



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:09 PM UTC

PDB ID : 4KQW / pdb_00004kqw
Title : The structure of the Slackia exigua KARI in complex with NADP
Authors : Brinkmann-Chen, S.; Flock, T.; Cahn, J.K.B.; Snow, C.D.; Brustad, E.M.;
Mcintosh, J.A.; Meinhold, P.; Zhang, L.; Arnold, F.H.
Deposited on : 2013-05-15
Resolution : 1.39 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

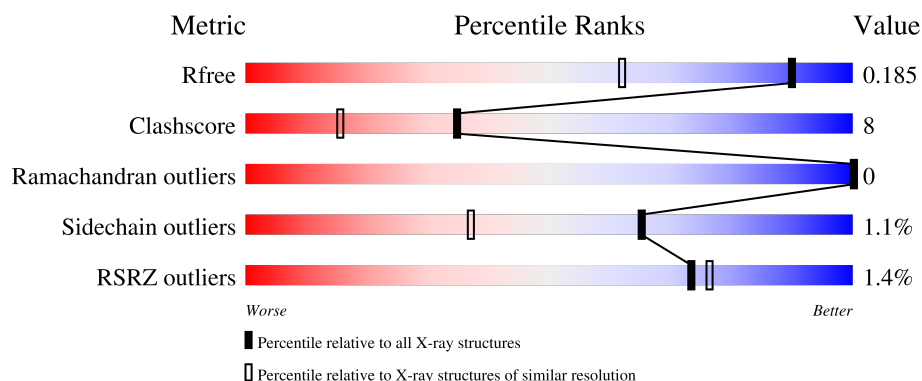
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	350	
1	B	350	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TLA	A	402	-	X	-	-
3	TLA	B	401	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6253 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.

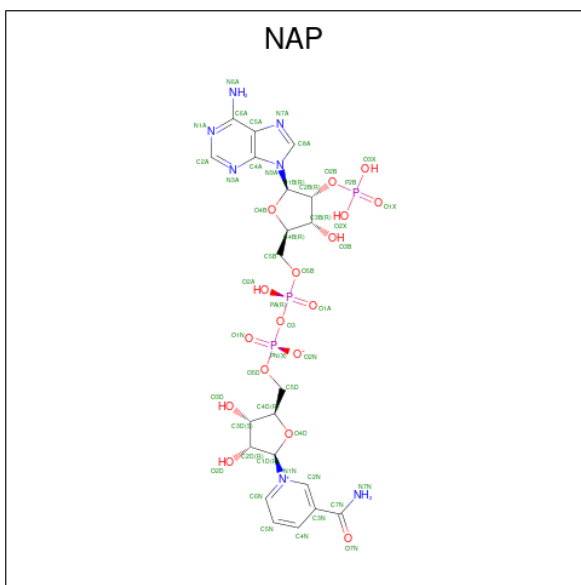
- Molecule 1 is a protein called Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	18	0
			2631	1674	429	507	21			
1	B	325	Total	C	N	O	S	0	12	0
			2596	1642	426	510	18			

There are 16 discrepancies between the modelled and reference sequences:

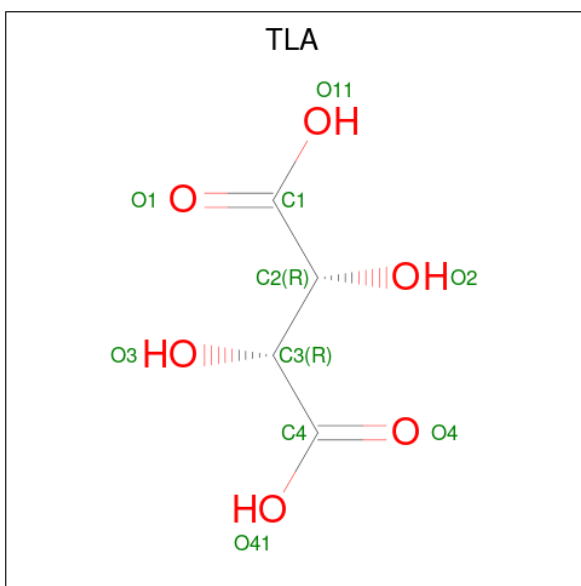
Chain	Residue	Modelled	Actual	Comment	Reference
A	343	LEU	-	expression tag	UNP D0WGK0
A	344	GLU	-	expression tag	UNP D0WGK0
A	345	HIS	-	expression tag	UNP D0WGK0
A	346	HIS	-	expression tag	UNP D0WGK0
A	347	HIS	-	expression tag	UNP D0WGK0
A	348	HIS	-	expression tag	UNP D0WGK0
A	349	HIS	-	expression tag	UNP D0WGK0
A	350	HIS	-	expression tag	UNP D0WGK0
B	343	LEU	-	expression tag	UNP D0WGK0
B	344	GLU	-	expression tag	UNP D0WGK0
B	345	HIS	-	expression tag	UNP D0WGK0
B	346	HIS	-	expression tag	UNP D0WGK0
B	347	HIS	-	expression tag	UNP D0WGK0
B	348	HIS	-	expression tag	UNP D0WGK0
B	349	HIS	-	expression tag	UNP D0WGK0
B	350	HIS	-	expression tag	UNP D0WGK0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 4 6	0	0
3	A	1	Total C O 10 4 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		

