
4	GOL	D	2	-	-	3/4/4/4	-
4	GOL	D	5	-	-	4/4/4/4	-
4	GOL	D	1	-	-	2/4/4/4	-
2	NAP	D	301	-	-	8/35/67/67	0/5/5/5
4	GOL	D	8	-	-	4/4/4/4	-
4	GOL	D	7	-	-	2/4/4/4	-
2	NAP	A	301	-	-	8/35/67/67	0/5/5/5
4	GOL	B	4	-	-	3/4/4/4	-
4	GOL	B	6	-	-	2/4/4/4	-
2	NAP	B	301	-	-	8/35/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	O7N-C7N	9.22	1.41	1.24
2	A	301	NAP	O7N-C7N	8.94	1.40	1.24
2	C	301	NAP	O7N-C7N	8.92	1.40	1.24
2	D	301	NAP	O7N-C7N	8.86	1.40	1.24
2	C	301	NAP	C2A-N1A	2.71	1.38	1.33
2	D	301	NAP	C2A-N3A	2.64	1.38	1.33
2	D	301	NAP	C2A-N1A	2.63	1.38	1.33
2	C	301	NAP	C2A-N3A	2.63	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C2A-N3A	2.60	1.38	1.33
2	A	301	NAP	C2A-N1A	2.50	1.38	1.33
2	A	301	NAP	C8A-N7A	2.50	1.36	1.31
2	B	301	NAP	C2A-N1A	2.47	1.38	1.33
2	C	301	NAP	C8A-N7A	2.41	1.36	1.31
2	B	301	NAP	C2A-N3A	2.24	1.37	1.33
2	B	301	NAP	C8A-N7A	2.22	1.35	1.31
2	B	301	NAP	C2N-N1N	2.00	1.37	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	N3A-C2A-N1A	-5.70	119.95	128.58
