



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:47 PM UTC

PDB ID : 8YP9 / pdb_00008yp9
Title : the crystal structure of wildtype Magnaporthe grisea oxidoreductase in complex with NADP
Authors : Huang, X.; Jiang, H.; Tang, D.; Lin, S.
Deposited on : 2024-03-15
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

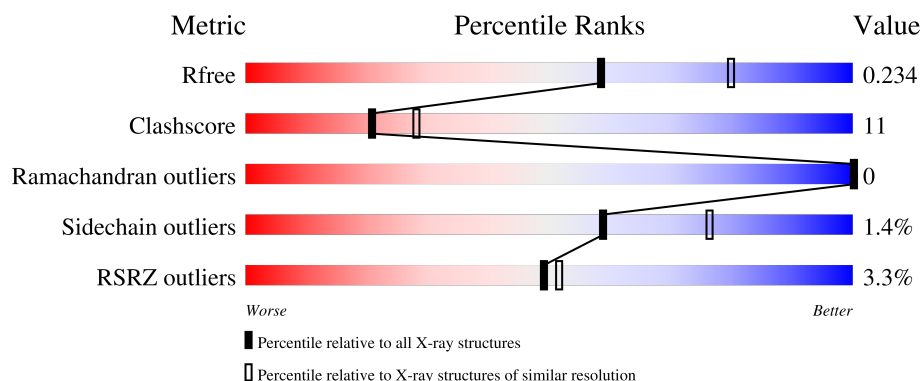
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

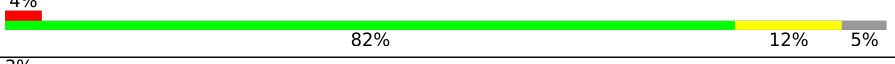
The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	332	
1	B	332	
1	C	332	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8343 atoms, of which 75 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 NADP-dependent oxidoreductase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2590	1649	444	488	9			
1	B	314	Total	C	N	O	S	0	0	0
			2502	1594	431	470	7			
1	C	321	Total	C	N	O	S	0	0	0
			2550	1623	439	481	7			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A6P8AP13
A	4	ALA	SER	conflict	UNP A0A6P8AP13
A	7	ALA	SER	conflict	UNP A0A6P8AP13
A	38	ALA	SER	conflict	UNP A0A6P8AP13
A	56	PHE	TYR	conflict	UNP A0A6P8AP13
A	103	ASP	GLU	conflict	UNP A0A6P8AP13
A	110	ARG	LYS	conflict	UNP A0A6P8AP13
A	145	HIS	LYS	conflict	UNP A0A6P8AP13
A	186	VAL	ILE	conflict	UNP A0A6P8AP13
A	252	MET	LEU	conflict	UNP A0A6P8AP13
A	290	GLU	ASP	conflict	UNP A0A6P8AP13
A	292	ASP	ASN	conflict	UNP A0A6P8AP13
A	294	GLN	GLU	conflict	UNP A0A6P8AP13
A	322	GLU	ASP	conflict	UNP A0A6P8AP13
A	325	LEU	-	expression tag	UNP A0A6P8AP13
A	326	GLU	-	expression tag	UNP A0A6P8AP13
A	327	HIS	-	expression tag	UNP A0A6P8AP13
A	328	HIS	-	expression tag	UNP A0A6P8AP13
A	329	HIS	-	expression tag	UNP A0A6P8AP13
A	330	HIS	-	expression tag	UNP A0A6P8AP13
A	331	HIS	-	expression tag	UNP A0A6P8AP13
A	332	HIS	-	expression tag	UNP A0A6P8AP13
B	1	MET	-	initiating methionine	UNP A0A6P8AP13

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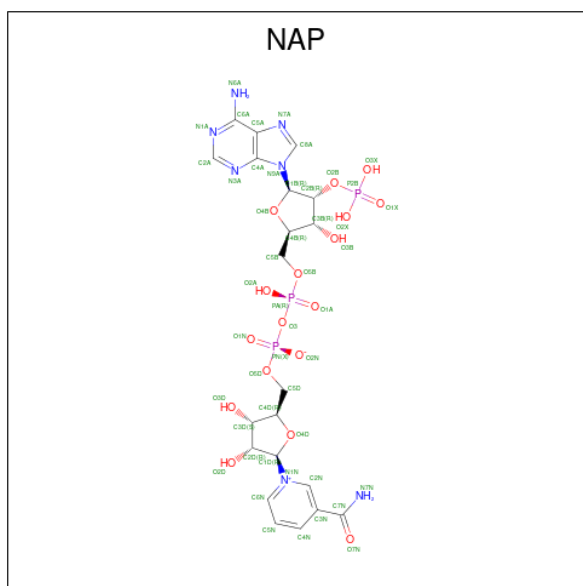
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ALA	SER	conflict	UNP A0A6P8AP13
B	7	ALA	SER	conflict	UNP A0A6P8AP13
B	38	ALA	SER	conflict	UNP A0A6P8AP13
B	56	PHE	TYR	conflict	UNP A0A6P8AP13
B	103	ASP	GLU	conflict	UNP A0A6P8AP13
B	110	ARG	LYS	conflict	UNP A0A6P8AP13
B	145	HIS	LYS	conflict	UNP A0A6P8AP13
B	186	VAL	ILE	conflict	UNP A0A6P8AP13
B	252	MET	LEU	conflict	UNP A0A6P8AP13
B	290	GLU	ASP	conflict	UNP A0A6P8AP13
B	292	ASP	ASN	conflict	UNP A0A6P8AP13
B	294	GLN	GLU	conflict	UNP A0A6P8AP13
B	322	GLU	ASP	conflict	UNP A0A6P8AP13
B	325	LEU	-	expression tag	UNP A0A6P8AP13
B	326	GLU	-	expression tag	UNP A0A6P8AP13
B	327	HIS	-	expression tag	UNP A0A6P8AP13
B	328	HIS	-	expression tag	UNP A0A6P8AP13
B	329	HIS	-	expression tag	UNP A0A6P8AP13
B	330	HIS	-	expression tag	UNP A0A6P8AP13
B	331	HIS	-	expression tag	UNP A0A6P8AP13
B	332	HIS	-	expression tag	UNP A0A6P8AP13
C	1	MET	-	initiating methionine	UNP A0A6P8AP13
C	4	ALA	SER	conflict	UNP A0A6P8AP13
C	7	ALA	SER	conflict	UNP A0A6P8AP13
C	38	ALA	SER	conflict	UNP A0A6P8AP13
C	56	PHE	TYR	conflict	UNP A0A6P8AP13
C	103	ASP	GLU	conflict	UNP A0A6P8AP13
C	110	ARG	LYS	conflict	UNP A0A6P8AP13
C	145	HIS	LYS	conflict	UNP A0A6P8AP13
C	186	VAL	ILE	conflict	UNP A0A6P8AP13
C	252	MET	LEU	conflict	UNP A0A6P8AP13
C	290	GLU	ASP	conflict	UNP A0A6P8AP13
C	292	ASP	ASN	conflict	UNP A0A6P8AP13
C	294	GLN	GLU	conflict	UNP A0A6P8AP13
C	322	GLU	ASP	conflict	UNP A0A6P8AP13
C	325	LEU	-	expression tag	UNP A0A6P8AP13
C	326	GLU	-	expression tag	UNP A0A6P8AP13
C	327	HIS	-	expression tag	UNP A0A6P8AP13
C	328	HIS	-	expression tag	UNP A0A6P8AP13
C	329	HIS	-	expression tag	UNP A0A6P8AP13
C	330	HIS	-	expression tag	UNP A0A6P8AP13
C	331	HIS	-	expression tag	UNP A0A6P8AP13

