Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 05:03 AM EDT

PDB ID	:	2O7P
Title	:	The crystal structure of RibD from Escherichia coli in complex with the oxidised NADP+ cofactor in the active site of the reductase domain
Authors	:	Moche, M.; Stenmark, P.; Gurmu, D.; Nordlund, P.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2006-12-11
Resolution	:	3.00 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36
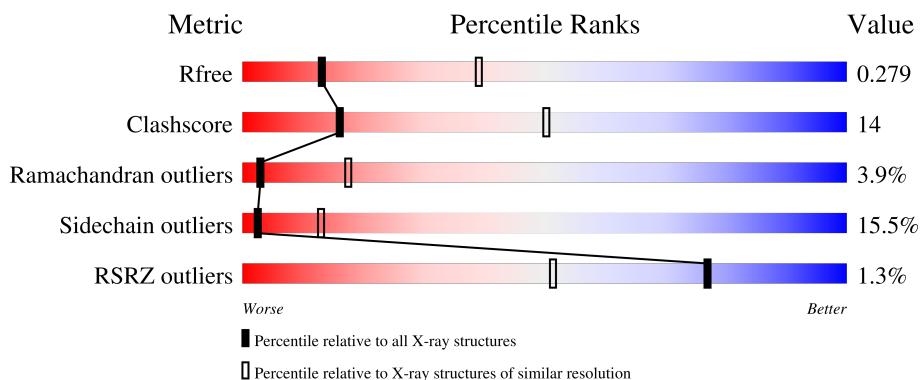
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
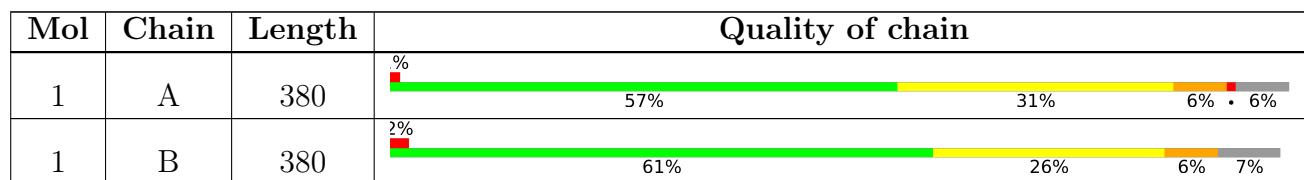
The reported resolution of this entry is 3.00 Å.

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		0.279
Clashscore		14
Ramachandran outliers		3.9%
Sidechain outliers		15.5%
RSRZ outliers		1.3%

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	380	% 57% 31% 6% · 6%
1	B	380	2% 61% 26% 6% 7%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 5523 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 Riboflavin biosynthesis protein ribD.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	Se		0	0	0
			2733	1720	495	503	6	9				
1	B	353	Total	C	N	O	S	Se		0	0	0
			2694	1698	489	496	3	8				

There are 28 discrepancies between the modelled and reference sequences:
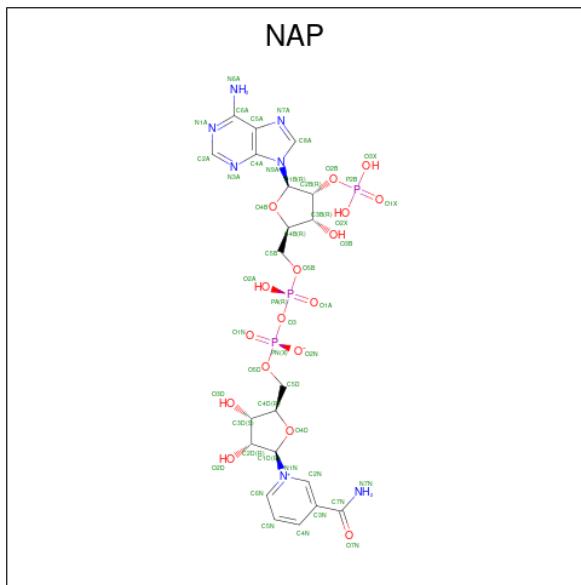
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	THR	-	cloning artifact	UNP P25539
A	-3	LEU	-	cloning artifact	UNP P25539
A	-2	TYR	-	cloning artifact	UNP P25539
A	-1	ILE	-	cloning artifact	UNP P25539
A	0	GLN	-	cloning artifact	UNP P25539
A	1	GLY	-	cloning artifact	UNP P25539
A	368	SER	-	cloning artifact	UNP P25539
A	369	THR	-	cloning artifact	UNP P25539
A	370	HIS	-	expression tag	UNP P25539
A	371	HIS	-	expression tag	UNP P25539
A	372	HIS	-	expression tag	UNP P25539
A	373	HIS	-	expression tag	UNP P25539
A	374	HIS	-	expression tag	UNP P25539
A	375	HIS	-	expression tag	UNP P25539
B	-4	THR	-	cloning artifact	UNP P25539
B	-3	LEU	-	cloning artifact	UNP P25539
B	-2	TYR	-	cloning artifact	UNP P25539
B	-1	ILE	-	cloning artifact	UNP P25539
B	0	GLN	-	cloning artifact	UNP P25539
B	1	GLY	-	cloning artifact	UNP P25539
B	368	SER	-	cloning artifact	UNP P25539
B	369	THR	-	cloning artifact	UNP P25539
B	370	HIS	-	expression tag	UNP P25539
B	371	HIS	-	expression tag	UNP P25539
B	372	HIS	-	expression tag	UNP P25539

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	373	HIS	-	expression tag	UNP P25539
B	374	HIS	-	expression tag	UNP P25539
B	375	HIS	-	expression tag	UNP P25539