2	A	301	NAP	N3A-C2A-N1A	-5.70	119.96	128.58
2	D	301	NAP	N3A-C2A-N1A	-5.44	120.34	128.58
2	B	301	NAP	N3A-C2A-N1A	-5.19	120.72	128.58
2	A	301	NAP	C5A-C4A-N3A	-4.46	120.58	126.72
2	D	301	NAP	C5A-C4A-N3A	-4.35	120.72	126.72
2	C	301	NAP	C5A-C4A-N3A	-4.35	120.73	126.72
2	D	301	NAP	N9A-C8A-N7A	-4.01	108.25	113.94
2	B	301	NAP	C5A-C4A-N3A	-4.00	121.20	126.72
2	B	301	NAP	O4B-C1B-N9A	3.89	115.57	108.09
2	C	301	NAP	O4B-C1B-N9A	3.88	115.54	108.09
2	B	301	NAP	N9A-C8A-N7A	-3.86	108.47	113.94
2	A	301	NAP	O4B-C1B-N9A	3.82	115.43	108.09
2	A	301	NAP	N9A-C8A-N7A	-3.81	108.53	113.94
2	D	301	NAP	O4B-C1B-N9A	3.76	115.32	108.09
2	C	301	NAP	N9A-C8A-N7A	-3.74	108.63	113.94
2	A	301	NAP	C2A-N3A-C4A	3.59	120.59	111.83
2	D	301	NAP	C5A-N7A-C8A	3.58	109.08	103.45
2	C	301	NAP	C2A-N3A-C4A	3.46	120.28	111.83
2	D	301	NAP	C2A-N3A-C4A	3.38	120.08	111.83
2	B	301	NAP	C5A-N7A-C8A	3.35	108.71	103.45
