



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 10:00 AM UTC

PDB ID : 4BMS / pdb_00004bms
Title : Short chain alcohol dehydrogenase from Ralstonia sp. DSM 6428 in complex with NADPH
Authors : Man, H.; Kulig, J.; Rother, D.; Grogan, G.
Deposited on : 2013-05-10
Resolution : 2.89 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

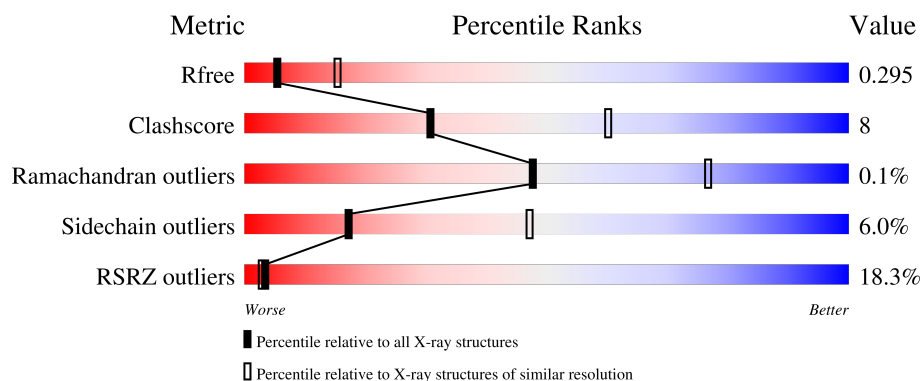
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	249	
1	B	249	
1	C	249	
1	E	249	
1	F	249	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	249	30% 84% 15%

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

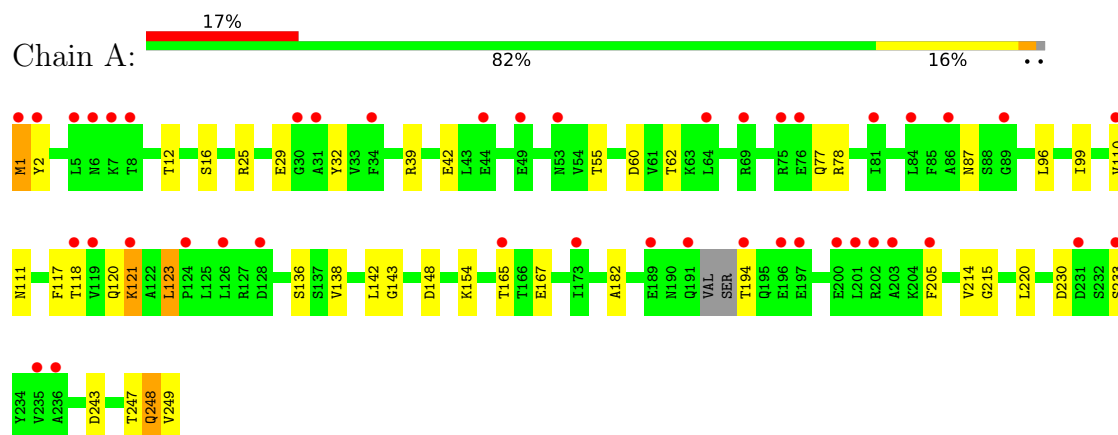
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	9	Total	O	0	0
			9	9		
3	C	9	Total	O	0	0
			9	9		
3	E	8	Total	O	0	0
			8	8		
3	F	1	Total	O	0	0
			1	1		
3	K	6	Total	O	0	0
			6	6		

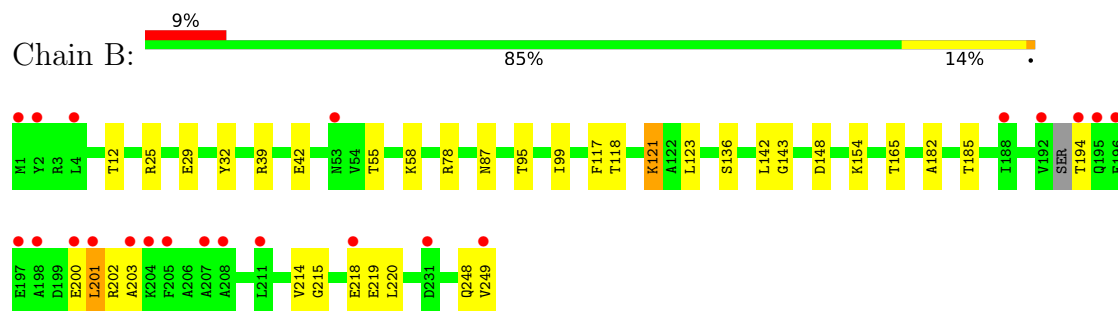
3 Residue-property plots [i](#)

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.

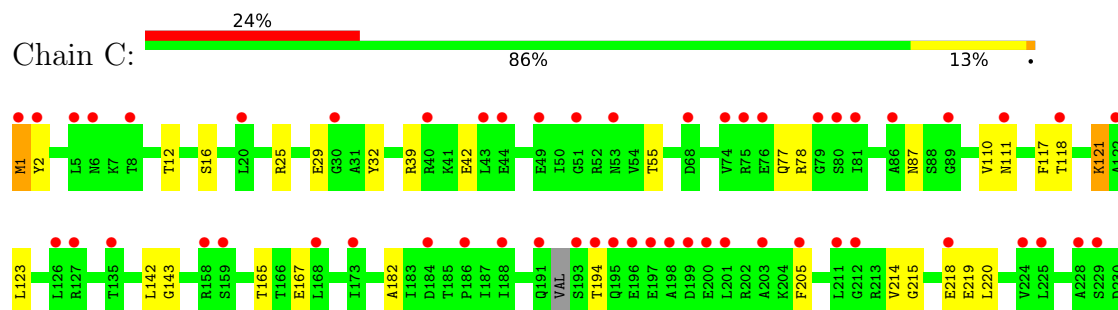
• Molecule 1: ALCLOHOL DEHYDROGENASE/SHORT-CHAIN DEHYDROGENASE



• Molecule 1: ALCLOHOL DEHYDROGENASE/SHORT-CHAIN DEHYDROGENASE

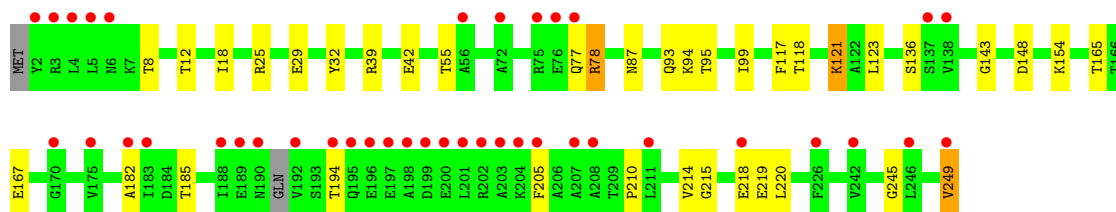
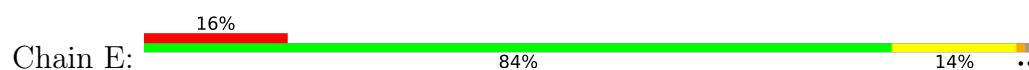


• Molecule 1: ALCLOHOL DEHYDROGENASE/SHORT-CHAIN DEHYDROGENASE

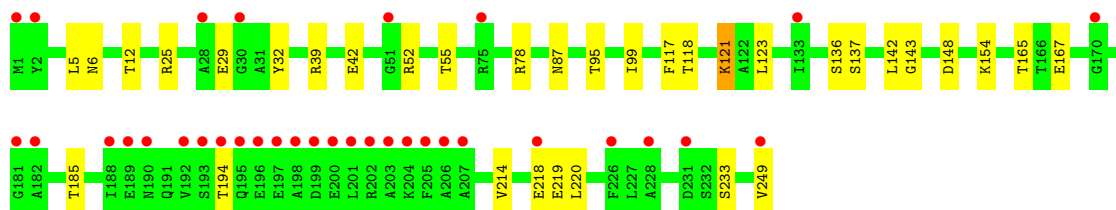
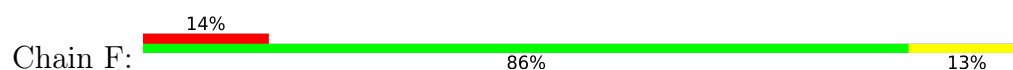




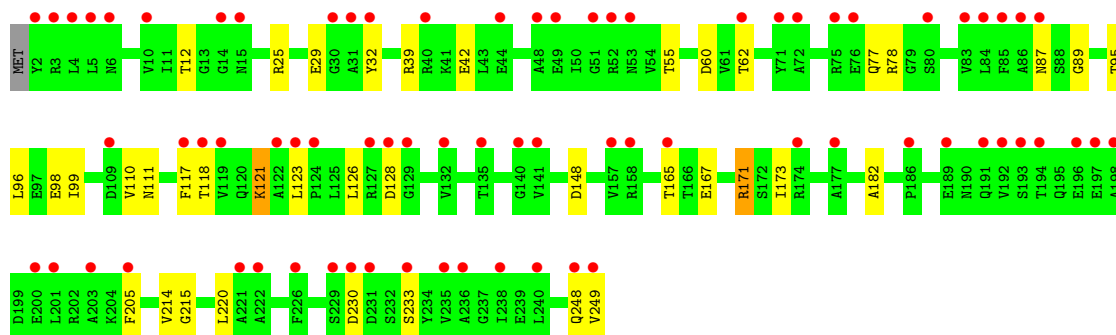
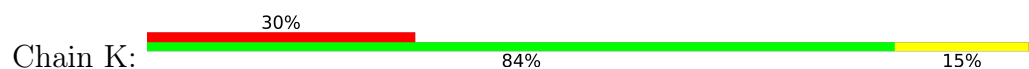
- Molecule 1: ALCLOHOL DEHYDROGENASE/SHORT-CHAIN DEHYDROGENASE



- Molecule 1: ALCLOHOL DEHYDROGENASE/SHORT-CHAIN DEHYDROGENASE



- Molecule 1: ALCLOHOL DEHYDROGENASE/SHORT-CHAIN DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.26Å 135.62Å 93.58Å 90.00° 100.12° 90.00°	Depositor
Resolution (Å)	74.54 – 2.89 74.54 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.1 (74.54-2.89) 99.1 (74.54-2.89)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0029	Depositor
R, R_{free}	0.268 , 0.293 0.272 , 0.295	Depositor DCC
R_{free} test set	2675 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11313	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5942e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.77	0/1843	0.96	3/2502 (0.1%)
1	B	0.71	0/1856	0.91	0/2519
1	C	0.75	0/1870	0.94	0/2535
1	E	0.71	0/1845	0.93	0/2506
1	F	0.71	0/1853	0.92	0/2519
1	K	0.79	0/1852	0.96	0/2515
All	All	0.74	0/11119	0.94	3/15096 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	248	GLN	N-CA-C	6.92	121.56	113.18
1	A	248	GLN	CA-C-N	6.42	133.26	121.70
1	A	248	GLN	C-N-CA	6.42	133.26	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	GLN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1821	0	1824	64	0
1	B	1835	0	1839	42	0
1	C	1848	0	1862	61	0
1	E	1823	0	1823	20	2
1	F	1831	0	1833	40	0
1	K	1829	0	1823	27	1
2	A	48	0	25	2	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	E	48	0	25	2	0
2	F	48	0	25	2	0
2	K	48	0	25	2	0
3	A	5	0	0	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	E	8	0	0	0	0
3	F	1	0	0	0	0
3	K	6	0	0	1	0
All	All	11313	0	11154	186	2

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 8.

