



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:38 PM UTC

PDB ID : 3RHO / pdb_00003rho
Title : Crystal structure of the E673Q MUTANT OF C-Terminal domain of 10'FOR MYLTETRAHYDROFOLATE DEHYDROGENASE in complex with NADP
Authors : Tsybovsky, Y.
Deposited on : 2011-04-11
Resolution : 2.26 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

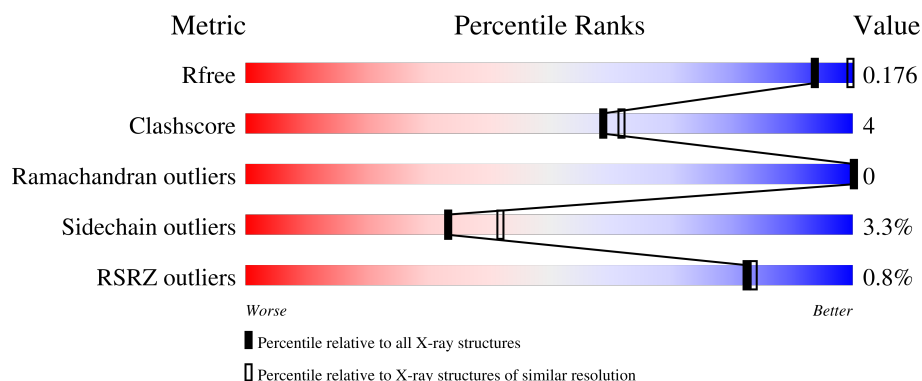
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	517	% 76% 18% • •
1	B	517	% 77% 17% • • •
1	C	517	% 72% 21% • •
1	D	517	% 74% 19% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17496 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 Aldehyde dehydrogenase 1 family, member L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	4	19	0
			3906	2478	672	735	21			
1	B	498	Total	C	N	O	S	0	19	0
			3906	2478	672	735	21			
1	C	498	Total	C	N	O	S	0	19	0
			3906	2478	672	735	21			
1	D	498	Total	C	N	O	S	0	19	0
			3906	2478	672	735	21			

There are 48 discrepancies between the modelled and reference sequences:

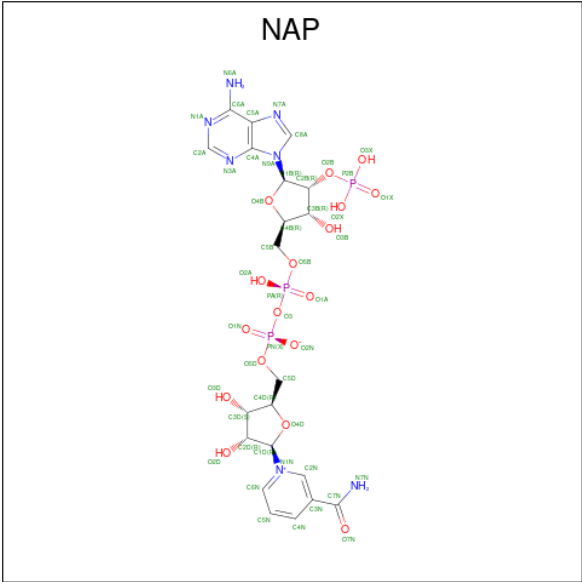
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	MET	-	expression tag	UNP Q5HQB2
A	387	ARG	-	expression tag	UNP Q5HQB2
A	388	GLY	-	expression tag	UNP Q5HQB2
A	389	SER	-	expression tag	UNP Q5HQB2
A	390	HIS	-	expression tag	UNP Q5HQB2
A	391	HIS	-	expression tag	UNP Q5HQB2
A	392	HIS	-	expression tag	UNP Q5HQB2
A	393	HIS	-	expression tag	UNP Q5HQB2
A	394	HIS	-	expression tag	UNP Q5HQB2
A	395	THR	-	expression tag	UNP Q5HQB2
A	396	THR	-	expression tag	UNP Q5HQB2
A	673	GLN	GLU	engineered mutation	UNP Q5HQB2
B	386	MET	-	expression tag	UNP Q5HQB2
B	387	ARG	-	expression tag	UNP Q5HQB2
B	388	GLY	-	expression tag	UNP Q5HQB2
B	389	SER	-	expression tag	UNP Q5HQB2
B	390	HIS	-	expression tag	UNP Q5HQB2
B	391	HIS	-	expression tag	UNP Q5HQB2
B	392	HIS	-	expression tag	UNP Q5HQB2
B	393	HIS	-	expression tag	UNP Q5HQB2
B	394	HIS	-	expression tag	UNP Q5HQB2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	395	THR	-	expression tag	UNP Q5HQB2
B	396	THR	-	expression tag	UNP Q5HQB2
B	673	GLN	GLU	engineered mutation	UNP Q5HQB2
C	386	MET	-	expression tag	UNP Q5HQB2
C	387	ARG	-	expression tag	UNP Q5HQB2
C	388	GLY	-	expression tag	UNP Q5HQB2
C	389	SER	-	expression tag	UNP Q5HQB2
C	390	HIS	-	expression tag	UNP Q5HQB2
C	391	HIS	-	expression tag	UNP Q5HQB2
C	392	HIS	-	expression tag	UNP Q5HQB2
C	393	HIS	-	expression tag	UNP Q5HQB2
C	394	HIS	-	expression tag	UNP Q5HQB2
C	395	THR	-	expression tag	UNP Q5HQB2
C	396	THR	-	expression tag	UNP Q5HQB2
C	673	GLN	GLU	engineered mutation	UNP Q5HQB2
D	386	MET	-	expression tag	UNP Q5HQB2
D	387	ARG	-	expression tag	UNP Q5HQB2
D	388	GLY	-	expression tag	UNP Q5HQB2
D	389	SER	-	expression tag	UNP Q5HQB2
D	390	HIS	-	expression tag	UNP Q5HQB2
D	391	HIS	-	expression tag	UNP Q5HQB2
D	392	HIS	-	expression tag	UNP Q5HQB2
D	393	HIS	-	expression tag	UNP Q5HQB2
D	394	HIS	-	expression tag	UNP Q5HQB2
D	395	THR	-	expression tag	UNP Q5HQB2
D	396	THR	-	expression tag	UNP Q5HQB2
D	673	GLN	GLU	engineered mutation	UNP Q5HQB2

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



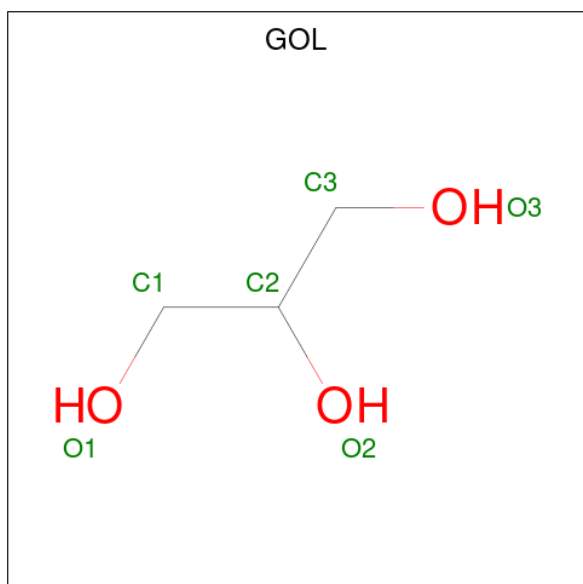
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

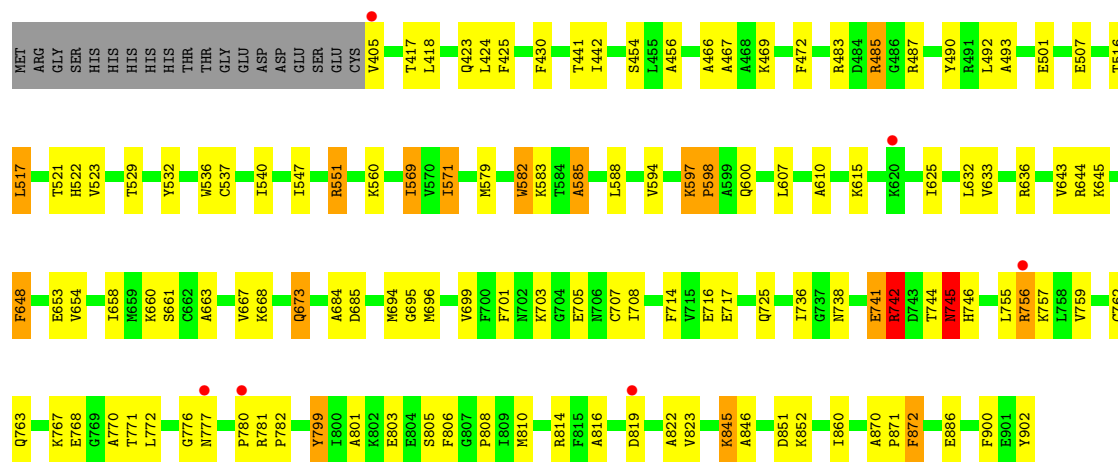
- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



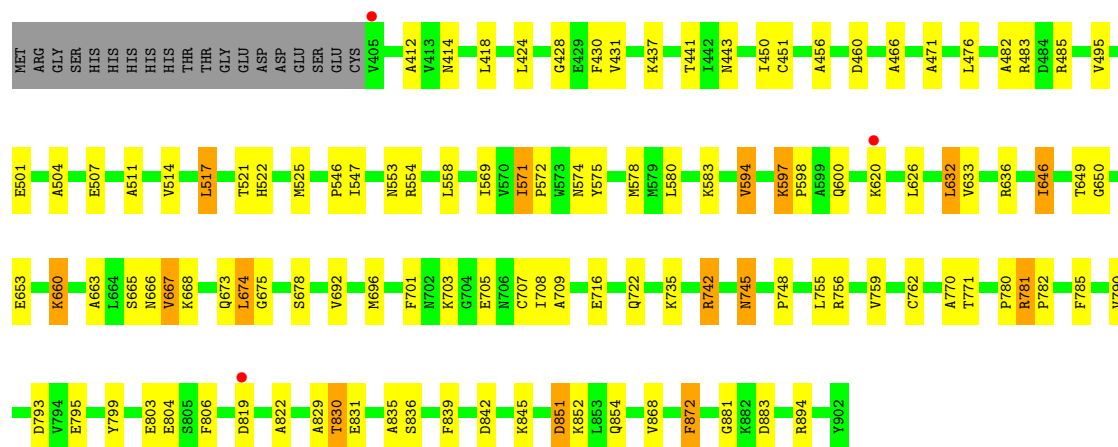
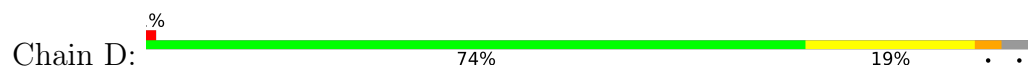
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	377	Total 377	O 377	0	4
5	B	336	Total 336	O 336	0	3
5	C	394	Total 394	O 394	0	3
5	D	377	Total 377	O 377	0	3



- Molecule 1: Aldehyde dehydrogenase 1 family, member L1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.90Å 194.40Å 97.22Å 90.00° 109.09° 90.00°	Depositor
Resolution (Å)	49.15 – 2.26 49.15 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.15-2.26) 99.5 (49.15-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.149 , 0.178 0.149 , 0.176	Depositor DCC
R_{free} test set	10652 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17496	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: SO4, GOL, 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	1.89	61/4066 (1.5%)	1.30	9/5496 (0.2%)
1	B	1.89	64/4066 (1.6%)	1.28	11/5496 (0.2%)
1	C	2.02	84/4066 (2.1%)	1.34	13/5496 (0.2%)
1	D	1.90	70/4066 (1.7%)	1.27	11/5496 (0.2%)
All	All	1.93	279/16264 (1.7%)	1.30	44/21984 (0.2%)

