W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:16 PM GMT

PDB ID	:	1SUW
Title	:	Crystal structure of a NAD kinase from Archaeoglobus fulgidus in complex with its substrate and product: Insights into the catalysis of NAD kinase
Authors	:	Liu, J.; Lou, Y.; Yokota, H.; Adams, P.D.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2004-03-26
Resolution	:	2.45 Å(reported)

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

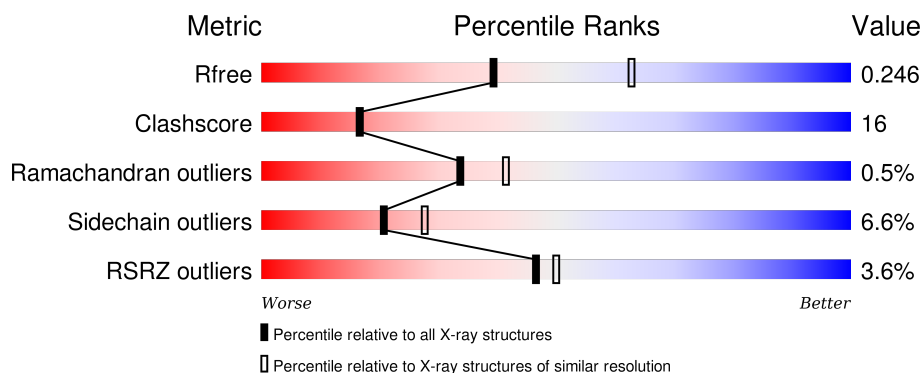|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.45 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		0.246
Clashscore		16
Ramachandran outliers		0.5%
Sidechain outliers		6.6%
RSRZ outliers		3.6%

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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	249	4% / 65% / 32% / •
1	B	249	4% / 60% / 37% / •
1	C	249	4% / 64% / 33% / •
1	D	249	2% / 67% / 32% / •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8351 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 Probable inorganic polyphosphate/ATP-NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1964	1266	334	356	8	0	0	0
1	B	249	Total	C	N	O	S	0	0	0
			1964	1266	334	356	8			
1	C	249	Total	C	N	O	S	0	0	0
			1964	1266	334	356	8			
1	D	249	Total	C	N	O	S	0	0	0
			1964	1266	334	356	8			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
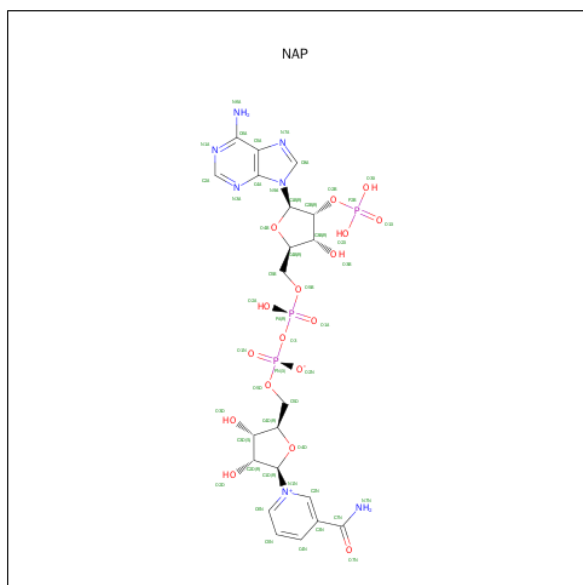
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	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	70	Total	O	0	0
			70	70		
3	B	67	Total	O	0	0
			67	67		
3	C	83	Total	O	0	0
			83	83		
3	D	83	Total	O	0	0
			83	83		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the secon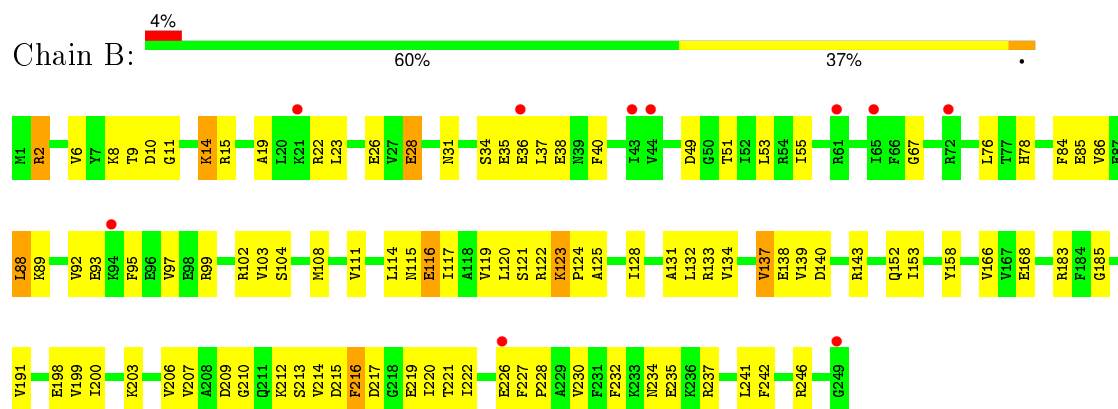d graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above 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: Probable inorganic polyphosphate/ATP-NAD kinase
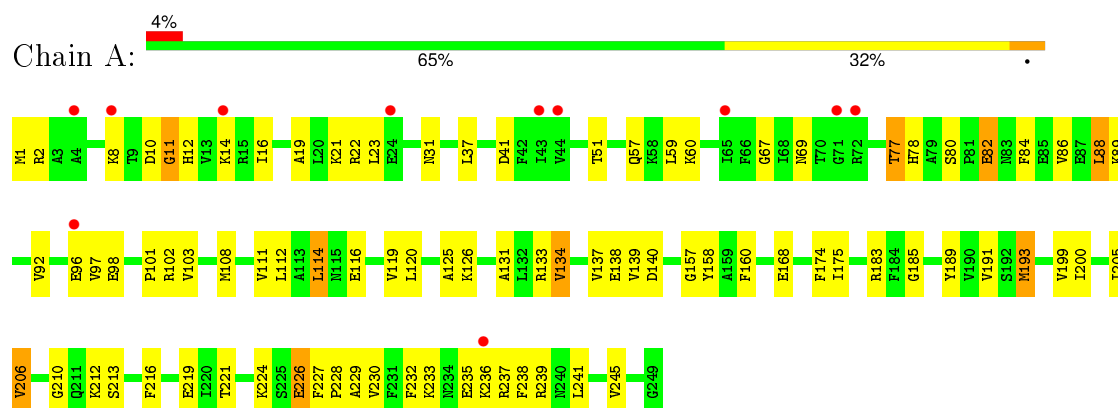
- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

