



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:28 AM UTC

PDB ID : 3F8R / pdb_00003f8r
Title : Crystal structure of Sulfolobus solfataricus Thioredoxin reductase B3 in complex with two NADP molecules
Authors : Ruggiero, A.; Masullo, M.; Ruocco, M.R.; Arcari, P.; Zagari, A.; Vitagliano, L.
Deposited on : 2008-11-13
Resolution : 1.95 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:

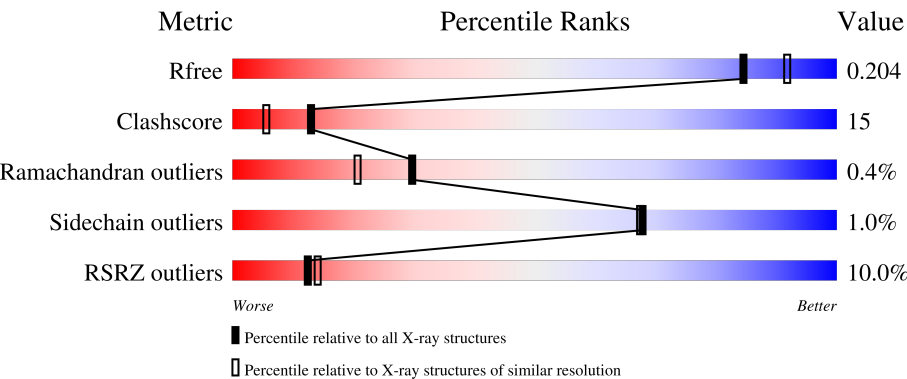
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	323	5% 75%20%• 5%
1	B	323	10% 67%26%• •
1	C	323	9% 70%25%5%
1	D	323	14% 67%24%• 8%

2 Entry composition ⓘ

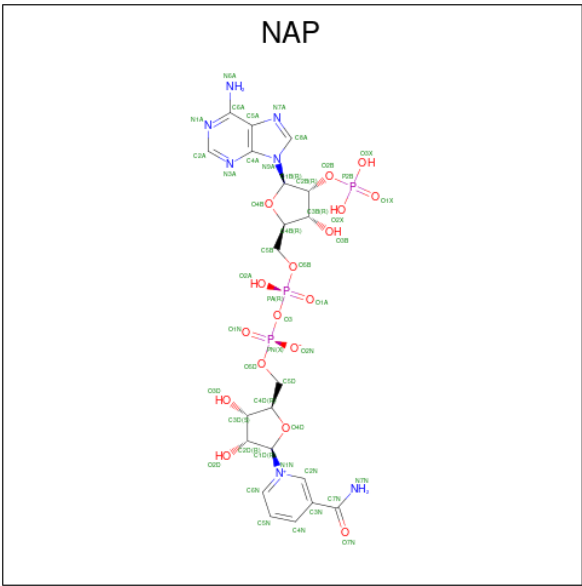
There are 3 unique types of molecules in this entry. The entry contains 10058 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thioredoxin reductase (TrxB-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2367	1523	395	443	6			
1	B	309	Total	C	N	O	S	0	0	0
			2375	1527	396	446	6			
1	C	307	Total	C	N	O	S	0	0	0
			2356	1517	391	442	6			
1	D	298	Total	C	N	O	S	0	0	0
			2285	1469	381	429	6			

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



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

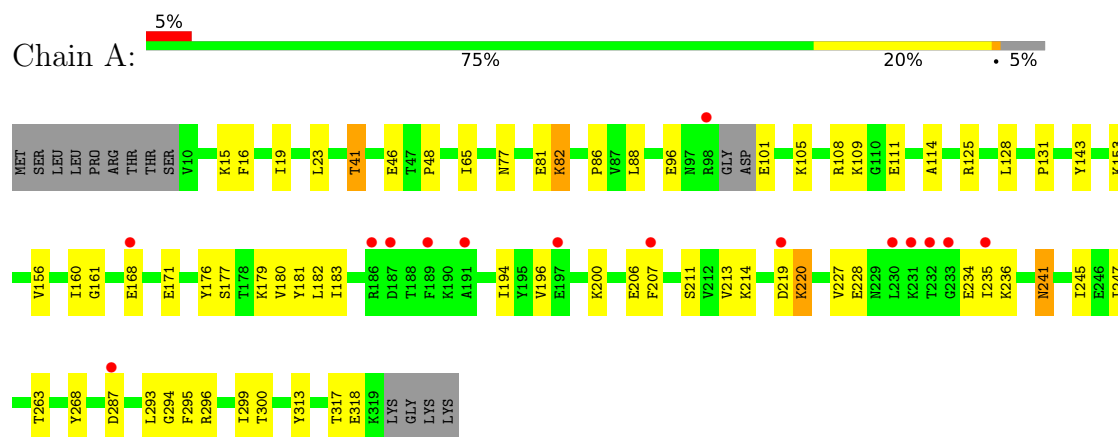
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total	O	0	0
			88	88		
3	B	82	Total	O	0	0
			82	82		
3	C	89	Total	O	0	0
			89	89		
3	D	101	Total	O	0	0
			101	101		

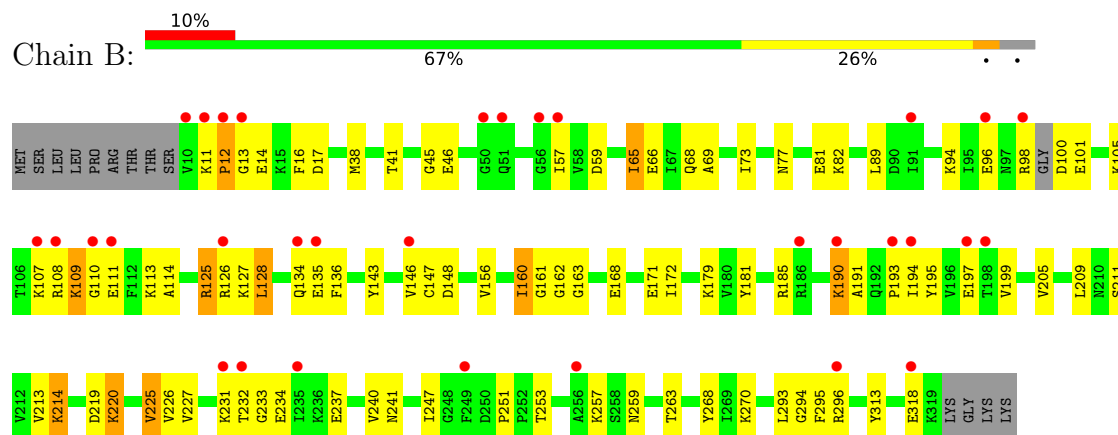
3 Residue-property plots [i](#)

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

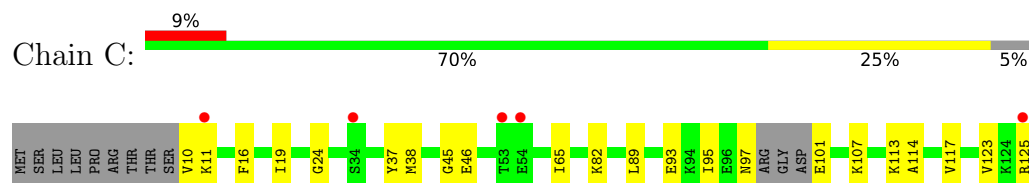
• Molecule 1: Thioredoxin reductase (TrxB-3)

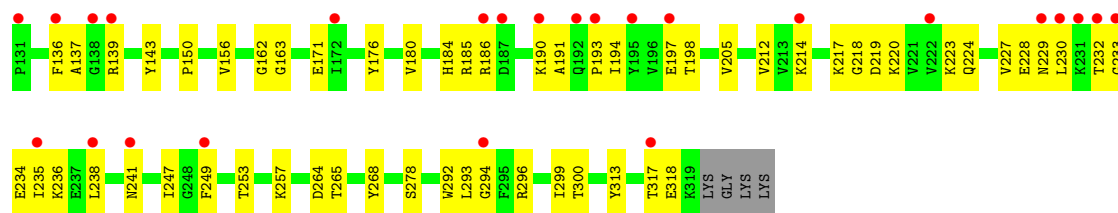


• Molecule 1: Thioredoxin reductase (TrxB-3)

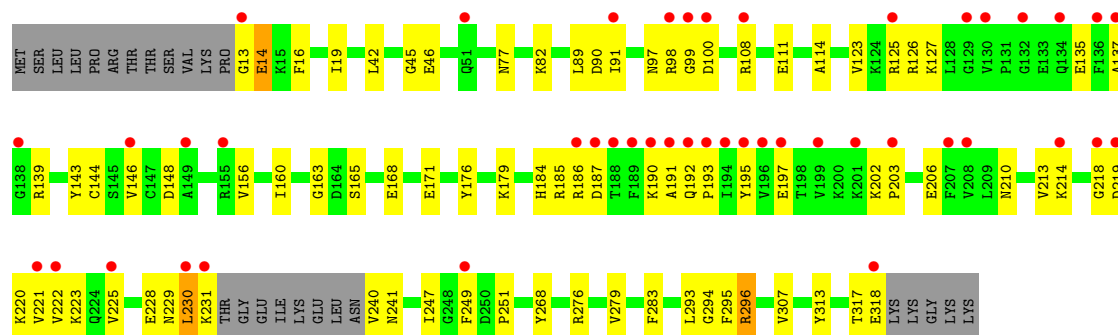


• Molecule 1: Thioredoxin reductase (TrxB-3)





● Molecule 1: Thioredoxin reductase (TrxB-3)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.87Å 123.42Å 127.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.95) 86.3 (15.00-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.94Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.257 0.181 , 0.204	Depositor DCC
R_{free} test set	776 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10058	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	0/2407	1.02	7/3252 (0.2%)
1	B	0.64	0/2415	1.05	15/3263 (0.5%)
1	C	0.69	0/2396	1.04	9/3238 (0.3%)
1	D	0.66	0/2324	1.04	7/3141 (0.2%)
All	All	0.66	0/9542	1.04	38/12894 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	GLY	N-CA-C	-8.16	103.21	114.64
1	B	41	THR	N-CA-C	6.63	120.21	109.40
1	D	148	ASP	N-CA-C	6.52	121.40	113.38
1	A	65	ILE	N-CA-C	6.26	117.10	108.84
1	B	12	PRO	N-CA-C	-6.19	101.17	111.26
1	B	251	PRO	CA-C-N	-6.08	115.52	121.65
1	B	251	PRO	C-N-CA	-6.08	115.52	121.65
1	A	287	ASP	N-CA-C	6.04	120.34	113.15
1	C	128	LEU	N-CA-C	-6.01	104.30	111.69
1	C	37	TYR	N-CA-C	-5.95	105.78	113.16
1	D	202	LYS	CA-C-N	5.92	126.03	119.87
1	D	202	LYS	C-N-CA	5.92	126.03	119.87
1	A	177	SER	N-CA-C	5.91	118.15	110.53
1	D	203	PRO	N-CA-C	5.89	121.28	114.03
1	B	65	ILE	N-CA-C	5.83	116.59	109.30
1	B	17	ASP	N-CA-C	-5.76	105.14	111.82
1	C	24	GLY	CA-C-N	5.70	125.17	119.24
1	C	24	GLY	C-N-CA	5.70	125.17	119.24
1	B	148	ASP	N-CA-C	5.67	120.35	113.38
1	D	82	LYS	N-CA-C	-5.56	105.76	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ILE	N-CA-C	5.51	115.79	107.80
1	C	65	ILE	N-CA-C	5.50	116.10	108.84
1	A	241	ASN	N-CA-C	-5.49	106.94	113.97
1	C	278	SER	CA-C-N	-5.48	118.65	122.59
1	C	278	SER	C-N-CA	-5.48	118.65	122.59
1	A	220	LYS	N-CA-C	-5.44	105.00	111.69
1	D	135	GLU	N-CA-C	5.43	117.95	111.71
1	A	41	THR	N-CA-C	5.36	118.22	109.59
1	B	13	GLY	N-CA-C	-5.32	100.57	113.18
1	B	147	CYS	N-CA-C	5.32	116.88	111.14
1	A	295	PHE	N-CA-C	-5.30	100.45	108.67
1	B	82	LYS	N-CA-C	-5.28	105.70	111.82
1	B	209	LEU	N-CA-C	5.28	117.34	110.53
1	B	136	PHE	N-CA-C	5.27	118.73	112.72
1	C	82	LYS	N-CA-C	-5.24	105.69	111.71
1	B	220	LYS	N-CA-C	-5.23	106.40	112.89
1	B	214	LYS	N-CA-C	-5.08	107.64	113.88
1	D	279	VAL	N-CA-C	5.07	113.45	107.77

