



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 05:38 AM EDT

PDB ID : 3O4R / pdb_00003o4r
Title : Crystal Structure of Human Dehydrogenase/Reductase (SDR family) member 4 (DHRS4)
Authors : Ugochukwu, E.; Bhatia, C.; Krojer, T.; Vollmar, M.; Yue, W.W.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; von Delft, F.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2010-07-27
Resolution : 1.70 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

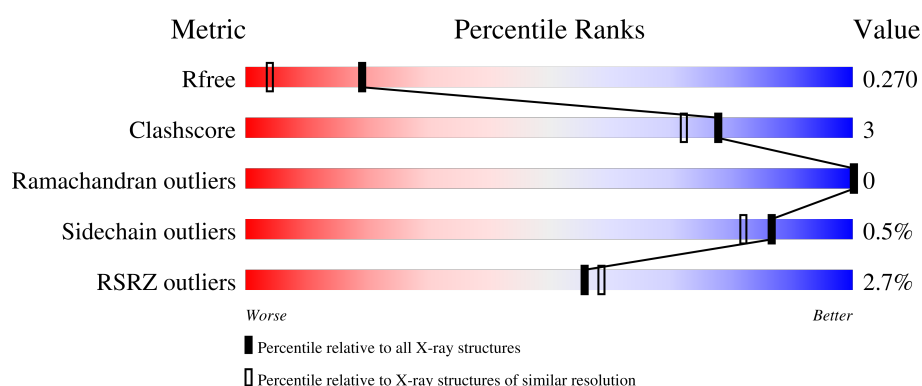
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	261	
1	B	261	
1	C	261	
1	D	261	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8296 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 Dehydrogenase/reductase SDR family member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	2	0
			1871	1173	324	363	11			
1	B	252	Total	C	N	O	S	0	5	0
			1878	1181	322	364	11			
1	C	253	Total	C	N	O	S	0	0	0
			1850	1163	319	358	10			
1	D	251	Total	C	N	O	S	0	1	0
			1856	1168	321	356	11			

There are 4 discrepancies between the modelled and reference sequences:

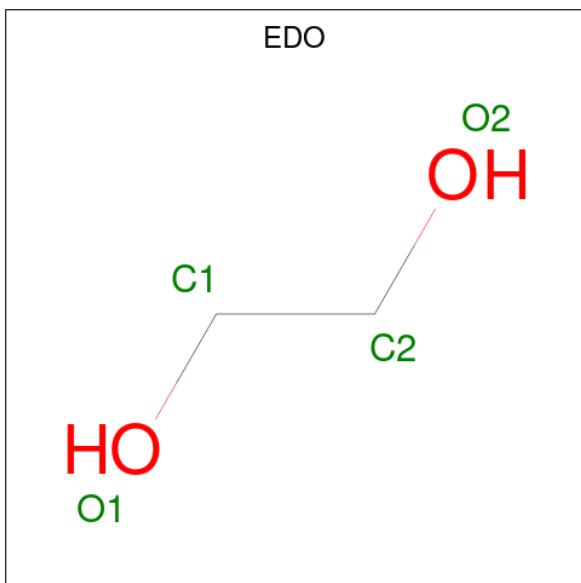
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	SER	-	expression tag	UNP Q9BTZ2
B	18	SER	-	expression tag	UNP Q9BTZ2
C	18	SER	-	expression tag	UNP Q9BTZ2
D	18	SER	-	expression tag	UNP Q9BTZ2

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



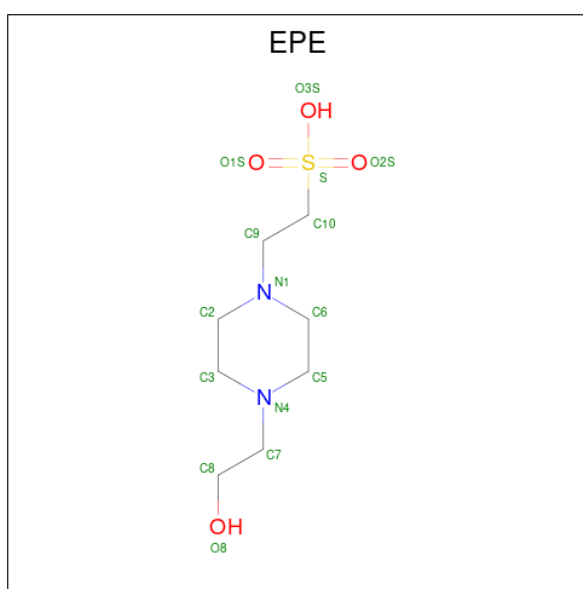
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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



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

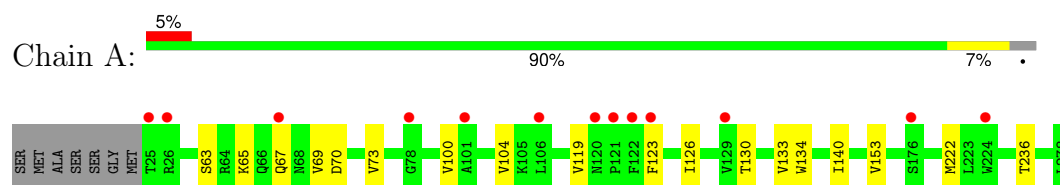
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	152	Total	O	0	0
			152	152		
6	B	177	Total	O	0	0
			177	177		
6	C	123	Total	O	0	0
			123	123		
6	D	154	Total	O	0	0
			154	154		

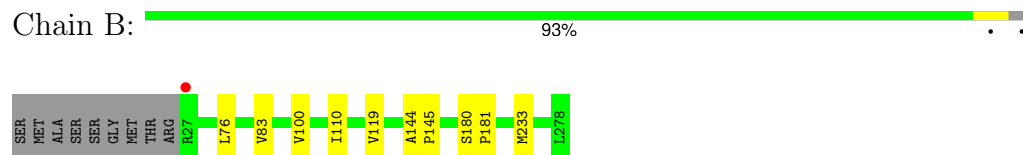
3 Residue-property plots [i](#)

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.

