



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 PM UTC

PDB ID : 2H63 / pdb_00002h63
Title : Crystal Structure of Human Biliverdin Reductase A
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Weigelt, J.; Edwards, A.; von Delft, F.; Oppermann, U.; Structural Genomics
Consortium (SGC)
Deposited on : 2006-05-30
Resolution : 2.70 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](#) ①) were used in the production of this report:

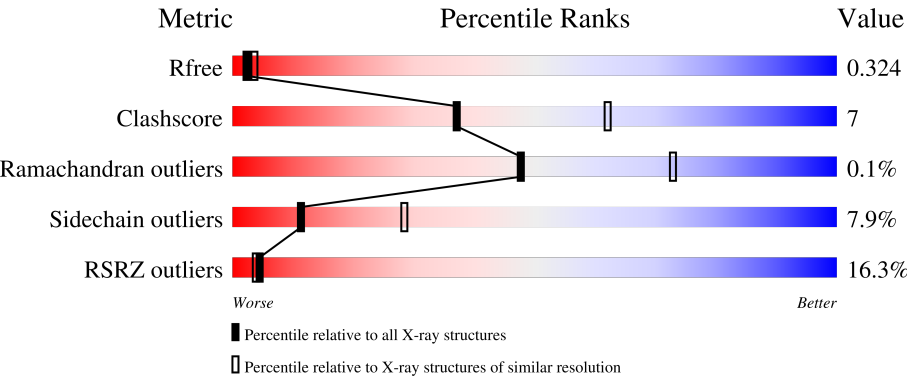
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	292	
1	B	292	
1	C	292	
1	D	292	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8668 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.

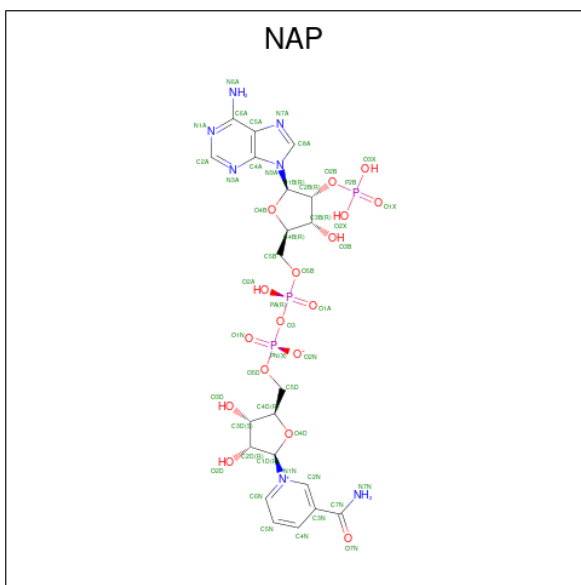
- Molecule 1 is a protein called Biliverdin reductase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2140	1379	364	388	9			
1	B	279	Total	C	N	O	S	0	0	0
			2087	1342	359	378	8			
1	C	283	Total	C	N	O	S	0	0	0
			2097	1351	360	378	8			
1	D	285	Total	C	N	O	S	0	0	0
			2129	1375	360	385	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	-	cloning artifact	UNP P53004
A	6	MET	-	cloning artifact	UNP P53004
B	5	SER	-	cloning artifact	UNP P53004
B	6	MET	-	cloning artifact	UNP P53004
C	5	SER	-	cloning artifact	UNP P53004
C	6	MET	-	cloning artifact	UNP P53004
D	5	SER	-	cloning artifact	UNP P53004
D	6	MET	-	cloning artifact	UNP P53004

- 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

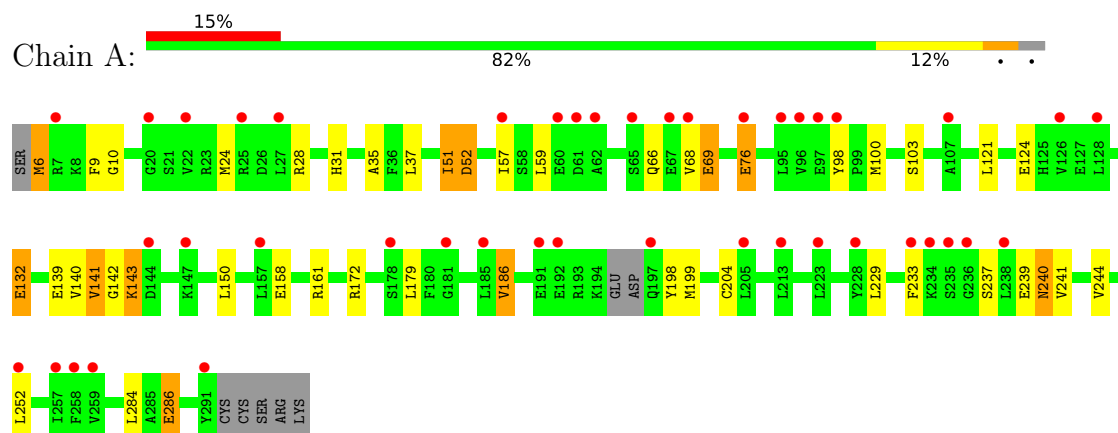
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	4	Total O 4 4	0	0
3	C	5	Total O 5 5	0	0
3	D	6	Total O 6 6	0	0

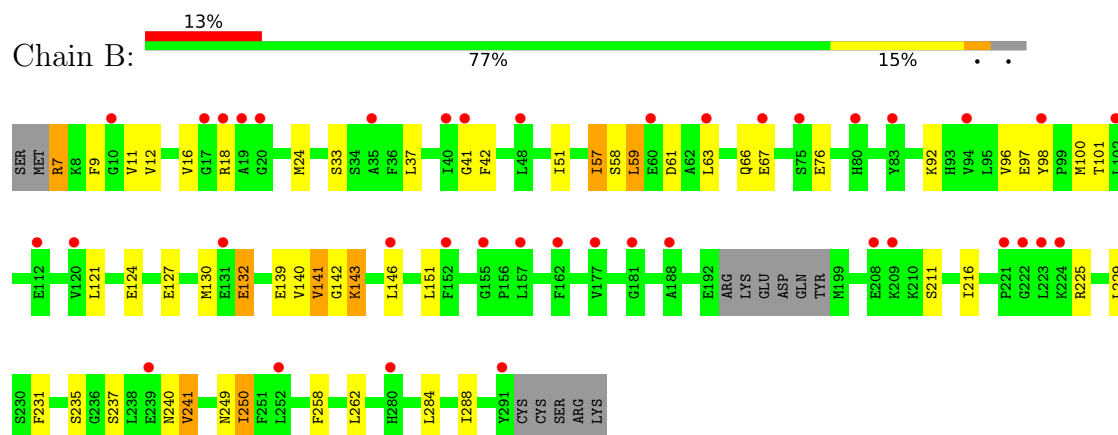
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