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	2367	0	2428	62	0
1	B	2375	0	2432	82	0
1	C	2356	0	2415	83	0
1	D	2285	0	2330	75	0
2	A	79	0	36	7	0
2	B	79	0	36	8	0
2	C	79	0	36	10	0
2	D	78	0	36	5	0
3	A	88	0	0	11	0
3	B	82	0	0	13	0
3	C	89	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	101	0	0	8	0
All	All	10058	0	9749	291	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 15.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:H	1:B:241:ASN:ND2	1.61	0.97
1:A:219:ASP:CG	1:A:220:LYS:H	1.77	0.93
1:A:105:LYS:HG2	1:A:111:GLU:HG2	1.52	0.90
1:C:190:LYS:H	1:C:190:LYS:HD3	1.36	0.89
1:D:214:LYS:HD2	1:D:228:GLU:HB2	1.55	0.89
1:C:219:ASP:CG	1:C:220:LYS:H	1.82	0.87
1:B:156:VAL:H	1:B:241:ASN:HD22	0.91	0.87
2:A:4001:NAP:H2D	3:A:5128:HOH:O	1.77	0.85
1:B:125:ARG:HH12	1:B:127:LYS:HB3	1.43	0.84
1:A:179:LYS:HE2	1:A:181:TYR:CE1	2.14	0.82
1:B:156:VAL:N	1:B:241:ASN:HD22	1.74	0.82
1:A:179:LYS:HE2	1:A:181:TYR:CZ	2.14	0.81
1:B:190:LYS:HE3	2:B:4002:NAP:H4B	1.62	0.81
1:D:146:VAL:HG13	3:D:5318:HOH:O	1.82	0.80
1:A:88:LEU:HD11	1:A:109:LYS:HD3	1.64	0.80
1:B:109:LYS:H	1:B:109:LYS:HD2	1.46	0.80
1:D:214:LYS:HD2	1:D:228:GLU:CB	2.10	0.79
1:C:232:THR:HG21	1:C:234:GLU:HB2	1.64	0.78
1:B:193:PRO:O	1:B:197:GLU:HG2	1.82	0.77
1:B:162:GLY:C	1:B:190:LYS:HE2	2.10	0.77
1:B:195:TYR:O	1:B:199:VAL:HG23	1.84	0.77
1:C:125:ARG:HD2	1:C:143:TYR:CD1	2.21	0.75
1:A:96:GLU:OE1	1:A:105:LYS:HE3	1.87	0.74
1:C:214:LYS:HE3	1:C:228:GLU:HB2	1.68	0.74
1:B:125:ARG:HD2	1:B:143:TYR:CD1	2.21	0.74
1:B:190:LYS:CE	2:B:4002:NAP:H4B	2.17	0.74
1:A:88:LEU:HD11	1:A:109:LYS:CD	2.17	0.74
1:B:126:ARG:NH1	3:B:5025:HOH:O	2.20	0.74
1:C:232:THR:CG2	1:C:234:GLU:HB2	2.18	0.73
1:B:190:LYS:HD3	3:B:5090:HOH:O	1.89	0.73
1:C:190:LYS:CE	2:C:4003:NAP:H4B	2.19	0.72
1:A:156:VAL:H	1:A:241:ASN:HD22	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASP:CG	1:A:220:LYS:N	2.48	0.71
1:C:313:TYR:OH	1:D:171:GLU:HG3	1.90	0.71
1:D:156:VAL:H	1:D:241:ASN:HD22	1.38	0.71
1:B:190:LYS:NZ	2:B:4002:NAP:H4B	2.05	0.71
1:B:185:ARG:HG2	3:B:5001:HOH:O	1.90	0.70
1:C:194:ILE:HG12	1:D:318:GLU:HG2	1.74	0.70
1:B:105:LYS:HG3	1:B:111:GLU:HG2	1.74	0.69
1:B:226:VAL:HG22	1:B:237:GLU:HG2	1.75	0.69
1:B:98:ARG:HB2	3:B:5210:HOH:O	1.91	0.69
1:B:163:GLY:N	1:B:190:LYS:HE2	2.08	0.68
1:A:179:LYS:NZ	1:A:206:GLU:OE1	2.22	0.68
1:C:214:LYS:HE3	1:C:235:ILE:HD12	1.75	0.67
1:C:194:ILE:CG1	1:D:318:GLU:HG2	2.25	0.67
1:B:294:GLY:C	3:B:5127:HOH:O	2.38	0.67
1:C:234:GLU:O	1:C:235:ILE:HD13	1.95	0.67
1:B:190:LYS:HZ1	2:B:4002:NAP:H4B	1.58	0.66
1:D:225:VAL:HG13	1:D:240:VAL:HG21	1.78	0.66
1:C:163:GLY:N	1:C:190:LYS:HE2	2.11	0.65
1:A:128:LEU:HD13	3:A:5057:HOH:O	1.94	0.65
1:A:171:GLU:HG3	1:B:313:TYR:OH	1.97	0.65
2:B:4002:NAP:H8A	3:B:5025:HOH:O	1.97	0.65
1:D:184:HIS:NE2	1:D:186:ARG:HB2	2.12	0.65
1:B:109:LYS:HD2	1:B:109:LYS:N	2.10	0.64
1:D:190:LYS:NZ	2:D:4004:NAP:H4B	2.12	0.64
1:C:185:ARG:HG2	3:C:5012:HOH:O	1.97	0.64
1:C:11:LYS:HD2	1:C:11:LYS:N	2.13	0.64
1:B:98:ARG:HB3	1:B:101:GLU:O	1.97	0.63
1:B:125:ARG:NH1	1:B:127:LYS:HB3	2.11	0.63
1:B:125:ARG:HD2	1:B:143:TYR:CE1	2.33	0.63
1:D:160:ILE:CD1	1:D:213:VAL:HG21	2.28	0.63
1:D:168:GLU:HB2	1:D:195:TYR:HE2	1.63	0.63
1:D:90:ASP:OD1	1:D:108:ARG:HD2	1.98	0.63
1:B:125:ARG:HH22	1:B:127:LYS:HD3	1.63	0.62
1:D:268:TYR:OH	1:D:296:ARG:NH2	2.24	0.62
1:B:268:TYR:OH	1:B:296:ARG:NH2	2.33	0.62
1:C:229:ASN:HB3	1:C:232:THR:HB	1.82	0.62
1:A:313:TYR:OH	1:B:171:GLU:HG3	2.00	0.62
1:A:82:LYS:HE2	1:B:59:ASP:OD2	1.99	0.61
1:A:105:LYS:HG2	1:A:111:GLU:CG	2.29	0.61
1:C:93:GLU:OE2	1:C:107:LYS:HG3	2.00	0.61
1:C:219:ASP:CG	1:C:220:LYS:N	2.51	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LYS:HZ1	2:D:4004:NAP:H4B	1.64	0.61
1:B:163:GLY:CA	1:B:190:LYS:HE2	2.30	0.61
1:B:179:LYS:HE3	1:B:181:TYR:CZ	2.36	0.61
1:B:101:GLU:OE1	1:B:113:LYS:HD3	2.01	0.61
1:C:190:LYS:HZ1	2:C:4003:NAP:H4B	1.65	0.61
1:C:190:LYS:HD3	1:C:190:LYS:N	2.13	0.61
1:A:234:GLU:OE1	1:A:236:LYS:HE3	2.00	0.61
1:A:77:ASN:HB2	3:A:5213:HOH:O	1.99	0.61
2:B:4002:NAP:H3B	3:B:5025:HOH:O	2.00	0.60
1:C:190:LYS:HE3	2:C:4003:NAP:O3B	2.00	0.60
1:D:219:ASP:CG	1:D:220:LYS:H	2.07	0.60
1:C:218:GLY:HA2	1:C:223:LYS:HB2	1.83	0.60
1:B:161:GLY:HA3	3:B:5045:HOH:O	2.01	0.60
1:C:268:TYR:OH	1:C:296:ARG:NH2	2.34	0.60
1:D:125:ARG:HD2	1:D:143:TYR:CE1	2.36	0.60
1:C:190:LYS:NZ	2:C:4003:NAP:H4B	2.16	0.60
1:C:214:LYS:CE	1:C:235:ILE:HD12	2.32	0.60
1:A:168:GLU:OE2	2:A:4001:NAP:H4N	2.02	0.60
1:B:125:ARG:HH12	1:B:127:LYS:CB	2.14	0.59
1:C:318:GLU:HG3	3:C:5292:HOH:O	2.01	0.59
1:A:161:GLY:HA3	3:A:5067:HOH:O	2.02	0.59
1:C:125:ARG:HD2	1:C:143:TYR:CE1	2.37	0.59
1:B:105:LYS:CG	1:B:111:GLU:HG2	2.33	0.58
1:D:230:LEU:O	1:D:231:LYS:HG3	2.03	0.58
1:D:125:ARG:HD2	1:D:143:TYR:CZ	2.38	0.58
1:A:214:LYS:HD2	1:A:228:GLU:HB2	1.86	0.58
1:C:253:THR:HG22	1:C:257:LYS:HE3	1.85	0.58
1:A:101:GLU:N	3:A:5130:HOH:O	2.37	0.58
1:B:57:ILE:HD13	1:B:68:GLN:OE1	2.04	0.58
1:A:82:LYS:NZ	1:B:66:GLU:OE2	2.32	0.57
1:C:227:VAL:HG12	1:C:228:GLU:N	2.17	0.57
1:C:101:GLU:OE2	1:C:113:LYS:HD2	2.04	0.57
1:A:125:ARG:HD2	1:A:143:TYR:CD1	2.40	0.57
1:B:128:LEU:HD13	1:B:247:ILE:HD13	1.86	0.57
1:B:160:ILE:CD1	1:B:213:VAL:HG21	2.34	0.57
1:B:163:GLY:C	1:B:191:ALA:HB2	2.30	0.57
1:A:153:LYS:HG3	3:A:5208:HOH:O	2.05	0.56
1:C:156:VAL:H	1:C:241:ASN:HD22	1.52	0.56
2:C:4003:NAP:H3D	2:C:4003:NAP:O2N	2.05	0.56
1:D:165:SER:HB2	2:D:4004:NAP:O1N	2.06	0.56
1:A:296:ARG:HH22	2:A:4001:NAP:H51N	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:MET:HG2	1:D:176:TYR:CZ	2.40	0.56
1:A:15:LYS:HG3	1:A:16:PHE:N	2.20	0.56
1:A:294:GLY:HA3	2:A:4001:NAP:H1D	1.87	0.56
1:B:214:LYS:HE2	1:B:214:LYS:HA	1.87	0.55
1:A:108:ARG:NH1	1:A:109:LYS:HE3	2.21	0.55
1:D:91:ILE:HD12	1:D:91:ILE:N	2.21	0.55
1:D:206:GLU:HB2	3:D:5155:HOH:O	2.06	0.55
1:A:160:ILE:HD12	1:A:245:ILE:HG12	1.89	0.54
1:D:190:LYS:HE3	3:D:5154:HOH:O	2.07	0.54
1:B:232:THR:C	1:B:234:GLU:H	2.15	0.54
1:C:162:GLY:C	1:C:190:LYS:HE2	2.33	0.54
1:C:313:TYR:O	1:C:317:THR:HG23	2.07	0.54
1:D:13:GLY:O	1:D:14:GLU:HB3	2.08	0.54
1:D:144:CYS:SG	1:D:146:VAL:HG22	2.48	0.54
1:D:218:GLY:HA2	1:D:223:LYS:HB2	1.90	0.53
1:A:194:ILE:HG12	1:B:318:GLU:HG2	1.90	0.53
1:C:163:GLY:C	1:C:191:ALA:HB2	2.34	0.53
1:D:193:PRO:O	1:D:197:GLU:HG2	2.08	0.53
1:A:194:ILE:CG1	1:B:318:GLU:HG2	2.39	0.53
1:C:97:ASN:C	1:C:97:ASN:HD22	2.16	0.53
1:A:179:LYS:HG2	1:A:180:VAL:N	2.24	0.53
1:C:214:LYS:HZ2	1:C:235:ILE:HG21	1.74	0.53
1:A:108:ARG:HH12	1:A:109:LYS:HE3	1.73	0.52
1:A:108:ARG:CZ	3:A:5156:HOH:O	2.56	0.52
1:C:171:GLU:HG3	1:D:313:TYR:OH	2.10	0.52
1:C:162:GLY:O	1:C:190:LYS:HD3	2.09	0.52
1:C:214:LYS:NZ	1:C:235:ILE:HD12	2.25	0.52
1:A:161:GLY:CA	3:A:5067:HOH:O	2.57	0.52
1:C:10:VAL:C	1:C:11:LYS:HD2	2.34	0.52
1:D:125:ARG:HH12	1:D:127:LYS:HG2	1.75	0.51