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Chain	Residue	Modelled	Actual	Comment	Reference
C	332	HIS	-	expression tag	UNP A0A6P8AP13

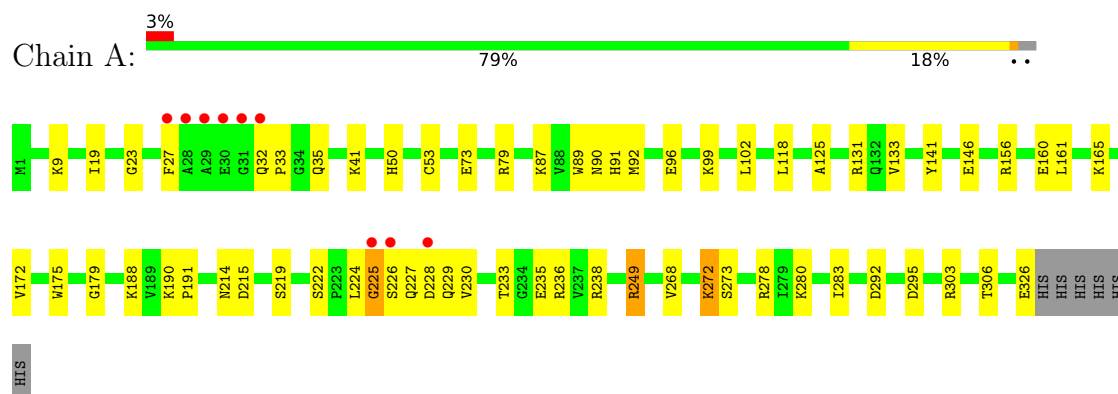
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



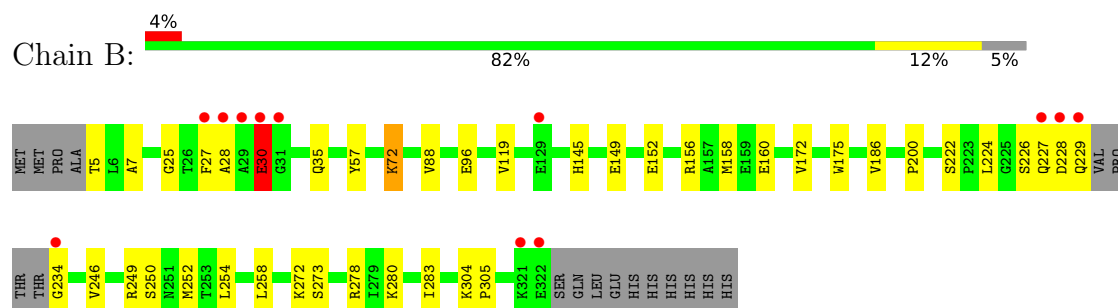
3 Residue-property plots

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.

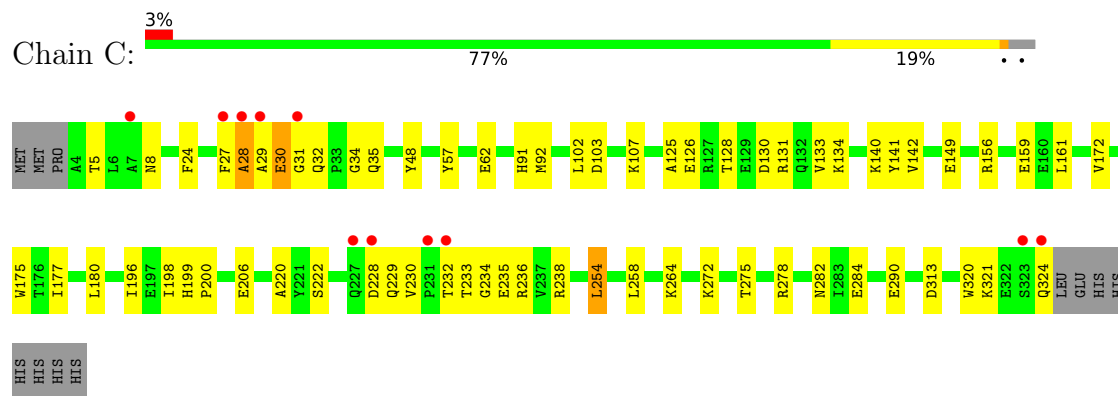
- Molecule 1: NADP-dependent oxidoreductase domain-containing protein



- Molecule 1: NADP-dependent oxidoreductase domain-containing protein



- Molecule 1: NADP-dependent oxidoreductase domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.62Å 111.45Å 171.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.15 – 2.30 25.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (25.15-2.30) 88.6 (25.15-2.30)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.183 , 0.233 0.183 , 0.234	Depositor DCC
R_{free} test set	1990 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8343	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/2655	0.60	2/3611 (0.1%)
1	B	0.37	0/2564	0.56	0/3484
1	C	0.38	0/2614	0.60	2/3556 (0.1%)
All	All	0.38	0/7833	0.59	4/10651 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	ALA	CA-C-N	8.34	136.72	121.70
1	C	28	ALA	C-N-CA	8.34	136.72	121.70
1	A	225	GLY	CA-C-N	-6.30	109.37	122.03
1	A	225	GLY	C-N-CA	-6.30	109.37	122.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	30	GLU	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	2590	0	2544	55	0
1	B	2502	0	2450	44	0
1	C	2550	0	2499	71	0
2	A	48	25	23	11	0
2	B	48	25	23	11	0
2	C	48	25	24	9	0
3	A	178	0	0	6	1
3	B	153	0	0	1	0
3	C	151	0	0	5	1
All	All	8268	75	7563	171	1

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 11.