All (279) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	540	ILE	CA-CB	12.25	1.68	1.54
1	C	699	VAL	CA-CB	11.05	1.68	1.54
1	C	466	ALA	CA-CB	10.27	1.69	1.53
1	C	808	PRO	CA-C	9.85	1.61	1.52
1	D	790	VAL	CA-CB	-9.82	1.42	1.54
1	D	829	ALA	CA-CB	9.60	1.65	1.52
1	B	800	ILE	CA-C	9.24	1.62	1.52
1	A	540	ILE	CA-CB	9.06	1.64	1.54
1	C	507	GLU	CA-C	8.99	1.64	1.52
1	B	810	MET	N-CA	-8.94	1.35	1.46
1	B	819	ASP	C-O	8.68	1.34	1.23
1	D	511	ALA	CA-CB	8.57	1.66	1.53
1	B	667	VAL	CA-CB	8.43	1.66	1.54
1	C	742	ARG	CD-NE	-8.16	1.34	1.46
1	B	857	THR	C-O	7.99	1.32	1.23
1	B	565	GLY	C-O	7.89	1.28	1.24
1	C	745	ASN	CB-CG	-7.74	1.32	1.52
1	C	762	CYS	CA-C	7.73	1.62	1.52
1	B	738	ASN	CA-C	7.67	1.61	1.53
1	C	501	GLU	CD-OE2	7.67	1.40	1.25
1	A	413	VAL	CA-CB	7.58	1.64	1.54
1	C	781[A]	ARG	CA-C	-7.55	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	781[B]	ARG	CA-C	-7.55	1.43	1.52
1	C	661	SER	C-O	7.53	1.33	1.24
1	C	777	ASN	CB-CG	7.51	1.70	1.52
1	B	789	THR	C-O	7.47	1.33	1.23
1	D	822	ALA	CA-CB	7.47	1.65	1.53
1	C	780	PRO	CA-C	7.46	1.62	1.52
1	A	546	PRO	CA-C	7.45	1.59	1.52
1	C	523	VAL	CA-CB	7.41	1.62	1.55
1	A	599	ALA	C-O	7.33	1.32	1.23
1	A	466	ALA	CA-CB	7.29	1.64	1.53
1	C	717	GLU	C-O	-7.24	1.15	1.24
1	C	886	GLU	CA-C	7.24	1.62	1.52
1	B	524	GLY	CA-C	7.20	1.60	1.52
1	A	898	VAL	CA-CB	-7.17	1.45	1.54
1	A	622	VAL	CA-CB	7.12	1.63	1.54
1	B	823	VAL	CA-C	7.10	1.62	1.52
1	B	822	ALA	CA-CB	7.10	1.64	1.53
1	D	722	GLN	CA-C	7.09	1.61	1.52
1	A	656	LYS	N-CA	7.08	1.54	1.46
1	B	691	ALA	CA-CB	-7.03	1.42	1.53
1	C	870	ALA	CA-C	6.98	1.60	1.52
1	C	441	THR	CA-CB	6.96	1.65	1.53
1	A	463	LYS	CA-C	6.95	1.61	1.52
1	A	550	ALA	CA-C	6.91	1.61	1.53
1	B	575	TYR	N-CA	6.90	1.54	1.46
1	C	492	LEU	CA-C	6.88	1.61	1.52
1	C	746	HIS	N-CA	-6.82	1.38	1.46
1	D	716	GLU	CA-C	6.82	1.61	1.52
1	D	504	ALA	CA-C	6.81	1.61	1.52
1	C	900	PHE	C-O	6.81	1.31	1.23
1	C	516	THR	CA-CB	6.79	1.64	1.53
1	A	412	ALA	CA-CB	6.75	1.62	1.53
1	B	678	SER	CA-C	-6.73	1.45	1.52
1	B	709	ALA	CA-CB	6.73	1.64	1.53
1	A	782	PRO	CA-C	6.70	1.60	1.52
1	C	472	PHE	CA-C	6.70	1.61	1.52
1	A	719	ILE	CA-CB	6.66	1.61	1.54
1	A	542	GLY	C-O	6.65	1.30	1.23
1	B	860	ILE	C-O	6.65	1.31	1.24
1	A	654	VAL	CA-C	6.65	1.61	1.52
1	B	719	ILE	CA-CB	6.61	1.62	1.54
1	B	782	PRO	CA-C	6.61	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	LYS	CE-NZ	6.60	1.69	1.49
1	D	759	VAL	CA-CB	6.57	1.62	1.54
1	D	517	LEU	N-CA	-6.55	1.38	1.46
1	D	495	VAL	N-CA	-6.54	1.39	1.46
1	B	445	THR	CA-C	6.53	1.61	1.52
1	C	585	ALA	CA-CB	6.52	1.63	1.53
1	A	735	LYS	N-CA	-6.52	1.38	1.46
1	C	801	ALA	CA-C	6.52	1.61	1.52
1	D	868	VAL	CA-CB	6.46	1.62	1.54
1	D	460	ASP	CB-CG	6.46	1.68	1.52
1	C	799	TYR	CA-C	6.44	1.61	1.52
1	B	871	PRO	C-O	-6.44	1.16	1.23
1	C	645	LYS	CD-CE	6.43	1.71	1.52
1	C	716	GLU	CA-C	6.43	1.60	1.52
1	B	716	GLU	CA-C	6.42	1.61	1.52
1	A	822	ALA	CA-CB	6.38	1.63	1.53
1	C	767	LYS	N-CA	-6.33	1.38	1.46
1	A	589	ALA	CA-CB	6.33	1.63	1.53
1	B	466	ALA	CA-CB	6.33	1.63	1.53
1	B	580	LEU	CA-C	6.31	1.60	1.52
1	C	819	ASP	C-O	6.30	1.31	1.23
1	C	648	PHE	C-O	6.28	1.31	1.23
1	C	822	ALA	CA-CB	6.26	1.63	1.53
1	C	871	PRO	C-O	6.26	1.30	1.23
1	C	469	LYS	CE-NZ	-6.26	1.30	1.49
1	B	482	ALA	CA-CB	6.25	1.63	1.53
1	D	583	LYS	N-CA	-6.23	1.38	1.46
1	D	646	ILE	CA-CB	6.21	1.61	1.54
1	C	823	VAL	CA-C	6.19	1.60	1.52
1	C	771	THR	CA-C	6.17	1.60	1.52
1	A	571	ILE	CA-CB	-6.16	1.48	1.55
1	A	509	LEU	C-O	-6.12	1.16	1.24
1	D	795[A]	GLU	C-O	6.12	1.31	1.23
1	D	795[B]	GLU	C-O	6.12	1.31	1.23
1	A	762	CYS	CA-C	6.11	1.60	1.52
1	C	517	LEU	CG-CD1	6.10	1.72	1.52
1	D	666	ASN	C-O	6.07	1.31	1.24
1	D	842	ASP	CA-C	6.06	1.60	1.52
1	D	501	GLU	N-CA	6.06	1.53	1.46
1	C	694	MET	CB-CG	6.05	1.70	1.52
1	A	562	GLU	N-CA	6.01	1.50	1.45
1	C	756	ARG	CZ-NH1	6.00	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	756	ARG	NE-CZ	5.98	1.39	1.33
1	C	551	ARG	CA-C	5.98	1.59	1.53
1	D	748	PRO	CA-C	5.97	1.59	1.52
1	A	740	LEU	C-O	-5.97	1.16	1.24
1	C	782	PRO	CA-C	5.97	1.59	1.52
1	D	441	THR	CA-CB	5.94	1.64	1.53
1	B	869	ALA	CA-C	5.93	1.60	1.52
1	D	575	TYR	N-CA	5.93	1.53	1.46
1	B	844	ASN	C-O	5.93	1.31	1.24
1	A	485	ARG	CG-CD	5.91	1.70	1.52
1	D	649	THR	CA-C	5.89	1.59	1.52
1	C	846	ALA	CA-C	5.87	1.60	1.52
1	C	759	VAL	CA-CB	5.87	1.61	1.54
1	B	504	ALA	CA-C	5.86	1.60	1.52
1	D	437	LYS	C-O	5.86	1.31	1.23
1	A	595	VAL	CA-CB	5.85	1.61	1.54
1	A	551	ARG	CA-C	5.84	1.60	1.52
1	D	514	VAL	CA-C	5.83	1.58	1.52
1	B	831	GLU	CG-CD	5.82	1.66	1.52
1	D	663	ALA	CA-CB	5.82	1.62	1.53
1	A	571	ILE	CA-C	5.81	1.57	1.52
1	B	836	SER	C-O	5.81	1.30	1.23
1	C	696	MET	CB-CG	5.77	1.69	1.52
1	D	705	GLU	CA-C	5.77	1.59	1.53
1	C	772	LEU	C-O	-5.77	1.16	1.23
1	D	466	ALA	CA-CB	5.77	1.62	1.53
1	A	724	VAL	CA-CB	-5.76	1.47	1.54
1	C	763	GLN	CG-CD	5.76	1.66	1.52
1	C	653	GLU	CG-CD	5.75	1.66	1.52
1	B	826	ARG	N-CA	5.75	1.53	1.46
1	C	598	PRO	C-O	5.71	1.30	1.23
1	A	594	VAL	CA-CB	5.69	1.63	1.55
1	D	771	THR	N-CA	-5.69	1.39	1.46
1	D	632	LEU	CA-C	5.68	1.57	1.52
1	A	797	HIS	N-CA	5.68	1.53	1.46
1	C	814	ARG	CD-NE	5.68	1.54	1.46
1	D	476	LEU	CA-C	5.68	1.60	1.52
1	A	871	PRO	C-O	5.67	1.30	1.23
1	B	495	VAL	N-CA	-5.67	1.40	1.46
1	C	780	PRO	C-O	5.66	1.31	1.24
1	B	707[A]	CYS	N-CA	5.65	1.53	1.46
1	B	707[B]	CYS	N-CA	5.65	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	571	ILE	CA-C	5.64	1.57	1.52
1	A	622	VAL	CA-C	-5.60	1.45	1.52
1	D	546	PRO	CA-C	5.59	1.58	1.52
1	C	644	ARG	CZ-NH1	5.57	1.40	1.32
1	A	756	ARG	CD-NE	5.57	1.54	1.46
1	D	709	ALA	CA-CB	5.56	1.62	1.53
1	D	636	ARG	CA-C	5.55	1.59	1.52
1	A	529	THR	CA-CB	5.54	1.61	1.53
1	B	712	ARG	CD-NE	5.54	1.54	1.46
1	A	498	GLN	CG-CD	5.54	1.66	1.52
1	B	469	LYS	C-O	5.54	1.30	1.24
1	C	695	GLY	CA-C	-5.54	1.45	1.52
1	D	839	PHE	C-O	5.54	1.30	1.24
1	A	883	ASP	CG-OD1	5.54	1.35	1.25
1	C	487	ARG	CA-CB	5.54	1.61	1.53
1	C	493	ALA	CA-CB	5.53	1.61	1.53
1	C	442	ILE	CA-CB	5.53	1.61	1.54
1	A	409	VAL	CA-CB	-5.52	1.47	1.54
1	D	742	ARG	CG-CD	5.52	1.69	1.52
1	A	441	THR	C-O	-5.51	1.17	1.24
1	D	804	GLU	CG-CD	5.51	1.65	1.52
1	B	858	VAL	CA-CB	-5.51	1.47	1.54
1	B	742	ARG	CG-CD	5.50	1.69	1.52
1	D	770	ALA	CA-CB	5.50	1.62	1.53
1	C	860	ILE	CA-CB	-5.49	1.46	1.53
1	A	716	GLU	CA-C	5.49	1.59	1.52
1	D	653	GLU	CB-CG	5.47	1.68	1.52
1	D	793	ASP	CA-CB	5.47	1.61	1.53
1	C	776	GLY	CA-C	-5.47	1.43	1.51
1	A	550	ALA	N-CA	5.47	1.53	1.46
1	C	745	ASN	C-O	-5.47	1.16	1.24
1	B	655	GLY	N-CA	5.46	1.52	1.45
1	A	471	ALA	CA-C	5.46	1.59	1.52
1	A	756	ARG	CZ-NH1	5.45	1.40	1.32
1	D	667	VAL	CA-CB	5.44	1.61	1.54
1	A	754	HIS	CA-CB	5.44	1.62	1.53
1	B	701	PHE	CA-C	-5.43	1.46	1.52
1	B	682	ILE	CA-CB	5.42	1.60	1.53
1	D	780	PRO	N-CA	5.42	1.54	1.47
1	B	569	ILE	C-O	-5.42	1.18	1.24
1	C	636	ARG	CA-C	5.42	1.59	1.52
1	B	711	GLY	C-O	5.42	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	768[A]	GLU	N-CA	5.42	1.53	1.46
1	B	768[B]	GLU	N-CA	5.42	1.53	1.46
1	D	675	GLY	C-O	5.42	1.29	1.23
1	A	735	LYS	CG-CD	5.40	1.68	1.52
1	D	782	PRO	CA-C	5.40	1.59	1.52
1	A	791	PHE	C-O	5.39	1.30	1.23
1	B	554	ARG	CZ-NH1	5.39	1.40	1.32
1	D	485	ARG	CG-CD	5.38	1.68	1.52
1	C	872	PHE	CA-C	5.37	1.58	1.52
1	C	736	ILE	N-CA	-5.37	1.39	1.46
1	C	714	PHE	N-CA	-5.36	1.39	1.46
1	D	830	THR	CA-C	5.36	1.59	1.52
1	B	501	GLU	CD-OE2	5.36	1.35	1.25
1	A	521	THR	CA-CB	5.35	1.60	1.53
1	B	630	GLY	C-O	5.33	1.30	1.23
1	A	779	VAL	CA-C	5.33	1.57	1.53
1	A	800	ILE	CA-C	5.33	1.59	1.52
1	A	756	ARG	NE-CZ	5.32	1.39	1.33
1	A	819	ASP	C-O	5.32	1.30	1.23
1	C	653	GLU	CD-OE1	5.31	1.35	1.25
1	C	770	ALA	CA-CB	5.31	1.61	1.53
1	B	636	ARG	CA-C	5.30	1.59	1.52
1	B	577	LEU	CA-C	5.30	1.59	1.52
1	D	501	GLU	CD-OE2	5.30	1.35	1.25
1	B	656	LYS	N-CA	5.30	1.52	1.46
1	D	836	SER	CA-C	-5.30	1.46	1.52
1	C	694	MET	CG-SD	5.29	1.94	1.80
1	C	490[A]	TYR	N-CA	5.29	1.52	1.46
1	C	490[B]	TYR	N-CA	5.29	1.52	1.46
1	C	582	TRP	C-O	5.29	1.30	1.24
1	C	684	ALA	CA-CB	5.29	1.62	1.53
1	B	753	ALA	CA-CB	5.29	1.62	1.53
1	D	762	CYS	CA-CB	-5.29	1.44	1.53
1	A	639	ASP	CA-CB	5.28	1.62	1.53
1	C	417	THR	CA-CB	5.28	1.59	1.53
1	A	694	MET	CG-SD	5.26	1.93	1.80
1	A	421	PRO	N-CA	5.25	1.53	1.47
1	B	853	LEU	C-O	5.25	1.30	1.23
1	C	816	ALA	CA-C	-5.25	1.46	1.52
1	C	654	VAL	C-O	5.24	1.30	1.24
1	B	675	GLY	C-O	5.24	1.29	1.23
1	B	706	ASN	N-CA	-5.23	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	532	TYR	CA-C	5.23	1.59	1.52
1	D	471	ALA	CA-C	5.23	1.59	1.52
1	D	431	VAL	C-O	5.23	1.29	1.23
1	D	835	ALA	CA-CB	5.20	1.61	1.53
1	D	653	GLU	CD-OE1	5.20	1.35	1.25
1	B	823	VAL	C-O	5.19	1.30	1.24
1	D	831	GLU	CG-CD	5.19	1.65	1.52
1	D	894	ARG	C-O	5.19	1.30	1.23
1	D	451	CYS	CA-C	-5.18	1.46	1.52
1	C	705	GLU	CA-C	5.18	1.59	1.53
1	A	834	LEU	N-CA	-5.18	1.40	1.46
1	B	871	PRO	CA-C	5.17	1.58	1.52
1	C	569	ILE	CG1-CD1	5.17	1.72	1.51
1	A	467	ALA	CA-C	5.15	1.59	1.52
1	A	756	ARG	CB-CG	5.15	1.67	1.52
1	B	566	VAL	CA-CB	5.15	1.60	1.54
1	C	653	GLU	CB-CG	5.15	1.67	1.52
1	A	469	LYS	CE-NZ	-5.13	1.33	1.49
1	D	571	ILE	C-O	5.12	1.29	1.24
1	B	857	THR	CA-C	-5.09	1.46	1.52
1	D	507	GLU	CA-C	5.09	1.59	1.52
1	D	883	ASP	CG-OD1	5.08	1.35	1.25
1	C	663	ALA	CA-CB	5.08	1.61	1.53
1	C	810	MET	CA-CB	5.08	1.60	1.53
1	D	872	PHE	N-CA	-5.08	1.40	1.46
1	D	525	MET	SD-CE	5.08	1.92	1.79
1	D	665	SER	CA-C	5.07	1.59	1.52
1	A	725[A]	GLN	CA-CB	5.07	1.61	1.53
1	A	725[B]	GLN	CA-CB	5.07	1.61	1.53
1	B	653	GLU	CD-OE1	5.07	1.34	1.25
1	B	785	PHE	C-O	5.06	1.30	1.23
1	B	879	GLY	CA-C	5.06	1.57	1.52
1	C	744	THR	CA-CB	-5.06	1.45	1.53
1	D	443	ASN	CA-C	5.05	1.58	1.52
1	C	467	ALA	CA-C	5.05	1.59	1.52
1	D	872	PHE	CA-C	5.04	1.58	1.52
1	D	412	ALA	CA-CB	5.03	1.60	1.53
1	B	416	LEU	CA-C	-5.03	1.46	1.52
1	B	829	ALA	CA-C	-5.03	1.47	1.53
1	D	854	GLN	CA-CB	5.02	1.59	1.52
1	D	626	LEU	N-CA	-5.02	1.41	1.46
1	B	441	THR	CA-CB	5.02	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	781[A]	ARG	CA-C	-5.01	1.45	1.53
1	D	781[B]	ARG	CA-C	-5.01	1.45	1.53
1	A	459	SER	CA-C	5.01	1.59	1.52
1	C	485	ARG	CG-CD	5.01	1.67	1.52
1	D	819	ASP	C-O	5.00	1.30	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	742	ARG	NE-CZ-NH2	-8.84	111.25	119.20
1	D	450	ILE	N-CA-C	-8.79	102.30	110.82
1	D	674	LEU	CA-C-N	-7.26	111.16	121.54
1	D	674	LEU	C-N-CA	-7.26	111.16	121.54
1	A	776	GLY	N-CA-C	-7.22	105.88	114.48
1	D	881	GLY	N-CA-C	-6.89	104.58	112.29
1	A	708	ILE	N-CA-C	6.72	118.61	112.29
1	C	742	ARG	CD-NE-CZ	6.72	133.80	124.40
1	C	597	LYS	CB-CA-C	-6.63	102.81	110.17
1	B	694	MET	CG-SD-CE	6.43	115.05	100.90
1	B	873	GLY	CA-C-N	-6.41	115.77	122.69
1	B	873	GLY	C-N-CA	-6.41	115.77	122.69
1	C	763	GLN	N-CA-C	-6.37	103.62	111.33
1	B	855	ALA	CA-C-N	6.17	127.86	120.14
1	B	855	ALA	C-N-CA	6.17	127.86	120.14
1	A	812	ILE	N-CA-C	6.13	116.76	108.17
1	B	523	VAL	N-CA-C	-6.13	106.28	111.56
1	A	571	ILE	N-CA-C	6.10	115.77	108.45
1	C	851	ASP	CB-CA-C	-6.00	100.83	110.79
1	B	708	ILE	N-CA-C	5.87	117.81	112.29
1	C	777	ASN	N-CA-CB	-5.81	101.45	111.55
1	C	571	ILE	N-CA-C	5.70	115.29	108.45
1	D	851	ASP	CB-CA-C	-5.68	101.36	110.79
1	C	696	MET	CA-CB-CG	5.65	125.40	114.10
1	B	830	THR	N-CA-C	-5.51	100.35	108.99
1	A	694	MET	CG-SD-CE	5.38	112.75	100.90
1	D	482	ALA	N-CA-C	-5.37	105.43	111.28
1	C	768[A]	GLU	N-CA-C	-5.35	106.43	113.17
1	C	768[B]	GLU	N-CA-C	-5.35	106.43	113.17
1	A	655	GLY	N-CA-C	-5.28	106.40	112.73
1	B	667	VAL	CB-CA-C	-5.23	102.72	111.29
1	A	674	LEU	CA-C-N	-5.19	114.12	121.54
1	A	674	LEU	C-N-CA	-5.19	114.12	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	594	VAL	N-CA-C	5.09	115.08	108.35
1	D	574	ASN	N-CA-C	5.08	116.89	111.36
1	C	745	ASN	CB-CG-ND2	-5.06	108.80	116.40
1	A	696	MET	CG-SD-CE	5.03	111.97	100.90
1	C	725[A]	GLN	N-CA-C	-5.02	105.69	111.07
1	C	725[B]	GLN	N-CA-C	-5.02	105.69	111.07
1	B	696	MET	CG-SD-CE	5.02	111.95	100.90
1	D	678	SER	N-CA-C	5.02	116.85	109.42
1	D	553	ASN	N-CA-C	5.02	117.00	110.53
1	D	822	ALA	N-CA-C	-5.01	105.90	111.36
1	B	553	ASN	N-CA-C	5.01	116.99	110.53