1:D:160:ILE:HD13	1:D:213:VAL:HG21	1.91	0.51
1:B:160:ILE:HD13	1:B:213:VAL:HG21	1.92	0.51
1:C:190:LYS:H	1:C:190:LYS:CD	2.18	0.51
1:B:270:LYS:HE3	3:B:5269:HOH:O	2.09	0.51
1:C:137:ALA:O	1:C:139:ARG:HG3	2.11	0.51
1:D:249:PHE:CD1	1:D:296:ARG:NH1	2.79	0.51
1:C:313:TYR:HH	1:D:171:GLU:HG3	1.75	0.51
1:D:214:LYS:HD2	1:D:228:GLU:HB3	1.91	0.50
1:C:162:GLY:H	1:C:190:LYS:HZ1	1.58	0.50
1:A:183:ILE:HD13	1:A:227:VAL:HG21	1.94	0.50
1:C:180:VAL:HB	1:C:205:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:H	1:A:241:ASN:ND2	2.09	0.49
1:D:97:ASN:C	1:D:99:GLY:H	2.20	0.49
1:C:293:LEU:HD13	1:C:294:GLY:N	2.28	0.49
1:B:107:LYS:NZ	3:B:5015:HOH:O	2.22	0.49
1:D:191:ALA:O	1:D:192:GLN:C	2.56	0.49
1:B:125:ARG:HH12	1:B:127:LYS:HD3	1.76	0.49
1:B:295:PHE:N	3:B:5127:HOH:O	2.45	0.49
1:C:184:HIS:CE1	1:C:190:LYS:HZ3	2.30	0.49
1:B:16:PHE:O	1:B:114:ALA:HA	2.13	0.48
1:D:125:ARG:NH1	1:D:127:LYS:HG2	2.28	0.48
1:A:23:LEU:HG	1:A:48:PRO:HA	1.95	0.48
1:A:247:ILE:HG21	3:A:5057:HOH:O	2.13	0.48
1:B:98:ARG:C	1:B:100:ASP:N	2.71	0.48
1:C:19:ILE:HG13	1:C:114:ALA:HB2	1.95	0.48
1:D:160:ILE:HD11	1:D:213:VAL:HG21	1.96	0.48
1:A:88:LEU:HD11	1:A:109:LYS:HD2	1.91	0.48
1:A:211:SER:HB3	1:A:227:VAL:CG1	2.43	0.48
1:C:214:LYS:HZ2	1:C:235:ILE:CG2	2.26	0.48
1:D:313:TYR:O	1:D:317:THR:HG23	2.14	0.48
1:D:229:ASN:C	1:D:231:LYS:H	2.22	0.47
1:A:131:PRO:HD2	1:A:214:LYS:O	2.15	0.47
1:D:230:LEU:C	1:D:231:LYS:HG3	2.39	0.47
1:B:45:GLY:O	1:B:89:LEU:HA	2.14	0.47
1:B:125:ARG:NH2	1:B:127:LYS:HD3	2.29	0.47
1:B:199:VAL:HG12	1:B:205:VAL:HG11	1.96	0.47
1:C:93:GLU:CD	1:C:107:LYS:HA	2.40	0.47
1:C:126:ARG:HD2	1:C:247:ILE:O	2.14	0.47
1:C:123:VAL:HG23	1:C:249:PHE:CD2	2.49	0.47
1:A:46:GLU:HB3	2:A:4005:NAP:O3X	2.15	0.46
1:D:45:GLY:O	1:D:89:LEU:HA	2.15	0.46
1:D:123:VAL:HG12	1:D:251:PRO:HA	1.98	0.46
1:D:137:ALA:C	1:D:139:ARG:H	2.22	0.46
1:D:190:LYS:HE3	1:D:190:LYS:HB3	1.79	0.46
1:D:126:ARG:HD2	1:D:247:ILE:O	2.16	0.46
1:B:263:THR:HA	1:B:268:TYR:O	2.16	0.46
1:C:45:GLY:O	1:C:89:LEU:HA	2.16	0.46
1:C:184:HIS:NE2	1:C:186:ARG:HB2	2.30	0.46
1:C:162:GLY:C	1:C:190:LYS:CE	2.89	0.46
1:D:185:ARG:O	1:D:210:ASN:HA	2.16	0.46
1:B:225:VAL:HG22	1:B:240:VAL:CG2	2.46	0.46
1:C:190:LYS:NZ	2:C:4003:NAP:O2B	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:TYR:CE1	1:D:317:THR:HG21	2.51	0.46
1:A:19:ILE:HG13	1:A:114:ALA:HB2	1.98	0.45
1:A:160:ILE:CG2	3:A:5057:HOH:O	2.63	0.45
1:B:65:ILE:O	1:B:66:GLU:C	2.59	0.45
1:D:190:LYS:HE2	2:D:4004:NAP:O3B	2.16	0.45
1:C:125:ARG:NH1	1:C:126:ARG:O	2.49	0.45
1:B:11:LYS:O	1:B:12:PRO:C	2.56	0.45
1:B:98:ARG:HD2	3:B:5210:HOH:O	2.16	0.45
1:C:46:GLU:HB3	2:C:4007:NAP:O3X	2.16	0.45
1:A:196:VAL:O	1:A:200:LYS:HB2	2.17	0.45
1:B:69:ALA:O	1:B:73:ILE:HG13	2.16	0.45
1:B:94:LYS:HD2	1:B:259:ASN:OD1	2.17	0.45
1:C:163:GLY:CA	1:C:190:LYS:HE2	2.46	0.45
1:B:211:SER:HB3	1:B:227:VAL:CG1	2.46	0.45
1:C:217:LYS:HB2	1:C:224:GLN:HG3	1.99	0.45
1:C:130:VAL:HB	1:C:214:LYS:O	2.17	0.45
1:D:98:ARG:O	1:D:98:ARG:HG2	2.16	0.45
1:D:163:GLY:C	1:D:191:ALA:HB2	2.42	0.45
1:C:171:GLU:OE1	1:C:198:THR:HG22	2.16	0.45
1:D:13:GLY:O	1:D:14:GLU:CB	2.64	0.45
2:A:4001:NAP:O2N	2:A:4001:NAP:H3D	2.17	0.44
1:B:77:ASN:O	1:B:81:GLU:HG2	2.16	0.44
1:A:77:ASN:O	1:A:81:GLU:HG2	2.16	0.44
1:C:95:ILE:HD13	1:C:117:VAL:HG11	1.99	0.44
1:D:294:GLY:C	3:D:5058:HOH:O	2.60	0.44
1:B:108:ARG:O	1:B:110:GLY:N	2.50	0.44
1:B:190:LYS:HE3	2:B:4002:NAP:C4B	2.41	0.44
1:D:139:ARG:NH1	3:D:5274:HOH:O	2.49	0.44
1:B:194:ILE:HG23	1:B:195:TYR:N	2.33	0.44
1:C:136:PHE:HZ	1:C:218:GLY:O	2.00	0.44
1:C:264:ASP:OD1	1:C:264:ASP:C	2.61	0.44
1:C:292:TRP:CE2	1:D:307:VAL:HG21	2.53	0.44
1:A:160:ILE:HG21	3:A:5057:HOH:O	2.18	0.43
1:B:168:GLU:CD	3:B:5050:HOH:O	2.61	0.43
1:D:19:ILE:HG13	1:D:114:ALA:HB2	2.01	0.43
1:D:137:ALA:C	1:D:139:ARG:N	2.74	0.43
1:C:293:LEU:HD13	1:C:293:LEU:C	2.44	0.43
1:D:13:GLY:HA3	1:D:111:GLU:O	2.18	0.43
1:C:162:GLY:HA3	1:C:190:LYS:HZ3	1.84	0.43
1:B:226:VAL:HG22	1:B:237:GLU:CG	2.47	0.43
1:D:16:PHE:CE2	1:D:42:LEU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:O	1:A:86:PRO:HD2	2.17	0.43
1:A:219:ASP:OD2	1:A:220:LYS:HE2	2.18	0.43
1:B:232:THR:C	1:B:234:GLU:N	2.76	0.43
1:C:227:VAL:CG1	1:C:228:GLU:N	2.82	0.43
1:C:16:PHE:O	1:C:114:ALA:HA	2.19	0.43
1:D:91:ILE:HD13	1:D:108:ARG:NH1	2.34	0.43
1:B:46:GLU:HB3	2:B:4006:NAP:O3X	2.19	0.42
1:C:162:GLY:CA	1:C:190:LYS:HZ3	2.33	0.42
1:C:194:ILE:HG13	1:D:318:GLU:HG2	2.01	0.42
1:D:16:PHE:O	1:D:114:ALA:HA	2.19	0.42
1:A:16:PHE:O	1:A:114:ALA:HA	2.20	0.42
1:A:294:GLY:HA3	2:A:4001:NAP:C1D	2.49	0.42
1:D:225:VAL:HG13	1:D:240:VAL:CG2	2.46	0.42
1:C:150:PRO:HG3	1:C:176:TYR:CZ	2.54	0.42
1:C:190:LYS:HE3	2:C:4003:NAP:H4B	1.98	0.42
1:D:219:ASP:OD1	1:D:223:LYS:HE3	2.20	0.42
2:C:4003:NAP:H52A	3:C:5113:HOH:O	2.19	0.42
1:B:219:ASP:HB3	1:B:220:LYS:H	1.67	0.41
1:A:182:LEU:HD23	1:A:207:PHE:CE1	2.55	0.41
1:A:263:THR:HA	1:A:268:TYR:O	2.20	0.41
1:C:212:VAL:HG22	1:C:230:LEU:HD21	2.02	0.41
1:B:160:ILE:HD11	1:B:213:VAL:HG21	2.02	0.41
1:D:125:ARG:HD2	1:D:143:TYR:CD1	2.55	0.41
1:B:146:VAL:HG12	1:B:172:ILE:CD1	2.50	0.41
1:C:227:VAL:HG12	1:C:228:GLU:H	1.85	0.41
1:D:295:PHE:N	3:D:5058:HOH:O	2.53	0.41
1:B:253:THR:O	1:B:257:LYS:HG3	2.20	0.41
1:D:98:ARG:O	1:D:100:ASP:N	2.53	0.41
1:A:313:TYR:CE1	1:A:317:THR:HG21	2.56	0.41
1:D:168:GLU:HB2	1:D:195:TYR:CE2	2.48	0.41
1:A:318:GLU:HG2	1:B:194:ILE:CG1	2.50	0.41
1:B:96:GLU:CD	1:B:105:LYS:HZ1	2.28	0.41
1:C:38:MET:HG2	1:D:176:TYR:CE2	2.56	0.41
1:C:236:LYS:HE2	1:C:238:LEU:HD21	2.02	0.41
1:C:247:ILE:HB	2:C:4003:NAP:C8A	2.51	0.41
1:C:299:ILE:HG23	1:C:300:THR:N	2.35	0.41
1:D:179:LYS:HE3	3:D:5155:HOH:O	2.21	0.41
1:D:276:ARG:HG2	1:D:283:PHE:CE2	2.56	0.41
1:D:293:LEU:HD13	1:D:293:LEU:C	2.46	0.41
1:B:231:LYS:HB3	1:B:231:LYS:HE2	1.79	0.41
1:A:228:GLU:HB2	1:A:235:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:HG23	1:A:300:THR:N	2.34	0.40
1:A:176:TYR:CZ	1:B:38:MET:HG3	2.56	0.40
1:B:179:LYS:HE3	1:B:181:TYR:CE1	2.55	0.40
1:C:193:PRO:O	1:C:197:GLU:HG2	2.21	0.40
1:D:46:GLU:HB3	2:D:4008:NAP:O3X	2.21	0.40
1:A:179:LYS:HG2	1:A:180:VAL:H	1.86	0.40
1:C:253:THR:CG2	1:C:257:LYS:HE3	2.49	0.40
1:D:77:ASN:CB	3:D:5137:HOH:O	2.70	0.40
1:B:134:GLN:O	1:B:135:GLU:C	2.64	0.40
1:B:296:ARG:HH11	1:B:296:ARG:HG3	1.87	0.40
1:A:125:ARG:HG2	1:A:125:ARG:HH11	1.87	0.40
1:A:160:ILE:CD1	1:A:213:VAL:HG21	2.52	0.40
1:D:221:VAL:O	1:D:222:VAL:C	2.64	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	304/323 (94%)	295 (97%)	9 (3%)	0	100	100
1	B	305/323 (94%)	288 (94%)	14 (5%)	3 (1%)	12	5
1	C	303/323 (94%)	293 (97%)	10 (3%)	0	100	100
1	D	294/323 (91%)	278 (95%)	14 (5%)	2 (1%)	18	10
All	All	1206/1292 (93%)	1154 (96%)	47 (4%)	5 (0%)	30	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	LYS
1	B	14	GLU