All (171) 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)
2:A:401:NAP:O4D	2:A:401:NAP:C1D	1.64	1.25
2:C:401:NAP:O4D	2:C:401:NAP:C1D	1.64	1.20
2:C:401:NAP:C1B	2:C:401:NAP:O4B	1.64	1.15
1:B:30:GLU:HG3	1:C:232:THR:HB	1.10	1.10
1:A:188:LYS:NZ	3:A:501:HOH:O	1.89	1.03
1:B:304:LYS:HD3	1:B:305:PRO:HD2	1.38	1.02
1:B:30:GLU:CG	1:C:232:THR:HB	1.91	1.00
1:B:222:SER:HA	2:B:401:NAP:O3	1.66	0.96
1:B:30:GLU:HG3	1:C:232:THR:CB	1.95	0.95
1:B:25:GLY:O	1:B:272:LYS:HG2	1.74	0.88
1:C:30:GLU:HB2	1:C:35:GLN:HE22	1.39	0.87
1:A:229:GLN:OE1	1:A:236:ARG:NH2	2.10	0.83
1:C:8:ASN:ND2	3:C:502:HOH:O	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:CE1	1:A:272:LYS:HG2	2.14	0.81
1:B:304:LYS:HD3	1:B:305:PRO:CD	2.11	0.81
1:C:29:ALA:HB1	1:C:30:GLU:HA	1.61	0.81
1:B:280:LYS:NZ	3:B:501:HOH:O	2.07	0.80
1:B:222:SER:H	2:B:401:NAP:H51N	1.46	0.80
1:A:27:PHE:HE1	2:A:401:NAP:O2N	1.65	0.78
1:B:156:ARG:O	1:B:160:GLU:HG3	1.86	0.76
1:C:103:ASP:OD2	3:C:501:HOH:O	2.04	0.75
1:B:27:PHE:CE2	1:B:28:ALA:HB2	2.25	0.71
1:A:92:MET:HE1	1:A:131:ARG:HD3	1.73	0.70
1:B:272:LYS:HD2	1:B:273:SER:N	2.05	0.70
1:B:229:GLN:HG2	1:B:234:GLY:HA2	1.74	0.70
1:A:32:GLN:HG2	1:A:35:GLN:HG3	1.75	0.69
1:B:27:PHE:CD2	1:B:28:ALA:HB2	2.27	0.69
1:C:278:ARG:HD2	2:C:401:NAP:C6A	2.23	0.69
1:C:29:ALA:HA	1:C:30:GLU:C	2.16	0.69
1:B:96:GLU:H	1:B:96:GLU:CD	2.00	0.69
1:C:134:LYS:HE3	3:C:612:HOH:O	1.92	0.69
2:C:401:NAP:N3A	2:C:401:NAP:H2B	2.06	0.68
1:A:236:ARG:NH2	3:A:503:HOH:O	2.26	0.67
1:C:133:VAL:HG11	1:C:141:TYR:CE2	2.30	0.67
1:C:32:GLN:H	1:C:35:GLN:HE21	1.43	0.66
1:C:229:GLN:HE21	1:C:236:ARG:NH1	1.94	0.66
1:A:27:PHE:CE1	2:A:401:NAP:O2N	2.49	0.66
1:A:27:PHE:HD1	2:A:401:NAP:O3D	1.78	0.66
1:C:32:GLN:H	1:C:35:GLN:NE2	1.95	0.65
1:A:272:LYS:NZ	2:A:401:NAP:O1X	2.29	0.64
1:A:272:LYS:HD2	1:A:273:SER:N	2.12	0.64
1:C:222:SER:HA	2:C:401:NAP:O3	1.97	0.64
1:C:103:ASP:O	1:C:107:LYS:HG2	1.98	0.63
1:C:198:ILE:HD12	1:C:220:ALA:HB2	1.81	0.63
1:C:229:GLN:HG2	1:C:234:GLY:HA2	1.80	0.63
1:B:119:VAL:HG23	1:B:158:MET:HE2	1.80	0.62
1:B:280:LYS:O	1:B:283:ILE:HG22	1.99	0.62
1:C:32:GLN:HB2	1:C:35:GLN:NE2	2.16	0.61
1:B:35:GLN:OE1	1:C:233:THR:HG21	2.00	0.61
1:B:5:THR:HG22	1:B:7:ALA:H	1.66	0.61
1:C:92:MET:HE1	1:C:131:ARG:CB	2.31	0.61
1:C:27:PHE:HE2	1:C:272:LYS:HD2	1.66	0.60
1:A:280:LYS:O	1:A:283:ILE:HG22	2.01	0.60
1:C:172:VAL:HB	1:C:175:TRP:CE3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PHE:HB2	1:B:57:TYR:CZ	2.38	0.59
1:C:29:ALA:CB	1:C:30:GLU:HA	2.27	0.58
1:C:282:ASN:OD1	2:C:401:NAP:H2A	2.04	0.58
1:C:92:MET:HE1	1:C:131:ARG:HB3	1.84	0.58
1:C:27:PHE:HB2	1:C:57:TYR:CE2	2.39	0.58
1:C:200:PRO:HG2	1:C:258:LEU:HD22	1.85	0.58
1:B:30:GLU:CG	1:C:232:THR:CB	2.69	0.57
1:B:272:LYS:O	2:B:401:NAP:H8A	2.05	0.57
1:C:29:ALA:HA	1:C:31:GLY:N	2.19	0.57
1:A:226:SER:HB3	1:A:228:ASP:HB2	1.87	0.56
1:A:214:ASN:O	1:A:215:ASP:HB2	2.05	0.56
1:B:27:PHE:HB2	1:B:57:TYR:CE2	2.40	0.56
1:A:133:VAL:HG11	1:A:141:TYR:CE1	2.40	0.56
1:C:230:VAL:HG23	1:C:235:GLU:O	2.06	0.56
1:C:238:ARG:HG2	1:C:254:LEU:HD12	1.88	0.56
1:C:28:ALA:HB1	1:C:29:ALA:C	2.31	0.56
1:A:172:VAL:HB	1:A:175:TRP:CE3	2.42	0.54
1:C:32:GLN:HB2	1:C:35:GLN:CD	2.32	0.54
1:A:226:SER:C	1:A:228:ASP:H	2.15	0.54
1:A:156:ARG:NH1	1:A:188:LYS:HG3	2.23	0.54
1:A:230:VAL:HG23	1:A:235:GLU:O	2.09	0.53
1:B:145:HIS:O	1:B:149:GLU:HG3	2.08	0.53
1:C:27:PHE:HB2	1:C:57:TYR:CZ	2.43	0.53
1:C:229:GLN:HB2	1:C:236:ARG:NH1	2.23	0.53
2:B:401:NAP:H6N	2:B:401:NAP:H3D	1.90	0.53
1:C:92:MET:CE	1:C:131:ARG:HB3	2.38	0.53
2:A:401:NAP:H6N	2:A:401:NAP:H3D	1.90	0.52
1:B:27:PHE:HE1	2:B:401:NAP:O1N	1.92	0.52
1:C:278:ARG:HB3	2:C:401:NAP:N1A	2.25	0.52
1:A:32:GLN:HB2	1:A:33:PRO:HD2	1.91	0.52
1:B:119:VAL:CG2	1:B:158:MET:HE2	2.39	0.52
1:B:152:GLU:HG3	1:B:186:VAL:HB	1.92	0.51