F216 I220 T221 I222 E226 F227 P228 A229 F232 K233 N234 E235 K236 R237 F238 R239 R246 G249

• Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

Chain D:

M1 R2 V6 G11 K14 R15 I16 E17 E18 A19 L20 K21 R22 L23 E26 T43 V44 I55 L59 K60 R61 C62 P63 P64 I65 F66 G67 I68 N69 T70 G71 R72 H78 A79 S80 P81 F84 E85 V86 E87 L88 K89 K90 A91 V92 E93 K94 F95 E96 V97 E98

R99 R102 V103 S104 C105 M108 V111 L114 N115 E116 L120 S121 A125 A131 L132 R133 V134 V137 E138 V139 D140 Q152 S155 Y158 V166 V167 E168 P169 Y170 I175 L176 R183 F184 G185 K196 I197 I200 D209 G210 V214 D215

E219 I220 T221 I222 E223 F227 V230 F231 F232 E235 K236 R237 F238 R239 N240 L241 F242 G243 K244 G249
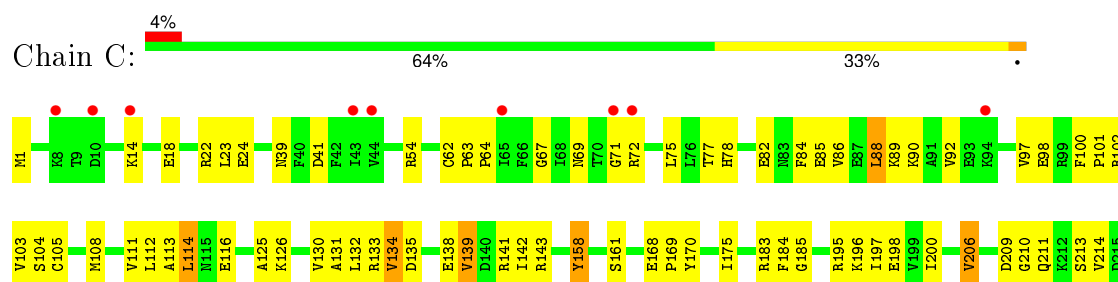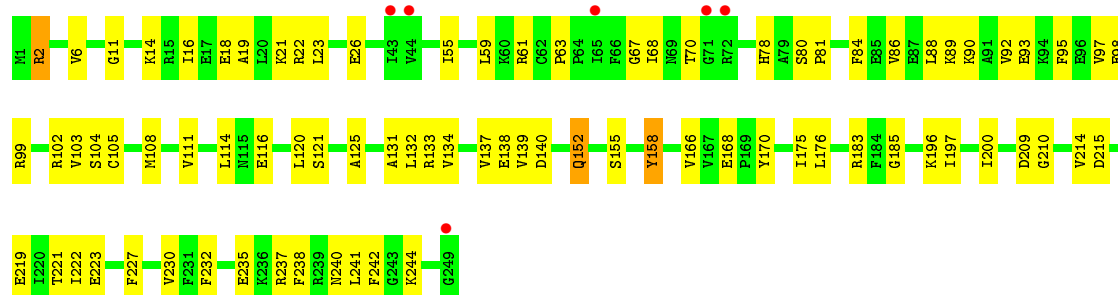
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.14Å 122.14Å 198.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 19.98 – 2.34	Depositor EDS
% Data completeness (in resolution range)	82.5 (20.00-2.45) 80.0 (19.98-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.20 (at 2.35Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.252 0.213 , 0.246	Depositor DCC
R_{free} test set	2790 reflections (6.37%)	DCC
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\lvert L\rvert> = 0.50, <L^2> = 0.34$	Xtriage
Outliers	2 of 62718 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8351	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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 49.35 % 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 7.5493e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.40	0/2002	0.63	0/2699
1	B	0.39	0/2002	0.62	0/2699
1	C	0.40	0/2002	0.71	2/2699 (0.1%)
1	D	0.41	0/2002	0.65	1/2699 (0.0%)
All	All	0.40	0/8008	0.65	3/10796 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	71	GLY	N-CA-C	11.68	142.31	113.10
1	C	72	ARG	N-CA-CB	-10.00	92.60	110.60
1	D	61	ARG	N-CA-C	-5.65	95.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1964	0	2015	73	0
1	B	1964	0	2015	88	0
1	C	1964	0	2015	67	0
1	D	1964	0	2015	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	48	0	25	3	0
2	B	48	0	25	3	0
2	C	48	0	25	6	0
2	D	48	0	25	4	0
3	A	70	0	0	5	0
3	B	67	0	0	4	0
3	C	83	0	0	5	0
3	D	83	0	0	2	0
All	All	8351	0	8160	267	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 16.

