



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:19 AM UTC

PDB ID : 3BUV / pdb_00003buv
Title : Crystal structure of human Delta(4)-3-ketosteroid 5-beta-reductase in complex with NADP and HEPES. Resolution: 1.35 Å.
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Deposited on : 2008-01-03
Resolution : 1.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

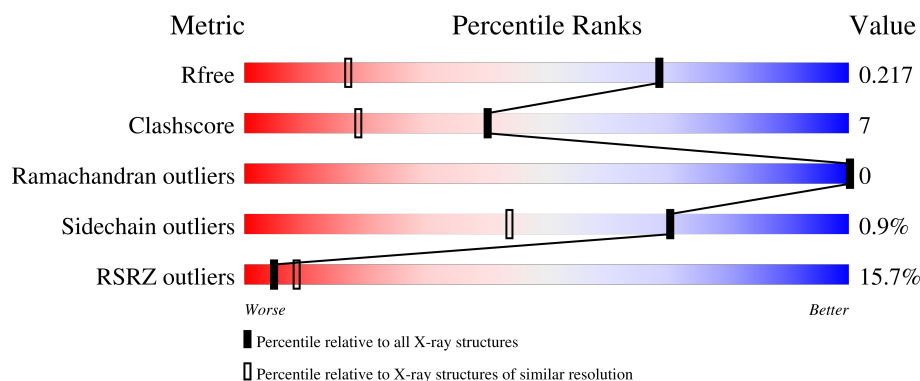
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	326	25% 84% 16%
1	B	326	6% 86% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

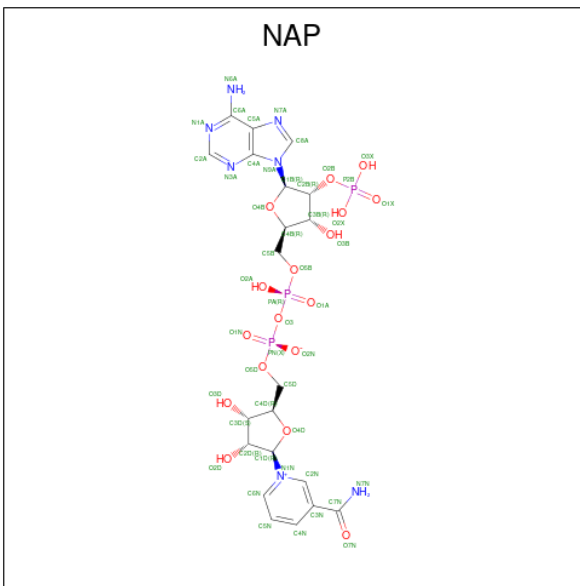
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	330	-	-	-	X

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 3-oxo-5-beta-steroid 4-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	325	Total 2627	C 1680	N 455	O 481	S 11	0	0	0
1	A	325	Total 2627	C 1680	N 455	O 481	S 11	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

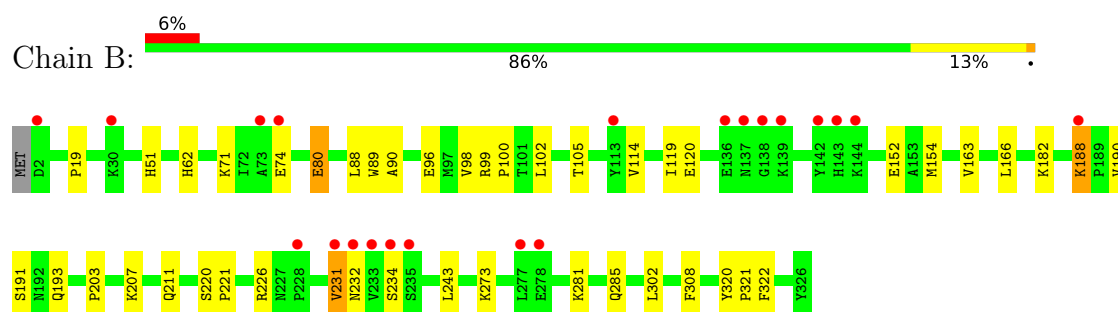
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	304	Total 304	O 304	0	0
5	A	252	Total 252	O 252	0	0