1:A:303:ARG:HH12	1:A:306:THR:HG23	1.76	0.51
1:C:30:GLU:O	1:C:35:GLN:NE2	2.44	0.51
1:A:27:PHE:HE1	1:A:272:LYS:HG2	1.71	0.51
1:C:91:HIS:HA	1:C:125:ALA:O	2.11	0.51
1:C:27:PHE:CD2	2:C:401:NAP:O3D	2.64	0.51
1:A:303:ARG:HH12	1:A:306:THR:CG2	2.23	0.50
1:B:200:PRO:HG2	1:B:258:LEU:HD22	1.93	0.50
1:B:250:SER:HB2	1:B:252:MET:HE3	1.93	0.50
1:C:228:ASP:CG	1:C:229:GLN:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:HG3	1:A:33:PRO:O	2.11	0.50
1:A:278:ARG:HD3	2:A:401:NAP:C5A	2.42	0.50
1:C:91:HIS:NE2	1:C:92:MET:HE2	2.27	0.49
1:C:199:HIS:HB2	1:C:200:PRO:CD	2.42	0.49
1:C:324:GLN:HA	1:C:324:GLN:OE1	2.12	0.49
1:A:222:SER:H	2:A:401:NAP:H51N	1.77	0.49
1:C:284:GLU:OE1	3:C:503:HOH:O	2.20	0.49
1:A:215:ASP:OD2	3:A:502:HOH:O	2.20	0.49
1:A:278:ARG:HD3	2:A:401:NAP:C4A	2.42	0.49
1:B:227:GLN:O	1:B:227:GLN:HG3	2.13	0.49
1:C:196:ILE:O	1:C:220:ALA:HA	2.13	0.49
1:C:133:VAL:HG11	1:C:141:TYR:CZ	2.47	0.48
1:A:227:GLN:HB3	1:A:238:ARG:NH2	2.28	0.48
1:C:91:HIS:CD2	1:C:92:MET:HE2	2.48	0.48
1:A:9:LYS:HE2	3:A:631:HOH:O	2.14	0.48
1:C:156:ARG:NH1	1:C:159:GLU:OE1	2.45	0.48
1:A:179:GLY:HA3	3:A:649:HOH:O	2.13	0.48
1:A:87:LYS:HG2	1:A:118:LEU:HB2	1.96	0.48
1:A:224:LEU:C	1:A:225:GLY:O	2.52	0.48
1:B:27:PHE:CE1	2:B:401:NAP:O1N	2.67	0.48
1:B:278:ARG:HD2	2:B:401:NAP:O1X	2.14	0.47
1:C:230:VAL:HB	1:C:235:GLU:H	1.78	0.47
1:B:272:LYS:HD2	1:B:273:SER:H	1.80	0.47
1:C:275:THR:HG22	3:C:564:HOH:O	2.14	0.47
1:B:27:PHE:CD1	1:B:272:LYS:HG3	2.50	0.47
1:B:246:VAL:HA	1:B:249:ARG:HG2	1.95	0.47
1:A:23:GLY:HA2	1:A:50:HIS:HB3	1.96	0.47
1:C:282:ASN:OD1	2:C:401:NAP:C2A	2.63	0.47
1:B:224:LEU:HB2	2:B:401:NAP:O1A	2.14	0.47
1:C:229:GLN:CG	1:C:234:GLY:HA2	2.44	0.47
1:B:27:PHE:HD1	2:B:401:NAP:O3D	1.98	0.47
1:A:92:MET:HE1	1:A:131:ARG:CD	2.43	0.46
1:A:190:LYS:HG2	1:A:191:PRO:HD2	1.98	0.46
1:A:233:THR:OG1	1:A:235:GLU:HG2	2.16	0.46
1:A:99:LYS:NZ	1:A:160:GLU:OE1	2.45	0.45
1:C:180:LEU:HA	1:C:180:LEU:HD23	1.83	0.45
1:A:41:LYS:NZ	1:A:73:GLU:OE1	2.49	0.45
1:A:326:GLU:HA	1:A:326:GLU:OE1	2.15	0.45
1:A:219:SER:HB3	1:A:268:VAL:HB	1.98	0.45
1:B:249:ARG:HG3	1:B:250:SER:N	2.31	0.45
1:C:229:GLN:HE21	1:C:236:ARG:HH12	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLN:HG2	1:B:234:GLY:CA	2.44	0.45
1:A:224:LEU:O	1:A:225:GLY:O	2.35	0.44
1:A:249:ARG:NH1	1:A:292:ASP:OD1	2.49	0.44
1:C:27:PHE:CE2	1:C:272:LYS:HD2	2.49	0.44
1:B:172:VAL:HB	1:B:175:TRP:CE3	2.53	0.44
1:C:24:PHE:HB2	1:C:48:TYR:CD2	2.53	0.43
1:B:27:PHE:HB3	2:B:401:NAP:H2D	1.99	0.43
1:B:226:SER:OG	1:B:228:ASP:HB2	2.18	0.43
1:C:92:MET:HE1	1:C:131:ARG:HG2	1.99	0.43
1:C:128:THR:OG1	1:C:130:ASP:OD2	2.36	0.43
1:C:92:MET:HE1	1:C:131:ARG:CG	2.49	0.43
1:C:290:GLU:HA	1:C:290:GLU:OE1	2.19	0.43
1:A:228:ASP:O	1:A:229:GLN:HB3	2.18	0.43
1:B:72:LYS:O	1:B:72:LYS:HG3	2.19	0.43
1:A:92:MET:HE1	1:A:131:ARG:CG	2.49	0.42
1:A:102:LEU:CD2	1:A:161:LEU:HD13	2.49	0.42
1:A:165:LYS:HE2	1:C:149:GLU:OE2	2.19	0.42
1:A:215:ASP:HA	3:A:502:HOH:O	2.18	0.42
1:A:19:ILE:HD11	1:A:50:HIS:CE1	2.54	0.42
1:B:27:PHE:CD1	2:B:401:NAP:H3D	2.54	0.42
1:C:102:LEU:HD23	1:C:161:LEU:HD22	2.01	0.42
1:A:96:GLU:H	1:A:96:GLU:CD	2.28	0.42
1:A:89:TRP:CG	1:A:90:ASN:H	2.39	0.41
1:C:177:ILE:HD11	1:C:206:GLU:HG2	2.03	0.41
1:C:27:PHE:CD2	1:C:272:LYS:HG3	2.56	0.41
1:C:126:GLU:HB2	1:C:142:VAL:HB	2.03	0.41
1:A:146:GLU:HA	1:A:146:GLU:OE1	2.20	0.41
2:A:401:NAP:H6N	2:A:401:NAP:C3D	2.51	0.41
1:A:91:HIS:HA	1:A:125:ALA:O	2.21	0.41
1:A:222:SER:HA	2:A:401:NAP:O3	2.20	0.41
1:A:249:ARG:NH2	1:A:295:ASP:OD2	2.39	0.40
1:C:28:ALA:HA	1:C:29:ALA:O	2.22	0.40
1:C:34:GLY:H	1:C:62:GLU:CD	2.27	0.40
1:C:140:LYS:HE2	1:C:313:ASP:O	2.22	0.40
1:C:320:TRP:O	1:C:321:LYS:C	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:678:HOH:O	3:C:646:HOH:O[3_655]	2.19	0.01

