



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 4H8A / pdb_00004h8a
Title : Crystal structure of ureidoglycolate dehydrogenase in binary complex with NADH
Authors : Rhee, S.; Shin, I.; Kim, M.
Deposited on : 2012-09-22
Resolution : 1.64 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

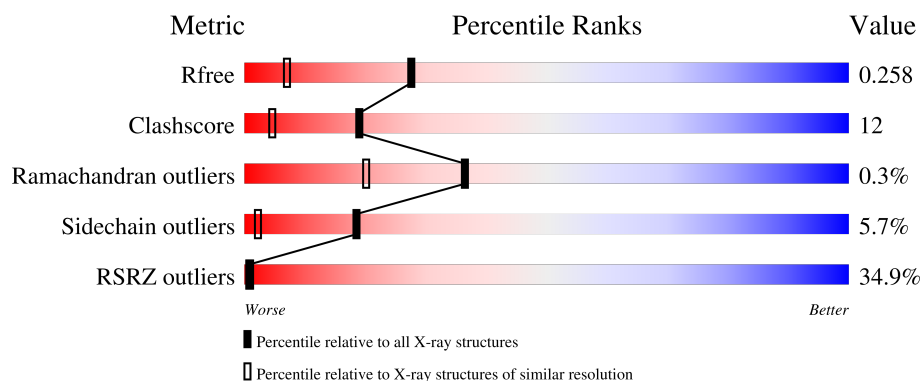
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	339	34% 85% 14% ..
1	B	339	33% 73% 17% • 8%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5749 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.

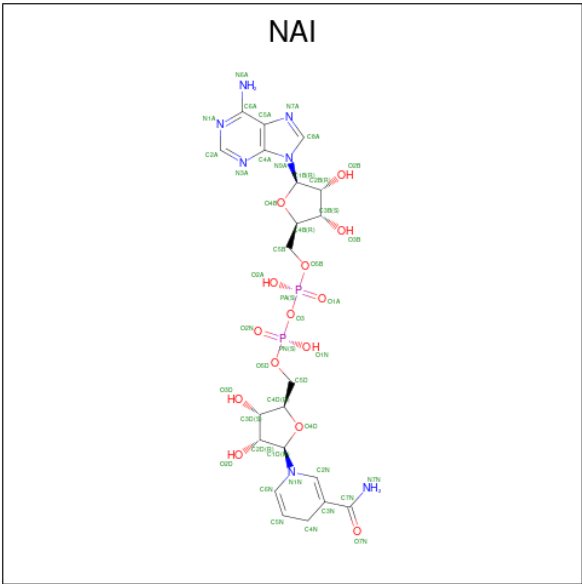
- Molecule 1 is a protein called Ureidoglycolate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2571	1621	450	484	16			
1	B	313	Total	C	N	O	S	0	0	0
			2379	1496	424	444	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P77555
A	0	HIS	-	expression tag	UNP P77555
B	-1	GLY	-	expression tag	UNP P77555
B	0	HIS	-	expression tag	UNP P77555

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

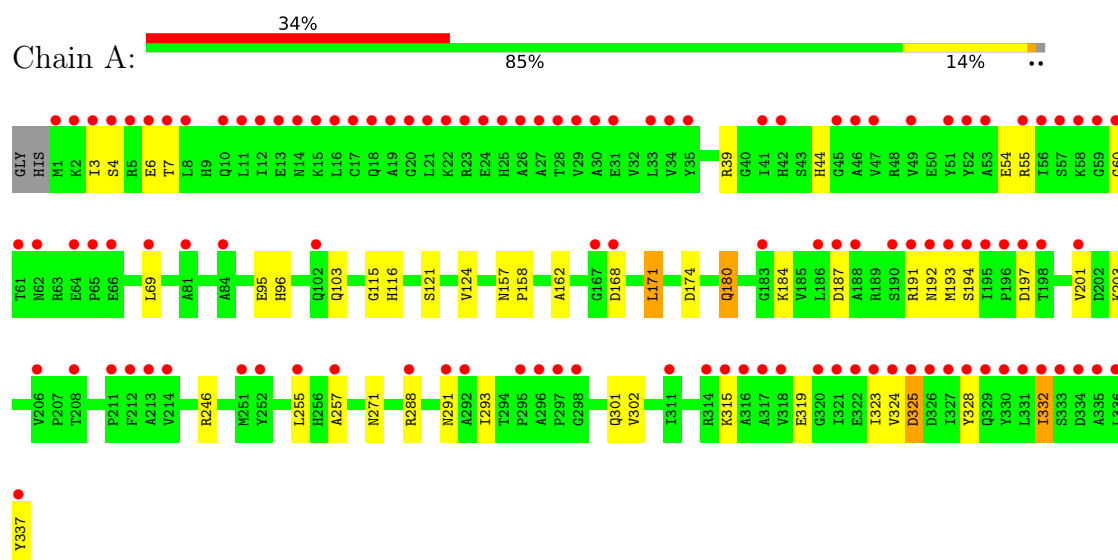
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	341	Total 341	O 341	0	0
3	B	370	Total 370	O 370	0	0

