



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:18 PM UTC

PDB ID : 2O7P / pdb\_00002o7p  
Title : The crystal structure of RibD from Escherichia coli in complex with the oxidised NADP<sup>+</sup> 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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

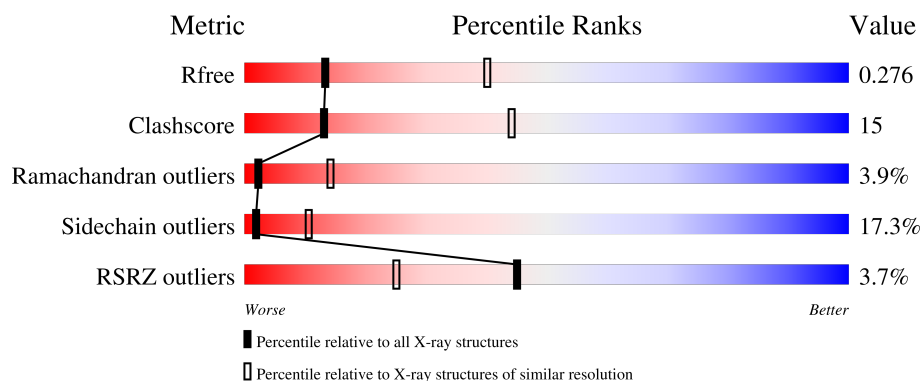
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	380	 3% 56% 31% 7% 6%
1	B	380	 4% 57% 28% 6% 7%

## 2 Entry composition [i](#)

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:

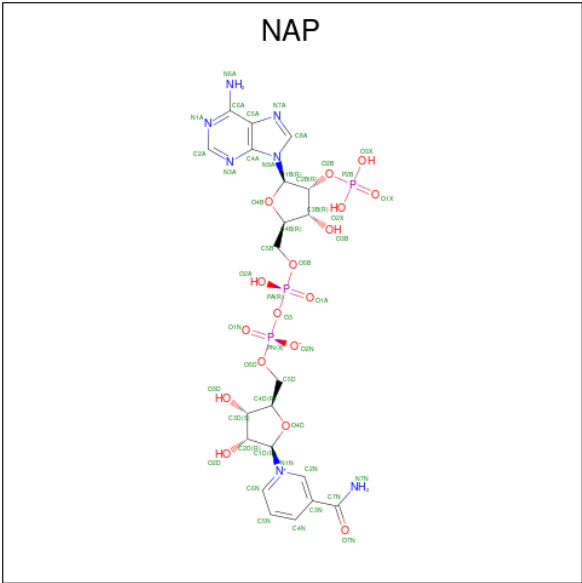
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	THR	-	cloning artifact	UNP P25539
A	-3	LEU	-	cloning artifact	UNP P25539
A	-2	TYR	-	cloning artifact	UNP P25539
A	-1	ILE	-	cloning artifact	UNP P25539
A	0	GLN	-	cloning artifact	UNP P25539
A	1	GLY	-	cloning artifact	UNP P25539
A	368	SER	-	cloning artifact	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

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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 (CCD ID: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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



