



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 07:57 PM UTC

PDB ID : 5MSR / pdb_00005msr
Title : Structure of the unmodified PCP-R domain of carboxylic acid reductase (CAR) from *Segniliparus rugosus* in complex with NADPH, P43 form
Authors : Gahloth, D.; Leys, D.
Deposited on : 2017-01-05
Resolution : 2.37 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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

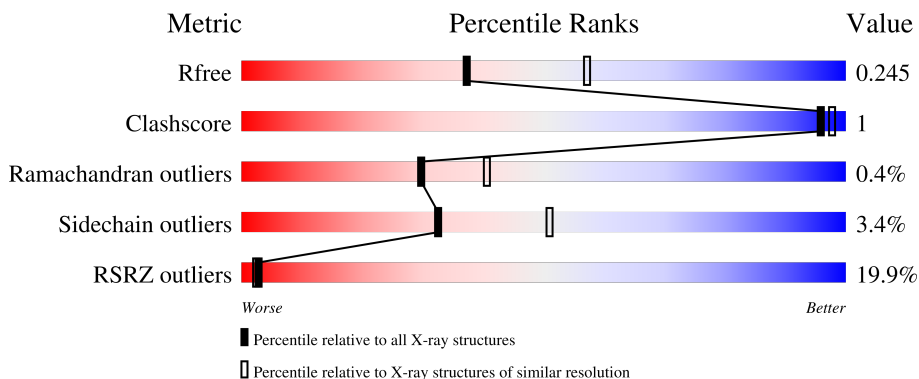
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	1188	 8% 41% 57%
1	B	1188	 7% 42% 56%
1	C	1188	 8% 41% 57%
1	D	1188	 12% 40% 58%

2 Entry composition [i](#)

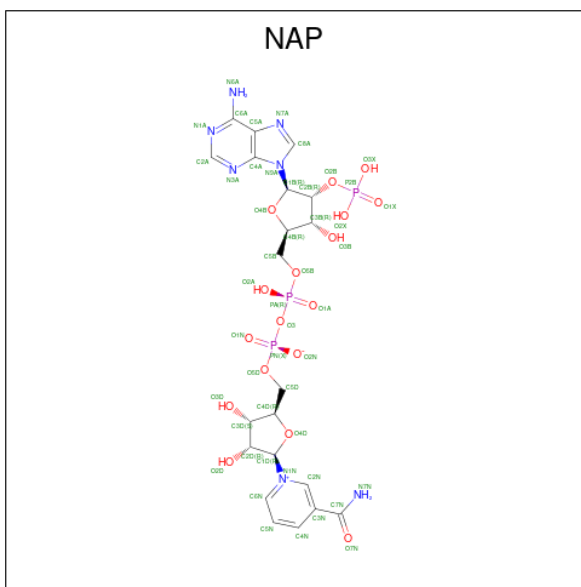
There are 3 unique types of molecules in this entry. The entry contains 16105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thioester reductase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	0	0
			3926	2492	687	746	1			
1	B	520	Total	C	N	O	S	0	0	0
			3973	2519	693	760	1			
1	C	516	Total	C	N	O	S	0	0	0
			3944	2504	689	750	1			
1	D	504	Total	C	N	O	S	0	0	0
			3869	2461	676	731	1			

- 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	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			40	15	6	16	3		
2	B	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			40	15	6	16	3		
2	D	1	Total	C	N	O	P	0	0
			40	15	6	16	3		

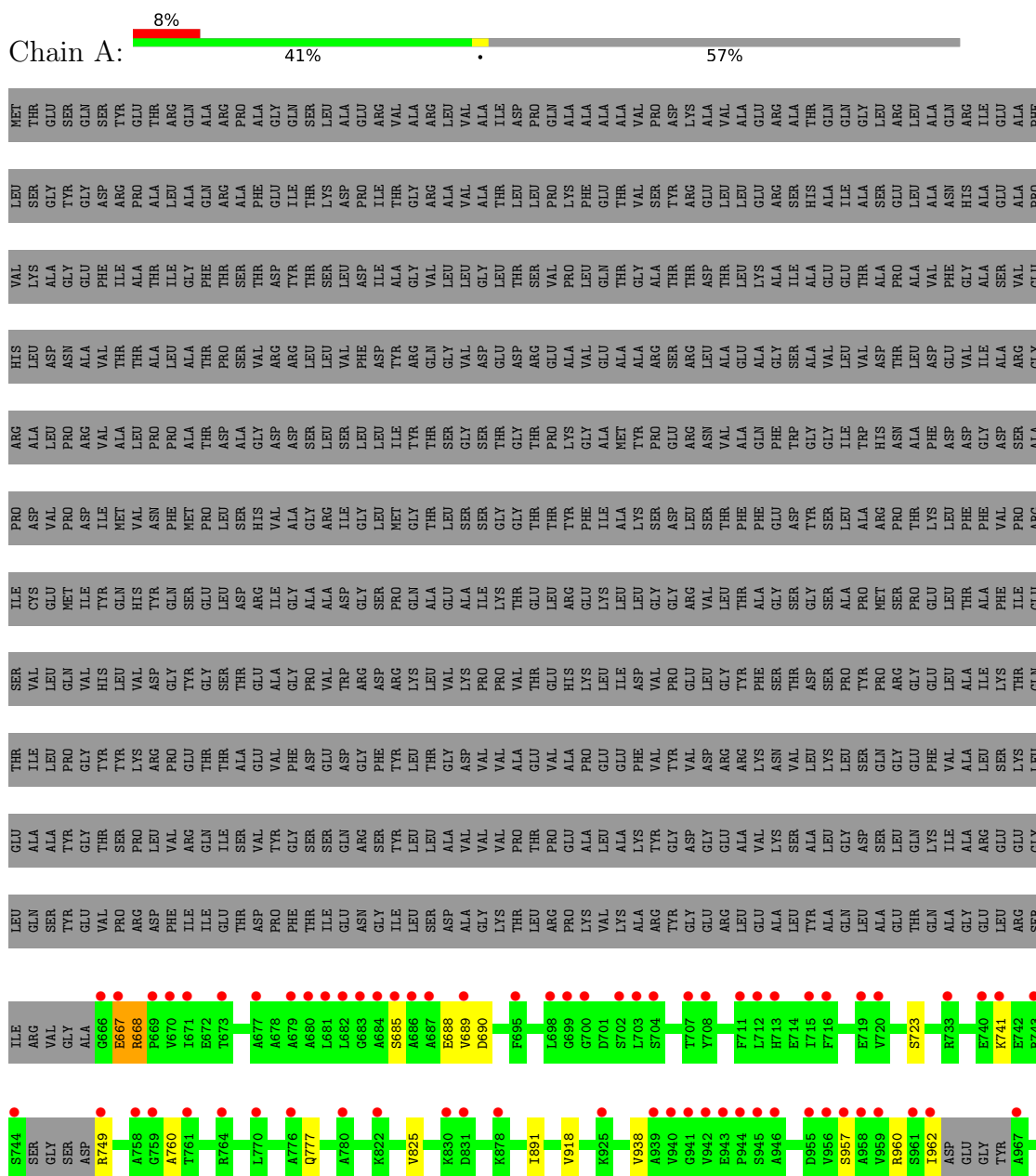
- Molecule 3 is water.

