Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 03:33 PM EDT

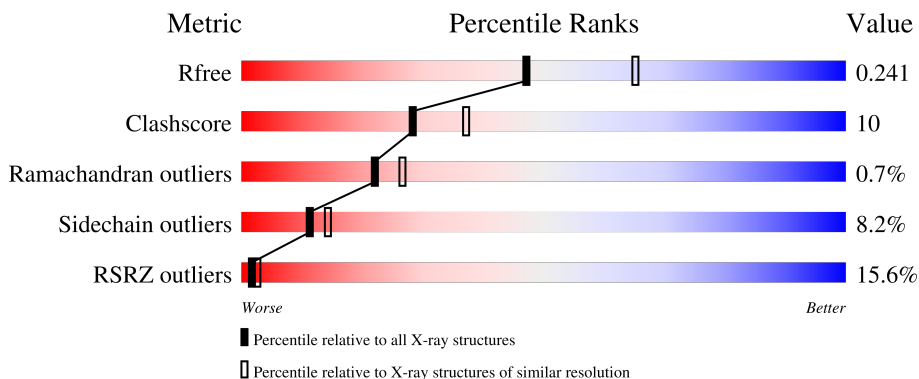|		
PDB ID	:	1XKD
Title	:	Ternary complex of Isocitrate dehydrogenase from the hyperthermophile Aeropyrum pernix
Authors	:	Karlstrom, M.; Stokke, R.; Steen, I.H.; Birkeland, N.-K.; Ladenstein, R.
Deposited on	:	2004-09-28
Resolution	:	2.30 Å(reported)

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 2.30 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		10
Ramachandran outliers		0.7%
Sidechain outliers		8.2%
RSRZ outliers		15.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	435	6% 81% 14% · ·
1	B	435	24% 68% 26% · ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6888 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.
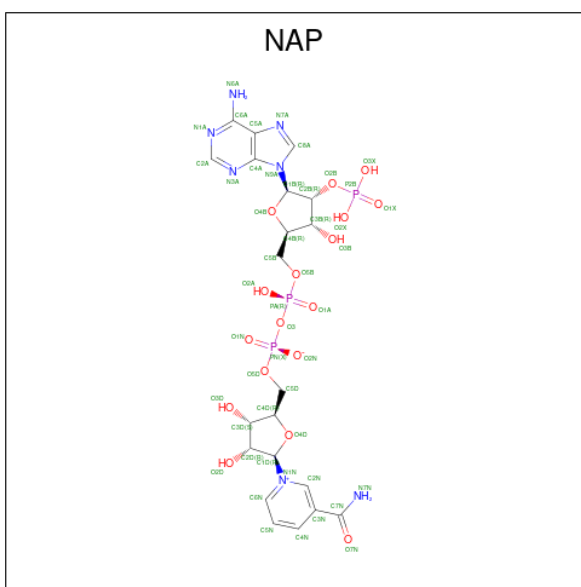
- Molecule 1 is a protein called isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	11	0	0
			3314	2100	588	613	13			
1	B	419	Total	C	N	O	S	88	0	0
			3254	2064	575	602	13			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
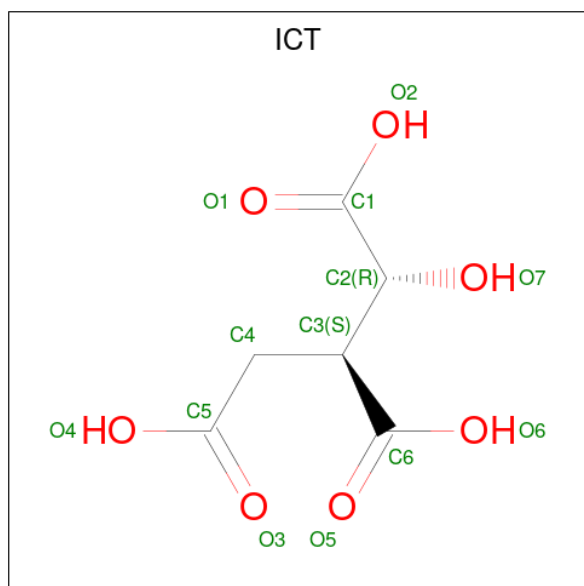

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$).

| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 6	O 7	0	0
4	B	1	Total 13	C 6	O 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total 131	O 131	0	0
5	B	65	Total 65	O 65	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: isocitrate dehydrogenase
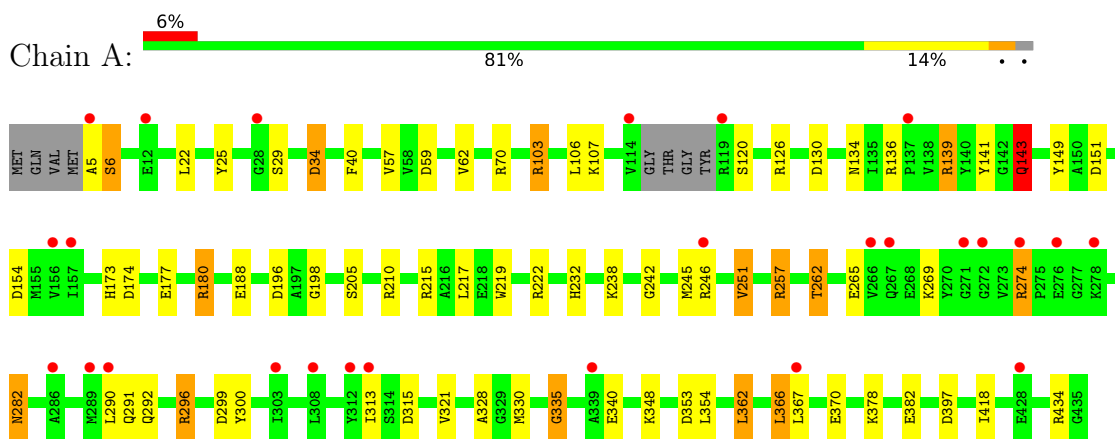
- Molecule 1: isocitrate dehydrogenase
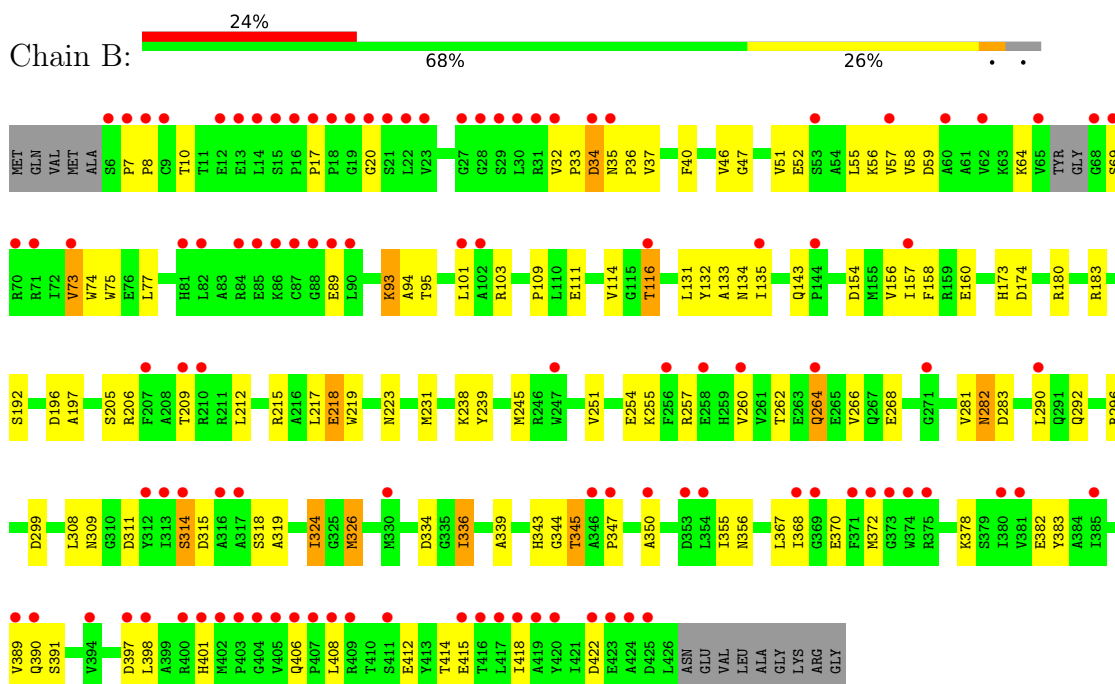
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.58Å 107.58Å 171.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.30 39.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.70-2.30) 99.8 (39.74-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.248 0.219 , 0.241	Depositor DCC
R_{free} test set	2289 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6888	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 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.61	0/3382	0.84	10/4585 (0.2%)
1	B	0.60	1/3322 (0.0%)	0.77	9/4507 (0.2%)
All	All	0.61	1/6704 (0.0%)	0.81	19/9092 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	GLU	CG-CD	5.59	1.60	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	ASP	CB-CG-OD2	7.95	125.45	118.30
1	A	174	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	154	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	311	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	299	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	299	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	174	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	353	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	196	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	154	ASP	CB-CG-OD2	5.62	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	34	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	151	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	315	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	334	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	283	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	143	GLN	CB-CA-C	-5.14	100.11	110.40
1	B	397	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	130	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	GLY	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	3314	0	3337	63	0
1	B	3254	0	3273	80	0
2	A	2	0	0	0	0
3	A	48	0	25	1	0
3	B	48	0	25	5	0
4	A	13	0	4	0	0
4	B	13	0	4	2	0
5	A	131	0	0	4	0
5	B	65	0	0	7	0
All	All	6888	0	6668	128	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 10.