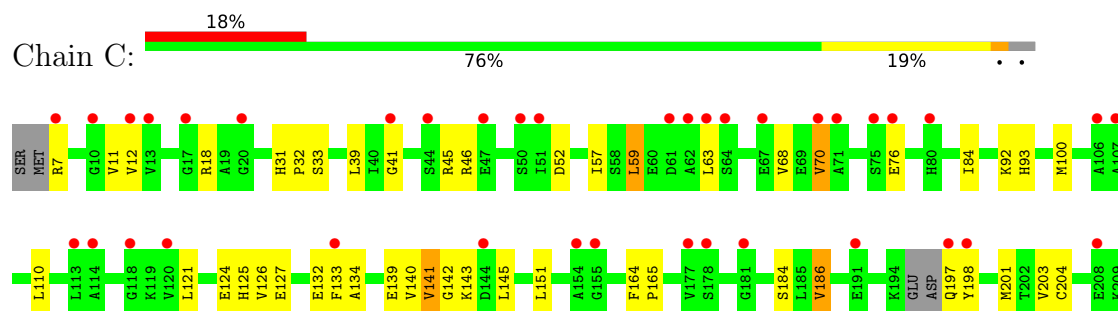
• Molecule 1: Biliverdin reductase A

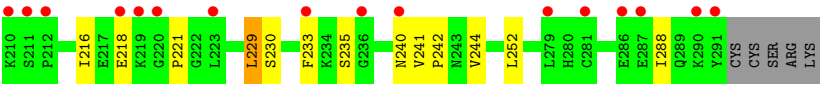


• Molecule 1: Biliverdin reductase A

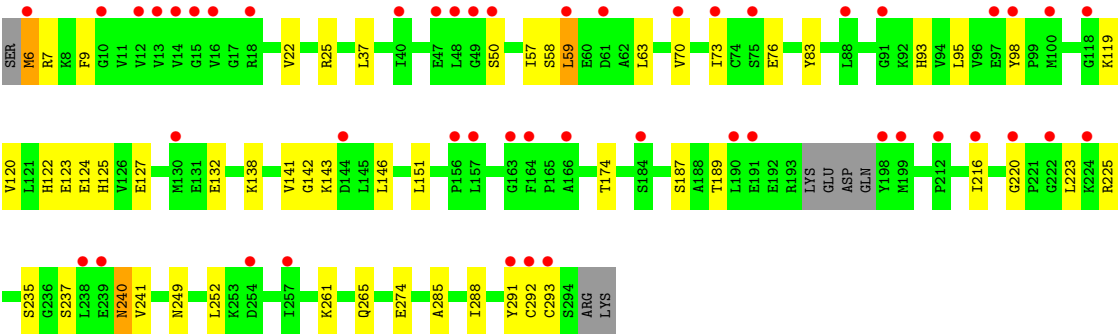
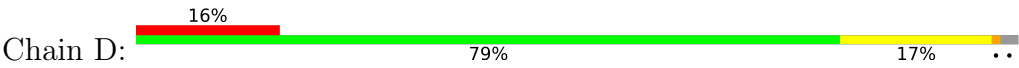


• Molecule 1: Biliverdin reductase A





● Molecule 1: Biliverdin reductase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.79Å 92.75Å 147.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-2.70) 96.4 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.237 , 0.287 0.281 , 0.324	Depositor DCC
R_{free} test set	1399 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8668	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.83% 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: 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	0.89	0/2179	0.92	3/2944 (0.1%)
1	B	0.87	0/2125	0.93	1/2873 (0.0%)
1	C	0.83	0/2137	0.93	2/2895 (0.1%)
1	D	0.89	0/2169	0.96	2/2933 (0.1%)
All	All	0.87	0/8610	0.94	8/11645 (0.1%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	LYS	N-CA-C	6.65	120.36	109.85
1	B	143	LYS	N-CA-C	6.15	119.56	109.85
1	A	143	LYS	N-CA-C	5.86	119.11	109.85
1	D	120	VAL	CB-CA-C	-5.84	103.67	110.91
1	C	143	LYS	N-CA-C	5.65	118.77	109.85
1	C	33	SER	CB-CA-C	-5.25	102.13	110.84
1	A	6	MET	CA-C-N	5.08	131.25	121.54
1	A	6	MET	C-N-CA	5.08	131.25	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	ASN	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	2140	0	2092	25	0
1	B	2087	0	2030	30	0
1	C	2097	0	2014	42	0
1	D	2129	0	2066	25	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	1	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
3	C	5	0	0	0	0
3	D	6	0	0	0	0
All	All	8668	0	8302	120	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 7.

All (120) 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:7:ARG:N	1:B:7:ARG:HD2	1.50	1.16
1:B:7:ARG:N	1:B:7:ARG:CD	2.19	1.06
1:C:242:PRO:O	1:C:244:VAL:HG23	1.80	0.80
1:C:229:LEU:C	1:C:229:LEU:HD23	2.07	0.79
1:D:132:GLU:HG3	1:D:241:VAL:HG11	1.67	0.77
1:C:229:LEU:HD23	1:C:230:SER:N	2.02	0.75
1:A:132:GLU:HG3	1:A:241:VAL:HG11	1.70	0.73
1:C:203:VAL:HG21	1:C:288:ILE:HD13	1.71	0.72
1:B:98:TYR:CE2	2:B:501:NAP:H5N	2.25	0.71
1:B:132:GLU:HG3	1:B:241:VAL:HG11	1.73	0.70
1:B:258:PHE:CE2	1:B:262:LEU:HD11	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:HG13	1:A:204:CYS:HB3	1.76	0.65
1:B:141:VAL:CG1	1:B:142:GLY:N	2.60	0.65
1:C:59:LEU:HD22	1:C:63:LEU:HD11	1.78	0.64
1:D:141:VAL:HG13	1:D:142:GLY:N	2.13	0.64
1:D:70:VAL:HG22	1:D:93:HIS:HB2	1.80	0.62
1:C:244:VAL:HG12	1:C:244:VAL:O	1.99	0.61
1:B:42:PHE:CE1	1:B:51:ILE:HD12	2.35	0.61
1:B:24:MET:HE1	1:B:51:ILE:HD13	1.84	0.60
1:D:123:GLU:OE1	1:D:125:HIS:NE2	2.35	0.60
1:C:132:GLU:HG3	1:C:241:VAL:HG11	1.83	0.60
1:C:229:LEU:C	1:C:229:LEU:CD2	2.76	0.59
1:D:291:TYR:O	1:D:293:CYS:N	2.37	0.57
1:D:285:ALA:HA	1:D:288:ILE:HD12	1.87	0.57
1:C:59:LEU:HD22	1:C:63:LEU:CD1	2.33	0.57
1:C:141:VAL:CG1	1:C:142:GLY:N	2.68	0.57
1:A:98:TYR:CE2	2:A:501:NAP:H5N	2.40	0.56
1:A:229:LEU:HD23	1:A:229:LEU:C	2.30	0.56
1:A:24:MET:CE	1:A:51:ILE:HG21	2.36	0.56
1:C:201:MET:HE3	1:C:203:VAL:CG2	2.36	0.56
1:C:18:ARG:HD3	2:C:501:NAP:O2A	2.06	0.55
1:D:138:LYS:O	1:D:141:VAL:HG12	2.05	0.55
1:B:141:VAL:HG21	1:D:265:GLN:CG	2.35	0.55
1:A:150:LEU:HD21	1:A:172:ARG:HG3	1.89	0.55
1:C:145:LEU:HD12	1:C:233:PHE:CE1	2.42	0.55
1:C:84:ILE:CG2	1:C:110:LEU:HD13	2.37	0.55
1:C:100:MET:HE1	1:C:121:LEU:HD21	1.89	0.55
1:C:164:PHE:CD1	1:C:165:PRO:HD2	2.42	0.55
1:A:24:MET:HE3	1:A:51:ILE:HG21	1.89	0.54
1:C:141:VAL:HG13	1:C:142:GLY:N	2.22	0.54
1:C:84:ILE:HG21	1:C:110:LEU:HD13	1.90	0.54
1:C:12:VAL:HG23	1:C:41:GLY:O	2.08	0.54
1:D:151:LEU:HD13	1:D:216:ILE:HB	1.90	0.54
1:C:201:MET:HE3	1:C:203:VAL:HG23	1.90	0.53
1:D:6:MET:HE2	1:D:7:ARG:N	2.24	0.52
1:A:100:MET:HE1	1:A:121:LEU:HD21	1.92	0.52
1:A:6:MET:HE2	1:A:35:ALA:O	2.08	0.52
1:B:100:MET:HG3	1:B:101:THR:HG23	1.92	0.52
1:D:291:TYR:C	1:D:293:CYS:H	2.17	0.52
1:C:198:TYR:OH	1:C:218:GLU:OE2	2.26	0.51
1:C:59:LEU:CD2	1:C:63:LEU:HD11	2.41	0.51
1:C:46:ARG:NE	2:C:501:NAP:O1X	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:VAL:O	1:C:39:LEU:HD12	2.13	0.49
1:A:51:ILE:HG22	1:A:52:ASP:N	2.26	0.49
1:B:12:VAL:HG23	1:B:41:GLY:O	2.12	0.49
1:B:229:LEU:HD21	1:B:231:PHE:CE2	2.48	0.49
1:B:57:ILE:HD12	1:B:58:SER:H	1.78	0.49
1:C:70:VAL:HG22	1:C:93:HIS:HB2	1.94	0.49
1:C:7:ARG:N	1:C:7:ARG:CD	2.76	0.49
1:B:59:LEU:HD22	1:B:63:LEU:CD1	2.43	0.48
1:A:244:VAL:HG22	1:C:32:PRO:N	2.28	0.48
1:A:9:PHE:HB2	1:A:37:LEU:HD23	1.96	0.48
1:D:220:GLY:N	1:D:223:LEU:HD12	2.30	0.47
1:A:198:TYR:CD2	1:A:199:MET:N	2.83	0.47
1:C:197:GLN:O	1:C:221:PRO:HD3	2.15	0.47
1:B:151:LEU:HD13	1:B:216:ILE:HB	1.96	0.47
1:B:229:LEU:C	1:B:229:LEU:HD23	2.39	0.47
1:C:31:HIS:CG	1:C:252:LEU:HD21	2.51	0.46
1:D:249:ASN:HB3	1:D:252:LEU:HB3	1.97	0.46
1:B:141:VAL:HG12	1:B:142:GLY:N	2.29	0.46
1:D:141:VAL:CG1	1:D:142:GLY:N	2.79	0.46
1:B:11:VAL:CG2	1:B:37:LEU:HD22	2.46	0.46
1:A:103:SER:HA	1:A:286:GLU:OE2	2.16	0.45
1:B:9:PHE:HB2	1:B:37:LEU:HD23	1.97	0.45
1:C:186:VAL:HG13	1:C:204:CYS:HB3	1.99	0.45
1:B:141:VAL:HG13	1:B:142:GLY:N	2.32	0.45
1:C:68:VAL:O	1:C:92:LYS:NZ	2.40	0.45
1:A:240:ASN:N	1:A:240:ASN:HD22	2.14	0.44
1:C:151:LEU:HD13	1:C:216:ILE:CG2	2.47	0.44
1:D:98:TYR:CE2	2:D:501:NAP:H5N	2.52	0.44
1:C:45:ARG:NE	2:C:501:NAP:O3X	2.50	0.44
1:A:31:HIS:CG	1:A:252:LEU:HD21	2.53	0.44
1:C:125:HIS:ND1	1:C:127:GLU:OE2	2.51	0.44
1:B:57:ILE:HD12	1:B:58:SER:N	2.33	0.44
1:D:127:GLU:OE2	1:D:174:THR:HG21	2.18	0.44
1:D:261:LYS:NZ	1:D:274:GLU:OE1	2.51	0.43
1:A:143:LYS:HB3	1:A:233:PHE:CD1	2.53	0.43
1:D:22:VAL:HG13	1:D:25:ARG:NH2	2.33	0.43
1:A:140:VAL:HG21	1:A:179:LEU:HD22	1.99	0.43
1:A:186:VAL:HG13	1:A:204:CYS:CB	2.48	0.43
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.75	0.43
1:B:241:VAL:O	1:B:241:VAL:HG12	2.18	0.43
1:D:93:HIS:CE1	1:D:119:LYS:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:HG22	1:B:97:GLU:O	2.19	0.43
1:B:100:MET:CE	1:B:121:LEU:HD21	2.48	0.43
1:C:186:VAL:HG13	1:C:204:CYS:CB	2.49	0.43
1:B:57:ILE:HD11	1:B:61:ASP:CB	2.49	0.42
1:C:203:VAL:CG2	1:C:288:ILE:HD13	2.43	0.42
1:B:18:ARG:HB2	2:B:501:NAP:O1N	2.20	0.42
1:D:240:ASN:ND2	1:D:240:ASN:N	2.67	0.42
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.89	0.42
1:D:73:ILE:HD12	1:D:83:TYR:HB3	2.01	0.42
1:D:122:HIS:ND1	1:D:261:LYS:NZ	2.58	0.42
1:D:291:TYR:C	1:D:293:CYS:N	2.78	0.42
1:A:239:GLU:C	1:A:240:ASN:HD22	2.28	0.42
1:A:10:GLY:H	1:A:69:GLU:HG3	1.84	0.42
1:A:141:VAL:CG1	1:A:142:GLY:N	2.83	0.42
1:C:124:GLU:CD	1:C:126:VAL:HG13	2.45	0.42
1:D:59:LEU:HD22	1:D:63:LEU:HD11	2.02	0.41
1:B:127:GLU:HA	1:B:130:MET:HE3	2.02	0.41
1:C:203:VAL:HG12	1:C:204:CYS:N	2.35	0.41
1:C:127:GLU:OE1	1:C:127:GLU:N	2.47	0.41
1:B:249:ASN:O	1:B:250:ILE:C	2.62	0.41
1:B:16:VAL:O	1:B:16:VAL:HG12	2.21	0.41
1:C:133:PHE:O	1:C:134:ALA:C	2.63	0.41
1:C:201:MET:HE3	1:C:203:VAL:HG21	2.03	0.41
1:D:9:PHE:HB2	1:D:37:LEU:HD23	2.03	0.41
1:B:284:LEU:O	1:B:288:ILE:HG13	2.21	0.40
1:A:76:GLU:HG2	1:A:161:ARG:CZ	2.51	0.40
1:C:125:HIS:C	1:C:127:GLU:OE1	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/292 (96%)	264 (94%)	16 (6%)	0	100	100
1	B	275/292 (94%)	264 (96%)	11 (4%)	0	100	100
1	C	279/292 (96%)	268 (96%)	11 (4%)	0	100	100
1	D	281/292 (96%)	268 (95%)	12 (4%)	1 (0%)	30	54
All	All	1115/1168 (96%)	1064 (95%)	50 (4%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	292	CYS