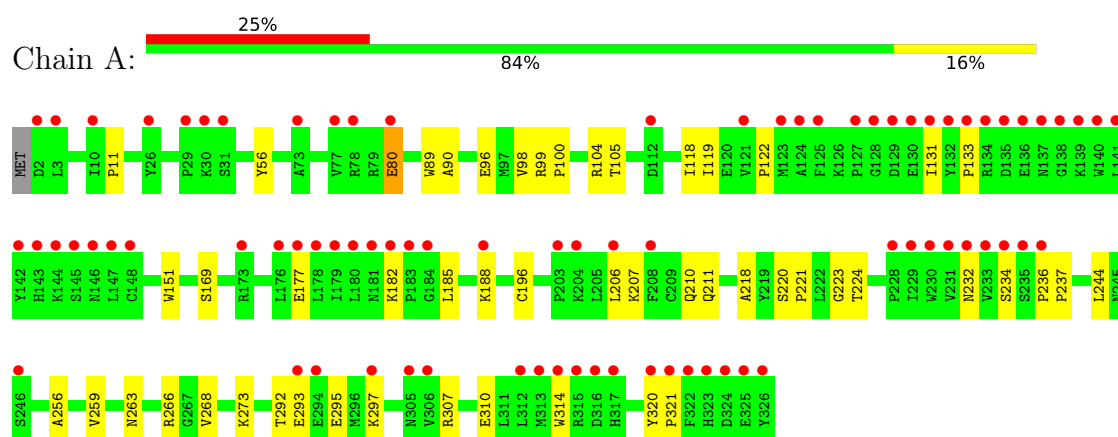
3 Residue-property plots

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

- Molecule 1: 3-oxo-5-beta-steroid 4-dehydrogenase



- Molecule 1: 3-oxo-5-beta-steroid 4-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.71Å 109.80Å 128.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.69 – 1.35 33.69 – 1.35	Depositor EDS
% Data completeness (in resolution range)	91.0 (33.69-1.35) 95.6 (33.69-1.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.35Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.218 , 0.232 0.215 , 0.217	Depositor DCC
R_{free} test set	7402 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5933	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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, EPE, GOL

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	0.33	0/2692	0.78	3/3649 (0.1%)
1	B	0.35	0/2692	0.84	7/3649 (0.2%)
All	All	0.34	0/5384	0.81	10/7298 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	VAL	N-CA-C	7.06	119.60	108.87
1	B	322	PHE	N-CA-C	6.40	120.70	113.02
1	B	98	VAL	N-CA-C	6.33	116.49	110.42
1	B	321	PRO	N-CA-C	5.90	122.38	114.18
1	B	308	PHE	N-CA-C	-5.67	105.47	112.90
1	B	120	GLU	N-CA-C	5.39	117.16	111.28
1	A	119	ILE	N-CA-C	-5.34	101.79	108.84
1	A	98	VAL	N-CA-C	5.17	115.32	110.30
1	B	320	TYR	N-CA-C	-5.07	102.18	109.48
1	A	11	PRO	N-CA-C	5.01	119.05	111.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2622	34	0
1	B	2627	0	2622	33	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
3	B	12	0	16	1	0
4	A	15	0	17	4	0
5	A	252	0	0	4	0
5	B	304	0	0	5	0
All	All	5933	0	5327	71	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 (71) 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)
4:A:3999:EPE:N1	4:A:3999:EPE:C2	1.70	1.48
4:A:3999:EPE:C2	4:A:3999:EPE:C6	2.44	0.95
1:B:114:VAL:HG22	1:B:163:VAL:HG22	1.57	0.84
4:A:3999:EPE:C2	4:A:3999:EPE:C9	2.56	0.84
1:B:102:LEU:HD21	1:B:163:VAL:HG23	1.61	0.81
1:A:232:ASN:HD21	1:A:234:SER:HB3	1.50	0.76
1:A:263:ASN:O	1:A:266:ARG:HG2	1.85	0.75
1:B:114:VAL:CG2	1:B:163:VAL:HG22	2.19	0.72
1:B:152:GLU:HG3	1:B:182:LYS:HE3	1.70	0.71
1:A:263:ASN:OD1	1:A:266:ARG:HD3	1.92	0.68
4:A:3999:EPE:N1	4:A:3999:EPE:C3	2.59	0.64
1:A:232:ASN:ND2	1:A:234:SER:HB3	2.12	0.63
1:A:185:LEU:HD21	1:A:188:LYS:HG2	1.80	0.63
1:A:206:LEU:O	1:A:210:GLN:HG3	2.00	0.62
1:B:188:LYS:HE2	5:B:3958:HOH:O	2.03	0.58
1:B:80:GLU:H	1:B:80:GLU:CD	2.12	0.57
1:A:122:PRO:HG3	1:A:321:PRO:HG3	1.86	0.57
1:B:88:LEU:HD22	1:B:154:MET:HE2	1.87	0.56
1:A:122:PRO:CG	1:A:321:PRO:HG3	2.35	0.56