All (128) 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:64:LYS:HE3	1:B:422:ASP:HA	1.42	1.01
1:A:143:GLN:HE21	1:A:143:GLN:H	1.02	0.99
1:B:324:ILE:HG12	1:B:343:HIS:HB3	1.44	0.99
1:A:141:TYR:H	1:A:143:GLN:HE22	1.07	0.94
3:B:1003:NAP:C4N	4:B:1004:ICT:H2	2.08	0.82
1:A:173:HIS:HD2	5:A:1078:HOH:O	1.63	0.81
1:B:262:THR:HG22	1:B:264:GLN:H	1.46	0.81
1:A:139:ARG:NH2	1:A:370:GLU:OE2	2.13	0.80
1:A:143:GLN:H	1:A:143:GLN:NE2	1.80	0.79
1:A:238:LYS:HD3	5:B:1064:HOH:O	1.84	0.77
1:A:246:ARG:HH22	1:B:116:THR:HG23	1.50	0.75
1:A:246:ARG:HH22	1:B:116:THR:CG2	2.00	0.74
1:A:141:TYR:N	1:A:143:GLN:HE22	1.85	0.74
1:A:296:ARG:CG	1:A:296:ARG:HH11	2.03	0.71
1:B:205:SER:O	1:B:209:THR:HG23	1.91	0.70
1:A:274:ARG:HG3	1:A:274:ARG:O	1.92	0.69
1:A:210:ARG:NH1	1:A:251:VAL:HG13	2.09	0.68
1:A:188:GLU:OE1	1:B:180:ARG:NH1	2.26	0.68
1:B:46:VAL:HG11	1:B:355:ILE:HD13	1.77	0.66
1:A:246:ARG:HH12	1:B:116:THR:HG23	1.62	0.64
1:A:257:ARG:NH2	1:A:265:GLU:OE1	2.32	0.63
1:A:291:GLN:HE22	1:B:324:ILE:HD12	1.62	0.62
1:B:143:GLN:HB2	1:B:398:LEU:HD22	1.79	0.62
1:A:330:MET:HB2	1:A:366:LEU:HD13	1.81	0.62
1:B:368:ILE:HD13	1:B:372:MET:SD	2.42	0.60
1:A:246:ARG:NH2	1:B:116:THR:HG23	2.17	0.59
1:B:64:LYS:HE3	1:B:422:ASP:CA	2.28	0.59
1:A:141:TYR:H	1:A:143:GLN:NE2	1.90	0.59
1:A:328:ALA:HB2	1:A:362:LEU:HB3	1.85	0.58
1:B:254:GLU:OE2	1:B:255:LYS:HE3	2.04	0.57
1:B:157:ILE:HD13	1:B:314:SER:HA	1.85	0.57
1:A:232:HIS:CE1	1:B:114:VAL:HG11	2.41	0.56
1:A:291:GLN:NE2	1:B:324:ILE:HD12	2.20	0.56
1:A:262:THR:HG22	1:A:265:GLU:H	1.70	0.56
1:A:232:HIS:HE1	1:B:114:VAL:HG11	1.70	0.56
1:B:47:GLY:O	1:B:51:VAL:HG23	2.06	0.55
1:B:77:LEU:HB3	1:B:95:THR:HG23	1.87	0.55
1:B:326:MET:HE1	1:B:356:ASN:HD21	1.72	0.55
1:B:339:ALA:HB2	1:B:367:LEU:HB2	1.89	0.54
1:A:149:TYR:OH	1:B:401:HIS:HD2	1.90	0.54
1:A:180:ARG:CG	1:A:180:ARG:HH11	2.20	0.54
1:A:34:ASP:OD1	1:A:70:ARG:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.71	0.54
3:B:1003:NAP:C5N	4:B:1004:ICT:H2	2.38	0.54
1:A:290:LEU:HD23	1:A:313:ILE:HD12	1.91	0.53
1:B:131:LEU:HD21	1:B:336:ILE:HG12	1.89	0.53
1:B:219:TRP:O	1:B:223:ASN:ND2	2.39	0.53
1:B:345:THR:HG22	1:B:347:PRO:HD3	1.90	0.52
1:B:408:LEU:HB3	1:B:412:GLU:HG3	1.92	0.52
1:B:292:GLN:HE22	1:B:296:ARG:HD3	1.74	0.52
1:B:17:PRO:HD2	1:B:37:VAL:CG2	2.40	0.52
1:A:103:ARG:HD3	1:A:335:GLY:O	2.09	0.51
1:A:25:TYR:CD2	1:A:335:GLY:HA3	2.45	0.51
1:B:344:GLY:HA3	3:B:1003:NAP:C6N	2.40	0.51
1:A:180:ARG:HH11	1:A:180:ARG:HG3	1.76	0.51
1:A:246:ARG:NH1	1:B:116:THR:HG23	2.26	0.51
1:A:291:GLN:HG3	1:B:319:ALA:HB2	1.93	0.51
1:B:40:PHE:CD2	1:B:74:TRP:HB3	2.47	0.50
1:B:33:PRO:C	1:B:35:ASN:H	2.15	0.50
1:A:126:ARG:NH2	1:A:340:GLU:OE2	2.44	0.50
1:B:57:VAL:HA	1:B:418:ILE:HD11	1.94	0.50
1:B:46:VAL:HG22	1:B:345:THR:O	2.12	0.49
1:B:231:MET:CE	1:B:309:ASN:HB3	2.42	0.49
1:A:242:GLY:O	1:A:246:ARG:HG3	2.12	0.49
1:B:157:ILE:HD13	1:B:314:SER:CA	2.43	0.49
1:B:109:PRO:HB3	1:B:344:GLY:HA2	1.95	0.49
1:B:262:THR:HG22	1:B:264:GLN:N	2.23	0.48
1:B:132:TYR:HB2	5:B:1027:HOH:O	2.13	0.48
1:B:318:SER:HB2	1:B:324:ILE:HG22	1.96	0.48
1:B:58:VAL:CG1	1:B:74:TRP:HZ2	2.27	0.48
1:B:135:ILE:HD12	1:B:158:PHE:CE1	2.49	0.47
1:A:180:ARG:HG3	1:A:180:ARG:NH1	2.30	0.47
1:A:196:ASP:HA	5:A:1078:HOH:O	2.15	0.47
1:B:35:ASN:N	1:B:36:PRO:HD3	2.29	0.47
1:B:262:THR:O	1:B:266:VAL:HG23	2.15	0.47
1:A:296:ARG:HH11	1:A:296:ARG:HG3	1.75	0.47
1:B:34:ASP:C	1:B:36:PRO:HD3	2.35	0.47
1:B:157:ILE:CD1	1:B:314:SER:HA	2.45	0.46
1:B:173:HIS:HD2	5:B:1025:HOH:O	1.97	0.46
1:A:177:GLU:HA	1:A:180:ARG:NH1	2.31	0.46
1:A:291:GLN:NE2	1:B:324:ILE:H	2.14	0.46
1:B:326:MET:CE	1:B:356:ASN:HD21	2.28	0.46
1:B:215:ARG:NH1	1:B:218:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ALA:O	1:A:6:SER:HB3	2.16	0.45
1:A:57:VAL:HA	1:A:418:ILE:HD11	1.98	0.45
1:B:10:THR:C	1:B:94:ALA:HB2	2.37	0.45
1:B:17:PRO:HD2	1:B:37:VAL:HG22	1.98	0.45
1:B:93:LYS:HD2	1:B:93:LYS:HA	1.65	0.45
1:A:57:VAL:HA	1:A:418:ILE:CD1	2.46	0.45
1:B:324:ILE:HG12	1:B:343:HIS:CB	2.32	0.45
5:A:1073:HOH:O	1:B:308:LEU:HD21	2.17	0.44
1:B:32:VAL:HA	1:B:33:PRO:HD3	1.79	0.44
1:B:378:LYS:O	1:B:382:GLU:HG3	2.17	0.44
1:A:205:SER:HA	1:B:197:ALA:HA	2.00	0.44
1:A:282:ASN:C	1:A:282:ASN:HD22	2.20	0.44
1:B:262:THR:HG21	5:B:1061:HOH:O	2.17	0.44
1:B:324:ILE:HD11	3:B:1003:NAP:C8A	2.48	0.44
1:B:156:VAL:HG21	1:B:219:TRP:HE1	1.83	0.44
1:A:292:GLN:HB3	1:A:300:TYR:CE2	2.53	0.44
1:A:397:ASP:HB3	3:A:1001:NAP:H2A	1.99	0.43
1:A:107:LYS:NZ	1:A:340:GLU:OE1	2.51	0.43
1:B:356:ASN:HB3	3:B:1003:NAP:N1A	2.34	0.43
1:A:134:ASN:HD21	1:A:136:ARG:HE	1.64	0.43
1:A:378:LYS:O	1:A:382:GLU:HG3	2.19	0.42
1:A:219:TRP:HH2	1:A:366:LEU:CD2	2.32	0.42
1:B:209:THR:HG22	5:B:1033:HOH:O	2.20	0.42
1:A:348:LYS:HG2	5:A:1031:HOH:O	2.18	0.42
1:A:177:GLU:HA	1:A:180:ARG:HH12	1.84	0.42
1:A:198:GLY:HA3	1:B:239:TYR:O	2.20	0.42
1:A:210:ARG:CZ	1:A:251:VAL:HG13	2.49	0.42
1:A:40:PHE:HA	1:A:106:LEU:O	2.20	0.42
1:B:245:MET:CE	5:B:1032:HOH:O	2.67	0.42
1:B:160:GLU:HB2	1:B:212:LEU:HD22	2.01	0.41
1:A:257:ARG:O	1:A:257:ARG:HD3	2.20	0.41
1:B:7:PRO:HA	1:B:8:PRO:HD3	1.81	0.41
1:B:20:GLY:HA3	1:B:73:VAL:HG21	2.01	0.41
1:B:160:GLU:HG3	5:B:1033:HOH:O	2.20	0.41
1:B:412:GLU:HA	1:B:415:GLU:HG2	2.02	0.41
1:B:260:VAL:HG22	1:B:281:VAL:CG2	2.49	0.41
1:B:17:PRO:CG	1:B:75:TRP:HB2	2.51	0.41
1:A:134:ASN:HD21	1:A:136:ARG:NE	2.18	0.41
1:A:274:ARG:O	1:A:274:ARG:CG	2.66	0.41
1:A:291:GLN:HE22	1:B:324:ILE:H	1.70	0.40
1:A:180:ARG:CG	1:A:180:ARG:NH1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TYR:OH	1:B:401:HIS:CD2	2.72	0.40
1:B:282:ASN:C	1:B:282:ASN:HD22	2.25	0.40
1:B:133:ALA:HB1	1:B:135:ILE:HD11	2.03	0.40
1:B:389:VAL:C	1:B:391:SER:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/435 (97%)	406 (96%)	15 (4%)	2 (0%)	29	35
1	B	415/435 (95%)	382 (92%)	29 (7%)	4 (1%)	15	17
All	All	838/870 (96%)	788 (94%)	44 (5%)	6 (1%)	22	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	SER
1	B	268	GLU
1	A	6	SER
1	B	69	SER
1	B	350	ALA
1	B	390	GLN