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	216/255 (85%)	198 (92%)	18 (8%)	10	26
1	B	209/255 (82%)	188 (90%)	21 (10%)	7	19
1	C	206/255 (81%)	193 (94%)	13 (6%)	16	39
1	D	212/255 (83%)	197 (93%)	15 (7%)	13	33
All	All	843/1020 (83%)	776 (92%)	67 (8%)	11	28

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	51	ILE
1	A	52	ASP
1	A	57	ILE
1	A	59	LEU
1	A	66	GLN
1	A	68	VAL
1	A	69	GLU
1	A	76	GLU
1	A	124	GLU

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Mol	Chain	Res	Type
1	A	132	GLU
1	A	139	GLU
1	A	141	VAL
1	A	158	GLU
1	A	186	VAL
1	A	237	SER
1	A	240	ASN
1	A	286	GLU
1	B	7	ARG
1	B	33	SER
1	B	57	ILE
1	B	59	LEU
1	B	66	GLN
1	B	67	GLU
1	B	76	GLU
1	B	92	LYS
1	B	124	GLU
1	B	132	GLU
1	B	139	GLU
1	B	140	VAL
1	B	141	VAL
1	B	143	LYS
1	B	146	LEU
1	B	211	SER
1	B	225	ARG
1	B	235	SER
1	B	237	SER
1	B	241	VAL
1	B	250	ILE
1	C	52	ASP
1	C	57	ILE
1	C	59	LEU
1	C	70	VAL
1	C	76	GLU
1	C	139	GLU
1	C	140	VAL
1	C	141	VAL
1	C	184	SER
1	C	186	VAL
1	C	229	LEU
1	C	235	SER
1	C	240	ASN

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Mol	Chain	Res	Type
1	D	6	MET
1	D	50	SER
1	D	57	ILE
1	D	58	SER
1	D	59	LEU
1	D	76	GLU
1	D	95	LEU
1	D	124	GLU
1	D	146	LEU
1	D	187	SER
1	D	189	THR
1	D	225	ARG
1	D	235	SER
1	D	237	SER
1	D	240	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	256	ASN
1	A	260	GLN
1	B	31	HIS
1	B	55	GLN
1	B	86	GLN
1	B	243	ASN
1	B	247	ASN
1	C	255	GLN
1	D	240	ASN
1	D	260	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	501	-	50,52,52	1.63	10 (20%)	71,80,80	1.77	14 (19%)
2	NAP	B	501	-	50,52,52	1.68	9 (18%)	71,80,80	1.88	19 (26%)
2	NAP	A	501	-	50,52,52	1.65	9 (18%)	71,80,80	1.89	17 (23%)
2	NAP	D	501	-	50,52,52	1.91	10 (20%)	71,80,80	1.87	14 (19%)