G366
A367
SER
THR
HIS
HIS
HIS
HIS
HIS
HIS
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.00Å 173.00Å 77.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.93 – 3.00 28.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.93-3.00) 99.8 (28.93-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.212 , 0.267 0.235 , 0.276	Depositor DCC
$R_{free}$ test set	1359 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.01	3/2776 (0.1%)	1.18	9/3753 (0.2%)
1	B	1.03	13/2736 (0.5%)	1.15	12/3703 (0.3%)
All	All	1.02	16/5512 (0.3%)	1.16	21/7456 (0.3%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	GLN	CD-OE1	9.80	1.42	1.23
1	B	116	GLN	CD-NE2	9.57	1.53	1.33
1	B	215	THR	CA-CB	9.46	1.69	1.53
1	B	275	HIS	CE1-NE2	8.81	1.41	1.32
1	B	87	ALA	C-O	6.49	1.32	1.24
1	A	297	TRP	CD2-CE3	6.45	1.50	1.40
1	B	91	ALA	C-O	6.08	1.31	1.24
1	B	275	HIS	CG-ND1	5.99	1.44	1.38
1	B	62	LYS	CD-CE	5.80	1.69	1.52
1	A	334	CYS	CA-C	5.74	1.60	1.52
1	B	116	GLN	C-O	5.62	1.30	1.24
1	B	213	GLU	N-CA	5.46	1.52	1.46
1	B	119	GLY	C-O	5.31	1.31	1.23
1	A	297	TRP	CD1-NE1	5.28	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	ALA	C-N	5.14	1.41	1.33
1	B	275	HIS	CG-CD2	5.07	1.41	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	GLN	OE1-CD-NE2	12.45	135.05	122.60
1	A	67	THR	N-CA-C	9.01	129.99	110.80
1	B	116	GLN	CG-CD-OE1	-7.45	105.90	120.80
1	B	218	LEU	N-CA-C	-6.25	97.48	110.80
1	B	102	ASP	CA-C-N	6.08	125.47	118.85
1	B	102	ASP	C-N-CA	6.08	125.47	118.85
1	B	216	GLN	N-CA-C	6.02	120.68	112.68
1	B	214	GLN	N-CA-C	-6.01	104.85	111.82
1	A	66	ALA	CA-C-N	5.74	132.50	121.54
1	A	66	ALA	C-N-CA	5.74	132.50	121.54
1	B	124	HIS	N-CA-C	5.56	117.08	110.19
1	B	331	ARG	N-CA-C	5.47	119.95	112.68
1	A	348	PHE	N-CA-C	5.40	117.61	109.41
1	A	213	GLU	N-CA-C	5.39	118.66	112.57
1	A	260	SER	N-CA-C	5.31	119.85	112.90
1	B	300	ALA	N-CA-C	5.23	115.44	108.38
1	B	332	GLY	N-CA-C	5.22	125.55	113.18
1	A	162	ALA	N-CA-C	5.20	121.88	110.80
1	B	149	ILE	N-CA-C	5.16	115.28	107.80
1	A	231	VAL	CB-CA-C	-5.11	103.07	110.63
1	A	16	ARG	N-CA-C	-5.10	106.16	112.38

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	85	0
1	B	2694	0	2686	81	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
All	All	5523	0	5463	163	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (163) 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
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:A:170:TRP:HH2	1:A:200:ASP:CG	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:TRP:CH2	1:A:200:ASP:CG	2.71	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: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
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:214:GLN:H	1:B:214:GLN:CD	2.10	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:B:212:ASP:CG	1:B:213:GLU:H	2.16	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:102:ASP:CG	1:A:103:PRO:HD2	2.32	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ALA:C	1:B:120:ILE:H	2.17	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:B:214:GLN:N	1:B:214:GLN:CD	2.67	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:B:207:ARG:NH1	1:B:210:GLU:OE1	2.41	0.50
1:B:33:LYS:HZ1	1:B:65:GLY:HA3	1.76	0.50
1:B:170:TRP:HA	1:B:170:TRP:HE3	1.75	0.50
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:B:31:ILE:HD13	1:B:56:LEU:HD13	1.94	0.48
1:A:72:LEU:O	1:A:73:GLU:C	2.55	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:271:LEU:C	1:A:272:ILE:HD12	2.39	0.47
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:238:VAL:HG12	1:A:239:THR:N	2.32	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: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
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:259:ASP:OD2	1:A:259:ASP:C	2.62	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:A:212:ASP:CG	1:A:213:GLU:N	2.76	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:342:LEU:C	1:B:344:ASP:H	2.28	0.42
1:B:214:GLN:O	1:B:215:THR:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:15:GLN:C	1:B:17:GLY:N	2.77	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:A:15:GLN:C	1:A:17:GLY:N	2.76	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 ⓘ

### 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	350/380 (92%)	309 (88%)	29 (8%)	12 (3%)	3	17
1	B	345/380 (91%)	295 (86%)	35 (10%)	15 (4%)	2	12
All	All	695/760 (91%)	604 (87%)	64 (9%)	27 (4%)	2	14

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	THR

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Mol	Chain	Res	Type
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
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%)	236 (83%)	48 (17%)	2	11
1	B	277/302 (92%)	228 (82%)	49 (18%)	2	10
All	All	561/604 (93%)	464 (83%)	97 (17%)	2	10

All (97) 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	21	THR
1	A	33	LYS
1	A	48	GLU
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	116	GLN
1	A	126	LEU
1	A	141	ARG
1	A	143	ARG
1	A	146	PHE
1	A	149	ILE
1	A	152	LYS
1	A	153	LEU
1	A	161	THR
1	A	168	SER
1	A	170	TRP
1	A	183	LEU
1	A	187	SER
1	A	198	LEU
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