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	344/350 (98%)	320 (93%)	24 (7%)	15	19
1	B	339/350 (97%)	307 (91%)	32 (9%)	8	10
All	All	683/700 (98%)	627 (92%)	56 (8%)	11	14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	29	SER
1	A	62	VAL
1	A	103	ARG
1	A	139	ARG
1	A	143	GLN
1	A	180	ARG
1	A	215	ARG
1	A	217	LEU
1	A	222	ARG
1	A	245	MET
1	A	251	VAL
1	A	257	ARG
1	A	262	THR
1	A	269	LYS
1	A	274	ARG
1	A	282	ASN
1	A	296	ARG
1	A	321	VAL
1	A	354	LEU
1	A	362	LEU
1	A	366	LEU
1	A	367	LEU
1	A	434	ARG
1	B	34	ASP
1	B	52	GLU
1	B	55	LEU
1	B	56	LYS
1	B	73	VAL
1	B	89	GLU
1	B	93	LYS
1	B	101	LEU
1	B	103	ARG
1	B	111	GLU

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Mol	Chain	Res	Type
1	B	116	THR
1	B	134	ASN
1	B	183	ARG
1	B	192	SER
1	B	206	ARG
1	B	217	LEU
1	B	238	LYS
1	B	251	VAL
1	B	257	ARG
1	B	264	GLN
1	B	282	ASN
1	B	290	LEU
1	B	314	SER
1	B	315	ASP
1	B	324	ILE
1	B	326	MET
1	B	336	ILE
1	B	345	THR
1	B	370	GLU
1	B	383	TYR
1	B	406	GLN
1	B	414	THR

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	134	ASN
1	A	143	GLN
1	A	147	HIS
1	A	173	HIS
1	A	282	ASN
1	A	288	ASN
1	A	291	GLN
1	B	134	ASN
1	B	173	HIS
1	B	282	ASN
1	B	292	GLN
1	B	401	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	NAP	A	1001	-	45,52,52	1.80	5 (11%)	56,80,80	1.27	5 (8%)
3	NAP	B	1003	-	45,52,52	1.69	4 (8%)	56,80,80	1.10	3 (5%)
4	ICT	B	1004	2	12,12,12	1.05	0	13,16,16	1.30	2 (15%)
4	ICT	A	1002	2	12,12,12	1.15	0	13,16,16	1.41	2 (15%)