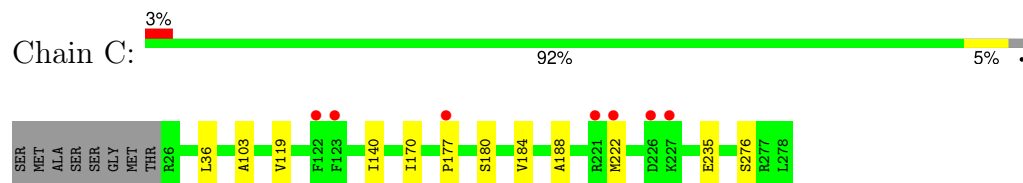
- Molecule 1: Dehydrogenase/reductase SDR family member 4



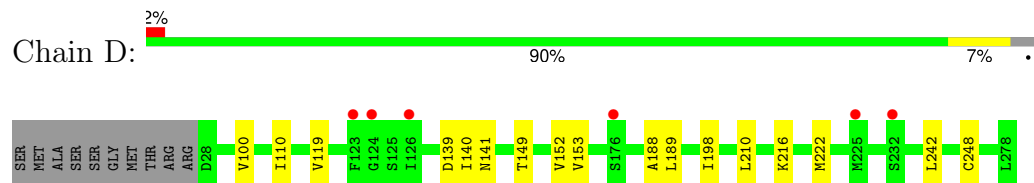
- Molecule 1: Dehydrogenase/reductase SDR family member 4



- Molecule 1: Dehydrogenase/reductase SDR family member 4



- Molecule 1: Dehydrogenase/reductase SDR family member 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.07Å 132.20Å 133.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.29 – 1.70 29.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.29-1.70) 98.6 (29.29-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.250 0.230 , 0.270	Depositor DCC
R_{free} test set	5820 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8296	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, NAP, GOL, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	1/1902 (0.1%)	0.80	0/2580
1	B	0.66	0/1919	0.82	0/2603
1	C	0.63	0/1876	0.81	0/2547
1	D	0.69	1/1885 (0.1%)	0.82	0/2555
All	All	0.67	2/7582 (0.0%)	0.81	0/10285

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	VAL	CA-CB	6.28	1.57	1.54
1	D	153	VAL	CA-CB	5.49	1.57	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1871	0	1895	15	0
1	B	1878	0	1911	9	0
1	C	1850	0	1865	8	0
1	D	1856	0	1894	11	0
2	A	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	D	4	0	6	0	0
4	A	15	0	17	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
6	A	152	0	0	7	0
6	B	177	0	0	3	0
6	C	123	0	0	2	0
6	D	154	0	0	2	0
All	All	8296	0	7722	41	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 3.

All (41) 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:119:VAL:HG23	6:B:303:HOH:O	1.60	1.02
1:B:119:VAL:CG2	6:B:303:HOH:O	2.12	0.97
1:A:67:GLN:O	6:A:593:HOH:O	1.92	0.87
1:A:119:VAL:HG23	6:A:373:HOH:O	1.80	0.80
1:A:119:VAL:O	6:A:373:HOH:O	2.12	0.68
1:C:119:VAL:HG23	6:C:425:HOH:O	1.93	0.67
1:D:222[B]:MET:HE3	6:D:611:HOH:O	1.97	0.65
1:A:70:ASP:N	6:A:593:HOH:O	2.31	0.63
1:A:119:VAL:CG2	6:A:373:HOH:O	2.43	0.62
1:D:100:VAL:HG13	1:D:110:ILE:CD1	2.31	0.60
1:A:126:ILE:HD11	1:A:134:TRP:HZ2	1.68	0.57
1:A:100:VAL:O	1:A:104:VAL:HG23	2.05	0.57
1:C:188:ALA:HB2	1:D:188:ALA:HB2	1.86	0.56
1:A:63:SER:OG	2:A:601:NAP:O2X	2.25	0.55
1:B:233[A]:MET:HA	1:B:233[A]:MET:HE2	1.89	0.54
1:C:177:PRO:HD3	1:D:198:ILE:HG21	1.95	0.49
1:A:69:VAL:O	1:A:73:VAL:HG23	2.14	0.48
1:A:67:GLN:C	6:A:593:HOH:O	2.49	0.48
1:C:119:VAL:HG13	1:C:140:ILE:HB	1.96	0.48
1:A:123:PHE:CD2	1:A:222[A]:MET:HE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:VAL:HG13	1:D:110:ILE:HD11	1.97	0.47
1:A:119:VAL:HG13	1:A:140:ILE:HB	1.97	0.47
1:B:180[B]:SER:OG	1:B:181:PRO:HD3	2.15	0.46
1:B:100:VAL:HG13	1:B:110:ILE:CD1	2.46	0.46
1:C:119:VAL:CG2	6:C:425:HOH:O	2.58	0.46
1:C:170:ILE:HD11	1:C:276:SER:HB3	1.98	0.46
1:D:119:VAL:HG13	1:D:140:ILE:HB	1.97	0.46
1:B:100:VAL:HG13	1:B:110:ILE:HD12	1.99	0.45
1:C:180:SER:O	1:C:184:VAL:HG23	2.17	0.44
1:D:149:THR:O	1:D:152:VAL:HG22	2.18	0.43
1:D:216:LYS:HG2	1:D:242:LEU:HD23	2.00	0.43
1:D:139:ASP:HB2	6:D:319:HOH:O	2.19	0.42
1:D:210:LEU:HD21	1:D:248:CYS:HB3	2.01	0.42
1:A:70:ASP:HB2	6:A:593:HOH:O	2.20	0.42
1:B:144:ALA:HB3	1:B:145:PRO:HD3	2.02	0.42
1:A:126:ILE:HD11	1:A:134:TRP:CZ2	2.53	0.42
1:A:130:THR:OG1	1:A:133:VAL:HG23	2.21	0.41
1:B:76:LEU:HD12	1:B:83:VAL:HG11	2.03	0.40
1:D:141:ASN:O	1:D:189:LEU:HD21	2.21	0.40
1:B:233[A]:MET:HE3	6:B:474:HOH:O	2.22	0.40
1:C:36:LEU:HD21	1:C:103:ALA:HB2	2.04	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	254/261 (97%)	248 (98%)	6 (2%)	0	100	100
1	B	255/261 (98%)	250 (98%)	5 (2%)	0	100	100
1	C	251/261 (96%)	247 (98%)	4 (2%)	0	100	100
1	D	250/261 (96%)	246 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1010/1044 (97%)	991 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/212 (94%)	198 (99%)	2 (1%)	73	64
1	B	203/212 (96%)	203 (100%)	0	100	100
1	C	196/212 (92%)	194 (99%)	2 (1%)	73	64
1	D	199/212 (94%)	199 (100%)	0	100	100
All	All	798/848 (94%)	794 (100%)	4 (0%)	86	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	236	THR
1	C	222	MET
1	C	235	GLU