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	501	-	-	3/35/67/67	0/5/5/5
2	NAP	B	501	-	-	5/35/67/67	0/5/5/5
2	NAP	A	501	-	-	3/35/67/67	0/5/5/5
2	NAP	D	501	-	-	8/35/67/67	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAP	C2N-N1N	6.37	1.42	1.35
2	D	501	NAP	PA-O3	5.92	1.65	1.59
2	A	501	NAP	PA-O3	5.50	1.65	1.59
2	D	501	NAP	P2B-O1X	5.39	1.67	1.50
2	C	501	NAP	C2N-N1N	4.71	1.40	1.35
2	B	501	NAP	C2N-N1N	4.62	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAP	P2B-O1X	4.55	1.64	1.50
2	A	501	NAP	PN-O3	4.51	1.64	1.59
2	C	501	NAP	P2B-O1X	4.26	1.63	1.50
2	A	501	NAP	C2N-N1N	4.09	1.39	1.35
2	C	501	NAP	PA-O3	4.04	1.63	1.59
2	B	501	NAP	PN-O3	3.98	1.63	1.59
2	B	501	NAP	C5A-N7A	-3.90	1.32	1.39
2	C	501	NAP	C3N-C7N	3.67	1.56	1.50
2	D	501	NAP	C5A-N7A	-3.40	1.32	1.39
2	A	501	NAP	P2B-O1X	3.36	1.60	1.50
2	A	501	NAP	C5A-N7A	-3.22	1.33	1.39
2	C	501	NAP	C5A-N7A	-3.10	1.33	1.39
2	B	501	NAP	O4D-C1D	3.09	1.44	1.40
2	B	501	NAP	PA-O3	3.06	1.62	1.59
2	D	501	NAP	C3N-C7N	2.96	1.55	1.50
2	C	501	NAP	PN-O3	2.64	1.62	1.59
2	D	501	NAP	C6N-N1N	2.63	1.41	1.35
2	D	501	NAP	P2B-O2X	2.49	1.64	1.54
2	B	501	NAP	C4A-N9A	-2.47	1.32	1.37
2	D	501	NAP	C4A-N9A	-2.42	1.32	1.37
2	A	501	NAP	C4A-N9A	-2.37	1.32	1.37
2	B	501	NAP	P2B-O3X	-2.34	1.46	1.54
2	C	501	NAP	C6N-N1N	2.30	1.40	1.35
2	A	501	NAP	C6N-N1N	2.29	1.40	1.35
2	C	501	NAP	C5B-C4B	2.25	1.58	1.51
2	A	501	NAP	P2B-O2X	2.21	1.63	1.54
2	B	501	NAP	C6N-N1N	2.19	1.40	1.35
2	C	501	NAP	O4D-C1D	2.12	1.43	1.40
2	C	501	NAP	O5D-C5D	-2.12	1.36	1.44
2	D	501	NAP	C8A-N9A	-2.07	1.34	1.37
2	D	501	NAP	O4B-C4B	-2.05	1.40	1.45
2	A	501	NAP	PA-O2A	-2.04	1.45	1.55

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAP	O4B-C1B-N9A	-6.48	95.65	108.09
2	B	501	NAP	C5A-C4A-N3A	-6.15	118.24	126.72
2	D	501	NAP	O4B-C1B-N9A	-5.95	96.65	108.09
2	D	501	NAP	C5A-C4A-N3A	-5.58	119.04	126.72
2	C	501	NAP	C5A-C4A-N3A	-5.52	119.12	126.72
2	C	501	NAP	C4D-O4D-C1D	-5.25	105.12	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAP	C4D-O4D-C1D	-5.21	105.16	109.92
2	A	501	NAP	C5A-C4A-N3A	-4.77	120.15	126.72
2	D	501	NAP	N3A-C2A-N1A	-4.52	121.73	128.58
2	C	501	NAP	N3A-C2A-N1A	-4.24	122.16	128.58
2	B	501	NAP	N3A-C4A-N9A	4.13	134.19	127.17
2	B	501	NAP	C2N-C3N-C4N	3.98	122.89	118.26
2	A	501	NAP	P2B-O2B-C2B	-3.96	112.86	123.43
2	A	501	NAP	C2B-C1B-N9A	3.84	120.08	113.75
2	D	501	NAP	N3A-C4A-N9A	3.78	133.60	127.17
2	C	501	NAP	N3A-C4A-N9A	3.72	133.49	127.17
2	D	501	NAP	C2A-N3A-C4A	3.71	120.89	111.83
2	A	501	NAP	O2B-P2B-O1X	-3.61	96.46	109.33
2	D	501	NAP	O3-PA-O1A	-3.61	99.84	110.70
2	C	501	NAP	C2A-N3A-C4A	3.59	120.59	111.83
2	B	501	NAP	N3A-C2A-N1A	-3.56	123.19	128.58
2	A	501	NAP	N3A-C4A-N9A	3.56	133.22	127.17
2	A	501	NAP	C2N-C3N-C4N	3.49	122.31	118.26
2	B	501	NAP	C2A-N3A-C4A	3.35	120.02	111.83
2	A	501	NAP	O3X-P2B-O2B	3.35	118.89	105.85
2	A	501	NAP	C4D-O4D-C1D	-3.34	106.87	109.92
2	A	501	NAP	N3A-C2A-N1A	-3.25	123.66	128.58
2	C	501	NAP	O2A-PA-O3	3.15	115.79	107.27
2	D	501	NAP	N9A-C8A-N7A	-3.08	109.56	113.94
2	C	501	NAP	C5N-C4N-C3N	2.98	123.29	120.36
2	C	501	NAP	N9A-C8A-N7A	-2.83	109.92	113.94
2	D	501	NAP	C4D-O4D-C1D	-2.81	107.35	109.92
2	A	501	NAP	N9A-C8A-N7A	-2.65	110.18	113.94
2	B	501	NAP	O3X-P2B-O1X	2.63	121.09	110.83
2	A	501	NAP	C2A-N3A-C4A	2.63	118.25	111.83
2	D	501	NAP	C5A-N7A-C8A	2.63	107.58	103.45
2	B	501	NAP	O3-PN-O1N	-2.61	102.84	110.70
2	B	501	NAP	N9A-C8A-N7A	-2.59	110.25	113.94
2	D	501	NAP	C5D-C4D-C3D	-2.59	105.88	115.21
2	C	501	NAP	C5A-N7A-C8A	2.59	107.52	103.45
2	D	501	NAP	O2B-P2B-O1X	-2.58	100.14	109.33
2	D	501	NAP	C4A-C5A-N7A	-2.56	107.65	110.58
2	B	501	NAP	C6N-N1N-C2N	-2.56	119.70	121.88
2	B	501	NAP	O7N-C7N-N7N	2.54	126.29	122.62
2	B	501	NAP	C3N-C7N-N7N	-2.54	114.61	117.74
2	C	501	NAP	O3-PA-O1A	-2.53	103.09	110.70
2	C	501	NAP	C4A-C5A-N7A	-2.44	107.80	110.58
2	B	501	NAP	C5A-N7A-C8A	2.37	107.18	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAP	O2A-PA-O1A	2.35	123.37	112.44
2	C	501	NAP	O2D-C2D-C3D	-2.32	104.37	111.82
2	B	501	NAP	C6A-C5A-C4A	2.30	120.32	117.18
2	A	501	NAP	O3-PA-O1A	-2.26	103.92	110.70
2	B	501	NAP	C2B-C1B-N9A	2.24	117.44	113.75
2	B	501	NAP	C4A-C5A-N7A	-2.24	108.02	110.58
2	A	501	NAP	C5D-C4D-C3D	-2.23	107.18	115.21
2	D	501	NAP	C6N-N1N-C2N	-2.21	120.00	121.88
2	A	501	NAP	C4B-O4B-C1B	-2.20	104.60	109.47
2	C	501	NAP	O3X-P2B-O1X	2.18	119.33	110.83
2	A	501	NAP	C5A-N7A-C8A	2.16	106.84	103.45
2	C	501	NAP	O4D-C4D-C5D	-2.13	102.52	109.33
2	A	501	NAP	C4A-N9A-C8A	2.11	107.95	105.74
2	B	501	NAP	O3-PA-O1A	-2.08	104.45	110.70
2	B	501	NAP	O2N-PN-O3	2.05	112.82	107.27
2	B	501	NAP	C5D-C4D-C3D	-2.02	107.93	115.21

There are no chirality outliers.

