



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:58 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

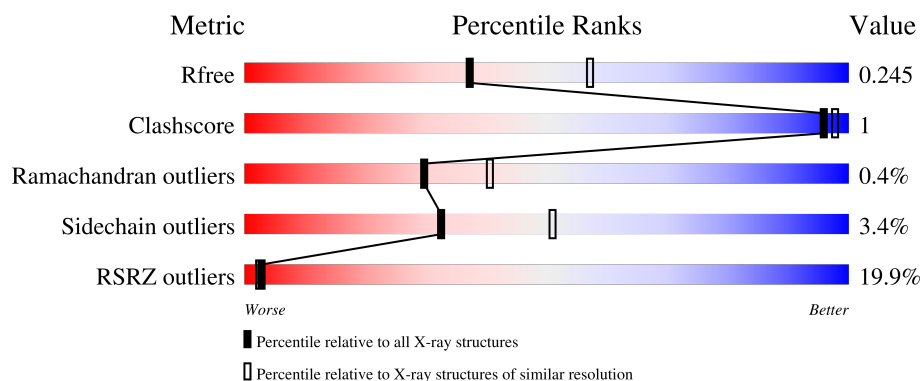
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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 ⓘ

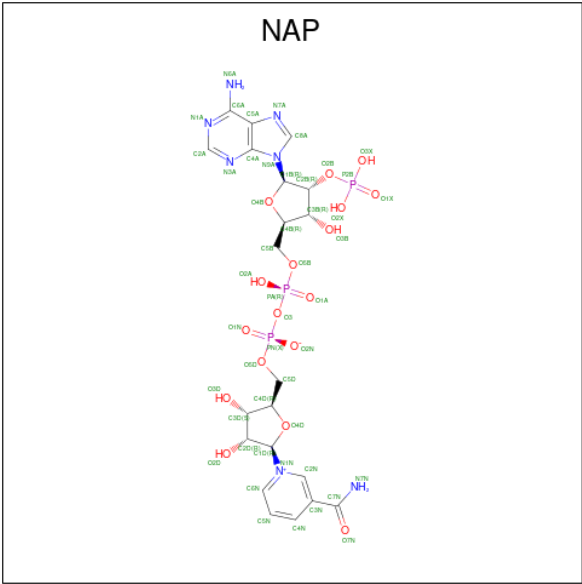
There are 3 unique types of molecules in this entry. The entry contains 16105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
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: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

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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		

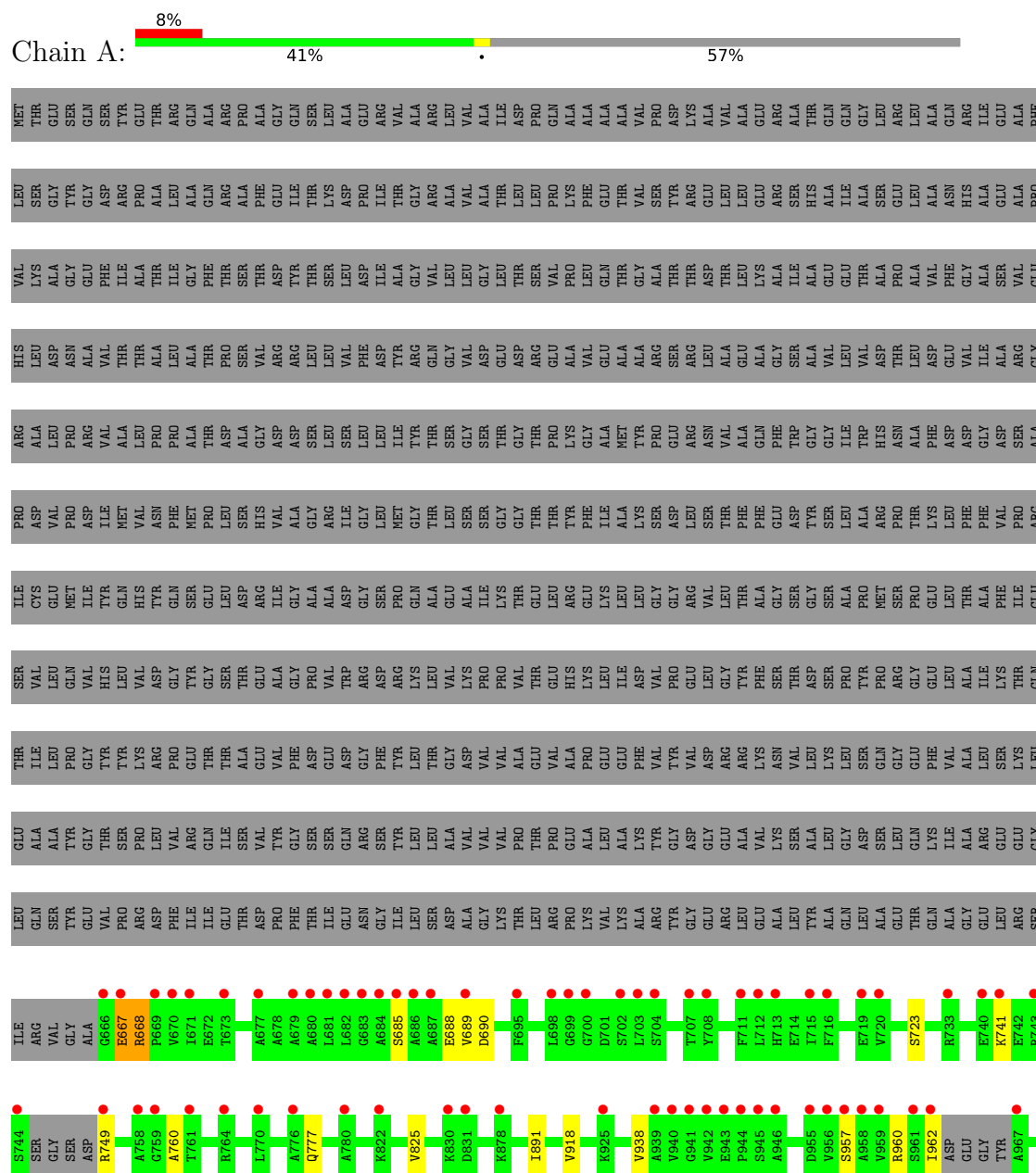
- Molecule 3 is water.