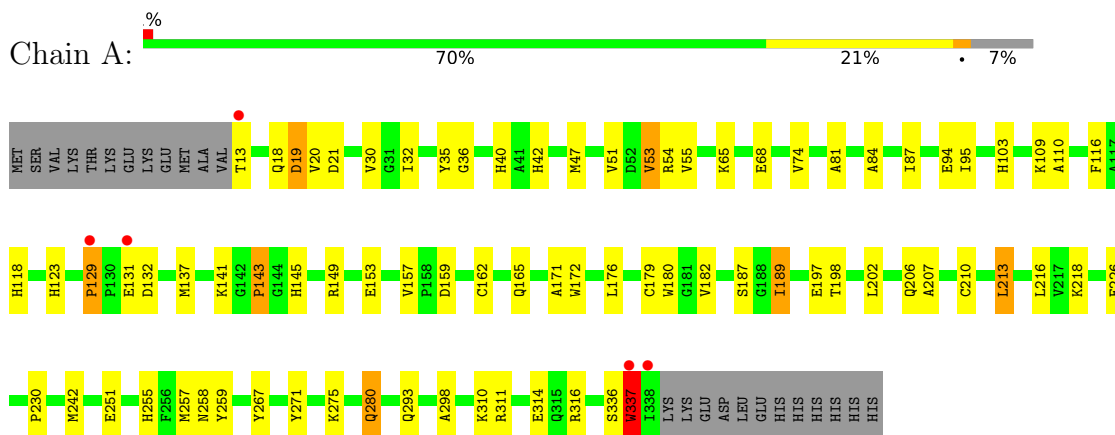
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	431	Total	O	0	0
			431	431		
5	B	455	Total	O	0	0
			455	455		

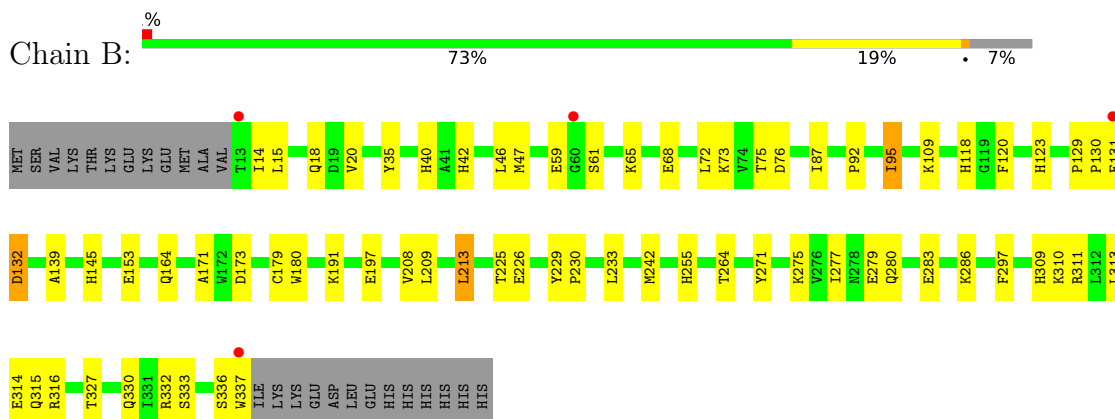
3 Residue-property plots [i](#)

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: Ketol-acid reductoisomerase



- Molecule 1: Ketol-acid reductoisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.20Å 118.93Å 62.16Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	60.98 – 1.39 60.98 – 1.39	Depositor EDS
% Data completeness (in resolution range)	92.9 (60.98-1.39) 92.9 (60.98-1.39)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.160 , 0.187 0.158 , 0.185	Depositor DCC
R_{free} test set	6865 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6253	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.96% 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: TLA, NAP, MG

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	1.85	43/2730 (1.6%)	1.51	13/3698 (0.4%)
1	B	1.84	41/2678 (1.5%)	1.53	12/3627 (0.3%)
All	All	1.85	84/5408 (1.6%)	1.52	25/7325 (0.3%)