All (19) torsion outliers are listed below:

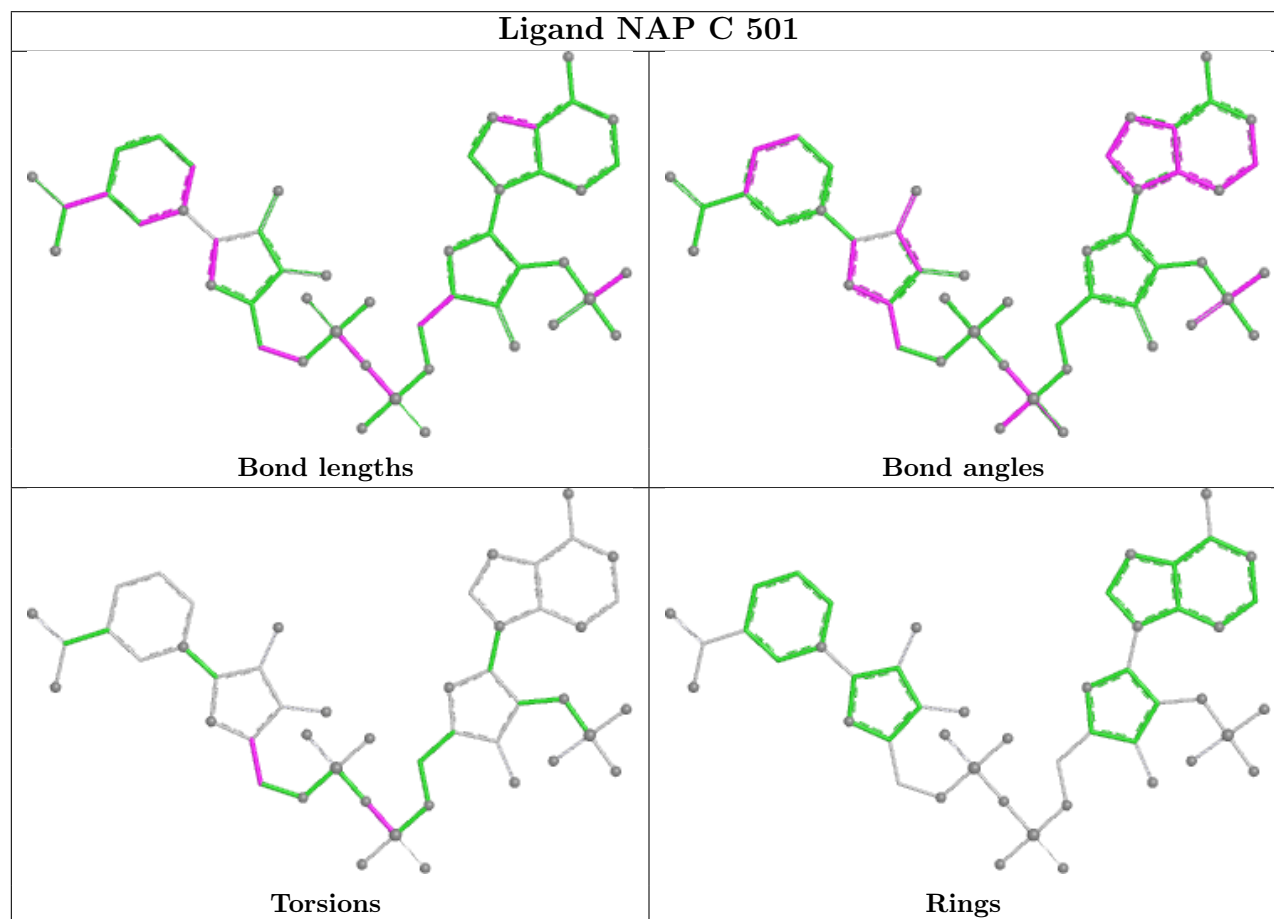
Mol	Chain	Res	Type	Atoms
2	B	501	NAP	O4D-C4D-C5D-O5D
2	D	501	NAP	C2N-C3N-C7N-O7N
2	C	501	NAP	PN-O3-PA-O1A
2	D	501	NAP	C4N-C3N-C7N-O7N
2	D	501	NAP	C3B-C4B-C5B-O5B
2	D	501	NAP	C4N-C3N-C7N-N7N
2	A	501	NAP	PN-O3-PA-O2A
2	D	501	NAP	C2N-C3N-C7N-N7N
2	A	501	NAP	C5B-O5B-PA-O1A
2	C	501	NAP	PN-O3-PA-O2A
2	D	501	NAP	C2B-C1B-N9A-C8A
2	B	501	NAP	C3D-C4D-C5D-O5D
2	D	501	NAP	C2B-C1B-N9A-C4A
2	B	501	NAP	O4B-C1B-N9A-C8A
2	D	501	NAP	O4B-C1B-N9A-C8A
2	A	501	NAP	PN-O3-PA-O1A
2	B	501	NAP	C2B-C1B-N9A-C8A
2	B	501	NAP	C3B-C4B-C5B-O5B
2	C	501	NAP	O4D-C4D-C5D-O5D

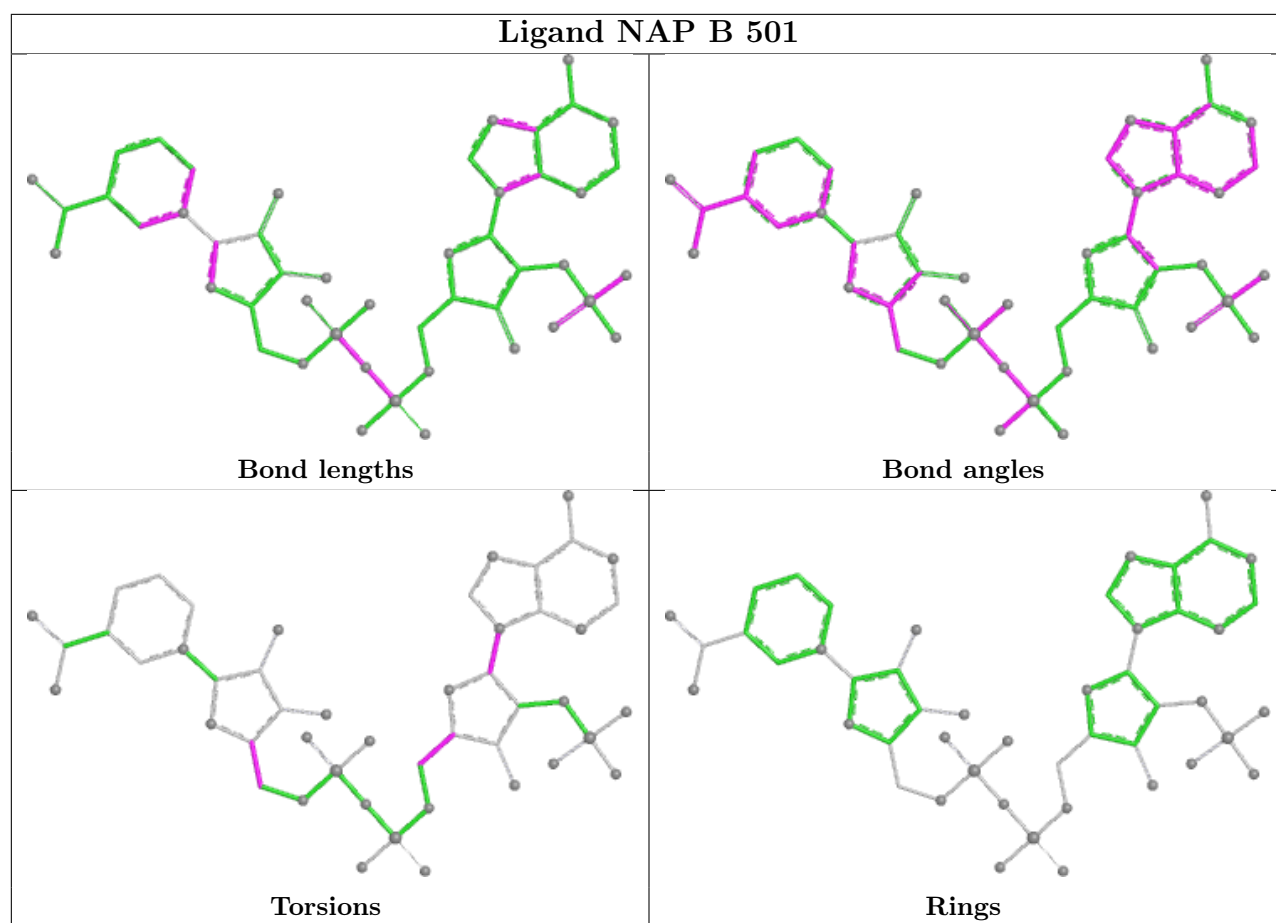
There are no ring outliers.