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	324/332 (98%)	314 (97%)	10 (3%)	0	100	100
1	B	310/332 (93%)	300 (97%)	10 (3%)	0	100	100
1	C	319/332 (96%)	312 (98%)	7 (2%)	0	100	100
All	All	953/996 (96%)	926 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	276/282 (98%)	273 (99%)	3 (1%)	65	81
1	B	265/282 (94%)	261 (98%)	4 (2%)	57	75
1	C	271/282 (96%)	267 (98%)	4 (2%)	57	75
All	All	812/846 (96%)	801 (99%)	11 (1%)	59	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	249	ARG
1	A	272	LYS
1	B	30	GLU
1	B	72	LYS

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Mol	Chain	Res	Type
1	B	88	VAL
1	B	254	LEU
1	C	5	THR
1	C	30	GLU
1	C	254	LEU
1	C	264	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	58	GLN
1	A	74	ASN
1	B	58	GLN
1	B	244	ASN
1	C	32	GLN
1	C	35	GLN
1	C	229	GLN
1	C	248	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	401	-	50,52,52	4.06	19 (38%)	71,80,80	2.05	17 (23%)
2	NAP	B	401	-	50,52,52	3.89	16 (32%)	71,80,80	2.10	17 (23%)
2	NAP	C	401	-	50,52,52	4.04	16 (32%)	71,80,80	1.86	10 (14%)

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	401	-	-	7/35/67/67	0/5/5/5
2	NAP	B	401	-	-	12/35/67/67	0/5/5/5
2	NAP	C	401	-	-	6/35/67/67	0/5/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	O4D-C1D	17.65	1.64	1.40
2	A	401	NAP	O4D-C1D	17.62	1.64	1.40
2	B	401	NAP	O4D-C1D	17.15	1.63	1.40
2	C	401	NAP	O4B-C1B	9.73	1.64	1.42
2	C	401	NAP	C2B-C1B	-9.11	1.30	1.53
2	B	401	NAP	O4B-C1B	8.82	1.62	1.42
2	A	401	NAP	O4B-C1B	8.70	1.62	1.42
2	B	401	NAP	C2B-C1B	-8.61	1.31	1.53
2	A	401	NAP	C2B-C1B	-8.21	1.32	1.53
2	A	401	NAP	C7N-N7N	7.80	1.47	1.33
2	A	401	NAP	PA-O3	7.25	1.67	1.59
2	C	401	NAP	C7N-N7N	7.25	1.46	1.33
2	C	401	NAP	PA-O3	6.79	1.66	1.59
2	B	401	NAP	PN-O3	6.61	1.66	1.59
2	A	401	NAP	O4B-C4B	-6.59	1.30	1.45
2	B	401	NAP	O4B-C4B	-6.54	1.30	1.45
2	C	401	NAP	PN-O3	6.48	1.66	1.59
2	B	401	NAP	C7N-N7N	6.46	1.44	1.33
2	A	401	NAP	PN-O3	6.21	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAP	O4D-C4D	-5.88	1.31	1.45
2	B	401	NAP	O4D-C4D	-5.84	1.32	1.45
2	C	401	NAP	O4B-C4B	-5.58	1.32	1.45
2	A	401	NAP	O4D-C4D	-5.35	1.33	1.45
2	B	401	NAP	PA-O3	5.30	1.65	1.59
2	A	401	NAP	P2B-O2B	5.03	1.68	1.59
2	A	401	NAP	C6A-N6A	4.45	1.45	1.34
2	B	401	NAP	C6A-N6A	4.28	1.45	1.34
2	C	401	NAP	C6A-N6A	4.20	1.44	1.34
2	C	401	NAP	O2D-C2D	3.44	1.51	1.43
2	C	401	NAP	P2B-O2B	3.39	1.65	1.59
2	B	401	NAP	P2B-O2B	3.39	1.65	1.59
2	A	401	NAP	O2D-C2D	3.33	1.51	1.43
2	A	401	NAP	C5A-N7A	-3.07	1.33	1.39
2	C	401	NAP	O3D-C3D	-3.00	1.35	1.43
2	B	401	NAP	O2D-C2D	2.99	1.50	1.43
2	A	401	NAP	O3D-C3D	-2.96	1.35	1.43
2	A	401	NAP	O3B-C3B	-2.96	1.35	1.43
2	B	401	NAP	O3D-C3D	-2.80	1.36	1.43
2	C	401	NAP	C5A-C4A	-2.70	1.34	1.39
2	B	401	NAP	C5A-N7A	-2.68	1.34	1.39
2	B	401	NAP	C5A-C4A	-2.63	1.34	1.39
2	C	401	NAP	C5A-N7A	-2.60	1.34	1.39
2	B	401	NAP	O3B-C3B	-2.59	1.36	1.43
2	A	401	NAP	C5A-C4A	-2.56	1.34	1.39
2	B	401	NAP	C3N-C7N	2.55	1.54	1.50
2	A	401	NAP	O2B-C2B	2.42	1.52	1.44
2	A	401	NAP	C3N-C7N	2.34	1.54	1.50
2	C	401	NAP	C4N-C3N	-2.20	1.36	1.39
2	A	401	NAP	C5D-C4D	2.11	1.57	1.51
2	A	401	NAP	C4N-C3N	-2.05	1.36	1.39
2	C	401	NAP	O3B-C3B	-2.04	1.37	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAP	N6A-C6A-N1A	-7.98	100.61	118.38
2	C	401	NAP	N6A-C6A-N1A	-7.17	102.41	118.38
2	B	401	NAP	C5A-C6A-N6A	6.44	139.24	123.29
2	A	401	NAP	N6A-C6A-N1A	-6.24	104.48	118.38
2	C	401	NAP	C5A-C6A-N6A	6.15	138.52	123.29
2	C	401	NAP	N3A-C2A-N1A	-5.85	119.73	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAP	N3A-C2A-N1A	-5.49	120.27	128.58
2	A	401	NAP	C5A-C4A-N3A	-5.48	119.17	126.72
2	B	401	NAP	C5A-C4A-N3A	-5.23	119.51	126.72
2	A	401	NAP	C5A-C6A-N6A	5.17	136.08	123.29
2	A	401	NAP	N3A-C2A-N1A	-4.79	121.34	128.58
2	A	401	NAP	C2B-C1B-N9A	-4.75	105.93	113.75
2	A	401	NAP	C6N-N1N-C2N	-4.08	118.41	121.88
2	B	401	NAP	N9A-C8A-N7A	-3.99	108.27	113.94
2	C	401	NAP	C5A-C4A-N3A	-3.79	121.50	126.72
2	C	401	NAP	C2B-C3B-C4B	3.53	109.59	101.99
2	B	401	NAP	C2B-C1B-N9A	-3.43	108.11	113.75
2	B	401	NAP	C2A-N3A-C4A	3.37	120.07	111.83
2	B	401	NAP	C6N-N1N-C2N	-3.36	119.02	121.88
2	A	401	NAP	N3A-C4A-N9A	3.33	132.84	127.17
2	C	401	NAP	N9A-C8A-N7A	-3.29	109.27	113.94
2	B	401	NAP	C5A-N7A-C8A	3.26	108.57	103.45
2	A	401	NAP	C6A-C5A-C4A	3.19	121.54	117.18
2	A	401	NAP	O2A-PA-O3	3.14	115.76	107.27
2	A	401	NAP	C2A-N3A-C4A	3.12	119.45	111.83
2	A	401	NAP	N9A-C8A-N7A	-3.08	109.57	113.94
2	C	401	NAP	C2A-N3A-C4A	2.95	119.05	111.83
2	B	401	NAP	C4A-N9A-C1B	-2.90	119.85	126.63
2	A	401	NAP	O3-PA-O1A	-2.87	102.08	110.70
2	B	401	NAP	N3A-C4A-N9A	2.83	131.99	127.17
2	A	401	NAP	O2B-C2B-C1B	2.80	119.88	110.05
2	B	401	NAP	C4A-C5A-N7A	-2.75	107.44	110.58
2	A	401	NAP	O4B-C1B-C2B	2.74	111.31	106.59
2	A	401	NAP	C5A-N7A-C8A	2.67	107.65	103.45
2	B	401	NAP	C1B-N9A-C8A	2.63	132.92	127.09
2	A	401	NAP	C2B-C3B-C4B	2.56	107.50	101.99
2	C	401	NAP	C6N-N1N-C2N	-2.52	119.73	121.88
2	B	401	NAP	C5A-C4A-N9A	2.47	108.50	105.81
2	B	401	NAP	O7N-C7N-C3N	2.46	122.61	119.60
2	C	401	NAP	O3B-C3B-C4B	-2.36	104.31	111.08
2	C	401	NAP	N3A-C4A-N9A	2.34	131.15	127.17
2	B	401	NAP	P2B-O2B-C2B	-2.28	117.34	123.43
2	B	401	NAP	C6A-C5A-C4A	2.20	120.18	117.18
2	A	401	NAP	C5A-C4A-N9A	2.00	107.99	105.81