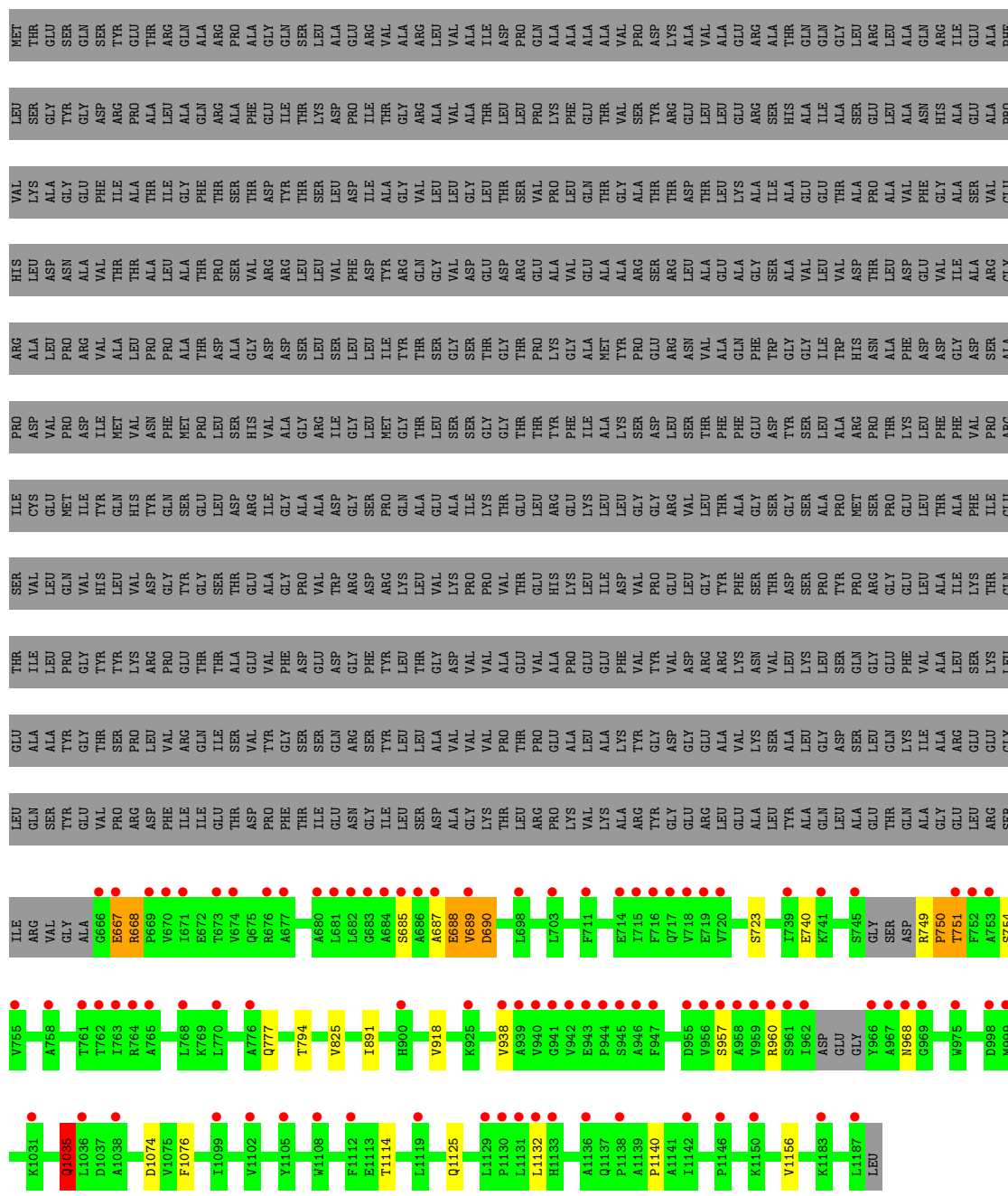
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	75	Total	O	0	0
			75	75		
3	C	58	Total	O	0	0
			58	58		
3	D	37	Total	O	0	0
			37	37		

3 Residue-property plots [i](#)

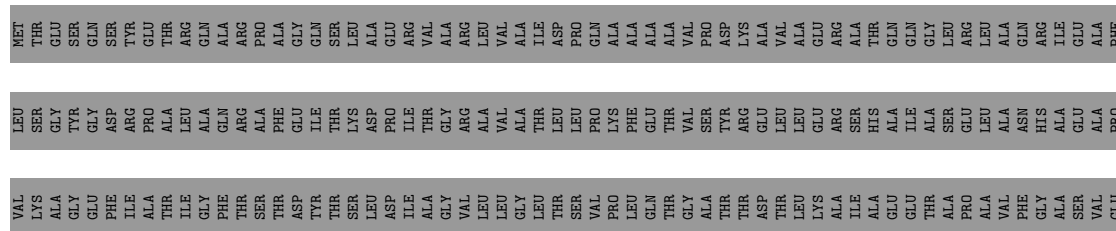
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Thioester reductase domain-containing protein