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	3906	0	3923	37	0
1	B	3906	0	3922	28	0
1	C	3906	0	3923	42	0
1	D	3906	0	3923	32	0
2	A	56	0	14	1	0
2	B	56	0	14	1	0
2	C	56	0	14	1	0
2	D	56	0	14	1	0
3	A	35	0	0	0	0
3	B	40	0	0	1	0
3	C	40	0	0	2	0
3	D	25	0	0	1	0
4	A	6	0	8	0	0
4	B	6	0	8	2	0
4	C	6	0	8	0	0
4	D	6	0	8	1	0
5	A	377	0	0	6	0
5	B	336	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	394	0	0	6	0
5	D	377	0	0	3	0
All	All	17496	0	15779	140	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 4.

All (140) 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:A:669:LYS:CE	1:A:669:LYS:NZ	1.69	1.50
1:B:799:TYR:CE2	1:B:803[A]:GLU:HG3	2.14	0.83
1:D:742:ARG:HD2	5:D:1465:HOH:O	1.83	0.78
1:A:569:ILE:HD12	1:A:594:VAL:HG21	1.69	0.74
1:B:706:ASN:HD21	4:B:3026:GOL:H12	1.53	0.73
1:B:673:GLN:HB2	5:B:1472:HOH:O	1.89	0.72
1:A:799:TYR:CE2	1:A:803[A]:GLU:HG3	2.27	0.70
1:C:745:ASN:HD22	1:C:745:ASN:C	2.02	0.68
1:B:414:ASN:OD1	1:B:742:ARG:NH2	2.27	0.66
1:D:708:ILE:CG2	1:D:872:PHE:HE1	2.08	0.66
1:D:799:TYR:CE2	1:D:803[A]:GLU:HG3	2.32	0.65
1:B:569:ILE:HD12	1:B:594:VAL:HG21	1.79	0.64
1:C:852:LYS:NZ	3:C:3002:SO4:O3	2.29	0.63
1:D:735:LYS:H	1:D:745:ASN:HD21	1.45	0.63
1:A:600:GLN:NE2	5:A:1208:HOH:O	2.27	0.62
1:D:708:ILE:CG2	1:D:872:PHE:CE1	2.83	0.61
1:C:756:ARG:NH2	5:C:1221:HOH:O	2.34	0.61
1:A:632:LEU:C	1:A:632:LEU:HD23	2.25	0.61
2:D:903[B]:NAP:H6N	2:D:903[B]:NAP:H52N	1.82	0.61
2:B:903[B]:NAP:H6N	2:B:903[B]:NAP:H52N	1.83	0.60
1:C:742:ARG:HD2	3:C:3028:SO4:O4	2.01	0.60
1:C:799:TYR:CE2	1:C:803[A]:GLU:HG3	2.36	0.60
1:A:517:LEU:HD11	1:A:701:PHE:CZ	2.37	0.60
1:A:777:ASN:H	1:A:787:GLN:HE21	1.50	0.59
1:B:756:ARG:NH2	5:B:1282:HOH:O	2.35	0.59
1:B:692:VAL:O	1:B:696:MET:HG3	2.03	0.59
1:B:735:LYS:H	1:B:745:ASN:HD21	1.51	0.58
1:C:632:LEU:C	1:C:632:LEU:HD23	2.28	0.58
2:C:903[B]:NAP:H52N	2:C:903[B]:NAP:H6N	1.84	0.57
1:B:706:ASN:ND2	4:B:3026:GOL:H12	2.18	0.57
1:C:521:THR:O	1:C:522:HIS:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:GLU:OE2	1:A:814:ARG:HD3	2.05	0.57
1:B:799:TYR:CZ	1:B:803[A]:GLU:HG3	2.42	0.55
1:D:428:GLY:HA3	1:D:620[A]:LYS:HG2	1.89	0.55
1:D:632:LEU:C	1:D:632:LEU:HD23	2.32	0.54
1:D:600:GLN:NE2	5:D:352:HOH:O	2.38	0.54
1:C:456:ALA:HB3	1:C:633:VAL:HG21	1.90	0.54
1:D:521:THR:O	1:D:522:HIS:C	2.51	0.53
1:C:424:LEU:O	1:C:430:PHE:HA	2.09	0.53
1:D:756:ARG:NH2	5:D:1384:HOH:O	2.41	0.53
1:D:781[B]:ARG:HD2	1:D:785:PHE:CD2	2.44	0.53
1:C:648:PHE:CD1	1:C:658:ILE:HD12	2.44	0.53
1:D:414:ASN:OD1	1:D:742:ARG:NH2	2.37	0.52
1:C:569:ILE:HD12	1:C:594:VAL:HG21	1.91	0.52
1:B:708:ILE:CG2	1:B:872:PHE:HE1	2.23	0.52
1:C:425:PHE:CD2	1:C:610:ALA:HB1	2.45	0.52
1:C:597:LYS:HD2	1:C:598:PRO:O	2.10	0.52
1:C:560[B]:LYS:NZ	5:C:1072:HOH:O	2.33	0.51
1:C:643:VAL:O	1:C:668:LYS:HE3	2.11	0.51
1:D:424:LEU:O	1:D:430:PHE:HA	2.10	0.51
1:A:777:ASN:H	1:A:787:GLN:NE2	2.08	0.50
5:B:77:HOH:O	1:D:483:ARG:HD3	2.11	0.50
1:B:521:THR:O	1:B:522:HIS:C	2.53	0.50
1:C:685:ASP:OD2	1:C:845:LYS:NZ	2.44	0.50
1:B:600:GLN:NE2	5:B:974:HOH:O	2.45	0.49
1:A:851:ASP:OD2	1:C:902:TYR:OH	2.25	0.49
1:C:600:GLN:NE2	5:C:930:HOH:O	2.43	0.49
2:A:903[B]:NAP:H6N	2:A:903[B]:NAP:H52N	1.93	0.49
1:D:554:ARG:NE	3:D:3020:SO4:O4	2.31	0.49
5:A:1015:HOH:O	1:C:483:ARG:HD3	2.13	0.49
1:D:558:LEU:HD12	1:D:558:LEU:C	2.37	0.49
1:A:824:LEU:HD21	1:A:849:VAL:HG13	1.95	0.48
1:A:569:ILE:HG23	1:A:583:LYS:HD3	1.95	0.48
1:C:615:LYS:NZ	5:C:1327:HOH:O	2.46	0.48
1:C:738:ASN:HB3	1:C:741[A]:GLU:CG	2.43	0.48
1:A:648:PHE:CD1	1:A:658:ILE:HD12	2.47	0.48
1:A:479:LYS:NZ	5:A:1367:HOH:O	2.46	0.47
1:A:692:VAL:O	1:A:696:MET:CG	2.62	0.47
1:B:684:ALA:HA	1:B:719:ILE:HD13	1.95	0.47
1:B:902:TYR:OH	1:D:851:ASP:OD2	2.23	0.47
1:A:571:ILE:HB	1:A:572:PRO:HD2	1.96	0.47
1:A:413:VAL:CG1	1:A:418:LEU:HD22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ILE:CG2	1:B:872:PHE:CE1	2.98	0.47
1:D:578:MET:HE1	4:D:3028:GOL:H11	1.97	0.47
1:D:456:ALA:HB3	1:D:633:VAL:HG21	1.98	0.46
1:D:692:VAL:O	1:D:696:MET:HG2	2.15	0.46
1:A:735:LYS:H	1:A:745:ASN:HD21	1.63	0.45
1:B:424:LEU:O	1:B:430:PHE:HA	2.17	0.45
1:B:735:LYS:H	1:B:745:ASN:ND2	2.14	0.45
1:C:423:GLN:HA	1:C:454:SER:OG	2.16	0.45
1:C:648:PHE:CD1	1:C:658:ILE:CD1	3.00	0.45
1:D:646:ILE:HG12	1:D:668:LYS:HD3	1.97	0.45
1:D:571:ILE:HB	1:D:572:PRO:HD2	1.98	0.45
1:D:597:LYS:HD2	1:D:598:PRO:O	2.17	0.45
3:B:3003:SO4:O1	1:D:852:LYS:NZ	2.43	0.45
1:C:517:LEU:HD11	1:C:701:PHE:CZ	2.52	0.45
1:A:533:PHE:HB3	1:A:589:ALA:HB2	1.99	0.44
1:A:692:VAL:O	1:A:696:MET:HG3	2.17	0.44
1:B:646:ILE:HG12	1:B:668:LYS:HD3	1.98	0.44
1:B:745:ASN:C	1:B:745:ASN:HD22	2.25	0.44
1:C:610:ALA:HB2	1:C:625:ILE:HD12	1.99	0.44
1:C:757:LYS:HE2	1:C:805:SER:O	2.17	0.44
1:D:735:LYS:N	1:D:745:ASN:HD21	2.11	0.44
1:A:547:ILE:H	1:A:547:ILE:HD13	1.83	0.44
1:B:666:ASN:C	1:B:667:VAL:HG23	2.43	0.44
1:C:571:ILE:HG13	1:C:598:PRO:HA	2.00	0.43
1:C:579:MET:HE1	1:C:582:TRP:CZ3	2.53	0.43
1:C:673:GLN:OE1	1:C:872:PHE:CE2	2.71	0.43
1:C:738:ASN:HB3	1:C:741[A]:GLU:HG3	2.00	0.43
1:D:580:LEU:C	1:D:580:LEU:HD23	2.43	0.43
1:A:529:THR:HG21	1:A:582:TRP:HA	1.99	0.43
1:A:571:ILE:HB	1:A:572:PRO:CD	2.49	0.43
1:D:735:LYS:H	1:D:745:ASN:ND2	2.15	0.43
1:A:781[B]:ARG:HD2	1:A:785:PHE:CE2	2.54	0.43
1:A:645:LYS:HE3	1:A:892:TYR:CE1	2.54	0.42
1:C:551:ARG:HD3	5:C:1259:HOH:O	2.19	0.42
1:C:660:LYS:HG3	1:D:660:LYS:HG3	2.01	0.42
1:A:745:ASN:C	1:A:745:ASN:HD22	2.26	0.42
1:C:741[B]:GLU:OE1	5:C:939:HOH:O	2.21	0.42
1:D:571:ILE:HB	1:D:572:PRO:CD	2.49	0.42
1:A:708:ILE:CG2	1:A:872:PHE:HE1	2.32	0.42
1:C:708:ILE:CG2	1:C:872:PHE:HE1	2.32	0.42
1:B:424:LEU:CD2	1:B:627:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ARG:HD3	1:C:588:LEU:O	2.19	0.42
1:A:521:THR:O	1:A:522:HIS:C	2.60	0.42
1:D:517:LEU:HD11	1:D:701:PHE:CZ	2.54	0.42
1:D:569:ILE:HD12	1:D:594:VAL:HG21	2.02	0.41
1:C:673:GLN:OE1	1:C:872:PHE:HE2	2.03	0.41
1:A:465:VAL:HG11	1:A:640:HIS:CE1	2.55	0.41
1:B:797:HIS:HD2	5:B:954:HOH:O	2.02	0.41
1:A:560[B]:LYS:CD	5:A:1267:HOH:O	2.68	0.41
1:A:560[B]:LYS:HD3	5:A:1267:HOH:O	2.21	0.41
1:A:690:LYS:HD2	1:A:694:MET:HG2	2.01	0.41
1:C:569:ILE:HG23	1:C:583:LYS:HD3	2.03	0.41
1:B:643:VAL:O	1:B:668:LYS:HE3	2.21	0.41
1:C:799:TYR:CD2	1:C:803[A]:GLU:HG3	2.56	0.41
1:A:536:TRP:CG	1:A:889:LEU:HD11	2.56	0.41
1:A:799:TYR:CD2	1:A:803[A]:GLU:HG3	2.56	0.41
1:B:799:TYR:CD2	1:B:803[A]:GLU:HG3	2.55	0.41
1:B:672:LEU:HB3	1:B:674:LEU:HD21	2.03	0.40
1:C:425:PHE:CG	1:C:610:ALA:HB1	2.57	0.40
1:C:529:THR:HG22	1:C:585:ALA:HB3	2.03	0.40
1:B:547:ILE:H	1:B:547:ILE:HD13	1.86	0.40
1:B:735:LYS:N	1:B:745:ASN:HD21	2.17	0.40
1:C:607:LEU:HD23	1:C:607:LEU:HA	1.91	0.40
1:A:580:LEU:HD23	1:A:580:LEU:C	2.47	0.40
1:A:854:GLN:HG3	5:A:1262:HOH:O	2.20	0.40
1:D:650:GLY:O	1:D:674:LEU:HA	2.22	0.40
1:A:643:VAL:O	1:A:668:LYS:HE3	2.22	0.40
1:C:536:TRP:O	1:C:537:CYS:C	2.65	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	515/517 (100%)	501 (97%)	14 (3%)	0	100	100
1	B	515/517 (100%)	495 (96%)	20 (4%)	0	100	100
1	C	515/517 (100%)	492 (96%)	23 (4%)	0	100	100
1	D	515/517 (100%)	497 (96%)	18 (4%)	0	100	100
All	All	2060/2068 (100%)	1985 (96%)	75 (4%)	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	428/426 (100%)	413 (96%)	15 (4%)	32	39
1	B	428/426 (100%)	412 (96%)	16 (4%)	30	37
1	C	428/426 (100%)	413 (96%)	15 (4%)	32	39
1	D	428/426 (100%)	414 (97%)	14 (3%)	33	42
All	All	1712/1704 (100%)	1652 (96%)	60 (4%)	33	39