2	A	301	NAP	C5A-N7A-C8A	3.22	108.52	103.45
2	B	301	NAP	C2A-N3A-C4A	3.15	119.53	111.83
2	C	301	NAP	C5A-N7A-C8A	3.13	108.36	103.45
2	C	301	NAP	N3A-C4A-N9A	2.73	131.81	127.17
2	A	301	NAP	N3A-C4A-N9A	2.73	131.80	127.17
2	C	301	NAP	C2B-C1B-N9A	-2.72	109.27	113.75
2	D	301	NAP	C4A-C5A-N7A	-2.69	107.50	110.58
2	D	301	NAP	N3A-C4A-N9A	2.68	131.73	127.17
2	A	301	NAP	C2B-C1B-N9A	-2.63	109.42	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	C2B-C1B-N9A	-2.60	109.47	113.75
2	B	301	NAP	C4A-C5A-N7A	-2.51	107.71	110.58
2	B	301	NAP	C2B-C1B-N9A	-2.50	109.64	113.75
2	B	301	NAP	N3A-C4A-N9A	2.49	131.40	127.17
2	A	301	NAP	C4A-C5A-N7A	-2.41	107.83	110.58
2	C	301	NAP	C4A-C5A-N7A	-2.37	107.87	110.58
2	C	301	NAP	C3N-C7N-N7N	2.03	120.24	117.74
2	C	301	NAP	C2N-C3N-C4N	2.01	120.59	118.26

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4	GOL	O1-C1-C2-C3
4	B	6	GOL	O1-C1-C2-C3
4	D	2	GOL	O1-C1-C2-C3
4	D	5	GOL	C1-C2-C3-O3
4	D	7	GOL	O1-C1-C2-C3
4	D	8	GOL	O1-C1-C2-C3