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
3	NAP	A	1001	-	-	13/31/67/67	0/5/5/5
3	NAP	B	1003	-	-	13/31/67/67	0/5/5/5
4	ICT	B	1004	2	-	4/16/16/16	-
4	ICT	A	1002	2	-	5/16/16/16	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAP	O7N-C7N	9.45	1.42	1.24
3	B	1003	NAP	O7N-C7N	9.26	1.41	1.24
3	A	1001	NAP	C2A-N3A	4.46	1.39	1.32
3	B	1003	NAP	C2N-N1N	3.41	1.39	1.35
3	B	1003	NAP	C8A-N7A	-2.36	1.30	1.34
3	A	1001	NAP	C2N-N1N	2.30	1.37	1.35
3	B	1003	NAP	O4B-C1B	2.28	1.44	1.41
3	A	1001	NAP	C2A-N1A	2.24	1.38	1.33
3	A	1001	NAP	P2B-O2B	2.08	1.63	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	NAP	N3A-C2A-N1A	-5.48	120.11	128.68
3	A	1001	NAP	O7N-C7N-C3N	-3.03	116.00	119.63
4	A	1002	ICT	C4-C3-C2	2.72	117.94	110.29
3	A	1001	NAP	C3N-C7N-N7N	2.71	121.00	117.75
3	B	1003	NAP	O2B-C2B-C1B	-2.66	100.54	110.10
3	A	1001	NAP	PN-O3-PA	-2.65	123.73	132.83
3	B	1003	NAP	C1B-N9A-C4A	2.58	131.18	126.64
4	B	1004	ICT	O2-C1-C2	2.46	119.93	113.27
4	A	1002	ICT	O7-C2-C1	-2.41	105.62	110.66
3	A	1001	NAP	C3D-C2D-C1D	2.38	104.56	100.98
3	B	1003	NAP	C4N-C3N-C7N	-2.36	114.71	121.04
4	B	1004	ICT	O4-C5-C4	2.04	120.60	114.07

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	NAP	C5D-O5D-PN-O3
3	A	1001	NAP	C5D-O5D-PN-O1N
3	A	1001	NAP	C5D-O5D-PN-O2N
3	A	1001	NAP	O4D-C1D-N1N-C2N
3	A	1001	NAP	O4D-C1D-N1N-C6N
3	A	1001	NAP	C2D-C1D-N1N-C2N
3	A	1001	NAP	C2D-C1D-N1N-C6N
3	B	1003	NAP	O4D-C1D-N1N-C2N
3	B	1003	NAP	O4D-C1D-N1N-C6N
3	B	1003	NAP	C2D-C1D-N1N-C2N
3	B	1003	NAP	C2N-C3N-C7N-O7N