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

Mol	Chain	Res	Type
1	B	120	ASN
1	C	71	GLN

5.3.3 RNA ⓘ

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](#)

11 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	A	601	-	46,52,52	1.18	1 (2%)	61,80,80	1.37	9 (14%)
3	EDO	B	702	-	3,3,3	0.46	0	2,2,2	0.19	0
4	EPE	A	705	-	15,15,15	0.86	1 (6%)	19,20,20	1.98	6 (31%)
3	EDO	D	701	-	3,3,3	0.44	0	2,2,2	0.31	0
5	GOL	C	706	-	5,5,5	0.36	0	5,5,5	0.26	0
3	EDO	B	704	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	A	703	-	3,3,3	0.41	0	2,2,2	0.42	0
2	NAP	B	602	-	46,52,52	1.22	3 (6%)	61,80,80	1.44	7 (11%)
5	GOL	B	707	-	5,5,5	0.40	0	5,5,5	0.37	0
2	NAP	C	604	-	46,52,52	1.18	4 (8%)	61,80,80	1.51	8 (13%)
2	NAP	D	603	-	46,52,52	1.35	5 (10%)	61,80,80	1.52	10 (16%)

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	A	601	-	-	2/31/67/67	0/5/5/5
3	EDO	B	702	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	A	705	-	-	4/9/19/19	0/1/1/1
3	EDO	D	701	-	-	0/1/1/1	-
5	GOL	C	706	-	-	3/4/4/4	-
3	EDO	B	704	-	-	0/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-
2	NAP	B	602	-	-	0/31/67/67	0/5/5/5
5	GOL	B	707	-	-	2/4/4/4	-
2	NAP	C	604	-	-	2/31/67/67	0/5/5/5
2	NAP	D	603	-	-	4/31/67/67	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	603	NAP	O7N-C7N	5.91	1.35	1.24
2	A	601	NAP	O7N-C7N	5.53	1.34	1.24
2	B	602	NAP	O7N-C7N	5.19	1.33	1.24
2	C	604	NAP	O7N-C7N	4.59	1.32	1.24
2	D	603	NAP	PN-O3	3.55	1.63	1.59
2	C	604	NAP	PA-O3	3.52	1.63	1.59
4	A	705	EPE	C10-S	2.98	1.81	1.77
2	B	602	NAP	PN-O3	2.89	1.62	1.59
2	D	603	NAP	C8A-N7A	2.63	1.39	1.34
2	B	602	NAP	O4B-C1B	2.47	1.44	1.40
2	C	604	NAP	PN-O3	2.38	1.62	1.59
2	C	604	NAP	O4D-C1D	2.30	1.43	1.40
2	D	603	NAP	O4B-C1B	2.12	1.43	1.40
2	D	603	NAP	PA-O3	2.08	1.61	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	603	NAP	N3A-C2A-N1A	-6.27	120.16	128.67
2	C	604	NAP	N3A-C2A-N1A	-6.03	120.49	128.67
4	A	705	EPE	C6-C5-N4	4.75	120.23	110.65
2	A	601	NAP	N3A-C2A-N1A	-4.66	122.34	128.67
2	B	602	NAP	N3A-C2A-N1A	-4.54	122.51	128.67
2	C	604	NAP	C2B-C1B-N9A	4.01	121.47	112.56
4	A	705	EPE	C5-N4-C3	3.71	116.84	108.84
2	D	603	NAP	O2A-PA-O3	3.62	117.07	107.27
2	B	602	NAP	C2B-C1B-N9A	3.34	119.98	112.56
2	B	602	NAP	C4D-O4D-C1D	-3.23	106.97	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NAP	C5D-C4D-C3D	-3.11	104.00	115.21
2	A	601	NAP	C2B-C1B-N9A	3.10	119.44	112.56
2	C	604	NAP	C3N-C7N-N7N	3.01	121.45	117.74
2	D	603	NAP	C2B-C1B-N9A	2.93	119.06	112.56
2	A	601	NAP	C4A-C5A-N7A	-2.92	106.25	109.34
2	C	604	NAP	O3X-P2B-O2X	2.76	118.16	107.80
2	D	603	NAP	C4D-O4D-C1D	-2.65	107.50	109.92
2	A	601	NAP	O3X-P2B-O2X	2.62	117.63	107.80
2	A	601	NAP	C4D-O4D-C1D	-2.59	107.55	109.92
4	A	705	EPE	C5-C6-N1	2.53	115.76	110.65
2	C	604	NAP	C4D-O4D-C1D	-2.51	107.63	109.92
4	A	705	EPE	O3S-S-C10	2.45	110.81	106.00
4	A	705	EPE	C2-C3-N4	2.44	115.57	110.65
2	D	603	NAP	O7N-C7N-C3N	2.38	122.51	119.60
4	A	705	EPE	C9-N1-C6	2.38	117.57	111.24
2	A	601	NAP	O5D-PN-O1N	-2.32	99.76	108.94
2	C	604	NAP	O4B-C1B-N9A	-2.30	105.69	108.75
2	A	601	NAP	O4B-C1B-N9A	-2.29	105.71	108.75
2	D	603	NAP	O2N-PN-O5D	2.28	117.89	107.57
2	B	602	NAP	O7N-C7N-C3N	2.25	122.34	119.60
2	C	604	NAP	O7N-C7N-N7N	-2.21	119.42	122.62
2	C	604	NAP	O4B-C1B-C2B	-2.18	102.88	106.61
2	A	601	NAP	O2N-PN-O1N	2.18	122.57	112.44
2	D	603	NAP	C1B-N9A-C4A	-2.14	122.89	126.64
2	D	603	NAP	C3B-C2B-C1B	-2.13	98.73	102.81
2	D	603	NAP	O5D-PN-O1N	-2.10	100.60	108.94
2	A	601	NAP	C5D-C4D-C3D	-2.10	107.65	115.21
2	D	603	NAP	O3-PA-O1A	-2.08	104.44	110.70
2	B	602	NAP	C2D-C3D-C4D	-2.06	98.62	102.61
2	B	602	NAP	O2N-PN-O3	2.01	112.71	107.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	603	NAP	C5D-O5D-PN-O3
2	D	603	NAP	C5D-O5D-PN-O2N
4	A	705	EPE	C10-C9-N1-C6
5	C	706	GOL	O1-C1-C2-O2
5	B	707	GOL	C1-C2-C3-O3
5	C	706	GOL	O1-C1-C2-C3
5	B	707	GOL	O2-C2-C3-O3