2	A	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C3B-C4B-C5B-O5B
4	D	2	GOL	O1-C1-C2-O2
4	D	7	GOL	O1-C1-C2-O2
2	A	301	NAP	C3B-C4B-C5B-O5B
2	B	301	NAP	C3B-C4B-C5B-O5B
2	C	301	NAP	C3B-C4B-C5B-O5B
4	A	9	GOL	O1-C1-C2-C3
4	D	1	GOL	C1-C2-C3-O3
4	D	5	GOL	O1-C1-C2-C3
4	D	8	GOL	C1-C2-C3-O3
4	B	4	GOL	O1-C1-C2-O2
4	D	1	GOL	O2-C2-C3-O3
4	D	5	GOL	O2-C2-C3-O3
4	D	8	GOL	O1-C1-C2-O2
4	A	9	GOL	O1-C1-C2-O2
4	B	6	GOL	O1-C1-C2-O2
2	A	301	NAP	C5B-O5B-PA-O1A
2	A	301	NAP	C5B-O5B-PA-O2A
2	A	301	NAP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	B	301	NAP	C5B-O5B-PA-O1A
2	B	301	NAP	C5B-O5B-PA-O2A
2	B	301	NAP	C5B-O5B-PA-O3
2	C	301	NAP	C5B-O5B-PA-O1A
2	C	301	NAP	C5B-O5B-PA-O2A
2	C	301	NAP	C5B-O5B-PA-O3
2	D	301	NAP	C5B-O5B-PA-O1A
2	D	301	NAP	C5B-O5B-PA-O2A
2	D	301	NAP	C5B-O5B-PA-O3
4	B	4	GOL	C1-C2-C3-O3
4	D	2	GOL	C1-C2-C3-O3
4	D	5	GOL	O1-C1-C2-O2
4	D	8	GOL	O2-C2-C3-O3
2	A	301	NAP	PN-O3-PA-O2A
2	B	301	NAP	PN-O3-PA-O2A