All (186) 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:142:LEU:CA	1:C:249:VAL:HG21	1.45	1.44
1:A:249:VAL:CG2	1:C:143:GLY:H	1.32	1.43
1:A:142:LEU:CD2	1:C:249:VAL:HG11	1.54	1.37
1:A:142:LEU:HA	1:C:249:VAL:CG2	1.57	1.32
1:K:128:ASP:OD1	1:K:171:ARG:HD3	1.39	1.19
1:B:142:LEU:HA	1:F:249:VAL:CG2	1.73	1.18
1:A:142:LEU:HD22	1:C:249:VAL:HG11	1.19	1.16
1:B:142:LEU:CA	1:F:249:VAL:HG21	1.79	1.12
1:A:142:LEU:CD2	1:C:249:VAL:CG1	2.29	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HG12	1:F:143:GLY:H	1.09	1.10
1:A:249:VAL:CG2	1:C:143:GLY:N	2.15	1.10
1:A:249:VAL:HG11	1:C:142:LEU:HD22	1.17	1.10
1:A:142:LEU:HD22	1:C:249:VAL:CG1	1.84	1.08
1:A:233:SER:OG	1:B:219:GLU:OE2	1.72	1.06
1:A:249:VAL:HG23	1:C:143:GLY:H	1.17	1.05
1:A:249:VAL:CG1	1:C:142:LEU:HD22	1.86	1.03
1:B:249:VAL:HG11	1:F:142:LEU:HB3	1.41	1.03
1:B:142:LEU:HA	1:F:249:VAL:HG21	1.02	1.00
1:B:142:LEU:HD22	1:F:249:VAL:HG11	1.44	0.99
1:K:126:LEU:O	1:K:171:ARG:NH1	1.95	0.98
1:A:142:LEU:HD23	1:C:249:VAL:HG11	1.46	0.95
1:K:249:VAL:OXT	1:K:249:VAL:HG23	1.68	0.94
1:A:142:LEU:HD23	1:C:249:VAL:CG1	1.97	0.93
1:B:249:VAL:HG21	1:F:142:LEU:HD23	1.50	0.93
1:B:249:VAL:HG21	1:F:142:LEU:CD2	1.99	0.91
1:K:128:ASP:OD1	1:K:171:ARG:CD	2.18	0.90
1:A:249:VAL:HG22	1:C:142:LEU:HA	1.54	0.89
1:A:249:VAL:CG1	1:C:142:LEU:CD2	2.52	0.88
1:A:249:VAL:HG11	1:C:142:LEU:CD2	2.05	0.86
1:B:249:VAL:HG11	1:F:142:LEU:CB	2.06	0.85
1:A:249:VAL:HG21	1:C:142:LEU:HB3	1.60	0.83
1:B:248:GLN:O	1:B:249:VAL:OXT	1.95	0.82
1:A:142:LEU:C	1:C:249:VAL:HG21	2.04	0.82
1:A:249:VAL:HG21	1:C:143:GLY:H	1.41	0.79
1:A:249:VAL:HG23	1:C:143:GLY:N	1.91	0.77
1:B:142:LEU:CD2	1:F:249:VAL:HG11	2.13	0.76
1:B:249:VAL:HG12	1:F:143:GLY:N	1.95	0.75
1:A:249:VAL:HG22	1:C:142:LEU:CA	2.17	0.75
1:A:143:GLY:N	1:C:249:VAL:CG2	2.50	0.75
1:A:249:VAL:HG13	1:C:142:LEU:CD2	2.18	0.74
1:A:249:VAL:HG13	1:C:142:LEU:HD23	1.70	0.74
1:B:200:GLU:O	1:B:202:ARG:N	2.23	0.71
1:B:249:VAL:CG1	1:F:142:LEU:HB3	2.20	0.69
1:K:249:VAL:OXT	1:K:249:VAL:CG2	2.40	0.69
1:C:1:MET:C	1:C:2:TYR:HD1	2.00	0.69
1:A:249:VAL:HG22	1:C:143:GLY:N	2.05	0.68
1:B:249:VAL:CG1	1:F:143:GLY:H	1.97	0.68
1:A:142:LEU:HA	1:C:249:VAL:HG21	0.71	0.67
1:C:233:SER:OG	1:F:219:GLU:OE2	2.11	0.67
1:B:200:GLU:O	1:B:203:ALA:N	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLN:O	1:E:94:LYS:HG2	1.95	0.66
1:A:142:LEU:CA	1:C:249:VAL:CG2	2.41	0.65
1:B:32:TYR:OH	1:B:55:THR:HG23	1.98	0.64
1:A:142:LEU:HD23	1:C:249:VAL:HG13	1.79	0.64
1:C:2:TYR:HB3	1:C:29:GLU:O	1.98	0.64
1:E:32:TYR:OH	1:E:55:THR:CG2	2.46	0.64
1:A:55:THR:HG21	1:A:77:GLN:HE22	1.63	0.63
1:E:32:TYR:OH	1:E:55:THR:HG23	1.98	0.63
1:F:32:TYR:OH	1:F:55:THR:CG2	2.47	0.63
1:F:32:TYR:OH	1:F:55:THR:HG23	1.98	0.62
1:K:32:TYR:OH	1:K:55:THR:HG23	1.98	0.62
1:A:32:TYR:OH	1:A:55:THR:HG23	1.99	0.62
1:C:32:TYR:OH	1:C:55:THR:HG23	1.99	0.62
1:K:32:TYR:OH	1:K:55:THR:CG2	2.48	0.62
1:C:55:THR:HG21	1:C:77:GLN:HE22	1.63	0.62
1:B:32:TYR:OH	1:B:55:THR:CG2	2.47	0.62
1:A:32:TYR:OH	1:A:55:THR:CG2	2.48	0.62
1:C:32:TYR:OH	1:C:55:THR:CG2	2.48	0.62
1:E:55:THR:HG21	1:E:77:GLN:HE22	1.64	0.61
1:A:143:GLY:H	1:C:249:VAL:CG2	2.13	0.61
1:K:55:THR:HG21	1:K:77:GLN:HE22	1.65	0.61
1:A:243:ASP:OD2	1:A:247:THR:HG23	2.00	0.61
1:A:2:TYR:N	1:A:2:TYR:CD1	2.69	0.60
1:A:143:GLY:N	1:C:249:VAL:HG23	2.17	0.59
1:A:143:GLY:N	1:C:249:VAL:HG21	2.14	0.59
1:B:200:GLU:O	1:B:201:LEU:C	2.43	0.58
1:A:142:LEU:C	1:C:249:VAL:CG2	2.75	0.58
1:B:142:LEU:CB	1:F:249:VAL:HG21	2.34	0.57
1:B:249:VAL:HG21	1:F:142:LEU:HD22	1.85	0.57
1:K:248:GLN:O	1:K:249:VAL:HG22	2.06	0.55
1:B:249:VAL:HG11	1:F:142:LEU:CD2	2.36	0.55
1:A:1:MET:C	1:A:2:TYR:CD1	2.85	0.55
1:A:142:LEU:CG	1:C:249:VAL:HG11	2.35	0.53
1:B:249:VAL:HG11	1:F:142:LEU:HD22	1.91	0.53
1:F:185:THR:HG21	2:F:1250:NAP:O2N	2.08	0.53
2:K:1250:NAP:H52A	2:K:1250:NAP:H52N	1.91	0.53
1:A:249:VAL:CG2	1:C:142:LEU:CA	2.85	0.52
1:B:142:LEU:CA	1:F:249:VAL:CG2	2.59	0.52
1:C:219:GLU:OE2	1:F:233:SER:OG	2.21	0.51
1:A:25:ARG:O	1:A:29:GLU:HG2	2.11	0.51
1:A:138:VAL:HG12	1:A:247:THR:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:ARG:O	1:K:29:GLU:HG2	2.11	0.50
1:C:1:MET:O	1:C:1:MET:HG3	2.12	0.50
1:F:25:ARG:O	1:F:29:GLU:HG2	2.12	0.50
1:A:16:SER:OG	2:A:1250:NAP:O1A	2.26	0.50
1:A:148:ASP:OD1	1:F:167:GLU:OE2	2.30	0.50
1:C:248:GLN:O	1:C:249:VAL:HG22	2.12	0.49
1:E:25:ARG:O	1:E:29:GLU:HG2	2.11	0.49
1:A:1:MET:C	1:A:2:TYR:HD1	2.19	0.49
1:B:25:ARG:O	1:B:29:GLU:HG2	2.12	0.49
1:C:39:ARG:CB	1:C:42:GLU:HG2	2.43	0.49
1:B:249:VAL:HB	1:F:142:LEU:HA	1.94	0.49
1:C:25:ARG:O	1:C:29:GLU:HG2	2.13	0.49
1:A:249:VAL:CG2	1:C:142:LEU:HB3	2.36	0.48
1:F:87:ASN:CG	1:F:87:ASN:O	2.56	0.48
1:A:55:THR:HG21	1:A:77:GLN:NE2	2.29	0.48
1:C:2:TYR:CD1	1:C:2:TYR:N	2.81	0.48
1:C:87:ASN:CG	1:C:87:ASN:O	2.56	0.48
1:E:55:THR:HG21	1:E:77:GLN:NE2	2.29	0.48
1:B:185:THR:HG21	2:B:1250:NAP:O2N	2.14	0.48
1:K:87:ASN:CG	1:K:87:ASN:O	2.55	0.48
1:B:143:GLY:N	1:F:249:VAL:HG23	2.29	0.47
1:K:89:GLY:HA3	2:K:1250:NAP:O3D	2.13	0.47
1:C:39:ARG:CZ	1:C:42:GLU:HG3	2.44	0.47
1:E:18:ILE:HG12	2:E:1250:NAP:O2N	2.14	0.47
1:K:39:ARG:CB	1:K:42:GLU:HG2	2.45	0.47
1:B:58:LYS:HD2	1:K:98:GLU:OE2	2.14	0.47
1:C:55:THR:HG21	1:C:77:GLN:NE2	2.28	0.47
1:K:39:ARG:CZ	1:K:42:GLU:HG3	2.45	0.47
1:K:230:ASP:OD1	3:K:2005:HOH:O	2.21	0.46
1:A:142:LEU:CB	1:C:249:VAL:HG11	2.44	0.46
1:E:39:ARG:CB	1:E:42:GLU:HG2	2.45	0.46
1:A:39:ARG:CB	1:A:42:GLU:HG2	2.45	0.46
1:C:182:ALA:O	1:C:215:GLY:N	2.46	0.46
1:A:87:ASN:O	1:A:87:ASN:CG	2.58	0.46
1:B:87:ASN:O	1:B:87:ASN:CG	2.58	0.46
1:B:148:ASP:OD1	1:C:167:GLU:OE2	2.34	0.46
1:K:55:THR:HG21	1:K:77:GLN:NE2	2.30	0.46
1:F:39:ARG:CZ	1:F:42:GLU:HG3	2.46	0.46
1:C:248:GLN:O	1:C:249:VAL:CG2	2.64	0.46
1:A:182:ALA:O	1:A:215:GLY:N	2.47	0.45
1:B:39:ARG:CB	1:B:42:GLU:HG2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:H	1:F:249:VAL:CG2	2.29	0.45
1:A:39:ARG:CZ	1:A:42:GLU:HG3	2.46	0.45
1:E:39:ARG:CZ	1:E:42:GLU:HG3	2.47	0.45
1:F:39:ARG:CB	1:F:42:GLU:HG2	2.46	0.45
1:C:16:SER:OG	2:C:1250:NAP:O1A	2.29	0.45
1:K:110:VAL:HG13	1:K:111:ASN:N	2.32	0.45
1:A:230:ASP:O	1:A:233:SER:HB3	2.16	0.44
1:A:249:VAL:HG23	1:C:143:GLY:CA	2.47	0.44
1:B:39:ARG:CZ	1:B:42:GLU:HG3	2.46	0.44
1:K:171:ARG:HD2	1:K:173:ILE:CD1	2.47	0.44
1:C:39:ARG:HB2	1:C:42:GLU:HG2	1.99	0.44
1:A:110:VAL:HG13	1:A:111:ASN:N	2.33	0.44
1:B:117:PHE:O	1:B:121:LYS:HG3	2.18	0.44
1:B:136:SER:HA	1:B:154:LYS:HD2	2.00	0.44
1:B:143:GLY:N	1:F:249:VAL:CG2	2.81	0.43
1:E:87:ASN:O	1:E:87:ASN:CG	2.61	0.43
1:E:117:PHE:O	1:E:121:LYS:HG3	2.18	0.43
1:K:39:ARG:HB2	1:K:42:GLU:HG2	2.01	0.43
1:E:148:ASP:OD1	1:K:167:GLU:OE2	2.36	0.43
1:A:167:GLU:OE2	1:F:148:ASP:OD1	2.35	0.43
1:E:185:THR:HG21	2:E:1250:NAP:O2N	2.17	0.43
1:C:117:PHE:O	1:C:121:LYS:HG3	2.18	0.43
1:F:117:PHE:O	1:F:121:LYS:HG3	2.19	0.43
1:C:1:MET:C	1:C:2:TYR:CD1	2.90	0.43
1:E:167:GLU:OE2	1:K:148:ASP:OD1	2.37	0.43
1:C:110:VAL:HG13	1:C:111:ASN:N	2.34	0.42
1:A:117:PHE:O	1:A:121:LYS:HG3	2.19	0.42
1:K:117:PHE:O	1:K:121:LYS:HG3	2.19	0.42
1:F:136:SER:HA	1:F:154:LYS:HD2	2.01	0.42
2:A:1250:NAP:H52A	2:A:1250:NAP:H52N	2.02	0.42
1:E:95:THR:O	1:E:99:ILE:HG13	2.20	0.42
1:E:136:SER:HA	1:E:154:LYS:HD2	2.02	0.42
1:K:60:ASP:OD1	1:K:62:THR:OG1	2.35	0.42
1:E:39:ARG:HB2	1:E:42:GLU:HG2	2.02	0.42
1:E:182:ALA:O	1:E:215:GLY:N	2.48	0.41
1:F:95:THR:O	1:F:99:ILE:HG13	2.20	0.41
1:A:39:ARG:HB2	1:A:42:GLU:HG2	2.01	0.41
1:F:39:ARG:HB2	1:F:42:GLU:HG2	2.02	0.41
1:A:136:SER:HA	1:A:154:LYS:HD2	2.02	0.41
1:B:95:THR:O	1:B:99:ILE:HG13	2.21	0.41
1:E:210:PRO:HG2	1:E:245:GLY:HA3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:OD1	1:A:62:THR:OG1	2.36	0.41
1:F:137:SER:OG	2:F:1250:NAP:H5N	2.21	0.41
1:K:182:ALA:O	1:K:215:GLY:N	2.48	0.41
1:B:182:ALA:O	1:B:215:GLY:N	2.45	0.41
1:B:249:VAL:CG1	1:F:142:LEU:CB	2.90	0.41
1:A:249:VAL:HG22	1:C:142:LEU:C	2.46	0.40
1:K:95:THR:O	1:K:99:ILE:HG13	2.20	0.40
1:A:96:LEU:HA	1:A:99:ILE:HD12	2.04	0.40
1:B:39:ARG:HB2	1:B:42:GLU:HG2	2.03	0.40
1:A:120:GLN:O	1:A:123:LEU:HB2	2.21	0.40
1:E:8:THR:OG1	1:E:78:ARG:NH1	2.54	0.40
1:K:96:LEU:HA	1:K:99:ILE:HD12	2.03	0.40
1:F:5:LEU:O	1:F:6:ASN:HB2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:GLY:N	1:E:249:VAL:CG1[2_555]	2.05	0.15
1:E:219:GLU:OE2	1:K:233:SER:OG[2_555]	2.08	0.12