● Molecule 1: Thioester reductase domain-containing protein



Q1153	B1048	V938	S747	I1153	LEU
V1156	E1057	A939	D748	ARG	GLN
Q1157	L1064	V940	R749	VAL	TYR
E1158	L1064	G941	GLY	ALA	THR
B1181	F1076	V942	A753	GLY	THR
L1187	F1076	E943	S754	GLY	PRO
LEU	V1093	P944	V755	ARG	ARG
	E1094	S945	H756	ASP	PRO
	A1095	A946	G757	PHE	LEU
	I1099	F947	A758	ILE	VAL
	S1100	E948	G759	ILE	GLN
	R1101	I953	A760	THR	LEU
	V1105	R954	T761	THR	ASP
	A1106	D955	I762	ASP	VAL
	E1107	D955	I763	TYR	GLY
	V1108	V956	R764	PHE	GLY
	V1109	S957	A677	THR	ALA
	F1112	A958	A679	SER	PRO
	E1113	R960	A680	VAL	ALA
	T1114	R962	L681	TRP	ALA
	S1115	I962	L682	ASP	GLY
	L1116	ASP	L770	GLY	LEU
	P1119	GLY	L774	LEU	LEU
	L1120	GLY	Q777	ALA	ALA
	E1121	Y966	I778	VAL	VAL
	A1122	A967	L779	GLY	ILE
	Q1125	N968	A780	LYS	VAL
	H1126	R982	A781	THR	PRO
	L1129	R982	A782	THR	ALA
	P1130	D998	L785	LEU	THR
	L1131	M999	L785	ARG	PRO
	H1133	D1014	V792	LYS	ALA
	A1134	L1023	R793	VAL	LEU
	F1135	L1024	T798	ALA	ALA
	A1136	A1025	F715	LYS	LYS
	Q1137	T1026	F716	THR	ILE
	P1138	G1027	E714	ARG	LEU
	A1139	I1028	I715	VAL	LEU
	A1141	K1031	F717	ASP	LEU
	I1142	Y1034	Q717	GLY	VAL
	D1143	GLN	G820	GLY	THR
	G1144	LEU	G821	ARG	VAL
	S1145	ASP	K822	VAL	ALA
	P1146	ALA	V825	VAL	LYS
	F1147	LEU	K833	THR	ASN
	Q1148	LEU	D859	VAL	VAL
	T1149	ASP	D886	THR	ASP
	K1150	ALA	D886	GLY	TRP
	M1151	GLY	I891	THR	ASN
	F1152	GLY	V818	THR	THR
		R1042	E742	THR	ALA
		Q1043	K741	LEU	LEU
		R1044	E742	ALA	ASP
		A1045	R743	LEU	ASP
		H1046	S744	GLY	ASP
		Y1047	S744	LEU	ALA
			GLY	THR	ALA
				LEU	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	94.94Å 94.94Å 335.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 2.37 94.94 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.7 (200.00-2.37) 98.7 (94.94-2.37)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.219 , 0.241 0.229 , 0.245	Depositor DCC
R_{free} test set	5667 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtrriage
Anisotropy	0.011	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16105	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: 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	0.61	0/4011	0.86	2/5457 (0.0%)
1	B	0.61	0/4060	0.91	4/5525 (0.1%)
1	C	0.61	0/4030	0.89	7/5483 (0.1%)
1	D	0.61	1/3953 (0.0%)	0.87	1/5376 (0.0%)
All	All	0.61	1/16054 (0.0%)	0.88	14/21841 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	999	MET	CA-CB	5.32	1.61	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	940	VAL	N-CA-C	13.02	125.46	110.62
1	C	688	GLU	CA-C-N	8.59	137.16	121.70
1	C	688	GLU	C-N-CA	8.59	137.16	121.70
1	D	1149	THR	CB-CA-C	-7.54	96.82	109.03
1	C	750	PRO	N-CA-C	7.14	127.17	112.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	924	THR	Peptide

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	3926	0	3880	5	0
1	B	3973	0	3912	4	1
1	C	3944	0	3894	9	1
1	D	3869	0	3825	16	0
2	A	40	0	19	0	0
2	B	40	0	19	0	0
2	C	40	0	19	0	0
2	D	40	0	19	0	0
3	A	63	0	0	0	0
3	B	75	0	0	0	0
3	C	58	0	0	0	0
3	D	37	0	0	0	0
All	All	16105	0	15587	34	1

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 1.

The worst 5 of 34 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:782:ALA:HA	1:D:785:LEU:HD12	1.57	0.86
1:C:750:PRO:O	1:C:754:SER:OG	2.05	0.75
1:D:785:LEU:HD23	1:D:926:ARG:HA	1.67	0.74
1:A:667:GLU:HB2	1:A:668:ARG:HB2	1.75	0.69
1:D:1076:PHE:CE1	1:D:1149:THR:OG1	2.46	0.68

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:LYS:NZ	1:C:740:GLU:OE1[3_664]	2.14	0.06

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	508/1188 (43%)	491 (97%)	15 (3%)	2 (0%)	30 40
1	B	516/1188 (43%)	499 (97%)	15 (3%)	2 (0%)	30 40
1	C	510/1188 (43%)	490 (96%)	18 (4%)	2 (0%)	30 40
1	D	494/1188 (42%)	477 (97%)	14 (3%)	3 (1%)	21 30
All	All	2028/4752 (43%)	1957 (96%)	62 (3%)	9 (0%)	30 40

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	ARG
1	B	668	ARG
1	B	749	ARG
1	C	668	ARG
1	D	690	ASP

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	409/947 (43%)	396 (97%)	13 (3%)	34 53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	414/947 (44%)	401 (97%)	13 (3%)	35	54
1	C	411/947 (43%)	396 (96%)	15 (4%)	31	49
1	D	405/947 (43%)	391 (96%)	14 (4%)	32	50
All	All	1639/3788 (43%)	1584 (97%)	55 (3%)	32	51