2	C	301	NAP	PN-O3-PA-O2A
2	A	301	NAP	PN-O3-PA-O1A
2	B	301	NAP	PN-O3-PA-O1A
2	C	301	NAP	PN-O3-PA-O1A
2	D	301	NAP	PN-O3-PA-O1A
2	D	301	NAP	PN-O3-PA-O2A
2	A	301	NAP	C2B-O2B-P2B-O1X
2	B	301	NAP	C2B-O2B-P2B-O1X
2	C	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C2B-O2B-P2B-O1X

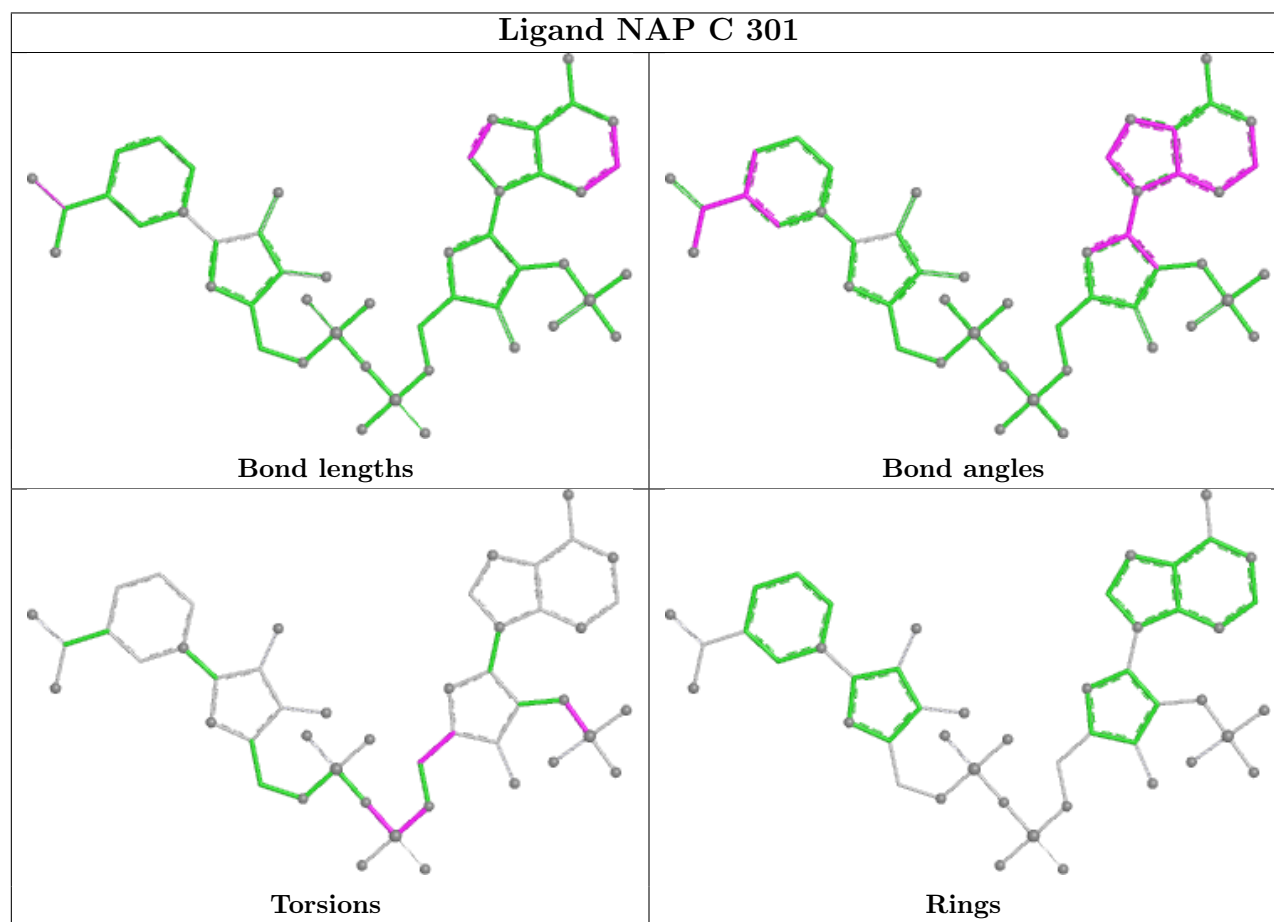
There are no ring outliers.

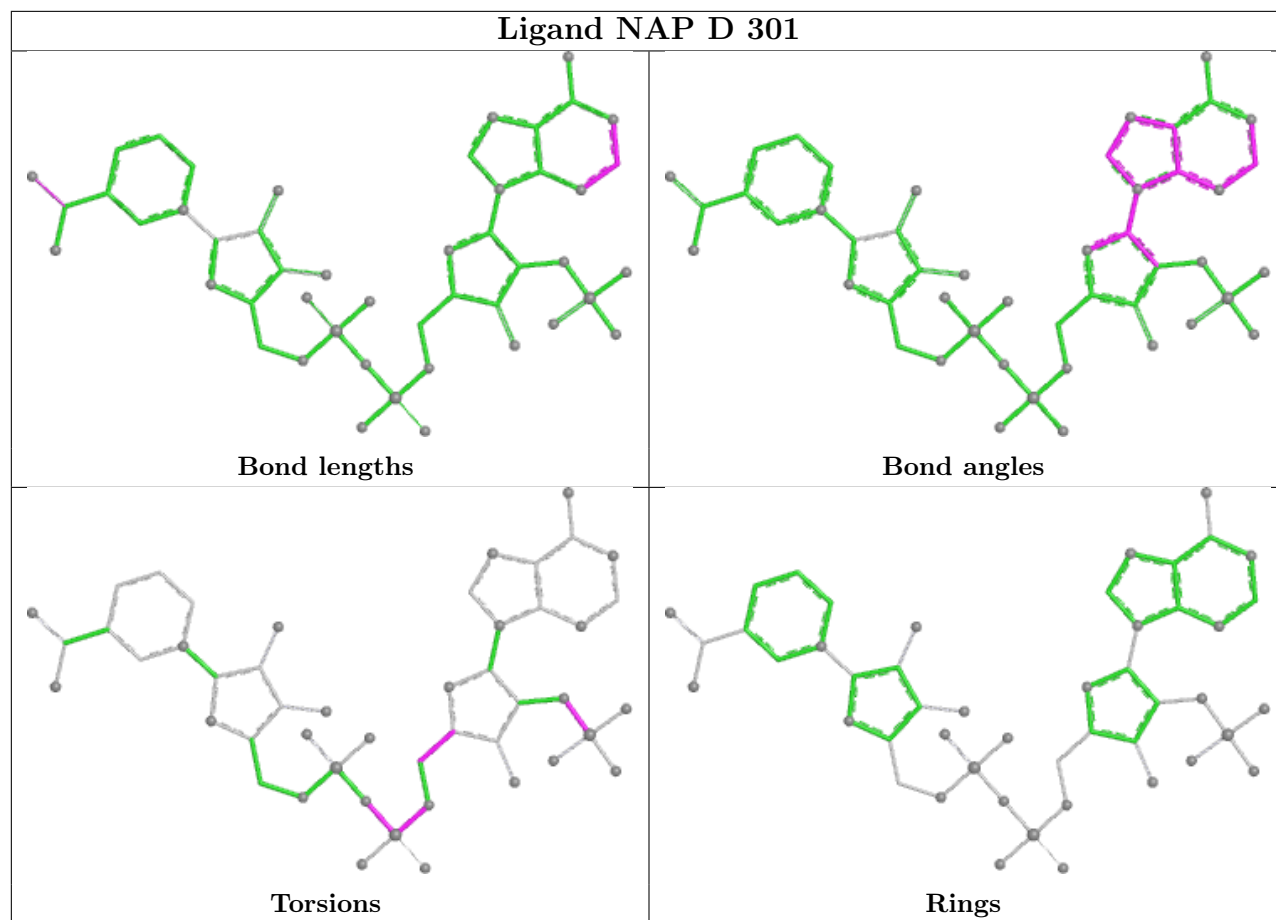
5 monomers are involved in 9 short contacts:

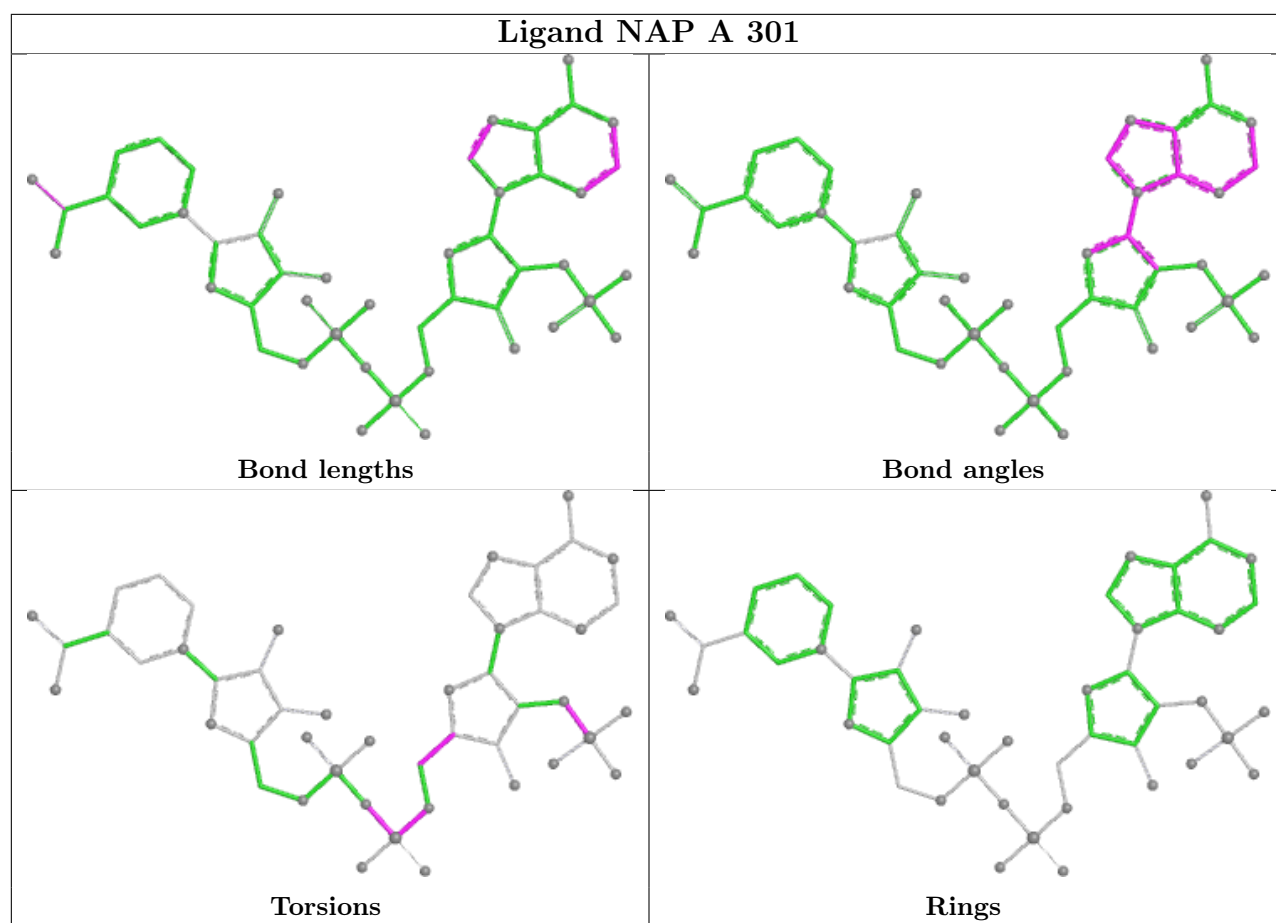
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	GOL	3	0
4	D	1	GOL	1	0
2	D	301	NAP	1	0
4	D	8	GOL	2	0
4	D	7	GOL	2	0

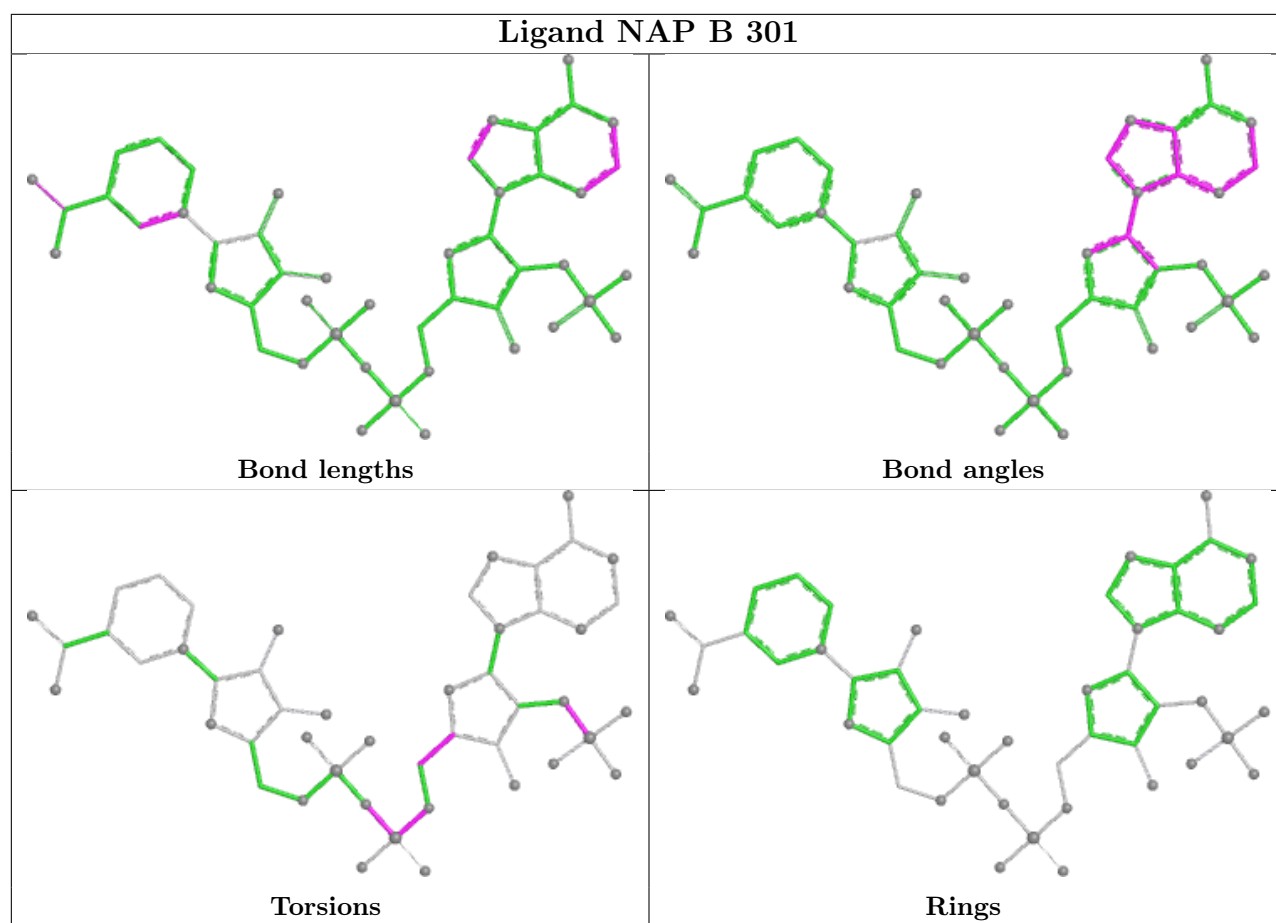
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	285:ASN	C	286:TRP	N	1.18
1	B	287:ASP	C	288:ASN	N	1.03
1	D	178:PRO	C	179:LEU	N	0.86

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	24:ASN	C	25:GLU	N	0.66

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	271/276 (98%)	0.04	6 (2%) 62 59	20, 37, 81, 153	0