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Mol	Chain	Res	Type
1	B	233	GLY
1	D	14	GLU
1	D	230	LEU

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	253/267 (95%)	251 (99%)	2 (1%)	73	74
1	B	254/267 (95%)	249 (98%)	5 (2%)	48	43
1	C	252/267 (94%)	251 (100%)	1 (0%)	84	85
1	D	243/267 (91%)	241 (99%)	2 (1%)	73	74
All	All	1002/1068 (94%)	992 (99%)	10 (1%)	68	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	293	LEU
1	B	125	ARG
1	B	128	LEU
1	B	190	LYS
1	B	225	VAL
1	B	293	LEU
1	C	265	THR
1	D	187	ASP
1	D	296	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	192	GLN
1	A	241	ASN

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Mol	Chain	Res	Type
1	A	266	ASN
1	B	210	ASN
1	B	241	ASN
1	B	266	ASN
1	B	297	GLN
1	C	97	ASN
1	C	184	HIS
1	C	192	GLN
1	C	241	ASN
1	D	241	ASN
1	D	297	GLN

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 ⓘ

8 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	D	4004	-	50,52,52	1.74	7 (14%)	71,80,80	1.26	7 (9%)
2	NAP	C	4003	-	50,52,52	1.66	5 (10%)	71,80,80	1.21	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	C	4007	-	32,33,52	1.89	6 (18%)	50,52,80	1.09	2 (4%)
2	NAP	D	4008	-	28,32,52	1.66	3 (10%)	44,49,80	1.08	3 (6%)
2	NAP	A	4001	-	50,52,52	1.65	5 (10%)	71,80,80	1.24	6 (8%)
2	NAP	B	4006	-	32,33,52	1.93	5 (15%)	50,52,80	1.03	1 (2%)
2	NAP	B	4002	-	50,52,52	1.73	8 (16%)	71,80,80	1.22	6 (8%)
2	NAP	A	4005	-	32,33,52	1.99	4 (12%)	50,52,80	1.06	2 (4%)

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	D	4004	-	-	4/35/67/67	0/5/5/5
2	NAP	C	4003	-	-	1/35/67/67	0/5/5/5
2	NAP	C	4007	-	-	0/21/37/67	0/3/3/5
2	NAP	D	4008	-	-	1/18/36/67	0/3/3/5
2	NAP	A	4001	-	-	5/35/67/67	0/5/5/5
2	NAP	B	4006	-	-	0/21/37/67	0/3/3/5
2	NAP	B	4002	-	-	6/35/67/67	0/5/5/5
2	NAP	A	4005	-	-	0/21/37/67	0/3/3/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4005	NAP	P2B-O2B	8.16	1.73	1.59
2	C	4007	NAP	P2B-O2B	6.83	1.71	1.59
2	A	4001	NAP	C2N-N1N	6.35	1.42	1.35
2	D	4004	NAP	C2N-N1N	6.34	1.41	1.35
2	D	4004	NAP	C3N-C7N	6.26	1.59	1.50
2	A	4001	NAP	C3N-C7N	6.22	1.59	1.50
2	C	4003	NAP	C2N-N1N	6.19	1.41	1.35
2	B	4006	NAP	P2B-O2B	6.15	1.70	1.59
2	C	4003	NAP	C3N-C7N	5.95	1.59	1.50
2	D	4008	NAP	P2B-O2B	5.88	1.69	1.59
2	B	4002	NAP	C3N-C7N	5.66	1.59	1.50
2	B	4006	NAP	PA-O3	5.50	1.65	1.59
2	B	4002	NAP	C2N-N1N	5.00	1.40	1.35
2	C	4007	NAP	P2B-O2X	-4.65	1.37	1.54
2	A	4005	NAP	P2B-O2X	-4.43	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4006	NAP	P2B-O2X	-4.42	1.38	1.54
2	B	4002	NAP	PA-O3	4.26	1.64	1.59
2	B	4002	NAP	PN-O3	4.19	1.64	1.59
2	D	4008	NAP	P2B-O2X	-4.18	1.39	1.54
2	B	4002	NAP	C6N-N1N	3.27	1.42	1.35
2	A	4005	NAP	PN-O5D	3.25	1.66	1.54
2	C	4003	NAP	O4D-C1D	3.18	1.45	1.40
2	A	4001	NAP	C6N-N1N	3.11	1.42	1.35
2	C	4003	NAP	C6N-N1N	3.04	1.42	1.35
2	D	4004	NAP	C6N-N1N	3.01	1.42	1.35
2	A	4001	NAP	O4D-C1D	2.97	1.44	1.40
2	C	4007	NAP	C4A-N3A	2.89	1.39	1.34
2	D	4004	NAP	O4D-C1D	2.84	1.44	1.40
2	B	4002	NAP	O4D-C1D	2.83	1.44	1.40
2	D	4004	NAP	PN-O3	2.78	1.62	1.59
2	C	4007	NAP	PN-O5D	2.73	1.65	1.54
2	B	4006	NAP	PN-O5D	2.67	1.64	1.54
2	A	4005	NAP	C4A-N3A	2.43	1.39	1.34
2	B	4002	NAP	C4A-N3A	2.37	1.38	1.34
2	D	4004	NAP	PA-O3	2.33	1.62	1.59
2	B	4002	NAP	P2B-O3X	-2.32	1.46	1.54
2	C	4003	NAP	C4A-N3A	2.27	1.38	1.34
2	D	4004	NAP	P2B-O2B	2.20	1.63	1.59
2	C	4007	NAP	PA-O2A	-2.16	1.45	1.55
2	A	4001	NAP	P2B-O2X	-2.11	1.46	1.54
2	D	4008	NAP	C4A-N3A	2.11	1.38	1.34
2	C	4007	NAP	PN-O1N	-2.07	1.44	1.50
2	B	4006	NAP	C4A-N3A	2.05	1.38	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4003	NAP	C3N-C7N-N7N	4.38	123.13	117.74
2	A	4001	NAP	C3N-C7N-N7N	4.28	123.01	117.74
2	D	4004	NAP	C3N-C7N-N7N	4.14	122.84	117.74
2	A	4001	NAP	C6N-N1N-C2N	-3.89	118.57	121.88
2	B	4002	NAP	C3N-C7N-N7N	3.81	122.44	117.74
2	C	4003	NAP	C6N-N1N-C2N	-3.57	118.84	121.88
2	B	4002	NAP	C6N-N1N-C2N	-3.46	118.93	121.88
2	D	4004	NAP	C6N-N1N-C2N	-3.46	118.94	121.88
2	C	4003	NAP	O7N-C7N-C3N	-2.93	116.01	119.60
2	D	4008	NAP	O4B-C1B-C2B	-2.84	101.69	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4002	NAP	C2B-C1B-N9A	-2.75	109.23	113.75
2	D	4004	NAP	O7N-C7N-C3N	-2.72	116.27	119.60
2	A	4001	NAP	O7N-C7N-C3N	-2.69	116.31	119.60
2	D	4008	NAP	O2X-P2B-O1X	2.65	121.17	110.83
2	B	4006	NAP	O2X-P2B-O1X	2.63	121.09	110.83
2	A	4005	NAP	O2X-P2B-O1X	2.63	121.08	110.83
2	C	4003	NAP	O5D-C5D-C4D	2.62	117.92	108.99
2	C	4007	NAP	O2X-P2B-O1X	2.57	120.83	110.83
2	D	4004	NAP	C2B-C1B-N9A	-2.56	109.54	113.75
2	A	4001	NAP	O5D-C5D-C4D	2.50	117.51	108.99
2	D	4004	NAP	O5D-C5D-C4D	2.46	117.38	108.99
2	C	4007	NAP	O4B-C1B-C2B	-2.46	102.35	106.59
2	A	4001	NAP	C5N-C4N-C3N	2.46	122.78	120.36
2	B	4002	NAP	O7N-C7N-C3N	-2.46	116.59	119.60
2	A	4001	NAP	C2B-C1B-N9A	-2.43	109.75	113.75
2	D	4004	NAP	O4B-C1B-N9A	2.32	112.55	108.09
2	B	4002	NAP	O3B-C3B-C4B	2.26	117.58	111.08
2	A	4005	NAP	O2B-C2B-C3B	2.15	119.38	111.68
2	D	4008	NAP	O5B-C5B-C4B	2.12	116.20	108.99
2	B	4002	NAP	O4B-C1B-N9A	2.08	112.09	108.09
2	D	4004	NAP	C5N-C4N-C3N	2.08	122.41	120.36
2	C	4003	NAP	C5N-C4N-C3N	2.02	122.36	120.36

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4002	NAP	C5D-O5D-PN-O1N
2	A	4001	NAP	O4D-C4D-C5D-O5D
2	A	4001	NAP	C3D-C4D-C5D-O5D
2	A	4001	NAP	C4D-C5D-O5D-PN
2	C	4003	NAP	C4D-C5D-O5D-PN
2	D	4004	NAP	C4D-C5D-O5D-PN
2	B	4002	NAP	PA-O3-PN-O1N
2	B	4002	NAP	C5D-O5D-PN-O3
2	B	4002	NAP	C5D-O5D-PN-O2N
2	D	4004	NAP	C2B-O2B-P2B-O2X
2	A	4001	NAP	C2D-C1D-N1N-C6N
2	D	4004	NAP	O4D-C4D-C5D-O5D
2	B	4002	NAP	C2B-O2B-P2B-O3X
2	D	4008	NAP	C2B-O2B-P2B-O2X
2	A	4001	NAP	O4B-C4B-C5B-O5B