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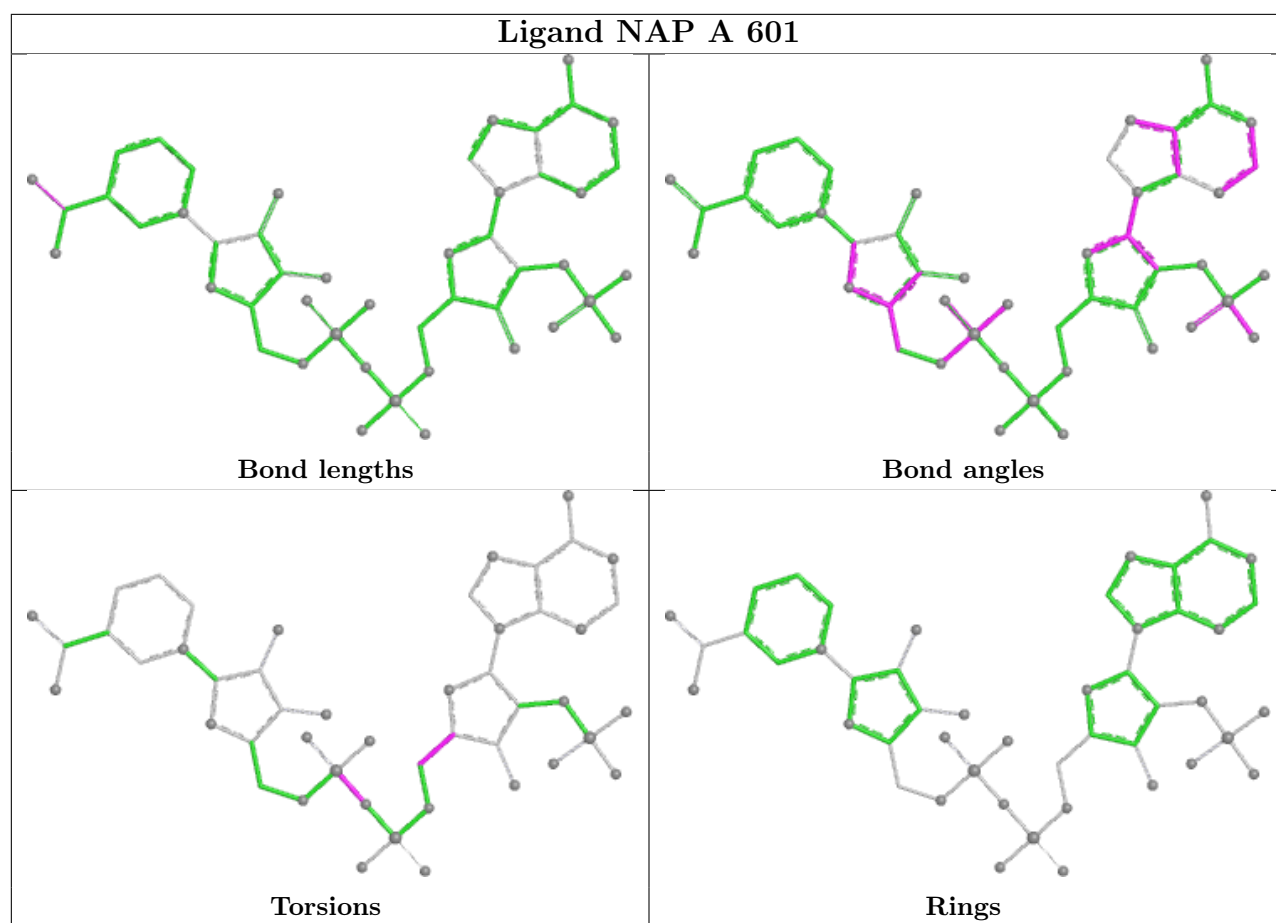
Mol	Chain	Res	Type	Atoms
2	D	603	NAP	C5D-O5D-PN-O1N
4	A	705	EPE	C10-C9-N1-C2
5	C	706	GOL	C1-C2-C3-O3
4	A	705	EPE	C9-C10-S-O3S
2	C	604	NAP	O4D-C4D-C5D-O5D
3	B	702	EDO	O1-C1-C2-O2
4	A	705	EPE	C9-C10-S-O1S
2	A	601	NAP	O4B-C4B-C5B-O5B
2	C	604	NAP	C3D-C4D-C5D-O5D
2	A	601	NAP	PA-O3-PN-O2N
2	D	603	NAP	PA-O3-PN-O1N