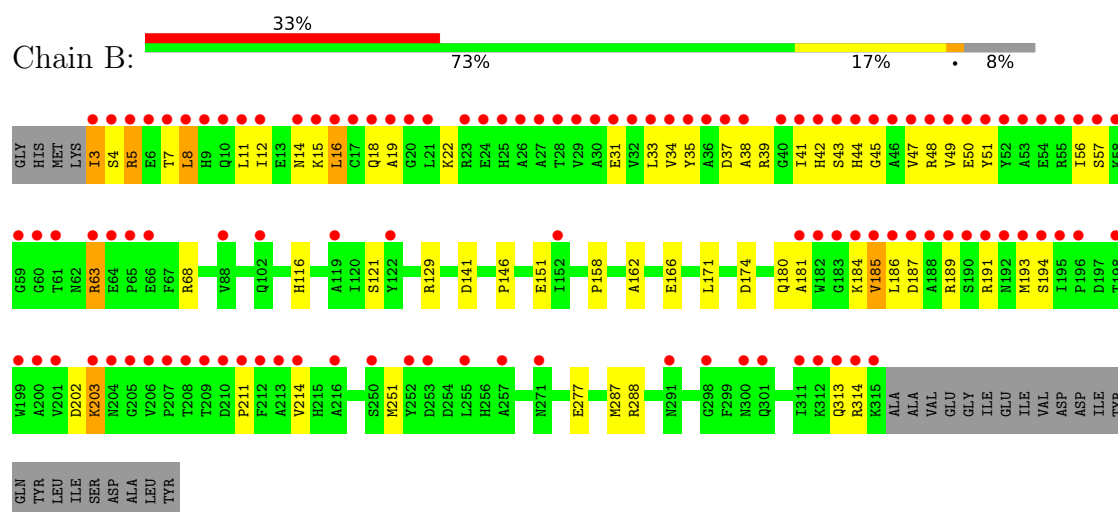
3 Residue-property plots

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

• Molecule 1: Ureidoglycolate dehydrogenase



• Molecule 1: Ureidoglycolate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	162.51Å 162.51Å 60.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.07 – 1.64 45.07 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.07-1.64) 94.3 (45.07-1.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.7.2 _869	Depositor
R, R_{free}	0.230 , 0.246 0.244 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5749	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/2626	0.74	0/3558
1	B	0.44	0/2431	0.80	1/3294 (0.0%)
All	All	0.44	0/5057	0.77	1/6852 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	VAL	N-CA-C	-5.39	105.87	111.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2571	0	2528	40	0
1	B	2379	0	2337	78	1
2	A	44	0	27	1	0
2	B	44	0	27	1	0
3	A	341	0	0	25	2
3	B	370	0	0	60	3
All	All	5749	0	4919	117	5