1:A:273:LYS:C	1:A:273:LYS:HD3	2.32	0.55
1:B:243:LEU:HD23	1:B:302:LEU:HD21	1.89	0.53
1:B:191:SER:HB2	5:B:4025:HOH:O	2.08	0.53
1:A:266:ARG:HG3	1:A:268:VAL:HG23	1.89	0.52
1:B:119:ILE:HG12	1:B:154:MET:CE	2.39	0.52
1:A:131:ILE:C	1:A:133:PRO:HD3	2.35	0.52
1:A:273:LYS:O	2:A:3902:NAP:H8A	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HA	1:B:74:GLU:HG2	1.92	0.51
1:A:307:ARG:HG3	1:A:310:GLU:HG2	1.91	0.51
1:A:207:LYS:O	1:A:211:GLN:HG3	2.09	0.51
1:B:273:LYS:O	2:B:3901:NAP:H8A	2.11	0.51
1:B:232:ASN:ND2	1:B:234:SER:OG	2.44	0.50
1:B:273:LYS:HD3	1:B:273:LYS:C	2.36	0.50
1:A:80:GLU:H	1:A:80:GLU:CD	2.18	0.50
1:A:185:LEU:CD2	1:A:188:LYS:HG2	2.42	0.50
1:A:99:ARG:HB3	1:A:100:PRO:HD3	1.93	0.50
1:A:293:GLU:HG3	1:A:297:LYS:HE3	1.94	0.49
1:B:99:ARG:HB3	1:B:100:PRO:HD3	1.95	0.49
1:B:207:LYS:O	1:B:211:GLN:HG3	2.13	0.49
1:A:256:ALA:O	1:A:259:VAL:HG22	2.11	0.49
1:A:118:ILE:HD12	1:A:169:SER:HB2	1.96	0.48
1:B:188:LYS:HB3	1:B:188:LYS:NZ	2.28	0.48
1:A:56:TYR:CD1	1:A:104:ARG:HD3	2.49	0.48
1:B:119:ILE:HG12	1:B:154:MET:HE2	1.96	0.47
1:B:62:HIS:HE1	5:B:4013:HOH:O	1.97	0.46
1:B:100:PRO:HB2	3:B:330:GOL:H11	1.97	0.46
1:B:203:PRO:HG2	5:B:3986:HOH:O	2.15	0.46
1:A:292:THR:OG1	1:A:295:GLU:HG3	2.17	0.45
1:A:196:CYS:HB3	1:A:218:ALA:CB	2.47	0.45
1:A:220:SER:N	1:A:221:PRO:CD	2.79	0.45
1:B:281:LYS:O	1:B:285:GLN:HG2	2.17	0.44
1:A:314:TRP:C	5:A:4142:HOH:O	2.61	0.43
1:A:151:TRP:HD1	1:A:182:LYS:NZ	2.16	0.43
1:A:223:GLY:C	1:A:224:THR:HG23	2.43	0.43
1:A:236:PRO:HG2	5:A:4018:HOH:O	2.17	0.43
1:A:236:PRO:HA	1:A:237:PRO:HD3	1.87	0.42
1:B:62:HIS:HD2	5:A:4004:HOH:O	2.01	0.42
1:B:119:ILE:CG1	1:B:154:MET:HE3	2.50	0.42
1:A:177:GLU:HG2	5:A:4139:HOH:O	2.18	0.42
1:B:232:ASN:HB2	5:B:4070:HOH:O	2.19	0.42
1:A:89:TRP:CG	1:A:90:ALA:N	2.87	0.42
1:B:226:ARG:HA	1:B:231:VAL:HG21	2.02	0.42
1:A:320:TYR:HA	1:A:321:PRO:HD3	1.87	0.41
1:B:220:SER:N	1:B:221:PRO:CD	2.82	0.41
1:B:193:GLN:OE1	2:B:3901:NAP:H2N	2.20	0.41
1:B:166:LEU:O	1:B:190:VAL:HG22	2.20	0.41
1:A:244:LEU:HD13	1:A:259:VAL:CG1	2.51	0.41
1:B:89:TRP:CG	1:B:90:ALA:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PRO:HB2	1:B:51:HIS:HB2	2.03	0.41
1:B:96:GLU:CD	1:B:96:GLU:H	2.29	0.41
1:A:96:GLU:CD	1:A:96:GLU:H	2.29	0.40
1:B:71:LYS:HA	1:B:71:LYS:HD3	1.93	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	323/326 (99%)	317 (98%)	6 (2%)	0	100	100
1	B	323/326 (99%)	317 (98%)	6 (2%)	0	100	100
All	All	646/652 (99%)	634 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	289/290 (100%)	287 (99%)	2 (1%)	76	54
1	B	289/290 (100%)	286 (99%)	3 (1%)	68	40
All	All	578/580 (100%)	573 (99%)	5 (1%)	70	44