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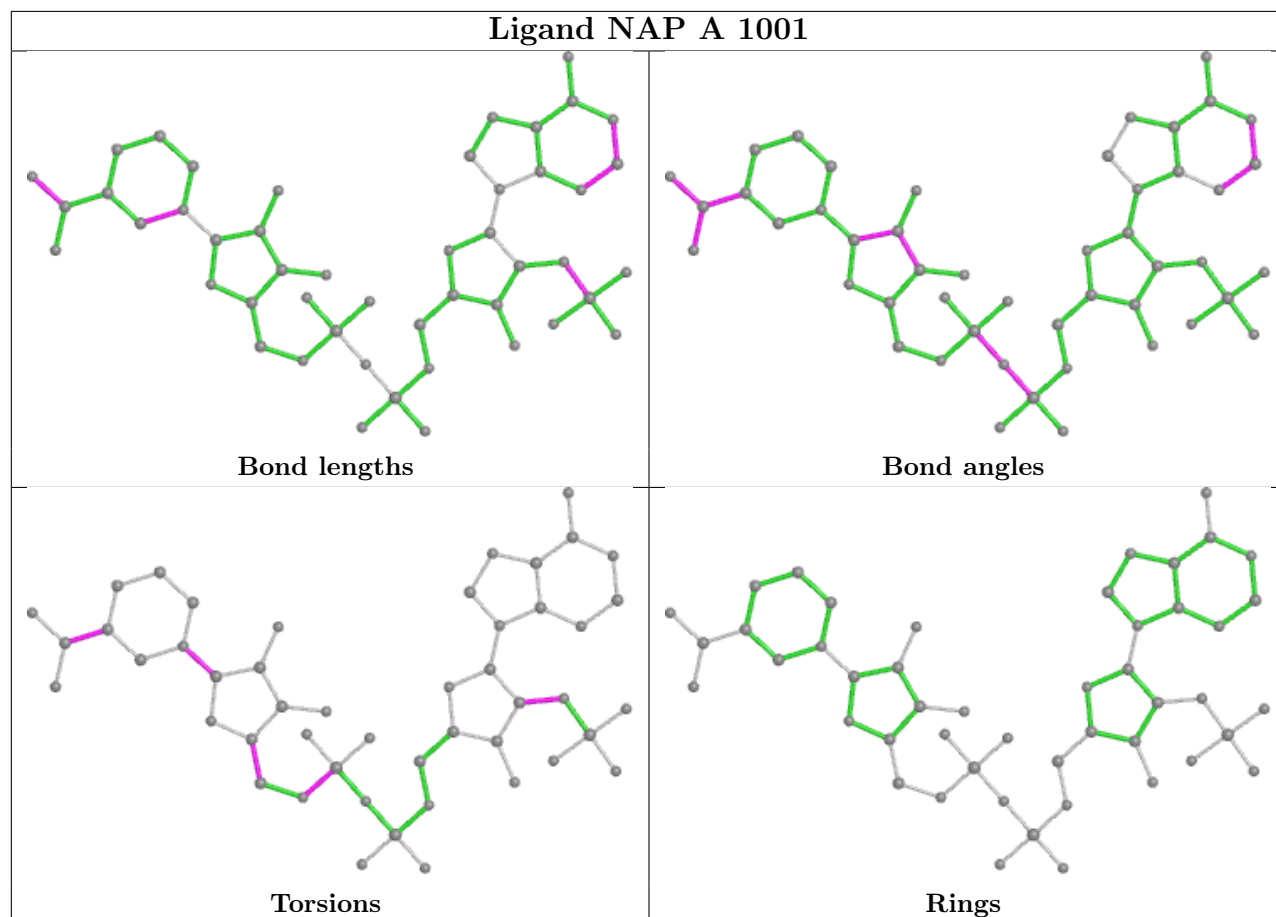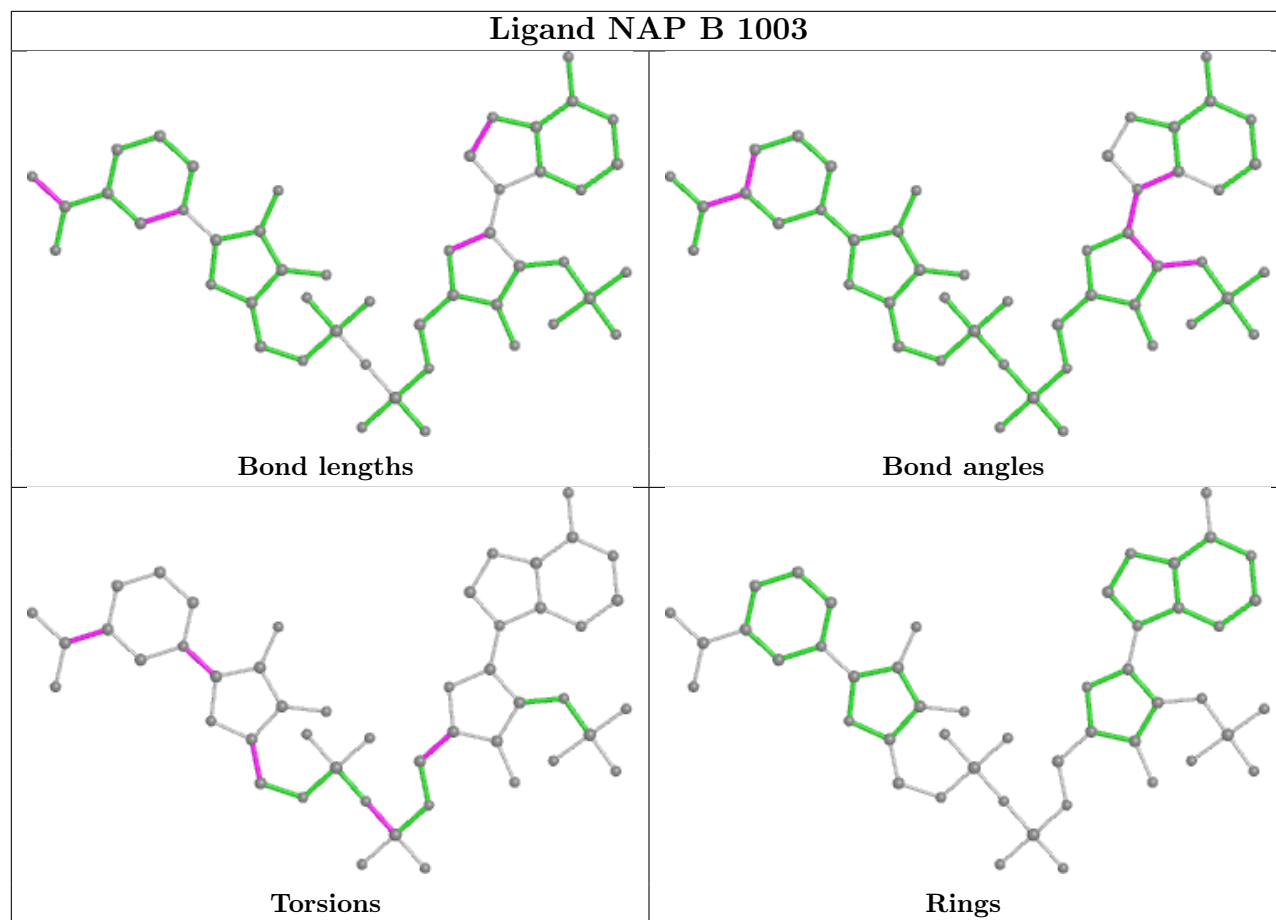| Mol	Chain	Res	Type	Atoms
3	B	1003	NAP	C2N-C3N-C7N-N7N
4	A	1002	ICT	C2-C3-C4-C5
4	A	1002	ICT	C6-C3-C4-C5
4	B	1004	ICT	C2-C3-C4-C5
4	B	1004	ICT	C6-C3-C4-C5
3	B	1003	NAP	C4N-C3N-C7N-O7N
3	B	1003	NAP	C4N-C3N-C7N-N7N
3	A	1001	NAP	O4D-C4D-C5D-O5D
3	A	1001	NAP	C3B-C2B-O2B-P2B
3	A	1001	NAP	C3D-C4D-C5D-O5D
3	B	1003	NAP	O4D-C4D-C5D-O5D
3	B	1003	NAP	O4B-C4B-C5B-O5B
3	B	1003	NAP	PN-O3-PA-O5B
4	B	1004	ICT	C4-C3-C6-O6
4	A	1002	ICT	O7-C2-C3-C4
3	A	1001	NAP	C2N-C3N-C7N-N7N
3	B	1003	NAP	C3D-C4D-C5D-O5D
3	A	1001	NAP	C2N-C3N-C7N-O7N
3	A	1001	NAP	C1B-C2B-O2B-P2B
3	B	1003	NAP	C3B-C4B-C5B-O5B
4	B	1004	ICT	C4-C3-C6-O5
3	B	1003	NAP	C2D-C1D-N1N-C6N
4	A	1002	ICT	C3-C4-C5-O3
4	A	1002	ICT	C3-C4-C5-O4

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	NAP	1	0
3	B	1003	NAP	5	0
4	B	1004	ICT	2	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 then 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 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 1003