1	B	275/276 (99%)	0.07	14 (5%) 33 30	20, 38, 83, 152	0
1	C	274/276 (99%)	0.06	5 (1%) 67 64	21, 41, 85, 153	0
1	D	275/276 (99%)	-0.04	3 (1%) 78 76	20, 37, 75, 151	0
All	All	1095/1104 (99%)	0.03	28 (2%) 57 54	20, 38, 82, 153	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	LEU	4.1
1	B	282	ALA	3.6
1	B	280	SER	3.5
1	A	177	TYR	3.2
1	B	266	TYR	3.1
1	C	292	ASN	3.0
1	B	284	TYR	2.8
1	B	289	VAL	2.8
1	D	298	ARG	2.7
1	C	294	LYS	2.7
1	B	295	LEU	2.6
1	B	281	ALA	2.5
1	B	292	ASN	2.5
1	D	299	TRP	2.5
1	B	283	GLU	2.5
1	B	299	TRP	2.5
1	C	124	ASN	2.5
1	B	286	TRP	2.4
1	B	123	TYR	2.4
1	B	279	LEU	2.4
1	A	298	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	298	ARG	2.4
1	A	202	LEU	2.4
1	A	293	GLU	2.3
1	B	297	GLY	2.2
1	A	124	ASN	2.1
1	A	284	TYR	2.1
1	D	281	ALA	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.

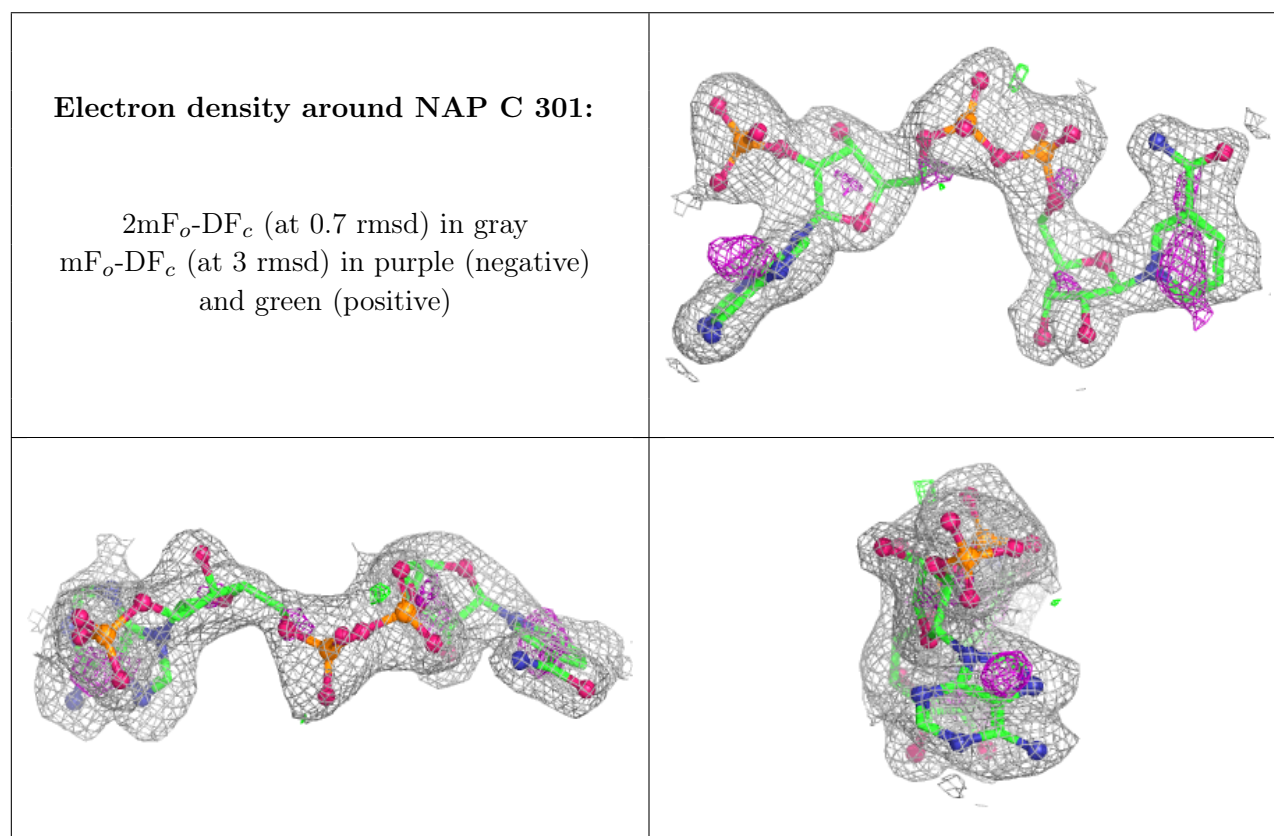
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	4	6/6	0.80	0.12	51,58,66,75	0