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	GLU
1	B	105	THR
1	B	188	LYS
1	A	80	GLU
1	A	105	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	HIS
1	B	92	ASN
1	B	93	HIS
1	B	170	ASN
1	B	232	ASN
1	A	92	ASN
1	A	146	ASN
1	A	210	GLN
1	A	211	GLN
1	A	232	ASN
1	A	285	GLN
1	A	323	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
3	GOL	B	329	-	5,5,5	0.52	0	5,5,5	0.70	0
3	GOL	B	330	-	5,5,5	0.50	0	5,5,5	0.74	0
2	NAP	A	3902	-	50,52,52	2.63	18 (36%)	71,80,80	1.92	19 (26%)
2	NAP	B	3901	-	50,52,52	2.65	19 (38%)	71,80,80	1.91	20 (28%)
4	EPE	A	3999	-	15,15,15	3.83	6 (40%)	19,20,20	3.27	9 (47%)

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
3	GOL	B	329	-	-	2/4/4/4	-
3	GOL	B	330	-	-	1/4/4/4	-
2	NAP	A	3902	-	-	7/35/67/67	0/5/5/5
2	NAP	B	3901	-	-	8/35/67/67	0/5/5/5
4	EPE	A	3999	-	-	5/9/19/19	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3999	EPE	C10-S	-8.91	1.65	1.77
4	A	3999	EPE	C2-N1	8.54	1.70	1.46
2	B	3901	NAP	PN-O3	-7.14	1.51	1.59
2	B	3901	NAP	C6N-N1N	6.83	1.50	1.35
2	A	3902	NAP	C6N-N1N	6.71	1.50	1.35
2	A	3902	NAP	C2N-N1N	6.25	1.41	1.35
2	B	3901	NAP	C4A-N3A	6.07	1.45	1.34
2	A	3902	NAP	C4A-N3A	5.98	1.45	1.34
2	A	3902	NAP	PN-O3	-5.94	1.53	1.59
2	B	3901	NAP	C2N-N1N	5.43	1.41	1.35
4	A	3999	EPE	O1S-S	-5.14	1.30	1.45
2	A	3902	NAP	O5B-C5B	-4.71	1.26	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3901	NAP	O5B-C5B	-4.51	1.27	1.44
2	A	3902	NAP	C5N-C4N	4.46	1.46	1.38
2	B	3901	NAP	C5N-C4N	4.36	1.46	1.38
4	A	3999	EPE	C7-N4	-4.20	1.37	1.47
2	B	3901	NAP	C4N-C3N	3.88	1.45	1.39
2	A	3902	NAP	C4N-C3N	3.77	1.45	1.39
2	A	3902	NAP	C2N-C3N	3.53	1.44	1.39
2	A	3902	NAP	O4D-C1D	3.49	1.45	1.40
2	B	3901	NAP	C8A-N7A	3.47	1.38	1.31
2	A	3902	NAP	C8A-N7A	3.44	1.38	1.31
2	B	3901	NAP	C6A-N1A	3.44	1.45	1.35
2	B	3901	NAP	O4D-C1D	3.43	1.45	1.40
2	A	3902	NAP	PN-O5D	-3.41	1.46	1.59
2	B	3901	NAP	PN-O5D	-3.39	1.46	1.59
2	A	3902	NAP	C6A-N1A	3.34	1.45	1.35
2	B	3901	NAP	C2N-C3N	3.16	1.44	1.39
2	B	3901	NAP	PN-O1N	-3.15	1.39	1.50
2	A	3902	NAP	PN-O1N	-3.13	1.40	1.50
4	A	3999	EPE	C5-N4	2.97	1.54	1.46
2	A	3902	NAP	C4A-N9A	-2.93	1.31	1.37
2	B	3901	NAP	C2A-N1A	2.89	1.39	1.33
2	A	3902	NAP	C2A-N1A	2.86	1.39	1.33
2	B	3901	NAP	C4A-N9A	-2.73	1.32	1.37
2	B	3901	NAP	PA-O1A	-2.70	1.41	1.50
2	A	3902	NAP	PA-O1A	-2.60	1.41	1.50
2	B	3901	NAP	C5A-N7A	-2.42	1.34	1.39
2	A	3902	NAP	C3N-C7N	2.26	1.54	1.50
4	A	3999	EPE	O2S-S	-2.17	1.39	1.45
2	B	3901	NAP	C3N-C7N	2.11	1.53	1.50
2	B	3901	NAP	C3D-C4D	2.08	1.58	1.53
2	A	3902	NAP	C5A-N7A	-2.03	1.35	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3999	EPE	O1S-S-C10	9.93	121.73	106.73
2	B	3901	NAP	N3A-C2A-N1A	-5.95	119.57	128.58
2	A	3902	NAP	N3A-C2A-N1A	-5.76	119.87	128.58
4	A	3999	EPE	C10-C9-N1	-5.05	93.24	112.36
2	A	3902	NAP	C3N-C7N-N7N	-4.91	111.68	117.74
2	B	3901	NAP	C3N-C7N-N7N	-4.79	111.83	117.74
2	B	3901	NAP	O7N-C7N-N7N	4.47	129.07	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3902	NAP	O7N-C7N-N7N	4.42	129.00	122.62
4	A	3999	EPE	O3S-S-O1S	-4.29	100.66	111.40
2	A	3902	NAP	C5A-C4A-N3A	-4.09	121.08	126.72
2	B	3901	NAP	C5A-C4A-N3A	-4.05	121.14	126.72
4	A	3999	EPE	C6-N1-C2	-3.51	101.29	108.84
2	A	3902	NAP	O3D-C3D-C2D	3.21	122.11	111.82
4	A	3999	EPE	O3S-S-C10	3.19	112.24	106.00
2	B	3901	NAP	O3D-C3D-C2D	3.17	121.98	111.82
2	B	3901	NAP	C2A-N3A-C4A	3.10	119.41	111.83
2	A	3902	NAP	C2A-N1A-C6A	3.04	123.72	118.73
2	B	3901	NAP	C2A-N1A-C6A	3.03	123.70	118.73
2	A	3902	NAP	C2A-N3A-C4A	2.97	119.08	111.83
2	A	3902	NAP	C6N-N1N-C2N	-2.95	119.37	121.88
2	A	3902	NAP	C6A-C5A-C4A	2.90	121.13	117.18
2	A	3902	NAP	PN-O5D-C5D	2.78	137.31	121.35
2	B	3901	NAP	C6A-C5A-C4A	2.77	120.97	117.18
4	A	3999	EPE	O2S-S-O1S	-2.71	105.01	113.82
2	B	3901	NAP	O5D-C5D-C4D	2.69	118.15	108.99
2	A	3902	NAP	C6A-C5A-N7A	-2.68	126.93	132.09
2	B	3901	NAP	C6N-N1N-C2N	-2.64	119.64	121.88
2	B	3901	NAP	C6A-C5A-N7A	-2.63	127.01	132.09
2	A	3902	NAP	O5D-C5D-C4D	2.63	117.95	108.99
2	B	3901	NAP	PN-O5D-C5D	2.57	136.10	121.35
2	A	3902	NAP	O4D-C4D-C3D	-2.55	100.10	105.15
4	A	3999	EPE	C5-N4-C3	-2.40	103.67	108.84
2	B	3901	NAP	O4D-C4D-C3D	-2.40	100.40	105.15
2	A	3902	NAP	C2B-C1B-N9A	2.33	117.59	113.75
2	A	3902	NAP	N3A-C4A-N9A	2.32	131.12	127.17
2	B	3901	NAP	C6N-C5N-C4N	-2.32	116.10	119.45
2	B	3901	NAP	N3A-C4A-N9A	2.31	131.10	127.17
4	A	3999	EPE	O3S-S-O2S	-2.24	105.80	111.40
2	A	3902	NAP	C6N-C5N-C4N	-2.21	116.27	119.45
4	A	3999	EPE	O2S-S-C10	2.16	109.99	106.73
2	B	3901	NAP	C2B-C1B-N9A	2.15	117.29	113.75
2	A	3902	NAP	C5A-C6A-N6A	2.12	128.54	123.29
2	A	3902	NAP	O5B-C5B-C4B	2.10	116.15	108.99
2	B	3901	NAP	C2N-C3N-C4N	2.09	120.69	118.26
2	B	3901	NAP	C5A-C6A-N6A	2.07	128.41	123.29
2	A	3902	NAP	C2N-C3N-C4N	2.06	120.65	118.26
2	B	3901	NAP	O5B-C5B-C4B	2.03	115.91	108.99
2	B	3901	NAP	C6N-N1N-C1D	2.02	123.69	119.73