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

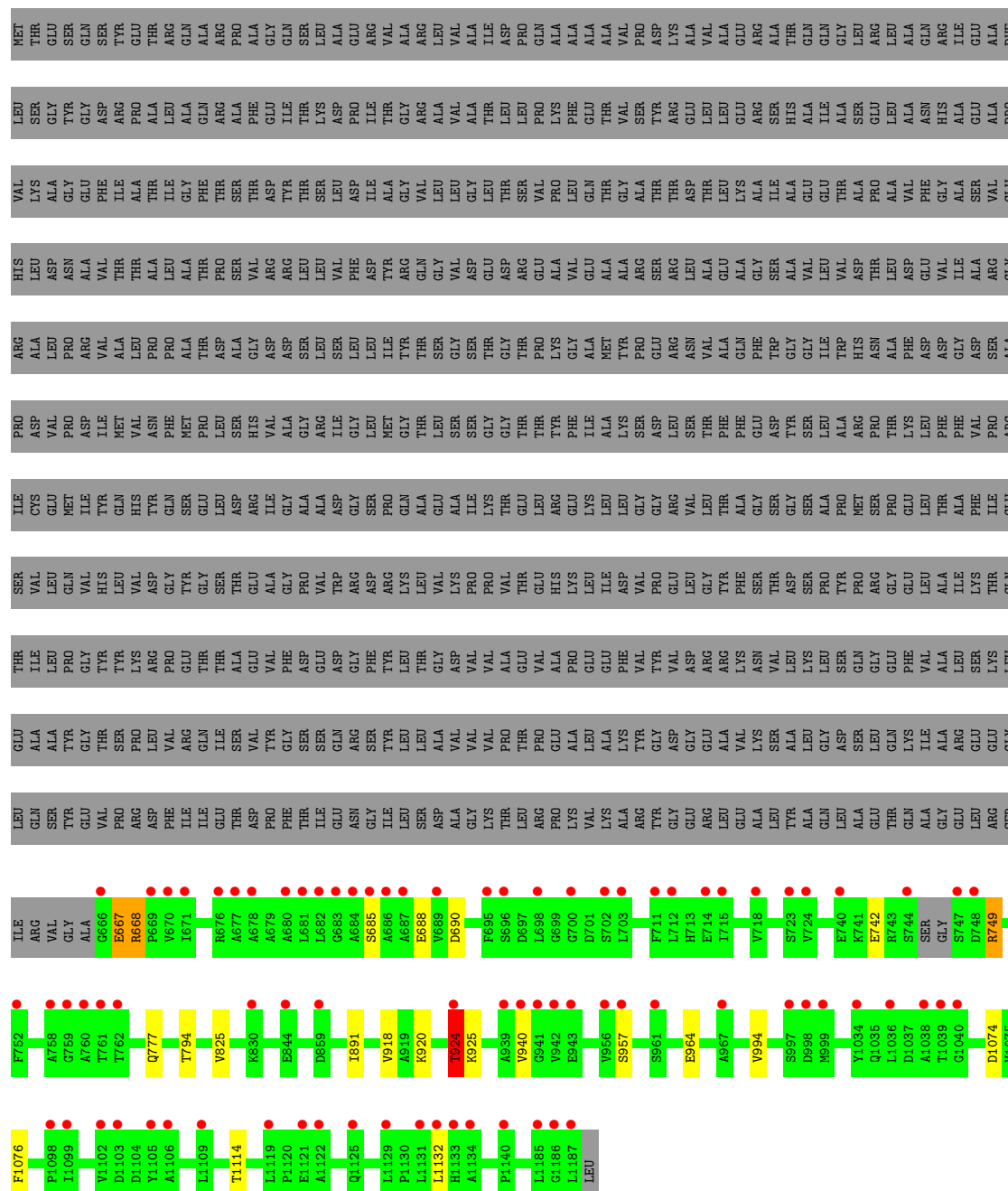
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Thioester reductase domain-containing protein



Q1153	D1048	V938	S747	ILE	LEU	GLU	THR	SER	ILE	PRO	ARG	ALA	ARG	HIS
V1156	E1057	A939	D748	ARG	GLN	ALA	ILE	VAL	CYS	ASP	ALA	LEU	ASP	LEU
Q1157	E1064	A940	R749	GLY	TYR	TYR	PRO	GLN	GLU	VAL	PRO	ASN	ASP	ASN
E1158	L1064	G941	F752	ALA	GLY	THR	GLY	VAL	TYR	ILE	VAL	ALA	ALA	VAL
D1181	F1076	V942	A753	GLY	VAL	SER	TYR	HIS	GLN	MET	ALA	THR	THR	THR
V1093	E1094	E943	S754	GLY	PRO	PRO	LYS	VAL	HIS	VAL	LEU	ALA	ALA	ALA
E1094	A1095	P944	H755	ARG	ARG	LEU	ARG	ASP	VAL	ASN	PRO	ALA	ALA	ALA
A1095	E948	S945	G757	PHE	ILE	VAL	PRO	GLY	GLN	GLY	THR	THR	THR	THR
T1099	S1100	F947	A758	ILE	ILE	GLN	THR	GLY	GLY	PRO	ASP	PRO	ASP	PRO
S1100	R1101	E948	G759	E672	ILE	ILE	ALA	SER	LEU	ASP	ALA	SER	SER	SER
R1101	V1105	T953	A760	E673	THR	SER	ALA	THR	ASP	GLY	GLY	GLY	GLY	GLY
V1105	A1106	R954	T761	V674	ASP	VAL	GLU	GLU	ARG	HIS	VAL	VAL	VAL	VAL
E1107	E1108	D955	I762	Q675	PRO	TYR	VAL	ILE	VAL	ASP	ALA	ASP	ARG	ARG
V1108	L1109	V956	R764	A677	PHE	GLY	PHE	ASP	GLY	ALA	ASP	ASP	ARG	ARG
L1109	E1112	S957	A765	A678	THR	SER	ASP	GLY	GLY	PRO	VAL	LEU	LEU	LEU
F1112	E1113	A958	L768	A679	ILE	ILE	ASP	TRP	ASP	ILE	ILE	SER	SER	SER
E1113	T1114	V959	K769	A680	GLU	ASN	GLY	ARG	GLY	LEU	VAL	SER	GLY	GLY
S1115	L1116	R960	L770	L681	GLY	ILE	TYR	ASP	PRO	MET	ILE	ASP	TYR	TYR
L1116	L1119	S961	L774	G682	LEU	LEU	THR	GLN	LYS	GLY	THR	ARG	ARG	ARG
L1119	P1120	I962	L774	G683	SER	LEU	GLY	LEU	ALA	THR	THR	GLN	GLY	GLY
P1120	E1121	ASP	L774	A684	ASP	ALA	GLY	VAL	VAL	LEU	SER	SER	GLY	GLY
E1121	A1122	GLY	L774	SER	ALA	ALA	ASP	LYS	VAL	LEU	SER	GLY	VAL	VAL
A1122	Q1125	Y966	Q777	ALA	ALA	VAL	VAL	GLY	VAL	ASP	LYS	VAL	ASP	ASP
Q1125	H1126	A967	T778	GLY	GLY	VAL	VAL	GLU	VAL	GLY	GLY	GLY	GLY	GLY
H1126	L1129	N968	L779	GLU	LYS	VAL	VAL	VAL	VAL	PRO	THR	THR	THR	THR
L1129	P1130	R982	A780	D690	THR	PRO	ALA	ALA	ALA	ALA	GLY	GLY	GLY	GLY
P1130	L1131	R982	A782	P691	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR
L1131	H1133	D998	L785	L703	ARG	PRO	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
H1133	A1134	M999	V792	F711	LYS	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
A1134	F1135	D1014	R793	L712	ALA	ALA	ALA	ILE	ILE	ILE	ILE	ILE	ILE	ILE
F1135	A1136	L1023	T798	H713	LYS	LYS	LYS	ASP	ASP	ASP	ASP	ASP	ASP	ASP
A1136	Q1137	L1024	P818	E714	ARG	TYR	TYR	VAL	VAL	VAL	VAL	VAL	VAL	VAL
Q1137	P1138	A1025	Q819	F715	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
P1138	A1139	T1026	G820	V716	ARG	GLY	ARG	GLY	VAL	VAL	VAL	VAL	VAL	VAL
A1139	P1140	G1027	G821	V717	LEU	ALA	ARG	TYR	THR	PHE	ALA	ALA	ALA	ALA
P1140	A1141	I1028	K822	V722	GLU	VAL	VAL	LYS	THR	THR	ALA	ALA	ALA	ALA
A1141	T1142	R1031	K822	S723	ALA	LYS	LYS	ASN	ASN	PHE	PHE	PHE	PHE	PHE
T1142	D1143	Y1034	V825	S724	LEU	SER	SER	VAL	VAL	GLY	GLY	GLY	GLY	GLY
D1143	G1144	GLN	K833	V732	TYR	ALA	ALA	LEU	LEU	THR	THR	THR	THR	THR
G1144	S1145	LEU	D859	L732	GLN	LEU	GLY	GLY	GLY	SER	SER	SER	SER	SER
S1145	P1146	ASP	D859	V735	LEU	ALA	ASP	GLY	GLY	PRO	PRO	PRO	PRO	PRO
P1146	F1147	ALA	D886	A736	ALA	SER	SER	GLN	GLN	GLY	GLY	GLY	GLY	GLY
F1147	Q1148	THR	D886	A737	THR	LEU	LEU	LYS	LYS	LYS	LYS	LYS	LYS	LYS
Q1148	T1149	GLY	I891	E740	GLN	GLN	GLN	ILE	ILE	ILE	ILE	ILE	ILE	ILE
T1149	K1150	R1042	V918	K741	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
K1150	N1151	Q1043	V918	E742	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
N1151	F1152	R1044	K925	R743	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
F1152		A1045	R926	S744	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU
		H1046	R926	S744	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
		Y1047	L927	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	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)	Xtriage
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	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
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

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

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

All (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
1	B	667	GLU	CA-C-N	6.69	133.74	121.70
1	B	667	GLU	C-N-CA	6.69	133.74	121.70
1	C	667	GLU	CA-C-N	6.55	133.49	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	667	GLU	C-N-CA	6.55	133.49	121.70
1	A	667	GLU	CA-C-N	6.51	133.41	121.70
1	A	667	GLU	C-N-CA	6.51	133.41	121.70
1	B	957	SER	N-CA-C	-6.35	97.27	110.80
1	C	1035	GLN	N-CA-CB	5.38	117.88	109.97
1	C	751	THR	N-CA-C	5.30	122.10	110.80

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 ⓘ

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.