All (267) 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:14:LYS:HA	1:B:14:LYS:HE3	1.42	1.01
1:A:67:GLY:H	1:A:78:HIS:HD2	1.05	0.97
1:D:183:ARG:HD2	1:D:185:GLY:O	1.73	0.89
1:C:67:GLY:H	1:C:78:HIS:HD2	1.19	0.88
1:A:67:GLY:H	1:A:78:HIS:CD2	1.94	0.83
1:D:133:ARG:HG2	1:D:138:GLU:HA	1.60	0.83
1:A:69:ASN:HB2	1:A:77:THR:HG21	1.60	0.81
1:D:67:GLY:H	1:D:78:HIS:HD2	1.26	0.80
1:C:142:ILE:HD12	1:C:143:ARG:H	1.47	0.77
1:D:23:LEU:HD13	1:D:92:VAL:HG11	1.65	0.77
1:B:183:ARG:HD2	1:B:185:GLY:O	1.86	0.75
1:B:198:GLU:HG2	1:B:221:THR:HG22	1.71	0.73
1:C:67:GLY:H	1:C:78:HIS:CD2	2.06	0.72
1:A:23:LEU:HD21	1:A:89:LYS:HG2	1.71	0.72
1:B:246:ARG:HD3	3:B:3103:HOH:O	1.90	0.71
1:C:23:LEU:HD13	1:C:92:VAL:HG11	1.74	0.69
1:D:89:LYS:O	1:D:93:GLU:HG2	1.91	0.69
1:B:2:ARG:HB3	1:B:26:GLU:HB3	1.75	0.69
1:B:102:ARG:HD3	1:B:227:PHE:O	1.92	0.68
1:B:67:GLY:H	1:B:78:HIS:HD2	1.40	0.68
1:B:122:ARG:HE	1:B:215:ASP:HB3	1.59	0.68
1:C:133:ARG:HG2	1:C:138:GLU:HA	1.75	0.67
1:A:23:LEU:HD13	1:A:92:VAL:HG11	1.76	0.66
1:B:134:VAL:O	1:B:137:VAL:HG13	1.94	0.66
1:A:86:VAL:HG23	3:A:3117:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:GLY:H	1:D:78:HIS:CD2	2.12	0.65
1:D:152:GLN:H	1:D:152:GLN:NE2	1.94	0.65
1:B:200:ILE:HD12	1:B:200:ILE:N	2.14	0.63
1:B:23:LEU:HD13	1:B:92:VAL:HG11	1.79	0.63
1:D:131:ALA:HB3	1:D:200:ILE:HB	1.80	0.63
1:A:102:ARG:HD3	1:A:227:PHE:O	2.00	0.62
1:C:24:GLU:HB2	3:C:3110:HOH:O	1.99	0.62
1:A:80:SER:OG	1:A:82:GLU:HG2	1.99	0.62
1:B:117:ILE:HG21	1:B:222:ILE:HD11	1.82	0.62
1:A:67:GLY:N	1:A:78:HIS:HD2	1.88	0.62
1:B:143:ARG:HD3	1:C:249:GLY:O	2.00	0.61
1:A:98:GLU:OE1	1:A:237:ARG:NH1	2.33	0.61
1:C:98:GLU:OE1	1:C:237:ARG:NH1	2.33	0.61
1:D:78:HIS:HE1	1:D:232:PHE:O	1.82	0.61
1:A:37:LEU:HB2	1:A:59:LEU:HD21	1.83	0.61
1:B:210:GLY:HA3	2:B:3076:NAP:H51N	1.81	0.60
1:D:152:GLN:H	1:D:152:GLN:HE21	1.50	0.60
1:C:210:GLY:HA3	2:C:3077:NAP:H51N	1.83	0.60
1:A:140:ASP:CG	1:B:246:ARG:HH21	2.06	0.59
1:B:99:ARG:HG2	1:B:230:VAL:HG22	1.85	0.58
1:A:189:TYR:HD2	1:B:166:VAL:HG22	1.67	0.58
1:D:19:ALA:O	1:D:23:LEU:HG	2.03	0.58
1:A:22:ARG:HD2	1:A:89:LYS:HZ1	1.68	0.58
1:B:120:LEU:CD1	1:C:125:ALA:HB2	2.34	0.58
1:A:57:GLN:HE21	1:A:212:LYS:HG3	1.69	0.58
1:A:22:ARG:HH11	1:A:89:LYS:HZ1	1.51	0.58
1:B:103:VAL:CG1	1:B:222:ILE:HG23	2.34	0.57
1:A:134:VAL:CG1	1:A:139:VAL:HG21	2.34	0.57
1:A:108:MET:O	1:A:111:VAL:HG22	2.05	0.57
1:C:142:ILE:HD11	1:C:183:ARG:HB2	1.87	0.56
1:D:99:ARG:HG2	1:D:230:VAL:HG22	1.87	0.56
1:D:139:VAL:O	1:D:140:ASP:HB2	2.03	0.56
1:B:206:VAL:HG21	1:B:220:ILE:HD13	1.88	0.56
1:A:88:LEU:O	1:A:92:VAL:HG12	2.05	0.56
1:D:86:VAL:HG12	1:D:90:LYS:HE3	1.87	0.56
1:C:142:ILE:HD12	1:C:143:ARG:N	2.20	0.56
1:B:84:PHE:O	1:B:88:LEU:HB2	2.05	0.56
1:D:105:CYS:HA	1:D:221:THR:O	2.05	0.56
1:B:53:LEU:HD11	1:B:115:ASN:ND2	2.21	0.56
1:D:103:VAL:CG1	1:D:104:SER:N	2.69	0.56
1:A:84:PHE:O	1:A:88:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LYS:O	1:B:93:GLU:HG3	2.05	0.55
1:B:207:VAL:HG22	1:B:213:SER:HB3	1.88	0.55