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	690	ASP
1	C	968	ASN
1	D	1156	VAL
1	D	957	SER
1	C	723	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1011	ASN
1	C	1125	GLN
1	D	1125	GLN
1	D	675	GLN
1	B	1148	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

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	A	1201	-	42,43,52	1.28	6 (14%)	62,67,80	1.64	10 (16%)
2	NAP	B	1201	-	42,43,52	1.26	6 (14%)	62,67,80	1.65	11 (17%)
2	NAP	D	1201	-	42,43,52	1.21	5 (11%)	62,67,80	1.67	12 (19%)
2	NAP	C	1201	-	42,43,52	1.29	5 (11%)	62,67,80	1.68	11 (17%)

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	1201	-	-	4/27/59/67	0/4/4/5
2	NAP	B	1201	-	-	3/27/59/67	0/4/4/5
2	NAP	D	1201	-	-	5/27/59/67	0/4/4/5
2	NAP	C	1201	-	-	3/27/59/67	0/4/4/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	NAP	C5A-C4A	4.71	1.47	1.39
2	A	1201	NAP	C5A-C4A	4.62	1.47	1.39
2	D	1201	NAP	C5A-C4A	4.54	1.47	1.39
2	B	1201	NAP	C5A-C4A	4.50	1.47	1.39
2	A	1201	NAP	C5A-C6A	2.82	1.48	1.41

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	NAP	C5A-C4A-N3A	-5.54	119.08	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	NAP	C5A-C4A-N3A	-5.52	119.12	126.72
2	C	1201	NAP	C5A-C4A-N3A	-5.39	119.29	126.72
2	D	1201	NAP	C5A-C4A-N3A	-5.08	119.72	126.72
2	B	1201	NAP	N3A-C4A-N9A	4.70	135.16	127.17

There are no chirality outliers.

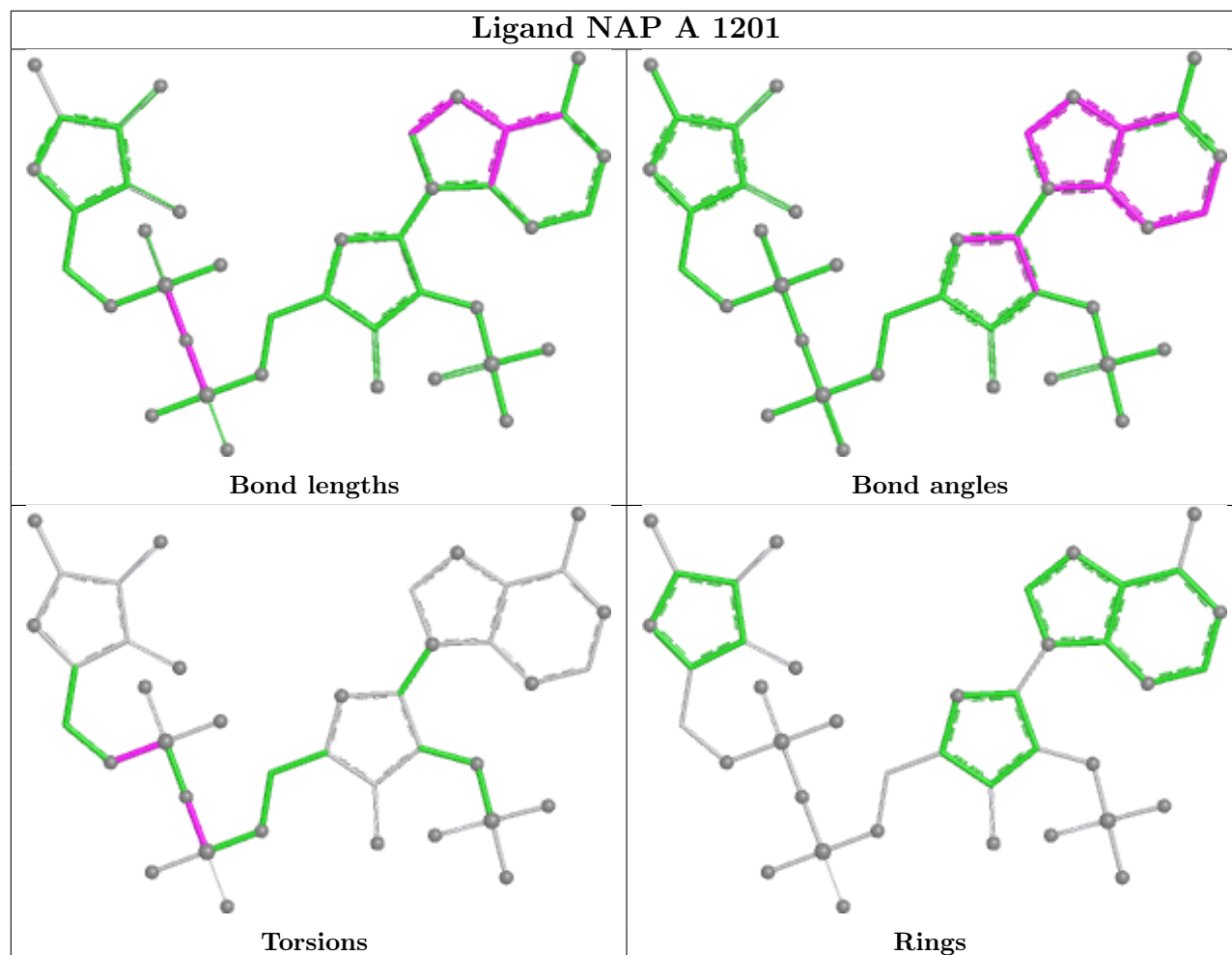
5 of 15 torsion outliers are listed below:

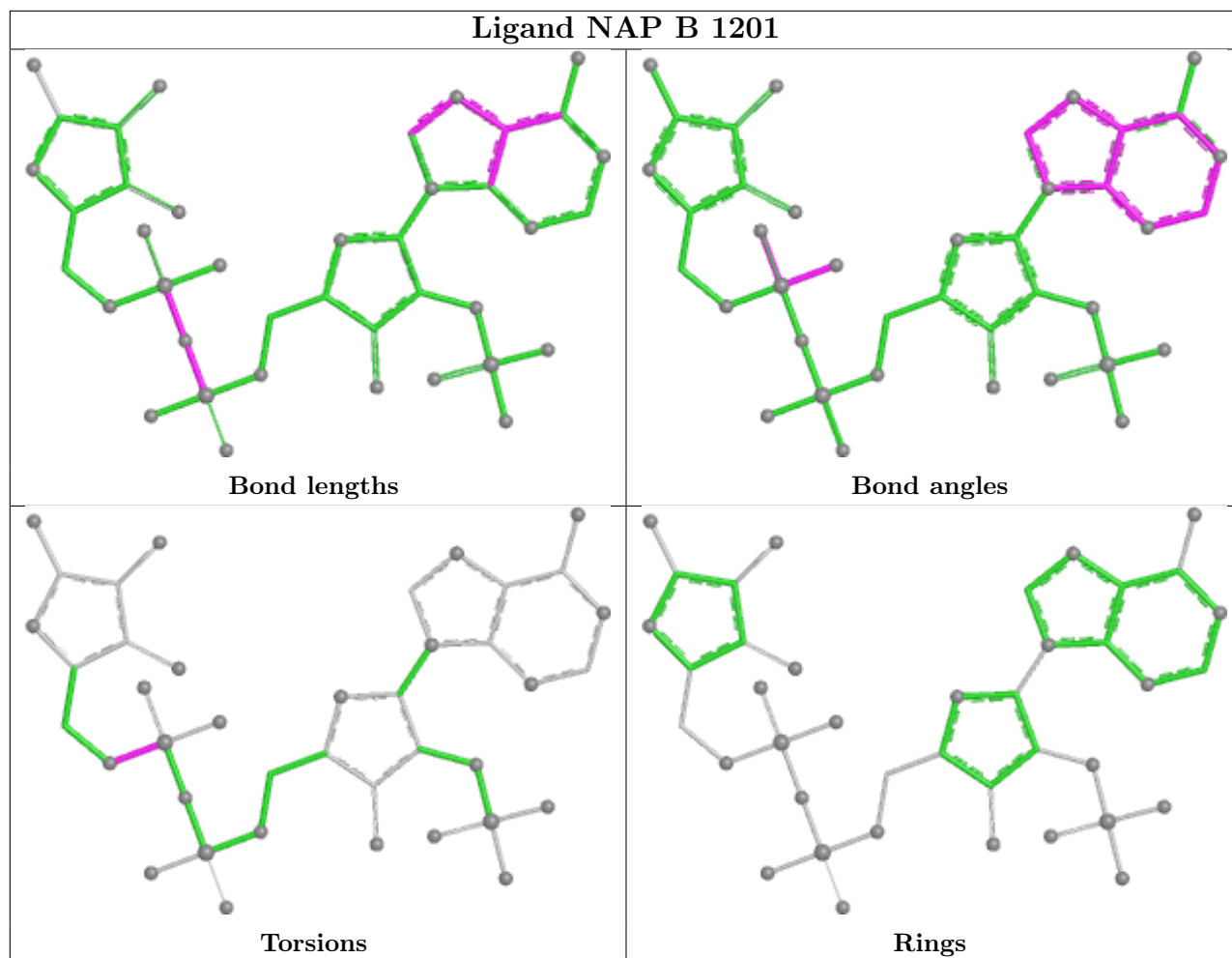
Mol	Chain	Res	Type	Atoms
2	A	1201	NAP	C5D-O5D-PN-O3
2	A	1201	NAP	C5D-O5D-PN-O2N
2	B	1201	NAP	C5D-O5D-PN-O3
2	B	1201	NAP	C5D-O5D-PN-O1N
2	B	1201	NAP	C5D-O5D-PN-O2N

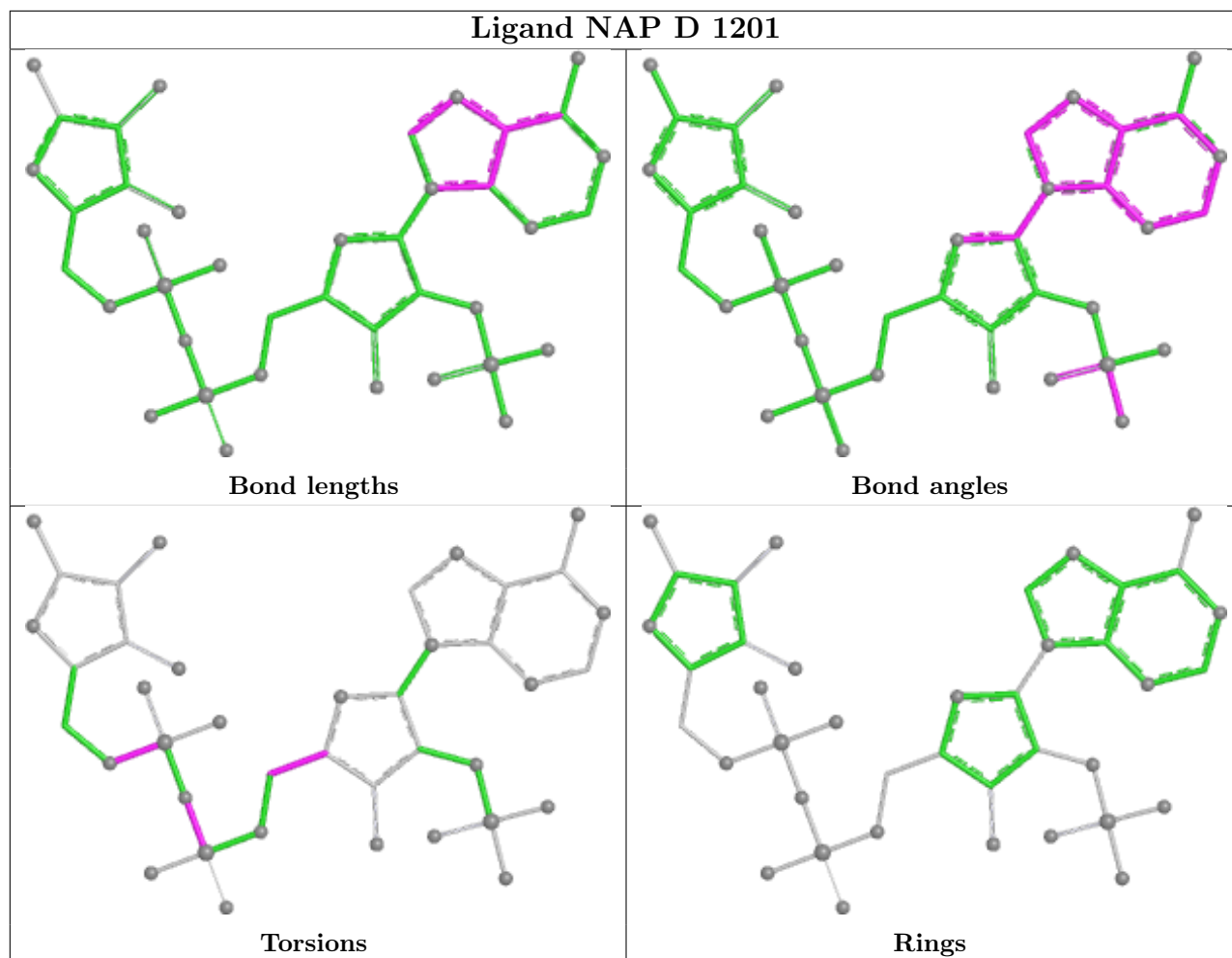
There are no ring outliers.