4	GOL	B	6	6/6	0.80	0.14	41,58,70,72	0
4	GOL	D	7	6/6	0.83	0.10	60,62,70,70	0
4	GOL	D	1	6/6	0.88	0.20	22,38,50,59	0
3	SO4	C	5	5/5	0.89	0.08	55,57,84,96	0
4	GOL	A	9	6/6	0.90	0.10	39,64,69,85	0
4	GOL	D	8	6/6	0.90	0.11	38,44,60,62	0
4	GOL	D	2	6/6	0.91	0.08	41,48,60,65	0
2	NAP	C	301	48/48	0.92	0.08	27,39,50,52	0
2	NAP	A	301	48/48	0.94	0.08	22,36,45,55	0
4	GOL	D	5	6/6	0.95	0.08	25,41,48,50	0
3	SO4	A	1	5/5	0.96	0.09	35,38,49,64	0
2	NAP	B	301	48/48	0.97	0.07	17,31,39,41	0
3	SO4	C	3	5/5	0.97	0.07	43,43,49,51	0
2	NAP	D	301	48/48	0.97	0.06	17,31,39,40	0
3	SO4	D	4	5/5	0.97	0.09	32,40,44,69	0

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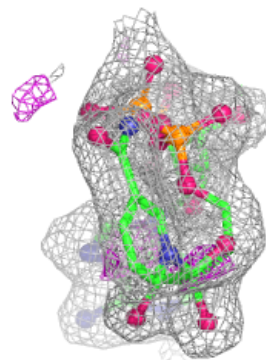
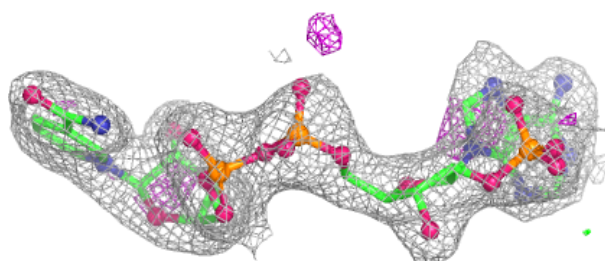
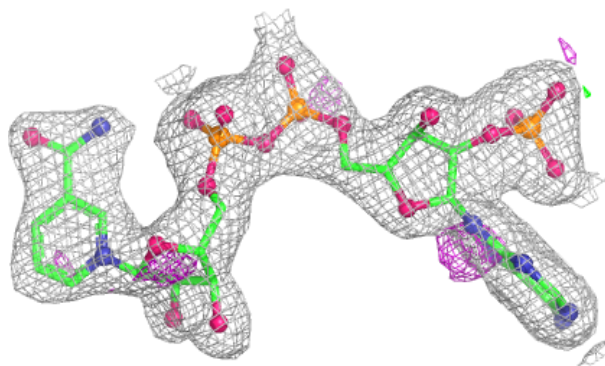
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	2	5/5	0.98	0.07	34,38,49,54	0

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.