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LEU
1	A	418	LEU
1	A	547	ILE
1	A	625	ILE
1	A	667	VAL
1	A	673	GLN
1	A	690	LYS
1	A	696	MET
1	A	703	LYS
1	A	707[A]	CYS
1	A	707[B]	CYS
1	A	725[A]	GLN
1	A	725[B]	GLN

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Mol	Chain	Res	Type
1	A	745	ASN
1	A	806	PHE
1	B	418	LEU
1	B	429	GLU
1	B	547	ILE
1	B	597	LYS
1	B	667	VAL
1	B	673	GLN
1	B	696	MET
1	B	703	LYS
1	B	707[A]	CYS
1	B	707[B]	CYS
1	B	742	ARG
1	B	745	ASN
1	B	755	LEU
1	B	788	PRO
1	B	830	THR
1	B	845	LYS
1	C	405	VAL
1	C	418	LEU
1	C	547	ILE
1	C	667	VAL
1	C	673	GLN
1	C	703	LYS
1	C	707[A]	CYS
1	C	707[B]	CYS
1	C	741[A]	GLU
1	C	741[B]	GLU
1	C	742	ARG
1	C	745	ASN
1	C	755	LEU
1	C	806	PHE
1	C	845	LYS
1	D	418	LEU
1	D	547	ILE
1	D	597	LYS
1	D	660	LYS
1	D	667	VAL
1	D	673	GLN
1	D	703	LYS
1	D	707[A]	CYS
1	D	707[B]	CYS

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Mol	Chain	Res	Type
1	D	745	ASN
1	D	755	LEU
1	D	806	PHE
1	D	830	THR
1	D	845	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	GLN
1	A	498	GLN
1	A	721	ASN
1	A	745	ASN
1	A	787	GLN
1	A	844	ASN
1	B	423	GLN
1	B	440	ASN
1	B	457	GLN
1	B	498	GLN
1	B	600	GLN
1	B	706	ASN
1	B	745	ASN
1	B	797	HIS
1	C	541	GLN
1	C	600	GLN
1	C	745	ASN
1	C	763	GLN
1	D	457	GLN
1	D	498	GLN
1	D	600	GLN
1	D	745	ASN

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 ⓘ

40 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	SO4	B	3022	-	4,4,4	0.41	0	6,6,6	0.88	0
2	NAP	A	903[A]	-	50,33,52	4.58	7 (14%)	71,52,80	1.88	12 (16%)
2	NAP	B	903[B]	-	50,52,52	3.36	7 (14%)	71,80,80	2.29	15 (21%)
2	NAP	C	903[A]	-	50,33,52	3.14	7 (14%)	71,52,80	2.03	15 (21%)
3	SO4	D	3008	-	4,4,4	0.67	0	6,6,6	1.51	1 (16%)
3	SO4	A	3015	-	4,4,4	0.55	0	6,6,6	1.29	1 (16%)
4	GOL	C	3029	-	5,5,5	0.68	0	5,5,5	1.35	1 (20%)
3	SO4	A	3001	-	4,4,4	0.47	0	6,6,6	0.48	0
4	GOL	B	3026	-	5,5,5	0.58	0	5,5,5	0.58	0
3	SO4	A	3021	-	4,4,4	0.49	0	6,6,6	0.96	0
2	NAP	B	903[A]	-	50,33,52	5.18	7 (14%)	71,52,80	2.54	16 (22%)
3	SO4	B	3004	-	4,4,4	0.45	0	6,6,6	0.33	0
3	SO4	C	3028	-	4,4,4	0.51	0	6,6,6	1.29	1 (16%)
3	SO4	D	3020	-	4,4,4	0.76	0	6,6,6	0.87	0
3	SO4	B	3019	-	4,4,4	0.57	0	6,6,6	0.58	0
2	NAP	D	903[B]	-	50,52,52	2.18	6 (12%)	71,80,80	1.53	9 (12%)
3	SO4	A	3024	-	4,4,4	0.29	0	6,6,6	0.45	0
3	SO4	D	3027	-	4,4,4	0.34	0	6,6,6	0.73	0
3	SO4	B	3009	-	4,4,4	0.36	0	6,6,6	0.46	0
3	SO4	B	3005	-	4,4,4	0.41	0	6,6,6	1.11	1 (16%)
4	GOL	A	3025	-	5,5,5	0.73	0	5,5,5	1.21	1 (20%)
3	SO4	C	3013	-	4,4,4	0.47	0	6,6,6	1.42	1 (16%)
3	SO4	B	3025	-	4,4,4	0.45	0	6,6,6	0.65	0
3	SO4	A	3011	-	4,4,4	0.28	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	3026	-	4,4,4	0.35	0	6,6,6	1.65	2 (33%)
2	NAP	A	903[B]	-	50,52,52	3.53	7 (14%)	71,80,80	1.56	11 (15%)
3	SO4	C	3023	-	4,4,4	0.35	0	6,6,6	0.70	0
3	SO4	D	3012	-	4,4,4	0.23	0	6,6,6	0.43	0
2	NAP	C	903[B]	-	50,52,52	2.35	7 (14%)	71,80,80	1.88	14 (19%)
3	SO4	A	3018	-	4,4,4	0.61	0	6,6,6	0.70	0
3	SO4	C	3007	-	4,4,4	0.33	0	6,6,6	1.31	1 (16%)
2	NAP	D	903[A]	-	50,33,52	3.11	7 (14%)	71,52,80	1.84	11 (15%)
3	SO4	A	3006	-	4,4,4	0.33	0	6,6,6	1.26	1 (16%)
3	SO4	B	3003	-	4,4,4	0.44	0	6,6,6	0.39	0
3	SO4	D	3016	-	4,4,4	0.77	0	6,6,6	1.16	1 (16%)
3	SO4	C	3017	-	4,4,4	0.41	0	6,6,6	0.79	0
4	GOL	D	3028	-	5,5,5	0.50	0	5,5,5	1.47	0
3	SO4	B	3014	-	4,4,4	0.38	0	6,6,6	1.28	2 (33%)
3	SO4	C	3010	-	4,4,4	0.25	0	6,6,6	0.46	0
3	SO4	C	3002	-	4,4,4	0.35	0	6,6,6	0.40	0

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
4	GOL	C	3029	-	-	3/4/4/4	-
2	NAP	A	903[B]	-	-	11/35/67/67	0/5/5/5
2	NAP	D	903[B]	-	-	11/35/67/67	0/5/5/5
2	NAP	C	903[B]	-	-	10/35/67/67	0/5/5/5
4	GOL	B	3026	-	-	1/4/4/4	-
2	NAP	A	903[A]	-	-	6/35/37/67	0/5/3/5
2	NAP	D	903[A]	-	-	8/35/37/67	0/5/3/5
2	NAP	B	903[B]	-	-	10/35/67/67	0/5/5/5
2	NAP	C	903[A]	-	-	4/35/37/67	0/5/3/5
4	GOL	D	3028	-	-	2/4/4/4	-
4	GOL	A	3025	-	-	4/4/4/4	-
2	NAP	B	903[A]	-	-	5/35/37/67	0/5/3/5

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	903[A]	NAP	O5D-C5D	28.00	2.50	1.44
2	A	903[A]	NAP	C3N-C7N	-21.87	1.18	1.50
2	A	903[B]	NAP	C3N-C7N	-21.87	1.18	1.50
2	A	903[A]	NAP	O5D-C5D	20.79	2.23	1.44
2	B	903[A]	NAP	C3N-C7N	-20.59	1.19	1.50
2	B	903[B]	NAP	C3N-C7N	-20.59	1.19	1.50
2	D	903[A]	NAP	O5D-C5D	15.65	2.03	1.44
2	C	903[A]	NAP	O5D-C5D	14.89	2.01	1.44
2	C	903[A]	NAP	C3N-C7N	-11.65	1.33	1.50
2	C	903[B]	NAP	C3N-C7N	-11.65	1.33	1.50
2	D	903[A]	NAP	C3N-C7N	-9.53	1.36	1.50
2	D	903[B]	NAP	C3N-C7N	-9.53	1.36	1.50
2	D	903[A]	NAP	O7N-C7N	9.53	1.41	1.24
2	D	903[B]	NAP	O7N-C7N	9.53	1.41	1.24
2	A	903[A]	NAP	O7N-C7N	9.13	1.41	1.24
2	A	903[B]	NAP	O7N-C7N	9.13	1.41	1.24
2	B	903[A]	NAP	O7N-C7N	9.12	1.41	1.24
2	B	903[B]	NAP	O7N-C7N	9.12	1.41	1.24
2	C	903[A]	NAP	O7N-C7N	9.10	1.41	1.24
2	C	903[B]	NAP	O7N-C7N	9.10	1.41	1.24
2	A	903[A]	NAP	C2A-N3A	2.67	1.38	1.33
2	A	903[B]	NAP	C2A-N3A	2.67	1.38	1.33
2	C	903[A]	NAP	C2N-N1N	2.64	1.37	1.35
2	C	903[B]	NAP	C2N-N1N	2.64	1.37	1.35
2	A	903[A]	NAP	C2N-N1N	2.64	1.37	1.35
2	A	903[B]	NAP	C2N-N1N	2.64	1.37	1.35
2	A	903[A]	NAP	C2A-N1A	2.58	1.38	1.33
2	A	903[B]	NAP	C2A-N1A	2.58	1.38	1.33
2	D	903[A]	NAP	C2N-N1N	2.57	1.37	1.35
2	D	903[B]	NAP	C2N-N1N	2.57	1.37	1.35
2	C	903[A]	NAP	C2A-N3A	2.55	1.38	1.33
2	C	903[B]	NAP	C2A-N3A	2.55	1.38	1.33
2	D	903[A]	NAP	C8A-N7A	2.51	1.36	1.31
2	D	903[B]	NAP	C8A-N7A	2.51	1.36	1.31
2	B	903[A]	NAP	C2N-N1N	2.50	1.37	1.35
2	B	903[B]	NAP	C2N-N1N	2.50	1.37	1.35
2	C	903[B]	NAP	PN-O3	2.49	1.62	1.59
2	B	903[A]	NAP	C2A-N1A	2.45	1.38	1.33
2	B	903[B]	NAP	C2A-N1A	2.45	1.38	1.33
2	A	903[B]	NAP	PN-O3	2.42	1.62	1.59
2	C	903[A]	NAP	C2A-N1A	2.38	1.38	1.33
2	C	903[B]	NAP	C2A-N1A	2.38	1.38	1.33
2	B	903[A]	NAP	C2A-N3A	2.31	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	903[B]	NAP	C2A-N3A	2.31	1.38	1.33
2	B	903[A]	NAP	C8A-N7A	2.30	1.36	1.31
2	B	903[B]	NAP	C8A-N7A	2.30	1.36	1.31
2	D	903[A]	NAP	C2A-N1A	2.29	1.38	1.33
2	D	903[B]	NAP	C2A-N1A	2.29	1.38	1.33
2	D	903[A]	NAP	C2A-N3A	2.26	1.37	1.33
2	D	903[B]	NAP	C2A-N3A	2.26	1.37	1.33
2	A	903[A]	NAP	C8A-N7A	2.25	1.36	1.31
2	A	903[B]	NAP	C8A-N7A	2.25	1.36	1.31
2	C	903[A]	NAP	C8A-N7A	2.24	1.36	1.31
2	C	903[B]	NAP	C8A-N7A	2.24	1.36	1.31
2	B	903[B]	NAP	PN-O3	2.23	1.61	1.59