All (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
1:C:667:GLU:HB2	1:C:668:ARG:HB2	1.75	0.67
1:B:667:GLU:HB2	1:B:668:ARG:HB2	1.76	0.67
1:D:1149:THR:HG22	1:D:1149:THR:O	2.00	0.60
1:D:785:LEU:HD23	1:D:926:ARG:CA	2.33	0.59
1:C:687:ALA:HA	1:C:688:GLU:HG2	1.86	0.57
1:D:1076:PHE:CZ	1:D:1147:PHE:O	2.59	0.56
1:C:938:VAL:O	1:C:960:ARG:NH2	2.42	0.52
1:D:1076:PHE:CZ	1:D:1149:THR:OG1	2.61	0.52
1:D:782:ALA:HA	1:D:785:LEU:CD1	2.37	0.51
1:A:938:VAL:O	1:A:960:ARG:NH2	2.43	0.51
1:D:1149:THR:O	1:D:1151:ASN:N	2.42	0.51
1:D:938:VAL:O	1:D:960:ARG:NH2	2.43	0.51
1:D:1149:THR:O	1:D:1149:THR:CG2	2.59	0.51
1:C:688:GLU:HB3	1:C:690:ASP:N	2.26	0.50
1:C:750:PRO:O	1:C:751:THR:HG22	2.11	0.50
1:D:1149:THR:HG22	1:D:1153:GLN:H	1.80	0.47
1:A:760:ALA:O	1:A:962:ILE:HD11	2.16	0.45
1:A:1074:ASP:HB3	1:A:1076:PHE:CE2	2.52	0.44
1:C:1074:ASP:HB3	1:C:1076:PHE:CE2	2.53	0.43
1:B:1074:ASP:HB3	1:B:1076:PHE:CE2	2.53	0.43
1:D:1149:THR:HG21	1:D:1153:GLN:HB2	1.99	0.43
1:B:891:ILE:HG21	1:B:918:VAL:HG13	2.01	0.42
1:D:891:ILE:HG21	1:D:918:VAL:HG13	2.00	0.42
1:C:1035:GLN:HG2	1:C:1140:PRO:HA	2.02	0.42
1:C:891:ILE:HG21	1:C:918:VAL:HG13	2.01	0.42
1:A:891:ILE:HG21	1:A:918:VAL:HG13	2.01	0.41
1:D:1149:THR:O	1:D:1150:LYS:C	2.62	0.41
1:B:920:LYS:O	1:B:924:THR:CG2	2.69	0.41
1:D:1076:PHE:HZ	1:D:1147:PHE:O	2.00	0.41

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (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
1	D	749	ARG
1	D	1150	LYS
1	A	689	VAL
1	C	689	VAL

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	409/947 (43%)	396 (97%)	13 (3%)	34	53
1	B	414/947 (44%)	401 (97%)	13 (3%)	35	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	685	SER
1	A	688	GLU
1	A	690	ASP
1	A	723	SER
1	A	741	LYS
1	A	749	ARG
1	A	777	GLN
1	A	825	VAL
1	A	957	SER
1	A	1114	THR
1	A	1125	GLN
1	A	1132	LEU
1	A	1156	VAL
1	B	685	SER
1	B	688	GLU
1	B	690	ASP
1	B	742	GLU
1	B	749	ARG
1	B	777	GLN
1	B	794	THR
1	B	825	VAL
1	B	924	THR
1	B	964	GLU
1	B	994	VAL
1	B	1114	THR
1	B	1132	LEU
1	C	685	SER
1	C	689	VAL
1	C	690	ASP
1	C	723	SER
1	C	749	ARG
1	C	777	GLN
1	C	794	THR
1	C	825	VAL

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Mol	Chain	Res	Type
1	C	957	SER
1	C	968	ASN
1	C	1035	GLN
1	C	1114	THR
1	C	1125	GLN
1	C	1132	LEU
1	C	1156	VAL
1	D	723	SER
1	D	742	GLU
1	D	749	ARG
1	D	774	LEU
1	D	777	GLN
1	D	785	LEU
1	D	793	ARG
1	D	825	VAL
1	D	957	SER
1	D	1057	GLU
1	D	1114	THR
1	D	1125	GLN
1	D	1132	LEU
1	D	1156	VAL

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	1080	HIS
1	A	1125	GLN
1	B	675	GLN
1	B	1126	HIS
1	B	1148	GLN
1	C	675	GLN
1	C	738	HIS
1	C	1011	ASN
1	C	1125	GLN
1	D	675	GLN
1	D	1125	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](#)

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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
2	C	1201	NAP	C5A-C6A	2.75	1.48	1.41
2	D	1201	NAP	C5A-C6A	2.73	1.48	1.41
2	B	1201	NAP	C5A-C6A	2.57	1.48	1.41
2	C	1201	NAP	PN-O3	2.57	1.62	1.59
2	B	1201	NAP	C8A-N7A	2.47	1.36	1.31
2	B	1201	NAP	C5A-N7A	-2.45	1.34	1.39
2	C	1201	NAP	C5A-N7A	-2.44	1.34	1.39
2	A	1201	NAP	C5A-N7A	-2.41	1.34	1.39
2	A	1201	NAP	C8A-N7A	2.35	1.36	1.31
2	C	1201	NAP	C8A-N7A	2.33	1.36	1.31
2	B	1201	NAP	PN-O3	2.30	1.62	1.59
2	D	1201	NAP	C8A-N7A	2.25	1.36	1.31
2	D	1201	NAP	C5A-N7A	-2.20	1.35	1.39
2	A	1201	NAP	PN-O3	2.20	1.61	1.59
2	B	1201	NAP	PA-O3	2.11	1.61	1.59
2	A	1201	NAP	PA-O3	2.07	1.61	1.59
2	D	1201	NAP	C4A-N9A	-2.04	1.33	1.37