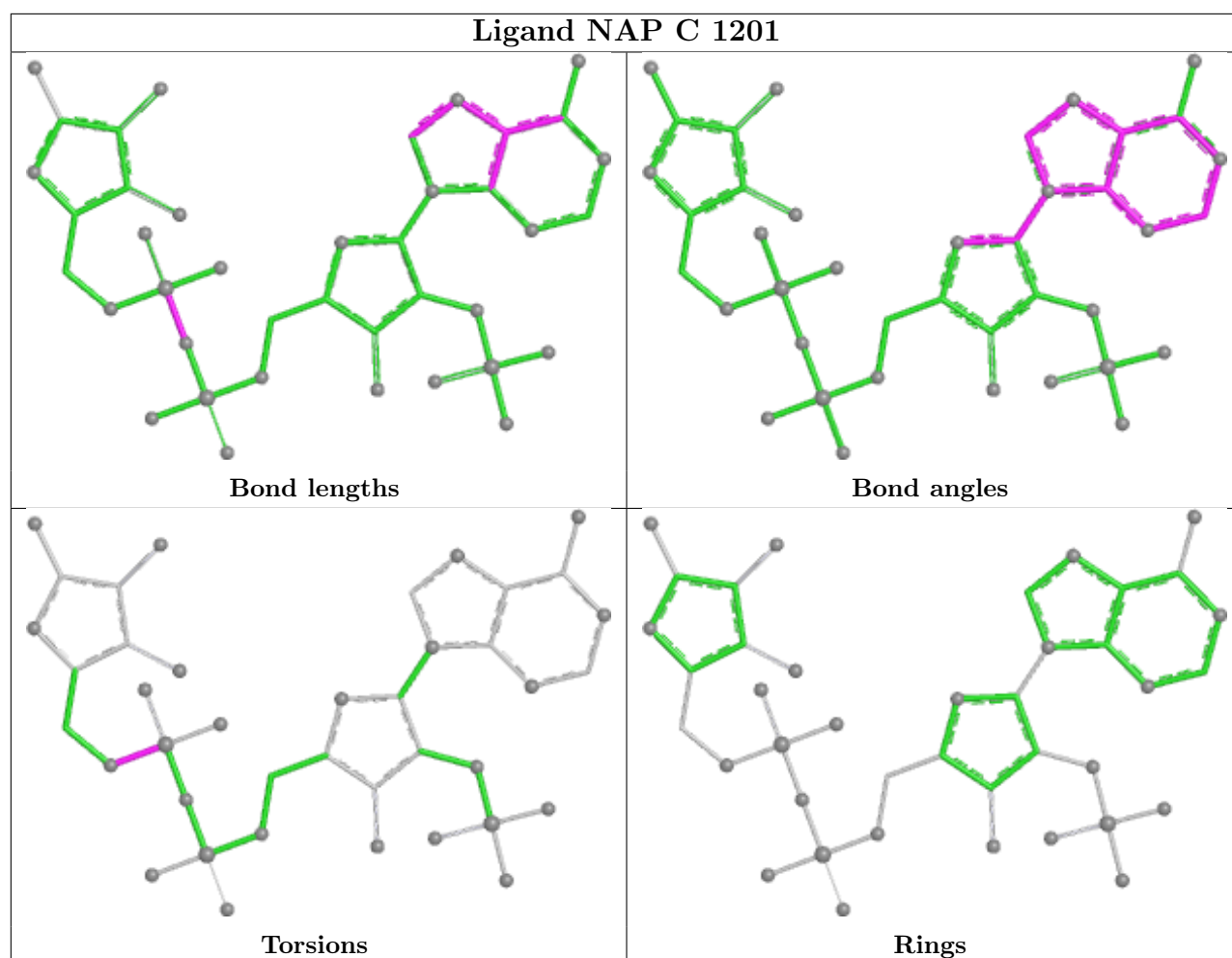
No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	514/1188 (43%)	0.96	91 (17%) 4 3	44, 79, 126, 182	0
1	B	520/1188 (43%)	0.98	80 (15%) 5 4	42, 75, 126, 187	0
1	C	516/1188 (43%)	1.11	92 (17%) 4 3	41, 84, 141, 203	0
1	D	504/1188 (42%)	1.57	145 (28%) 1 1	46, 93, 153, 185	0
All	All	2054/4752 (43%)	1.15	408 (19%) 3 2	41, 82, 142, 203	0