1:C:84:PHE:O	1:C:88:LEU:HB2	2.07	0.55
1:A:120:LEU:HD13	1:D:125:ALA:HB2	1.89	0.55
1:A:125:ALA:HB2	1:D:120:LEU:CD1	2.37	0.54
1:B:234:ASN:HB3	1:B:237:ARG:HH11	1.72	0.54
1:B:97:VAL:HG13	1:B:230:VAL:HG13	1.89	0.54
1:C:206:VAL:HG22	1:C:216:PHE:CD1	2.42	0.54
1:B:123:LYS:N	1:B:123:LYS:HD3	2.23	0.54
1:D:108:MET:O	1:D:111:VAL:HG22	2.08	0.54
1:C:184:PHE:HB3	3:C:3131:HOH:O	2.08	0.54
1:A:69:ASN:CB	1:A:77:THR:HG21	2.37	0.54
1:D:102:ARG:HD3	1:D:227:PHE:O	2.07	0.54
1:D:134:VAL:HG13	1:D:139:VAL:HG11	1.88	0.53
1:D:168:GLU:HG3	1:D:238:PHE:CE1	2.43	0.53
1:C:86:VAL:HG12	1:C:90:LYS:HE3	1.90	0.53
1:A:183:ARG:HD2	1:A:185:GLY:O	2.08	0.53
1:A:237:ARG:NH2	3:A:3097:HOH:O	2.41	0.53
1:C:175:ILE:HD12	1:C:175:ILE:N	2.23	0.53
1:B:122:ARG:NH2	1:B:217:ASP:OD2	2.40	0.53
1:A:238:PHE:HE2	1:B:134:VAL:HG23	1.73	0.53
1:C:246:ARG:NH2	1:D:139:VAL:O	2.41	0.53
1:B:206:VAL:CG2	1:B:220:ILE:HD13	2.38	0.53
1:D:19:ALA:HA	1:D:22:ARG:NH1	2.25	0.52
1:B:108:MET:O	1:B:111:VAL:HG22	2.09	0.52
1:C:139:VAL:HG23	1:D:242:PHE:CD2	2.44	0.52
1:B:9:THR:HG22	1:B:10:ASP:N	2.24	0.52
1:B:121:SER:HB3	1:B:128:ILE:HG23	1.91	0.52
1:B:8:LYS:HE3	1:B:51:THR:OG1	2.09	0.52
3:B:3108:HOH:O	1:C:126:LYS:HE2	2.10	0.52
1:B:131:ALA:HB3	1:B:200:ILE:HB	1.92	0.52
1:B:119:VAL:C	1:B:120:LEU:HD23	2.30	0.52
1:D:168:GLU:OE2	1:D:170:TYR:HB2	2.10	0.51
1:A:131:ALA:HB3	1:A:200:ILE:HB	1.91	0.51
1:C:103:VAL:CG1	1:C:104:SER:N	2.73	0.51
1:B:133:ARG:HG2	1:B:138:GLU:HA	1.90	0.51
1:D:84:PHE:O	1:D:88:LEU:HB2	2.10	0.51
1:A:77:THR:CG2	1:A:78:HIS:N	2.73	0.51
1:C:131:ALA:HB3	1:C:200:ILE:HB	1.92	0.51
1:B:210:GLY:HA3	2:B:3076:NAP:C5D	2.40	0.51
1:D:6:VAL:HB	1:D:55:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASN:HB2	1:C:77:THR:OG1	2.10	0.51
1:C:105:CYS:HA	1:C:221:THR:O	2.11	0.51
1:C:54:ARG:NH1	1:C:211:GLN:OE1	2.44	0.51
1:B:122:ARG:HB2	1:B:123:LYS:HD3	1.92	0.51
1:A:189:TYR:HD2	1:B:166:VAL:CG2	2.23	0.51
2:A:3075:NAP:H52N	2:A:3075:NAP:H6N	1.91	0.51
1:B:134:VAL:HG22	1:B:139:VAL:HG11	1.93	0.50
1:D:132:LEU:HD21	1:D:176:LEU:HD13	1.92	0.50
1:A:134:VAL:HG13	1:A:139:VAL:HG21	1.93	0.50
1:A:103:VAL:HG11	1:A:174:PHE:CE2	2.46	0.50
1:D:155:SER:HB3	1:D:175:ILE:CD1	2.42	0.50
1:C:85:GLU:O	1:C:89:LYS:HG3	2.11	0.50
1:C:168:GLU:OE2	1:C:170:TYR:HB2	2.12	0.50
1:C:78:HIS:HE1	1:C:232:PHE:O	1.95	0.49
1:B:103:VAL:CG1	1:B:104:SER:N	2.75	0.49
1:A:140:ASP:OD2	1:A:183:ARG:NH2	2.40	0.49
1:C:210:GLY:HA3	2:C:3077:NAP:C5D	2.43	0.49
1:C:103:VAL:HG12	1:C:104:SER:N	2.27	0.49
1:D:210:GLY:HA3	2:D:3078:NAP:C5D	2.43	0.49
1:C:206:VAL:O	1:C:213:SER:HA	2.13	0.49
1:A:78:HIS:HE1	1:A:232:PHE:O	1.96	0.49
1:D:210:GLY:HA3	2:D:3078:NAP:H52N	1.93	0.49
1:C:228:PRO:HG3	3:C:3125:HOH:O	2.13	0.48
1:B:103:VAL:HG11	1:B:222:ILE:HG23	1.95	0.48
1:C:102:ARG:HD2	1:C:229:ALA:HB2	1.95	0.48
1:B:140:ASP:CG	1:B:183:ARG:HH22	2.15	0.48
1:D:103:VAL:HG12	1:D:104:SER:N	2.27	0.48
1:A:191:VAL:HA	1:B:168:GLU:HG2	1.96	0.48
1:B:120:LEU:HD12	1:C:125:ALA:HB2	1.96	0.48
1:A:21:LYS:C	1:A:23:LEU:H	2.18	0.48
1:A:175:ILE:HD12	1:A:175:ILE:N	2.29	0.47