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903[A]	NAP	PN-O5D-C5D	-9.02	69.68	121.35
2	A	903[A]	NAP	PN-O5D-C5D	-8.70	71.49	121.35
2	B	903[A]	NAP	O7N-C7N-C3N	8.57	130.08	119.60
2	B	903[B]	NAP	O7N-C7N-C3N	8.57	130.08	119.60
2	D	903[A]	NAP	PN-O5D-C5D	-8.02	75.39	121.35
2	B	903[A]	NAP	C3N-C7N-N7N	-7.93	107.97	117.74
2	B	903[B]	NAP	C3N-C7N-N7N	-7.93	107.97	117.74
2	C	903[A]	NAP	O7N-C7N-C3N	6.64	127.71	119.60
2	C	903[B]	NAP	O7N-C7N-C3N	6.64	127.71	119.60
2	C	903[A]	NAP	PN-O5D-C5D	-6.27	85.41	121.35
2	B	903[A]	NAP	C4N-C3N-C7N	-6.17	104.26	121.06
2	B	903[B]	NAP	C4N-C3N-C7N	-6.17	104.26	121.06
2	D	903[A]	NAP	N3A-C2A-N1A	-5.92	119.63	128.58
2	D	903[B]	NAP	N3A-C2A-N1A	-5.92	119.63	128.58
2	C	903[A]	NAP	C3N-C7N-N7N	-5.81	110.58	117.74
2	C	903[B]	NAP	C3N-C7N-N7N	-5.81	110.58	117.74
2	B	903[A]	NAP	N3A-C2A-N1A	-5.44	120.35	128.58
2	B	903[B]	NAP	N3A-C2A-N1A	-5.44	120.35	128.58
2	B	903[A]	NAP	C2N-C3N-C7N	5.36	134.92	119.46
2	B	903[B]	NAP	C2N-C3N-C7N	5.36	134.92	119.46
2	A	903[A]	NAP	N3A-C2A-N1A	-5.20	120.71	128.58
2	A	903[B]	NAP	N3A-C2A-N1A	-5.20	120.71	128.58
2	C	903[A]	NAP	N3A-C2A-N1A	-5.06	120.93	128.58
2	C	903[B]	NAP	N3A-C2A-N1A	-5.06	120.93	128.58
2	A	903[A]	NAP	C5A-C4A-N3A	-4.56	120.44	126.72
2	A	903[B]	NAP	C5A-C4A-N3A	-4.56	120.44	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903[A]	NAP	N9A-C8A-N7A	-4.40	107.69	113.94
2	B	903[B]	NAP	N9A-C8A-N7A	-4.40	107.69	113.94
2	C	903[A]	NAP	C5A-C4A-N3A	-4.25	120.87	126.72
2	C	903[B]	NAP	C5A-C4A-N3A	-4.25	120.87	126.72
2	B	903[A]	NAP	C5A-C4A-N3A	-4.02	121.18	126.72
2	B	903[B]	NAP	C5A-C4A-N3A	-4.02	121.18	126.72
2	D	903[A]	NAP	N9A-C8A-N7A	-3.92	108.38	113.94
2	D	903[B]	NAP	N9A-C8A-N7A	-3.92	108.38	113.94
2	A	903[A]	NAP	N9A-C8A-N7A	-3.88	108.44	113.94
2	A	903[B]	NAP	N9A-C8A-N7A	-3.88	108.44	113.94
2	B	903[A]	NAP	C5A-N7A-C8A	3.68	109.24	103.45
2	B	903[B]	NAP	C5A-N7A-C8A	3.68	109.24	103.45
2	C	903[A]	NAP	N9A-C8A-N7A	-3.68	108.71	113.94
2	C	903[B]	NAP	N9A-C8A-N7A	-3.68	108.71	113.94
2	D	903[A]	NAP	C5A-C4A-N3A	-3.63	121.72	126.72
2	D	903[B]	NAP	C5A-C4A-N3A	-3.63	121.72	126.72
2	A	903[A]	NAP	C5A-N7A-C8A	3.59	109.09	103.45
2	A	903[B]	NAP	C5A-N7A-C8A	3.59	109.09	103.45
2	C	903[A]	NAP	C5A-N7A-C8A	3.43	108.84	103.45
2	C	903[B]	NAP	C5A-N7A-C8A	3.43	108.84	103.45
2	B	903[A]	NAP	C6N-N1N-C2N	-3.36	119.02	121.88
2	B	903[B]	NAP	C6N-N1N-C2N	-3.36	119.02	121.88
2	A	903[A]	NAP	C2A-N3A-C4A	3.33	119.97	111.83
2	A	903[B]	NAP	C2A-N3A-C4A	3.33	119.97	111.83
2	D	903[A]	NAP	C2A-N3A-C4A	3.31	119.92	111.83
2	D	903[B]	NAP	C2A-N3A-C4A	3.31	119.92	111.83
2	B	903[A]	NAP	C2A-N3A-C4A	3.26	119.81	111.83
2	B	903[B]	NAP	C2A-N3A-C4A	3.26	119.81	111.83
2	C	903[A]	NAP	C4N-C3N-C7N	-3.24	112.24	121.06
2	C	903[B]	NAP	C4N-C3N-C7N	-3.24	112.24	121.06
2	C	903[A]	NAP	C2A-N3A-C4A	3.19	119.61	111.83
2	C	903[B]	NAP	C2A-N3A-C4A	3.19	119.61	111.83
2	D	903[A]	NAP	C5A-N7A-C8A	3.18	108.44	103.45
2	D	903[B]	NAP	C5A-N7A-C8A	3.18	108.44	103.45
2	B	903[A]	NAP	O4B-C1B-N9A	3.16	114.16	108.09
2	B	903[B]	NAP	O4B-C1B-N9A	3.16	114.16	108.09
2	D	903[A]	NAP	C6N-N1N-C2N	-3.04	119.29	121.88
2	D	903[B]	NAP	C6N-N1N-C2N	-3.04	119.29	121.88
2	A	903[A]	NAP	C6N-N1N-C2N	-2.96	119.36	121.88
2	A	903[B]	NAP	C6N-N1N-C2N	-2.96	119.36	121.88
2	D	903[A]	NAP	O4B-C1B-N9A	2.91	113.68	108.09
2	D	903[B]	NAP	O4B-C1B-N9A	2.91	113.68	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	903[A]	NAP	C4A-C5A-N7A	-2.91	107.26	110.58
2	A	903[B]	NAP	C4A-C5A-N7A	-2.91	107.26	110.58
2	C	903[A]	NAP	C2N-C3N-C7N	2.90	127.82	119.46
2	C	903[B]	NAP	C2N-C3N-C7N	2.90	127.82	119.46
2	C	903[A]	NAP	O4B-C1B-N9A	2.89	113.65	108.09
2	C	903[B]	NAP	O4B-C1B-N9A	2.89	113.65	108.09
2	A	903[A]	NAP	O4B-C1B-N9A	2.87	113.59	108.09
2	A	903[B]	NAP	O4B-C1B-N9A	2.87	113.59	108.09
2	C	903[A]	NAP	C4D-O4D-C1D	2.82	112.51	109.92
2	C	903[B]	NAP	C4D-O4D-C1D	2.82	112.51	109.92
3	C	3013	SO4	O3-S-O2	-2.78	95.02	109.56
2	C	903[A]	NAP	C4A-C5A-N7A	-2.77	107.41	110.58
2	C	903[B]	NAP	C4A-C5A-N7A	-2.77	107.41	110.58
2	B	903[A]	NAP	C4A-C5A-N7A	-2.76	107.43	110.58
2	B	903[B]	NAP	C4A-C5A-N7A	-2.76	107.43	110.58
2	C	903[A]	NAP	C6N-N1N-C2N	-2.74	119.55	121.88
2	C	903[B]	NAP	C6N-N1N-C2N	-2.74	119.55	121.88
2	D	903[A]	NAP	C4D-O4D-C1D	2.74	112.43	109.92
2	D	903[B]	NAP	C4D-O4D-C1D	2.74	112.43	109.92
3	C	3026	SO4	O3-S-O2	2.66	123.48	109.56
2	A	903[A]	NAP	N3A-C4A-N9A	2.66	131.70	127.17
2	A	903[B]	NAP	N3A-C4A-N9A	2.66	131.70	127.17
3	C	3007	SO4	O4-S-O3	2.66	123.19	108.54
4	C	3029	GOL	C3-C2-C1	2.62	121.41	111.80
2	B	903[A]	NAP	C4D-O4D-C1D	2.61	112.32	109.92
2	B	903[B]	NAP	C4D-O4D-C1D	2.61	112.32	109.92
2	A	903[A]	NAP	C4D-O4D-C1D	2.57	112.28	109.92
2	A	903[B]	NAP	C4D-O4D-C1D	2.57	112.28	109.92
3	C	3028	SO4	O4-S-O2	-2.52	96.37	109.56
2	D	903[A]	NAP	C4A-C5A-N7A	-2.52	107.70	110.58
2	D	903[B]	NAP	C4A-C5A-N7A	-2.52	107.70	110.58
2	B	903[A]	NAP	N3A-C4A-N9A	2.45	131.34	127.17
2	B	903[B]	NAP	N3A-C4A-N9A	2.45	131.34	127.17
3	B	3005	SO4	O4-S-O2	2.42	122.19	109.56
2	C	903[A]	NAP	N3A-C4A-N9A	2.38	131.22	127.17
2	C	903[B]	NAP	N3A-C4A-N9A	2.38	131.22	127.17
4	A	3025	GOL	O3-C3-C2	2.38	121.08	110.38
3	D	3016	SO4	O3-S-O1	-2.34	97.30	109.56
2	B	903[A]	NAP	C4A-N9A-C8A	2.31	108.16	105.74
2	B	903[B]	NAP	C4A-N9A-C8A	2.31	108.16	105.74
3	A	3015	SO4	O4-S-O3	-2.29	95.93	108.54
2	A	903[A]	NAP	O4B-C1B-C2B	-2.25	102.72	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	903[B]	NAP	O4B-C1B-C2B	-2.25	102.72	106.59
2	D	903[A]	NAP	O5D-C5D-C4D	-2.22	101.43	108.99
3	C	3026	SO4	O4-S-O2	-2.21	98.01	109.56
3	B	3014	SO4	O4-S-O1	2.20	121.07	109.56
3	B	3014	SO4	O4-S-O3	-2.19	96.48	108.54
3	D	3008	SO4	O4-S-O2	-2.13	98.44	109.56
3	A	3006	SO4	O2-S-O1	2.03	123.36	109.06

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	903[A]	NAP	C5D-O5D-PN-O1N
2	A	903[B]	NAP	C5B-O5B-PA-O1A
2	A	903[B]	NAP	C5B-O5B-PA-O3
2	B	903[A]	NAP	C5D-O5D-PN-O1N
2	B	903[B]	NAP	C5B-O5B-PA-O1A
2	B	903[B]	NAP	C5B-O5B-PA-O3
2	C	903[A]	NAP	C5D-O5D-PN-O1N
2	C	903[B]	NAP	C5B-O5B-PA-O1A
2	C	903[B]	NAP	C5B-O5B-PA-O3
2	D	903[A]	NAP	C5D-O5D-PN-O3
2	D	903[A]	NAP	C5D-O5D-PN-O1N
2	D	903[B]	NAP	C5B-O5B-PA-O1A
2	D	903[B]	NAP	C5B-O5B-PA-O3
4	A	3025	GOL	O1-C1-C2-C3
4	A	3025	GOL	C1-C2-C3-O3
4	C	3029	GOL	C1-C2-C3-O3
4	C	3029	GOL	O2-C2-C3-O3
2	A	903[B]	NAP	C3D-C4D-C5D-O5D
2	B	903[B]	NAP	C3D-C4D-C5D-O5D
2	C	903[B]	NAP	C3D-C4D-C5D-O5D
2	D	903[B]	NAP	C3D-C4D-C5D-O5D
2	A	903[B]	NAP	O4D-C4D-C5D-O5D
4	A	3025	GOL	O1-C1-C2-O2
2	B	903[B]	NAP	O4D-C4D-C5D-O5D
2	C	903[B]	NAP	O4D-C4D-C5D-O5D
2	D	903[B]	NAP	O4D-C4D-C5D-O5D
2	D	903[A]	NAP	C4N-C3N-C7N-N7N
2	D	903[B]	NAP	C4N-C3N-C7N-N7N
2	D	903[A]	NAP	C4N-C3N-C7N-O7N
2	D	903[B]	NAP	C4N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
2	B	903[B]	NAP	PN-O3-PA-O1A
4	B	3026	GOL	O2-C2-C3-O3
4	C	3029	GOL	O1-C1-C2-O2
2	A	903[A]	NAP	C2B-C1B-N9A-C8A
2	A	903[B]	NAP	C2B-C1B-N9A-C8A
2	B	903[A]	NAP	C2B-C1B-N9A-C8A
2	B	903[B]	NAP	C2B-C1B-N9A-C8A
2	C	903[A]	NAP	C2B-C1B-N9A-C8A
2	C	903[B]	NAP	C2B-C1B-N9A-C8A
2	D	903[A]	NAP	C2B-C1B-N9A-C8A
2	D	903[B]	NAP	C2B-C1B-N9A-C8A
2	D	903[B]	NAP	PN-O3-PA-O1A
4	D	3028	GOL	O1-C1-C2-O2
2	D	903[A]	NAP	O4D-C4D-C5D-O5D
2	A	903[A]	NAP	C5D-O5D-PN-O3
2	A	903[B]	NAP	C5B-O5B-PA-O2A
2	B	903[B]	NAP	C5B-O5B-PA-O2A
2	C	903[B]	NAP	C5B-O5B-PA-O2A
2	D	903[A]	NAP	C5D-O5D-PN-O2N
2	D	903[B]	NAP	C5B-O5B-PA-O2A
2	A	903[B]	NAP	PN-O3-PA-O1A
2	A	903[B]	NAP	PN-O3-PA-O2A
2	C	903[B]	NAP	PN-O3-PA-O1A
2	B	903[A]	NAP	O4B-C1B-N9A-C8A
2	B	903[B]	NAP	O4B-C1B-N9A-C8A
4	A	3025	GOL	O2-C2-C3-O3
2	C	903[A]	NAP	O4D-C4D-C5D-O5D
4	D	3028	GOL	O2-C2-C3-O3
2	B	903[A]	NAP	C4N-C3N-C7N-O7N
2	B	903[B]	NAP	C4N-C3N-C7N-O7N
2	A	903[A]	NAP	O4B-C1B-N9A-C8A
2	A	903[B]	NAP	O4B-C1B-N9A-C8A
2	D	903[A]	NAP	O4B-C1B-N9A-C8A
2	D	903[B]	NAP	O4B-C1B-N9A-C8A
2	B	903[A]	NAP	O4D-C4D-C5D-O5D
2	B	903[B]	NAP	PN-O3-PA-O2A
2	C	903[B]	NAP	PN-O3-PA-O2A
2	C	903[B]	NAP	PA-O3-PN-O2N
2	A	903[A]	NAP	C4N-C3N-C7N-N7N
2	A	903[B]	NAP	C4N-C3N-C7N-N7N
2	C	903[A]	NAP	O4B-C1B-N9A-C8A
2	C	903[B]	NAP	O4B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	A	903[A]	NAP	C3B-C2B-O2B-P2B
2	A	903[B]	NAP	C3B-C2B-O2B-P2B
2	D	903[B]	NAP	PN-O3-PA-O2A

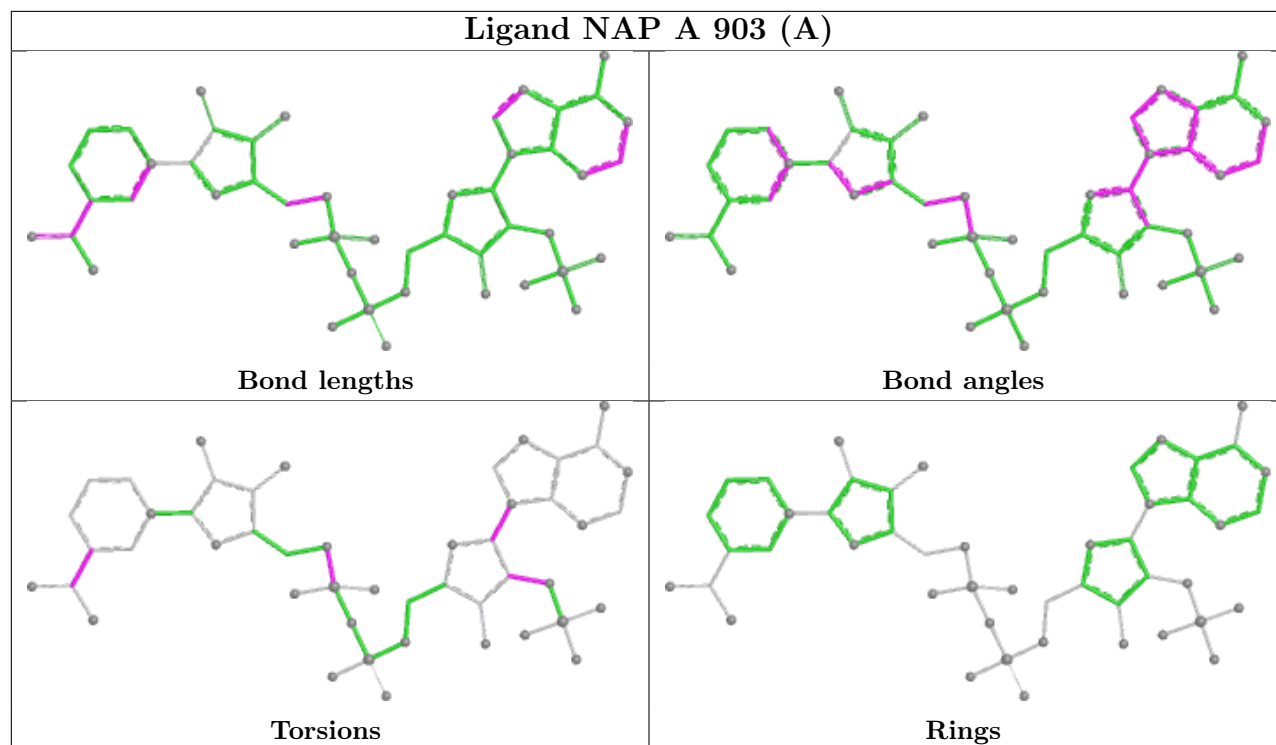
There are no ring outliers.