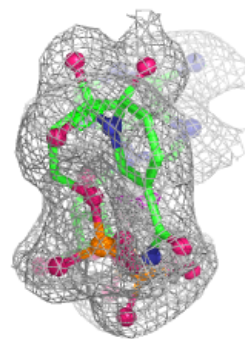
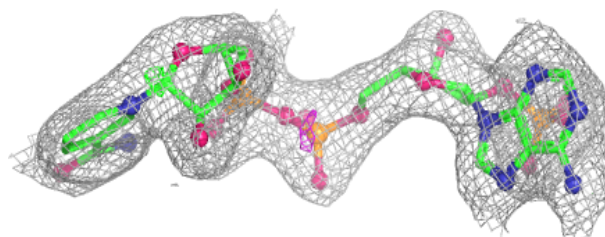
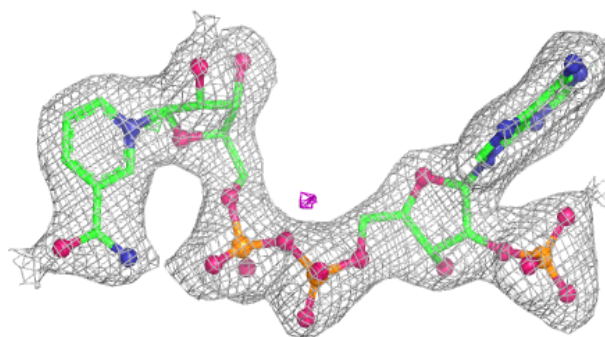


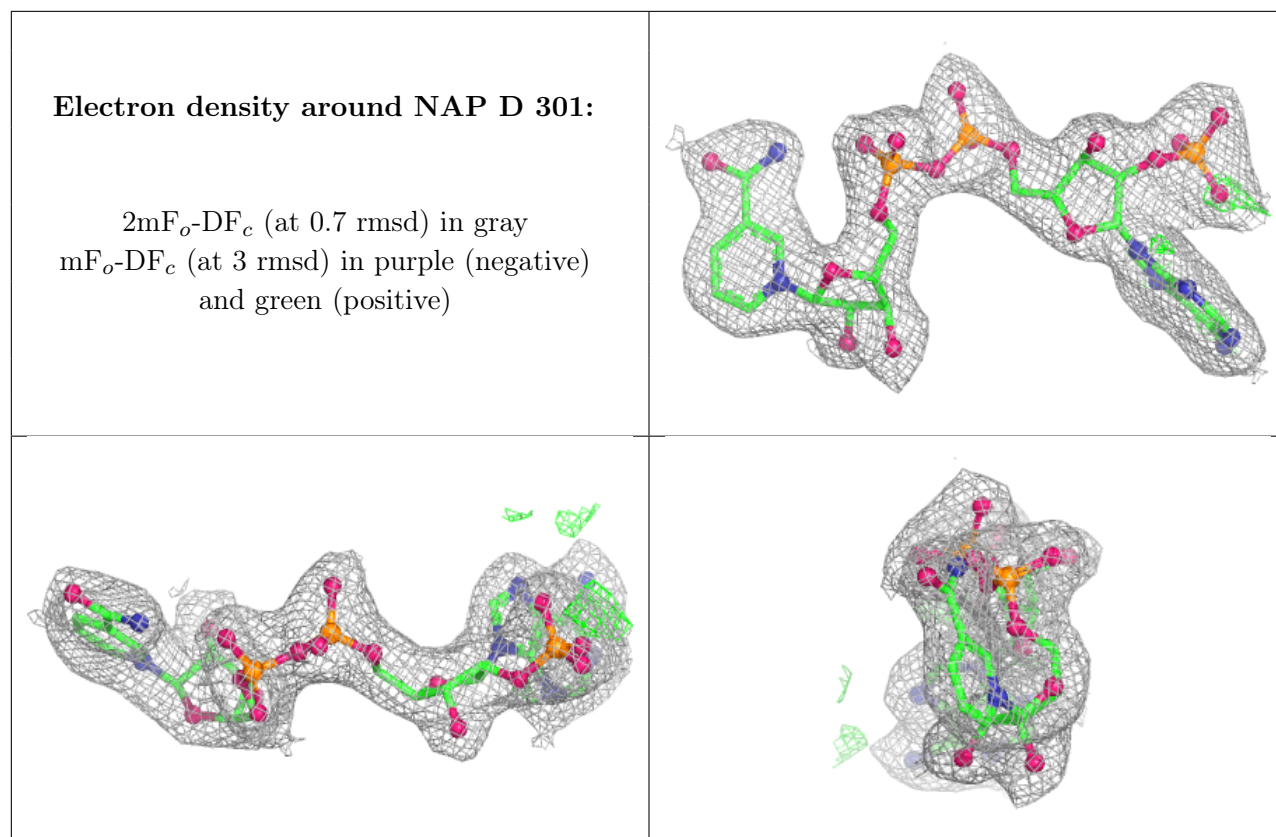
Electron density around NAP A 301:

$2mF_o-DF_c$ (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.