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 12.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:HIS:HA	3:B:768:HOH:O	1.35	1.24
1:B:48:ARG:CZ	3:B:853:HOH:O	1.90	1.19
1:B:287:MET:SD	3:B:780:HOH:O	1.95	1.19
1:B:42:HIS:CA	3:B:768:HOH:O	1.82	1.18
1:B:38:ALA:HB3	3:B:773:HOH:O	1.43	1.18
1:A:7:THR:HG21	3:A:840:HOH:O	1.45	1.14
1:B:48:ARG:NH2	3:B:853:HOH:O	1.81	1.14
1:B:51:TYR:HA	3:B:764:HOH:O	1.49	1.10
1:B:5:ARG:HB3	3:B:771:HOH:O	1.51	1.08
1:B:8:LEU:HB2	3:B:543:HOH:O	1.53	1.08
1:B:5:ARG:CA	3:B:771:HOH:O	2.04	1.06
1:A:323:ILE:HA	3:A:771:HOH:O	1.55	1.05
1:B:5:ARG:CB	3:B:771:HOH:O	2.05	1.03
1:B:48:ARG:NE	3:B:853:HOH:O	1.86	1.03
1:B:5:ARG:C	3:B:771:HOH:O	2.03	1.02
1:A:7:THR:CG2	3:A:840:HOH:O	2.02	0.97
1:B:37:ASP:OD1	3:B:768:HOH:O	1.80	0.97
1:B:5:ARG:O	3:B:771:HOH:O	1.84	0.95
1:B:39:ARG:N	3:B:773:HOH:O	2.01	0.93
1:A:95:GLU:OE1	3:A:781:HOH:O	1.87	0.91
1:B:129:ARG:NH1	3:B:834:HOH:O	1.85	0.90
1:B:15:LYS:NZ	3:B:698:HOH:O	2.04	0.90
1:A:301:GLN:CG	3:A:780:HOH:O	2.21	0.89
1:A:168:ASP:OD1	3:A:800:HOH:O	1.92	0.87
1:B:42:HIS:CB	3:B:768:HOH:O	2.10	0.87
1:A:60:GLY:C	3:A:778:HOH:O	2.19	0.86
1:B:38:ALA:CB	3:B:773:HOH:O	2.08	0.85
1:B:38:ALA:C	3:B:773:HOH:O	2.20	0.84
1:B:42:HIS:HB3	3:B:768:HOH:O	1.76	0.82
1:B:50:GLU:O	3:B:764:HOH:O	1.99	0.80
1:B:314:ARG:NH1	3:B:735:HOH:O	2.16	0.77
1:A:301:GLN:HG2	3:A:780:HOH:O	1.81	0.76
1:B:287:MET:CE	3:B:780:HOH:O	2.27	0.76
1:B:51:TYR:N	3:B:604:HOH:O	2.00	0.74
1:A:7:THR:CB	3:A:840:HOH:O	2.27	0.74
1:A:103:GLN:NE2	3:A:579:HOH:O	2.18	0.74
1:A:60:GLY:O	3:A:778:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:O	3:B:559:HOH:O	2.05	0.73
1:B:19:ALA:O	3:B:584:HOH:O	2.06	0.73
1:A:197:ASP:CG	3:A:783:HOH:O	2.30	0.73
1:A:301:GLN:HG3	3:A:780:HOH:O	1.87	0.73
1:B:37:ASP:OD1	3:B:767:HOH:O	2.07	0.72
1:B:129:ARG:NH2	3:B:718:HOH:O	2.22	0.72
1:B:180:GLN:OE1	3:B:798:HOH:O	2.05	0.72
1:B:34:VAL:HG11	3:B:771:HOH:O	1.88	0.72
1:A:325:ASP:OD1	1:A:325:ASP:N	2.19	0.72
1:A:180:GLN:HG3	1:A:184:LYS:HG3	1.73	0.71
1:B:166:GLU:OE2	3:B:708:HOH:O	2.09	0.71
1:A:337:TYR:OXT	3:A:766:HOH:O	2.09	0.70
1:A:323:ILE:C	3:A:817:HOH:O	2.35	0.70
1:B:50:GLU:C	3:B:764:HOH:O	2.34	0.69
1:B:43:SER:CB	3:B:779:HOH:O	2.39	0.69
1:B:181:ALA:HB3	3:B:789:HOH:O	1.92	0.69
1:B:38:ALA:CA	3:B:773:HOH:O	2.31	0.68
1:B:48:ARG:HH22	1:B:251:MET:HE1	1.58	0.67
1:B:186:LEU:HA	1:B:189:ARG:HB2	1.76	0.67
1:A:39:ARG:HG3	3:A:685:HOH:O	1.95	0.66
1:A:324:VAL:HA	3:A:817:HOH:O	1.94	0.66
1:B:43:SER:HB3	3:B:779:HOH:O	1.94	0.66
1:B:51:TYR:CA	3:B:764:HOH:O	2.23	0.64
1:B:202:ASP:HB2	3:B:807:HOH:O	2.00	0.62
1:A:271:ASN:ND2	3:A:610:HOH:O	2.29	0.61
1:B:287:MET:HE3	3:B:780:HOH:O	1.95	0.61
1:A:158:PRO:HD3	2:A:401:NAI:H42N	1.85	0.59
1:B:287:MET:CB	3:B:780:HOH:O	2.51	0.59
1:A:324:VAL:N	3:A:817:HOH:O	2.35	0.59
1:A:54:GLU:OE1	3:A:689:HOH:O	2.17	0.58
1:B:180:GLN:NE2	3:B:667:HOH:O	2.36	0.58
1:B:158:PRO:HD3	2:B:401:NAI:H42N	1.86	0.57
1:A:324:VAL:CA	3:A:817:HOH:O	2.50	0.56
1:B:35:TYR:HA	3:B:821:HOH:O	2.04	0.56
1:A:44:HIS:HD2	1:A:116:HIS:CE1	2.24	0.56
1:B:191:ARG:HH21	1:B:193:MET:HE3	1.70	0.56
1:B:14:ASN:ND2	3:B:863:HOH:O	2.39	0.55
1:B:184:LYS:HA	1:B:187:ASP:HB3	1.89	0.55
1:B:3:ILE:N	3:B:525:HOH:O	2.40	0.55
1:B:39:ARG:HG3	3:B:773:HOH:O	2.06	0.54
1:B:211:PRO:HA	1:B:214:VAL:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLN:C	3:B:844:HOH:O	2.51	0.52
1:A:55:ARG:NH1	1:A:257:ALA:O	2.41	0.52
1:B:4:SER:O	1:B:7:THR:HB	2.09	0.52
1:B:184:LYS:HB2	3:B:765:HOH:O	2.10	0.51
1:A:293:ILE:HG23	1:B:151:GLU:HB2	1.91	0.51
1:A:288:ARG:NH2	3:A:580:HOH:O	2.44	0.51
1:A:246:ARG:HD2	3:B:801:HOH:O	2.12	0.48
1:A:44:HIS:HD2	1:A:116:HIS:HE1	1.61	0.47
1:B:18:GLN:CB	3:B:844:HOH:O	2.61	0.47
1:A:69:LEU:HD21	1:A:96:HIS:CE1	2.50	0.46
1:B:288:ARG:HD3	3:B:826:HOH:O	2.15	0.46
1:A:328:TYR:O	1:A:332:ILE:HD13	2.15	0.46
1:B:57:SER:CA	3:B:584:HOH:O	2.63	0.45
1:B:288:ARG:CD	3:B:826:HOH:O	2.64	0.45
1:B:313:GLN:HG2	3:B:833:HOH:O	2.16	0.45
1:A:121:SER:HB3	1:A:174:ASP:HB2	1.99	0.44
1:B:18:GLN:HB3	3:B:844:HOH:O	2.17	0.44
1:B:50:GLU:HB3	3:B:604:HOH:O	2.17	0.44
1:B:121:SER:HB3	1:B:174:ASP:HB2	2.00	0.44
1:B:57:SER:HB3	3:B:584:HOH:O	2.17	0.44
1:B:189:ARG:HG3	1:B:211:PRO:HB2	2.00	0.43
1:B:68:ARG:NH2	3:B:692:HOH:O	2.15	0.43
1:B:44:HIS:HD2	1:B:116:HIS:HE1	1.67	0.42
1:B:146:PRO:HD2	1:B:151:GLU:O	2.19	0.42
1:B:44:HIS:CD2	1:B:116:HIS:HE1	2.37	0.42
1:A:121:SER:HA	1:A:124:VAL:HG22	2.00	0.42
1:B:3:ILE:HD11	1:B:8:LEU:HG	2.01	0.42
1:A:162:ALA:HA	1:A:171:LEU:O	2.20	0.42
1:A:315:LYS:HA	1:A:315:LYS:HD3	1.72	0.42
1:A:315:LYS:HD2	1:A:319:GLU:CD	2.45	0.42
1:B:33:LEU:HD22	1:B:45:GLY:O	2.20	0.42
1:B:12:ILE:HG12	1:B:49:VAL:HG21	2.02	0.41
1:A:54:GLU:HB2	3:A:689:HOH:O	2.21	0.41
1:A:302:VAL:N	3:A:780:HOH:O	2.42	0.41
1:A:115:GLY:HA3	3:A:698:HOH:O	2.20	0.41
1:B:16:LEU:HD13	3:B:689:HOH:O	2.19	0.41
1:B:56:ILE:O	1:B:63:ARG:NH1	2.54	0.41
1:B:162:ALA:HA	1:B:171:LEU:O	2.21	0.41
1:B:203:LYS:H	1:B:203:LYS:HG2	1.61	0.40