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Mol	Chain	Res	Type
1	A	304	LEU
1	A	317	LEU
1	A	333	LEU
1	A	349	LYS
1	A	365	VAL
1	B	-4	THR
1	B	-3	LEU
1	B	3	ASP
1	B	20	THR
1	B	33	LYS
1	B	56	LEU
1	B	62	LYS
1	B	70	VAL
1	B	71	THR
1	B	85	CYS
1	B	86	ASP
1	B	101	GLN
1	B	104	ASN
1	B	107	VAL
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	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	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	258	GLU

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Mol	Chain	Res	Type
1	B	260	SER
1	B	265	GLU
1	B	269	THR
1	B	272	ILE
1	B	278	HIS
1	B	286	MSE
1	B	304	LEU
1	B	321	ILE
1	B	333	LEU
1	B	352	GLU
1	B	354	ARG
1	B	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	116	GLN
1	A	186	GLN
1	A	188	HIS
1	A	226	GLN
1	A	247	GLN
1	A	294	ASN
1	B	24	ASN
1	B	43	HIS
1	B	101	GLN
1	B	104	ASN
1	B	106	GLN
1	B	116	GLN
1	B	150	GLN
1	B	188	HIS
1	B	214	GLN
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	-	50,52,52	1.74	5 (10%)	71,80,80	1.62	12 (16%)
2	NAP	B	1402	-	50,52,52	1.75	6 (12%)	71,80,80	1.43	9 (12%)

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	-	-	5/35/67/67	0/5/5/5
2	NAP	B	1402	-	-	16/35/67/67	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1402	NAP	O7N-C7N	9.79	1.42	1.24
2	A	402	NAP	O7N-C7N	9.34	1.41	1.24
2	B	1402	NAP	C2N-N1N	3.03	1.38	1.35
2	B	1402	NAP	C2A-N1A	2.95	1.39	1.33
2	A	402	NAP	C2N-N1N	2.91	1.38	1.35
2	A	402	NAP	C2A-N1A	2.90	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	NAP	C5A-N7A	-2.77	1.34	1.39
2	A	402	NAP	C2A-N3A	2.73	1.38	1.33
2	B	1402	NAP	C5A-N7A	-2.28	1.34	1.39
2	B	1402	NAP	C8A-N7A	2.17	1.35	1.31
2	B	1402	NAP	C2A-N3A	2.13	1.37	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	NAP	C5A-C4A-N3A	-5.14	119.64	126.72
2	B	1402	NAP	N3A-C2A-N1A	-5.12	120.83	128.58
2	A	402	NAP	N3A-C2A-N1A	-4.76	121.37	128.58
2	B	1402	NAP	C4D-O4D-C1D	-4.55	105.76	109.92
2	A	402	NAP	C2B-C1B-N9A	-4.22	106.81	113.75
2	B	1402	NAP	C5A-C4A-N3A	-3.65	121.69	126.72
2	A	402	NAP	N3A-C4A-N9A	3.40	132.95	127.17
2	A	402	NAP	C2A-N3A-C4A	3.19	119.62	111.83
2	A	402	NAP	C5A-N7A-C8A	3.17	108.44	103.45
2	A	402	NAP	N9A-C8A-N7A	-3.00	109.68	113.94
2	B	1402	NAP	C2A-N3A-C4A	2.79	118.64	111.83
2	B	1402	NAP	N9A-C8A-N7A	-2.77	110.00	113.94
2	A	402	NAP	C6A-C5A-C4A	2.76	120.95	117.18
2	B	1402	NAP	C6N-N1N-C2N	-2.58	119.69	121.88
2	A	402	NAP	C4D-O4D-C1D	-2.52	107.62	109.92
2	B	1402	NAP	C5A-N7A-C8A	2.51	107.40	103.45
2	A	402	NAP	O2N-PN-O1N	2.41	123.68	112.44
2	A	402	NAP	C4A-C5A-N7A	-2.17	108.10	110.58
2	B	1402	NAP	N3A-C4A-N9A	2.16	130.85	127.17
2	B	1402	NAP	C2N-C3N-C4N	2.15	120.75	118.26
2	A	402	NAP	O3D-C3D-C4D	-2.01	105.31	111.08

There are no chirality outliers.