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3901	NAP	PA-O3-PN-O5D
2	B	3901	NAP	C5D-O5D-PN-O2N
2	B	3901	NAP	O4D-C1D-N1N-C6N
2	A	3902	NAP	PA-O3-PN-O5D
2	A	3902	NAP	C5D-O5D-PN-O2N
4	A	3999	EPE	C10-C9-N1-C2
4	A	3999	EPE	C10-C9-N1-C6
2	B	3901	NAP	C4D-C5D-O5D-PN
2	A	3902	NAP	C4D-C5D-O5D-PN
4	A	3999	EPE	C9-C10-S-O3S
4	A	3999	EPE	C9-C10-S-O1S
3	B	329	GOL	C1-C2-C3-O3
2	B	3901	NAP	PN-O3-PA-O2A
2	A	3902	NAP	PN-O3-PA-O2A
2	B	3901	NAP	C5D-O5D-PN-O3
4	A	3999	EPE	N4-C7-C8-O8
2	B	3901	NAP	O4D-C1D-N1N-C2N
2	A	3902	NAP	O4D-C1D-N1N-C6N
2	A	3902	NAP	C2B-C1B-N9A-C8A
3	B	329	GOL	O2-C2-C3-O3
3	B	330	GOL	O1-C1-C2-O2
2	B	3901	NAP	PN-O3-PA-O1A
2	A	3902	NAP	PN-O3-PA-O1A

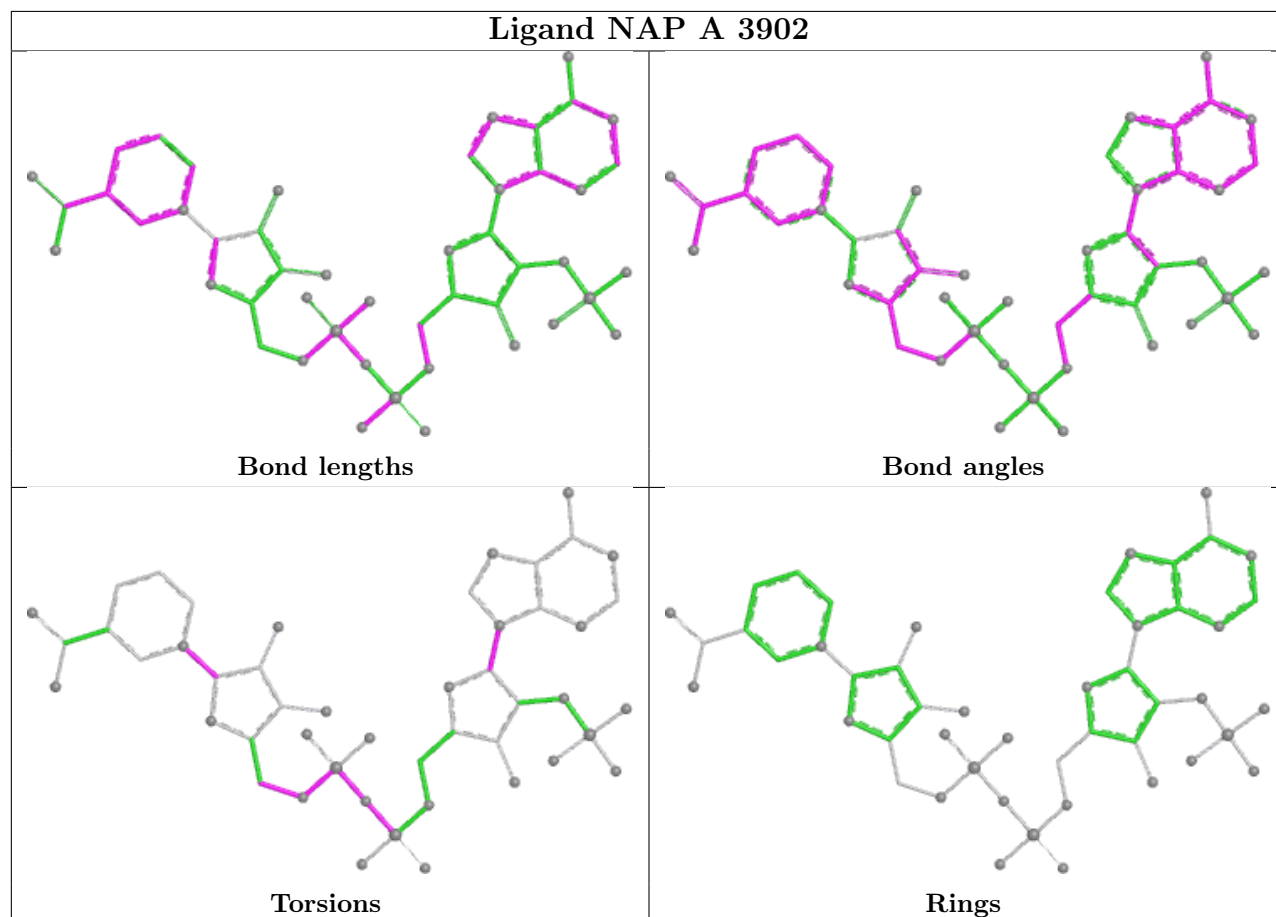
There are no ring outliers.