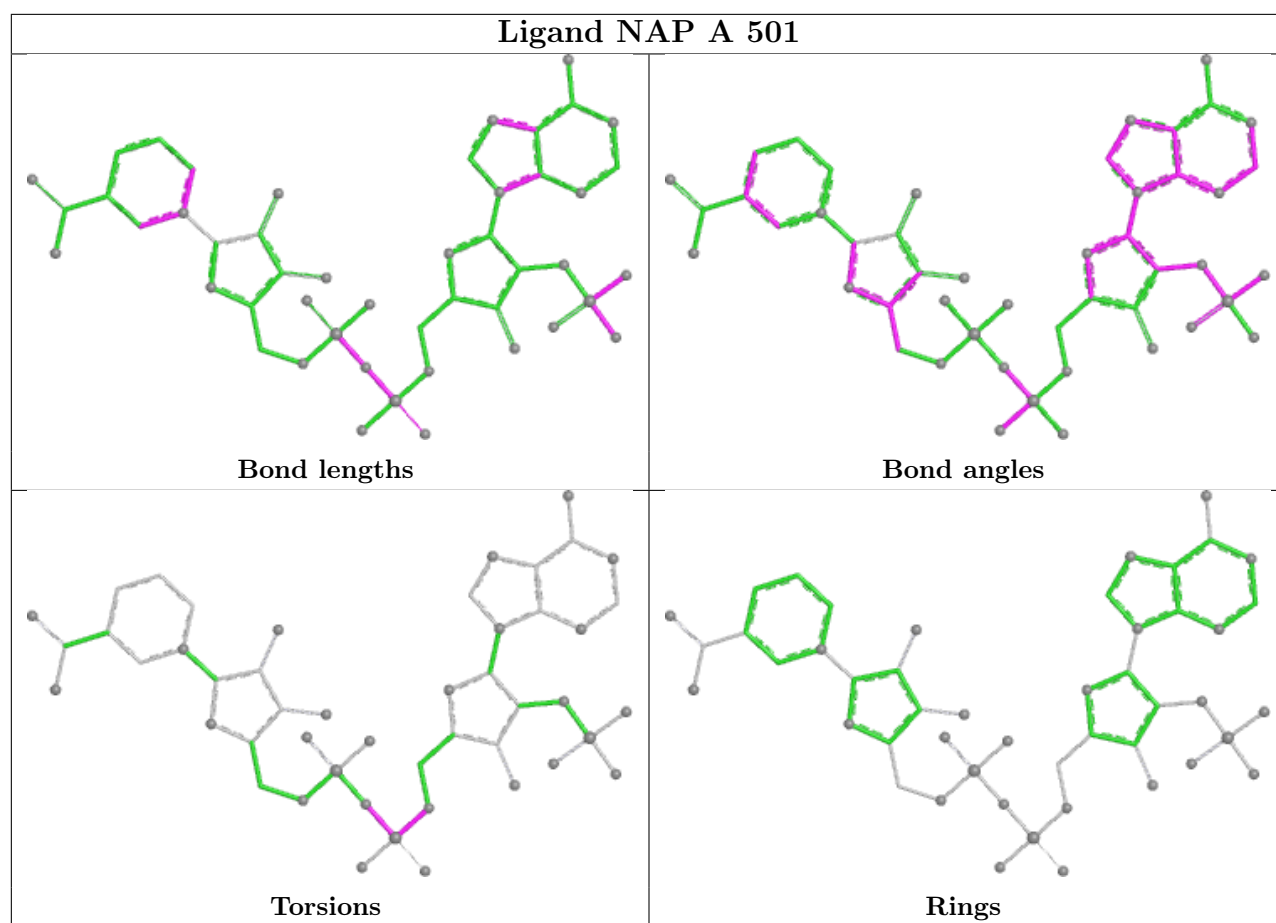
4 monomers are involved in 7 short contacts:

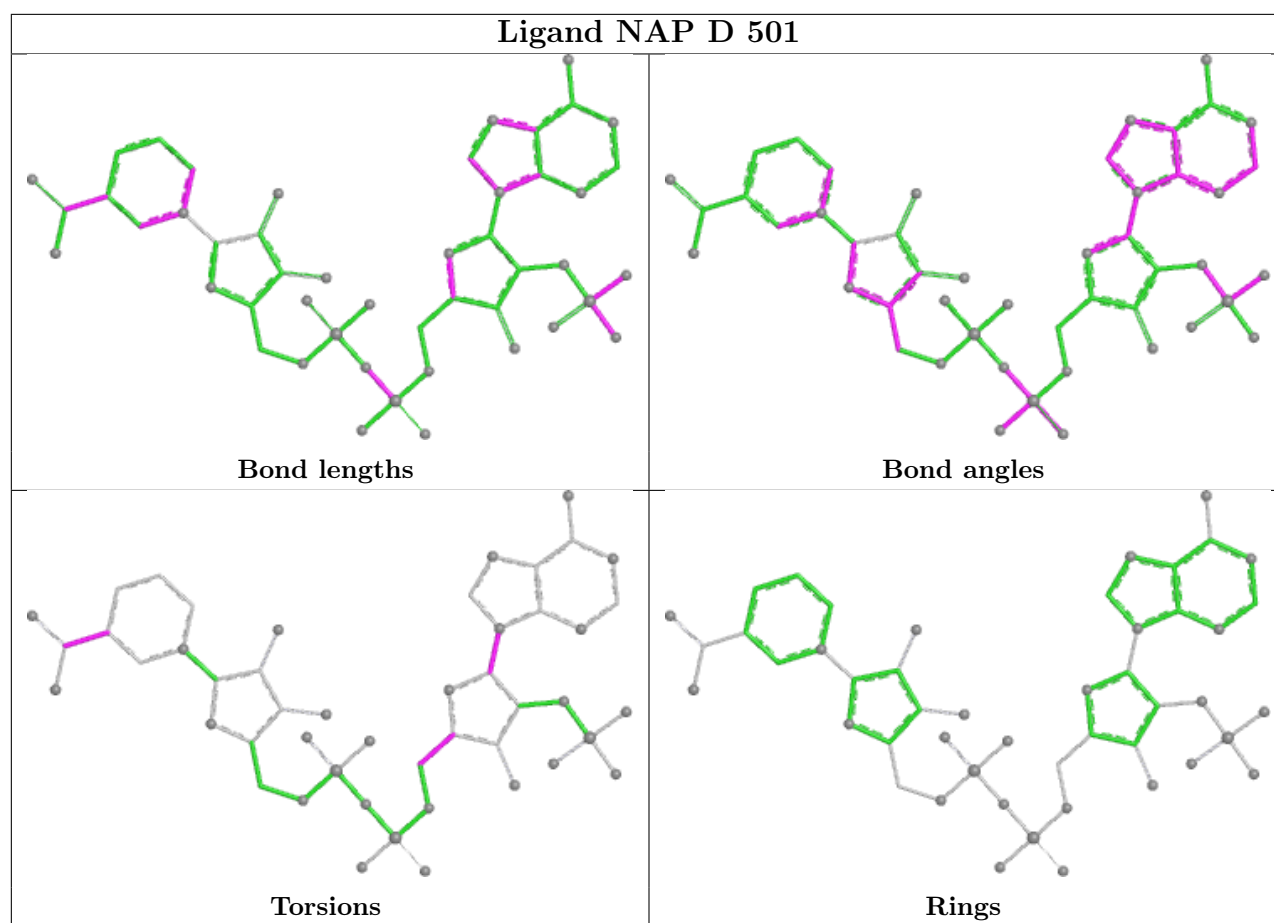
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAP	3	0
2	B	501	NAP	2	0
2	A	501	NAP	1	0
2	D	501	NAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	284/292 (97%)	1.23	43 (15%) 5 4	48, 71, 74, 79	0
1	B	279/292 (95%)	1.22	39 (13%) 6 5	48, 71, 74, 79	0
1	C	283/292 (96%)	1.38	54 (19%) 3 3	48, 71, 74, 79	0
1	D	285/292 (97%)	1.36	48 (16%) 4 3	49, 71, 74, 80	0
All	All	1131/1168 (96%)	1.30	184 (16%) 4 4	48, 71, 74, 80	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	198	TYR	5.6
1	D	49	GLY	5.5
1	A	234	LYS	4.4
1	C	61	ASP	4.2
1	C	220	GLY	4.2
1	C	281	CYS	4.0
1	A	205	LEU	3.8
1	C	219	LYS	3.8
1	A	61	ASP	3.7
1	B	224	LYS	3.7
1	D	10	GLY	3.6
1	C	197	GLN	3.6
1	C	212	PRO	3.5
1	C	114	ALA	3.5
1	B	112	GLU	3.5
1	D	239	GLU	3.5
1	A	233	PHE	3.4
1	C	75	SER	3.4
1	C	210	LYS	3.4
1	D	238	LEU	3.4
1	A	291	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	199	MET	3.3
1	B	291	TYR	3.3
1	C	50	SER	3.2
1	B	17	GLY	3.2
1	A	67	GLU	3.2
1	B	60	GLU	3.2
1	A	191	GLU	3.1
1	D	222	GLY	3.1
1	B	18	ARG	3.1
1	C	291	TYR	3.1
1	C	44	SER	3.1
1	B	20	GLY	3.1
1	D	292	CYS	3.1
1	D	47	GLU	3.0
1	C	71	ALA	3.0
1	B	40	ILE	3.0
1	D	163	GLY	3.0
1	C	70	VAL	3.0
1	D	75	SER	2.9
1	D	166	ALA	2.9
1	A	126	VAL	2.9
1	A	144	ASP	2.9
1	A	228	TYR	2.9
1	B	19	ALA	2.9
1	A	97	GLU	2.9
1	C	191	GLU	2.9
1	C	211	SER	2.9
1	A	20	GLY	2.9
1	C	279	LEU	2.9
1	B	181	GLY	2.8
1	A	258	PHE	2.8
1	C	41	GLY	2.8
1	A	238	LEU	2.8
1	D	291	TYR	2.8
1	A	95	LEU	2.8
1	A	223	LEU	2.7
1	C	113	LEU	2.7
1	B	80	HIS	2.7
1	A	96	VAL	2.7
1	D	13	VAL	2.7
1	A	157	LEU	2.7
1	D	212	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	177	VAL	2.7
1	D	61	ASP	2.7
1	B	131	GLU	2.6
1	D	220	GLY	2.6
1	C	62	ALA	2.6
1	A	192	GLU	2.6
1	C	154	ALA	2.6
1	B	146	LEU	2.6
1	B	223	LEU	2.6
1	D	157	LEU	2.6
1	B	155	GLY	2.6
1	D	48	LEU	2.6
1	A	98	TYR	2.6
1	D	144	ASP	2.5
1	B	188	ALA	2.5
1	C	107	ALA	2.5
1	A	178	SER	2.5
1	B	63	LEU	2.5
1	D	18	ARG	2.5
1	D	191	GLU	2.5
1	C	10	GLY	2.5
1	D	156	PRO	2.5
1	A	236	GLY	2.5
1	B	10	GLY	2.5
1	C	12	VAL	2.5
1	C	233	PHE	2.5
1	D	257	ILE	2.5
1	C	155	GLY	2.5
1	D	130	MET	2.5
1	C	13	VAL	2.5
1	A	25	ARG	2.4
1	B	75	SER	2.4
1	C	208	GLU	2.4
1	C	63	LEU	2.4
1	C	223	LEU	2.4
1	D	216	ILE	2.4
1	A	65	SER	2.4
1	D	6	MET	2.4
1	A	7	ARG	2.4
1	D	190	LEU	2.4
1	D	50	SER	2.4
1	D	100	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	224	LYS	2.4
1	D	293	CYS	2.4
1	A	128	LEU	2.3
1	C	218	GLU	2.3
1	A	197	GLN	2.3
1	B	222	GLY	2.3
1	D	118	GLY	2.3
1	A	257	ILE	2.3
1	C	67	GLU	2.3
1	C	290	LYS	2.3
1	D	14	VAL	2.3
1	A	185	LEU	2.3
1	B	48	LEU	2.3
1	A	235	SER	2.3
1	B	162	PHE	2.3
1	A	62	ALA	2.3
1	B	98	TYR	2.3
1	D	254	ASP	2.3
1	A	181	GLY	2.3
1	C	20	GLY	2.3
1	D	91	GLY	2.3
1	A	68	VAL	2.3
1	B	120	VAL	2.3
1	C	76	GLU	2.2
1	A	22	VAL	2.2
1	C	51	ILE	2.2
1	D	164	PHE	2.2
1	A	60	GLU	2.2
1	C	287	GLU	2.2
1	D	98	TYR	2.2
1	B	221	PRO	2.2
1	D	59	LEU	2.2
1	C	133	PHE	2.2
1	B	157	LEU	2.2
1	C	17	GLY	2.2
1	D	88	LEU	2.2
1	D	73	ILE	2.2
1	B	67	GLU	2.2
1	C	118	GLY	2.2
1	A	259	VAL	2.2
1	C	177	VAL	2.2
1	D	70	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	147	LYS	2.1
1	B	209	LYS	2.1
1	B	41	GLY	2.1
1	C	181	GLY	2.1
1	D	184	SER	2.1
1	C	236	GLY	2.1
1	D	15	GLY	2.1
1	B	94	VAL	2.1
1	C	64	SER	2.1
1	A	107	ALA	2.1
1	C	106	ALA	2.1
1	A	76	GLU	2.1
1	B	208	GLU	2.1
1	B	239	GLU	2.1
1	D	97	GLU	2.1
1	A	213	LEU	2.1
1	A	252	LEU	2.1
1	B	83	TYR	2.1
1	A	57	ILE	2.1
1	C	144	ASP	2.1
1	B	35	ALA	2.1
1	C	7	ARG	2.1
1	C	47	GLU	2.1
1	C	286	GLU	2.1
1	A	27	LEU	2.1
1	C	80	HIS	2.1
1	C	198	TYR	2.1
1	D	16	VAL	2.1
1	D	40	ILE	2.0
1	D	12	VAL	2.0
1	B	152	PHE	2.0
1	C	178	SER	2.0
1	B	102	LEU	2.0
1	B	252	LEU	2.0
1	B	280	HIS	2.0
1	C	240	ASN	2.0
1	C	120	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

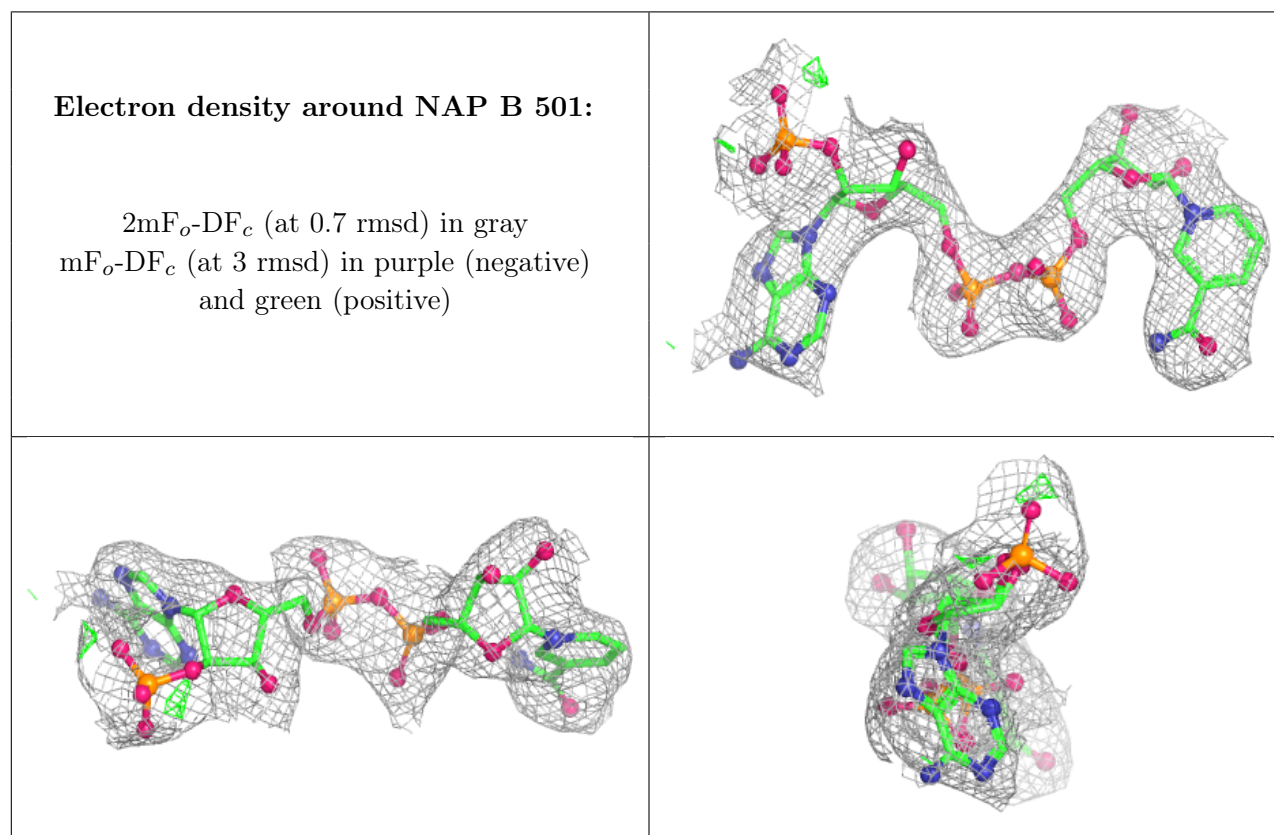
There are no oligosaccharides in this entry.