All (5) 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:818:HOH:O	3:B:869:HOH:O[8_555]	1.96	0.24
3:B:527:HOH:O	3:B:554:HOH:O[8_554]	2.06	0.14
3:B:766:HOH:O	3:B:774:HOH:O[7_555]	2.11	0.09
3:A:765:HOH:O	3:A:765:HOH:O[8_554]	2.18	0.02
1:B:7:THR:OG1	1:B:7:THR:OG1[7_555]	2.18	0.02

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	335/339 (99%)	325 (97%)	8 (2%)	2 (1%)	21	7
1	B	311/339 (92%)	297 (96%)	14 (4%)	0	100	100
All	All	646/678 (95%)	622 (96%)	22 (3%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	157	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/267 (100%)	251 (94%)	15 (6%)	19	2
1	B	246/267 (92%)	232 (94%)	14 (6%)	18	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	512/534 (96%)	483 (94%)	29 (6%)	18 2

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	4	SER
1	A	6	GLU
1	A	171	LEU
1	A	180	GLN
1	A	187	ASP
1	A	191	ARG
1	A	193	MET
1	A	194	SER
1	A	201	VAL
1	A	203	LYS
1	A	255	LEU
1	A	291	ASN
1	A	325	ASP
1	A	332	ILE
1	B	3	ILE
1	B	5	ARG
1	B	8	LEU
1	B	11	LEU
1	B	16	LEU
1	B	22	LYS
1	B	31	GLU
1	B	41	ILE
1	B	63	ARG
1	B	141	ASP
1	B	185	VAL
1	B	194	SER
1	B	203	LYS
1	B	277	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	44	HIS
1	A	291	ASN

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	307	GLN
1	B	42	HIS
1	B	44	HIS

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](#)

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	NAI	A	401	-	47,48,48	2.00	8 (17%)	64,73,73	1.71	11 (17%)
2	NAI	B	401	-	47,48,48	2.02	8 (17%)	64,73,73	1.73	13 (20%)