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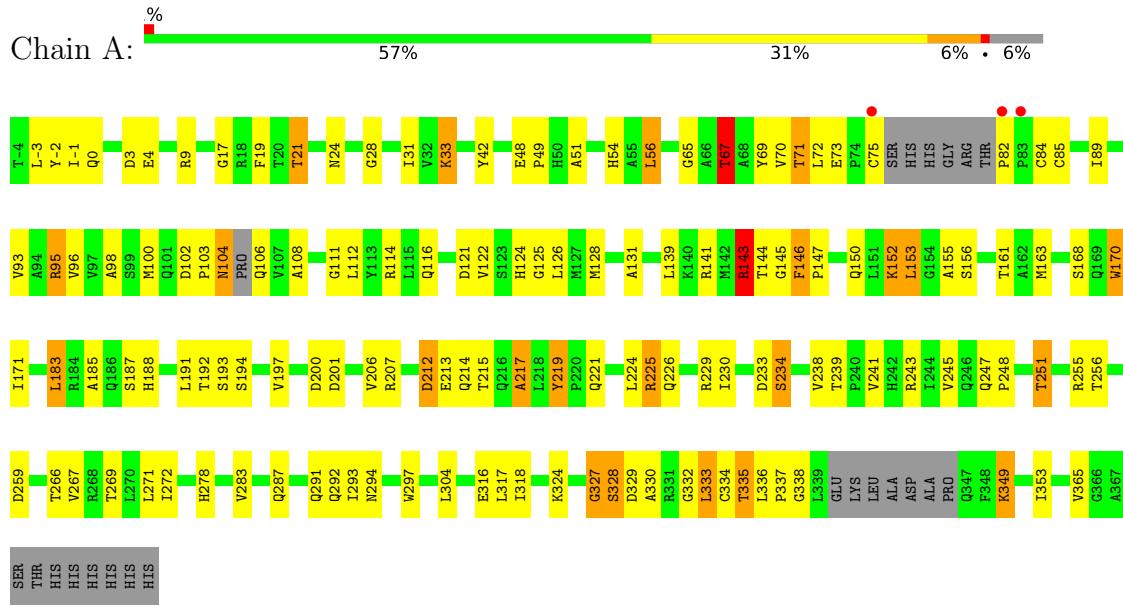
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
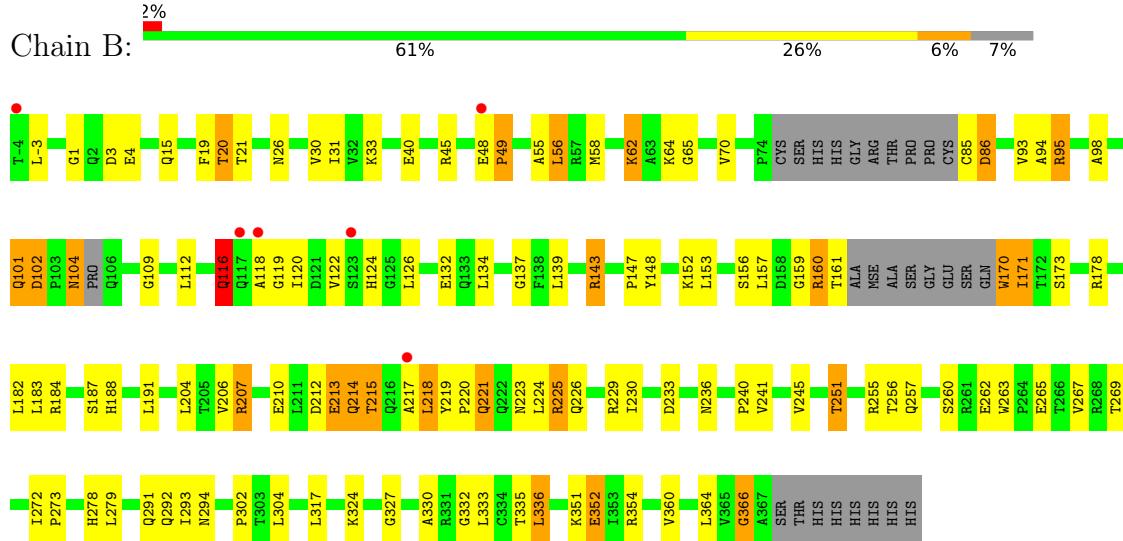
3 Residue-property plots ⓘ

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: Riboflavin biosynthesis protein ribD

• Molecule 1: Riboflavin biosynthesis protein ribD

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.00Å 173.00Å 77.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.93 – 3.00 28.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.93-3.00) 99.9 (28.92-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.267 0.234 , 0.279	Depositor DCC
R_{free} test set	1359 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	93.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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 ⓘ

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	0.82	4/2776 (0.1%)	0.87	3/3753 (0.1%)
1	B	0.82	7/2736 (0.3%)	0.83	4/3703 (0.1%)
All	All	0.82	11/5512 (0.2%)	0.85	7/7456 (0.1%)

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	2
1	B	0	3
All	All	0	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	GLN	CD-OE1	8.29	1.42	1.24
1	B	116	GLN	CD-NE2	8.20	1.53	1.32
1	B	62	LYS	CD-CE	7.45	1.69	1.51
1	A	297	TRP	CD2-CE3	6.82	1.50	1.40
1	A	297	TRP	CD1-NE1	6.46	1.49	1.38
1	B	215	THR	CA-CB	6.20	1.69	1.53
1	A	334	CYS	CB-SG	5.91	1.92	1.82
1	A	297	TRP	CD2-CE2	5.78	1.48	1.41
1	B	64	LYS	CD-CE	5.78	1.65	1.51
1	B	62	LYS	CE-NZ	5.68	1.63	1.49
1	B	262	GLU	CD-OE2	5.32	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	GLN	CG-CD-OE1	-7.85	105.90	121.60
1	A	67	THR	N-CA-C	7.03	129.99	111.00
1	B	116	GLN	OE1-CD-NE2	5.72	135.05	121.90
1	A	143	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	153	LEU	CA-CB-CG	5.19	127.23	115.30
1	B	333	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	218	LEU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLY	Peptide
1	A	217	ALA	Peptide
1	B	116	GLN	Sidechain
1	B	217	ALA	Peptide
1	B	366	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	2733	0	2727	83	0
1	B	2694	0	2686	78	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
All	All	5523	0	5463	158	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 14.