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	TYR	CA-CB	10.11	1.63	1.53
1	A	145	HIS	CE1-NE2	8.40	1.41	1.32
1	A	230	PRO	CA-C	8.39	1.59	1.52
1	A	255	HIS	ND1-CE1	8.32	1.40	1.32
1	A	189	ILE	CA-CB	-8.03	1.44	1.54
1	B	230	PRO	CA-C	7.79	1.59	1.52
1	B	255	HIS	ND1-CE1	7.39	1.40	1.32
1	B	120	PHE	C-O	7.31	1.32	1.24
1	B	129	PRO	C-O	7.26	1.32	1.24
1	A	251	GLU	N-CA	7.22	1.55	1.46
1	A	40	HIS	ND1-CE1	7.13	1.39	1.32
1	B	145	HIS	CE1-NE2	7.12	1.39	1.32
1	A	21	ASP	N-CA	7.05	1.55	1.46
1	A	123	HIS	ND1-CE1	6.89	1.39	1.32
1	B	95	ILE	CB-CG1	-6.84	1.39	1.53
1	A	129	PRO	C-O	6.79	1.32	1.24
1	A	109	LYS	N-CA	6.69	1.53	1.45
1	B	40	HIS	ND1-CE1	6.67	1.39	1.32
1	A	74	VAL	C-O	6.66	1.30	1.24
1	A	165	GLN	N-CA	6.62	1.54	1.46
1	A	95	ILE	CA-CB	6.62	1.62	1.54
1	B	92	PRO	N-CA	6.46	1.55	1.47
1	B	255	HIS	CG-CD2	6.41	1.42	1.35
1	A	118	HIS	ND1-CE1	6.39	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	ARG	CZ-NH2	6.38	1.41	1.33
1	B	42	HIS	ND1-CE1	6.37	1.39	1.32
1	A	40	HIS	CD2-NE2	6.32	1.44	1.37
1	B	179	CYS	N-CA	6.30	1.53	1.46
1	B	309	HIS	CG-ND1	-6.29	1.31	1.38
1	B	229	TYR	CA-CB	6.28	1.63	1.52
1	B	310	LYS	N-CA	-6.27	1.39	1.46
1	A	157	VAL	N-CA	6.14	1.53	1.47
1	A	337	TRP	CG-CD2	6.09	1.54	1.43
1	B	171	ALA	N-CA	6.01	1.53	1.46
1	A	123	HIS	N-CA	6.00	1.53	1.46
1	A	259	TYR	C-O	6.00	1.31	1.24
1	A	40	HIS	CE1-NE2	5.87	1.38	1.32
1	B	164	GLN	CG-CD	-5.85	1.37	1.52
1	A	55	VAL	C-N	-5.83	1.29	1.33
1	B	139	ALA	N-CA	5.81	1.52	1.46
1	B	209	LEU	CA-C	-5.79	1.45	1.52
1	B	333	SER	N-CA	5.77	1.53	1.46
1	B	208	VAL	N-CA	5.76	1.53	1.46
1	B	109	LYS	N-CA	5.75	1.52	1.45
1	A	143	PRO	N-CA	-5.75	1.40	1.47
1	B	118	HIS	ND1-CE1	5.73	1.38	1.32
1	B	197	GLU	C-O	5.71	1.30	1.24
1	B	132	ASP	N-CA	5.69	1.52	1.46
1	B	95	ILE	CA-CB	-5.68	1.47	1.54
1	A	103	HIS	ND1-CE1	5.67	1.38	1.32
1	B	336	SER	N-CA	5.66	1.53	1.46
1	A	206	GLN	C-O	5.65	1.30	1.24
1	A	53[A]	VAL	C-O	5.60	1.29	1.24
1	A	53[B]	VAL	C-O	5.60	1.29	1.24
1	B	264	THR	CB-OG1	5.50	1.52	1.43
1	B	68	GLU	CA-C	-5.50	1.45	1.52
1	B	226	GLU	CA-C	-5.50	1.45	1.52
1	A	36	GLY	N-CA	5.47	1.53	1.45
1	B	68	GLU	N-CA	5.42	1.53	1.46
1	A	172	TRP	C-O	5.39	1.30	1.24
1	A	171	ALA	N-CA	5.38	1.52	1.46
1	A	65	LYS	N-CA	-5.35	1.39	1.46
1	B	327	THR	C-O	5.34	1.30	1.24
1	B	72	LEU	N-CA	5.34	1.52	1.45
1	B	229	TYR	C-O	5.34	1.30	1.23
1	A	267	TYR	CA-CB	5.32	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	HIS	CE1-NE2	5.32	1.37	1.32
1	A	149	ARG	CD-NE	-5.31	1.38	1.46
1	B	14	ILE	CA-CB	-5.27	1.47	1.54
1	A	226	GLU	N-CA	5.26	1.52	1.46
1	A	19	ASP	N-CA	-5.23	1.39	1.46
1	A	316	ARG	CZ-NH1	5.21	1.40	1.32
1	B	123	HIS	ND1-CE1	5.16	1.37	1.32
1	A	189	ILE	N-CA	5.14	1.52	1.46
1	A	141	LYS	CA-CB	5.12	1.59	1.52
1	A	337	TRP	CD2-CE2	5.11	1.50	1.41
1	B	309	HIS	ND1-CE1	5.11	1.37	1.32
1	B	225	THR	C-O	5.05	1.30	1.24
1	A	207	ALA	CA-C	-5.02	1.45	1.52
1	A	202	LEU	N-CA	-5.01	1.40	1.46
1	A	218	LYS	C-O	5.01	1.29	1.24
1	B	35	TYR	CA-CB	5.01	1.60	1.53
1	B	277	ILE	CA-C	-5.00	1.48	1.53
1	B	286	LYS	CA-C	5.00	1.59	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	LYS	CD-CE-NZ	7.33	135.35	111.90
1	B	95	ILE	CB-CG1-CD1	-7.31	98.44	113.80
1	A	293	GLN	CA-C-O	-6.12	112.93	119.97
1	B	332	ARG	NE-CZ-NH2	-6.08	113.72	119.20
1	A	213	LEU	CD1-CG-CD2	5.97	123.93	110.80
1	B	332	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	B	209	LEU	N-CA-C	5.82	117.71	111.36
1	A	216	LEU	N-CA-C	-5.70	104.98	111.14
1	B	233	LEU	N-CA-C	-5.44	105.43	111.36
1	A	210	CYS	N-CA-C	-5.40	104.88	112.12
1	A	298	ALA	N-CA-C	-5.29	105.52	111.28
1	A	198	THR	N-CA-C	-5.29	105.52	111.28
1	B	129	PRO	O-C-N	5.25	127.66	121.46
1	B	297	PHE	CA-CB-CG	-5.25	108.56	113.80
1	B	316	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	A	13	THR	CA-C-N	-5.22	116.37	123.10
1	A	13	THR	C-N-CA	-5.22	116.37	123.10
1	B	46	LEU	CA-C-O	-5.17	114.94	120.42
1	A	110	ALA	CB-CA-C	-5.15	101.86	109.90
1	A	94	GLU	CA-C-N	5.14	128.78	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	GLU	C-N-CA	5.14	128.78	121.02
1	B	61	SER	N-CA-C	5.11	117.63	110.23
1	B	213	LEU	CD1-CG-CD2	5.10	122.02	110.80
1	A	32	ILE	CA-CB-CG1	5.09	119.06	110.40
1	B	73	LYS	CA-C-O	-5.03	114.75	120.58

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	2631	0	2568	49	0
1	B	2596	0	2504	33	0
2	A	48	0	25	3	0
2	B	48	0	25	0	0
3	A	20	0	6	1	0
3	B	20	0	7	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	431	0	0	18	0
5	B	455	0	0	16	0
All	All	6253	0	5135	79	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 8.