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	243/249 (98%)	228 (94%)	15 (6%)	0	100	100
1	B	244/249 (98%)	227 (93%)	16 (7%)	1 (0%)	30	59
1	C	244/249 (98%)	230 (94%)	14 (6%)	0	100	100
1	E	243/249 (98%)	229 (94%)	14 (6%)	0	100	100
1	F	247/249 (99%)	233 (94%)	14 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	246/249 (99%)	232 (94%)	14 (6%)	0	100	100
All	All	1467/1494 (98%)	1379 (94%)	87 (6%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	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	181/195 (93%)	170 (94%)	11 (6%)	17	46
1	B	183/195 (94%)	173 (94%)	10 (6%)	19	50
1	C	186/195 (95%)	174 (94%)	12 (6%)	15	44
1	E	182/195 (93%)	170 (93%)	12 (7%)	15	43
1	F	182/195 (93%)	171 (94%)	11 (6%)	17	47
1	K	180/195 (92%)	170 (94%)	10 (6%)	19	50
All	All	1094/1170 (94%)	1028 (94%)	66 (6%)	17	47

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	12	THR
1	A	78	ARG
1	A	118	THR
1	A	121	LYS
1	A	123	LEU
1	A	165	THR
1	A	194	THR
1	A	205	PHE
1	A	214	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	220	LEU
1	B	12	THR
1	B	78	ARG
1	B	118	THR
1	B	121	LYS
1	B	123	LEU
1	B	165	THR
1	B	194	THR
1	B	214	VAL
1	B	218	GLU
1	B	220	LEU
1	C	1	MET
1	C	12	THR
1	C	78	ARG
1	C	118	THR
1	C	121	LYS
1	C	123	LEU
1	C	165	THR
1	C	194	THR
1	C	205	PHE
1	C	214	VAL
1	C	218	GLU
1	C	220	LEU
1	E	12	THR
1	E	78	ARG
1	E	118	THR
1	E	121	LYS
1	E	123	LEU
1	E	165	THR
1	E	194	THR
1	E	205	PHE
1	E	214	VAL
1	E	218	GLU
1	E	220	LEU
1	E	249	VAL
1	F	12	THR
1	F	52	ARG
1	F	78	ARG
1	F	118	THR
1	F	121	LYS
1	F	123	LEU
1	F	165	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	194	THR
1	F	214	VAL
1	F	218	GLU
1	F	220	LEU
1	K	12	THR
1	K	78	ARG
1	K	118	THR
1	K	121	LYS
1	K	123	LEU
1	K	165	THR
1	K	171	ARG
1	K	205	PHE
1	K	214	VAL
1	K	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	145	GLN
1	A	191	GLN
1	A	248	GLN
1	B	191	GLN
1	C	77	GLN
1	C	191	GLN
1	E	77	GLN
1	F	191	GLN
1	K	77	GLN
1	K	191	GLN
1	K	248	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	E	1250	-	50,52,52	1.22	6 (12%)	71,80,80	1.77	19 (26%)
2	NAP	F	1250	-	50,52,52	1.25	6 (12%)	71,80,80	1.77	14 (19%)
2	NAP	K	1250	-	50,52,52	1.36	7 (14%)	71,80,80	1.82	15 (21%)
2	NAP	C	1250	-	50,52,52	1.59	10 (20%)	71,80,80	1.83	20 (28%)
2	NAP	A	1250	-	50,52,52	1.36	7 (14%)	71,80,80	1.79	17 (23%)
2	NAP	B	1250	-	50,52,52	1.25	6 (12%)	71,80,80	1.73	17 (23%)

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	E	1250	-	-	10/35/67/67	0/5/5/5
2	NAP	F	1250	-	-	9/35/67/67	0/5/5/5
2	NAP	K	1250	-	-	15/35/67/67	0/5/5/5
2	NAP	C	1250	-	-	12/35/67/67	0/5/5/5
2	NAP	A	1250	-	-	10/35/67/67	0/5/5/5
2	NAP	B	1250	-	-	11/35/67/67	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1250	NAP	C5A-C4A	5.07	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	NAP	C5A-C4A	4.67	1.47	1.39
2	F	1250	NAP	C5A-C4A	4.56	1.47	1.39
2	K	1250	NAP	PA-O3	4.28	1.64	1.59
2	B	1250	NAP	C5A-C4A	4.10	1.46	1.39
2	K	1250	NAP	C5A-C4A	3.93	1.46	1.39
2	E	1250	NAP	C5A-C4A	3.87	1.46	1.39
2	C	1250	NAP	PA-O3	3.48	1.63	1.59
2	C	1250	NAP	PN-O3	3.29	1.63	1.59
2	C	1250	NAP	O4D-C1D	3.28	1.45	1.40
2	C	1250	NAP	C8A-N7A	3.21	1.37	1.31
2	C	1250	NAP	C3N-C7N	3.00	1.55	1.50
2	E	1250	NAP	C5A-N7A	-2.98	1.33	1.39
2	K	1250	NAP	C5A-N7A	-2.93	1.33	1.39
2	B	1250	NAP	C5A-N7A	-2.93	1.33	1.39
2	A	1250	NAP	C8A-N7A	2.90	1.37	1.31
2	K	1250	NAP	O4D-C1D	2.88	1.44	1.40
2	A	1250	NAP	O4D-C1D	2.86	1.44	1.40
2	F	1250	NAP	PA-O3	2.76	1.62	1.59
2	A	1250	NAP	PA-O3	2.73	1.62	1.59
2	E	1250	NAP	C8A-N7A	2.69	1.36	1.31
2	A	1250	NAP	C4A-N9A	-2.69	1.32	1.37
2	K	1250	NAP	C8A-N7A	2.67	1.36	1.31
2	B	1250	NAP	C4A-N9A	-2.67	1.32	1.37
2	B	1250	NAP	O4D-C1D	2.63	1.44	1.40
2	F	1250	NAP	C5A-C6A	2.63	1.48	1.41
2	B	1250	NAP	C8A-N7A	2.62	1.36	1.31
2	F	1250	NAP	C8A-N7A	2.59	1.36	1.31
2	F	1250	NAP	C5A-N7A	-2.58	1.34	1.39
2	C	1250	NAP	C5A-N7A	-2.46	1.34	1.39
2	A	1250	NAP	P2B-O2B	2.43	1.63	1.59
2	E	1250	NAP	O4D-C1D	2.40	1.44	1.40
2	K	1250	NAP	C5A-C6A	2.36	1.47	1.41
2	A	1250	NAP	C5A-N7A	-2.32	1.34	1.39
2	E	1250	NAP	PA-O3	2.22	1.61	1.59
2	C	1250	NAP	C2N-N1N	2.20	1.37	1.35
2	K	1250	NAP	PN-O3	2.14	1.61	1.59
2	C	1250	NAP	P2B-O2B	2.13	1.63	1.59
2	C	1250	NAP	C5A-C6A	2.10	1.46	1.41
2	E	1250	NAP	C4A-N9A	-2.09	1.33	1.37
2	F	1250	NAP	C4A-N9A	-2.08	1.33	1.37
2	B	1250	NAP	P2B-O2B	2.04	1.63	1.59