All (158) 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:212:ASP:OD1	1:A:214:GLN:HG2	1.54	1.07
1:B:213:GLU:HA	1:B:213:GLU:OE1	1.59	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:SER:HB3	1:A:233:ASP:HB3	1.46	0.97
1:B:206:VAL:H	1:B:226:GLN:NE2	1.63	0.96
1:A:170:TRP:HH2	1:A:200:ASP:OD1	1.47	0.96
1:B:139:LEU:HB3	1:B:143:ARG:HH12	1.36	0.90
1:B:233:ASP:OD1	1:B:236:ASN:HA	1.81	0.81
1:B:214:GLN:H	1:B:214:GLN:NE2	1.79	0.80
1:A:206:VAL:H	1:A:226:GLN:NE2	1.80	0.79
1:B:139:LEU:HB3	1:B:143:ARG:NH1	1.96	0.79
1:A:188:HIS:HD2	1:A:294:ASN:H	1.31	0.78
1:B:132:GLU:OE2	1:B:143:ARG:NH2	2.16	0.77
1:A:170:TRP:HH2	1:A:200:ASP:CG	1.87	0.76
1:A:194:SER:CB	1:A:233:ASP:HB3	2.16	0.76
1:A:170:TRP:CH2	1:A:200:ASP:OD1	2.38	0.73
1:B:188:HIS:HD2	1:B:294:ASN:H	1.36	0.73
1:B:116:GLN:HE21	1:B:122:VAL:HG22	1.54	0.72
1:A:213:GLU:OE1	1:A:213:GLU:HA	1.90	0.72
1:A:201:ASP:O	1:A:243:ARG:HD3	1.91	0.70
1:B:33:LYS:NZ	1:B:65:GLY:HA3	2.07	0.69
1:A:141:ARG:HH11	1:A:294:ASN:HD21	1.39	0.68
1:B:171:ILE:O	1:B:171:ILE:HG22	1.94	0.66
1:A:139:LEU:O	1:A:143:ARG:HG2	1.94	0.66
1:A:95:ARG:HA	1:A:121:ASP:O	1.95	0.66
1:A:17:GLY:O	1:A:21:THR:HB	1.95	0.66
1:A:33:LYS:NZ	1:A:65:GLY:HA3	2.11	0.65
1:B:170:TRP:HA	1:B:170:TRP:CE3	2.31	0.65
1:B:214:GLN:H	1:B:214:GLN:HE21	1.44	0.64
1:A:327:GLY:O	1:A:328:SER:HB2	1.97	0.64
1:A:48:GLU:HG3	1:A:49:PRO:HD2	1.80	0.64
1:B:214:GLN:NE2	1:B:214:GLN:N	2.46	0.63
1:A:170:TRP:CH2	1:A:200:ASP:CG	2.71	0.63
1:A:229:ARG:NH2	1:A:248:PRO:O	2.31	0.63
1:A:193:SER:O	1:A:197:VAL:HG23	1.99	0.62
1:B:101:GLN:O	1:B:102:ASP:CB	2.47	0.62
1:B:213:GLU:H	1:B:214:GLN:HE21	1.47	0.62
1:B:15:GLN:HG2	1:B:134:LEU:HD11	1.81	0.61
1:B:139:LEU:O	1:B:143:ARG:HG2	2.00	0.61
1:A:146:PHE:N	1:A:146:PHE:CD1	2.68	0.60
1:B:245:VAL:HA	1:B:251:THR:HG21	1.84	0.60
1:B:206:VAL:H	1:B:226:GLN:HE22	1.43	0.59
1:B:45:ARG:NH1	1:B:223:ASN:O	2.33	0.59
1:B:116:GLN:NE2	1:B:122:VAL:HG22	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASN:HA	1:A:106:GLN:N	2.19	0.58
1:A:152:LYS:HE3	1:A:171:ILE:HD11	1.85	0.57
1:B:317:LEU:HB2	1:B:364:LEU:HB2	1.87	0.57
1:B:159:GLY:O	1:B:160:ARG:HB2	2.04	0.56
1:A:206:VAL:H	1:A:226:GLN:HE22	1.50	0.55
1:A:212:ASP:OD1	1:A:214:GLN:CG	2.44	0.54
1:B:272:ILE:HG23	1:B:273:PRO:HD2	1.87	0.54
1:A:234:SER:OG	2:A:402:NAP:O3X	2.23	0.54
1:B:1:GLY:HA2	1:B:4:GLU:HG3	1.89	0.54
1:A:150:GLN:HG2	1:A:316:GLU:CG	2.38	0.54
1:A:188:HIS:CD2	1:A:294:ASN:H	2.18	0.54
1:A:49:PRO:HG2	1:A:54:HIS:CE1	2.43	0.54
1:A:333:LEU:HD12	1:A:333:LEU:O	2.07	0.53
1:B:240:PRO:HA	1:B:263:TRP:CZ3	2.44	0.53
1:A:146:PHE:N	1:A:146:PHE:HD1	2.07	0.53
1:A:141:ARG:O	1:A:144:THR:O	2.27	0.53
1:A:329:ASP:OD2	1:A:330:ALA:N	2.42	0.52
1:A:156:SER:HB2	1:A:324:LYS:O	2.09	0.52
1:B:137:GLY:HA2	1:B:148:TYR:HB2	1.93	0.51
1:B:206:VAL:H	1:B:226:GLN:HE21	1.50	0.51
1:B:48:GLU:HG3	1:B:49:PRO:HD2	1.91	0.51
1:A:251:THR:HG23	1:A:267:VAL:HG22	1.92	0.51
1:A:191:LEU:HG	1:A:192:THR:N	2.25	0.51
1:B:93:VAL:O	1:B:120:ILE:HG12	2.10	0.51
1:A:150:GLN:HG2	1:A:316:GLU:HG2	1.93	0.51
1:A:82:PRO:HB2	1:A:84:CYS:N	2.26	0.51
1:A:21:THR:HG23	1:A:24:ASN:O	2.11	0.50
1:A:139:LEU:HB3	1:A:143:ARG:NH1	2.25	0.50
1:B:15:GLN:HG2	1:B:134:LEU:CD1	2.40	0.50
1:A:102:ASP:CG	1:A:103:PRO:HD2	2.32	0.50
1:B:207:ARG:NH1	1:B:210:GLU:OE1	2.41	0.50
1:B:170:TRP:HA	1:B:170:TRP:HE3	1.75	0.50
1:B:214:GLN:H	1:B:214:GLN:CD	2.10	0.50
1:B:212:ASP:CG	1:B:213:GLU:H	2.16	0.49
1:A:141:ARG:NH2	1:A:292:GLN:HG2	2.27	0.49
1:A:147:PRO:HB3	1:A:293:ILE:O	2.13	0.49
1:A:-3:LEU:O	1:A:0:GLN:HB3	2.12	0.49
1:A:188:HIS:CD2	1:A:293:ILE:HA	2.48	0.49