All (21) 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-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

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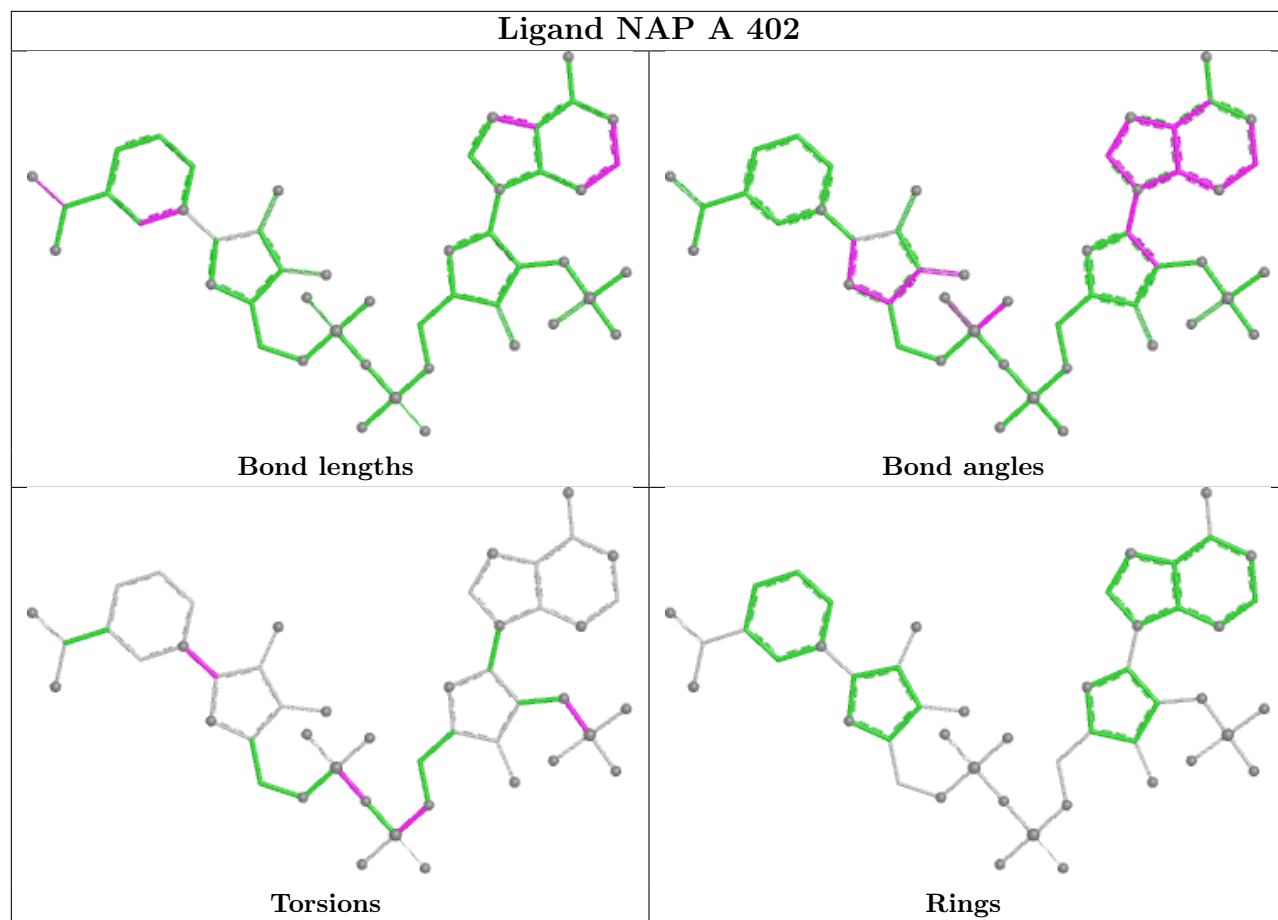
Mol	Chain	Res	Type	Atoms
2	B	1402	NAP	C4N-C3N-C7N-N7N
2	B	1402	NAP	C3D-C4D-C5D-O5D
2	B	1402	NAP	O4D-C4D-C5D-O5D
2	A	402	NAP	C5B-O5B-PA-O1A
2	B	1402	NAP	C5D-O5D-PN-O3
2	B	1402	NAP	C5D-O5D-PN-O2N
2	A	402	NAP	C2B-O2B-P2B-O3X
2	A	402	NAP	O4D-C1D-N1N-C2N
2	B	1402	NAP	C2B-O2B-P2B-O1X
2	A	402	NAP	PA-O3-PN-O5D
2	B	1402	NAP	C3B-C4B-C5B-O5B
2	B	1402	NAP	C2B-O2B-P2B-O2X
2	B	1402	NAP	C2B-O2B-P2B-O3X
2	B	1402	NAP	PA-O3-PN-O2N