10 monomers are involved in 11 short contacts:

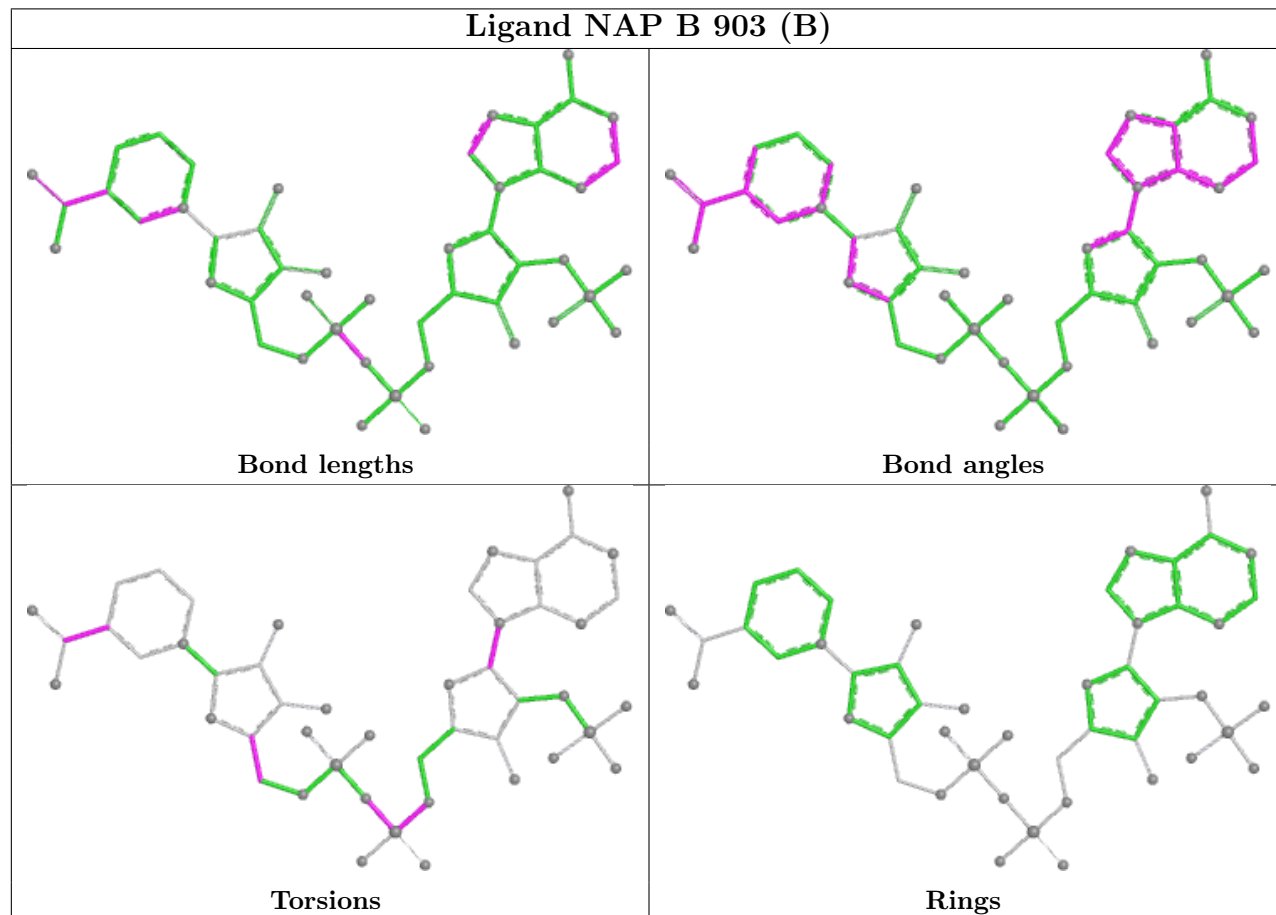
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	903[B]	NAP	1	0
4	B	3026	GOL	2	0
3	C	3028	SO4	1	0
3	D	3020	SO4	1	0
2	D	903[B]	NAP	1	0
2	A	903[B]	NAP	1	0
2	C	903[B]	NAP	1	0
3	B	3003	SO4	1	0
4	D	3028	GOL	1	0
3	C	3002	SO4	1	0

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.

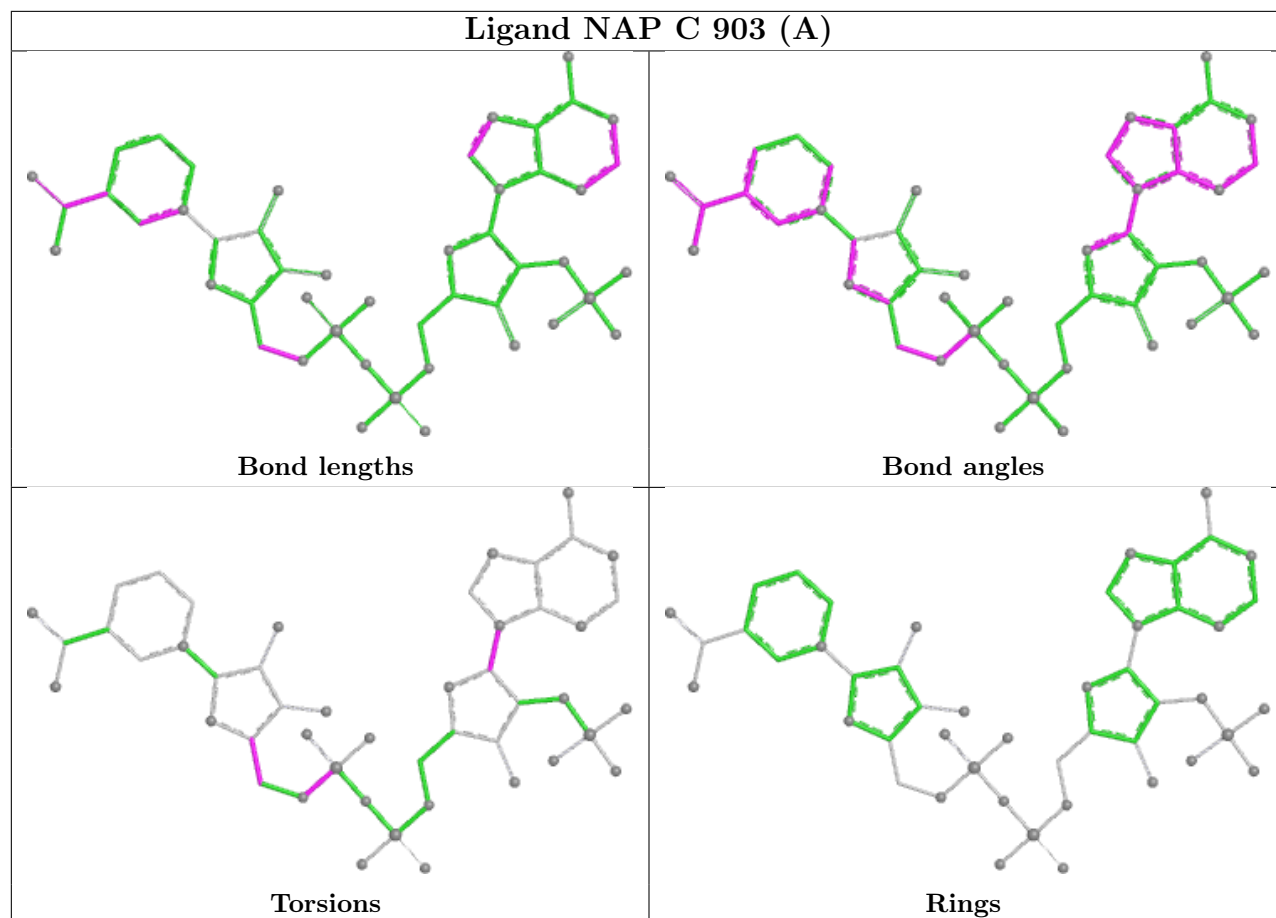
Ligand NAP A 903 (A)



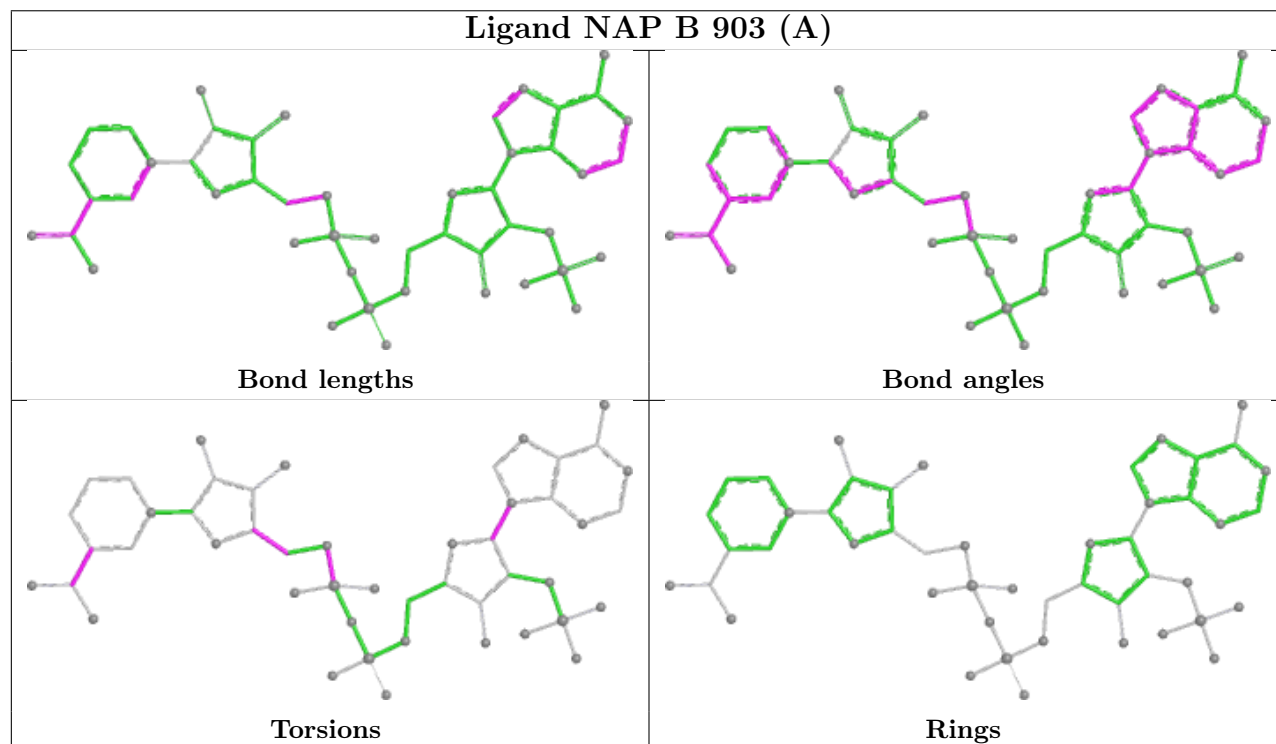
Ligand NAP B 903 (B)



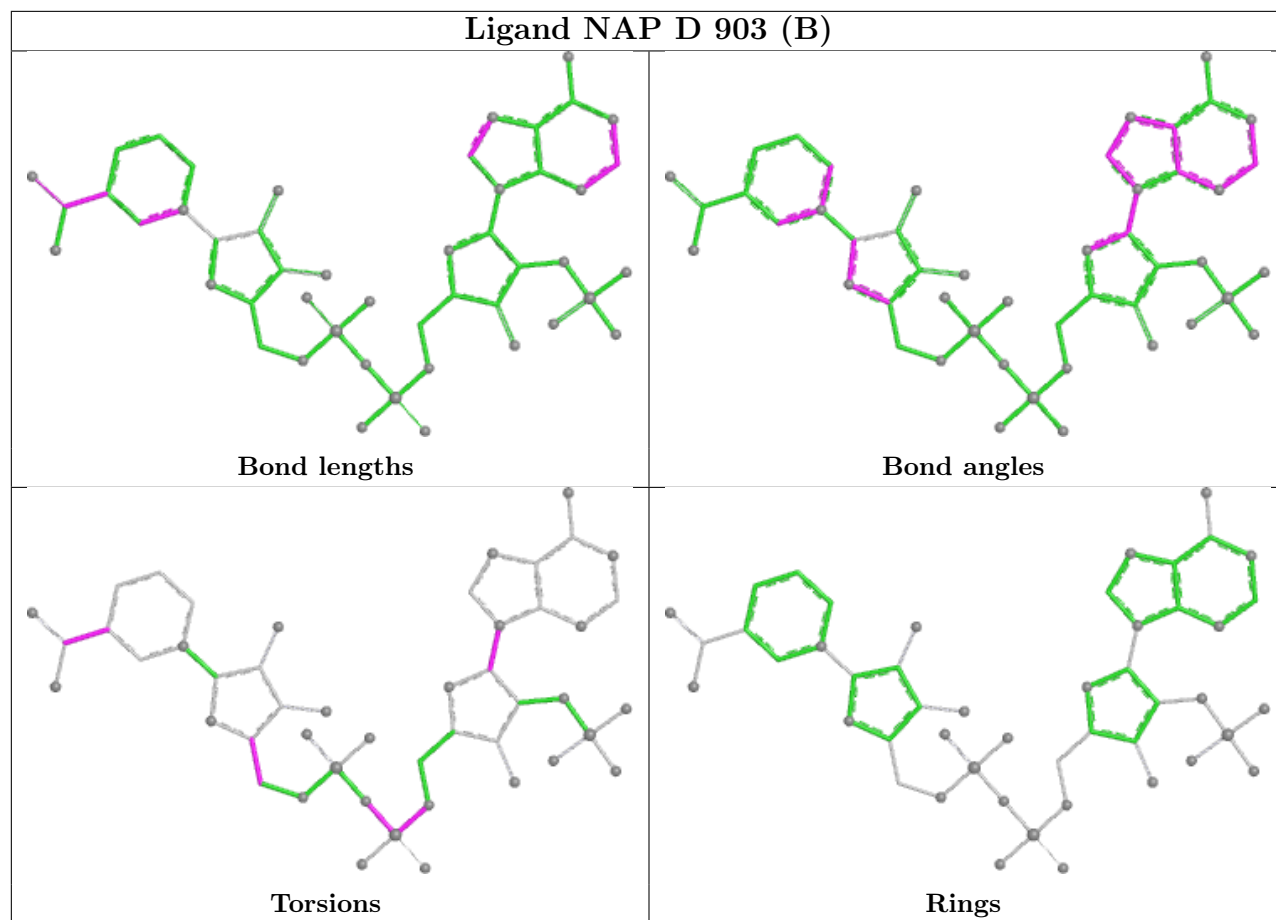
Ligand NAP C 903 (A)

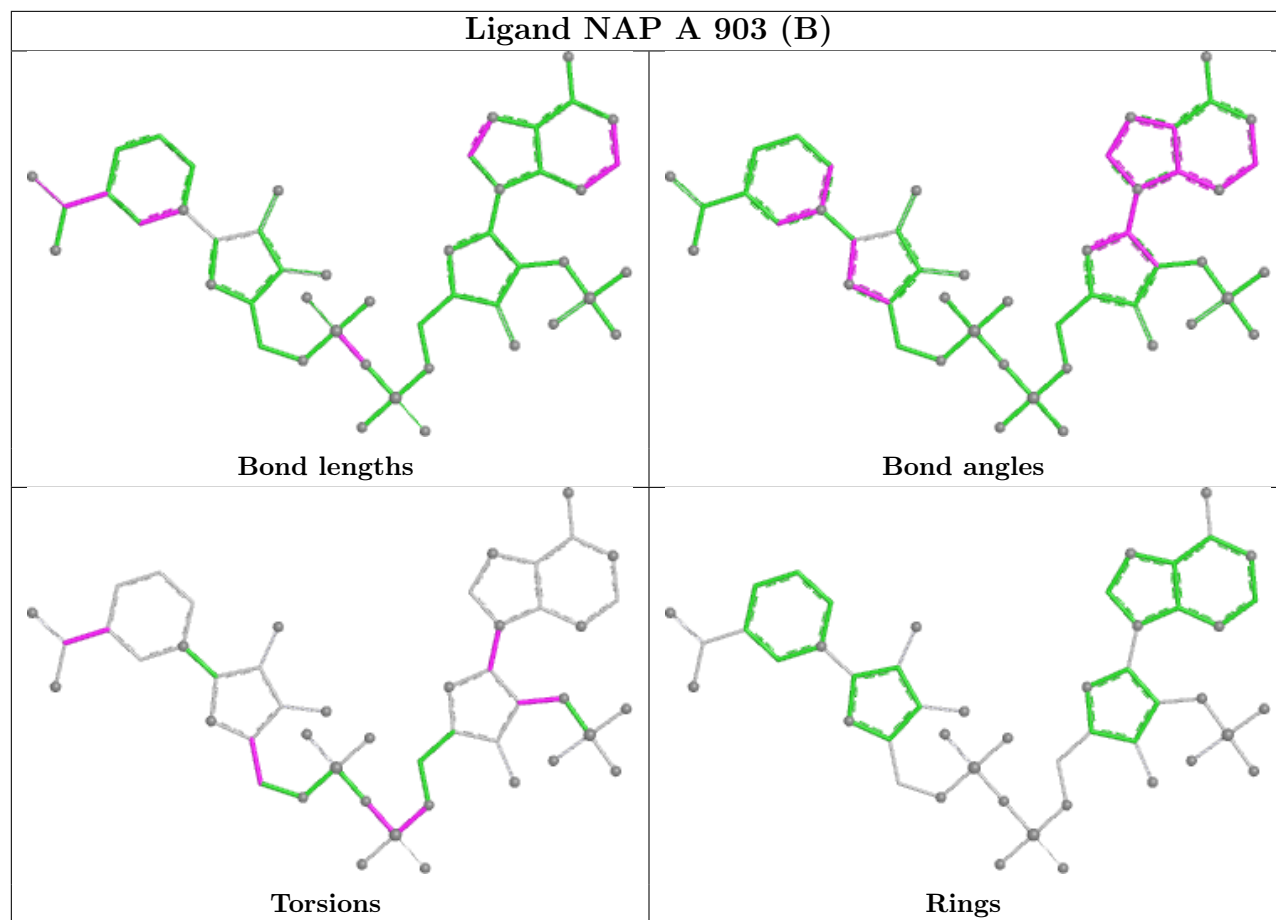


Ligand NAP B 903 (A)