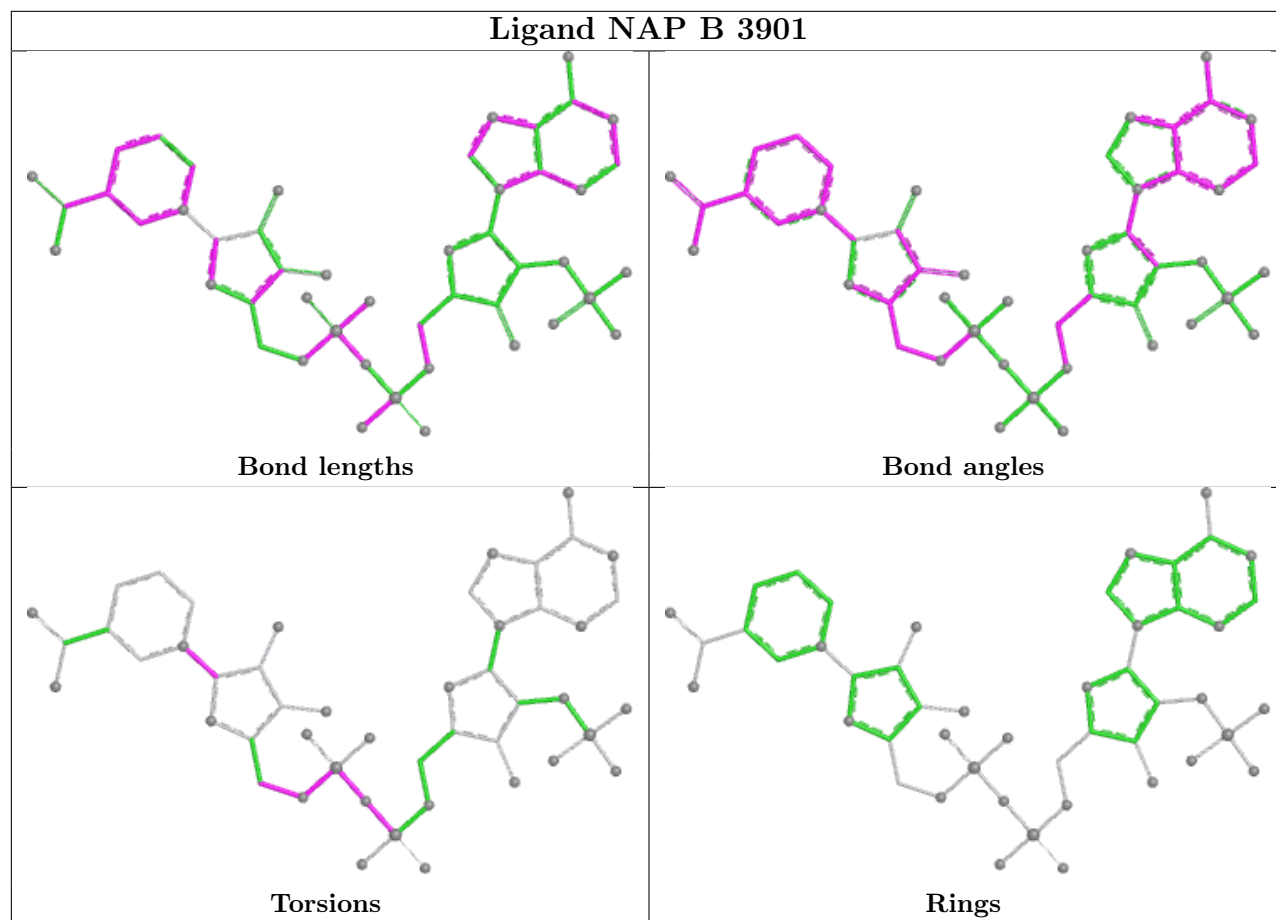
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	330	GOL	1	0
2	A	3902	NAP	1	0
2	B	3901	NAP	2	0
4	A	3999	EPE	4	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	325/326 (99%)	1.32	81 (24%) 2 2	10, 17, 36, 71	0
1	B	325/326 (99%)	0.63	21 (6%) 25 33	10, 14, 26, 41	0
All	All	650/652 (99%)	0.97	102 (15%) 5 8	10, 15, 33, 71	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	TYR	9.0
1	B	233	VAL	8.0
1	A	138	GLY	6.6
1	B	232	ASN	6.6
1	B	234	SER	6.3
1	B	231	VAL	6.3
1	A	140	TRP	6.3
1	A	233	VAL	6.2
1	A	323	HIS	5.9
1	A	178	LEU	5.9
1	B	235	SER	5.9
1	A	30	LYS	5.3
1	A	141	LEU	5.2
1	A	234	SER	5.1
1	B	138	GLY	4.7
1	A	147	LEU	4.7
1	A	133	PRO	4.7
1	A	135	ASP	4.6
1	A	173	ARG	4.6
1	A	188	LYS	4.5
1	B	144	LYS	4.4
1	A	321	PRO	4.4
1	A	125	PHE	4.3
1	A	2	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	136	GLU	4.2
1	A	139	LYS	4.1
1	A	229	ILE	4.1
1	A	130	GLU	4.1
1	A	142	TYR	4.0
1	A	137	ASN	4.0
1	A	26	TYR	3.9
1	A	143	HIS	3.9
1	A	177	GLU	3.9
1	A	183	PRO	3.9
1	B	30	LYS	3.8
1	A	129	ASP	3.7
1	A	131	ILE	3.7
1	A	134	ARG	3.3
1	B	143	HIS	3.3
1	A	236	PRO	3.3
1	A	145	SER	3.3
1	A	128	GLY	3.3
1	A	123	MET	3.2
1	A	232	ASN	3.2
1	B	136	GLU	3.2
1	A	316	ASP	3.2
1	A	182	LYS	3.2
1	B	228	PRO	3.2
1	B	73	ALA	3.2
1	B	139	LYS	3.1
1	A	181	ASN	3.1
1	A	204	LYS	3.1
1	A	184	GLY	3.1
1	B	137	ASN	3.1
1	A	231	VAL	3.1
1	B	2	ASP	3.1
1	A	297	LYS	3.0
1	A	29	PRO	3.0
1	A	326	TYR	2.9
1	A	306	VAL	2.9
1	A	146	ASN	2.9
1	A	31	SER	2.9
1	A	179	ILE	2.9
1	B	74	GLU	2.9
1	A	294	GLU	2.8
1	A	112	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	315	ARG	2.8
1	A	132	TYR	2.8
1	A	77	VAL	2.8
1	A	3	LEU	2.7
1	A	73	ALA	2.7
1	A	324	ASP	2.7
1	B	277	LEU	2.7
1	A	230	TRP	2.6
1	A	314	TRP	2.6
1	A	203	PRO	2.6
1	A	180	LEU	2.5
1	A	293	GLU	2.5
1	A	325	GLU	2.5
1	B	142	TYR	2.5
1	A	127	PRO	2.5
1	A	144	LYS	2.5
1	A	124	ALA	2.5
1	A	312	LEU	2.5
1	B	188	LYS	2.4
1	A	10	ILE	2.4
1	A	176	LEU	2.3
1	A	228	PRO	2.3
1	A	322	PHE	2.3
1	A	206	LEU	2.3
1	A	317	HIS	2.3
1	A	121	VAL	2.3
1	A	148	CYS	2.2
1	A	313	MET	2.2
1	A	305	ASN	2.2
1	A	208	PHE	2.2
1	A	246	SER	2.1
1	A	78	ARG	2.1
1	A	235	SER	2.0
1	B	278	GLU	2.0
1	A	80	GLU	2.0
1	B	113	TYR	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](#)