The worst 5 of 408 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	684	ALA	6.9
1	C	956	VAL	6.8
1	C	686	ALA	6.7
1	C	966	TYR	6.4
1	D	966	TYR	6.4

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](#)

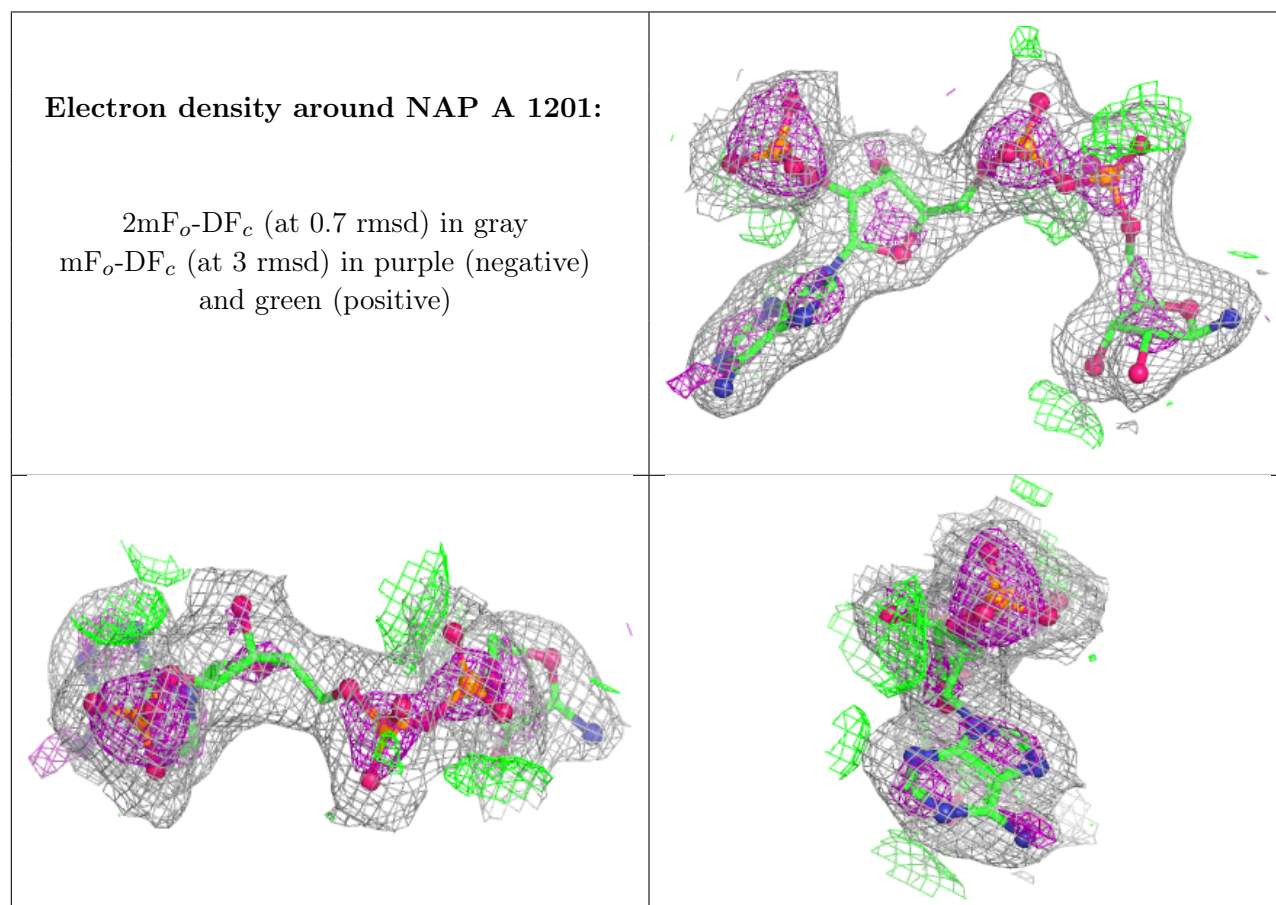
There are no oligosaccharides in this entry.

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.

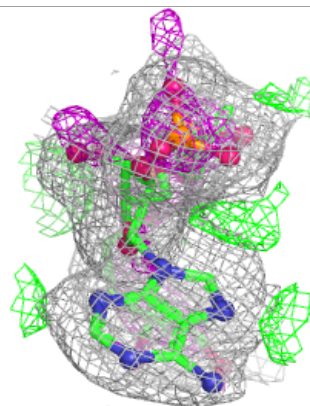
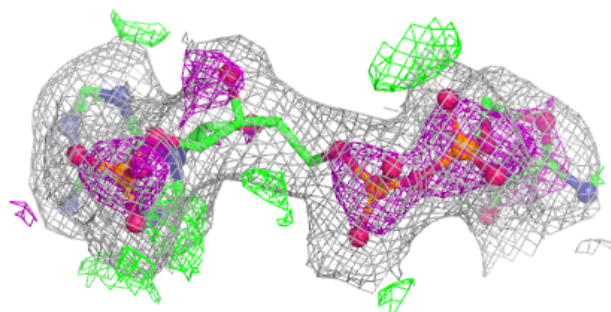
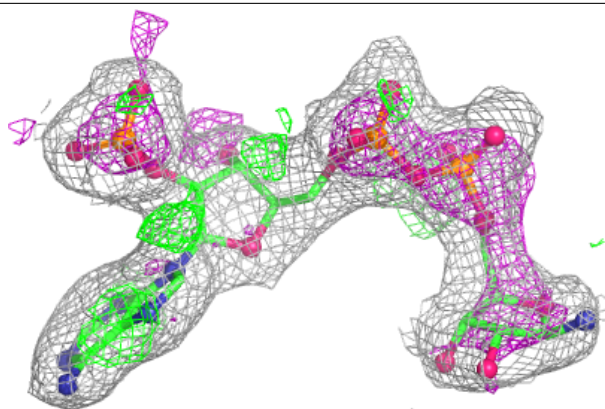
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	$Q < 0.9$
2	NAP	A	1201	40/48	0.95	0.09	37,43,60,60	0
2	NAP	C	1201	40/48	0.96	0.10	37,44,65,67	0
2	NAP	D	1201	40/48	0.96	0.09	37,42,66,68	0
2	NAP	B	1201	40/48	0.97	0.09	34,43,61,61	0

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.