All (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
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
2	A	1201	NAP	N3A-C4A-N9A	4.66	135.10	127.17
2	C	1201	NAP	N3A-C4A-N9A	4.63	135.05	127.17
2	D	1201	NAP	N3A-C4A-N9A	4.27	134.43	127.17
2	D	1201	NAP	N3A-C2A-N1A	-4.21	122.21	128.58
2	B	1201	NAP	N3A-C2A-N1A	-4.06	122.44	128.58
2	C	1201	NAP	N3A-C2A-N1A	-3.96	122.59	128.58
2	B	1201	NAP	C2A-N3A-C4A	3.85	121.24	111.83
2	D	1201	NAP	C2A-N3A-C4A	3.85	121.23	111.83
2	A	1201	NAP	C2A-N3A-C4A	3.81	121.15	111.83
2	A	1201	NAP	N3A-C2A-N1A	-3.79	122.84	128.58
2	C	1201	NAP	C2A-N3A-C4A	3.75	121.00	111.83
2	B	1201	NAP	C4A-N9A-C8A	3.57	109.48	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	NAP	C4A-N9A-C8A	3.49	109.41	105.74
2	D	1201	NAP	C4A-C5A-N7A	-3.38	106.71	110.58
2	A	1201	NAP	C4A-N9A-C8A	3.34	109.24	105.74
2	A	1201	NAP	C4A-C5A-N7A	-3.30	106.81	110.58
2	C	1201	NAP	C4A-N9A-C8A	3.30	109.20	105.74
2	B	1201	NAP	C4A-C5A-N7A	-3.29	106.82	110.58
2	C	1201	NAP	O4B-C1B-N9A	3.15	114.14	108.09
2	C	1201	NAP	C4A-C5A-N7A	-3.13	107.00	110.58
2	B	1201	NAP	C5A-N7A-C8A	2.86	107.94	103.45
2	D	1201	NAP	C5A-N7A-C8A	2.79	107.83	103.45
2	A	1201	NAP	C5A-N7A-C8A	2.77	107.81	103.45
2	B	1201	NAP	N9A-C8A-N7A	-2.76	110.03	113.94
2	C	1201	NAP	C5A-N7A-C8A	2.67	107.65	103.45
2	D	1201	NAP	C6A-C5A-N7A	2.64	137.18	132.09
2	D	1201	NAP	N9A-C8A-N7A	-2.64	110.19	113.94
2	A	1201	NAP	N9A-C8A-N7A	-2.54	110.33	113.94
2	C	1201	NAP	N9A-C8A-N7A	-2.44	110.48	113.94
2	D	1201	NAP	O3X-P2B-O2X	2.42	116.87	107.80
2	D	1201	NAP	O4B-C1B-N9A	2.32	112.55	108.09
2	B	1201	NAP	C6A-C5A-N7A	2.25	136.42	132.09
2	D	1201	NAP	C2A-N1A-C6A	2.24	122.41	118.73
2	A	1201	NAP	C6A-C5A-N7A	2.19	136.31	132.09
2	C	1201	NAP	C6A-C5A-N7A	2.15	136.23	132.09
2	C	1201	NAP	C2A-N1A-C6A	2.10	122.18	118.73
2	A	1201	NAP	O4B-C1B-C2B	-2.03	103.09	106.59
2	B	1201	NAP	C2A-N1A-C6A	2.03	122.06	118.73
2	B	1201	NAP	O2N-PN-O1N	2.03	121.87	112.44

There are no chirality outliers.

All (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
2	C	1201	NAP	C5D-O5D-PN-O3
2	C	1201	NAP	C5D-O5D-PN-O1N
2	C	1201	NAP	C5D-O5D-PN-O2N
2	D	1201	NAP	C5D-O5D-PN-O3
2	D	1201	NAP	C5D-O5D-PN-O2N

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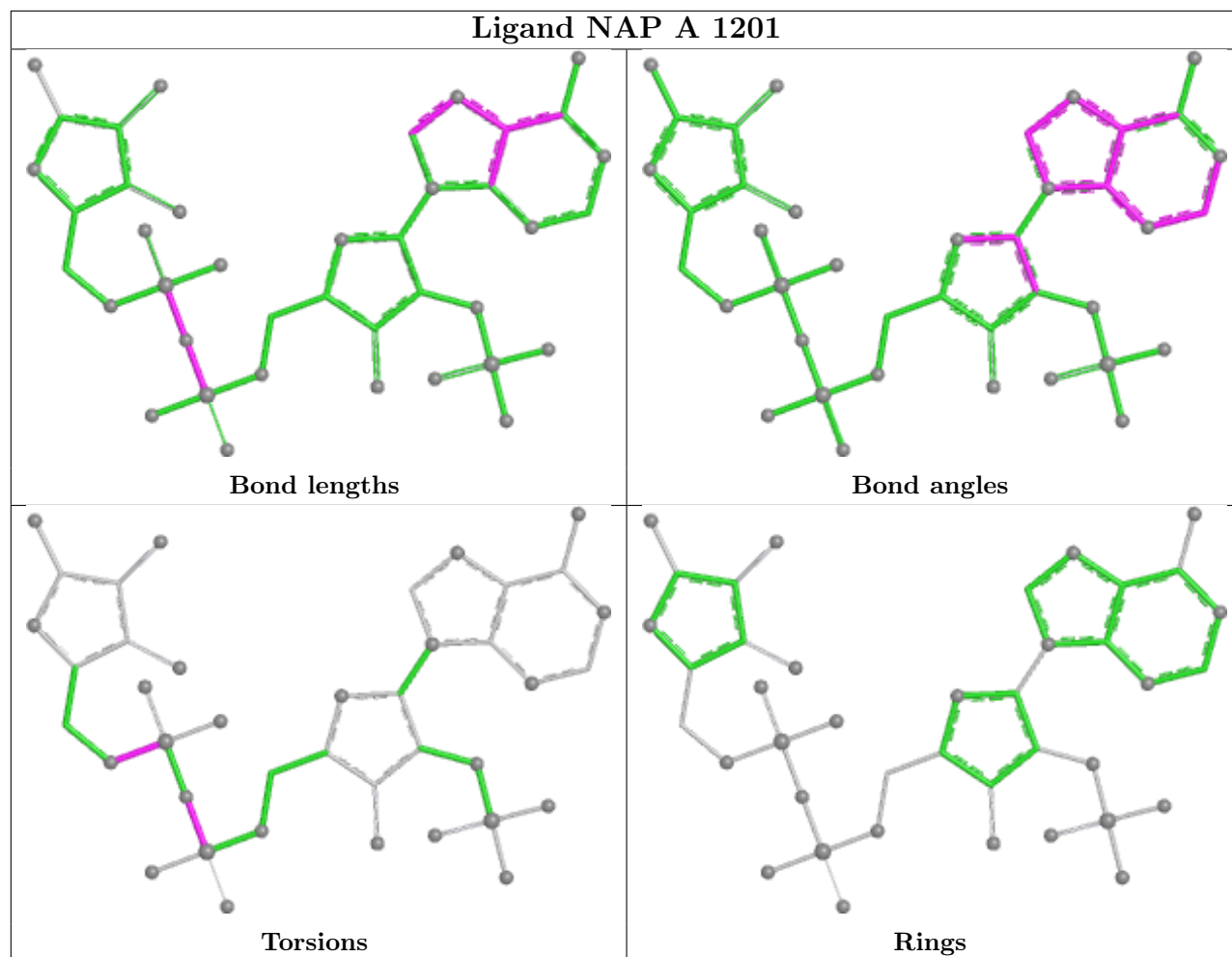
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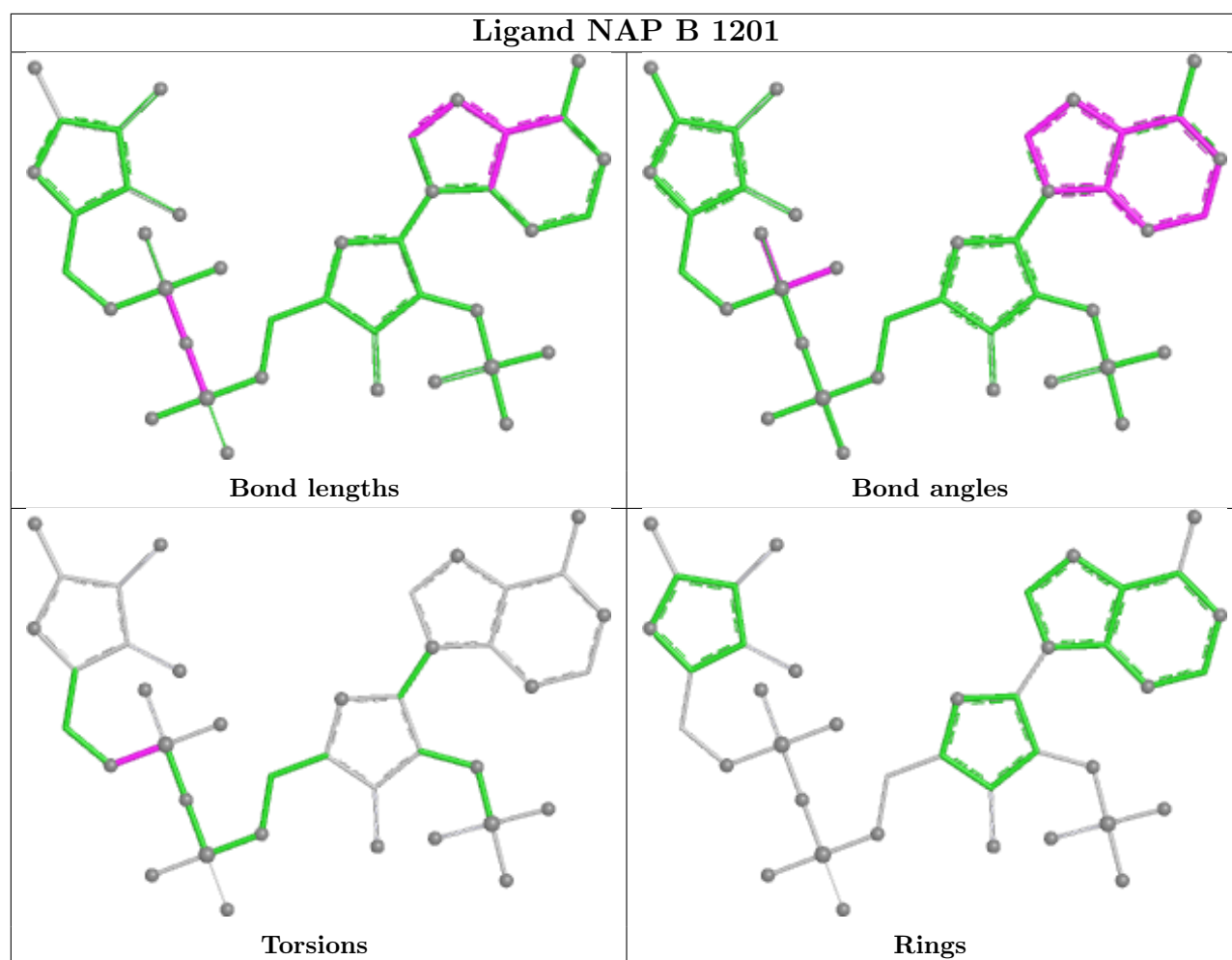
Mol	Chain	Res	Type	Atoms
2	A	1201	NAP	C5D-O5D-PN-O1N
2	D	1201	NAP	C5D-O5D-PN-O1N
2	A	1201	NAP	PN-O3-PA-O2A
2	D	1201	NAP	PN-O3-PA-O2A
2	D	1201	NAP	O4B-C4B-C5B-O5B