1:C:75:LEU:HD12	2:C:3077:NAP:C2A	2.44	0.47
1:A:60:LYS:HD3	3:A:3099:HOH:O	2.12	0.47
1:C:108:MET:O	1:C:111:VAL:HG22	2.14	0.47
1:C:18:GLU:O	1:C:22:ARG:HG3	2.15	0.47
1:A:12:HIS:O	1:A:16:ILE:HG13	2.13	0.47
1:A:139:VAL:HG13	1:B:242:PHE:CD2	2.50	0.47
1:A:103:VAL:HG11	1:A:174:PHE:HE2	1.80	0.47
1:C:102:ARG:NH2	1:C:112:LEU:HD12	2.30	0.47
1:D:197:ILE:HB	1:D:222:ILE:HB	1.96	0.47
1:C:113:ALA:HA	1:C:209:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:O	1:A:23:LEU:HG	2.15	0.47
1:B:134:VAL:HG23	1:B:134:VAL:O	2.15	0.46
1:A:125:ALA:HB2	1:D:120:LEU:HD11	1.97	0.46
1:A:226:GLU:O	1:A:228:PRO:HD3	2.15	0.46
1:A:14:LYS:HE3	1:A:14:LYS:HA	1.96	0.46
1:B:124:PRO:O	1:B:125:ALA:HB3	2.16	0.46
1:B:200:ILE:HG13	1:B:219:GLU:HG3	1.98	0.46
1:C:134:VAL:HA	1:C:196:LYS:O	2.14	0.46
1:B:226:GLU:O	1:B:228:PRO:HD3	2.16	0.46
1:B:6:VAL:HB	1:B:55:ILE:HD11	1.97	0.46
1:B:108:MET:HG2	1:B:214:VAL:HG21	1.97	0.46
1:B:120:LEU:HD11	1:C:125:ALA:HB2	1.97	0.46
1:C:134:VAL:HG12	1:C:139:VAL:HG11	1.98	0.46
1:A:133:ARG:HG2	1:A:138:GLU:HA	1.98	0.46
1:C:183:ARG:HD2	1:C:185:GLY:O	2.16	0.46
1:B:140:ASP:OD1	1:B:183:ARG:NH2	2.44	0.46
1:A:77:THR:HG23	1:A:78:HIS:N	2.31	0.46
1:A:22:ARG:NH1	1:A:89:LYS:HZ1	2.12	0.46
1:B:214:VAL:HG12	1:B:215:ASP:O	2.16	0.46
1:D:134:VAL:HA	1:D:196:LYS:O	2.15	0.45
1:C:41:ASP:O	1:C:64:PRO:HD2	2.16	0.45
1:D:121:SER:HB2	3:D:3157:HOH:O	2.15	0.45
1:A:22:ARG:HG2	1:A:22:ARG:O	2.16	0.45
1:B:97:VAL:CG1	1:B:230:VAL:HG13	2.46	0.45
1:A:69:ASN:HB2	1:A:77:THR:CG2	2.41	0.45
1:C:89:LYS:HA	1:C:92:VAL:HG12	1.99	0.45
1:B:132:LEU:O	1:B:139:VAL:HG22	2.16	0.45
1:B:115:ASN:HB3	1:B:116:GLU:OE2	2.16	0.45
1:C:206:VAL:HG22	1:C:216:PHE:CE1	2.52	0.45
1:A:233:LYS:HE2	3:A:3091:HOH:O	2.15	0.45
1:C:132:LEU:HG	1:C:139:VAL:CG1	2.45	0.45
1:B:152:GLN:HG2	1:B:153:ILE:N	2.32	0.45
1:A:102:ARG:NH2	1:A:112:LEU:HD12	2.32	0.45
1:A:97:VAL:CG1	1:A:98:GLU:N	2.80	0.45
1:B:122:ARG:NH1	1:B:203:LYS:HA	2.32	0.45
1:B:209:ASP:O	2:B:3076:NAP:H51N	2.18	0.44
1:A:97:VAL:HG13	1:A:230:VAL:HG13	1.98	0.44
1:C:198:GLU:HG2	1:C:221:THR:HG22	1.97	0.44
1:C:220:ILE:O	1:C:220:ILE:HG13	2.17	0.44
1:D:168:GLU:HG3	1:D:238:PHE:HE1	1.81	0.44
1:A:210:GLY:HA3	2:A:3075:NAP:H51N	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:HG23	3:B:3093:HOH:O	2.18	0.44
1:C:158:TYR:HB2	2:C:3077:NAP:H2D	1.99	0.44
1:C:88:LEU:O	1:C:92:VAL:HG12	2.17	0.44
1:B:117:ILE:CG2	1:B:222:ILE:HD11	2.45	0.44
1:B:14:LYS:HE3	1:B:14:LYS:CA	2.24	0.44
1:A:114:LEU:HD22	1:A:114:LEU:O	2.17	0.44
1:C:237:ARG:NH2	3:C:3087:HOH:O	2.47	0.44
1:B:15:ARG:HG2	1:B:15:ARG:HH11	1.82	0.44
1:D:18:GLU:O	1:D:21:LYS:HB3	2.18	0.43
1:B:103:VAL:HG11	1:B:222:ILE:CG2	2.48	0.43
1:A:228:PRO:HG3	3:A:3135:HOH:O	2.18	0.43
1:A:206:VAL:HG22	1:A:216:PHE:CE1	2.53	0.43
1:B:132:LEU:HG	1:B:139:VAL:CG2	2.48	0.43
1:B:216:PHE:CE2	1:B:220:ILE:HG23	2.53	0.43
1:D:200:ILE:HG12	1:D:219:GLU:HG3	2.00	0.43
1:B:111:VAL:HG12	1:B:212:LYS:HD2	1.99	0.43
1:B:35:GLU:O	1:B:38:GLU:HG3	2.18	0.43
1:C:169:PRO:HG3	3:C:3127:HOH:O	2.18	0.43