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	C5B-O5B-PA-O3
2	B	401	NAP	C5B-O5B-PA-O1A
2	B	401	NAP	C5B-O5B-PA-O3
2	B	401	NAP	O4B-C4B-C5B-O5B
2	B	401	NAP	C3B-C4B-C5B-O5B
2	B	401	NAP	C5D-O5D-PN-O1N
2	B	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	O4B-C4B-C5B-O5B
2	B	401	NAP	O4D-C4D-C5D-O5D
2	B	401	NAP	C3D-C4D-C5D-O5D
2	A	401	NAP	C3B-C4B-C5B-O5B
2	A	401	NAP	O4D-C4D-C5D-O5D
2	A	401	NAP	C3D-C4D-C5D-O5D
2	B	401	NAP	PN-O3-PA-O5B
2	B	401	NAP	PA-O3-PN-O1N
2	A	401	NAP	C5B-O5B-PA-O2A
2	C	401	NAP	C2B-C1B-N9A-C8A
2	B	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C2N
2	C	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	O4B-C1B-N9A-C8A
2	C	401	NAP	C1B-C2B-O2B-P2B
2	C	401	NAP	C2B-C1B-N9A-C4A
2	B	401	NAP	PA-O3-PN-O2N

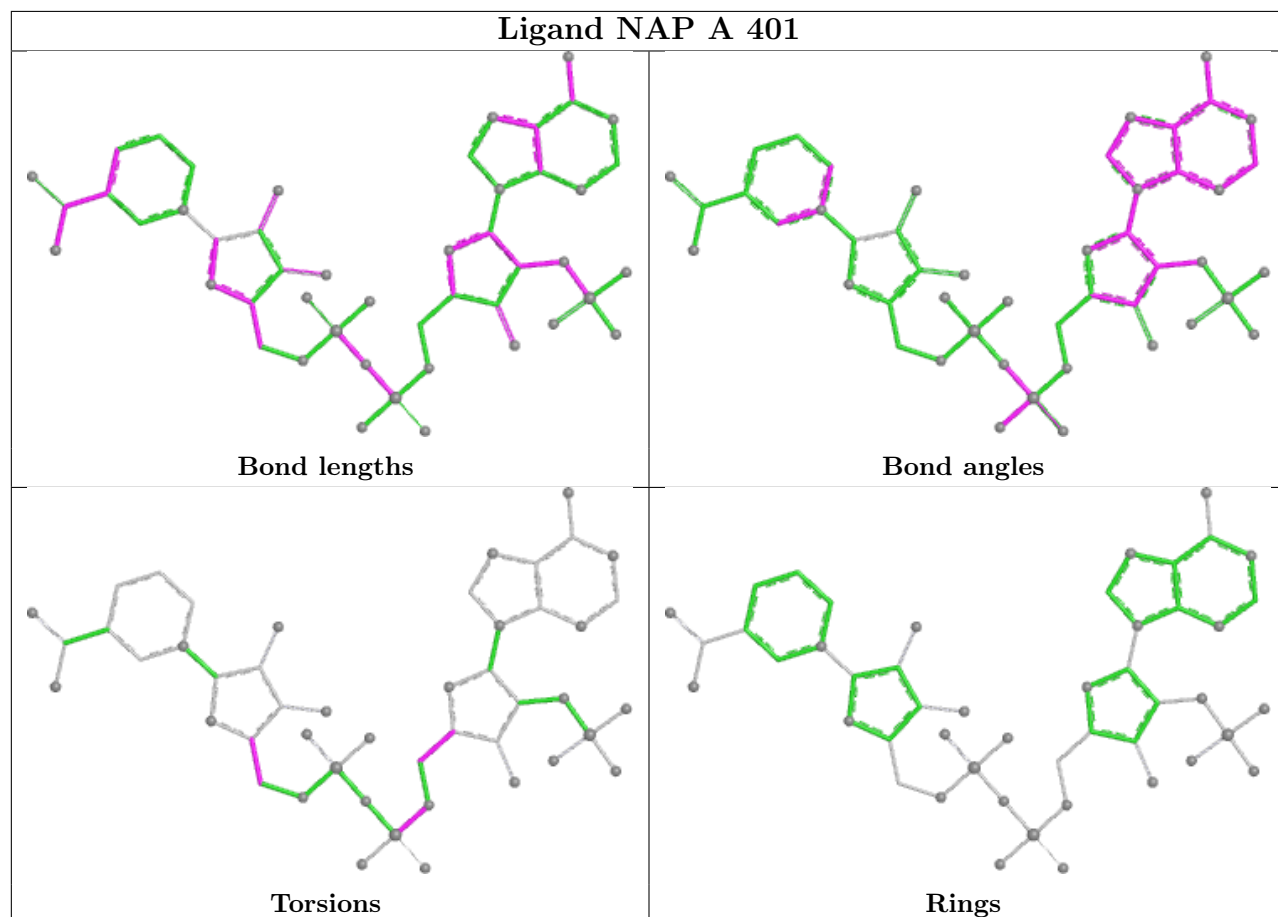
There are no ring outliers.