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1250	NAP	C5A-C4A-N3A	-6.43	117.86	126.72
2	F	1250	NAP	C5A-C4A-N3A	-5.33	119.38	126.72
2	E	1250	NAP	C5A-C4A-N3A	-4.80	120.11	126.72
2	C	1250	NAP	C5A-C4A-N3A	-4.79	120.12	126.72
2	E	1250	NAP	N3A-C2A-N1A	-4.79	121.34	128.58
2	B	1250	NAP	C5A-C4A-N3A	-4.48	120.54	126.72
2	B	1250	NAP	N3A-C2A-N1A	-4.45	121.85	128.58
2	A	1250	NAP	N3A-C2A-N1A	-4.44	121.86	128.58
2	F	1250	NAP	N3A-C2A-N1A	-4.38	121.95	128.58
2	K	1250	NAP	N3A-C4A-N9A	4.35	134.57	127.17
2	F	1250	NAP	N3A-C4A-N9A	4.34	134.54	127.17
2	E	1250	NAP	N3A-C4A-N9A	4.17	134.26	127.17
2	A	1250	NAP	C4A-N9A-C8A	4.05	109.99	105.74
2	K	1250	NAP	C4A-C5A-N7A	-3.99	106.02	110.58
2	F	1250	NAP	C2A-N3A-C4A	3.93	121.44	111.83
2	B	1250	NAP	C4D-O4D-C1D	-3.93	106.33	109.92
2	C	1250	NAP	N3A-C2A-N1A	-3.83	122.78	128.58
2	E	1250	NAP	C2A-N3A-C4A	3.81	121.13	111.83
2	K	1250	NAP	C2A-N3A-C4A	3.77	121.04	111.83
2	C	1250	NAP	N3A-C4A-N9A	3.76	133.56	127.17
2	B	1250	NAP	N3A-C4A-N9A	3.73	133.52	127.17
2	B	1250	NAP	O5D-C5D-C4D	3.68	121.51	108.99
2	F	1250	NAP	C4D-O4D-C1D	-3.66	106.57	109.92
2	B	1250	NAP	C2A-N3A-C4A	3.61	120.64	111.83
2	C	1250	NAP	C6N-N1N-C1D	-3.60	112.66	119.73
2	A	1250	NAP	O5D-C5D-C4D	3.55	121.06	108.99
2	A	1250	NAP	C3B-C2B-C1B	-3.38	96.34	102.81
2	F	1250	NAP	C3N-C7N-N7N	3.32	121.83	117.74
2	F	1250	NAP	C4A-C5A-N7A	-3.31	106.79	110.58
2	A	1250	NAP	C5A-C4A-N3A	-3.30	122.17	126.72
2	E	1250	NAP	O2A-PA-O3	3.29	116.17	107.27
2	C	1250	NAP	C2A-N3A-C4A	3.28	119.85	111.83
2	B	1250	NAP	C3N-C7N-N7N	3.28	121.78	117.74
2	E	1250	NAP	C4A-N9A-C8A	3.28	109.18	105.74
2	C	1250	NAP	O4B-C1B-N9A	3.28	114.38	108.09
2	F	1250	NAP	C4A-N9A-C8A	3.17	109.06	105.74
2	C	1250	NAP	O5D-C5D-C4D	3.16	119.77	108.99
2	A	1250	NAP	C2A-N1A-C6A	3.16	123.92	118.73
2	A	1250	NAP	N3A-C4A-N9A	3.14	132.50	127.17
2	K	1250	NAP	O3B-C3B-C2B	3.13	119.96	111.19
2	E	1250	NAP	C3N-C7N-N7N	3.13	121.60	117.74
2	B	1250	NAP	O4D-C4D-C5D	3.11	119.28	109.33
2	A	1250	NAP	C4A-N9A-C1B	-3.08	119.44	126.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	NAP	C2A-N3A-C4A	3.02	119.21	111.83
2	K	1250	NAP	O5D-C5D-C4D	2.98	119.12	108.99
2	K	1250	NAP	C5A-N7A-C8A	2.97	108.12	103.45
2	K	1250	NAP	N3A-C2A-N1A	-2.95	124.12	128.58
2	F	1250	NAP	O2A-PA-O3	2.94	115.23	107.27
2	B	1250	NAP	O2A-PA-O3	2.91	115.14	107.27
2	C	1250	NAP	C4D-O4D-C1D	-2.87	107.29	109.92
2	K	1250	NAP	C6N-N1N-C2N	-2.85	119.45	121.88
2	K	1250	NAP	C2B-C1B-N9A	2.83	118.42	113.75
2	B	1250	NAP	C4A-N9A-C8A	2.79	108.67	105.74
2	C	1250	NAP	C4A-C5A-N7A	-2.79	107.39	110.58
2	C	1250	NAP	C2N-N1N-C1D	2.74	125.19	119.13
2	K	1250	NAP	O2A-PA-O3	2.74	114.67	107.27
2	C	1250	NAP	O7N-C7N-N7N	-2.67	118.75	122.62
2	A	1250	NAP	N9A-C8A-N7A	-2.65	110.17	113.94
2	K	1250	NAP	O3X-P2B-O2X	2.65	117.75	107.80
2	C	1250	NAP	O2A-PA-O3	2.65	114.43	107.27
2	C	1250	NAP	C2N-C3N-C7N	2.64	127.08	119.46
2	E	1250	NAP	C2A-N1A-C6A	2.59	122.99	118.73
2	A	1250	NAP	O3X-P2B-O2X	2.59	117.50	107.80
2	C	1250	NAP	C2A-N1A-C6A	2.57	122.96	118.73
2	E	1250	NAP	O4D-C4D-C5D	2.57	117.57	109.33
2	C	1250	NAP	C4A-N9A-C8A	2.57	108.43	105.74
2	F	1250	NAP	C5A-N7A-C8A	2.56	107.47	103.45
2	F	1250	NAP	C6A-C5A-N7A	2.48	136.87	132.09
2	K	1250	NAP	C5N-C4N-C3N	-2.44	117.97	120.36
2	E	1250	NAP	O5D-C5D-C4D	2.42	117.23	108.99
2	E	1250	NAP	C4A-C5A-N7A	-2.41	107.82	110.58
2	E	1250	NAP	N9A-C8A-N7A	-2.41	110.52	113.94
2	A	1250	NAP	O7N-C7N-N7N	-2.41	119.14	122.62
2	A	1250	NAP	C6A-C5A-N7A	2.39	136.69	132.09
2	C	1250	NAP	O4B-C4B-C3B	2.37	109.86	105.15
2	F	1250	NAP	C2A-N1A-C6A	2.37	122.62	118.73
2	A	1250	NAP	O4D-C4D-C5D	2.36	116.91	109.33
2	F	1250	NAP	N9A-C8A-N7A	-2.34	110.61	113.94
2	K	1250	NAP	C2N-C3N-C4N	2.33	120.97	118.26
2	C	1250	NAP	O4D-C4D-C5D	2.30	116.69	109.33
2	A	1250	NAP	O2A-PA-O3	2.28	113.44	107.27
2	B	1250	NAP	O3-PA-O1A	-2.28	103.85	110.70
2	B	1250	NAP	O7N-C7N-N7N	-2.25	119.36	122.62
2	K	1250	NAP	N9A-C8A-N7A	-2.24	110.76	113.94
2	E	1250	NAP	C4D-O4D-C1D	-2.24	107.88	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
2	E	1250	NAP	C6N-N1N-C2N	-2.23	119.98	121.88
2	B	1250	NAP	C2A-N1A-C6A	2.23	122.39	118.73
2	F	1250	NAP	O5D-C5D-C4D	2.19	116.46	108.99
2	E	1250	NAP	C6A-C5A-N7A	2.19	136.31	132.09
2	E	1250	NAP	O3-PA-O1A	-2.17	104.18	110.70
2	E	1250	NAP	C5A-N7A-C8A	2.16	106.84	103.45
2	C	1250	NAP	C5A-N7A-C8A	2.14	106.82	103.45
2	B	1250	NAP	C6A-C5A-N7A	2.11	136.16	132.09
2	E	1250	NAP	C5D-C4D-C3D	-2.09	107.68	115.21
2	B	1250	NAP	C4A-C5A-N7A	-2.05	108.24	110.58
2	E	1250	NAP	O7N-C7N-C3N	-2.05	117.09	119.60
2	C	1250	NAP	N9A-C8A-N7A	-2.04	111.04	113.94
2	C	1250	NAP	C5B-C4B-C3B	-2.04	107.86	115.21
2	B	1250	NAP	C4A-N9A-C1B	-2.04	121.86	126.63
2	A	1250	NAP	C3N-C7N-N7N	2.02	120.23	117.74
2	B	1250	NAP	N9A-C8A-N7A	-2.01	111.09	113.94