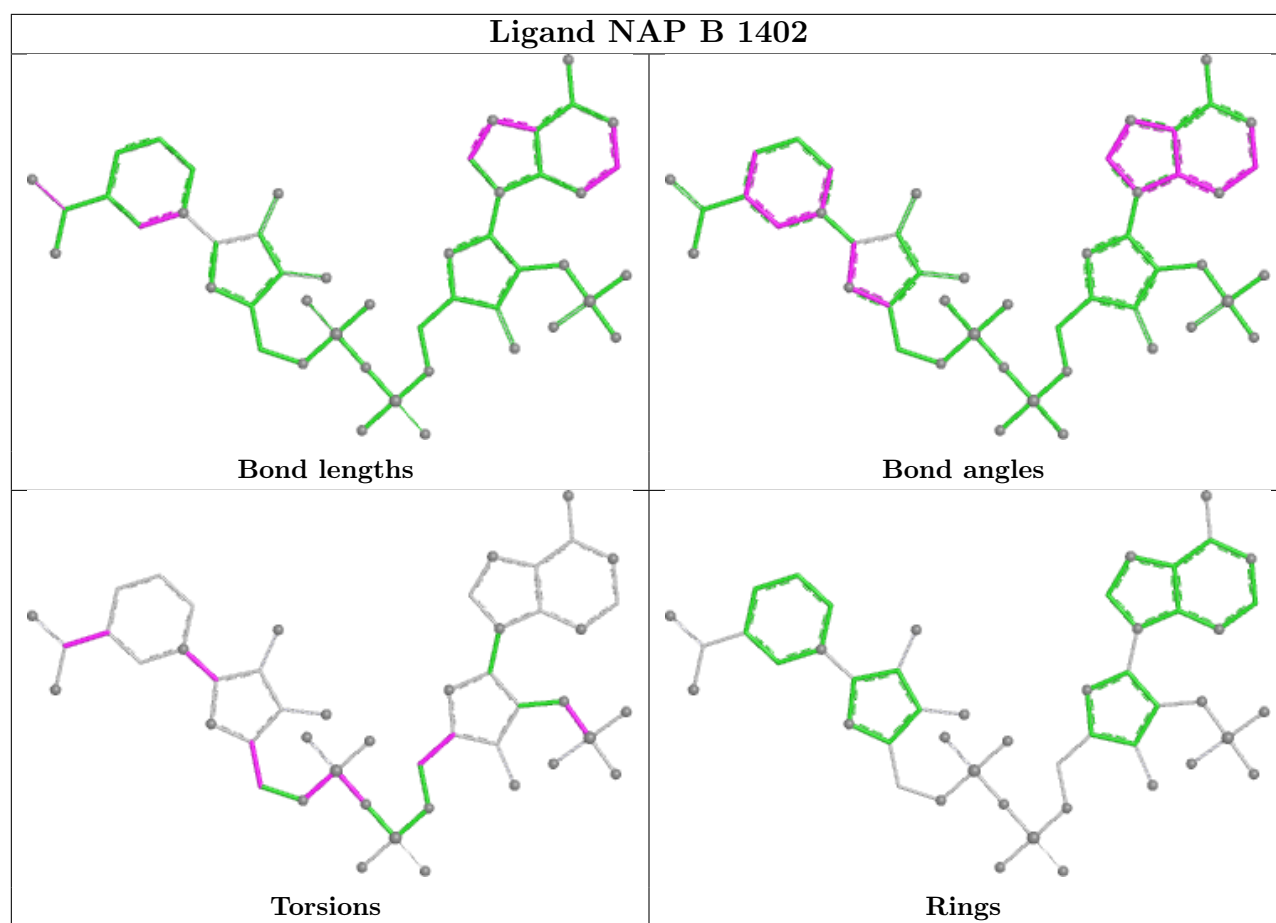
There are no ring outliers.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	349/380 (91%)	0.33	12 (3%)	48 27	68, 82, 108, 122	0
1	B	345/380 (90%)	0.24	14 (4%)	41 23	63, 81, 109, 118	0
All	All	694/760 (91%)	0.29	26 (3%)	45 25	63, 81, 109, 122	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	ILE	5.4
1	B	217	ALA	3.3
1	B	52	GLU	2.9
1	A	217	ALA	2.9
1	B	112	LEU	2.5
1	A	233	ASP	2.3
1	A	40	GLU	2.3
1	A	332	GLY	2.3
1	A	259	ASP	2.3
1	B	-3	LEU	2.3
1	B	274	GLU	2.2
1	A	218	LEU	2.2
1	A	-4	THR	2.2
1	B	0	GLN	2.2
1	B	170	TRP	2.2
1	B	89	ILE	2.2
1	A	75	CYS	2.2
1	A	366	GLY	2.2
1	A	74	PRO	2.1
1	A	260	SER	2.1
1	B	115	LEU	2.1
1	B	108	ALA	2.1
1	B	-4	THR	2.0
1	B	123	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	334	CYS	2.0
1	A	82	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