1:B:160:ARG:HD3	1:B:330:ALA:HB3	1.94	0.49
1:A:75:CYS:HG	1:A:85:CYS:HG	1.40	0.48
1:B:31:ILE:HD13	1:B:56:LEU:HD13	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:HZ1	1:B:65:GLY:HA3	1.78	0.48
1:B:213:GLU:N	1:B:214:GLN:HE21	2.10	0.48
1:B:20:THR:HG22	1:B:45:ARG:HH11	1.79	0.48
1:A:191:LEU:HD12	1:A:230:ILE:HB	1.96	0.48
1:A:42:TYR:HA	1:A:51:ALA:HB2	1.95	0.47
1:A:125:GLY:HA2	1:A:128:MSE:HE3	1.97	0.47
1:B:118:ALA:C	1:B:120:ILE:H	2.17	0.47
1:B:112:LEU:HD11	1:B:122:VAL:HB	1.96	0.47
1:B:279:LEU:O	2:B:1402:NAP:H2A	2.15	0.47
1:A:42:TYR:HA	1:A:51:ALA:CB	2.45	0.47
1:A:318:ILE:HD12	1:A:318:ILE:N	2.30	0.46
1:B:20:THR:CG2	1:B:45:ARG:HH11	2.29	0.46
1:B:214:GLN:N	1:B:214:GLN:CD	2.67	0.46
1:A:245:VAL:HA	1:A:251:THR:HG21	1.98	0.46
1:A:112:LEU:HD22	1:A:122:VAL:HB	1.97	0.46
1:B:188:HIS:CD2	1:B:293:ILE:HA	2.51	0.46
1:B:302:PRO:HB2	1:B:336:LEU:HD11	1.98	0.46
1:A:3:ASP:OD1	1:A:69:TYR:OH	2.27	0.46
1:B:191:LEU:HD12	1:B:230:ILE:HB	1.96	0.46
1:A:33:LYS:CE	1:A:65:GLY:HA3	2.45	0.45
1:A:33:LYS:HE3	1:A:65:GLY:HA3	1.98	0.45
1:B:31:ILE:CD1	1:B:56:LEU:HD13	2.45	0.45
1:B:147:PRO:HB3	1:B:293:ILE:O	2.16	0.45
1:B:291:GLN:O	1:B:292:GLN:HB2	2.16	0.45
1:A:100:MSE:HE2	1:A:131:ALA:HB1	1.99	0.45
1:A:155:ALA:HB2	1:A:333:LEU:CD2	2.46	0.45
1:A:219:TYR:HD1	1:A:219:TYR:HA	1.57	0.45
1:B:207:ARG:HB3	1:B:210:GLU:HG3	1.98	0.45
1:A:31:ILE:HD13	1:A:56:LEU:HD12	1.98	0.44
1:A:238:VAL:HG12	1:A:239:THR:N	2.32	0.44
1:B:30:VAL:HG22	1:B:40:GLU:HG2	1.99	0.44
1:A:335:THR:H	1:B:160:ARG:HH12	1.63	0.44
1:B:171:ILE:O	1:B:171:ILE:CG2	2.65	0.44
1:B:207:ARG:CB	1:B:210:GLU:HG3	2.47	0.44
1:B:212:ASP:OD1	1:B:214:GLN:NE2	2.49	0.44
1:A:98:ALA:O	1:A:124:HIS:HA	2.17	0.44
1:B:229:ARG:HH11	1:B:251:THR:HB	1.82	0.44
1:A:72:LEU:O	1:A:73:GLU:C	2.55	0.43
1:A:271:LEU:C	1:A:272:ILE:HD12	2.39	0.43
1:B:62:LYS:HE2	1:B:62:LYS:HB2	1.68	0.43
1:B:188:HIS:CD2	1:B:294:ASN:H	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:O	1:A:225:ARG:NH1	2.40	0.43
1:A:353:ILE:HG21	1:B:360:VAL:HG11	2.00	0.43
1:B:19:PHE:O	1:B:225:ARG:HD3	2.17	0.43
1:B:94:ALA:O	1:B:95:ARG:HB2	2.18	0.43
1:B:98:ALA:O	1:B:124:HIS:HA	2.19	0.43
1:B:251:THR:HG23	1:B:267:VAL:HG22	1.99	0.43
1:A:336:LEU:O	1:B:327:GLY:HA2	2.18	0.43
1:A:28:GLY:H	1:A:71:THR:HB	1.84	0.43
1:A:85:CYS:O	1:A:89:ILE:HG13	2.19	0.42
1:A:185:ALA:HA	1:A:206:VAL:HG21	2.01	0.42
1:B:31:ILE:HD12	1:B:55:ALA:HB1	2.01	0.42
1:A:102:ASP:HB3	1:A:108:ALA:O	2.19	0.42
1:A:349:LYS:HE3	1:A:349:LYS:HB3	1.67	0.42
1:B:104:ASN:ND2	1:B:104:ASN:H	2.18	0.42
1:B:31:ILE:HD13	1:B:56:LEU:CD1	2.50	0.42
1:B:101:GLN:O	1:B:102:ASP:HB3	2.18	0.42
1:B:48:GLU:HG3	1:B:49:PRO:CD	2.49	0.41
1:A:229:ARG:NH2	1:A:247:GLN:HB2	2.35	0.41
1:B:351:LYS:HB3	1:B:352:GLU:H	1.69	0.41
1:A:353:ILE:O	1:A:353:ILE:CG1	2.68	0.41
1:B:21:THR:HG21	1:B:26:ASN:OD1	2.20	0.41
1:B:184:ARG:NH1	1:B:204:LEU:HA	2.36	0.41
1:A:229:ARG:HH11	1:A:229:ARG:HD2	1.67	0.41
1:A:294:ASN:HD22	1:A:294:ASN:HA	1.66	0.41
1:B:33:LYS:CE	1:B:65:GLY:HA3	2.50	0.41
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.93	0.41
1:A:155:ALA:HB2	1:A:333:LEU:HD21	2.03	0.41
1:A:283:VAL:O	1:A:287:GLN:HB2	2.21	0.41
1:B:156:SER:HB2	1:B:324:LYS:O	2.21	0.41
1:A:139:LEU:HB3	1:A:143:ARG:HH12	1.86	0.40
1:A:183:LEU:HA	1:A:183:LEU:HD12	1.84	0.40
1:A:31:ILE:HD11	1:A:56:LEU:HD13	2.03	0.40
1:B:220:PRO:HD2	1:B:223:ASN:ND2	2.37	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	350/380 (92%)	309 (88%)	29 (8%)	12 (3%)	3	20
1	B	345/380 (91%)	295 (86%)	35 (10%)	15 (4%)	2	15
All	All	695/760 (91%)	604 (87%)	64 (9%)	27 (4%)	3	17