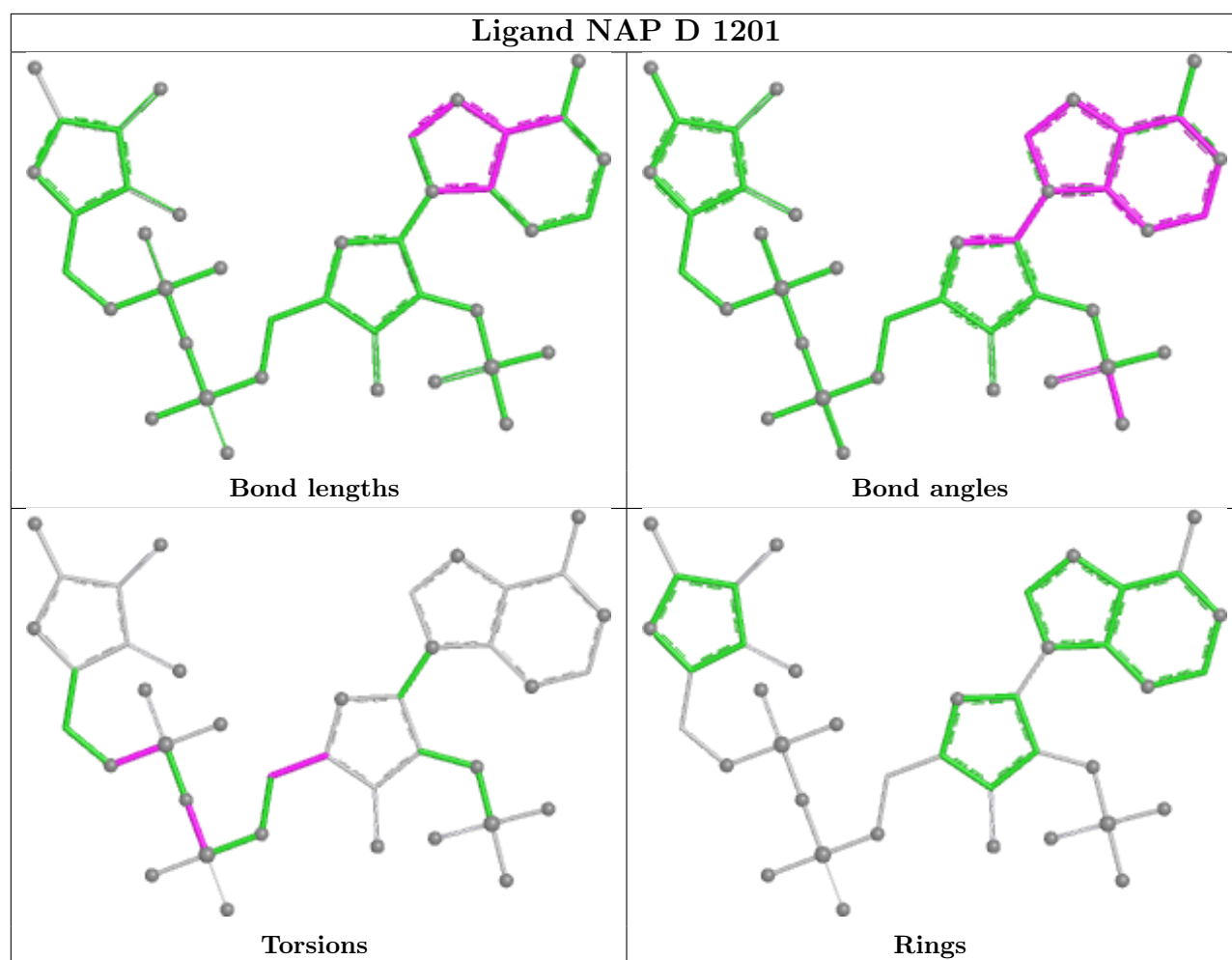
There are no ring outliers.