All (79) 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:47[B]:MET:HE1	5:A:699:HOH:O	1.38	1.20
1:B:18:GLN:OE1	5:B:730:HOH:O	1.56	1.19
3:B:401:TLA:H2	5:B:951:HOH:O	1.44	1.18
1:A:336:SER:O	1:A:337:TRP:HE3	1.30	1.13
1:A:336:SER:O	1:A:337:TRP:CE3	2.03	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ALA:HB3	1:A:87[B]:ILE:HD11	1.38	1.04
1:A:18:GLN:OE1	5:A:716:HOH:O	1.75	1.03
1:A:280[A]:GLN:HE22	1:B:280:GLN:HG2	1.23	1.03
1:A:179[B]:CYS:SG	1:A:189:ILE:HD13	1.99	1.03
3:A:402:TLA:H2	5:A:713:HOH:O	1.58	1.01
1:A:47[A]:MET:HE2	5:A:839:HOH:O	1.63	0.95
1:A:84:ALA:HB3	1:A:87[B]:ILE:CD1	1.96	0.94
1:A:131:GLU:HB2	5:A:923:HOH:O	1.68	0.93
1:B:173:ASP:OD2	5:B:656:HOH:O	1.89	0.90
1:B:47[B]:MET:HE3	5:B:532:HOH:O	1.72	0.89
1:B:314[B]:GLU:CA	1:B:315[B]:GLN:N	2.36	0.88
1:A:213:LEU:HD11	1:A:242[B]:MET:SD	2.14	0.88
1:A:280[A]:GLN:NE2	1:B:280:GLN:HG2	1.87	0.88
1:B:313:LEU:C	1:B:314[B]:GLU:CA	2.50	0.83
1:B:213:LEU:HD11	1:B:242[B]:MET:SD	2.19	0.82
1:B:330[C]:GLN:NE2	5:B:852:HOH:O	2.12	0.82
1:A:179[B]:CYS:SG	1:A:189:ILE:CD1	2.68	0.81
1:A:47[B]:MET:HE3	5:A:575:HOH:O	1.83	0.79
2:A:401:NAP:C4N	3:B:401:TLA:H3	2.13	0.79
1:A:30:VAL:HB	1:A:53[B]:VAL:HG12	1.62	0.79
1:B:75[A]:THR:HG23	1:B:76:ASP:O	1.86	0.75
1:B:47[B]:MET:CE	5:B:532:HOH:O	2.28	0.74
1:B:191:LYS:NZ	5:B:921:HOH:O	2.10	0.74
1:A:47[B]:MET:CE	5:A:699:HOH:O	2.12	0.72
1:A:153:GLU:OE2	5:A:704:HOH:O	2.07	0.72
1:A:257[B]:MET:HE2	1:A:258:ASN:OD1	1.92	0.70
1:B:153:GLU:OE2	5:B:878:HOH:O	2.09	0.70
1:B:132:ASP:N	5:B:520:HOH:O	1.87	0.70
1:A:47[B]:MET:CE	5:A:575:HOH:O	2.40	0.69
1:A:68:GLU:OE1	5:A:853:HOH:O	2.10	0.67
1:B:279[B]:GLU:O	1:B:283[B]:GLU:HG3	1.97	0.65
1:A:81:ALA:HA	1:A:87[B]:ILE:HD12	1.81	0.61
1:A:187[A]:SER:OG	1:B:337:TRP:CH2	2.52	0.61
1:A:132:ASP:N	5:A:847:HOH:O	1.93	0.58
1:B:311:ARG:HA	1:B:314[C]:GLU:HG2	1.84	0.58
2:A:401:NAP:H4N	3:B:401:TLA:H3	1.86	0.57
1:B:75[A]:THR:OG1	5:B:755:HOH:O	2.07	0.56
1:A:84:ALA:HB3	1:A:87[B]:ILE:HD13	1.85	0.55
1:A:81:ALA:HA	1:A:87[B]:ILE:CD1	2.36	0.55
1:B:311:ARG:O	1:B:314[C]:GLU:HG2	2.07	0.54
1:A:187[A]:SER:OG	1:B:337:TRP:HH2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280[B]:GLN:NE2	5:A:848:HOH:O	2.40	0.53
1:A:280[A]:GLN:NE2	1:B:280:GLN:CG	2.66	0.53
1:A:310:LYS:HD2	5:A:745:HOH:O	2.09	0.52
1:A:84:ALA:CB	1:A:87[B]:ILE:CD1	2.80	0.52
1:B:275:LYS:NZ	5:B:943:HOH:O	2.43	0.51
1:A:275:LYS:NZ	5:A:675:HOH:O	2.43	0.51
1:A:84:ALA:CB	1:A:87[B]:ILE:HD13	2.41	0.50
1:A:176:LEU:O	1:A:179[B]:CYS:SG	2.61	0.49
1:B:20:VAL:HG21	1:B:180:TRP:HB2	1.94	0.49
1:A:20:VAL:HG21	1:A:180:TRP:HB2	1.96	0.47
1:A:19:ASP:OD1	5:A:813:HOH:O	2.20	0.47
1:A:187[A]:SER:OG	1:B:337:TRP:CZ3	2.67	0.47
1:A:116:PHE:O	1:A:137[A]:MET:HG3	2.15	0.46
1:B:65:LYS:HG3	5:B:931:HOH:O	2.16	0.46
1:A:51:VAL:HG12	1:A:53[B]:VAL:HG13	1.97	0.45
1:B:330[C]:GLN:CD	5:B:852:HOH:O	2.55	0.45
1:B:59:GLU:HG2	5:B:757:HOH:O	2.17	0.45
1:A:47[B]:MET:HE3	5:A:652:HOH:O	2.17	0.44
1:A:159:ASP:OD2	1:A:179[B]:CYS:HB2	2.18	0.43
1:A:137[B]:MET:HB3	1:A:162:CYS:HB2	2.01	0.43
1:A:187[A]:SER:HG	1:B:337:TRP:HH2	1.57	0.42
1:B:15:LEU:HD11	1:B:191:LYS:HE3	2.00	0.42
1:B:87:ILE:HD12	1:B:87:ILE:N	2.34	0.42
1:A:129:PRO:HD2	5:A:805:HOH:O	2.20	0.42
1:B:131[A]:GLU:H	1:B:131[A]:GLU:HG2	1.44	0.42
1:B:130:PRO:HG3	5:B:886:HOH:O	2.19	0.41
1:A:131:GLU:HG2	5:A:885:HOH:O	2.19	0.41
1:A:311:ARG:NH1	1:A:314[B]:GLU:OE2	2.54	0.41
1:B:65:LYS:CG	5:B:931:HOH:O	2.68	0.41
1:A:137[B]:MET:SD	1:A:197:GLU:HG3	2.61	0.41
1:A:143:PRO:HA	2:A:401:NAP:O7N	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/350 (98%)	335 (98%)	7 (2%)	0	100	100
1	B	336/350 (96%)	329 (98%)	7 (2%)	0	100	100
All	All	678/700 (97%)	664 (98%)	14 (2%)	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	283/288 (98%)	278 (98%)	5 (2%)	51	20
1	B	277/288 (96%)	275 (99%)	2 (1%)	76	52
All	All	560/576 (97%)	553 (99%)	7 (1%)	65	30