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	95	ARG
1	A	217	ALA
1	A	328	SER
1	B	95	ARG
1	B	102	ASP
1	B	221	GLN
1	B	332	GLY
1	B	86	ASP
1	A	163	MSE
1	A	212	ASP
1	A	335	THR
1	B	335	THR
1	B	366	GLY
1	B	157	LEU
1	B	160	ARG
1	B	171	ILE
1	B	336	LEU
1	A	327	GLY
1	A	338	GLY
1	B	49	PRO
1	A	332	GLY
1	B	119	GLY
1	A	337	PRO
1	B	109	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	111	GLY
1	B	173	SER

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	284/302 (94%)	238 (84%)	46 (16%)	2	12
1	B	277/302 (92%)	236 (85%)	41 (15%)	3	14
All	All	561/604 (93%)	474 (84%)	87 (16%)	2	13

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	TYR
1	A	-1	ILE
1	A	4	GLU
1	A	9	ARG
1	A	21	THR
1	A	33	LYS
1	A	56	LEU
1	A	67	THR
1	A	70	VAL
1	A	71	THR
1	A	93	VAL
1	A	96	VAL
1	A	104	ASN
1	A	114	ARG
1	A	116	GLN
1	A	126	LEU
1	A	143	ARG
1	A	146	PHE
1	A	152	LYS
1	A	153	LEU
1	A	161	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	168	SER
1	A	170	TRP
1	A	183	LEU
1	A	187	SER
1	A	207	ARG
1	A	215	THR
1	A	219	TYR
1	A	221	GLN
1	A	224	LEU
1	A	225	ARG
1	A	234	SER
1	A	241	VAL
1	A	251	THR
1	A	255	ARG
1	A	256	THR
1	A	259	ASP
1	A	266	THR
1	A	269	THR
1	A	278	HIS
1	A	291	GLN
1	A	304	LEU
1	A	317	LEU
1	A	333	LEU
1	A	349	LYS
1	A	365	VAL
1	B	-3	LEU
1	B	3	ASP
1	B	20	THR
1	B	56	LEU
1	B	58	MSE
1	B	70	VAL
1	B	85	CYS
1	B	86	ASP
1	B	101	GLN
1	B	104	ASN
1	B	126	LEU
1	B	143	ARG
1	B	152	LYS
1	B	153	LEU
1	B	161	THR
1	B	170	TRP
1	B	178	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	LEU
1	B	183	LEU
1	B	187	SER
1	B	207	ARG
1	B	213	GLU
1	B	214	GLN
1	B	215	THR
1	B	218	LEU
1	B	219	TYR
1	B	221	GLN
1	B	224	LEU
1	B	225	ARG
1	B	241	VAL
1	B	251	THR
1	B	255	ARG
1	B	256	THR
1	B	257	GLN
1	B	260	SER
1	B	265	GLU
1	B	269	THR
1	B	278	HIS
1	B	304	LEU
1	B	352	GLU
1	B	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	104	ASN
1	A	116	GLN
1	A	150	GLN
1	A	186	GLN
1	A	188	HIS
1	A	226	GLN
1	A	247	GLN
1	A	294	ASN
1	B	104	ASN
1	B	116	GLN
1	B	150	GLN
1	B	188	HIS
1	B	214	GLN

Continued from previous page...