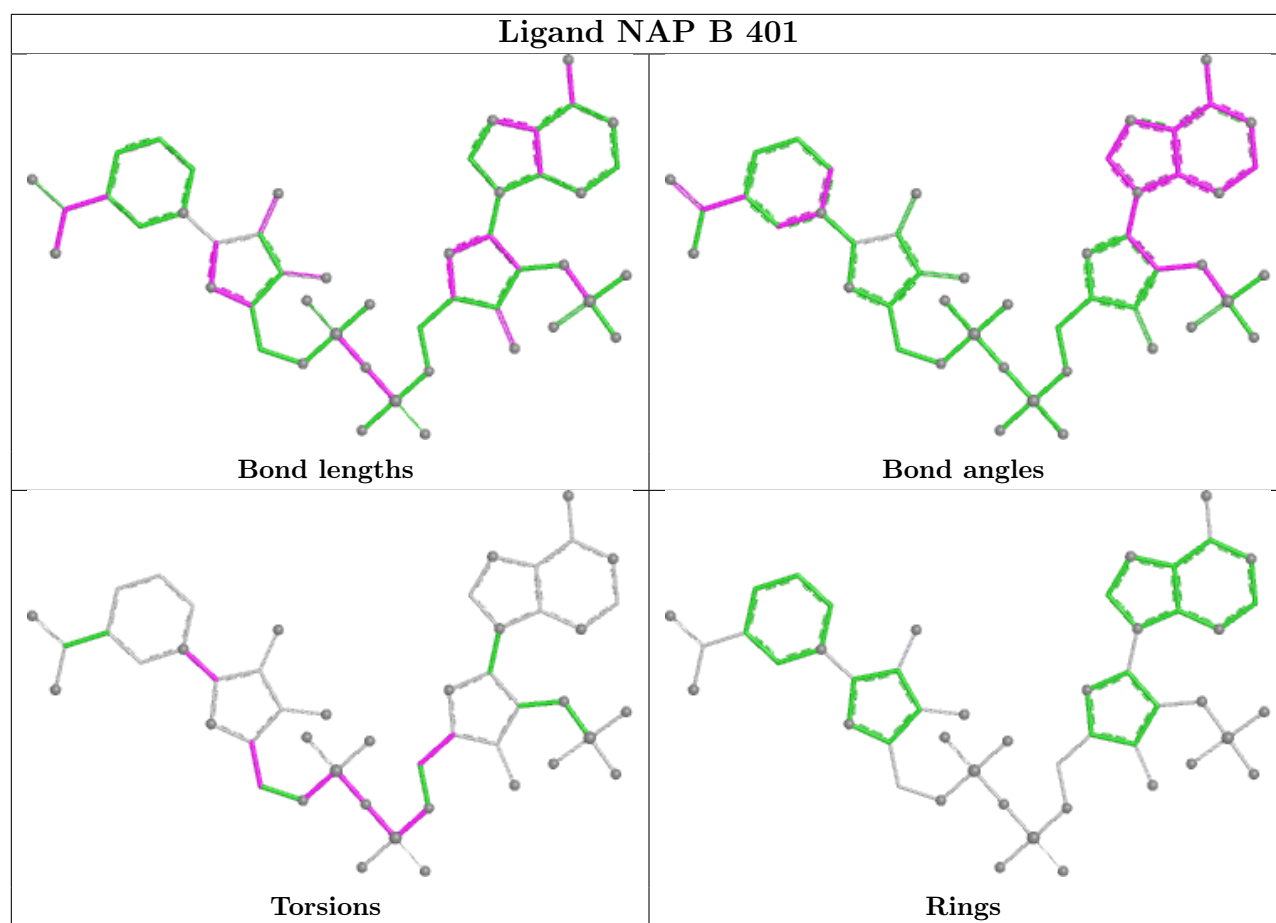
3 monomers are involved in 31 short contacts:

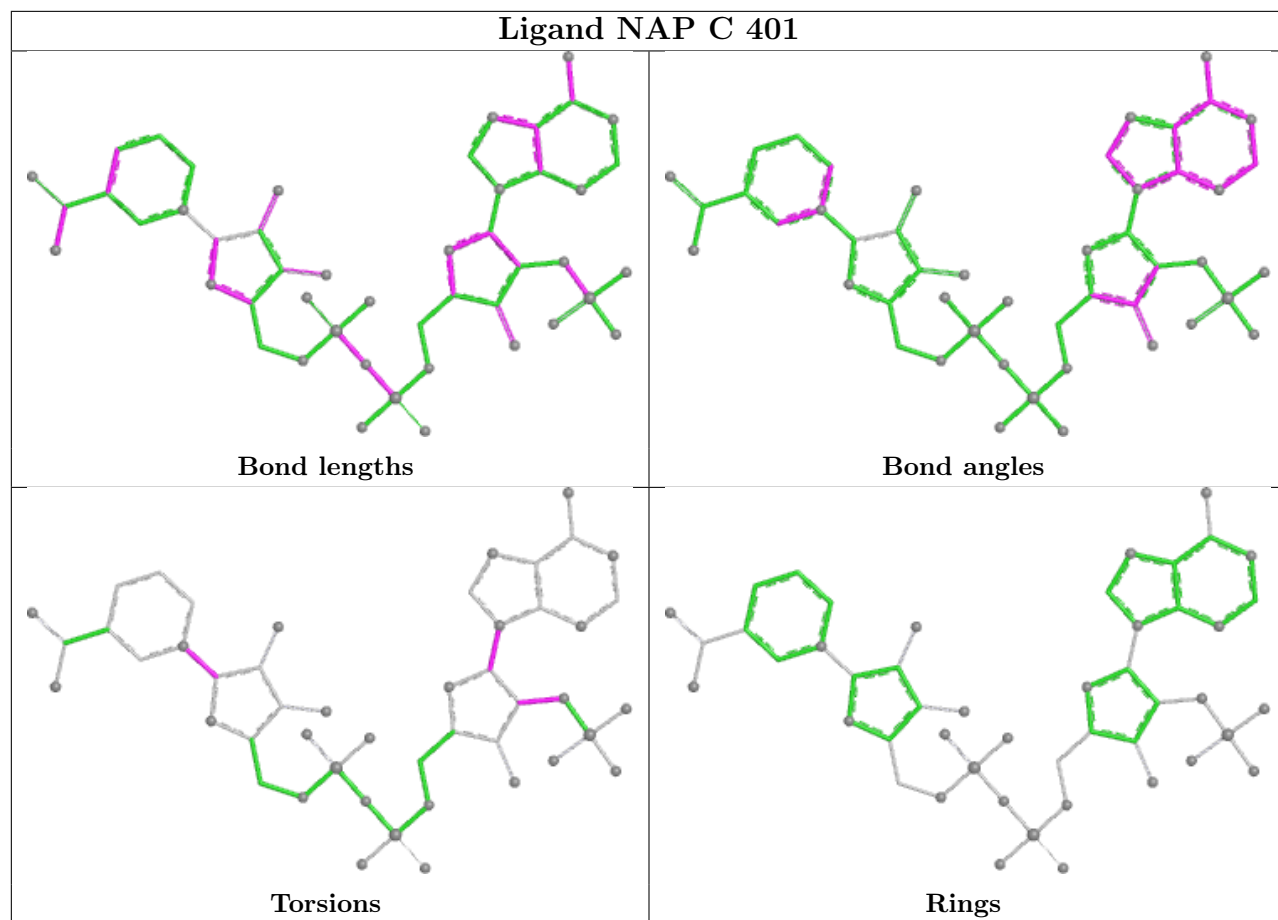
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	11	0
2	B	401	NAP	11	0
2	C	401	NAP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/332 (98%)	-0.21	9 (2%) 55 57	16, 25, 50, 76	0
1	B	314/332 (94%)	-0.16	12 (3%) 44 46	18, 27, 48, 80	0
1	C	321/332 (96%)	-0.02	11 (3%) 48 50	16, 30, 57, 77	0
All	All	961/996 (96%)	-0.13	32 (3%) 49 51	16, 27, 54, 80	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	PHE	5.6
1	B	28	ALA	5.0
1	C	27	PHE	4.8
1	C	232	THR	4.6
1	B	27	PHE	4.4
1	A	29	ALA	4.1
1	A	31	GLY	3.7
1	C	28	ALA	3.7
1	A	30	GLU	3.5
1	B	31	GLY	3.4
1	B	227	GLN	3.3
1	B	30	GLU	3.2
1	C	231	PRO	3.1
1	B	29	ALA	3.1
1	B	228	ASP	3.1
1	B	322	GLU	3.0
1	C	227	GLN	2.9
1	A	28	ALA	2.8
1	C	31	GLY	2.8
1	B	321	LYS	2.8
1	C	228	ASP	2.7
1	A	32	GLN	2.5
1	C	29	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	2.5
1	A	226	SER	2.4
1	A	225	GLY	2.3
1	B	229	GLN	2.3
1	C	324	GLN	2.3
1	B	129	GLU	2.1
1	C	323	SER	2.1
1	C	7	ALA	2.1
1	A	228	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