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	271	TYR
1	A	280[A]	GLN
1	A	280[B]	GLN
1	A	337	TRP
1	B	95	ILE
1	B	271	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	GLN
1	B	170	ASN
1	B	255	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	2.13	15 (30%)	71,80,80	2.59	23 (32%)
3	TLA	A	402	4	9,9,9	2.81	3 (33%)	12,12,12	3.99	10 (83%)
3	TLA	B	401	4	9,9,9	2.01	2 (22%)	12,12,12	2.27	7 (58%)
2	NAP	B	402	-	50,52,52	1.95	15 (30%)	71,80,80	2.16	17 (23%)
3	TLA	B	403	-	9,9,9	1.31	1 (11%)	12,12,12	2.21	7 (58%)
3	TLA	A	403	-	9,9,9	1.32	1 (11%)	12,12,12	2.18	5 (41%)

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	-	-	5/35/67/67	0/5/5/5
3	TLA	A	402	4	-	7/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TLA	B	401	4	-	5/12/12/12	-
2	NAP	B	402	-	-	5/35/67/67	0/5/5/5
3	TLA	B	403	-	-	0/12/12/12	-
3	TLA	A	403	-	-	4/12/12/12	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O4D-C1D	6.05	1.48	1.40
2	B	402	NAP	O4D-C1D	5.46	1.48	1.40
3	A	402	TLA	C3-C4	-5.19	1.45	1.52
2	A	401	NAP	C5A-C4A	5.05	1.48	1.39
2	A	401	NAP	C5A-C6A	4.80	1.54	1.41
2	B	402	NAP	C4N-C3N	4.80	1.46	1.39
3	A	402	TLA	C2-C1	-4.45	1.46	1.52
3	A	402	TLA	C3-C2	-3.90	1.41	1.53
2	A	401	NAP	P2B-O2B	3.81	1.66	1.59
2	B	402	NAP	C5A-C4A	3.65	1.45	1.39
2	A	401	NAP	C3N-C7N	-3.58	1.45	1.50
3	B	401	TLA	C3-C4	-3.58	1.47	1.52
3	B	401	TLA	C3-C2	-3.46	1.42	1.53
2	B	402	NAP	PN-O3	3.43	1.63	1.59
2	A	401	NAP	C2N-C3N	-3.30	1.33	1.39
2	B	402	NAP	C2N-C3N	-3.21	1.33	1.39
2	A	401	NAP	C4N-C3N	3.14	1.44	1.39
2	B	402	NAP	C8A-N7A	3.13	1.37	1.31
2	B	402	NAP	C2N-N1N	3.08	1.38	1.35
2	A	401	NAP	C4A-N3A	-3.00	1.28	1.34
2	B	402	NAP	C2A-N1A	2.94	1.39	1.33
2	A	401	NAP	C2A-N3A	2.85	1.39	1.33
2	A	401	NAP	C8A-N9A	-2.85	1.32	1.37
2	B	402	NAP	C5A-C6A	2.84	1.48	1.41
2	A	401	NAP	C5A-N7A	-2.72	1.34	1.39
2	B	402	NAP	C5N-C4N	2.62	1.43	1.38
2	B	402	NAP	P2B-O2B	2.57	1.64	1.59
2	B	402	NAP	C8A-N9A	-2.53	1.33	1.37
2	B	402	NAP	C6A-N1A	-2.47	1.28	1.35
3	B	403	TLA	C3-C4	-2.38	1.49	1.52
2	B	402	NAP	C7N-N7N	-2.36	1.28	1.33
2	A	401	NAP	PA-O3	-2.33	1.57	1.59
2	A	401	NAP	C6A-N1A	-2.28	1.29	1.35
2	B	402	NAP	C6N-C5N	-2.08	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	TLA	C2-C1	-2.05	1.49	1.52
2	A	401	NAP	C2N-N1N	2.05	1.37	1.35
2	A	401	NAP	P2B-O2X	-2.02	1.47	1.54