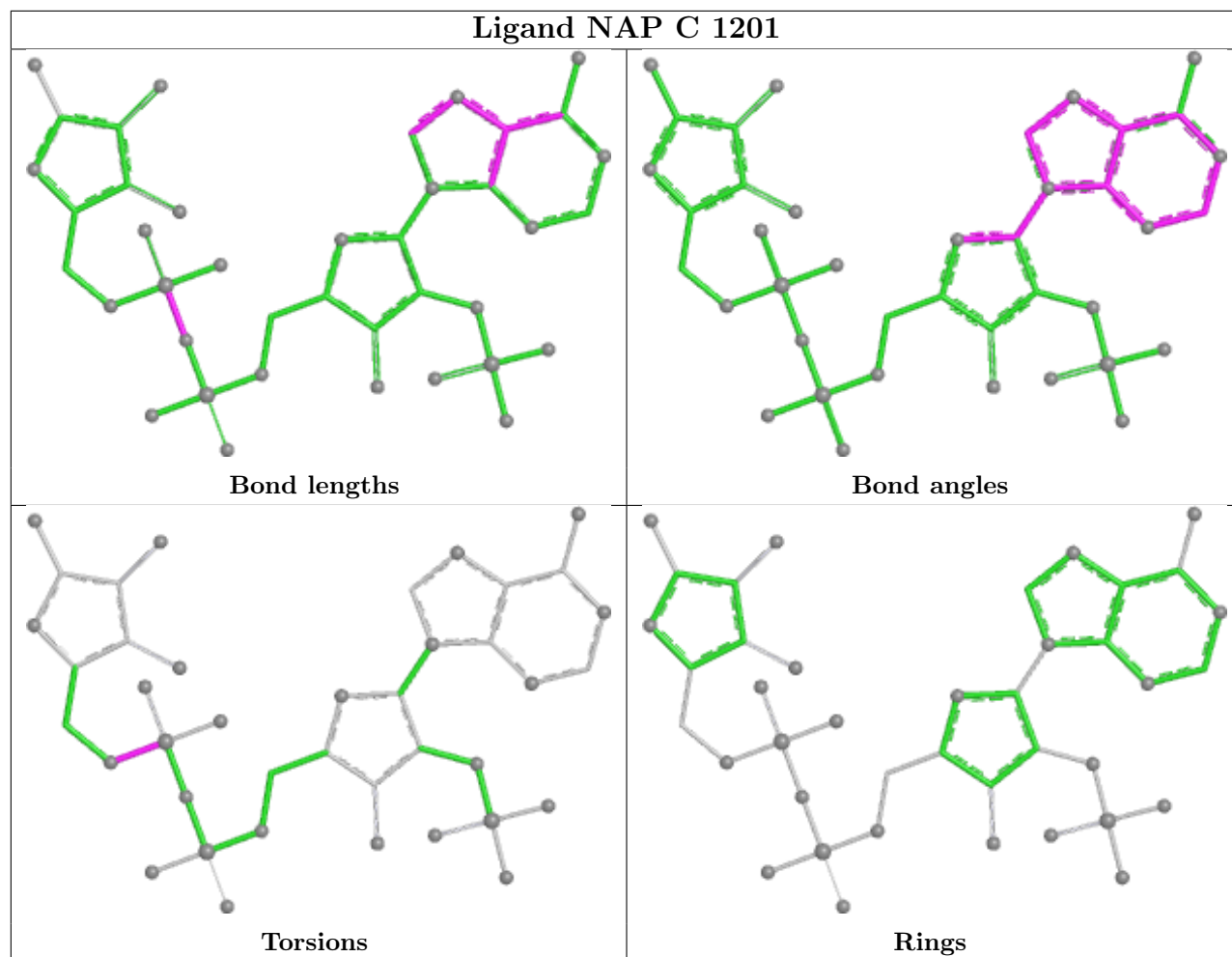
No monomer is involved in short contacts.

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

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	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