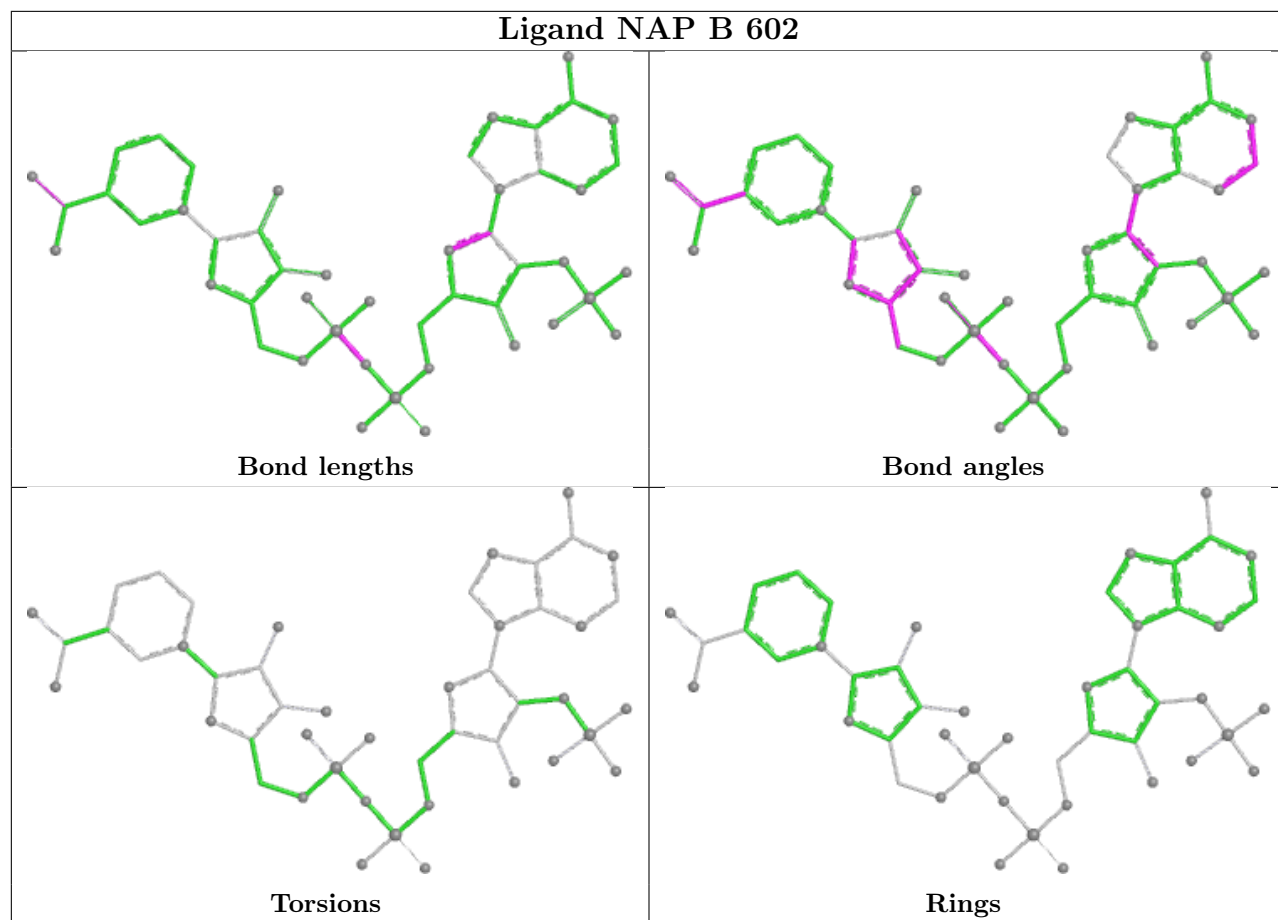
There are no ring outliers.