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	NAI	A	401	-	-	5/29/72/72	0/5/5/5
2	NAI	B	401	-	-	3/29/72/72	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAI	C7N-N7N	5.50	1.49	1.33
2	B	401	NAI	C7N-N7N	5.35	1.48	1.33
2	B	401	NAI	C4N-C3N	-5.18	1.40	1.50
2	B	401	NAI	C2D-C3D	-4.93	1.40	1.53
2	A	401	NAI	C2D-C3D	-4.80	1.40	1.53
2	A	401	NAI	C4N-C3N	-4.76	1.41	1.50
2	A	401	NAI	C2B-C3B	-4.21	1.42	1.53
2	A	401	NAI	PA-O3	-4.15	1.55	1.59
2	B	401	NAI	C2B-C3B	-3.99	1.42	1.53
2	B	401	NAI	PA-O3	-3.96	1.55	1.59
2	A	401	NAI	C4N-C5N	-3.53	1.39	1.49
2	B	401	NAI	C4N-C5N	-3.36	1.40	1.49
2	A	401	NAI	O4D-C4D	-2.84	1.38	1.45
2	B	401	NAI	O4D-C4D	-2.70	1.39	1.45
2	B	401	NAI	C6A-N6A	2.55	1.40	1.34
2	A	401	NAI	C6A-N6A	2.46	1.40	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAI	C5A-C4A-N3A	-5.44	119.22	126.72
2	B	401	NAI	C5A-C4A-N3A	-5.42	119.26	126.72
2	A	401	NAI	N3A-C2A-N1A	-4.51	121.76	128.58
2	B	401	NAI	N3A-C2A-N1A	-4.05	122.44	128.58
2	B	401	NAI	N3A-C4A-N9A	3.84	133.70	127.17
2	A	401	NAI	C4A-C5A-N7A	-3.82	106.21	110.58
2	B	401	NAI	N9A-C8A-N7A	-3.63	108.78	113.94
2	A	401	NAI	C2A-N3A-C4A	3.51	120.39	111.83
2	B	401	NAI	C5A-N7A-C8A	3.44	108.86	103.45
2	A	401	NAI	C5A-N7A-C8A	3.37	108.75	103.45
2	A	401	NAI	N3A-C4A-N9A	3.35	132.86	127.17
2	A	401	NAI	N9A-C8A-N7A	-3.33	109.21	113.94
2	B	401	NAI	C4A-C5A-N7A	-3.23	106.89	110.58
2	B	401	NAI	C6N-N1N-C2N	3.21	122.76	119.32
2	B	401	NAI	C2A-N3A-C4A	3.08	119.34	111.83
2	A	401	NAI	O2A-PA-O3	3.04	115.50	107.27
2	A	401	NAI	C6N-N1N-C2N	3.03	122.56	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAI	C3N-C2N-N1N	-2.95	118.88	123.20
2	B	401	NAI	O2A-PA-O3	2.93	115.19	107.27
2	B	401	NAI	O5D-C5D-C4D	2.73	118.29	108.99
2	B	401	NAI	C4A-N9A-C8A	2.57	108.43	105.74
2	B	401	NAI	O5B-C5B-C4B	2.45	117.33	108.99
2	A	401	NAI	C3N-C2N-N1N	-2.35	119.75	123.20
2	A	401	NAI	C4A-N9A-C8A	2.06	107.90	105.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAI	C5B-O5B-PA-O2A
2	A	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	A	401	NAI	C5B-O5B-PA-O3
2	B	401	NAI	C5D-O5D-PN-O3
2	A	401	NAI	PN-O3-PA-O1A
2	A	401	NAI	PN-O3-PA-O2A
2	B	401	NAI	O4D-C4D-C5D-O5D

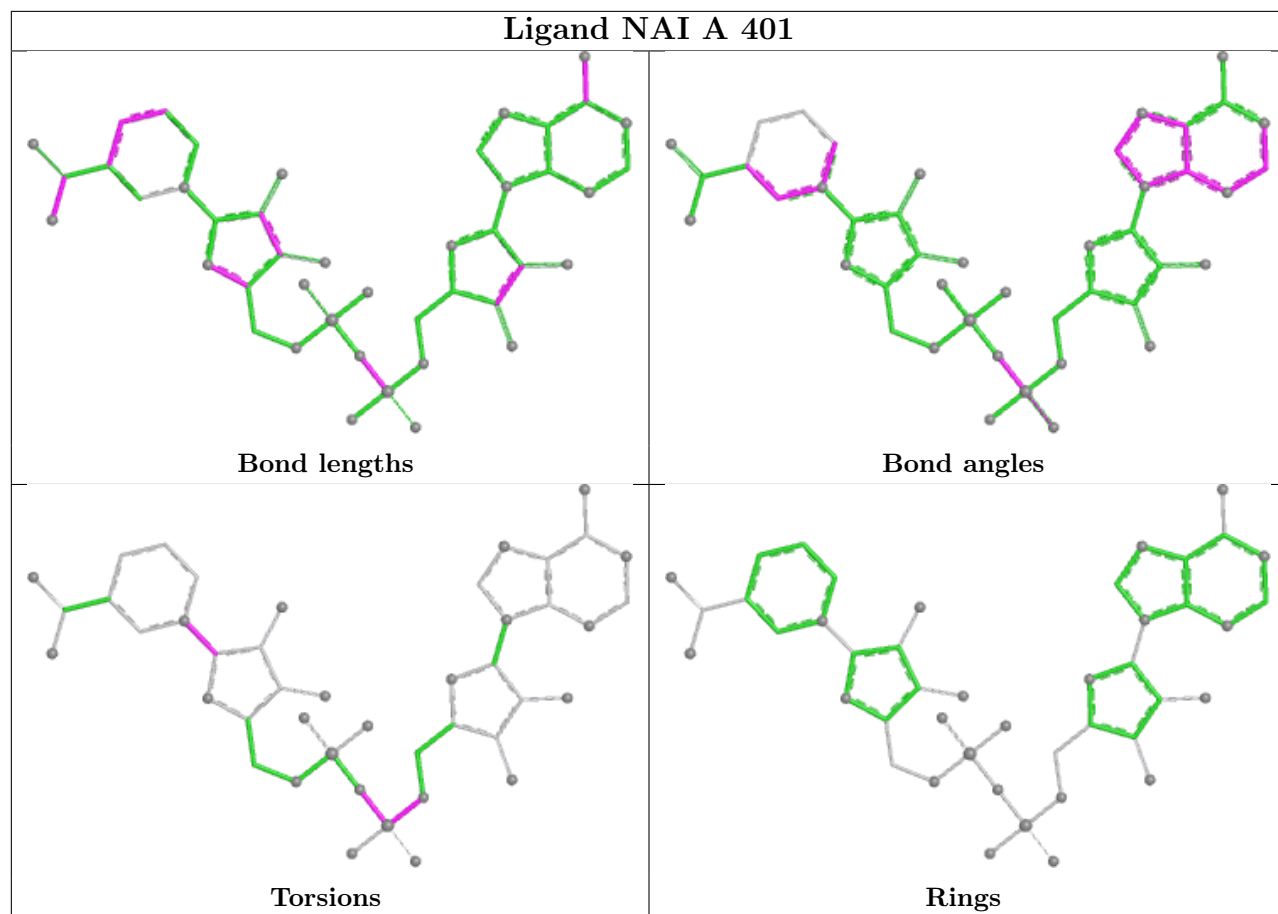
There are no ring outliers.