All (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
1	D	1147	PHE	5.9
1	D	1146	PRO	5.6
1	B	686	ALA	5.5
1	D	1076	PHE	5.3
1	D	1135	PHE	5.2
1	D	689	VAL	5.1
1	D	1149	THR	5.1
1	A	686	ALA	5.1
1	D	947	PHE	5.0
1	D	962	ILE	5.0
1	D	959	VAL	4.9
1	C	940	VAL	4.9
1	B	1133	HIS	4.8
1	A	956	VAL	4.8
1	D	956	VAL	4.8
1	B	957	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	745	SER	4.6
1	D	946	ALA	4.6
1	B	998	ASP	4.6
1	D	945	SER	4.6
1	C	967	ALA	4.5
1	A	962	ILE	4.5
1	D	1148	GLN	4.5
1	C	684	ALA	4.5
1	C	939	ALA	4.5
1	D	967	ALA	4.4
1	B	762	THR	4.3
1	D	670	VAL	4.3
1	A	943	GLU	4.3
1	D	999	MET	4.3
1	D	1142	ILE	4.3
1	D	758	ALA	4.2
1	D	957	SER	4.1
1	A	959	VAL	4.1
1	C	689	VAL	4.1
1	C	957	SER	4.1
1	D	942	VAL	4.1
1	C	683	GLY	4.0
1	D	818	PRO	4.0
1	A	680	ALA	4.0
1	A	666	GLY	4.0
1	C	715	ILE	4.0
1	D	940	VAL	4.0
1	D	744	SER	4.0
1	A	999	MET	4.0
1	C	947	PHE	3.9
1	A	687	ALA	3.9
1	D	762	THR	3.9
1	D	1034	TYR	3.8
1	C	680	ALA	3.8
1	C	959	VAL	3.8
1	B	684	ALA	3.7
1	D	763	ILE	3.7
1	B	940	VAL	3.7
1	D	761	THR	3.7
1	A	1187	LEU	3.6
1	B	687	ALA	3.6
1	A	744	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	957	SER	3.6
1	D	1131	LEU	3.6
1	A	711	PHE	3.6
1	C	711	PHE	3.6
1	D	774	LEU	3.6
1	D	968	ASN	3.6
1	D	1114	THR	3.6
1	A	669	PRO	3.6
1	B	703	LEU	3.5
1	A	677	ALA	3.5
1	D	944	PRO	3.5
1	A	940	VAL	3.5
1	D	1130	PRO	3.4
1	A	684	ALA	3.4
1	C	762	THR	3.4
1	C	1038	ALA	3.4
1	A	682	LEU	3.4
1	B	1122	ALA	3.4
1	D	1129	LEU	3.4
1	D	673	THR	3.4
1	A	958	ALA	3.4
1	D	1141	ALA	3.4
1	D	941	GLY	3.4
1	D	1043	GLN	3.4
1	C	673	THR	3.3
1	B	1187	LEU	3.3
1	B	941	GLY	3.3
1	C	941	GLY	3.3
1	D	1187	LEU	3.3
1	C	1036	LEU	3.3
1	C	763	ILE	3.3
1	A	925	LYS	3.3
1	D	1133	HIS	3.3
1	D	747	SER	3.3
1	C	677	ALA	3.2
1	A	703	LEU	3.2
1	B	1134	ALA	3.2
1	C	687	ALA	3.2
1	C	958	ALA	3.2
1	D	1105	TYR	3.2
1	A	822	LYS	3.2
1	C	1131	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	711	PHE	3.2
1	D	859	ASP	3.2
1	B	761	THR	3.2
1	A	945	SER	3.1
1	D	961	SER	3.1
1	A	942	VAL	3.1
1	B	689	VAL	3.1
1	B	859	ASP	3.1
1	A	681	LEU	3.1
1	D	1109	LEU	3.1
1	D	1138	PRO	3.1
1	D	1145	SER	3.1
1	B	670	VAL	3.1
1	D	681	LEU	3.1
1	D	1150	LYS	3.1
1	B	677	ALA	3.1
1	B	681	LEU	3.1
1	D	955	ASP	3.0
1	A	967	ALA	3.0
1	C	669	PRO	3.0
1	D	770	LEU	3.0
1	C	975	TRP	3.0
1	D	1143	ASP	3.0
1	B	999	MET	3.0
1	D	680	ALA	3.0
1	D	755	VAL	3.0
1	A	1133	HIS	3.0
1	C	666	GLY	3.0
1	D	669	PRO	3.0
1	D	948	GLU	3.0
1	B	956	VAL	3.0
1	C	942	VAL	3.0
1	D	1119	LEU	3.0
1	C	1133	HIS	3.0
1	A	1142	ILE	3.0
1	D	671	ILE	3.0
1	A	733	ARG	3.0
1	B	924	THR	3.0
1	B	666	GLY	3.0
1	D	1106	ALA	2.9
1	D	1134	ALA	2.9
1	B	1131	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	676	ARG	2.9
1	A	1105	TYR	2.9
1	C	968	ASN	2.9
1	A	1131	LEU	2.9
1	A	1132	LEU	2.9
1	D	939	ALA	2.9
1	C	670	VAL	2.9
1	C	925	LYS	2.9
1	A	695	PHE	2.9
1	C	1129	LEU	2.9
1	D	765	ALA	2.9
1	D	1064	LEU	2.9
1	A	689	VAL	2.9
1	C	719	GLU	2.9
1	B	680	ALA	2.9
1	B	711	PHE	2.9
1	C	1136	ALA	2.9
1	C	685	SER	2.8
1	B	942	VAL	2.8
1	D	674	VAL	2.8
1	D	1057	GLU	2.8
1	B	744	SER	2.8
1	C	681	LEU	2.8
1	D	753	ALA	2.8
1	D	925	LYS	2.8
1	B	669	PRO	2.8
1	D	1136	ALA	2.8
1	C	999	MET	2.8
1	D	716	PHE	2.8
1	C	938	VAL	2.8
1	B	715	ILE	2.8
1	C	962	ILE	2.8
1	A	998	ASP	2.8
1	B	1186	GLY	2.8
1	D	759	GLY	2.8
1	A	944	PRO	2.8
1	C	698	LEU	2.8
1	C	768	LEU	2.8
1	D	1025	ALA	2.8
1	D	752	PHE	2.8
1	B	1102	VAL	2.8
1	C	718	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	761	THR	2.7
1	A	1136	ALA	2.7
1	A	830	LYS	2.7
1	D	960	ARG	2.7
1	D	1044	ARG	2.7
1	B	758	ALA	2.7
1	C	752	PHE	2.7
1	D	1112	PHE	2.7
1	D	718	VAL	2.7
1	B	682	LEU	2.7
1	C	1187	LEU	2.7
1	A	1038	ALA	2.7
1	A	708	TYR	2.7
1	A	707	THR	2.7
1	B	830	LYS	2.7
1	C	764	ARG	2.7
1	C	946	ALA	2.6
1	D	677	ALA	2.6
1	D	1122	ALA	2.6
1	B	1105	TYR	2.6
1	A	670	VAL	2.6
1	D	1042	ARG	2.6
1	D	1099	ILE	2.6
1	B	1119	LEU	2.6
1	B	1132	LEU	2.6
1	D	782	ALA	2.6
1	C	944	PRO	2.6
1	D	1132	LEU	2.6
1	A	702	SER	2.6
1	D	717	GLN	2.6
1	B	714	GLU	2.6
1	B	676	ARG	2.6
1	A	761	THR	2.6
1	D	1140	PRO	2.5
1	A	1102	VAL	2.5
1	B	844	GLU	2.5
1	D	779	LEU	2.5
1	B	760	ALA	2.5
1	C	753	ALA	2.5
1	C	998	ASP	2.5
1	A	716	PHE	2.5
1	B	702	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	720	VAL	2.5
1	C	945	SER	2.5
1	A	667	GLU	2.5
1	C	682	LEU	2.5
1	A	741	LYS	2.5
1	A	1005	LYS	2.5
1	A	1039	THR	2.5
1	B	1039	THR	2.5
1	A	1112	PHE	2.5
1	C	716	PHE	2.5
1	C	1112	PHE	2.5
1	B	718	VAL	2.5
1	D	712	LEU	2.5
1	D	1023	LEU	2.5
1	D	1045	ALA	2.5
1	B	700	GLY	2.5
1	D	668	ARG	2.4
1	D	676	ARG	2.4
1	D	982	ARG	2.4
1	C	703	LEU	2.4
1	D	819	GLN	2.4
1	D	736	ALA	2.4
1	C	943	GLU	2.4
1	D	715	ILE	2.4
1	D	732	LEU	2.4
1	D	768	LEU	2.4
1	C	1138	PRO	2.4
1	C	751	THR	2.4
1	B	997	SER	2.4
1	A	715	ILE	2.4
1	B	671	ILE	2.4
1	B	1129	LEU	2.4
1	D	1108	TRP	2.4
1	C	765	ALA	2.4
1	C	671	ILE	2.4
1	C	1142	ILE	2.4
1	C	961	SER	2.3
1	B	724	VAL	2.3
1	D	792	VAL	2.3
1	A	749	ARG	2.3
1	C	1150	LYS	2.3
1	D	1120	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	678	ALA	2.3
1	C	755	VAL	2.3
1	D	756	HIS	2.3
1	B	1185	LEU	2.3
1	C	1132	LEU	2.3
1	D	1116	LEU	2.3
1	A	946	ALA	2.3
1	A	704	SER	2.3
1	B	685	SER	2.3
1	D	1126	HIS	2.3
1	C	667	GLU	2.3
1	C	717	GLN	2.3
1	D	953	ILE	2.3
1	C	1031	LYS	2.3
1	A	679	ALA	2.3
1	B	1038	ALA	2.3
1	D	737	ALA	2.3
1	D	958	ALA	2.3
1	A	673	THR	2.3
1	C	714	GLU	2.3
1	D	714	GLU	2.3
1	A	720	VAL	2.3
1	B	695	PHE	2.2
1	D	682	LEU	2.2
1	D	722	VAL	2.3
1	B	759	GLY	2.2
1	B	1040	GLY	2.2
1	D	1144	GLY	2.2
1	B	939	ALA	2.2
1	C	758	ALA	2.2
1	D	679	ALA	2.2
1	D	754	SER	2.2
1	C	739	ILE	2.2
1	A	712	LEU	2.2
1	B	712	LEU	2.2
1	A	1135	PHE	2.2
1	D	886	ASP	2.2
1	A	743	ARG	2.2
1	A	764	ARG	2.2
1	D	691	PRO	2.2
1	D	1101	ARG	2.2
1	A	758	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1183	LYS	2.2
1	D	1026	THR	2.2
1	A	685	SER	2.2
1	A	1119	LEU	2.2
1	A	759	GLY	2.2
1	A	941	GLY	2.2
1	D	740	GLU	2.2
1	A	939	ALA	2.2
1	B	967	ALA	2.2
1	C	776	ALA	2.2
1	D	780	ALA	2.2
1	A	1036	LEU	2.2
1	C	960	ARG	2.2
1	D	927	LEU	2.2
1	C	741	LYS	2.2
1	D	833	LYS	2.2
1	B	683	GLY	2.2
1	A	997	SER	2.2
1	A	671	ILE	2.1
1	C	770	LEU	2.1
1	D	703	LEU	2.1
1	C	955	ASP	2.1
1	D	1014	ASP	2.1
1	B	943	GLU	2.1
1	D	820	GLY	2.1
1	B	1106	ALA	2.1
1	D	1139	ALA	2.1
1	A	1109	LEU	2.1
1	B	1099	ILE	2.1
1	B	1109	LEU	2.1
1	C	1119	LEU	2.1
1	D	1028	ILE	2.1
1	A	955	ASP	2.1
1	B	1121	GLU	2.1
1	D	943	GLU	2.1
1	C	1102	VAL	2.1
1	D	1093	VAL	2.1
1	A	1137	GLN	2.1
1	A	1122	ALA	2.1
1	B	696	SER	2.1
1	B	723	SER	2.1
1	B	961	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	778	THR	2.1
1	D	822	LYS	2.1
1	B	740	GLU	2.1
1	D	785	LEU	2.1
1	A	831	ASP	2.1
1	A	1104	ASP	2.1
1	B	1034	TYR	2.1
1	D	1048	ASP	2.1
1	A	1125	GLN	2.1
1	C	1146	PRO	2.1
1	D	735	VAL	2.1
1	D	743	ARG	2.1
1	A	780	ALA	2.1
1	A	740	GLU	2.1
1	A	770	LEU	2.1
1	B	1036	LEU	2.1
1	C	1099	ILE	2.1
1	C	1105	TYR	2.1
1	C	674	VAL	2.1
1	C	969	GLY	2.1
1	C	1108	TRP	2.1
1	A	878	LYS	2.0
1	D	798	THR	2.0
1	A	719	GLU	2.0
1	D	742	GLU	2.0
1	A	713	HIS	2.0
1	B	1125	GLN	2.0
1	C	900	HIS	2.0
1	D	1046	HIS	2.0
1	D	1181	ASP	2.0
1	D	724	VAL	2.0
1	A	683	GLY	2.0
1	A	699	GLY	2.0
1	A	700	GLY	2.0
1	A	1040	GLY	2.0
1	B	752	PHE	2.0
1	A	961	SER	2.0
1	B	747	SER	2.0
1	D	1158	GLU	2.0
1	A	776	ALA	2.0
1	D	760	ALA	2.0
1	D	1095	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	698	LEU	2.0
1	B	698	LEU	2.0
1	B	748	ASP	2.0
1	B	1103	ASP	2.0
1	D	998	ASP	2.0
1	B	1098	PRO	2.0
1	B	1140	PRO	2.0
1	C	1130	PRO	2.0
1	D	1031	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