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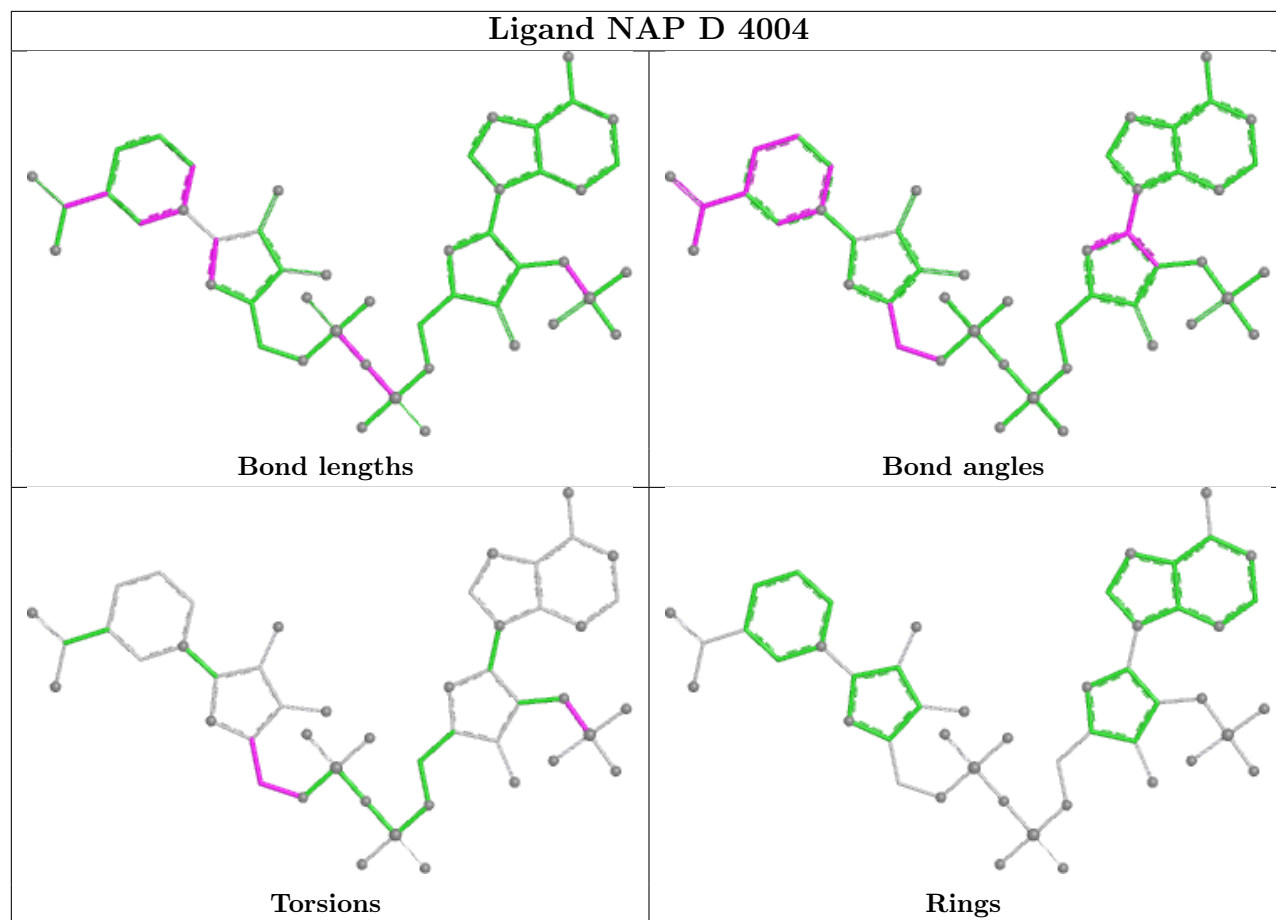
Mol	Chain	Res	Type	Atoms
2	D	4004	NAP	C3D-C4D-C5D-O5D
2	B	4002	NAP	PA-O3-PN-O2N

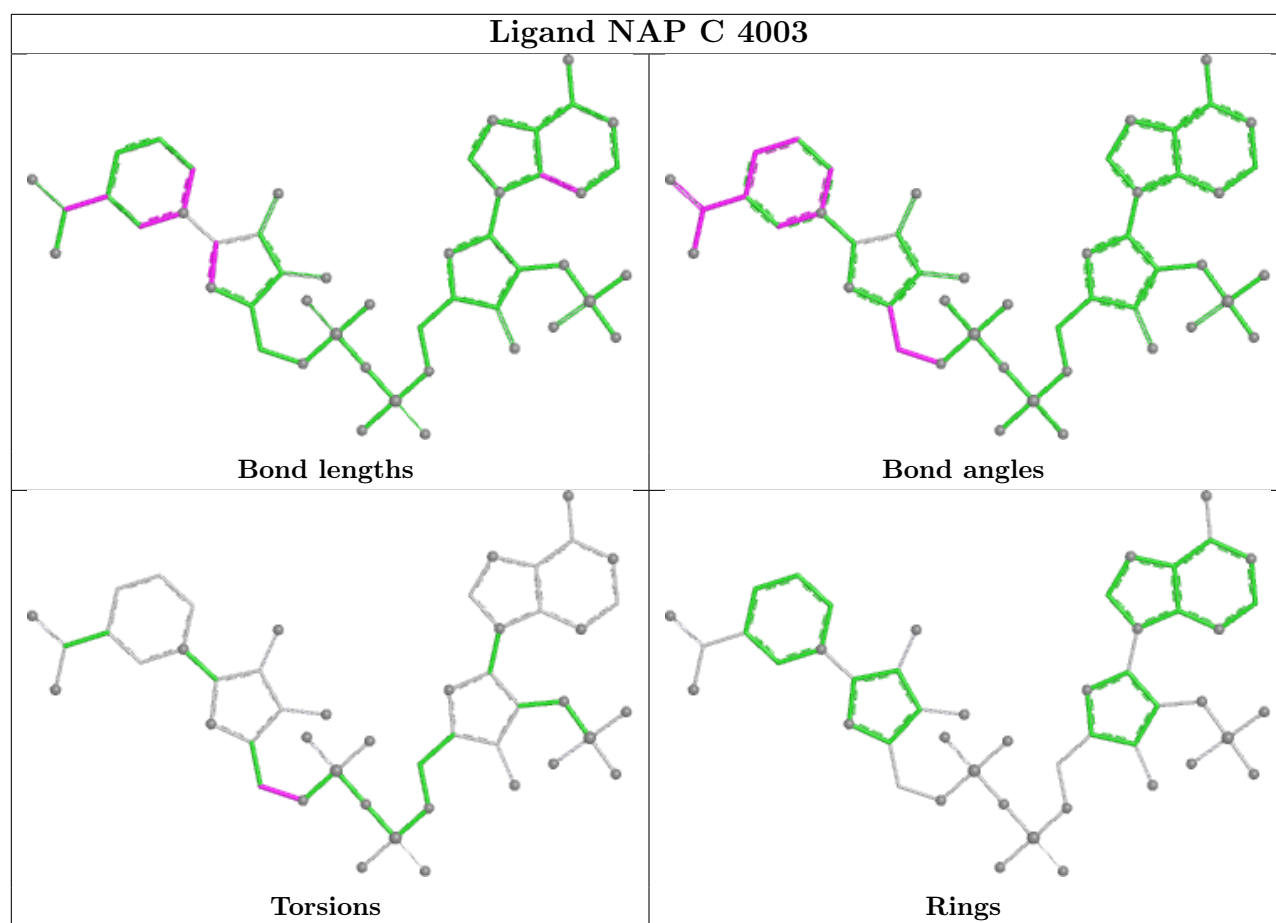
There are no ring outliers.

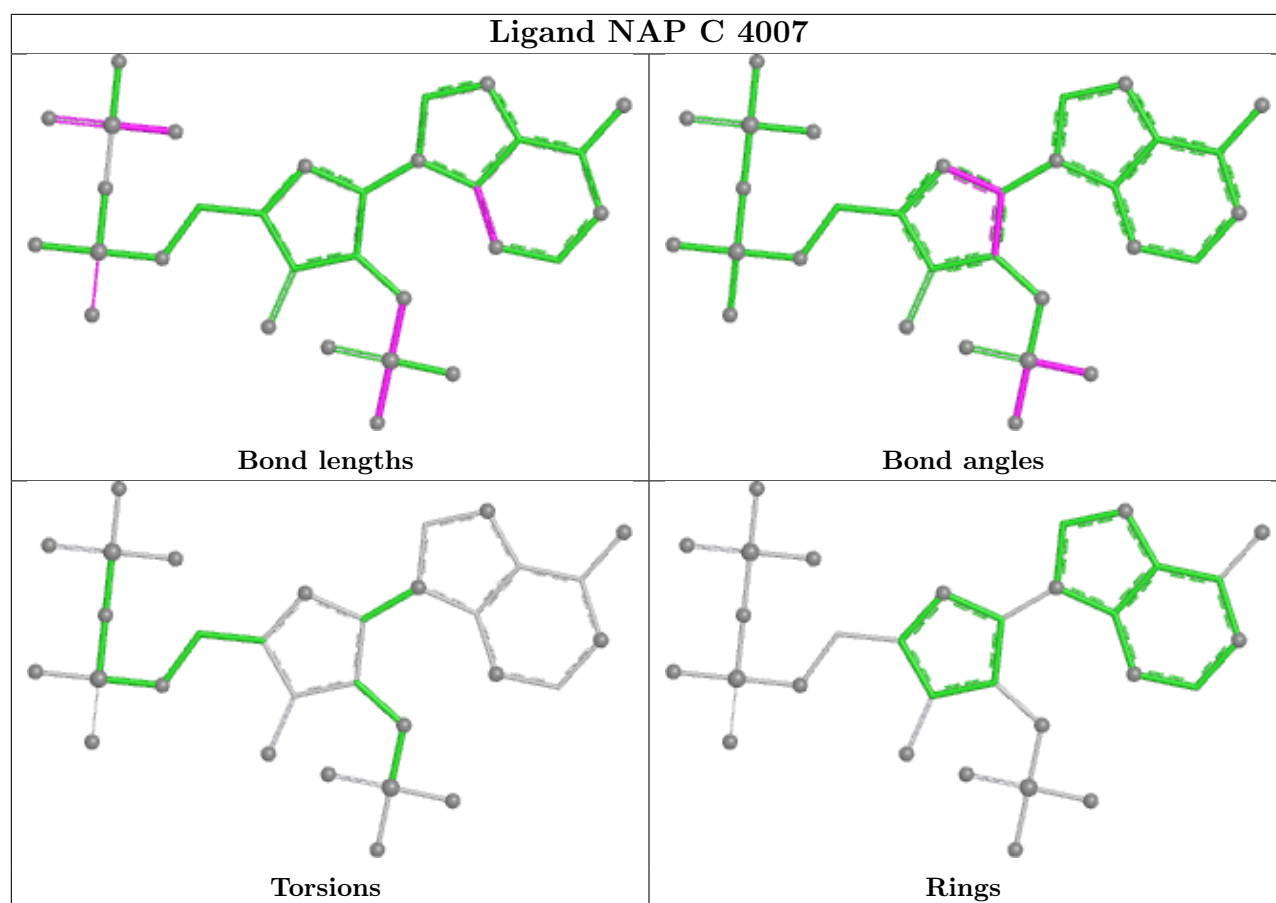
8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4004	NAP	4	0
2	C	4003	NAP	9	0
2	C	4007	NAP	1	0
2	D	4008	NAP	1	0
2	A	4001	NAP	6	0
2	B	4006	NAP	1	0
2	B	4002	NAP	7	0
2	A	4005	NAP	1	0