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.

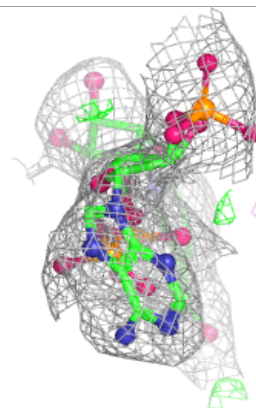
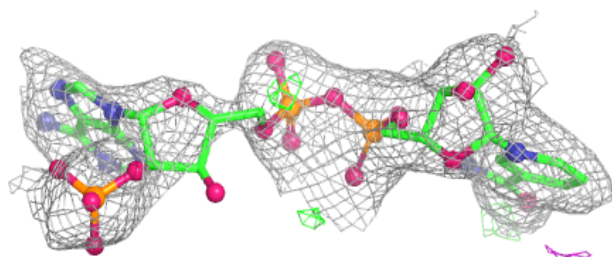
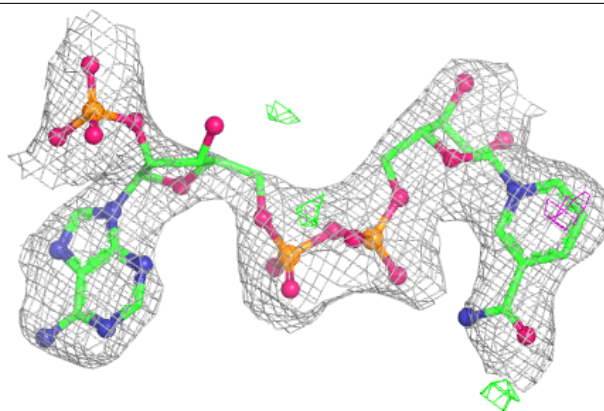
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	B	501	48/48	0.89	0.10	61,69,81,82	0
2	NAP	C	501	48/48	0.90	0.12	57,65,82,84	0
2	NAP	D	501	48/48	0.91	0.12	58,69,76,81	0
2	NAP	A	501	48/48	0.93	0.09	48,56,63,65	0

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.

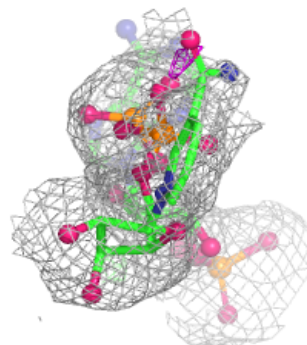
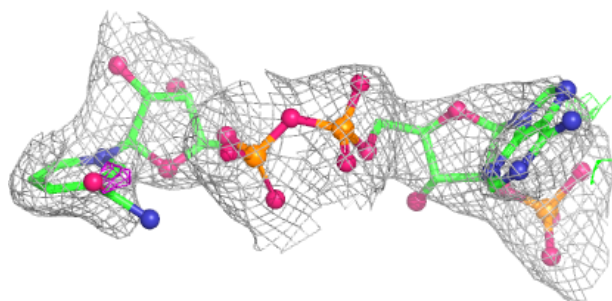
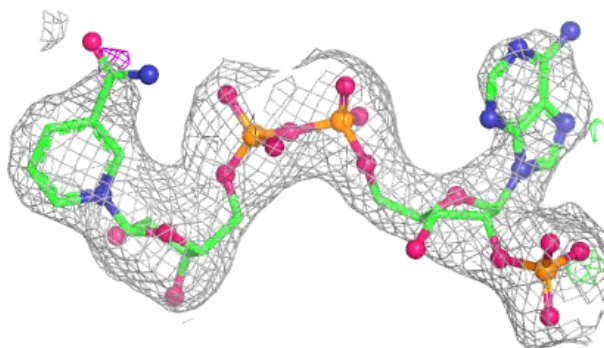


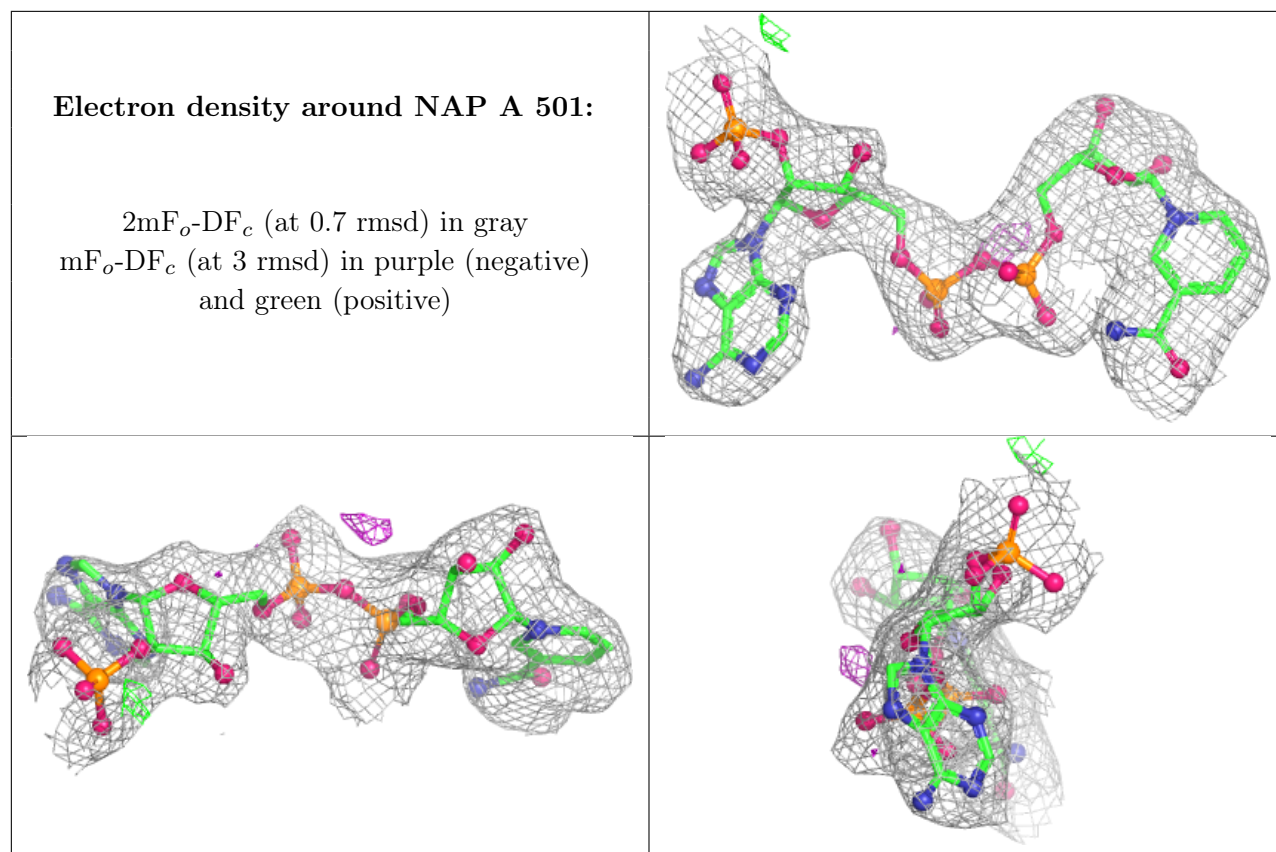
Electron density around NAP C 501:

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

**Electron density around NAP D 501:**

$2mF_o-DF_c$ (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.