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1250	NAP	C5B-O5B-PA-O1A
2	A	1250	NAP	C5B-O5B-PA-O2A
2	A	1250	NAP	C5B-O5B-PA-O3
2	A	1250	NAP	C5D-O5D-PN-O3
2	A	1250	NAP	C5D-O5D-PN-O1N
2	A	1250	NAP	O4D-C4D-C5D-O5D
2	B	1250	NAP	C5B-O5B-PA-O3
2	B	1250	NAP	PN-O3-PA-O5B
2	B	1250	NAP	C5D-O5D-PN-O3
2	B	1250	NAP	C5D-O5D-PN-O1N
2	B	1250	NAP	O4D-C4D-C5D-O5D
2	C	1250	NAP	C5B-O5B-PA-O1A
2	C	1250	NAP	C5B-O5B-PA-O2A
2	C	1250	NAP	C5B-O5B-PA-O3
2	C	1250	NAP	PN-O3-PA-O5B
2	C	1250	NAP	C5D-O5D-PN-O3
2	C	1250	NAP	C5D-O5D-PN-O1N
2	C	1250	NAP	O4D-C4D-C5D-O5D
2	C	1250	NAP	C3D-C4D-C5D-O5D
2	E	1250	NAP	C5B-O5B-PA-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	1250	NAP	C5D-O5D-PN-O3
2	E	1250	NAP	C5D-O5D-PN-O1N
2	F	1250	NAP	C5B-O5B-PA-O3
2	F	1250	NAP	C5D-O5D-PN-O1N
2	K	1250	NAP	C5B-O5B-PA-O1A
2	K	1250	NAP	C5B-O5B-PA-O2A
2	K	1250	NAP	C5B-O5B-PA-O3
2	K	1250	NAP	C5D-O5D-PN-O1N
2	K	1250	NAP	O4D-C4D-C5D-O5D
2	K	1250	NAP	C3D-C4D-C5D-O5D
2	A	1250	NAP	C3D-C4D-C5D-O5D
2	B	1250	NAP	C3D-C4D-C5D-O5D
2	F	1250	NAP	C3D-C4D-C5D-O5D
2	F	1250	NAP	O4D-C4D-C5D-O5D
2	C	1250	NAP	C4D-C5D-O5D-PN
2	E	1250	NAP	C3D-C4D-C5D-O5D
2	E	1250	NAP	O4D-C4D-C5D-O5D
2	A	1250	NAP	C4D-C5D-O5D-PN
2	B	1250	NAP	C4D-C5D-O5D-PN
2	K	1250	NAP	C4D-C5D-O5D-PN
2	E	1250	NAP	PN-O3-PA-O5B
2	E	1250	NAP	C4D-C5D-O5D-PN
2	B	1250	NAP	C2B-O2B-P2B-O1X
2	A	1250	NAP	C5D-O5D-PN-O2N
2	B	1250	NAP	C5B-O5B-PA-O1A
2	B	1250	NAP	C5D-O5D-PN-O2N
2	C	1250	NAP	C5D-O5D-PN-O2N
2	E	1250	NAP	C5B-O5B-PA-O1A
2	E	1250	NAP	C5D-O5D-PN-O2N
2	F	1250	NAP	C5B-O5B-PA-O1A
2	F	1250	NAP	C5D-O5D-PN-O3
2	F	1250	NAP	C5D-O5D-PN-O2N
2	K	1250	NAP	C5D-O5D-PN-O3
2	K	1250	NAP	C5D-O5D-PN-O2N
2	F	1250	NAP	C4D-C5D-O5D-PN
2	K	1250	NAP	O4D-C1D-N1N-C6N
2	C	1250	NAP	C2B-O2B-P2B-O1X
2	K	1250	NAP	PN-O3-PA-O1A
2	K	1250	NAP	PA-O3-PN-O1N
2	B	1250	NAP	O4B-C4B-C5B-O5B
2	K	1250	NAP	PN-O3-PA-O2A
2	K	1250	NAP	PA-O3-PN-O2N

Continued on next page...

Continued from previous page...

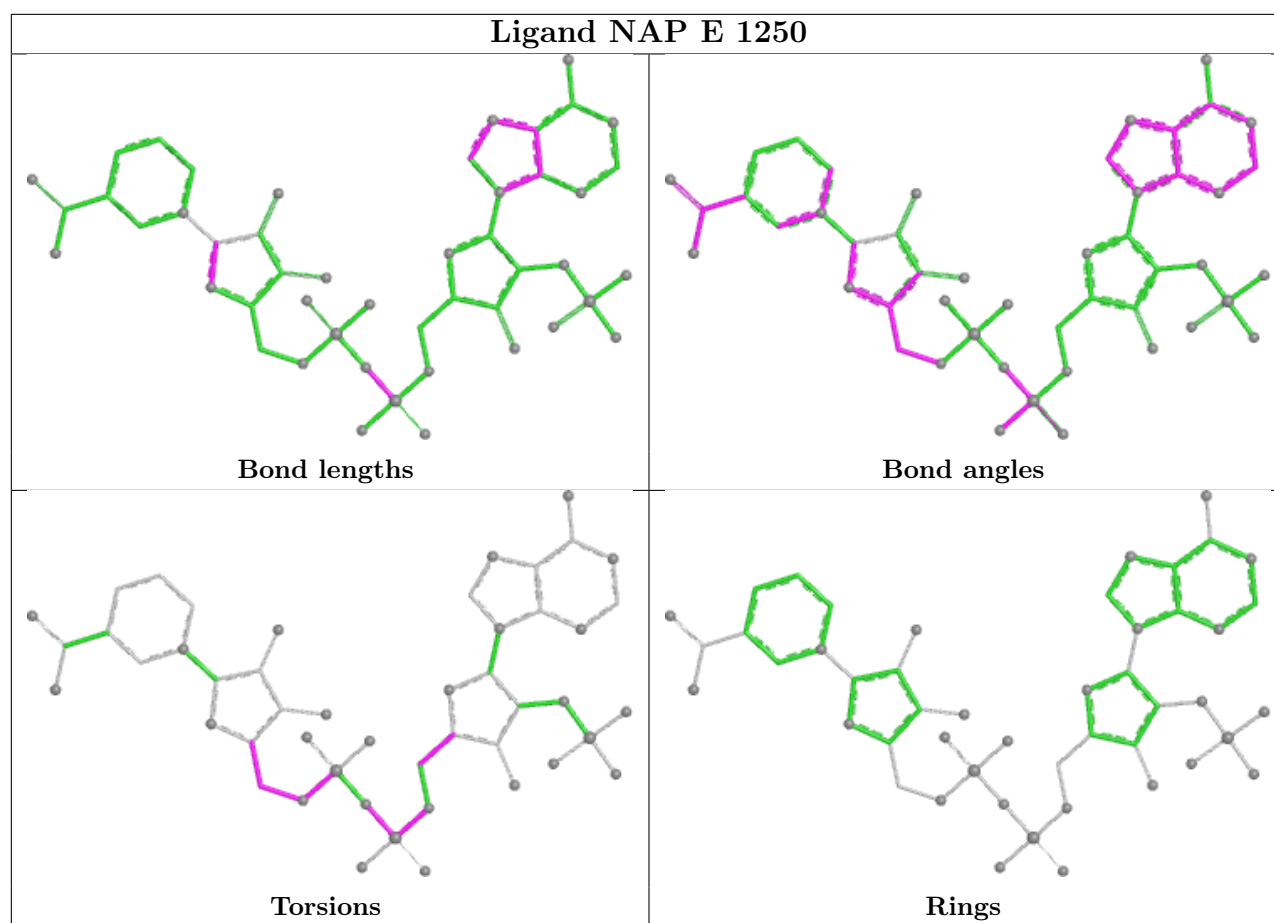
Mol	Chain	Res	Type	Atoms
2	C	1250	NAP	O4B-C4B-C5B-O5B
2	E	1250	NAP	O4B-C4B-C5B-O5B
2	K	1250	NAP	C2B-O2B-P2B-O2X
2	F	1250	NAP	O4B-C4B-C5B-O5B
2	A	1250	NAP	PA-O3-PN-O2N

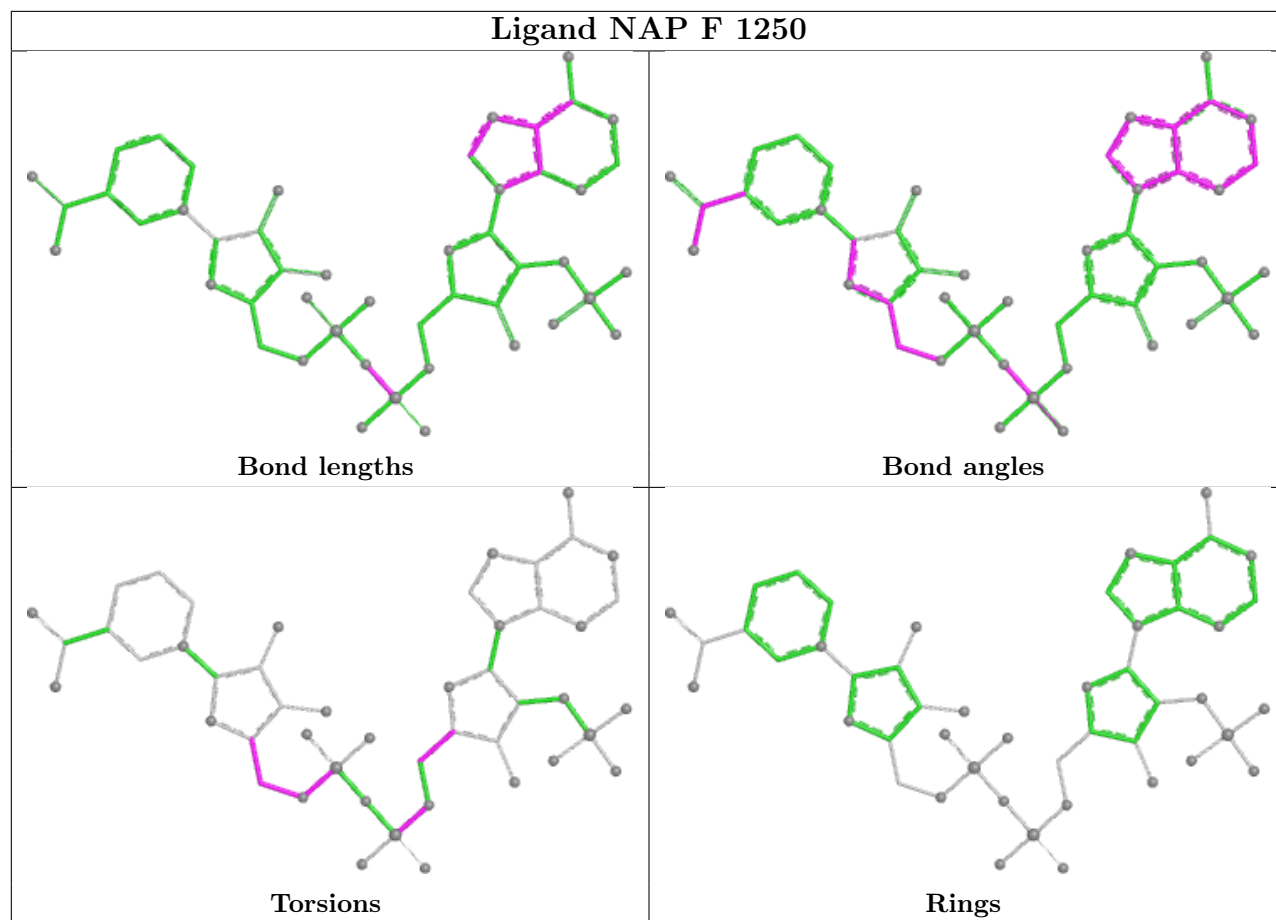
There are no ring outliers.