Bond lengths

Bond angles

Torsions

Rings

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(Å²)	Q<0.9
1	A	427/435 (98%)	0.26	26 (6%)	21	27	14, 24, 39, 47	3 (0%)
1	B	419/435 (96%)	1.22	106 (25%)	0	0	18, 29, 37, 42	21 (5%)
All	All	846/870 (97%)	0.74	132 (15%)	2	2	14, 27, 38, 47	24 (2%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	ALA	8.5
1	B	354	LEU	8.1
1	B	403	PRO	7.6
1	B	420	TYR	7.5
1	B	30	LEU	7.3
1	B	69	SER	6.8
1	B	7	PRO	6.5
1	B	372	MET	6.3
1	B	373	GLY	5.9
1	B	18	PRO	5.5
1	B	406	GLN	5.4
1	B	404	GLY	5.3
1	B	402	MET	5.2
1	B	405	VAL	5.2
1	B	17	PRO	5.1
1	B	368	ILE	5.1
1	A	276	GLU	5.0
1	B	21	SER	4.7
1	B	19	GLY	4.7
1	B	32	VAL	4.7
1	B	88	GLY	4.5
1	B	16	PRO	4.4
1	B	60	ALA	4.4
1	B	264	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	4.1
1	B	31	ARG	4.1
1	B	27	GLY	4.1
1	B	423	GLU	4.1
1	B	374	TRP	4.0
1	A	271	GLY	4.0
1	B	422	ASP	4.0
1	B	23	VAL	3.9
1	B	14	LEU	3.9
1	B	409	ARG	3.8
1	B	81	HIS	3.8
1	B	68	GLY	3.8
1	B	22	LEU	3.7
1	B	353	ASP	3.7
1	B	407	PRO	3.7
1	B	6	SER	3.7
1	B	86	LYS	3.6
1	B	35	ASN	3.6
1	B	271	GLY	3.5
1	B	316	ALA	3.5
1	B	401	HIS	3.5
1	B	415	GLU	3.5
1	B	398	LEU	3.5
1	B	400	ARG	3.4
1	A	157	ILE	3.4
1	B	381	VAL	3.3
1	B	390	GLN	3.3
1	B	346	ALA	3.3
1	B	425	ASP	3.2
1	A	313	ILE	3.2
1	B	84	ARG	3.2
1	B	256	PHE	3.2
1	B	371	PHE	3.2
1	B	247	TRP	3.2
1	B	9	CYS	3.2
1	B	210	ARG	3.1
1	B	101	LEU	3.1
1	A	272	GLY	3.1
1	B	57	VAL	3.0
1	B	85	GLU	3.0
1	B	408	LEU	3.0
1	B	71	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	144	PRO	2.9
1	B	347	PRO	2.9
1	A	286	ALA	2.9
1	B	89	GLU	2.8
1	B	385	ILE	2.8
1	B	20	GLY	2.8
1	B	394	VAL	2.8
1	A	156	VAL	2.8
1	B	258	GLU	2.8
1	B	135	ILE	2.8
1	B	73	VAL	2.8
1	B	157	ILE	2.8
1	B	380	ILE	2.8
1	B	317	ALA	2.7
1	B	116	THR	2.7
1	B	29	SER	2.7
1	B	13	GLU	2.6
1	B	207	PHE	2.6
1	B	416	THR	2.6
1	B	369	GLY	2.6
1	B	62	VAL	2.6
1	A	246	ARG	2.6
1	B	34	ASP	2.6
1	B	418	ILE	2.5
1	B	350	ALA	2.5
1	B	87	CYS	2.5
1	B	313	ILE	2.5
1	A	367	LEU	2.4
1	A	28	GLY	2.4
1	A	289	MET	2.4
1	B	102	ALA	2.4
1	B	8	PRO	2.4
1	A	5	ALA	2.4
1	B	397	ASP	2.4
1	B	28	GLY	2.3
1	B	290	LEU	2.3
1	B	314	SER	2.3
1	A	119	ARG	2.3
1	A	266	VAL	2.3
1	A	274	ARG	2.3
1	B	90	LEU	2.3
1	B	312	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	12	GLU	2.2
1	A	428	GLU	2.2
1	A	312	TYR	2.2
1	A	12	GLU	2.2
1	A	308	LEU	2.2
1	B	70	ARG	2.2
1	B	330	MET	2.2
1	B	389	VAL	2.2
1	B	375	ARG	2.1
1	B	260	VAL	2.1
1	B	411	SER	2.1
1	A	278	LYS	2.1
1	A	137	PRO	2.1
1	B	82	LEU	2.1
1	B	209	THR	2.1
1	A	114	VAL	2.1
1	B	15	SER	2.1
1	A	290	LEU	2.1
1	A	303	ILE	2.1
1	B	417	LEU	2.1
1	B	424	ALA	2.0
1	A	267	GLN	2.0
1	A	339	ALA	2.0
1	B	53	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

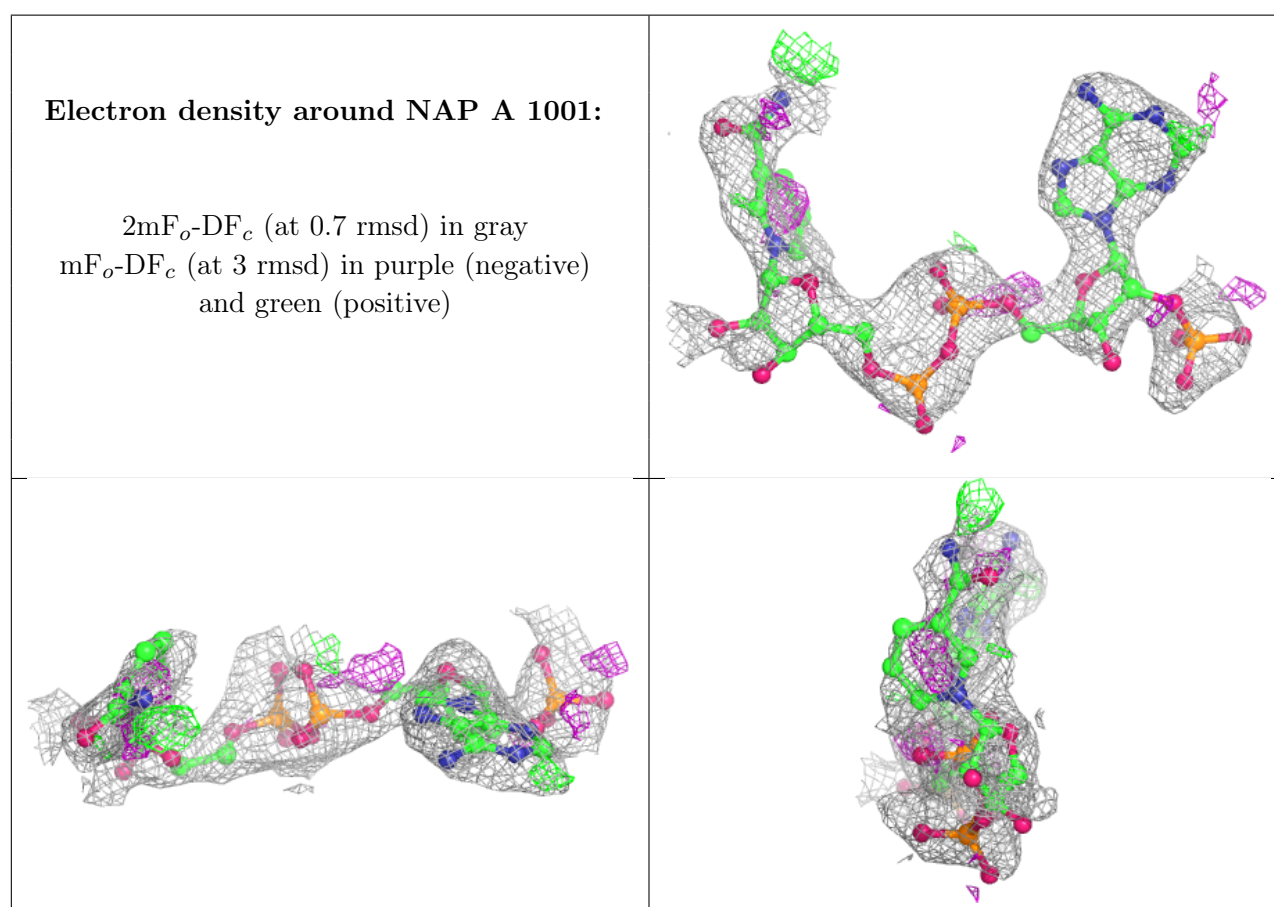There are no non-standard protein/DNA/RNA residues in this entry.