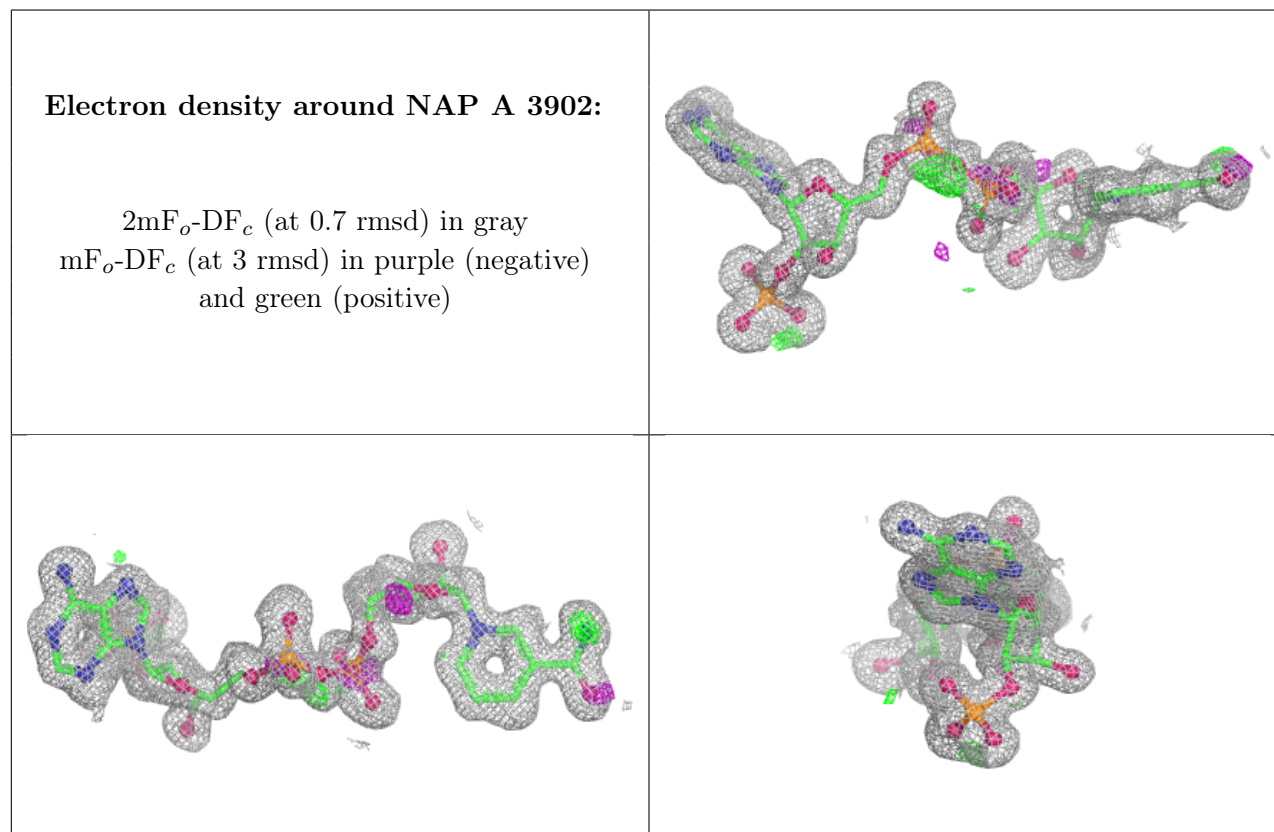
There are no oligosaccharides in this entry.