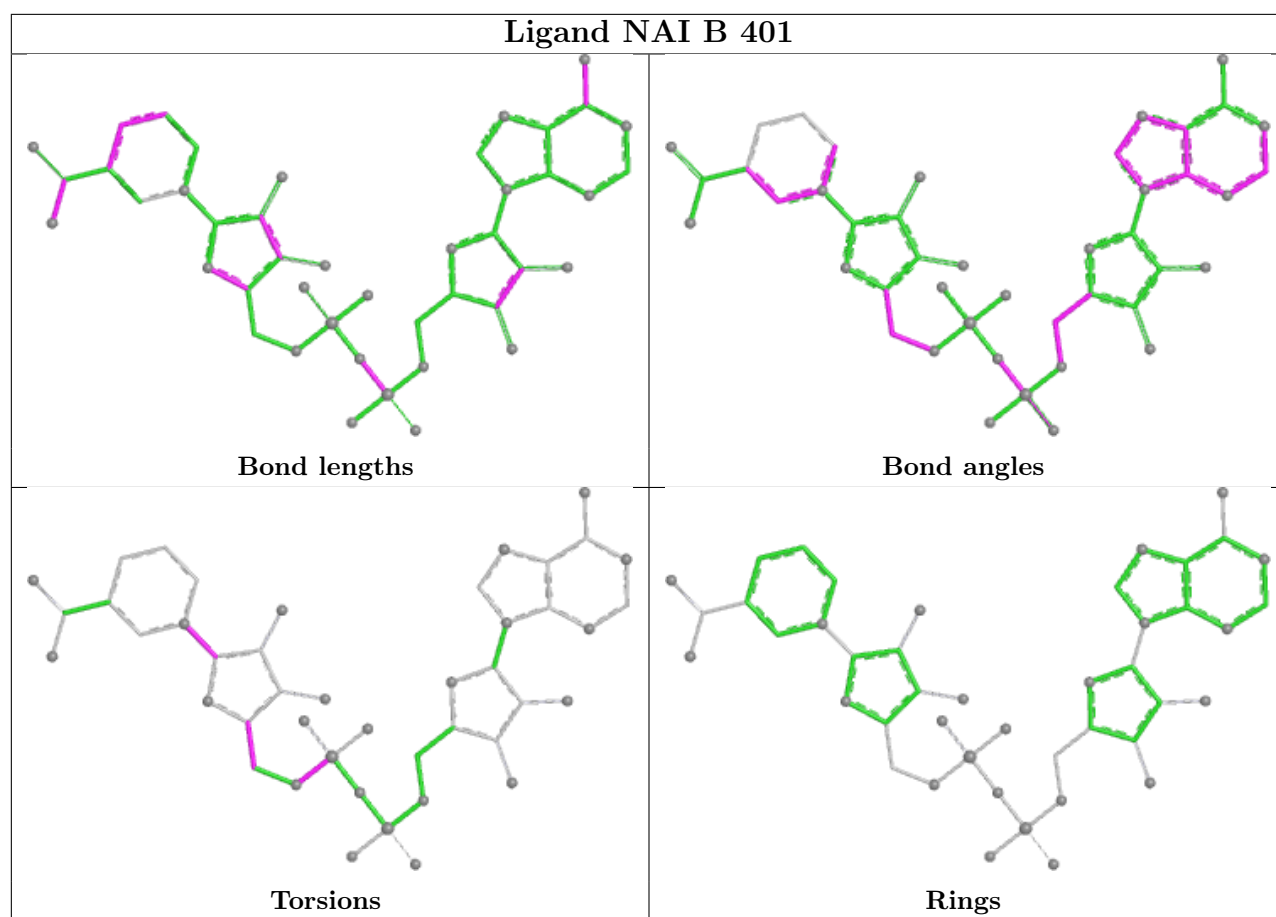
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAI	1	0
2	B	401	NAI	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.