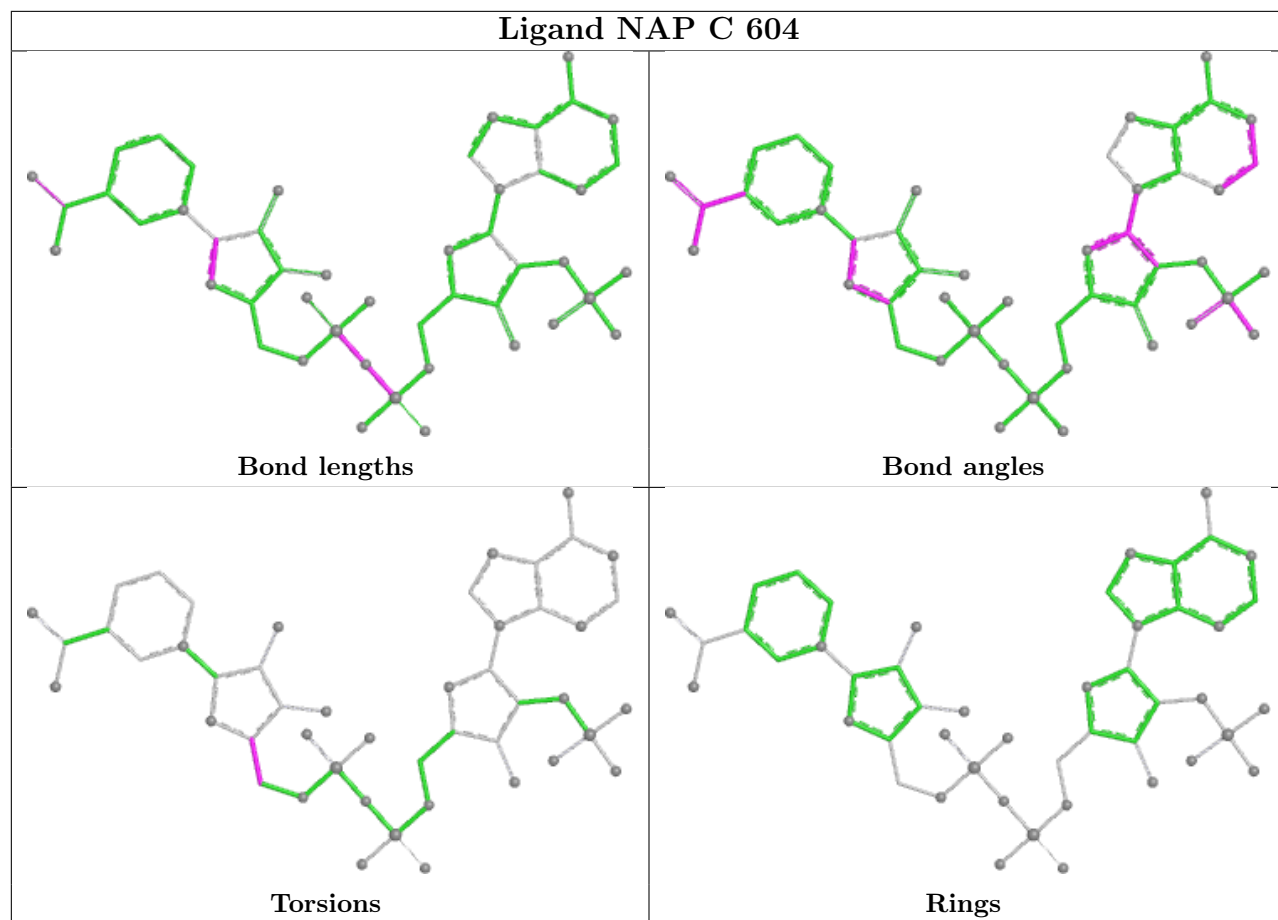
1 monomer is involved in 1 short contact:

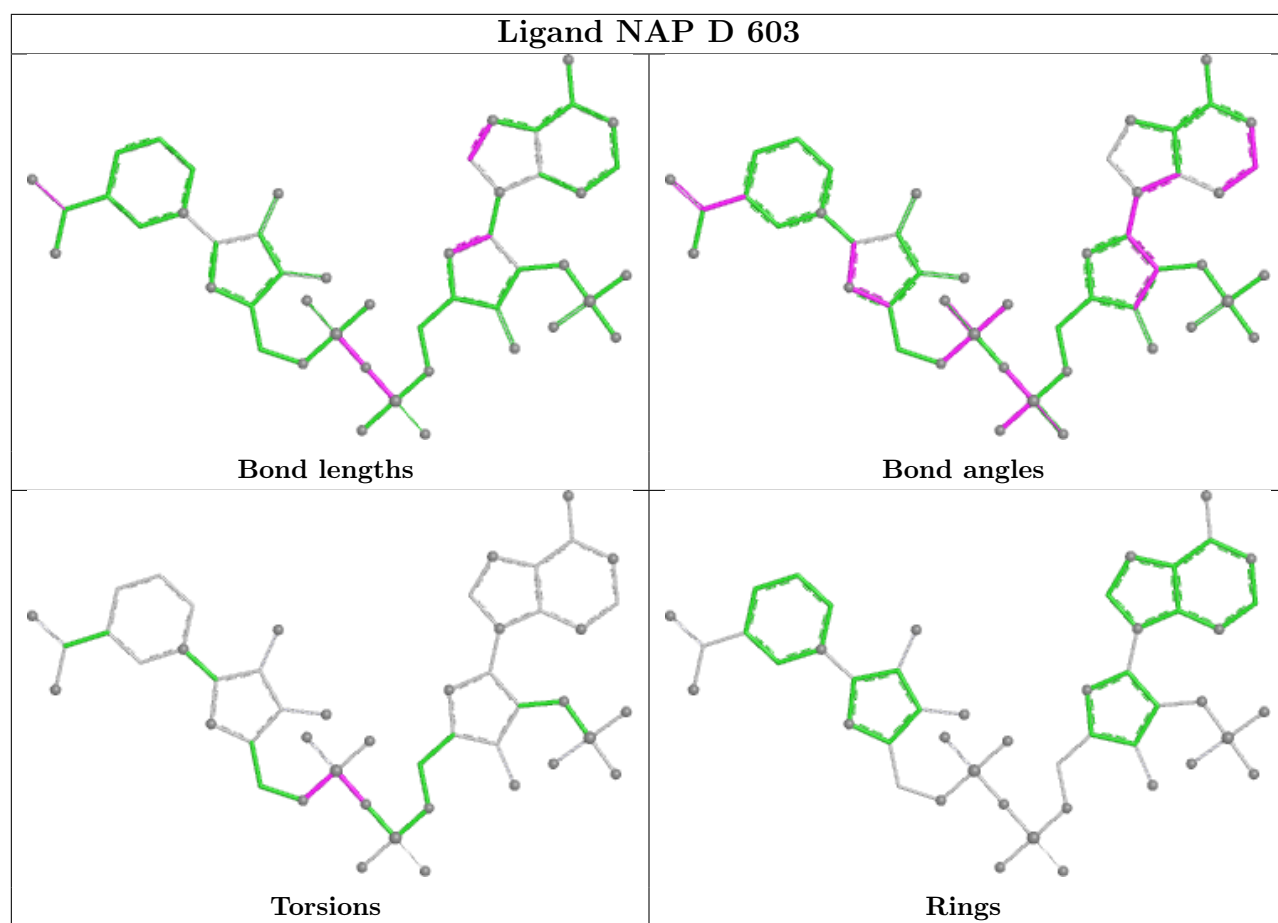
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAP	1	0