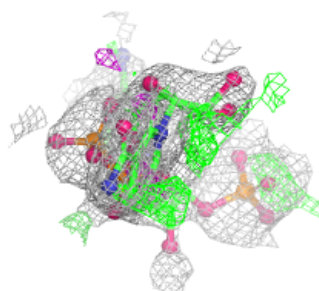
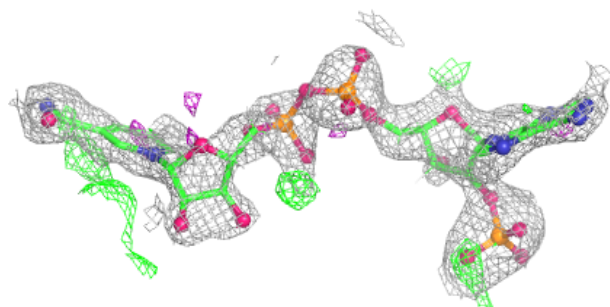
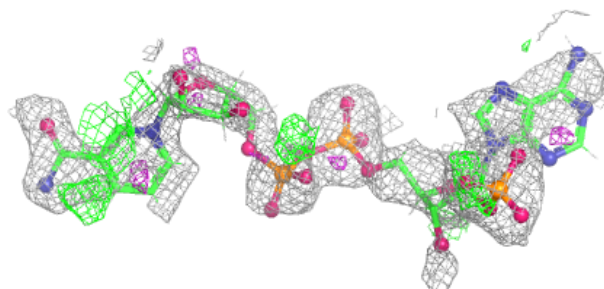
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	B	401	48/48	0.84	0.15	16,36,46,57	73
2	NAP	C	401	48/48	0.89	0.12	24,37,49,56	73
2	NAP	A	401	48/48	0.92	0.10	17,30,38,44	73

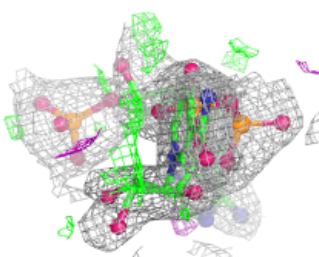
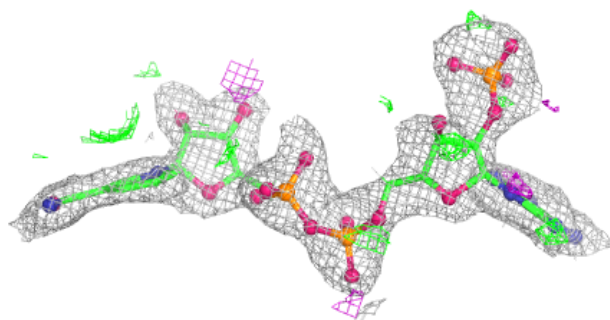
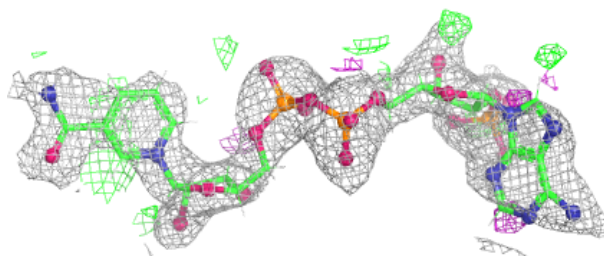
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 401:

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

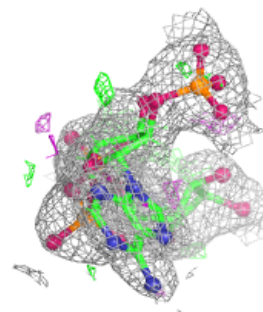
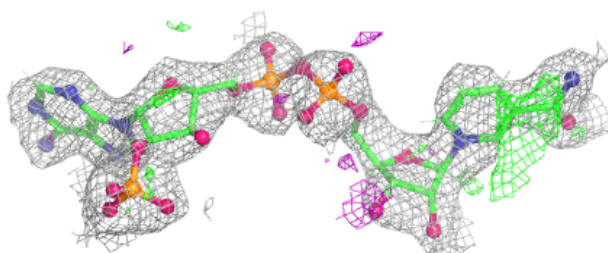
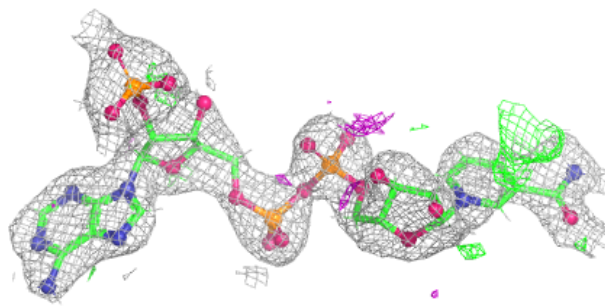
**Electron density around NAP C 401:**

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



Electron density around NAP A 401:

$2mF_o-DF_c$ (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.