Ligand NAI A 401





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	337/339 (99%)	1.35	114 (33%)  	14, 30, 59, 78	0
1	B	313/339 (92%)	1.64	113 (36%)  	13, 30, 60, 90	0
All	All	650/678 (95%)	1.49	227 (34%)  	13, 30, 60, 90	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ILE	14.3
1	B	7	THR	10.5
1	B	16	LEU	9.5
1	B	8	LEU	6.8
1	B	46	ALA	6.6
1	B	41	ILE	6.5
1	B	33	LEU	6.5
1	B	38	ALA	6.1
1	B	53	ALA	6.0
1	B	34	VAL	6.0
1	A	335	ALA	6.0
1	B	11	LEU	5.9
1	B	30	ALA	5.9
1	B	49	VAL	5.8
1	B	45	GLY	5.8
1	A	331	LEU	5.7
1	B	19	ALA	5.6
1	B	37	ASP	5.6
1	B	26	ALA	5.5
1	B	5	ARG	5.4
1	B	21	LEU	5.4
1	A	17	CYS	5.2
1	B	185	VAL	5.2
1	B	186	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	5.1
1	B	181	ALA	5.1
1	B	182	TRP	5.1
1	B	12	ILE	5.0
1	A	332	ILE	4.9
1	A	183	GLY	4.9
1	A	318	VAL	4.8
1	B	4	SER	4.8
1	A	56	ILE	4.6
1	B	212	PHE	4.4
1	B	56	ILE	4.4
1	B	47	VAL	4.3
1	B	29	VAL	4.3
1	B	213	ALA	4.3
1	A	336	LEU	4.2
1	B	188	ALA	4.2
1	A	11	LEU	4.2
1	A	327	ILE	4.2
1	B	36	ALA	4.2
1	A	323	ILE	4.2
1	B	18	GLN	4.1
1	B	211	PRO	4.1
1	B	20	GLY	4.1
1	B	51	TYR	4.1
1	B	190	SER	4.1
1	B	191	ARG	4.1
1	A	252	TYR	4.0
1	A	64	GLU	4.0
1	A	27	ALA	4.0
1	A	337	TYR	4.0
1	B	183	GLY	3.9
1	A	190	SER	3.9
1	B	43	SER	3.9
1	B	193	MET	3.9
1	B	298	GLY	3.9
1	A	329	GLN	3.8
1	B	252	TYR	3.8
1	B	6	GLU	3.8
1	A	334	ASP	3.8
1	B	32	VAL	3.8
1	B	35	TYR	3.8
1	A	14	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	7	THR	3.8
1	A	330	TYR	3.8
1	A	315	LYS	3.7
1	B	189	ARG	3.7
1	A	16	LEU	3.7
1	B	40	GLY	3.7
1	B	27	ALA	3.7
1	B	311	ILE	3.6
1	A	20	GLY	3.6
1	B	42	HIS	3.6
1	A	22	LYS	3.6
1	A	328	TYR	3.6
1	B	23	ARG	3.6
1	A	10	GLN	3.6
1	B	313	GLN	3.6
1	B	58	LYS	3.5
1	A	34	VAL	3.5
1	A	298	GLY	3.5
1	A	195	ILE	3.5
1	B	15	LYS	3.5
1	A	8	LEU	3.5
1	A	201	VAL	3.5
1	B	255	LEU	3.4
1	A	206	VAL	3.4
1	A	23	ARG	3.4
1	A	102	GLN	3.4
1	B	9	HIS	3.4
1	A	1	MET	3.4
1	A	19	ALA	3.3
1	A	46	ALA	3.3
1	B	152	ILE	3.3
1	B	195	ILE	3.3
1	A	191	ARG	3.3
1	B	17	CYS	3.3
1	B	57	SER	3.3
1	A	316	ALA	3.3
1	A	213	ALA	3.3
1	A	321	ILE	3.3
1	A	333	SER	3.3
1	A	59	GLY	3.2
1	A	193	MET	3.2
1	A	2	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	57	SER	3.2
1	A	255	LEU	3.2
1	B	209	THR	3.2
1	A	187	ASP	3.2
1	B	52	TYR	3.2
1	A	53	ALA	3.2
1	A	3	ILE	3.1
1	A	326	ASP	3.1
1	B	31	GLU	3.1
1	B	200	ALA	3.1
1	A	325	ASP	3.1
1	B	194	SER	3.0
1	A	18	GLN	3.0
1	A	45	GLY	3.0
1	B	24	GLU	3.0
1	A	30	ALA	3.0
1	B	250	SER	3.0
1	B	206	VAL	3.0
1	A	188	ALA	3.0
1	A	251	MET	3.0
1	B	50	GLU	3.0
1	B	14	ASN	3.0
1	A	29	VAL	2.9
1	A	12	ILE	2.9
1	B	196	PRO	2.9
1	B	54	GLU	2.9
1	A	65	PRO	2.9
1	A	211	PRO	2.9
1	B	44	HIS	2.8
1	B	48	ARG	2.8
1	B	59	GLY	2.8
1	A	324	VAL	2.8
1	B	300	ASN	2.8
1	A	4	SER	2.8
1	A	6	GLU	2.8
1	A	13	GLU	2.8
1	A	60	GLY	2.8
1	A	292	ALA	2.7
1	A	197	ASP	2.7
1	A	167	GLY	2.7
1	B	216	ALA	2.7
1	B	184	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	315	LYS	2.7
1	A	295	PRO	2.7
1	A	47	VAL	2.7
1	A	21	LEU	2.7
1	A	322	GLU	2.7
1	B	253	ASP	2.7
1	B	25	HIS	2.7
1	B	10	GLN	2.7
1	A	49	VAL	2.7
1	A	186	LEU	2.6
1	A	28	THR	2.6
1	B	314	ARG	2.6
1	A	58	LYS	2.6
1	B	65	PRO	2.6
1	B	60	GLY	2.5
1	A	198	THR	2.5
1	B	28	THR	2.5
1	A	42	HIS	2.5
1	A	297	PRO	2.5
1	B	207	PRO	2.5
1	B	257	ALA	2.5
1	A	61	THR	2.5
1	A	208	THR	2.5
1	B	61	THR	2.5
1	B	214	VAL	2.5
1	A	5	ARG	2.5
1	A	24	GLU	2.5
1	A	314	ARG	2.4
1	B	63	ARG	2.4
1	B	205	GLY	2.4
1	A	69	LEU	2.4
1	A	26	ALA	2.4
1	B	204	ASN	2.4
1	B	208	THR	2.4
1	B	291	ASN	2.4
1	A	214	VAL	2.4
1	B	192	ASN	2.3
1	B	119	ALA	2.3
1	A	52	TYR	2.3
1	B	201	VAL	2.3
1	A	288	ARG	2.3
1	A	196	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	312	LYS	2.3
1	A	41	ILE	2.3
1	A	291	ASN	2.3
1	B	271	ASN	2.3
1	B	199	TRP	2.3
1	A	317	ALA	2.3
1	A	168	ASP	2.3
1	B	187	ASP	2.3
1	B	301	GLN	2.2
1	B	122	TYR	2.2
1	B	55	ARG	2.2
1	A	62	ASN	2.2
1	A	194	SER	2.2
1	B	64	GLU	2.2
1	B	66	GLU	2.2
1	A	35	TYR	2.2
1	A	192	ASN	2.2
1	A	15	LYS	2.2
1	A	84	ALA	2.2
1	A	296	ALA	2.2
1	B	203	LYS	2.2
1	A	311	ILE	2.2
1	A	33	LEU	2.1
1	B	198	THR	2.1
1	B	210	ASP	2.1
1	A	31	GLU	2.1
1	A	66	GLU	2.1
1	B	102	GLN	2.1
1	A	55	ARG	2.1
1	A	320	GLY	2.0
1	A	51	TYR	2.0
1	A	81	ALA	2.0
1	A	257	ALA	2.0
1	B	88	VAL	2.0
1	A	25	HIS	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