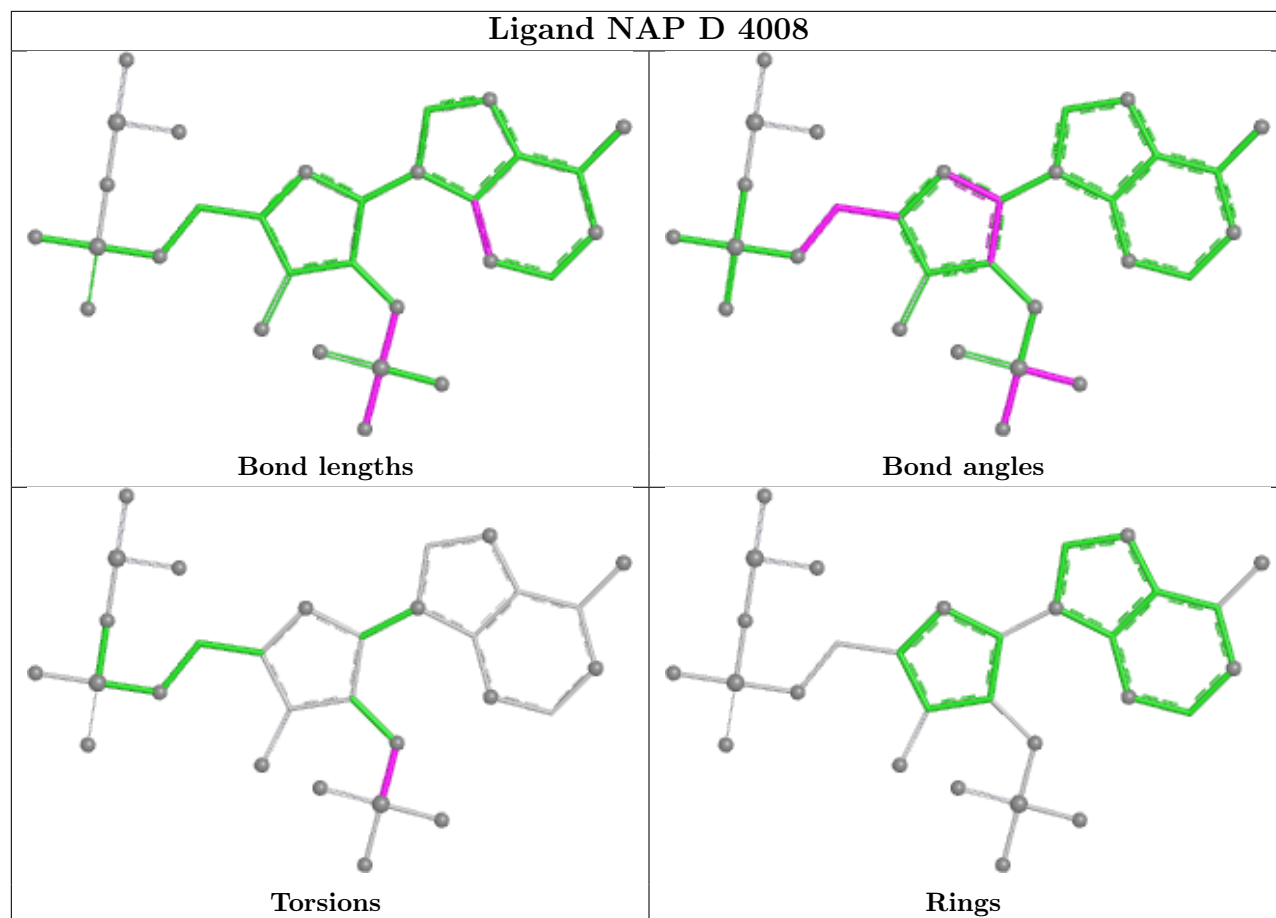
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