Mol	Chain	Res	Type
1	B	226	GLN
1	B	247	GLN
1	B	287	GLN
1	B	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	402	-	45,52,52	1.80	4 (8%)	56,80,80	1.17	2 (3%)
2	NAP	B	1402	-	45,52,52	1.78	4 (8%)	56,80,80	1.17	4 (7%)

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	402	-	-	5/31/67/67	0/5/5/5
2	NAP	B	1402	-	-	15/31/67/67	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1402	NAP	O7N-C7N	9.51	1.42	1.24
2	A	402	NAP	O7N-C7N	9.07	1.41	1.24
2	A	402	NAP	C2A-N3A	4.15	1.38	1.32
2	B	1402	NAP	C2A-N3A	3.49	1.37	1.32
2	B	1402	NAP	C2A-N1A	2.83	1.39	1.33
2	A	402	NAP	C2A-N1A	2.78	1.39	1.33
2	B	1402	NAP	C2N-N1N	2.75	1.38	1.35
2	A	402	NAP	C2N-N1N	2.64	1.38	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1402	NAP	N3A-C2A-N1A	-5.02	120.83	128.68
2	A	402	NAP	N3A-C2A-N1A	-4.67	121.37	128.68
2	B	1402	NAP	C6N-N1N-C2N	-2.51	119.69	121.97
2	B	1402	NAP	C3D-C2D-C1D	2.49	104.73	100.98
2	A	402	NAP	O2N-PN-O1N	2.31	123.68	112.24
2	B	1402	NAP	C2N-C3N-C4N	2.20	120.75	118.26