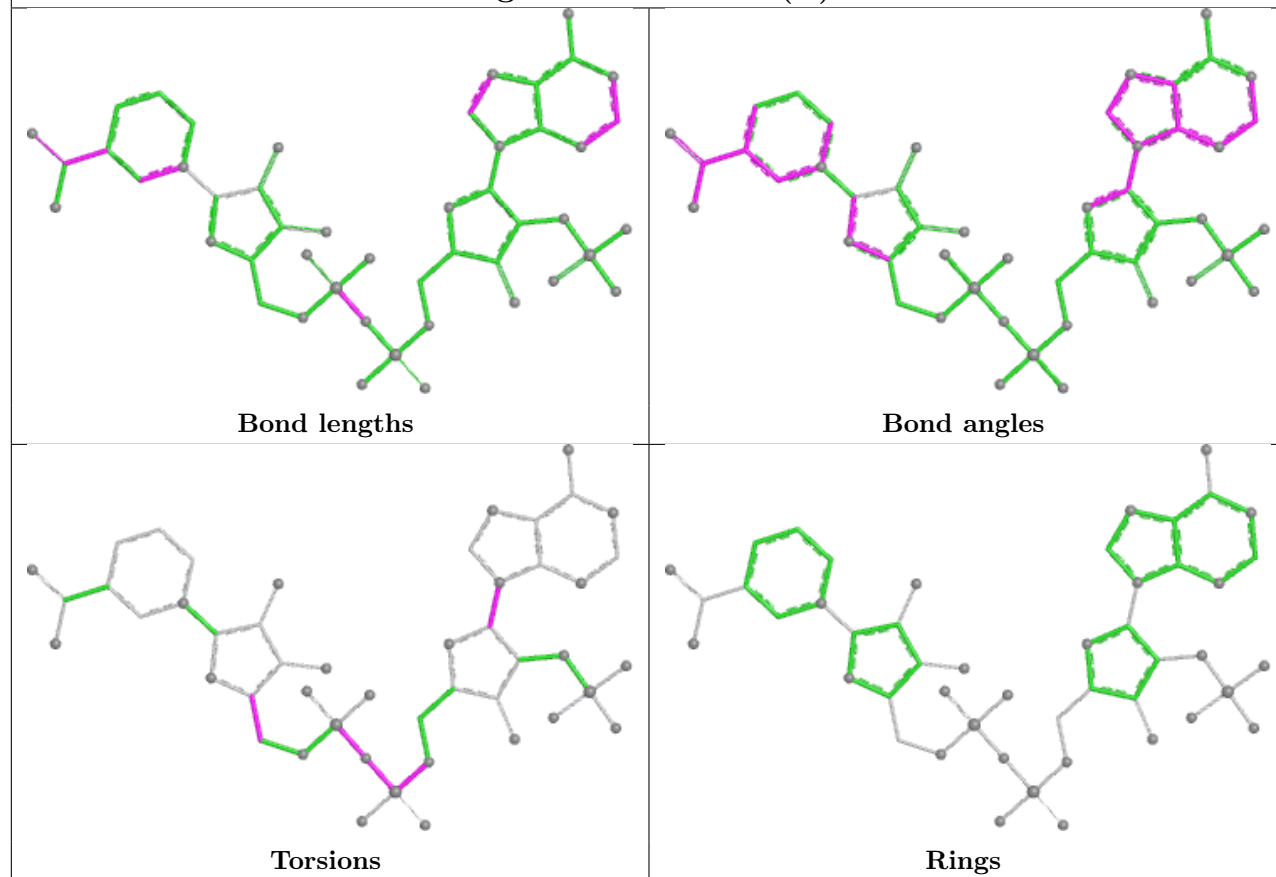


Ligand NAP D 903 (B)

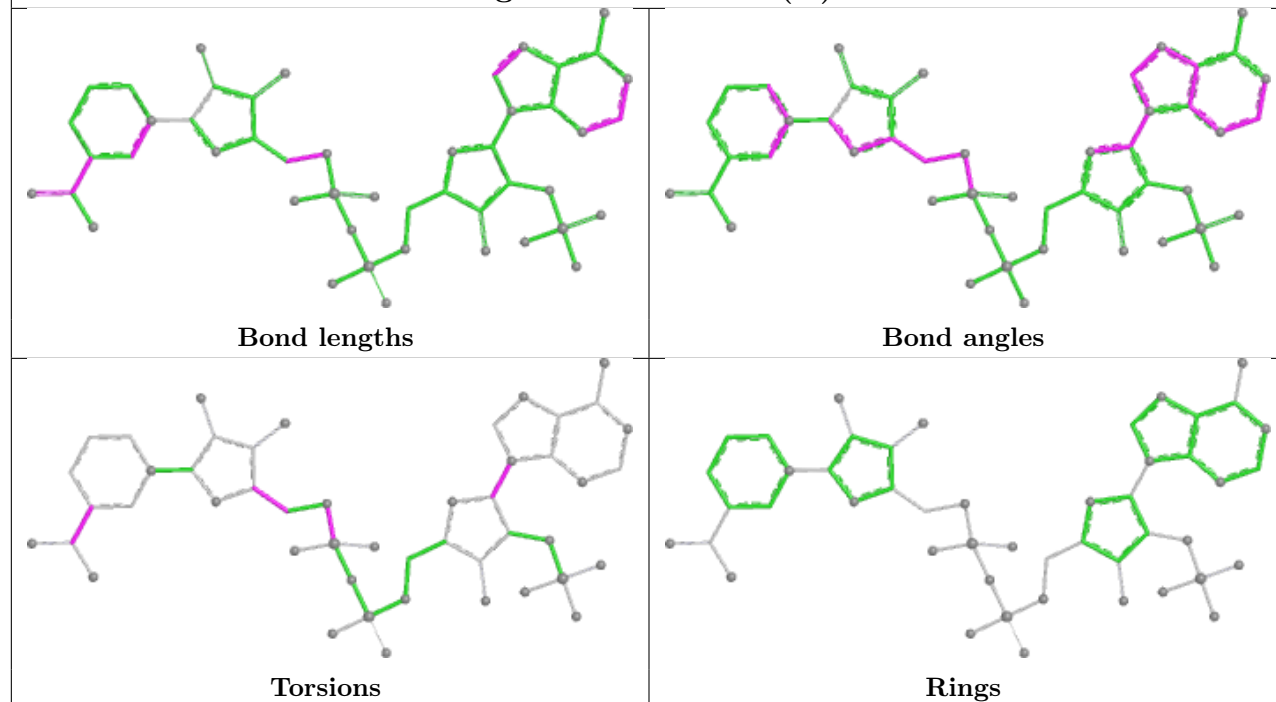




Ligand NAP C 903 (B)



Ligand NAP D 903 (A)



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	498/517 (96%)	-0.59	4 (0%) 82 84	9, 25, 38, 56	31 (6%)
1	B	498/517 (96%)	-0.51	3 (0%) 85 86	11, 28, 39, 63	33 (6%)
1	C	498/517 (96%)	-0.62	6 (1%) 76 77	8, 23, 35, 61	36 (7%)
1	D	498/517 (96%)	-0.57	3 (0%) 85 86	11, 26, 38, 60	34 (6%)
All	All	1992/2068 (96%)	-0.57	16 (0%) 82 84	8, 26, 38, 63	134 (6%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	405	VAL	5.9
1	A	405	VAL	5.0
1	D	620[A]	LYS	4.9
1	B	405	VAL	4.4
1	C	819	ASP	4.1
1	D	405	VAL	3.4
1	B	620[A]	LYS	3.2
1	B	819	ASP	2.9
1	C	620[A]	LYS	2.8
1	C	780	PRO	2.7
1	A	819	ASP	2.7
1	A	620[A]	LYS	2.5
1	D	819	ASP	2.4
1	C	756	ARG	2.2
1	A	756	ARG	2.0
1	C	777	ASN	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	SO4	D	3020	5/5	0.74	0.20	48,49,54,56	5
3	SO4	A	3018	5/5	0.77	0.19	50,51,54,55	5
3	SO4	D	3027	5/5	0.77	0.19	42,45,48,49	5
3	SO4	A	3021	5/5	0.82	0.22	42,50,55,56	5
3	SO4	C	3017	5/5	0.83	0.17	52,53,55,56	5
3	SO4	C	3026	5/5	0.83	0.19	45,47,49,51	5
3	SO4	D	3012	5/5	0.83	0.21	49,54,56,58	5
3	SO4	A	3011	5/5	0.83	0.20	58,59,62,64	5
3	SO4	B	3025	5/5	0.83	0.29	47,52,53,53	5
4	GOL	C	3029	6/6	0.83	0.23	59,66,72,75	0
3	SO4	B	3009	5/5	0.84	0.20	46,47,50,53	5
3	SO4	B	3019	5/5	0.85	0.15	50,50,54,56	5
3	SO4	C	3010	5/5	0.85	0.18	47,48,53,55	5
3	SO4	B	3022	5/5	0.86	0.18	37,46,48,50	5
3	SO4	C	3023	5/5	0.87	0.17	46,52,54,56	5
3	SO4	A	3024	5/5	0.87	0.28	57,58,60,60	5
4	GOL	D	3028	6/6	0.88	0.21	68,73,75,76	0
4	GOL	A	3025	6/6	0.91	0.18	59,65,68,70	0
4	GOL	B	3026	6/6	0.91	0.16	50,58,60,63	0
2	NAP	B	903[B]	48/48	0.91	0.15	31,37,39,46	25
2	NAP	B	903[A]	31/48	0.91	0.15	31,34,39,39	8
3	SO4	A	3001	5/5	0.92	0.11	59,60,62,62	5
2	NAP	A	903[B]	48/48	0.93	0.14	27,35,38,45	25
2	NAP	C	903[A]	31/48	0.93	0.12	26,29,34,35	8
2	NAP	C	903[B]	48/48	0.93	0.12	26,29,36,42	25
2	NAP	A	903[A]	31/48	0.93	0.14	27,31,35,35	8
3	SO4	D	3008	5/5	0.93	0.09	34,35,39,41	5
3	SO4	C	3002	5/5	0.93	0.10	40,42,47,47	5
3	SO4	B	3005	5/5	0.94	0.10	37,42,49,50	5
2	NAP	D	903[B]	48/48	0.94	0.12	26,29,36,40	25
2	NAP	D	903[A]	31/48	0.94	0.12	26,29,37,38	8
3	SO4	B	3004	5/5	0.95	0.08	35,41,42,42	5

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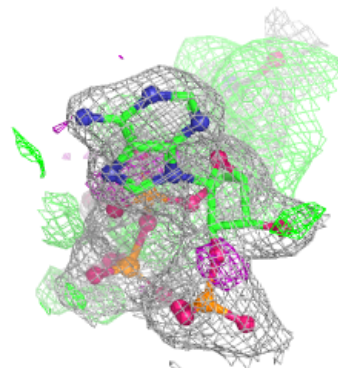
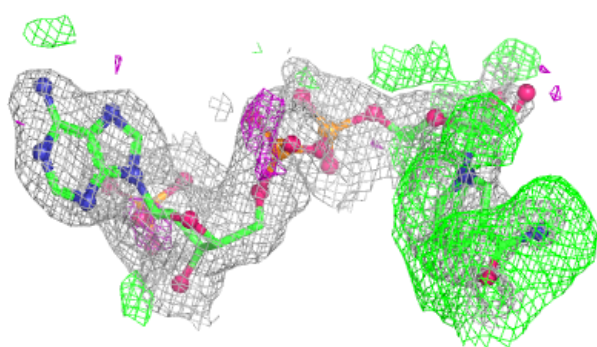
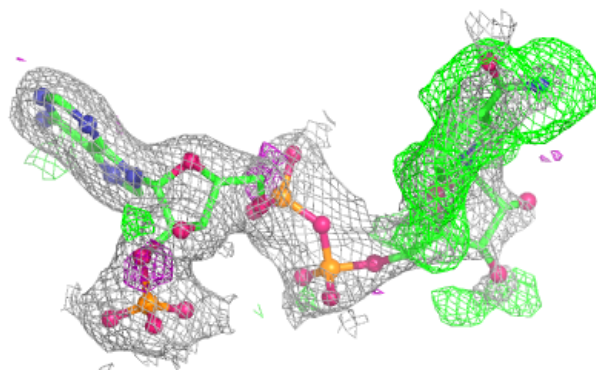
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	3007	5/5	0.96	0.09	38,40,46,49	5
3	SO4	C	3028	5/5	0.97	0.08	28,36,38,39	5
3	SO4	A	3006	5/5	0.97	0.07	31,34,41,45	5
3	SO4	A	3015	5/5	0.97	0.09	30,42,48,51	0
3	SO4	B	3014	5/5	0.98	0.06	34,45,48,54	0
3	SO4	C	3013	5/5	0.98	0.08	32,41,45,47	0
3	SO4	B	3003	5/5	0.98	0.10	28,28,32,33	5
3	SO4	D	3016	5/5	0.98	0.07	30,43,45,50	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.