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C2A-N1A-C6A	8.67	132.97	118.73
2	A	401	NAP	N3A-C2A-N1A	-8.41	115.86	128.58
2	A	401	NAP	C3N-C7N-N7N	7.52	127.01	117.74
2	B	402	NAP	C6N-N1N-C2N	-7.47	115.52	121.88
3	A	402	TLA	O1-C1-C2	-7.36	102.03	121.62
2	B	402	NAP	C5N-C4N-C3N	-6.27	114.20	120.36
3	A	402	TLA	C2-C3-C4	6.11	123.36	109.82
2	A	401	NAP	C6A-C5A-C4A	-5.29	109.96	117.18
2	B	402	NAP	N3A-C2A-N1A	-5.22	120.68	128.58
2	B	402	NAP	C2A-N1A-C6A	5.20	127.28	118.73
2	B	402	NAP	C3N-C7N-N7N	5.11	124.03	117.74
2	B	402	NAP	N6A-C6A-N1A	4.74	128.94	118.38
2	A	401	NAP	C5N-C4N-C3N	-4.68	115.77	120.36
2	A	401	NAP	C6N-N1N-C2N	-4.39	118.14	121.88
3	A	402	TLA	O2-C2-C3	4.36	119.05	110.17
2	A	401	NAP	O7N-C7N-N7N	-4.35	116.33	122.62
3	A	402	TLA	O11-C1-C2	4.13	124.78	113.31
3	A	402	TLA	O11-C1-O1	3.84	132.79	124.08
2	A	401	NAP	C5A-C4A-N9A	-3.84	101.63	105.81
2	A	401	NAP	O4B-C1B-C2B	-3.83	100.00	106.59
3	A	402	TLA	O2-C2-C1	3.79	118.79	110.69
2	B	402	NAP	O4B-C1B-C2B	-3.73	100.16	106.59
3	A	402	TLA	O3-C3-C4	3.66	118.52	110.69
2	A	401	NAP	C6A-C5A-N7A	3.58	138.99	132.09
2	A	401	NAP	N6A-C6A-N1A	3.47	126.11	118.38
2	A	401	NAP	C2B-C1B-N9A	-3.47	108.05	113.75
3	A	403	TLA	O1-C1-C2	-3.40	112.57	121.62
2	A	401	NAP	C5B-C4B-C3B	-3.37	103.09	115.21
3	B	401	TLA	O2-C2-C3	3.33	116.95	110.17
3	B	401	TLA	O2-C2-C1	3.27	117.67	110.69
3	A	403	TLA	O41-C4-C3	3.24	122.32	113.31
2	B	402	NAP	C5A-C6A-N6A	-3.24	115.27	123.29
3	B	401	TLA	C2-C3-C4	3.22	116.95	109.82
3	B	403	TLA	O41-C4-C3	3.20	122.20	113.31
2	B	402	NAP	C5N-C6N-N1N	3.18	124.73	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	TLA	C3-C2-C1	-3.15	102.85	109.82
3	B	401	TLA	O11-C1-C2	-3.04	104.86	113.31
3	A	403	TLA	O11-C1-C2	3.03	121.73	113.31
3	B	403	TLA	O3-C3-C2	-2.93	104.21	110.17
3	B	403	TLA	O2-C2-C1	2.86	116.80	110.69
3	B	403	TLA	O2-C2-C3	-2.81	104.44	110.17
2	B	402	NAP	O7N-C7N-C3N	-2.80	116.17	119.60
2	B	402	NAP	C6A-C5A-N7A	2.73	137.35	132.09
3	A	403	TLA	O3-C3-C2	-2.73	104.61	110.17
2	A	401	NAP	C4A-N9A-C8A	2.70	108.58	105.74
2	B	402	NAP	C6A-C5A-C4A	-2.70	113.50	117.18
3	A	403	TLA	O2-C2-C3	-2.67	104.74	110.17
2	A	401	NAP	O7N-C7N-C3N	-2.61	116.40	119.60
2	A	401	NAP	C4D-O4D-C1D	-2.57	107.57	109.92
2	B	402	NAP	C5B-C4B-C3B	-2.57	105.96	115.21
2	A	401	NAP	C5A-C4A-N3A	2.55	130.22	126.72
2	B	402	NAP	O3X-P2B-O2X	2.54	117.31	107.80
3	B	403	TLA	O11-C1-C2	2.44	120.10	113.31
2	B	402	NAP	C2B-C1B-N9A	-2.42	109.78	113.75
2	A	401	NAP	C2D-C3D-C4D	-2.38	98.01	102.61
2	B	402	NAP	C4D-O4D-C1D	-2.38	107.75	109.92
3	B	403	TLA	O3-C3-C4	-2.34	105.68	110.69
3	A	402	TLA	O4I-C4-O4	2.33	129.36	124.08
3	A	402	TLA	O4-C4-C3	-2.26	115.60	121.62
3	B	401	TLA	O3-C3-C4	2.23	115.46	110.69
3	B	401	TLA	O4-C4-C3	-2.17	115.84	121.62
2	A	401	NAP	C2A-N3A-C4A	2.16	117.11	111.83
2	A	401	NAP	C2N-N1N-C1D	2.11	123.80	119.13
3	B	403	TLA	O4-C4-C3	-2.09	116.04	121.62
2	A	401	NAP	O4D-C4D-C5D	2.08	116.01	109.33
2	A	401	NAP	O5B-C5B-C4B	-2.08	101.92	108.99
3	B	401	TLA	O1-C1-C2	2.07	127.14	121.62
2	A	401	NAP	C4A-N9A-C1B	-2.05	121.85	126.63
2	B	402	NAP	O7N-C7N-N7N	-2.01	119.71	122.62