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	NAP	O4D-C1D-N1N-C6N
2	B	1402	NAP	C5D-O5D-PN-O3
2	B	1402	NAP	C5D-O5D-PN-O1N
2	B	1402	NAP	C2D-C1D-N1N-C2N
2	B	1402	NAP	C2D-C1D-N1N-C6N
2	B	1402	NAP	C2N-C3N-C7N-O7N
2	B	1402	NAP	C2N-C3N-C7N-N7N
2	B	1402	NAP	C4N-C3N-C7N-O7N
2	B	1402	NAP	C4N-C3N-C7N-N7N
2	B	1402	NAP	O4D-C4D-C5D-O5D
2	B	1402	NAP	C3D-C4D-C5D-O5D
2	A	402	NAP	C2B-O2B-P2B-O3X
2	B	1402	NAP	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...
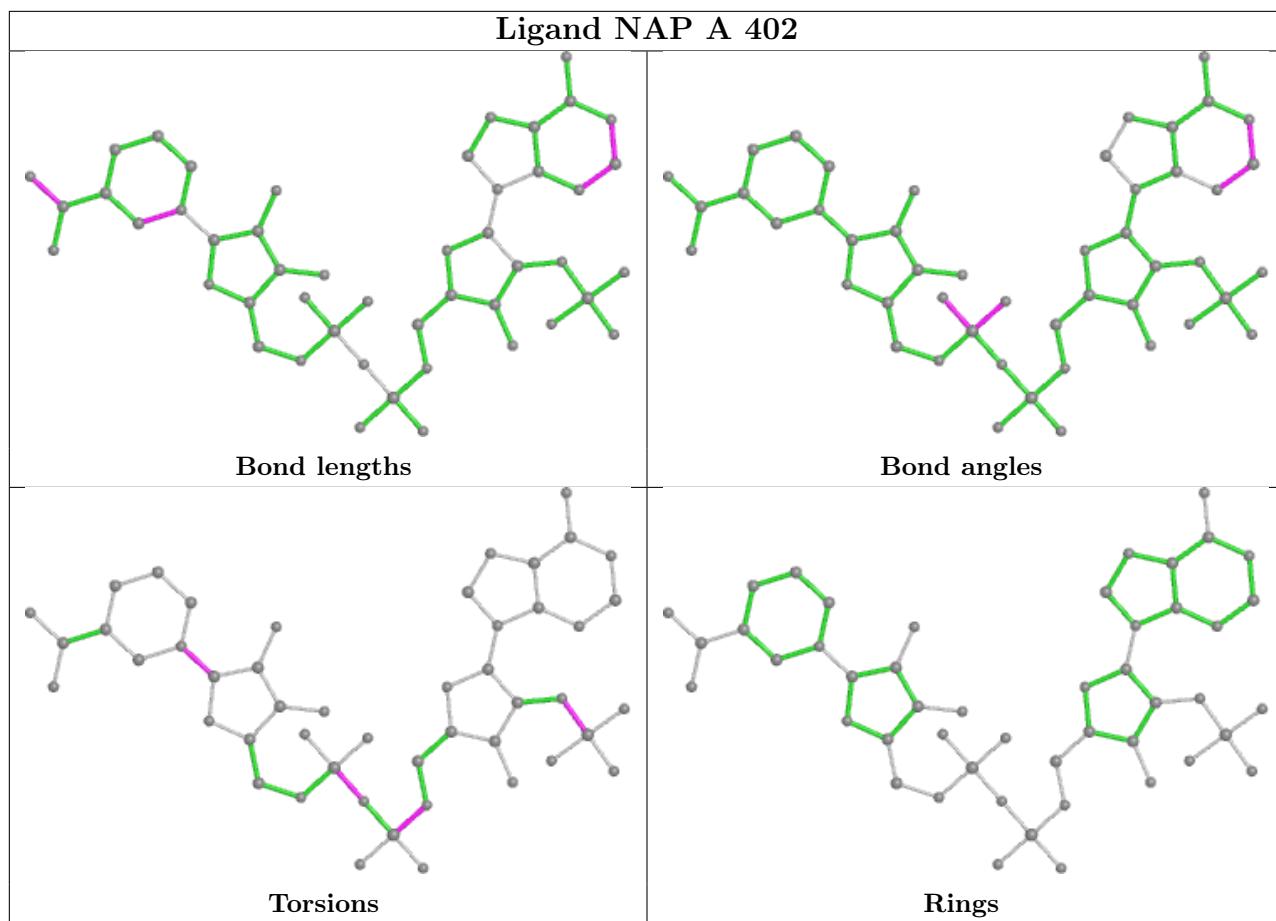
Mol	Chain	Res	Type	Atoms
2	A	402	NAP	PA-O3-PN-O5D
2	B	1402	NAP	C2B-O2B-P2B-O1X
2	B	1402	NAP	C3B-C4B-C5B-O5B
2	A	402	NAP	C2B-O2B-P2B-O2X
2	B	1402	NAP	C2B-O2B-P2B-O2X
2	B	1402	NAP	C2B-O2B-P2B-O3X
2	A	402	NAP	C5B-O5B-PA-O1A
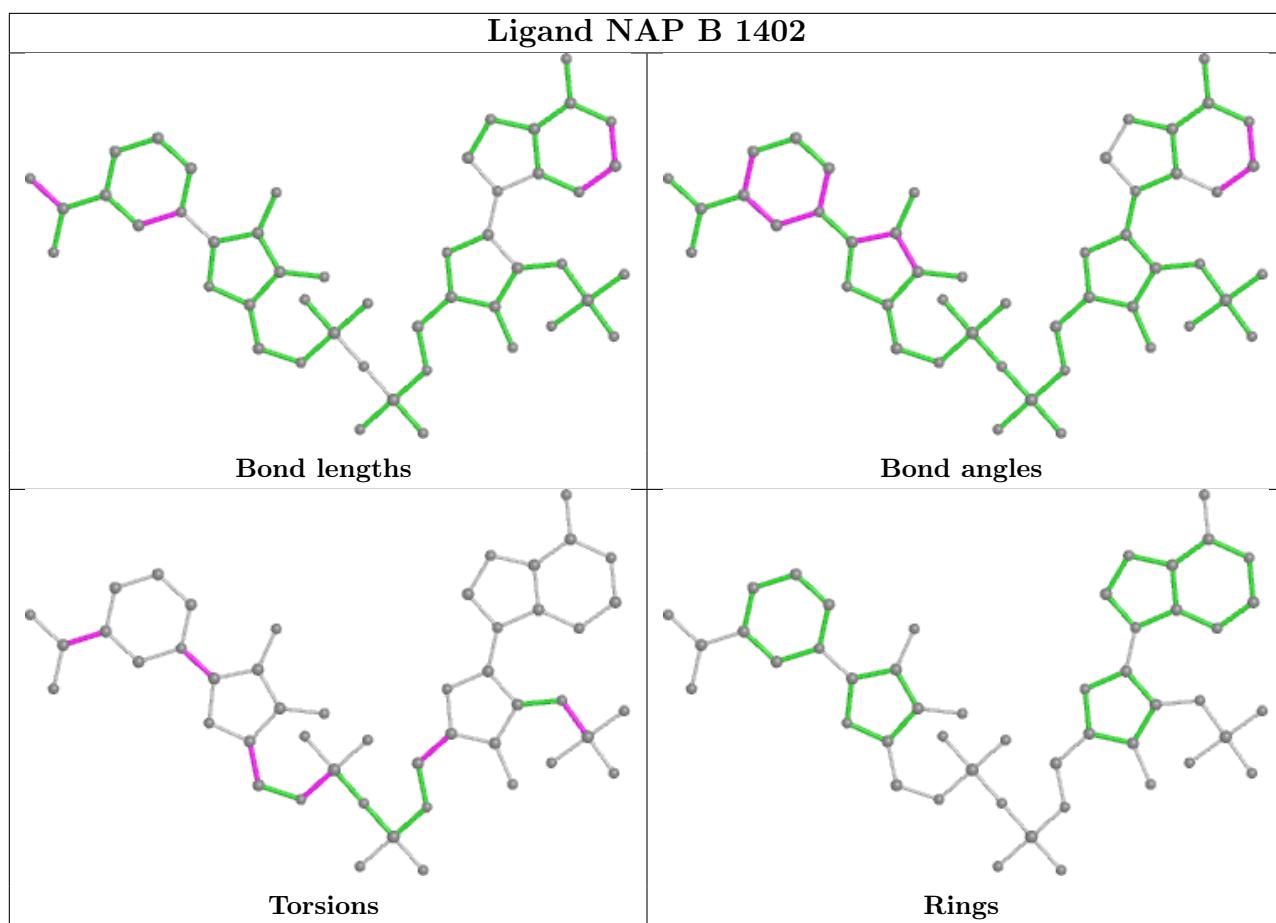
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	NAP	1	0
2	B	1402	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 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 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 1402