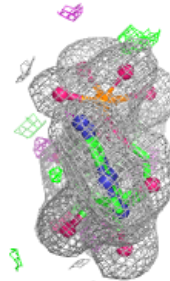
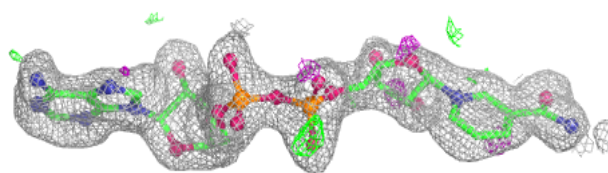
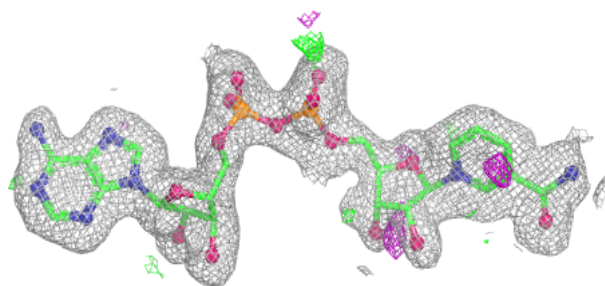
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAI	B	401	44/44	0.93	0.10	23,29,33,37	0
2	NAI	A	401	44/44	0.95	0.08	20,27,30,32	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.

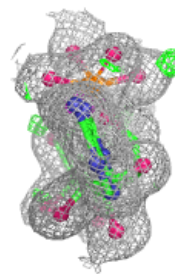
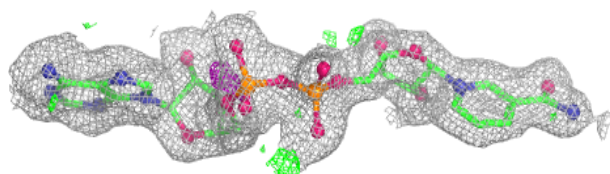
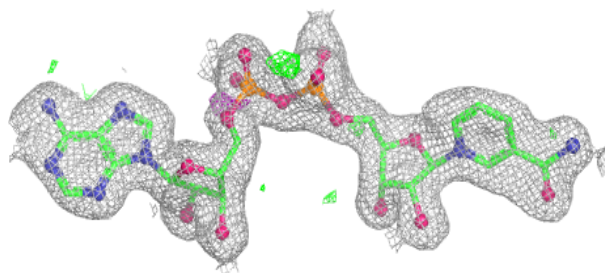
Electron density around NAI B 401:

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 NAI 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.