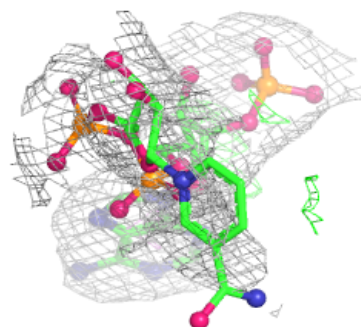
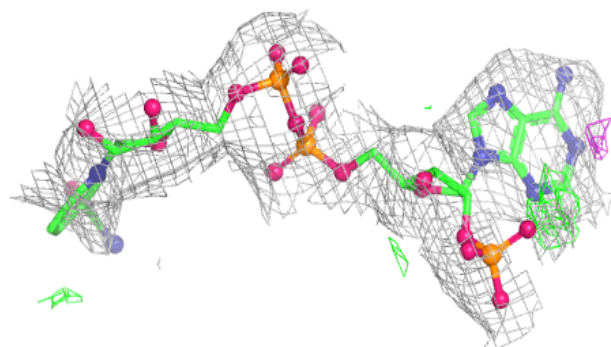
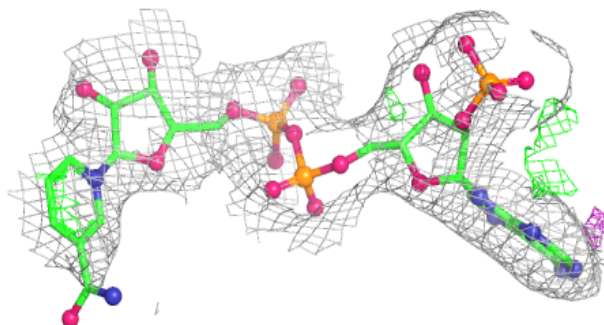
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	B	1402	48/48	0.87	0.10	95,107,141,143	0
2	NAP	A	402	48/48	0.95	0.08	71,81,89,93	0

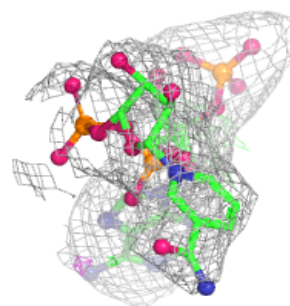
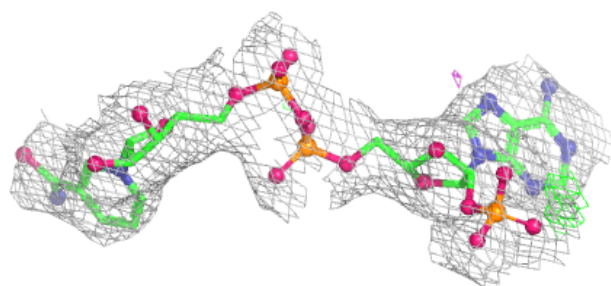
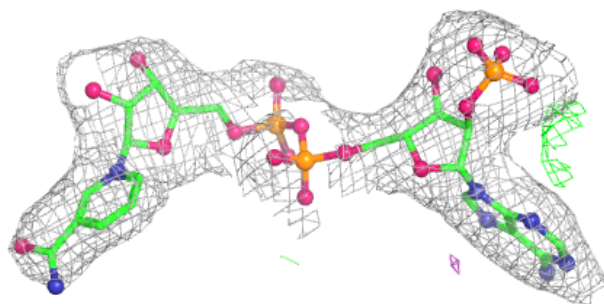
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP 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)

**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.