1:B:78:HIS:HE1	1:B:232:PHE:O	2.00	0.43
1:C:132:LEU:HG	1:C:139:VAL:HG13	2.01	0.43
2:A:3075:NAP:H5N	1:D:125:ALA:O	2.19	0.43
1:C:168:GLU:HG3	1:C:238:PHE:CE1	2.53	0.43
1:A:168:GLU:HG2	1:B:191:VAL:HA	1.99	0.43
1:C:239:ARG:CB	1:D:137:VAL:HG21	2.49	0.43
1:B:134:VAL:HG22	1:B:139:VAL:CG1	2.48	0.43
1:A:200:ILE:HG12	1:A:219:GLU:HG3	2.00	0.43
1:C:1:MET:HG3	1:C:41:ASP:CG	2.39	0.43
1:A:10:ASP:O	1:A:11:GLY:C	2.56	0.43
1:A:23:LEU:HD21	1:A:89:LYS:HE3	2.01	0.43
1:B:67:GLY:H	1:B:78:HIS:CD2	2.28	0.43
1:B:108:MET:SD	1:B:214:VAL:HG23	2.59	0.42
2:C:3077:NAP:H6N	2:C:3077:NAP:H52N	1.99	0.42
1:A:193:MET:HE2	1:A:224:LYS:HG3	2.01	0.42
1:D:14:LYS:O	1:D:18:GLU:HG3	2.19	0.42
1:D:2:ARG:HB3	1:D:26:GLU:HB3	2.01	0.42
1:B:85:GLU:HB2	3:B:3093:HOH:O	2.19	0.42
1:A:206:VAL:HG22	1:A:216:PHE:CD1	2.54	0.42
1:A:120:LEU:CD1	1:D:125:ALA:HB2	2.49	0.42
1:D:98:GLU:OE1	1:D:237:ARG:NH1	2.52	0.42
1:B:34:SER:C	1:B:36:GLU:N	2.73	0.42
1:B:200:ILE:CD1	1:B:200:ILE:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:LEU:HD22	1:D:63:PRO:HD2	2.02	0.42
1:B:119:VAL:HG21	1:B:199:VAL:HG11	2.02	0.42
1:B:28:GLU:HB2	1:B:40:PHE:HE2	1.85	0.42
1:A:157:GLY:O	1:A:160:PHE:HB3	2.20	0.42
1:D:86:VAL:O	1:D:90:LYS:HG3	2.20	0.42
1:A:236:LYS:HD3	1:A:239:ARG:HD2	2.01	0.42
1:B:19:ALA:O	1:B:23:LEU:HG	2.18	0.42
1:B:88:LEU:O	1:B:92:VAL:HG12	2.19	0.42
1:C:1:MET:HG3	1:C:41:ASP:OD2	2.19	0.42
1:A:205:ILE:HD11	1:A:213:SER:HB2	2.02	0.42
1:C:197:ILE:HB	1:C:222:ILE:HB	2.02	0.41
1:B:103:VAL:HG12	1:B:104:SER:N	2.36	0.41
1:D:209:ASP:O	2:D:3078:NAP:H51N	2.21	0.41
1:C:114:LEU:O	1:C:114:LEU:HD22	2.20	0.41
1:A:8:LYS:NZ	1:A:51:THR:HA	2.36	0.41
1:C:233:LYS:HE2	1:C:235:GLU:OE1	2.21	0.41
1:D:133:ARG:HH21	1:D:200:ILE:HD11	1.86	0.41
1:B:119:VAL:O	1:B:120:LEU:HD23	2.21	0.41
1:B:22:ARG:NH2	1:B:85:GLU:OE1	2.53	0.41
1:D:240:ASN:HB3	1:D:244:LYS:HE3	2.02	0.41
1:B:49:ASP:HB3	1:B:76:LEU:HD12	2.03	0.41
1:D:16:ILE:HD13	1:D:68:ILE:HD12	2.02	0.41
1:A:119:VAL:HG21	1:A:199:VAL:HG11	2.02	0.41
1:D:214:VAL:HG12	1:D:215:ASP:O	2.21	0.41
1:C:130:VAL:O	1:C:141:ARG:HA	2.21	0.41
1:A:126:LYS:HG2	3:D:3099:HOH:O	2.19	0.41
1:C:161:SER:OG	2:C:3077:NAP:N7N	2.52	0.40
1:C:134:VAL:HG22	1:D:238:PHE:CE2	2.57	0.40
1:C:100:PHE:HA	1:C:101:PRO:HD3	1.91	0.40
1:C:135:ASP:OD2	1:C:195:ARG:HG2	2.21	0.40
1:A:102:ARG:HD2	1:A:229:ALA:HB2	2.03	0.40
1:A:1:MET:HA	1:A:41:ASP:OD2	2.22	0.40
1:D:158:TYR:HB2	2:D:3078:NAP:H2D	2.03	0.40
1:A:101:PRO:HB2	1:A:193:MET:CE	2.51	0.40
1:B:28:GLU:HB2	1:B:40:PHE:CE2	2.56	0.40
1:C:62:CYS:HA	1:C:63:PRO:HD2	1.95	0.40
1:D:80:SER:HB2	1:D:81:PRO:CD	2.51	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	247/249 (99%)	237 (96%)	9 (4%)	1 (0%)	39	49
1	B	247/249 (99%)	231 (94%)	14 (6%)	2 (1%)	24	28
1	C	247/249 (99%)	230 (93%)	16 (6%)	1 (0%)	39	49
1	D	247/249 (99%)	233 (94%)	13 (5%)	1 (0%)	39	49
All	All	988/996 (99%)	931 (94%)	52 (5%)	5 (0%)	34	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11	GLY
1	D	11	GLY
1	A	11	GLY
1	B	37	LEU
1	C	214	VAL