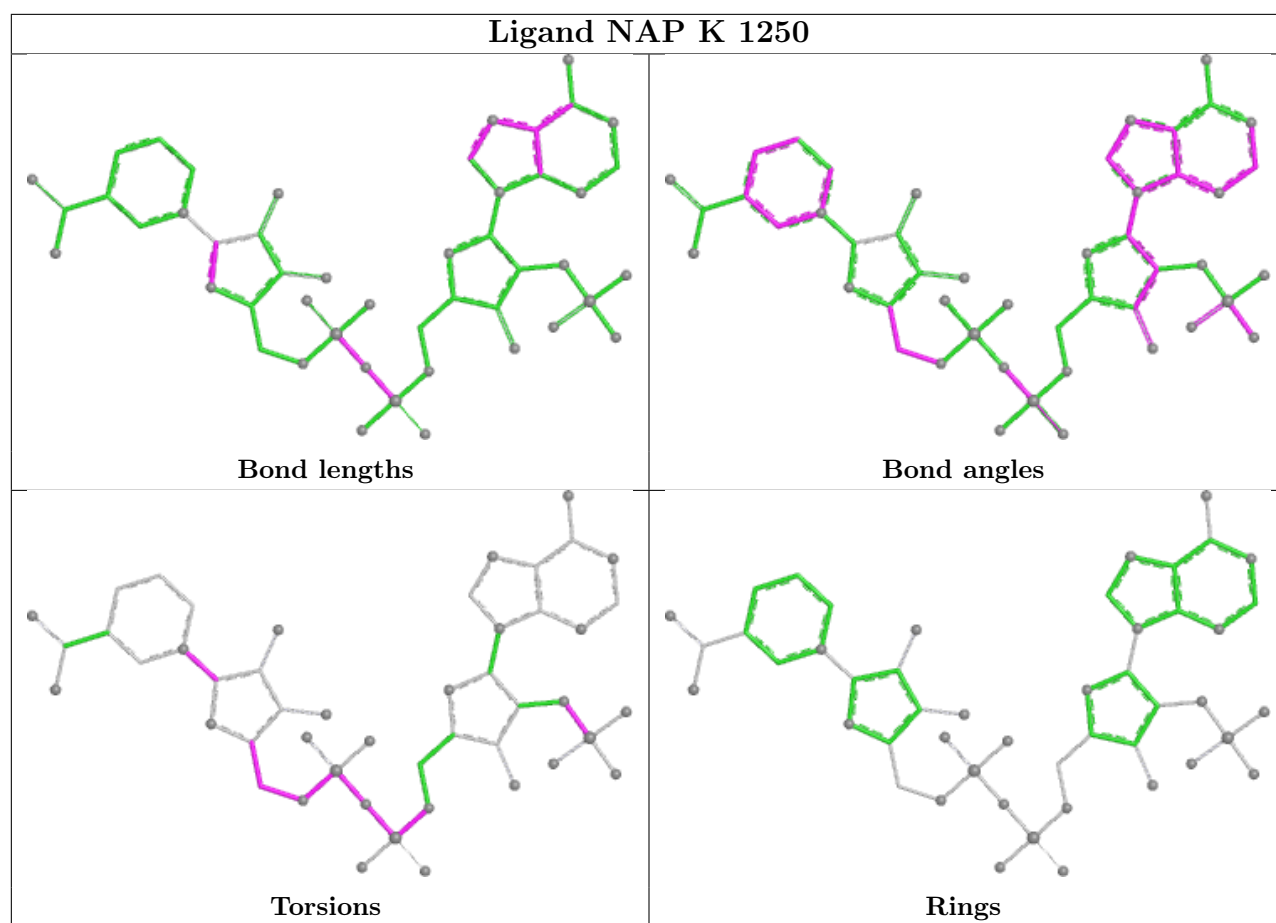
6 monomers are involved in 10 short contacts:

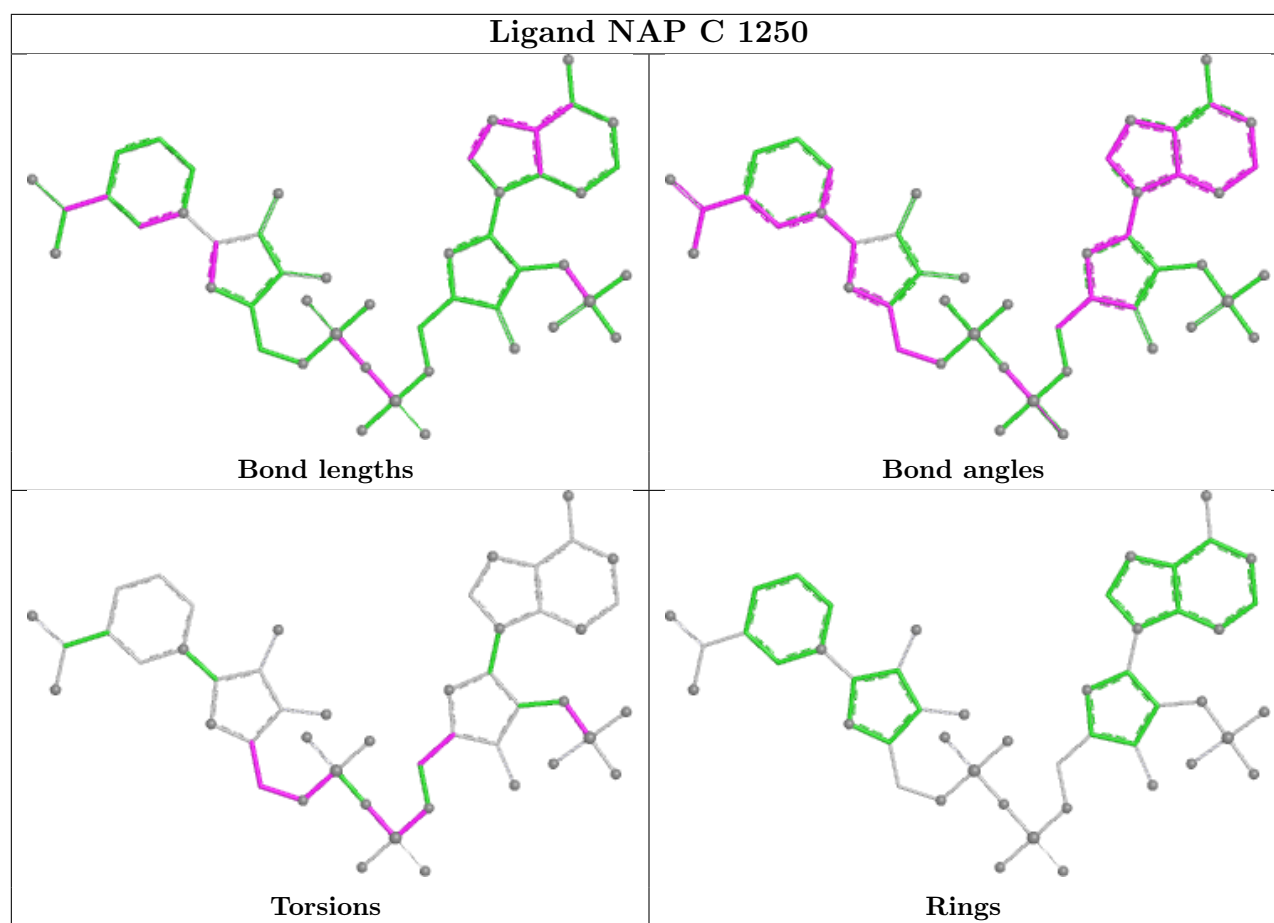
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1250	NAP	2	0
2	F	1250	NAP	2	0
2	K	1250	NAP	2	0
2	C	1250	NAP	1	0
2	A	1250	NAP	2	0
2	B	1250	NAP	1	0

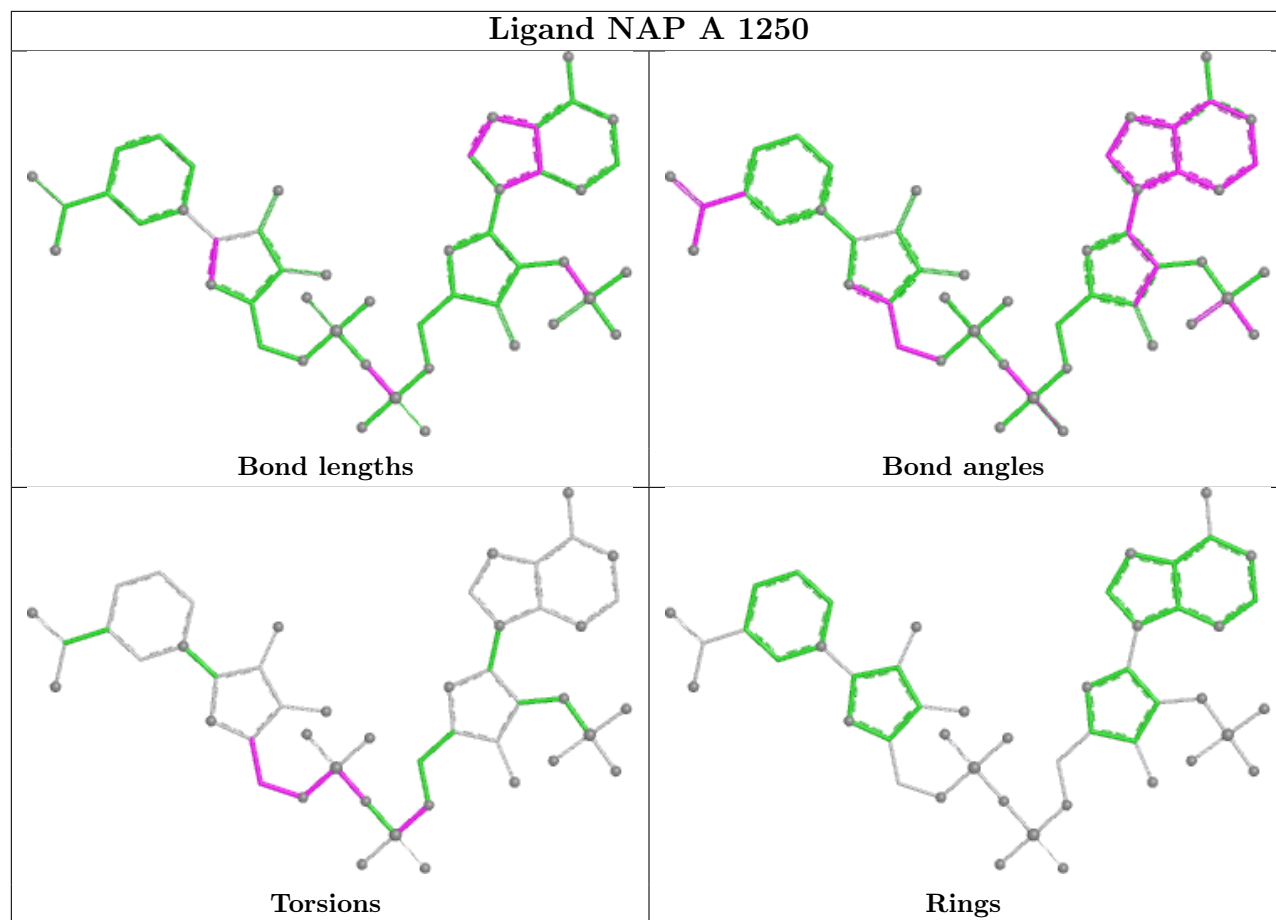
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