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	254/261 (97%)	0.34	13 (5%) 34 37	20, 31, 47, 66	2 (0%)
1	B	252/261 (96%)	0.27	1 (0%) 89 90	15, 31, 45, 63	5 (1%)
1	C	253/261 (96%)	0.33	7 (2%) 55 58	21, 32, 49, 70	0
1	D	251/261 (96%)	0.28	6 (2%) 59 62	21, 31, 44, 52	1 (0%)
All	All	1010/1044 (96%)	0.30	27 (2%) 56 58	15, 31, 46, 70	8 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	ASP	4.3
1	A	67	GLN	3.5
1	B	27	ARG	3.2
1	C	227	LYS	3.2
1	A	78	GLY	3.2
1	C	122	PHE	3.1
1	A	120	ASN	3.1
1	A	25	THR	3.1
1	A	122	PHE	2.9
1	C	123	PHE	2.8
1	C	177	PRO	2.8
1	A	123	PHE	2.7
1	A	121	PRO	2.6
1	C	222	MET	2.6
1	D	126	ILE	2.6
1	A	26	ARG	2.5
1	A	101	ALA	2.5
1	D	123	PHE	2.4
1	C	221	ARG	2.4
1	A	176	SER	2.4
1	A	129	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	124	GLY	2.3
1	D	232	SER	2.2
1	A	106	LEU	2.1
1	A	224	TRP	2.1
1	D	225	MET	2.0
1	D	176	SER	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 monosaccharides in this entry.

6.4 Ligands [i](#)

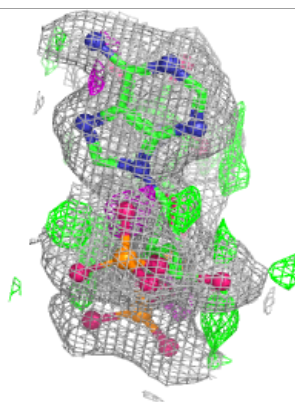
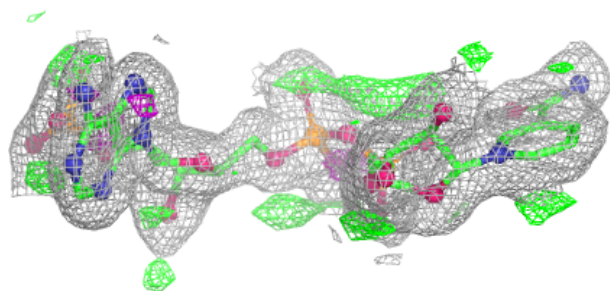
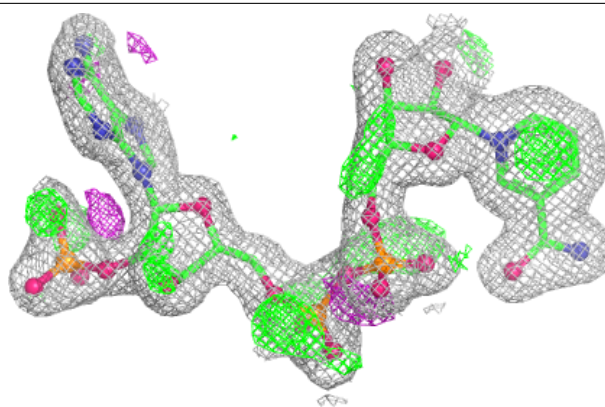
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	EPE	A	705	15/15	0.66	0.17	70,90,95,95	0
5	GOL	B	707	6/6	0.79	0.14	57,61,62,62	0
5	GOL	C	706	6/6	0.79	0.14	49,63,66,67	0
3	EDO	B	702	4/4	0.85	0.15	52,56,56,56	0
3	EDO	B	704	4/4	0.87	0.11	52,54,54,57	0
3	EDO	A	703	4/4	0.87	0.14	49,51,54,58	0
3	EDO	D	701	4/4	0.89	0.16	48,48,49,50	0
2	NAP	A	601	48/48	0.94	0.08	18,28,36,37	0
2	NAP	C	604	48/48	0.96	0.08	26,33,37,40	0
2	NAP	B	602	48/48	0.96	0.07	18,26,30,37	0
2	NAP	D	603	48/48	0.97	0.06	15,27,32,35	0