5.3.2 Protein sidechains (i)

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	213/213 (100%)	195 (92%)	18 (8%)	13	16
1	B	213/213 (100%)	199 (93%)	14 (7%)	21	28
1	C	213/213 (100%)	201 (94%)	12 (6%)	26	36
1	D	213/213 (100%)	201 (94%)	12 (6%)	26	36
All	All	852/852 (100%)	796 (93%)	56 (7%)	21	28

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

Mol	Chain	Res	Type
1	A	2	ARG
1	A	31	ASN
1	A	77	THR
1	A	82	GLU
1	A	88	LEU
1	A	96	GLU
1	A	114	LEU
1	A	116	GLU
1	A	134	VAL
1	A	137	VAL
1	A	158	TYR
1	A	193	MET
1	A	206	VAL
1	A	221	THR
1	A	226	GLU
1	A	235	GLU
1	A	241	LEU
1	A	245	VAL
1	B	2	ARG
1	B	14	LYS
1	B	28	GLU
1	B	31	ASN
1	B	88	LEU
1	B	95	PHE
1	B	114	LEU
1	B	116	GLU
1	B	123	LYS
1	B	137	VAL
1	B	158	TYR
1	B	216	PHE
1	B	235	GLU
1	B	241	LEU
1	C	14	LYS
1	C	39	ASN
1	C	82	GLU
1	C	88	LEU
1	C	97	VAL
1	C	114	LEU
1	C	116	GLU
1	C	134	VAL
1	C	139	VAL
1	C	158	TYR

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Mol	Chain	Res	Type
1	C	206	VAL
1	C	226	GLU
1	D	2	ARG
1	D	70	THR
1	D	95	PHE
1	D	97	VAL
1	D	114	LEU
1	D	116	GLU
1	D	152	GLN
1	D	158	TYR
1	D	166	VAL
1	D	223	GLU
1	D	235	GLU
1	D	241	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	78	HIS
1	B	57	GLN
1	B	78	HIS
1	C	39	ASN
1	C	57	GLN
1	C	78	HIS
1	D	57	GLN
1	D	78	HIS
1	D	152	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NAP	A	3075	-	42,52,52	1.71	7 (16%)	54,80,80	2.16	13 (24%)
2	NAP	B	3076	-	42,52,52	1.70	8 (19%)	54,80,80	2.22	14 (25%)
2	NAP	C	3077	-	42,52,52	1.66	10 (23%)	54,80,80	2.82	16 (29%)
2	NAP	D	3078	-	42,52,52	1.78	10 (23%)	54,80,80	2.81	16 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	3075	-	-	0/27/67/67	0/5/5/5
2	NAP	B	3076	-	-	0/27/67/67	0/5/5/5
2	NAP	C	3077	-	-	0/27/67/67	0/5/5/5
2	NAP	D	3078	-	-	0/27/67/67	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3075	NAP	PA-O1A	-2.78	1.41	1.51
2	B	3076	NAP	PA-O1A	-2.71	1.41	1.51
2	D	3078	NAP	PA-O1A	-2.68	1.41	1.51
2	C	3077	NAP	PA-O1A	-2.64	1.41	1.51
2	D	3078	NAP	C5B-C4B	2.00	1.58	1.51
2	D	3078	NAP	O4B-C1B	2.02	1.43	1.41
2	C	3077	NAP	C5N-C4N	2.04	1.43	1.38
2	A	3075	NAP	C4A-N3A	2.05	1.38	1.35
2	C	3077	NAP	C6N-C5N	2.07	1.43	1.38
2	B	3076	NAP	C6N-C5N	2.20	1.43	1.38
2	C	3077	NAP	C3N-C7N	2.37	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3077	NAP	C4A-N3A	2.37	1.39	1.35
2	D	3078	NAP	C4A-N3A	2.42	1.39	1.35
2	D	3078	NAP	C6N-C5N	2.51	1.44	1.38
2	B	3076	NAP	C4A-N3A	2.65	1.39	1.35
2	D	3078	NAP	O4D-C1D	3.15	1.45	1.41
2	B	3076	NAP	O4D-C1D	3.27	1.45	1.41
2	C	3077	NAP	O4D-C1D	3.30	1.45	1.41
2	C	3077	NAP	C2A-N3A	3.31	1.38	1.32
2	C	3077	NAP	C6N-N1N	3.36	1.44	1.35
2	B	3076	NAP	C6N-N1N	3.49	1.44	1.35
2	A	3075	NAP	C6N-N1N	3.50	1.44	1.35
2	A	3075	NAP	C2A-N1A	3.53	1.40	1.33
2	A	3075	NAP	O4D-C1D	3.57	1.45	1.41
2	B	3076	NAP	C2A-N1A	3.65	1.40	1.33
2	D	3078	NAP	C6N-N1N	3.70	1.45	1.35
2	A	3075	NAP	C2A-N3A	3.72	1.38	1.32
2	C	3077	NAP	C2A-N1A	3.80	1.41	1.33
2	D	3078	NAP	C2A-N3A	3.90	1.39	1.32
2	B	3076	NAP	C2A-N3A	3.93	1.39	1.32
2	D	3078	NAP	C2A-N1A	4.22	1.41	1.33
2	C	3077	NAP	C4N-C3N	4.56	1.47	1.39
2	A	3075	NAP	C4N-C3N	4.64	1.47	1.39
2	B	3076	NAP	C4N-C3N	4.75	1.47	1.39
2	D	3078	NAP	C4N-C3N	4.89	1.47	1.39