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C3B-C2B-O2B-P2B
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C2D-C1D-N1N-C6N
2	B	402	NAP	O4D-C1D-N1N-C2N
2	B	402	NAP	O4D-C1D-N1N-C6N
2	B	402	NAP	C2D-C1D-N1N-C6N
3	A	403	TLA	C2-C3-C4-O4
3	A	403	TLA	O3-C3-C4-O4
3	A	403	TLA	O3-C3-C4-O41
3	B	401	TLA	O1-C1-C2-O2
3	B	401	TLA	O11-C1-C2-O2
3	A	402	TLA	O2-C2-C3-O3
3	A	402	TLA	O1-C1-C2-O2
3	A	403	TLA	C2-C3-C4-O41
3	B	401	TLA	O2-C2-C3-O3
3	A	402	TLA	O11-C1-C2-O2
2	B	402	NAP	C3B-C2B-O2B-P2B
3	A	402	TLA	C2-C3-C4-O4
2	A	401	NAP	C1B-C2B-O2B-P2B
3	B	401	TLA	C1-C2-C3-C4
3	A	402	TLA	C1-C2-C3-C4
2	B	402	NAP	C1B-C2B-O2B-P2B
3	A	402	TLA	C2-C3-C4-O41
3	A	402	TLA	C1-C2-C3-O3
3	B	401	TLA	C2-C3-C4-O4

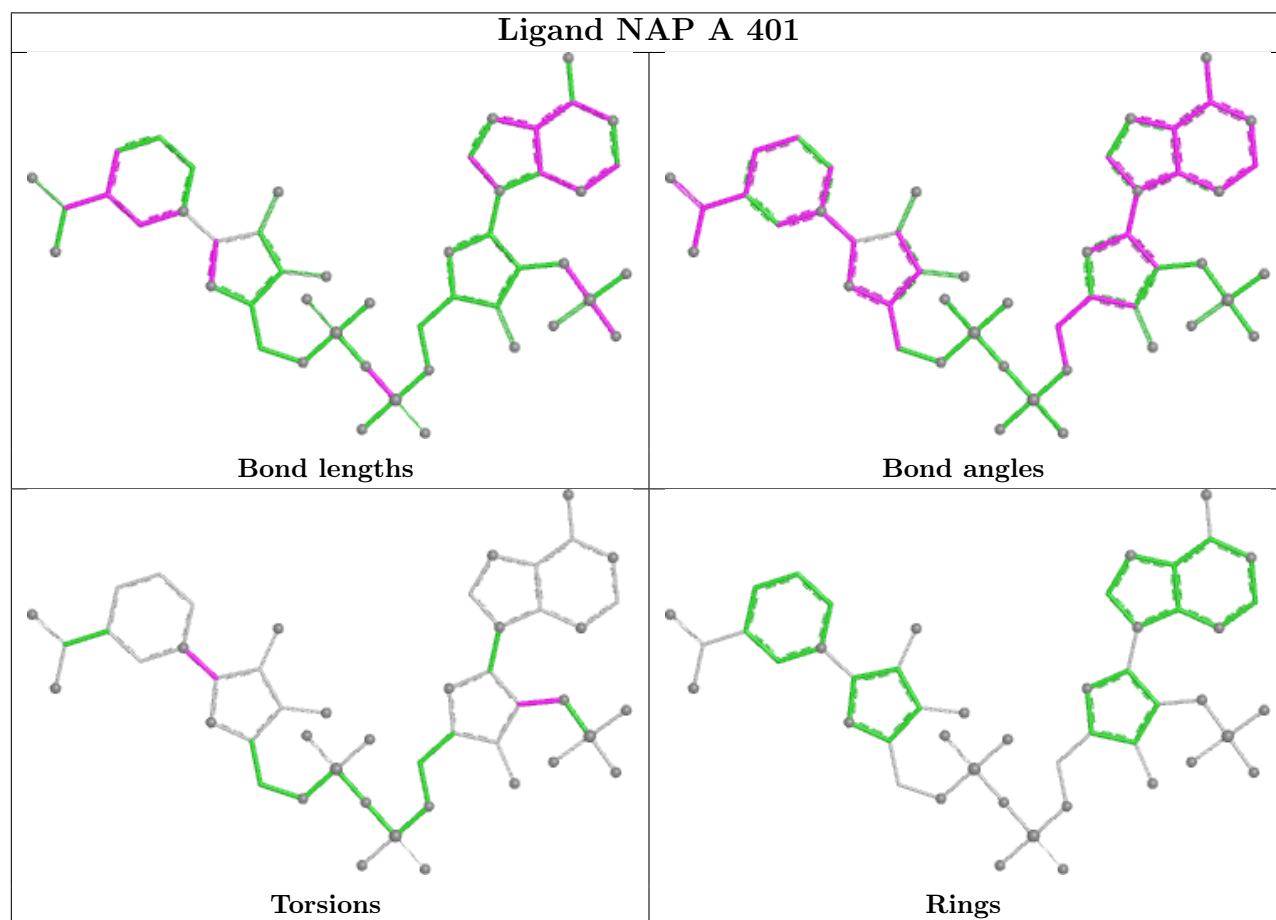
There are no ring outliers.