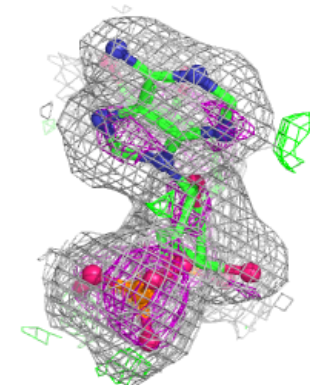
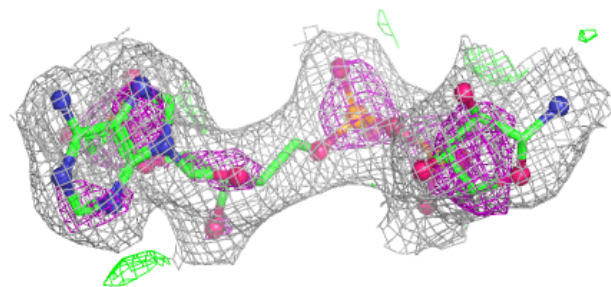
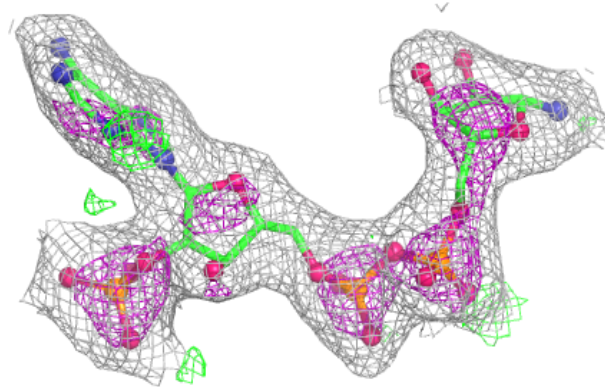


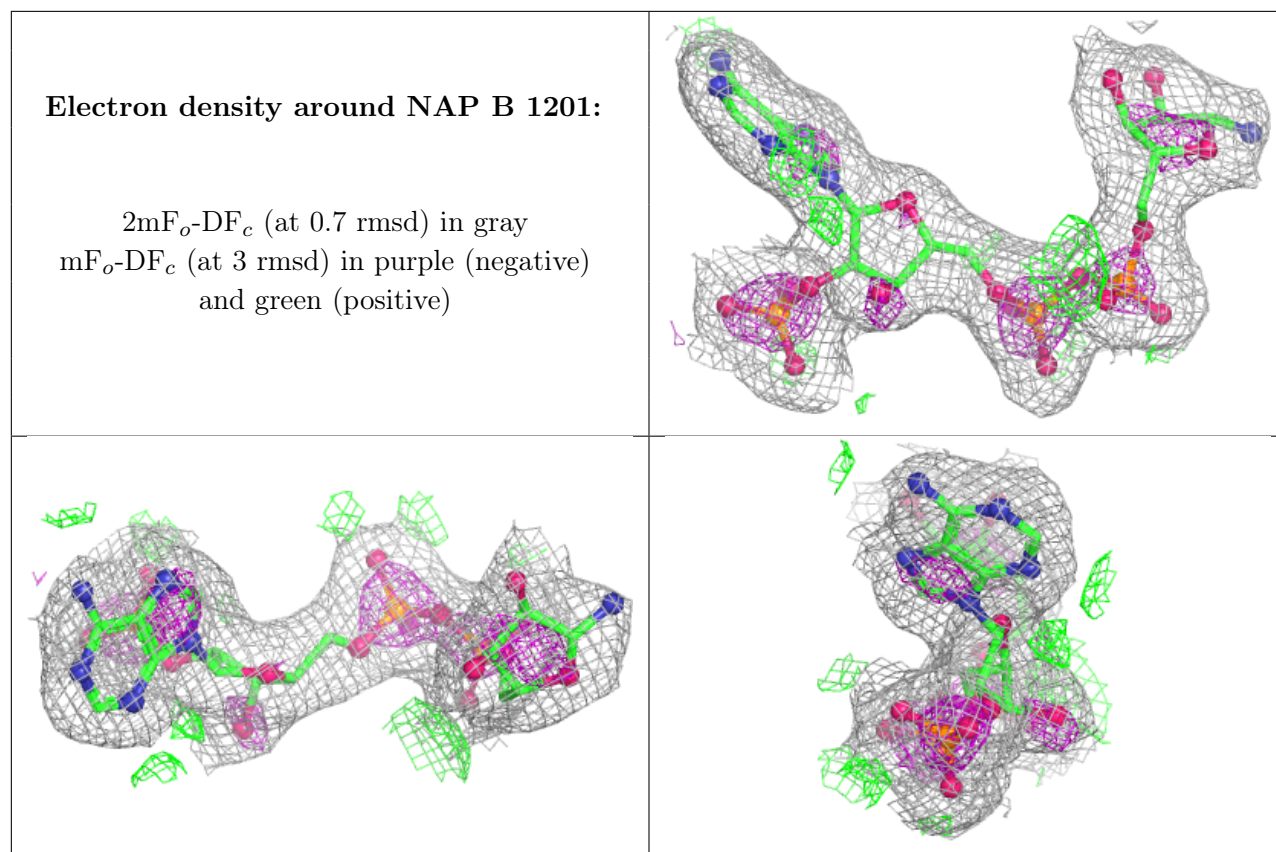
Electron density around NAP C 1201:

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

**Electron density around NAP D 1201:**

$2mF_o-DF_c$ (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.