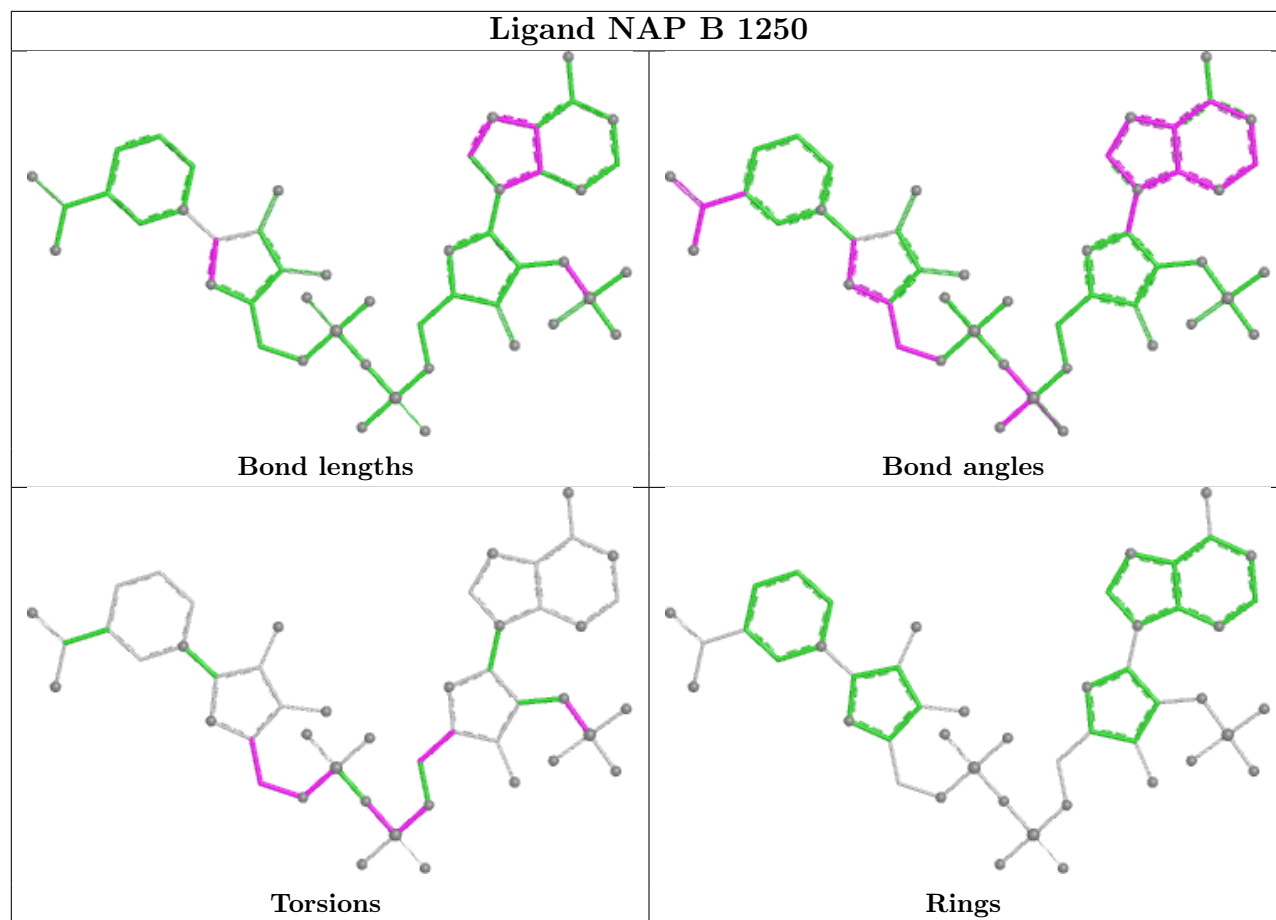












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	247/249 (99%)	1.13	43 (17%) 4 3	16, 33, 69, 99	0
1	B	248/249 (99%)	0.83	22 (8%) 15 13	16, 30, 66, 101	0
1	C	248/249 (99%)	1.32	59 (23%) 2 2	16, 33, 68, 106	0
1	E	247/249 (99%)	1.03	40 (16%) 4 4	16, 32, 74, 109	0
1	F	249/249 (100%)	0.89	34 (13%) 6 5	17, 31, 69, 104	0
1	K	248/249 (99%)	1.50	74 (29%) 1 1	18, 32, 70, 102	0
All	All	1487/1494 (99%)	1.11	272 (18%) 3 3	16, 32, 70, 109	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	205	PHE	8.6
1	F	1	MET	6.6
1	B	249	VAL	6.4
1	E	2	TYR	5.6
1	E	203	ALA	5.4
1	K	194	THR	5.4
1	B	195	GLN	5.2
1	F	205	PHE	5.2
1	E	192	VAL	5.1
1	B	196	GLU	4.9
1	K	86	ALA	4.9
1	F	207	ALA	4.8
1	A	86	ALA	4.8
1	B	207	ALA	4.8
1	F	195	GLN	4.7
1	K	249	VAL	4.7
1	E	197	GLU	4.5
1	B	192	VAL	4.5
1	C	86	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	200	GLU	4.4
1	B	1	MET	4.4
1	E	198	ALA	4.3
1	B	194	THR	4.2
1	C	195	GLN	4.2
1	C	75	ARG	4.2
1	A	201	LEU	4.2
1	E	202	ARG	4.2
1	K	76	GLU	4.2
1	B	197	GLU	4.1
1	F	196	GLU	4.1
1	F	197	GLU	4.1
1	B	201	LEU	4.1
1	F	203	ALA	4.1
1	K	75	ARG	4.0
1	K	193	SER	4.0
1	F	199	ASP	4.0
1	C	51	GLY	4.0
1	B	2	TYR	3.9
1	B	208	ALA	3.9
1	K	52	ARG	3.9
1	C	6	ASN	3.9
1	K	53	ASN	3.8
1	E	204	LYS	3.8
1	E	207	ALA	3.8
1	K	165	THR	3.8
1	C	80	SER	3.7
1	K	127	ARG	3.7
1	K	72	ALA	3.7
1	F	188	ILE	3.7
1	E	249	VAL	3.7
1	A	194	THR	3.6
1	C	168	LEU	3.6
1	A	165	THR	3.6
1	K	192	VAL	3.6
1	K	221	ALA	3.5
1	F	200	GLU	3.5
1	K	5	LEU	3.5
1	E	211	LEU	3.5
1	A	6	ASN	3.5
1	C	249	VAL	3.5
1	B	203	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	233	SER	3.4
1	C	2	TYR	3.4
1	K	2	TYR	3.4
1	E	195	GLN	3.4
1	K	189	GLU	3.4
1	C	49	GLU	3.3
1	F	198	ALA	3.3
1	A	205	PHE	3.3
1	C	193	SER	3.3
1	K	6	ASN	3.3
1	K	197	GLU	3.3
1	B	188	ILE	3.3
1	B	198	ALA	3.3
1	A	2	TYR	3.3
1	C	197	GLU	3.3
1	F	204	LYS	3.3
1	K	236	ALA	3.2
1	B	204	LYS	3.2
1	K	49	GLU	3.2
1	E	56	ALA	3.2
1	F	192	VAL	3.2
1	E	201	LEU	3.2
1	C	1	MET	3.2
1	K	124	PRO	3.2
1	C	231	ASP	3.1
1	C	127	ARG	3.1
1	A	76	GLU	3.1
1	A	196	GLU	3.1
1	E	208	ALA	3.0
1	F	28	ALA	3.0
1	F	201	LEU	3.0
1	K	201	LEU	3.0
1	K	240	LEU	3.0
1	E	76	GLU	3.0
1	C	218	GLU	3.0
1	F	30	GLY	2.9
1	K	51	GLY	2.9
1	K	129	GLY	2.9
1	B	205	PHE	2.9
1	B	200	GLU	2.9
1	C	44	GLU	2.9
1	A	53	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	242	VAL	2.9
1	K	118	THR	2.9
1	E	196	GLU	2.9
1	K	31	ALA	2.9
1	C	53	ASN	2.9
1	A	110	VAL	2.9
1	A	8	THR	2.9
1	E	4	LEU	2.8
1	A	197	GLU	2.8
1	E	188	ILE	2.8
1	F	194	THR	2.8
1	K	109	ASP	2.8
1	K	248	GLN	2.8
1	C	196	GLU	2.8
1	C	184	ASP	2.8
1	K	128	ASP	2.8
1	A	191	GLN	2.7
1	C	203	ALA	2.7
1	K	222	ALA	2.7
1	K	10	VAL	2.7
1	C	43	LEU	2.7
1	K	174	ARG	2.7
1	K	30	GLY	2.7
1	E	199	ASP	2.7
1	E	75	ARG	2.6
1	C	188	ILE	2.6
1	A	231	ASP	2.6
1	C	159	SER	2.6
1	A	30	GLY	2.6
1	A	173	ILE	2.6
1	C	30	GLY	2.6
1	F	2	TYR	2.6
1	A	5	LEU	2.6
1	K	196	GLU	2.6
1	C	81	ILE	2.5
1	E	200	GLU	2.5
1	K	200	GLU	2.5
1	A	236	ALA	2.5
1	F	202	ARG	2.5
1	F	231	ASP	2.5
1	E	246	LEU	2.5
1	F	51	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	81	ILE	2.5
1	F	249	VAL	2.5
1	C	191	GLN	2.5
1	A	7	LYS	2.5
1	A	49	GLU	2.5
1	C	76	GLU	2.5
1	F	182	ALA	2.5
1	C	211	LEU	2.5
1	A	233	SER	2.5
1	E	170	GLY	2.5
1	K	14	GLY	2.5
1	K	83	VAL	2.5
1	K	44	GLU	2.5
1	E	77	GLN	2.5
1	E	194	THR	2.5
1	E	190	ASN	2.5
1	A	202	ARG	2.4
1	F	75	ARG	2.4
1	K	84	LEU	2.4
1	C	68	ASP	2.4
1	K	40	ARG	2.4
1	K	158	ARG	2.4
1	C	20	LEU	2.4
1	K	85	PHE	2.4
1	K	117	PHE	2.4
1	C	8	THR	2.4
1	E	182	ALA	2.4
1	K	198	ALA	2.4
1	K	4	LEU	2.4
1	K	123	LEU	2.4
1	C	186	PRO	2.4
1	K	15	ASN	2.3
1	A	128	ASP	2.3
1	A	200	GLU	2.3
1	F	189	GLU	2.3
1	K	203	ALA	2.3
1	E	138	VAL	2.3
1	K	119	VAL	2.3
1	B	218	GLU	2.3
1	E	218	GLU	2.3
1	K	122	ALA	2.3
1	B	211	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	229	SER	2.3
1	E	3	ARG	2.3
1	E	137	SER	2.3
1	K	62	THR	2.3
1	F	170	GLY	2.3
1	B	53	ASN	2.3
1	C	236	ALA	2.3
1	F	218	GLU	2.3
1	A	75	ARG	2.3
1	A	119	VAL	2.3
1	A	89	GLY	2.3
1	C	212	GLY	2.3
1	F	181	GLY	2.3
1	C	205	PHE	2.2
1	E	226	PHE	2.2
1	C	198	ALA	2.2
1	C	5	LEU	2.2
1	C	201	LEU	2.2
1	K	230	ASP	2.2
1	A	69	ARG	2.2
1	C	234	TYR	2.2
1	F	193	SER	2.2
1	K	233	SER	2.2
1	C	122	ALA	2.2
1	A	64	LEU	2.2
1	A	126	LEU	2.2
1	F	226	PHE	2.2
1	B	4	LEU	2.2
1	E	72	ALA	2.2
1	C	40	ARG	2.2
1	K	191	GLN	2.2
1	C	199	ASP	2.2
1	K	231	ASP	2.2
1	K	141	VAL	2.2
1	A	1	MET	2.2
1	K	71	TYR	2.2
1	C	228	ALA	2.2
1	C	158	ARG	2.2
1	C	173	ILE	2.2
1	K	87	ASN	2.2
1	K	132	VAL	2.2
1	C	194	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	32	TYR	2.2
1	K	205	PHE	2.2
1	A	44	GLU	2.2
1	E	189	GLU	2.2
1	E	175	VAL	2.1
1	C	89	GLY	2.1
1	K	3	ARG	2.1
1	F	190	ASN	2.1
1	K	186	PRO	2.1
1	A	118	THR	2.1
1	C	79	GLY	2.1
1	C	126	LEU	2.1
1	K	238	ILE	2.1
1	A	84	LEU	2.1
1	A	34	PHE	2.1
1	C	135	THR	2.1
1	K	135	THR	2.1
1	A	31	ALA	2.1
1	A	203	ALA	2.1
1	F	206	ALA	2.1
1	K	48	ALA	2.1
1	A	189	GLU	2.1
1	K	80	SER	2.1
1	A	124	PRO	2.1
1	E	6	ASN	2.1
1	E	183	ILE	2.1
1	C	229	SER	2.0
1	C	74	VAL	2.0
1	K	157	VAL	2.0
1	K	235	VAL	2.0
1	K	140	GLY	2.0
1	B	231	ASP	2.0
1	F	228	ALA	2.0
1	K	177	ALA	2.0
1	A	121	LYS	2.0
1	C	225	LEU	2.0
1	E	5	LEU	2.0
1	C	111	ASN	2.0
1	K	226	PHE	2.0
1	F	133	ILE	2.0
1	C	118	THR	2.0
1	A	235	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	224	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](#)