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3077	NAP	O3X-P2B-O1X	-9.16	81.10	110.58
2	D	3078	NAP	O3X-P2B-O1X	-8.94	81.81	110.58
2	B	3076	NAP	N3A-C2A-N1A	-8.03	122.74	128.89
2	D	3078	NAP	N3A-C2A-N1A	-7.91	122.84	128.89
2	C	3077	NAP	N3A-C2A-N1A	-7.84	122.89	128.89
2	A	3075	NAP	N3A-C2A-N1A	-7.60	123.07	128.89
2	B	3076	NAP	O3-PA-O5B	-7.35	83.44	102.94
2	D	3078	NAP	O3-PA-O5B	-7.30	83.57	102.94
2	C	3077	NAP	O3-PA-O5B	-7.17	83.90	102.94
2	A	3075	NAP	O3-PA-O5B	-6.89	84.65	102.94
2	C	3077	NAP	O2A-PA-O3	-5.04	82.23	105.09
2	B	3076	NAP	O2A-PA-O3	-5.00	82.42	105.09
2	A	3075	NAP	O2A-PA-O3	-4.88	82.96	105.09
2	D	3078	NAP	O2A-PA-O3	-4.76	83.49	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3077	NAP	O3X-P2B-O2X	-4.35	90.81	107.38
2	D	3078	NAP	O3X-P2B-O2X	-4.26	91.14	107.38
2	C	3077	NAP	C1B-N9A-C4A	-3.18	122.14	126.94
2	B	3076	NAP	C1B-N9A-C4A	-3.09	122.28	126.94
2	D	3078	NAP	O4B-C1B-C2B	-2.87	101.40	106.60
2	B	3076	NAP	O4B-C4B-C5B	-2.75	99.48	109.32
2	D	3078	NAP	O3B-C3B-C4B	-2.74	102.84	111.05
2	B	3076	NAP	O3B-C3B-C4B	-2.66	103.08	111.05
2	A	3075	NAP	C1B-N9A-C4A	-2.64	122.97	126.94
2	D	3078	NAP	C1B-N9A-C4A	-2.63	122.97	126.94
2	D	3078	NAP	O4B-C4B-C5B	-2.61	99.99	109.32
2	A	3075	NAP	O3B-C3B-C4B	-2.47	103.63	111.05
2	D	3078	NAP	O7N-C7N-C3N	-2.38	116.99	119.59
2	A	3075	NAP	O4B-C4B-C5B	-2.36	100.87	109.32
2	C	3077	NAP	O4B-C4B-C5B	-2.32	101.01	109.32
2	B	3076	NAP	O4D-C1D-N1N	-2.31	105.59	108.13
2	C	3077	NAP	O7N-C7N-C3N	-2.30	117.07	119.59
2	A	3075	NAP	O7N-C7N-C3N	-2.30	117.07	119.59
2	B	3076	NAP	O7N-C7N-C3N	-2.23	117.15	119.59
2	C	3077	NAP	O3B-C3B-C4B	-2.19	104.48	111.05
2	B	3076	NAP	C5N-C4N-C3N	-2.02	117.79	120.33
2	C	3077	NAP	PN-O3-PA	2.02	138.41	132.73
2	B	3076	NAP	C3N-C7N-N7N	2.09	120.11	117.82
2	A	3075	NAP	PN-O3-PA	2.26	139.07	132.73
2	A	3075	NAP	C3N-C7N-N7N	2.28	120.32	117.82
2	A	3075	NAP	O3X-P2B-O2X	2.29	116.11	107.38
2	B	3076	NAP	O3X-P2B-O2X	2.30	116.14	107.38
2	D	3078	NAP	C3N-C7N-N7N	2.31	120.34	117.82
2	C	3077	NAP	C3N-C7N-N7N	2.42	120.47	117.82
2	D	3078	NAP	C4B-O4B-C1B	2.72	112.71	109.72
2	B	3076	NAP	C4B-O4B-C1B	2.87	112.88	109.72
2	C	3077	NAP	C2N-C3N-C4N	3.02	121.65	118.29
2	D	3078	NAP	O2X-P2B-O1X	3.04	120.38	110.58
2	A	3075	NAP	C2N-C3N-C4N	3.21	121.86	118.29
2	B	3076	NAP	C2N-C3N-C4N	3.25	121.91	118.29
2	D	3078	NAP	C2N-C3N-C4N	3.30	121.96	118.29
2	A	3075	NAP	C4B-O4B-C1B	3.44	113.50	109.72
2	C	3077	NAP	O2X-P2B-O1X	3.51	121.88	110.58
2	C	3077	NAP	C4B-O4B-C1B	3.83	113.93	109.72
2	D	3078	NAP	O2A-PA-O1A	4.76	138.35	112.53
2	A	3075	NAP	O2A-PA-O1A	4.82	138.67	112.53
2	B	3076	NAP	O2A-PA-O1A	4.86	138.85	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3077	NAP	O2A-PA-O1A	4.92	139.17	112.53
2	D	3078	NAP	O2B-P2B-O1X	7.58	126.04	107.11
2	C	3077	NAP	O2B-P2B-O1X	7.62	126.14	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3075	NAP	3	0
2	B	3076	NAP	3	0
2	C	3077	NAP	6	0
2	D	3078	NAP	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	249/249 (100%)	0.06	11 (4%)	38	41	36, 58, 97, 104	0
1	B	249/249 (100%)	0.08	10 (4%)	42	45	35, 62, 86, 95	0
1	C	249/249 (100%)	0.05	9 (3%)	46	50	32, 55, 92, 101	0
1	D	249/249 (100%)	-0.05	6 (2%)	62	65	34, 56, 77, 88	0
All	All	996/996 (100%)	0.03	36 (3%)	46	50	32, 58, 89, 104	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	ARG	6.0
1	B	249	GLY	5.5
1	A	72	ARG	4.9
1	D	72	ARG	4.7
1	C	72	ARG	4.3
1	A	43	ILE	4.1
1	C	44	VAL	3.9
1	A	44	VAL	3.9
1	B	44	VAL	3.6
1	C	43	ILE	3.5
1	B	65	ILE	3.2
1	A	14	LYS	3.0
1	D	44	VAL	3.0
1	C	71	GLY	2.8
1	A	96	GLU	2.8
1	A	8	LYS	2.8
1	D	65	ILE	2.7
1	C	8	LYS	2.7
1	B	36	GLU	2.6
1	B	43	ILE	2.6
1	C	65	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLY	2.5
1	A	24	GLU	2.5
1	D	71	GLY	2.4
1	C	14	LYS	2.4
1	C	10	ASP	2.3
1	A	236	LYS	2.3
1	D	43	ILE	2.2
1	B	226	GLU	2.2
1	D	249	GLY	2.2
1	B	94	LYS	2.2
1	C	94	LYS	2.2
1	B	21	LYS	2.1
1	A	4	ALA	2.1
1	A	65	ILE	2.1
1	B	61	ARG	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	NAP	D	3078	48/48	0.89	0.15	0.66	51,66,98,102	0
2	NAP	A	3075	48/48	0.94	0.11	-0.18	47,62,70,74	0
2	NAP	B	3076	48/48	0.93	0.12	-0.19	55,67,73,76	0
2	NAP	C	3077	48/48	0.94	0.12	-0.25	50,60,68,74	0

6.5 Other polymers (i)

There are no such residues in this entry.