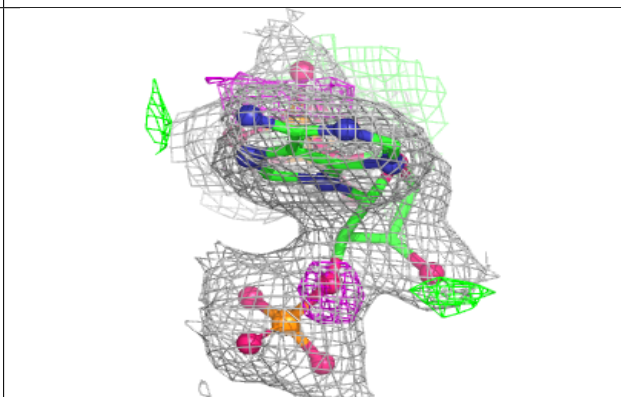
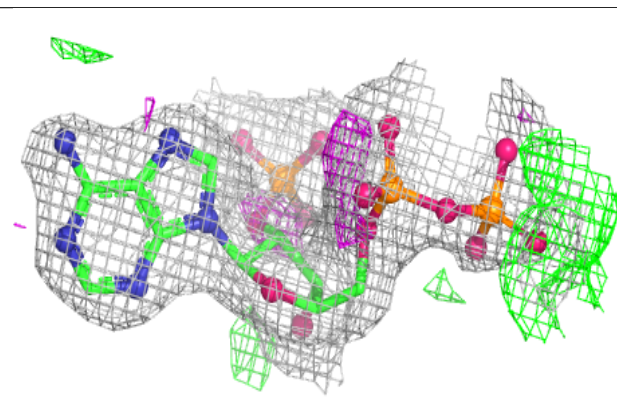
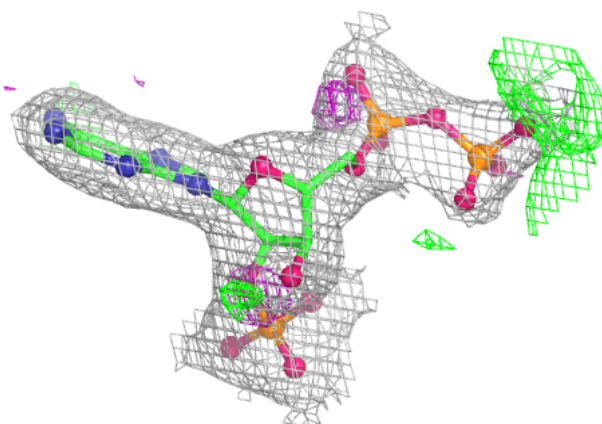
Electron density around NAP B 903 (B):

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

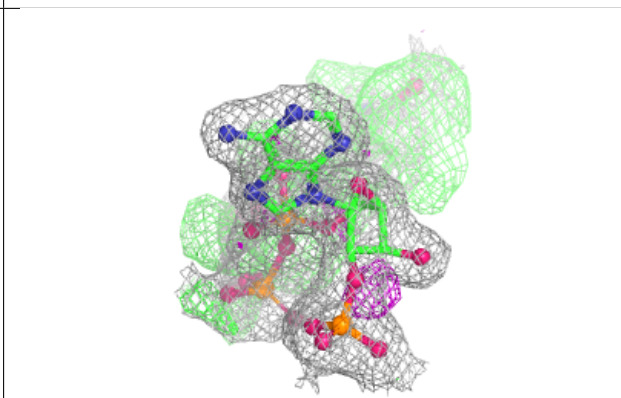
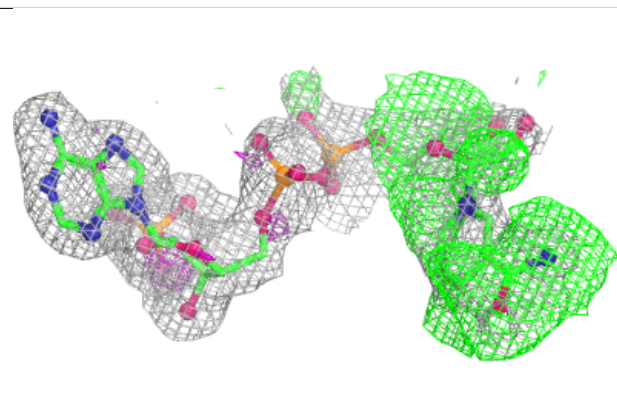
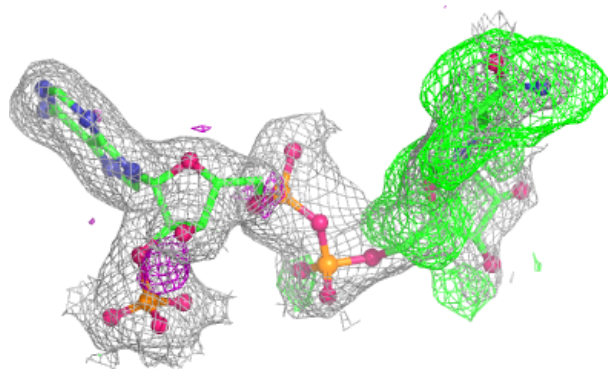


Electron density around NAP B 903 (A):

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

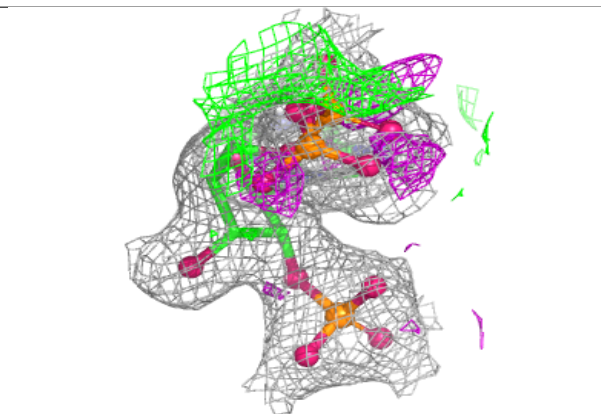
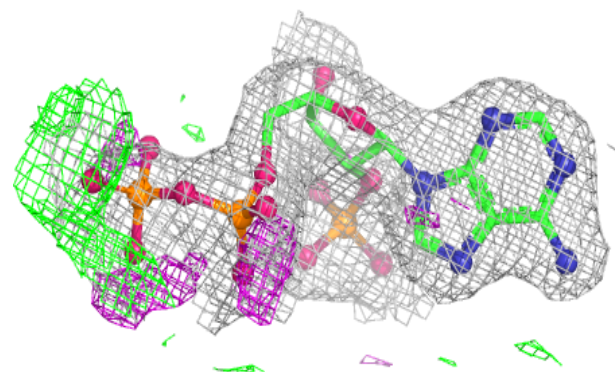
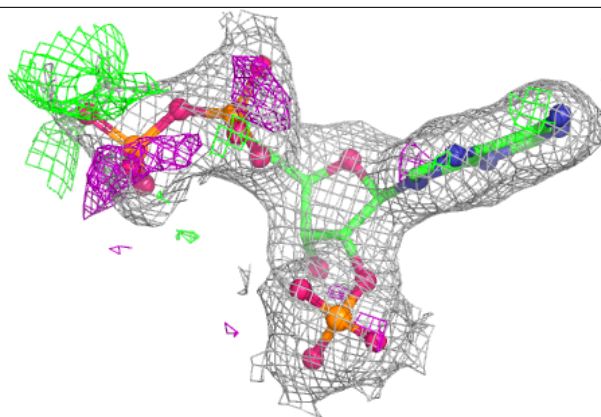
**Electron density around NAP A 903 (B):**

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and green (positive)

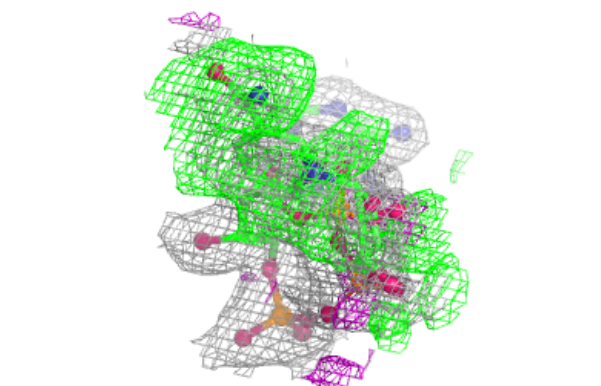
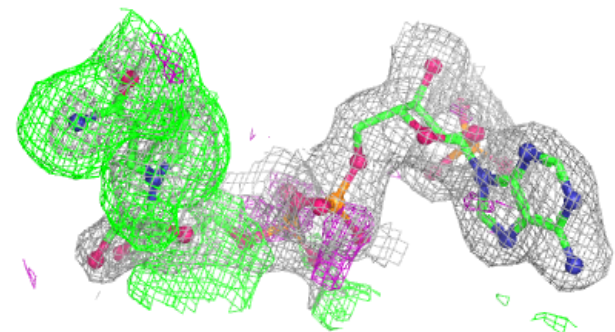
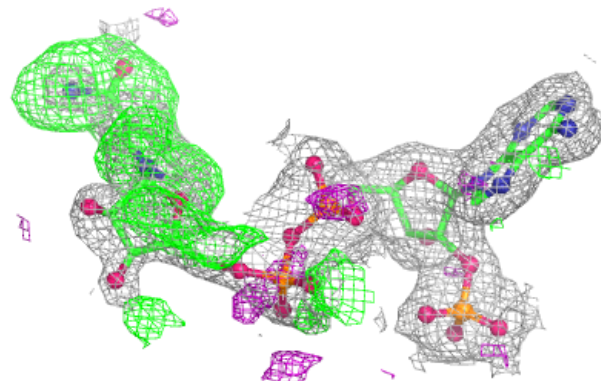


Electron density around NAP C 903 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

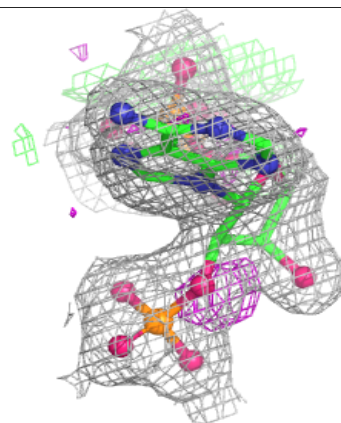
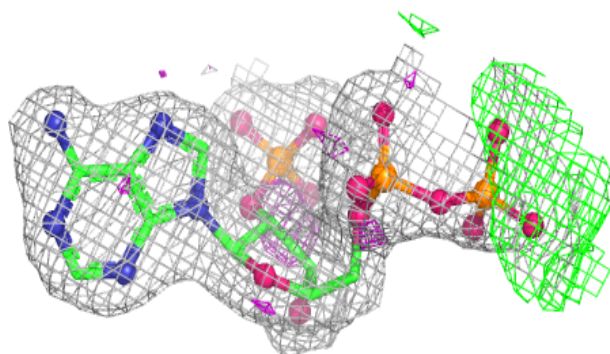
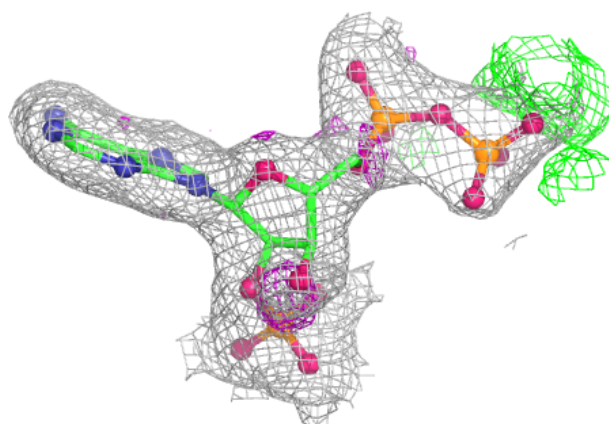
**Electron density around NAP C 903 (B):**

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

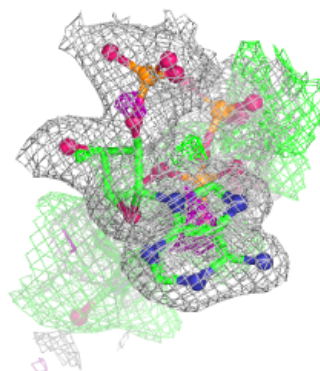
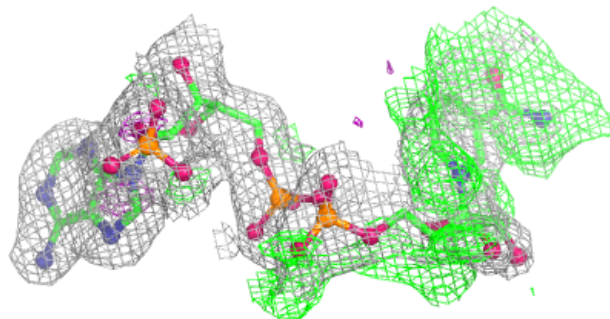
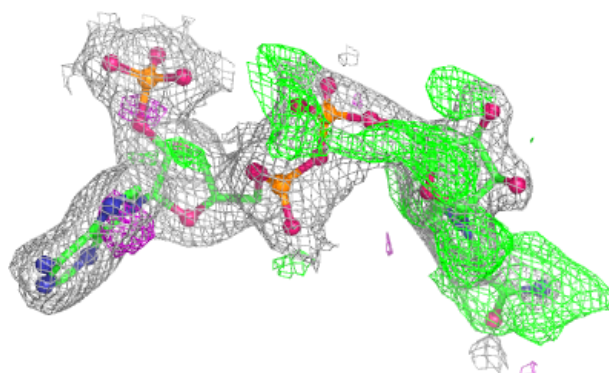


Electron density around NAP A 903 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

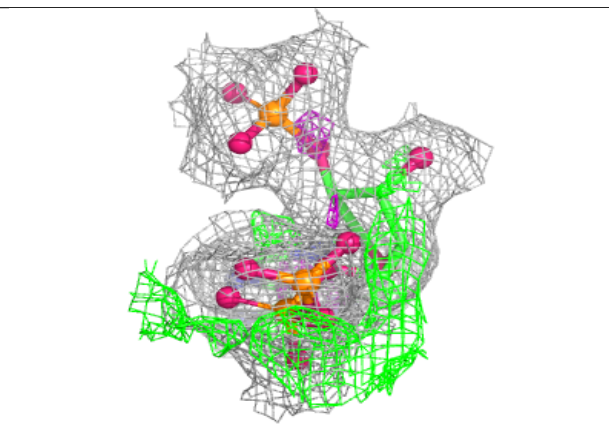
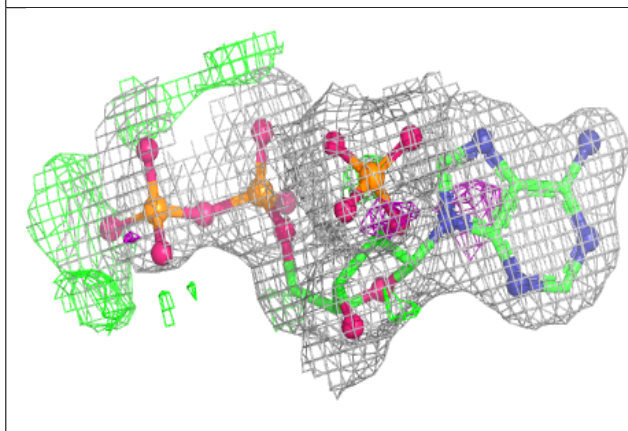
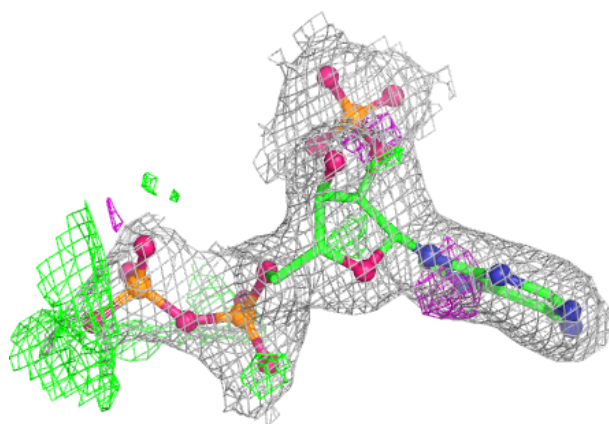
**Electron density around NAP D 903 (B):**

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



Electron density around NAP D 903 (A):

$2mF_o-DF_c$ (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.