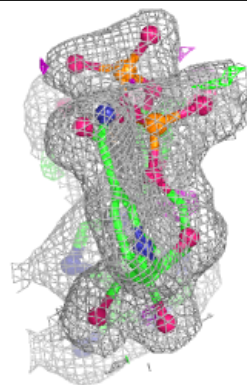
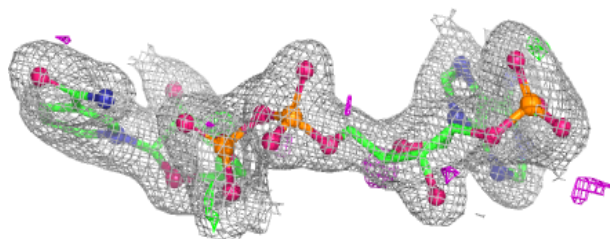
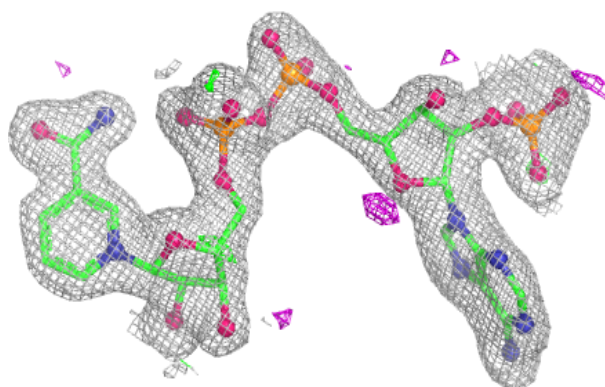
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 601:

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

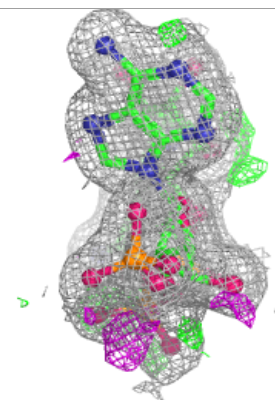
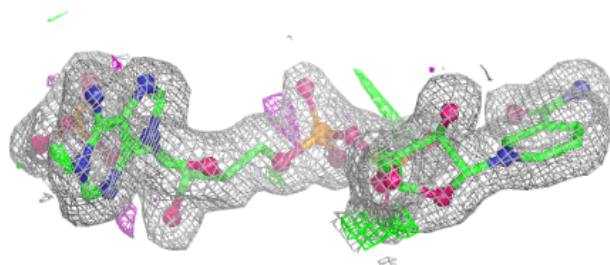
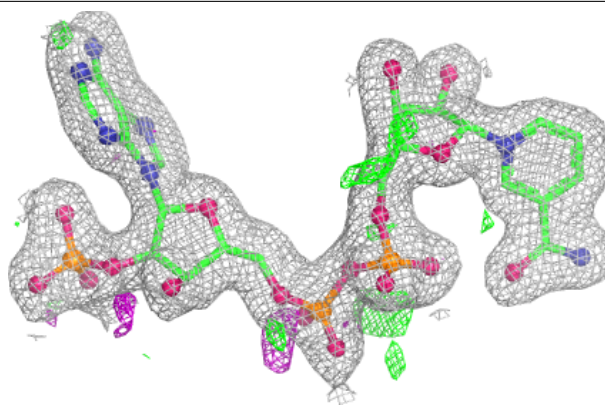
**Electron density around NAP C 604:**

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

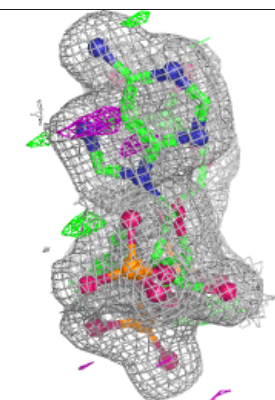
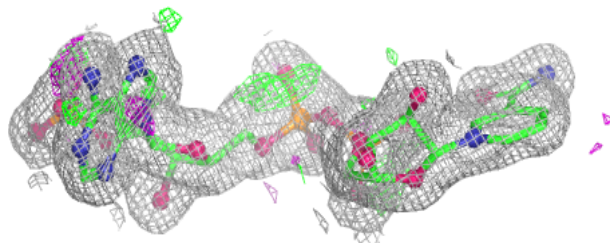
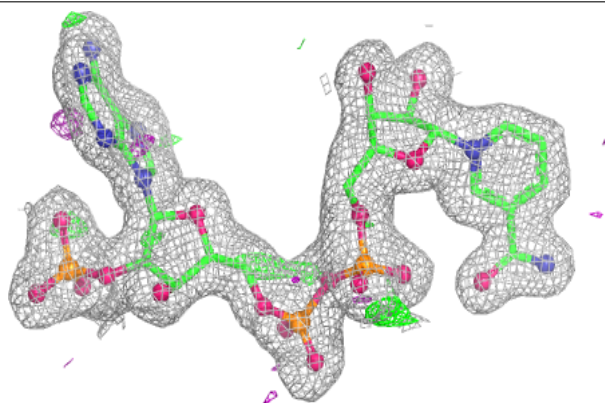


Electron density around NAP B 602:

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

**Electron density around NAP D 603:**

$2mF_o-DF_c$ (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.