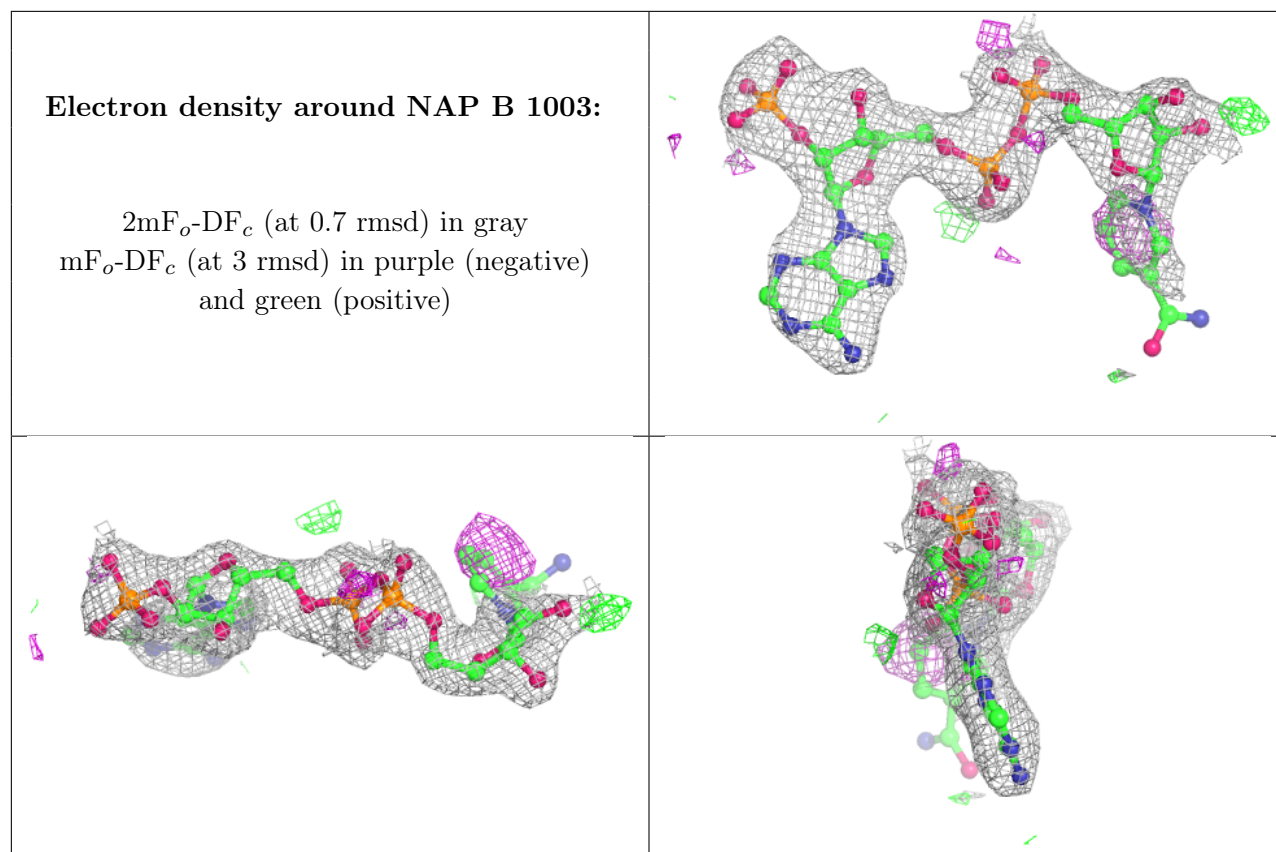## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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	NAP	A	1001	48/48	0.77	0.25	26,31,35,37	0
4	ICT	A	1002	13/13	0.88	0.20	25,29,31,32	0
3	NAP	B	1003	48/48	0.92	0.16	27,31,33,34	0
4	ICT	B	1004	13/13	0.92	0.18	20,24,27,29	0
2	CA	A	1005	1/1	0.96	0.15	30,30,30,30	0
2	CA	A	1006	1/1	0.99	0.21	23,23,23,23	0

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

Electron density around NAP A 1001:

$2mF_o$-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 1003:

$2mF_o$-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 ⓘ

There are no such residues in this entry.