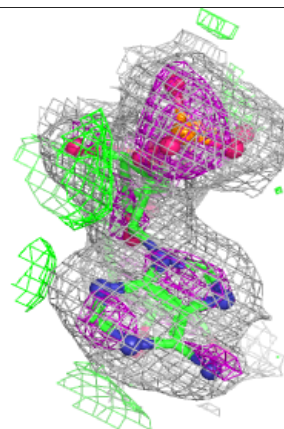
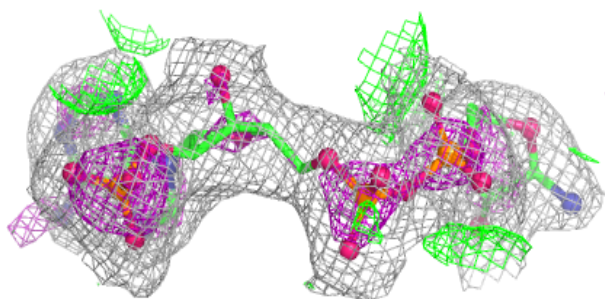
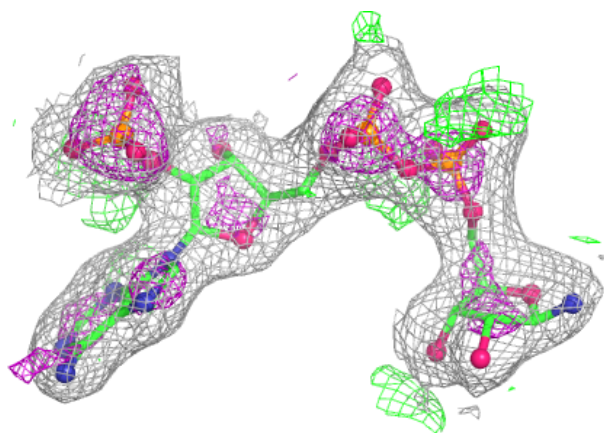
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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

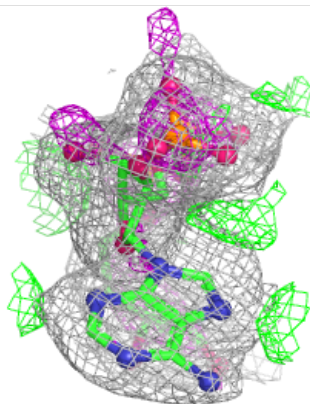
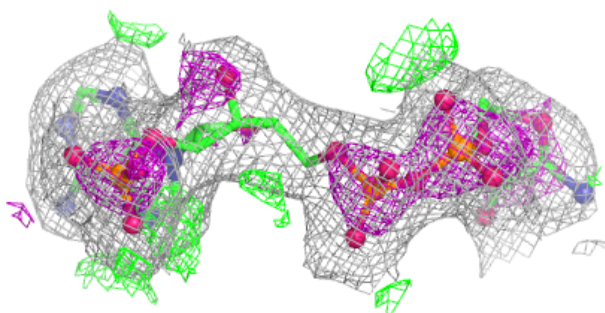
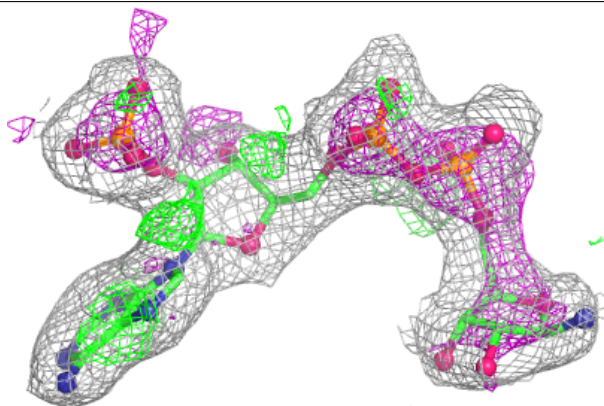
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 1201:

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

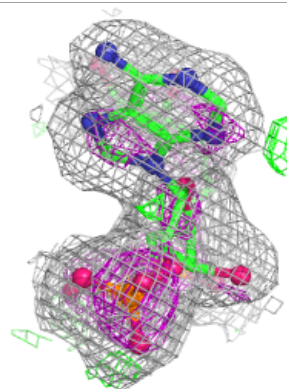
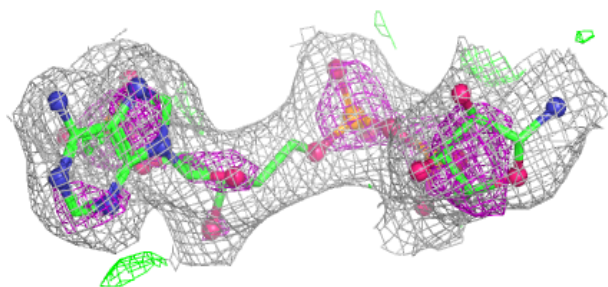
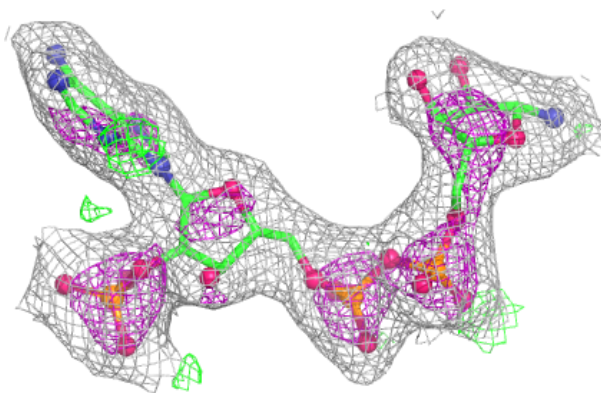
**Electron density around NAP C 1201:**

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

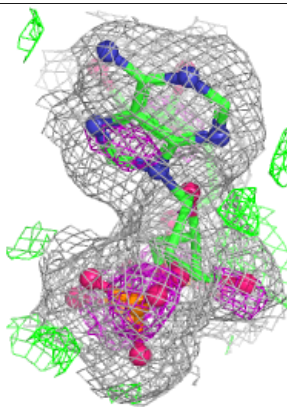
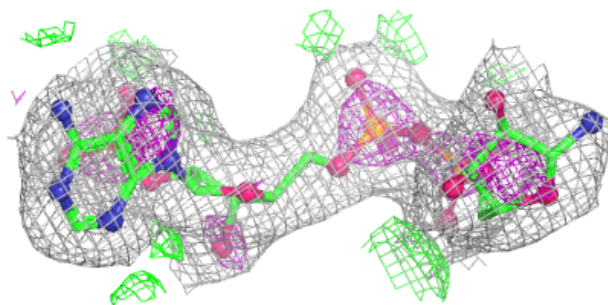
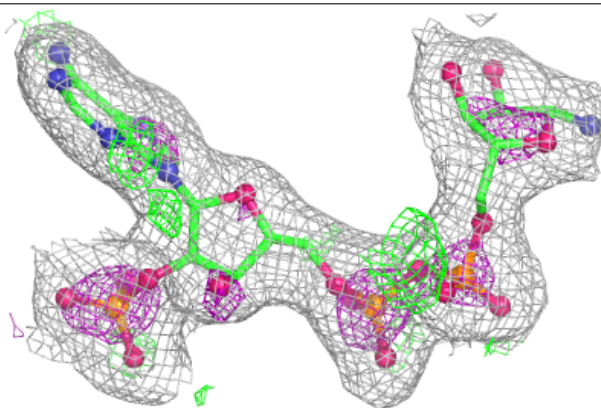


Electron density around NAP D 1201:

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

**Electron density around NAP B 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.