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	349/380 (91%)	-0.16	3 (0%)	84	63	68, 82, 108, 122	0
1	B	345/380 (90%)	-0.14	6 (1%)	70	41	63, 81, 109, 118	0
All	All	694/760 (91%)	-0.15	9 (1%)	77	51	63, 81, 109, 122	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-4	THR	3.9
1	A	75	CYS	3.0
1	B	217	ALA	2.6
1	B	118	ALA	2.6
1	B	123	SER	2.4
1	A	83	PRO	2.3
1	B	48	GLU	2.0
1	A	82	PRO	2.0
1	B	117	GLN	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.
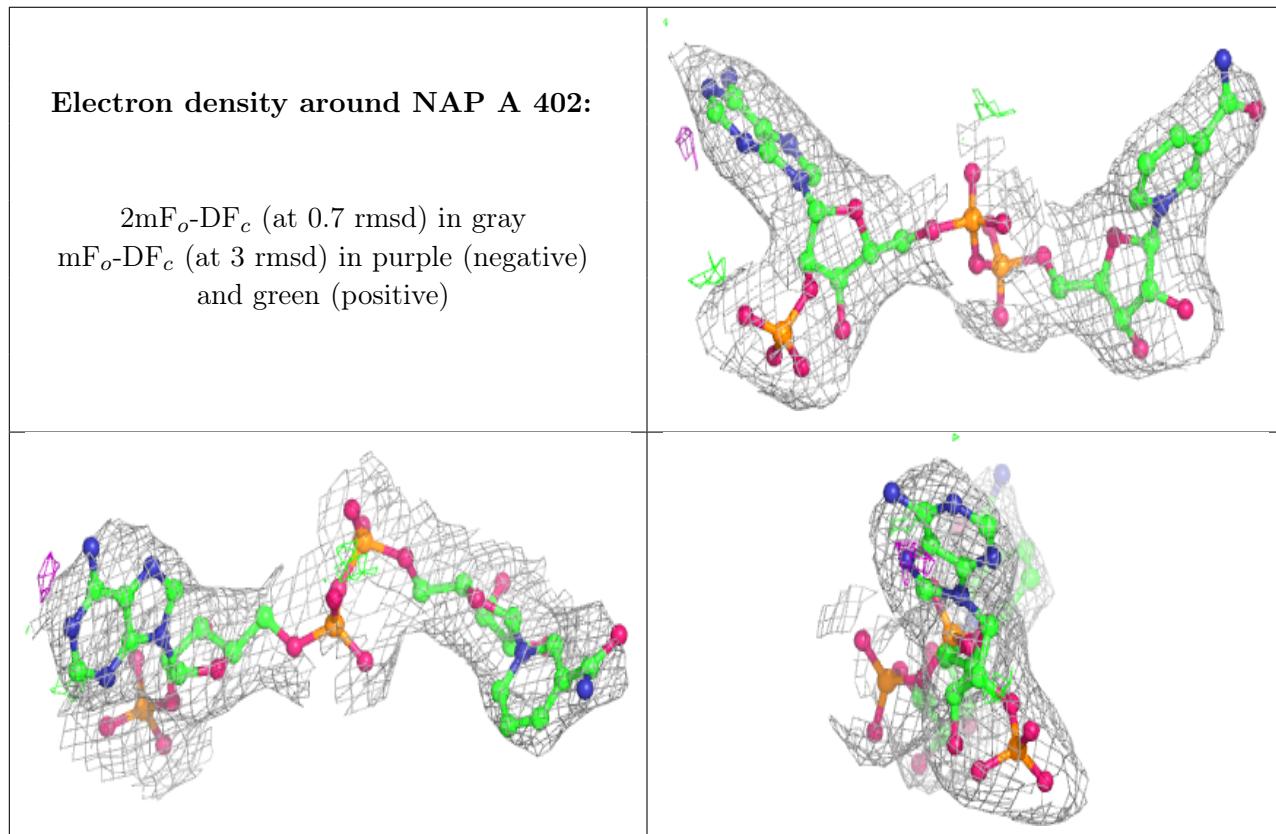
6.4   Ligands ⓘ
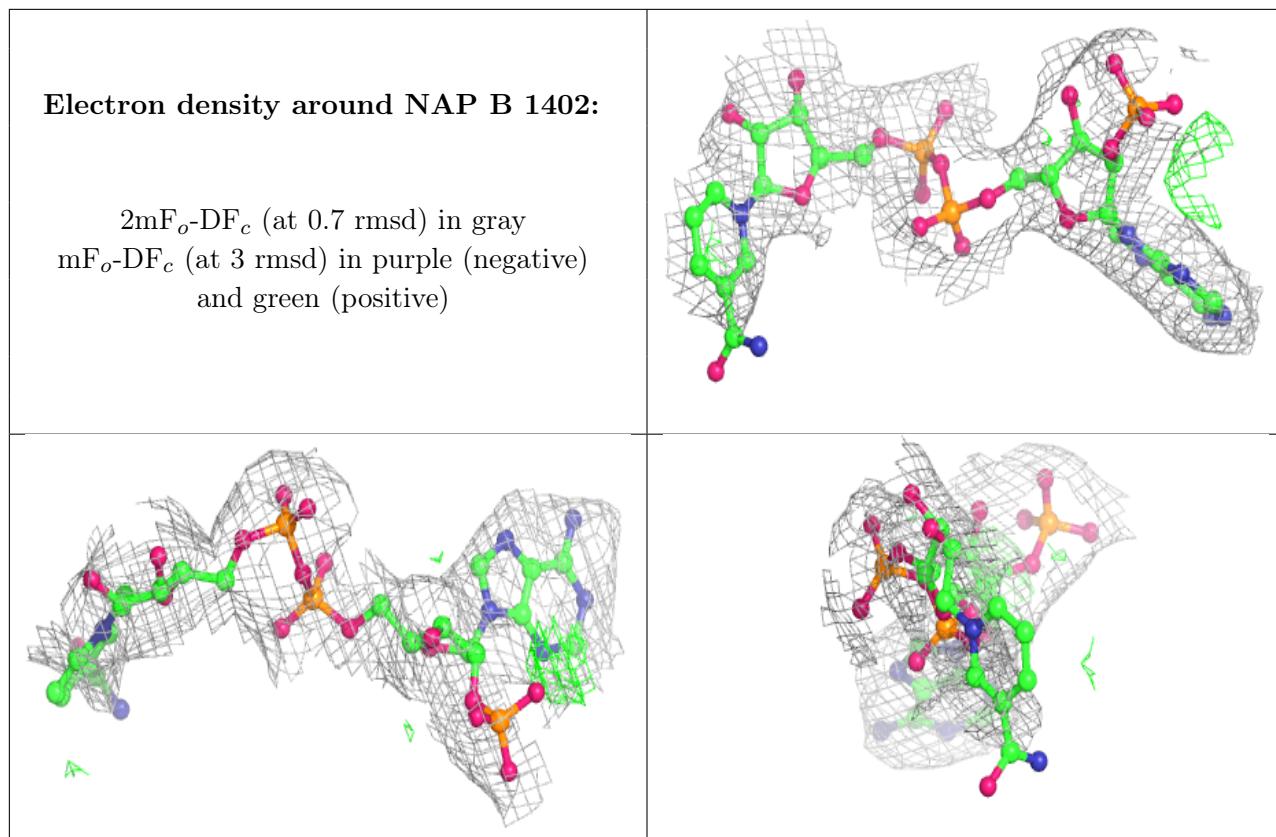
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
2	NAP	A	402	48/48	0.94	0.16	71,81,89,93	0
2	NAP	B	1402	48/48	0.94	0.14	95,107,141,143	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 402:

$2mF_o$-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 1402:

$2mF_o$-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.