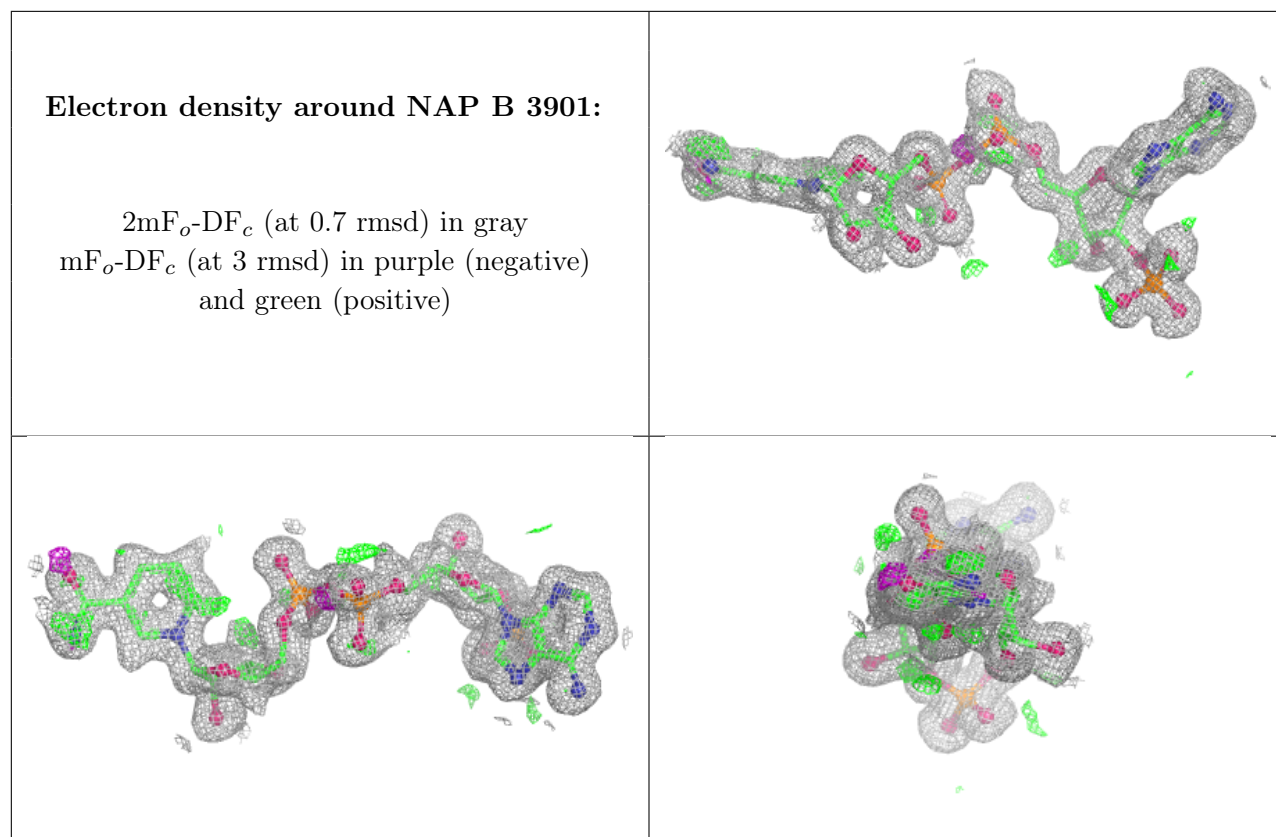
6.4 Ligands [i](#)

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
3	GOL	B	330	6/6	0.75	0.49	46,49,50,51	6
3	GOL	B	329	6/6	0.81	0.49	36,37,39,42	6
4	EPE	A	3999	15/15	0.84	0.15	30,34,35,35	0
2	NAP	A	3902	48/48	0.97	0.07	11,12,14,15	0
2	NAP	B	3901	48/48	0.97	0.06	9,12,14,14	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.