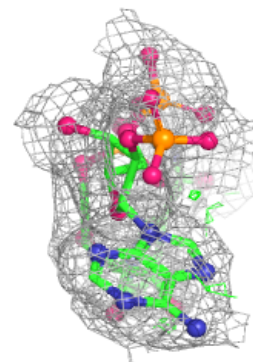
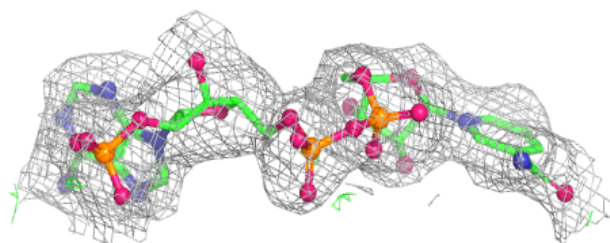
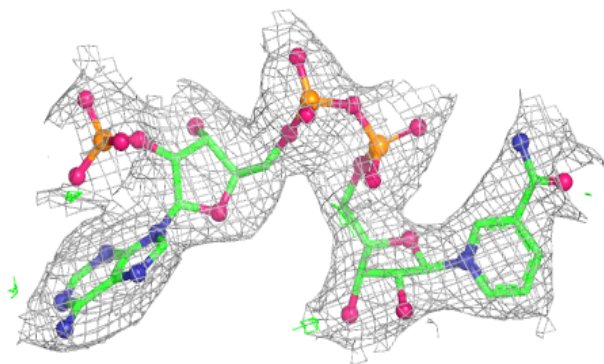
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	1250	48/48	0.92	0.11	29,34,38,42	0
2	NAP	K	1250	48/48	0.92	0.11	29,36,41,44	0
2	NAP	A	1250	48/48	0.93	0.10	29,33,37,44	0
2	NAP	F	1250	48/48	0.95	0.08	27,33,40,45	0
2	NAP	B	1250	48/48	0.96	0.08	22,28,39,40	0
2	NAP	E	1250	48/48	0.96	0.08	24,30,33,34	0

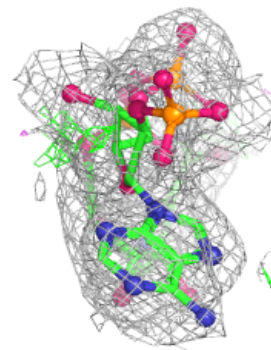
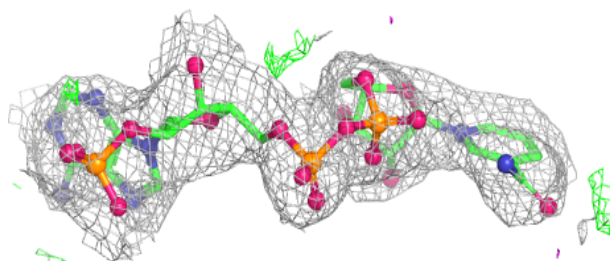
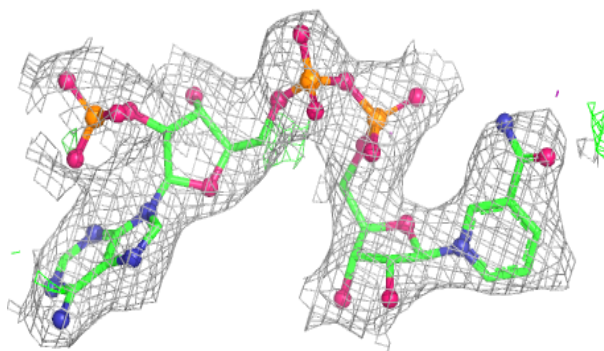
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP C 1250:

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

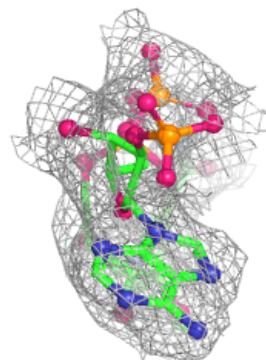
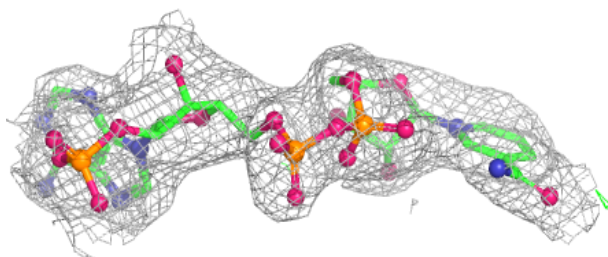
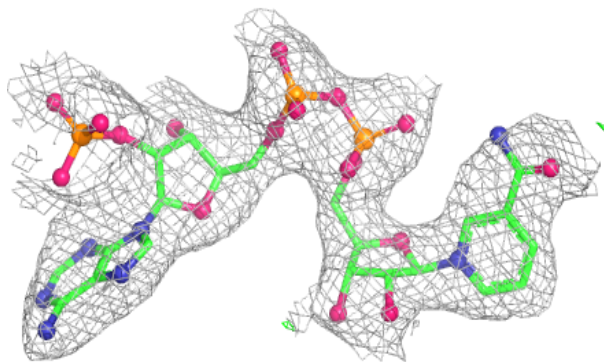
**Electron density around NAP K 1250:**

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

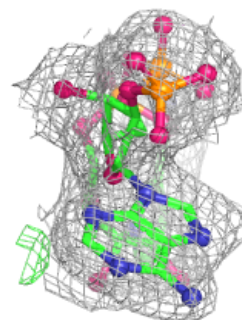
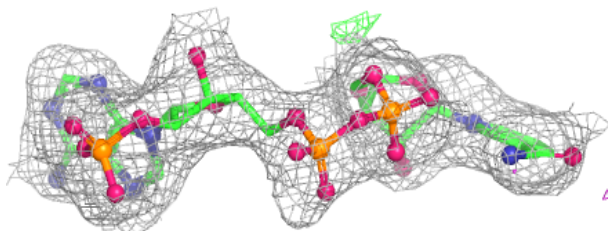
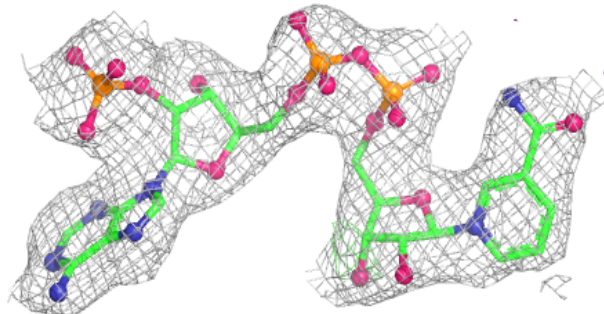


Electron density around NAP A 1250:

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

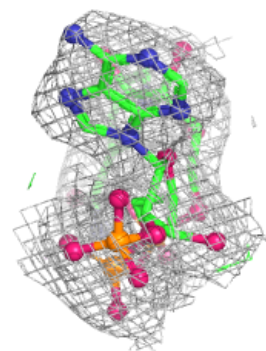
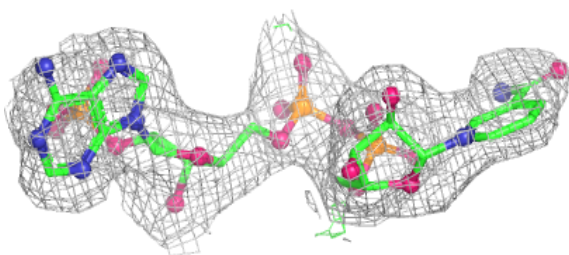
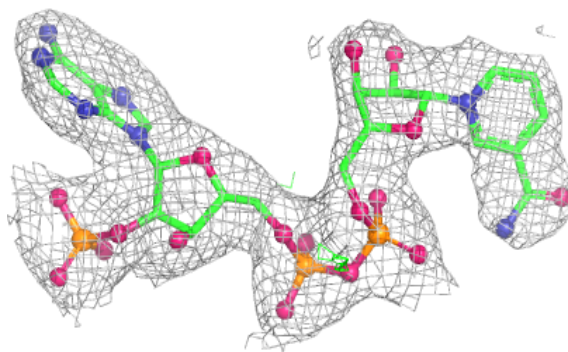
**Electron density around NAP F 1250:**

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

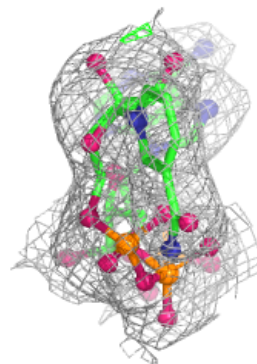
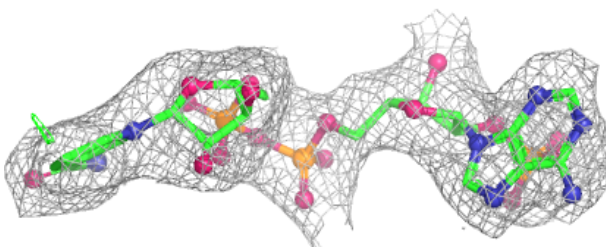
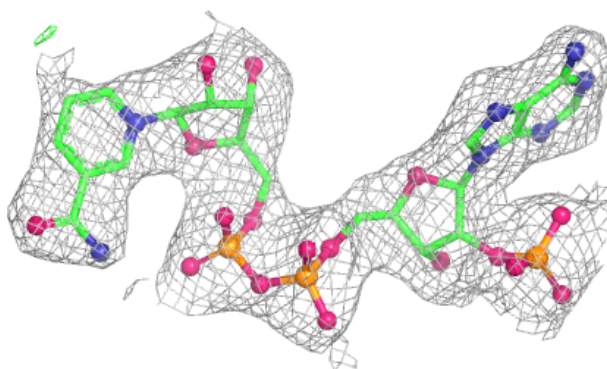


Electron density around NAP B 1250:

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

**Electron density around NAP E 1250:**

$2mF_o-DF_c$ (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.