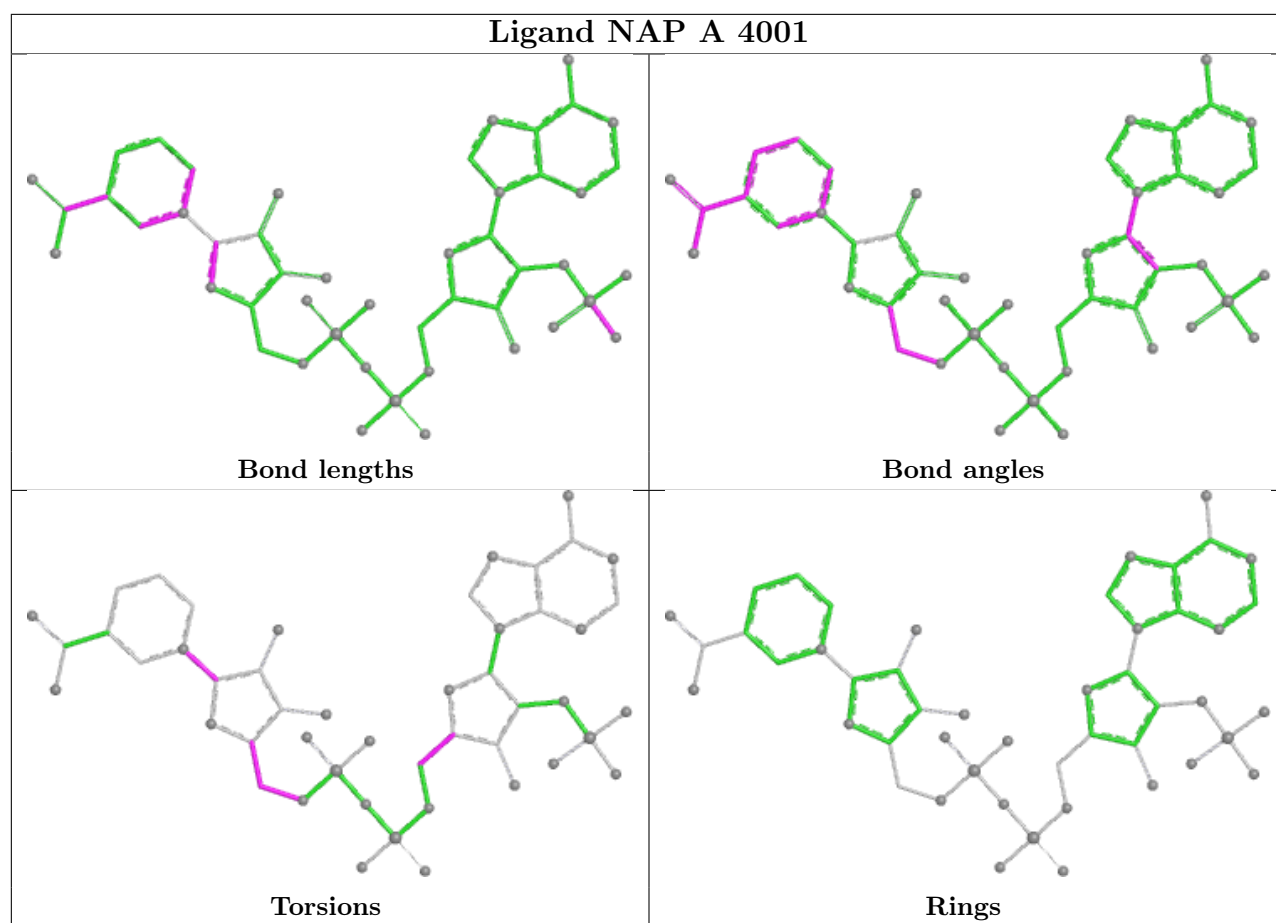


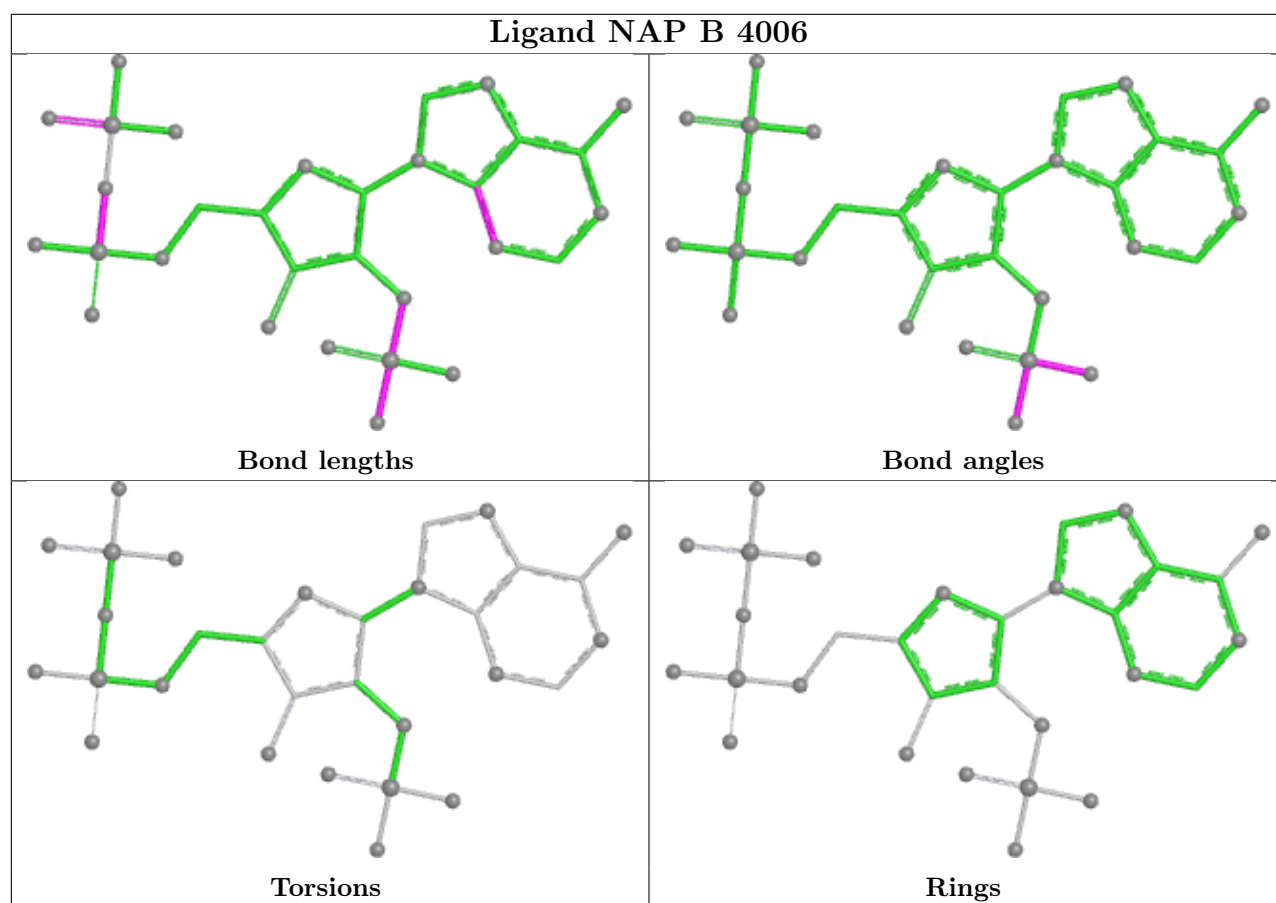


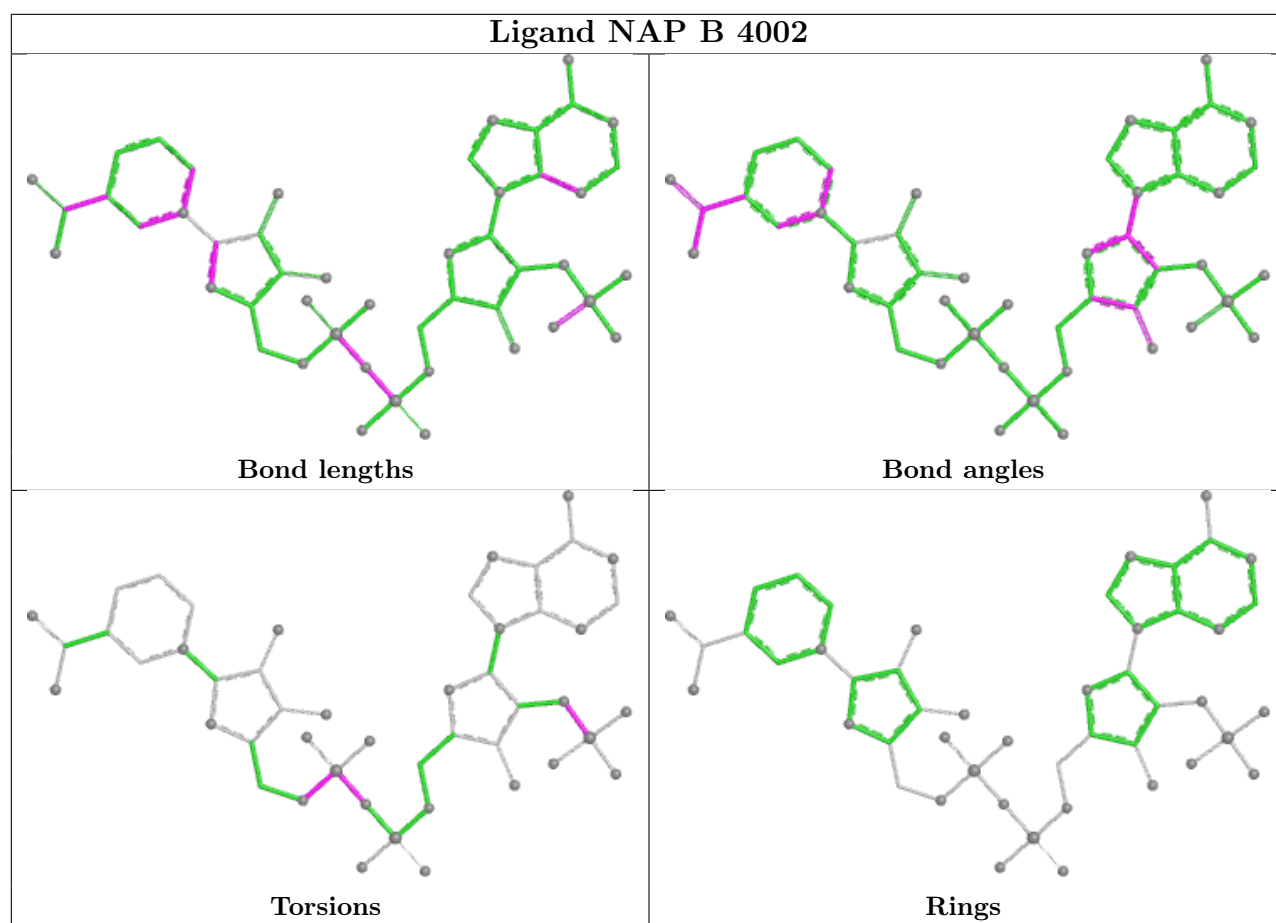


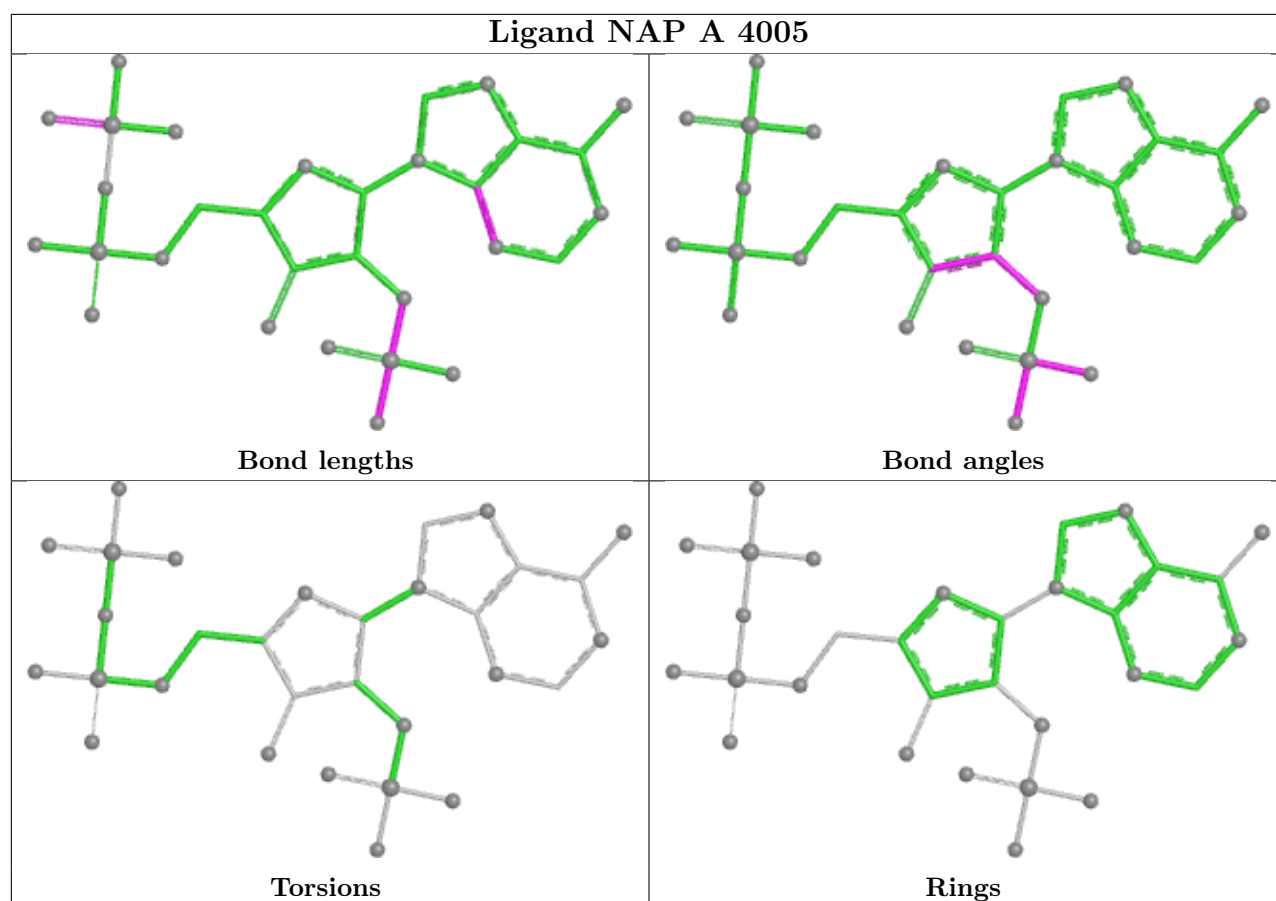
Ligand NAP D 4008











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	308/323 (95%)	0.80	15 (4%) 35 41	8, 22, 45, 59	0
1	B	309/323 (95%)	0.93	32 (10%) 11 13	9, 25, 48, 70	0
1	C	307/323 (95%)	0.94	30 (9%) 13 15	8, 21, 55, 68	0
1	D	298/323 (92%)	0.98	45 (15%) 5 6	7, 22, 57, 71	0
All	All	1222/1292 (94%)	0.91	122 (9%) 12 14	7, 23, 52, 71	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	GLY	6.4
1	D	190	LYS	5.0
1	D	193	PRO	4.6
1	C	190	LYS	4.6
1	D	13	GLY	4.5
1	D	194	ILE	4.4
1	C	233	GLY	4.2
1	D	195	TYR	4.0
1	B	186	ARG	3.8
1	D	129	GLY	3.6
1	B	12	PRO	3.6
1	B	232	THR	3.5
1	D	136	PHE	3.5
1	B	235	ILE	3.4
1	C	232	THR	3.4
1	B	57	ILE	3.3
1	B	194	ILE	3.3
1	D	137	ALA	3.3
1	B	190	LYS	3.3
1	D	191	ALA	3.3
1	D	231	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	136	PHE	3.2
1	B	51	GLN	3.1
1	D	99	GLY	3.1
1	C	186	ARG	3.1
1	C	294	GLY	3.0
1	C	235	ILE	3.0
1	D	221	VAL	3.0
1	D	100	ASP	3.0
1	A	235	ILE	3.0
1	C	193	PRO	2.9
1	D	186	ARG	2.9
1	C	172	ILE	2.9
1	C	238	LEU	2.9
1	B	135	GLU	2.9
1	B	318	GLU	2.9
1	D	189	PHE	2.8
1	D	138	GLY	2.8
1	D	98	ARG	2.8
1	C	230	LEU	2.8
1	B	98	ARG	2.8
1	C	231	LYS	2.8
1	B	134	GLN	2.7
1	A	207	PHE	2.7
1	A	230	LEU	2.7
1	D	222	VAL	2.7
1	C	249	PHE	2.7
1	D	207	PHE	2.7
1	D	230	LEU	2.7
1	D	91	ILE	2.7
1	D	214	LYS	2.7
1	A	287	ASP	2.6
1	B	107	LYS	2.6
1	B	10	VAL	2.6
1	B	108	ARG	2.6
1	B	126	ARG	2.6
1	A	233	GLY	2.6
1	C	222	VAL	2.6
1	D	208	VAL	2.5
1	A	191	ALA	2.5
1	D	225	VAL	2.5
1	D	192	GLN	2.4
1	B	110	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	249	PHE	2.4
1	D	187	ASP	2.4
1	A	186	ARG	2.4
1	A	98	ARG	2.4
1	A	168	GLU	2.4
1	C	197	GLU	2.4
1	D	134	GLN	2.4
1	D	196	VAL	2.4
1	D	155	ARG	2.3
1	A	189	PHE	2.3
1	A	197	GLU	2.3
1	B	111	GLU	2.3
1	D	203	PRO	2.3
1	C	229	ASN	2.3
1	C	138	GLY	2.3
1	C	192	GLN	2.3
1	B	50	GLY	2.2
1	D	318	GLU	2.2
1	C	241	ASN	2.2
1	C	214	LYS	2.2
1	D	130	VAL	2.2
1	C	187	ASP	2.2
1	D	132	GLY	2.2
1	C	195	TYR	2.2
1	D	199	VAL	2.2
1	D	149	ALA	2.2
1	D	51	GLN	2.1
1	A	187	ASP	2.1
1	A	219	ASP	2.1
1	C	34	SER	2.1
1	A	231	LYS	2.1
1	B	193	PRO	2.1
1	C	11	LYS	2.1
1	C	131	PRO	2.1
1	B	197	GLU	2.1
1	B	91	ILE	2.1
1	C	53	THR	2.1
1	B	56	GLY	2.1
1	B	11	LYS	2.1
1	C	54	GLU	2.1
1	B	256	ALA	2.1
1	D	108	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	198	THR	2.1
1	D	197	GLU	2.1
1	D	201	LYS	2.1
1	D	218	GLY	2.1
1	B	146	VAL	2.1
1	C	125	ARG	2.1
1	B	231	LYS	2.0
1	C	317	THR	2.0
1	D	188	THR	2.0
1	D	219	ASP	2.0
1	B	96	GLU	2.0
1	D	249	PHE	2.0
1	A	232	THR	2.0
1	B	296	ARG	2.0
1	C	139	ARG	2.0
1	D	125	ARG	2.0
1	D	146	VAL	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	D	4004	48/48	0.82	0.18	33,54,76,79	0
2	NAP	C	4003	48/48	0.84	0.17	33,42,74,76	0
2	NAP	A	4001	48/48	0.84	0.18	36,48,77,79	0
2	NAP	B	4002	48/48	0.87	0.15	28,39,70,72	0
2	NAP	C	4007	31/48	0.92	0.10	10,14,33,37	0
2	NAP	B	4006	31/48	0.92	0.11	13,25,48,50	0

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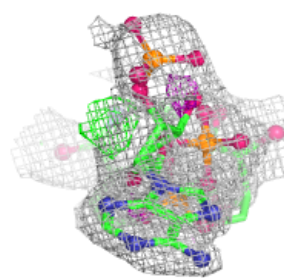
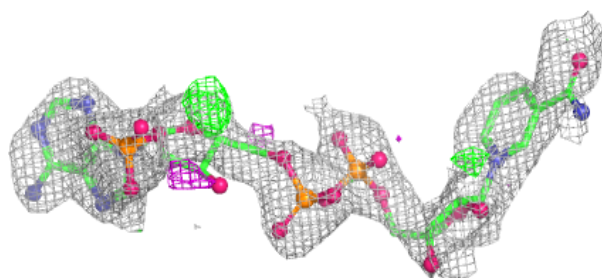
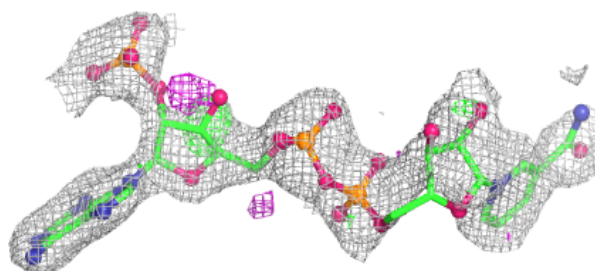
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	D	4008	30/48	0.92	0.11	11,18,53,55	0
2	NAP	A	4005	31/48	0.93	0.09	8,16,43,46	0

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.

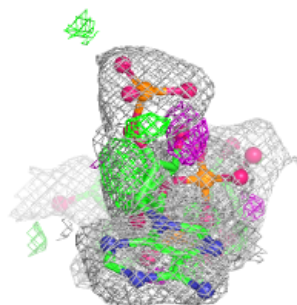
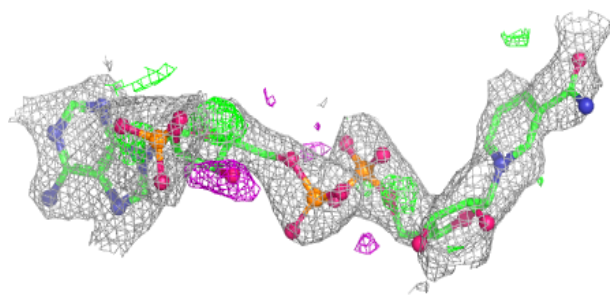
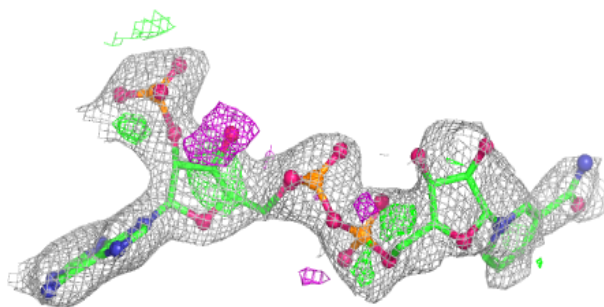
Electron density around NAP D 4004:

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

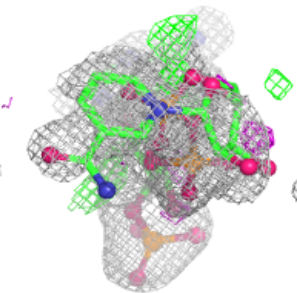
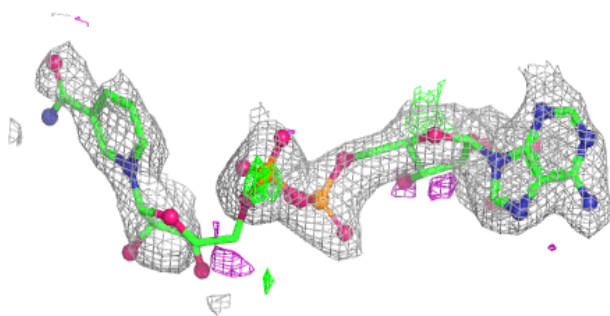
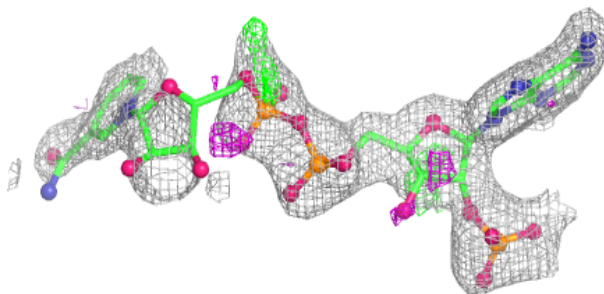


Electron density around NAP C 4003:

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

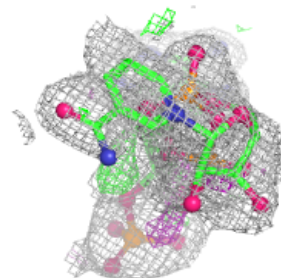
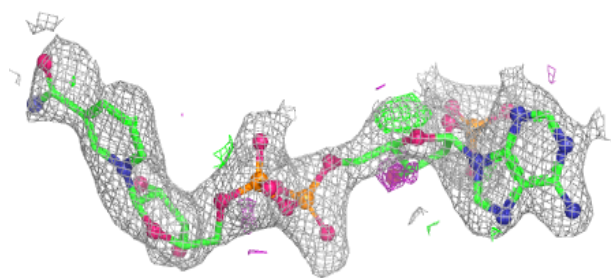
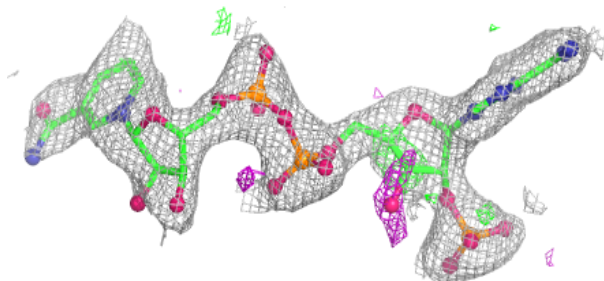
**Electron density around NAP A 4001:**

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

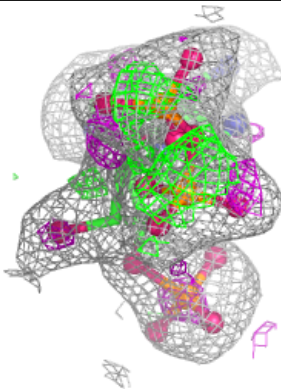
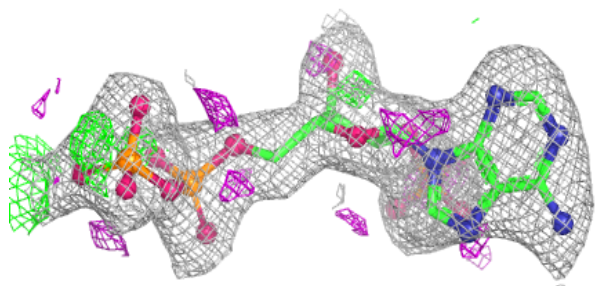
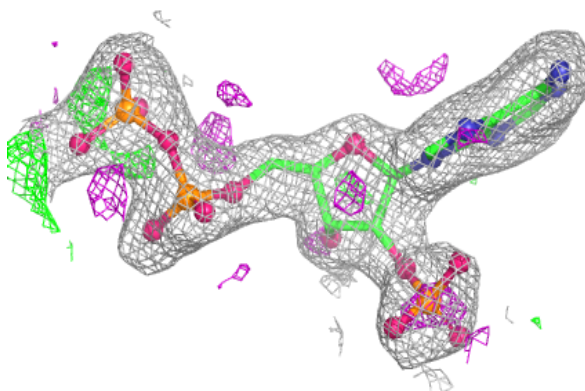


Electron density around NAP B 4002:

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

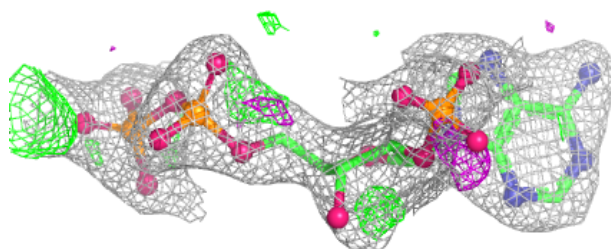
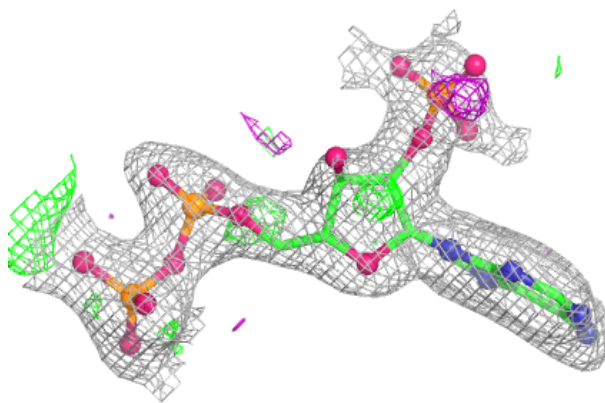
**Electron density around NAP C 4007:**

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

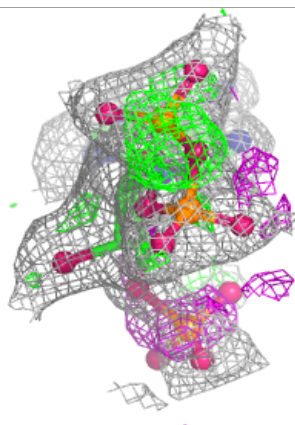
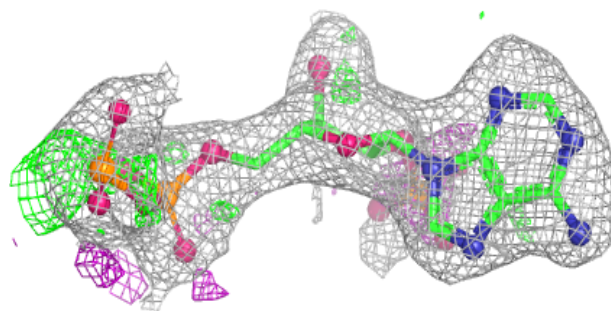
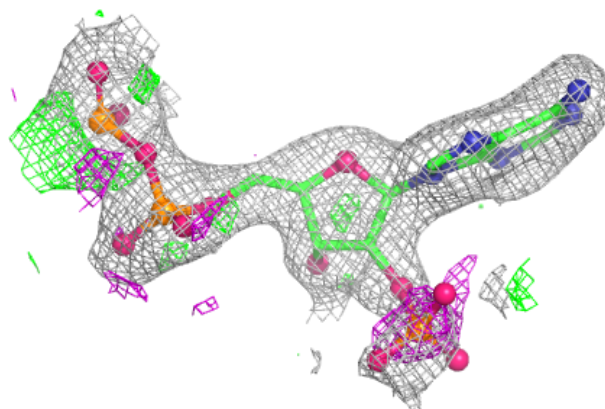


Electron density around NAP B 4006:

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

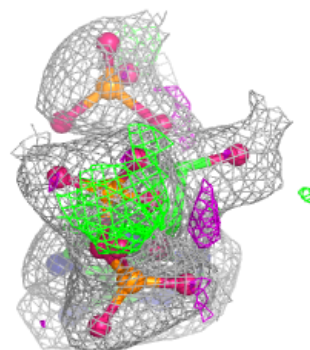
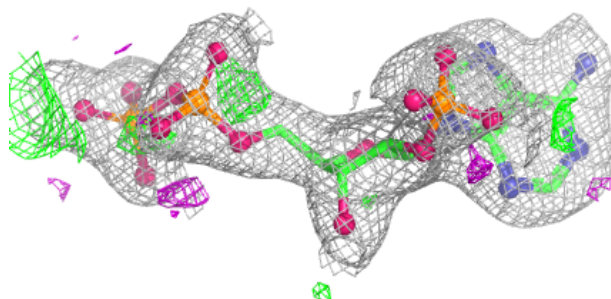
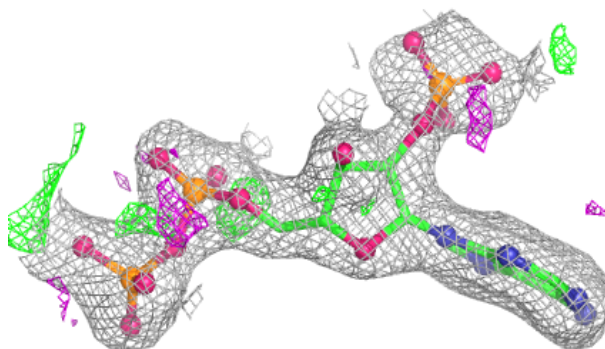
**Electron density around NAP D 4008:**

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



Electron density around NAP A 4005:

$2mF_o-DF_c$ (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.