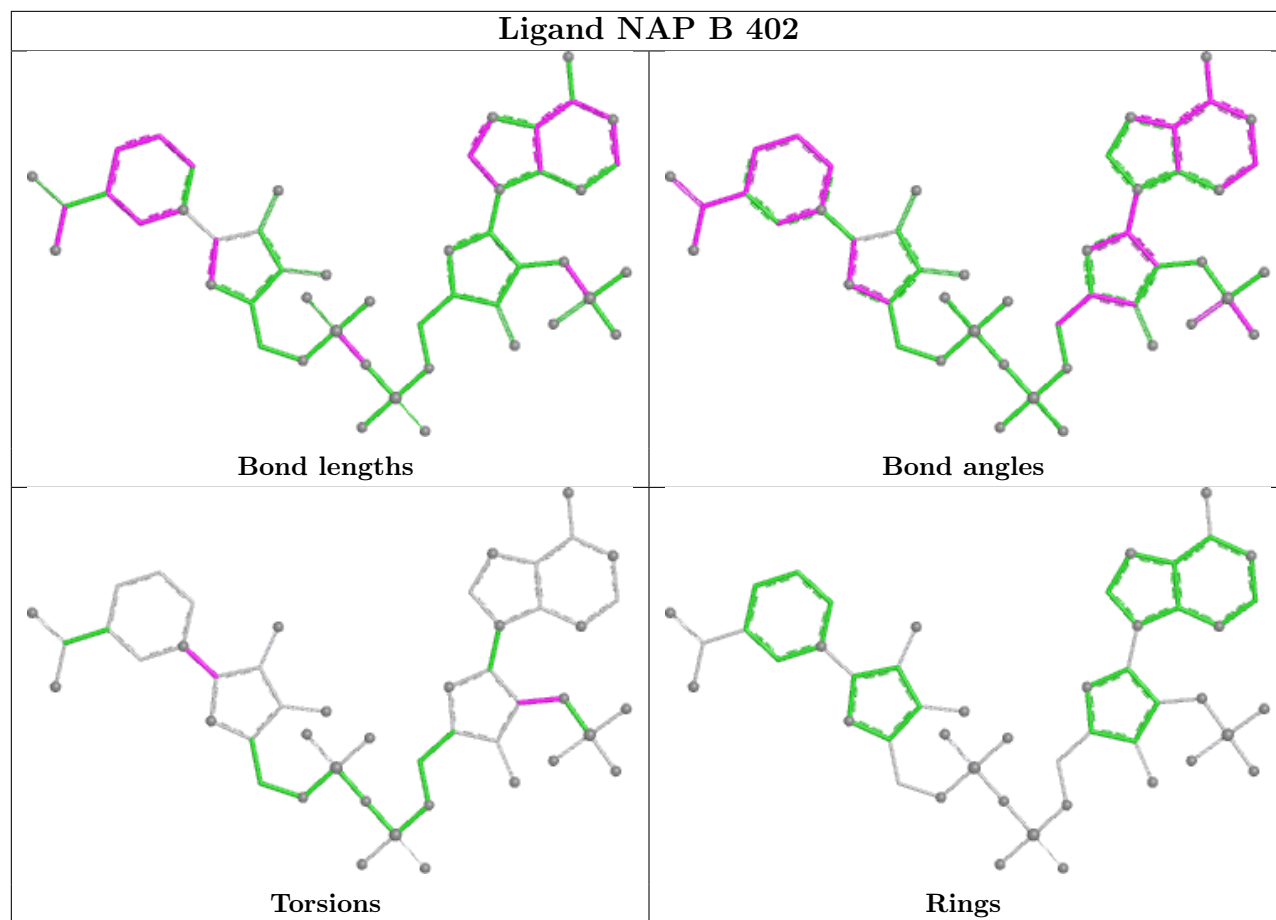
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	3	0
3	A	402	TLA	1	0
3	B	401	TLA	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/350 (93%)	-0.12	5 (1%) 72 75	6, 13, 24, 48	18 (5%)
1	B	325/350 (92%)	-0.12	4 (1%) 76 80	5, 13, 22, 40	13 (4%)
All	All	651/700 (93%)	-0.12	9 (1%) 73 76	5, 13, 23, 48	31 (4%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	ILE	5.6
1	A	337	TRP	5.4
1	B	337	TRP	2.8
1	B	13	THR	2.7
1	A	13	THR	2.4
1	B	60	GLY	2.2
1	A	129	PRO	2.2
1	B	131[A]	GLU	2.1
1	A	131	GLU	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.

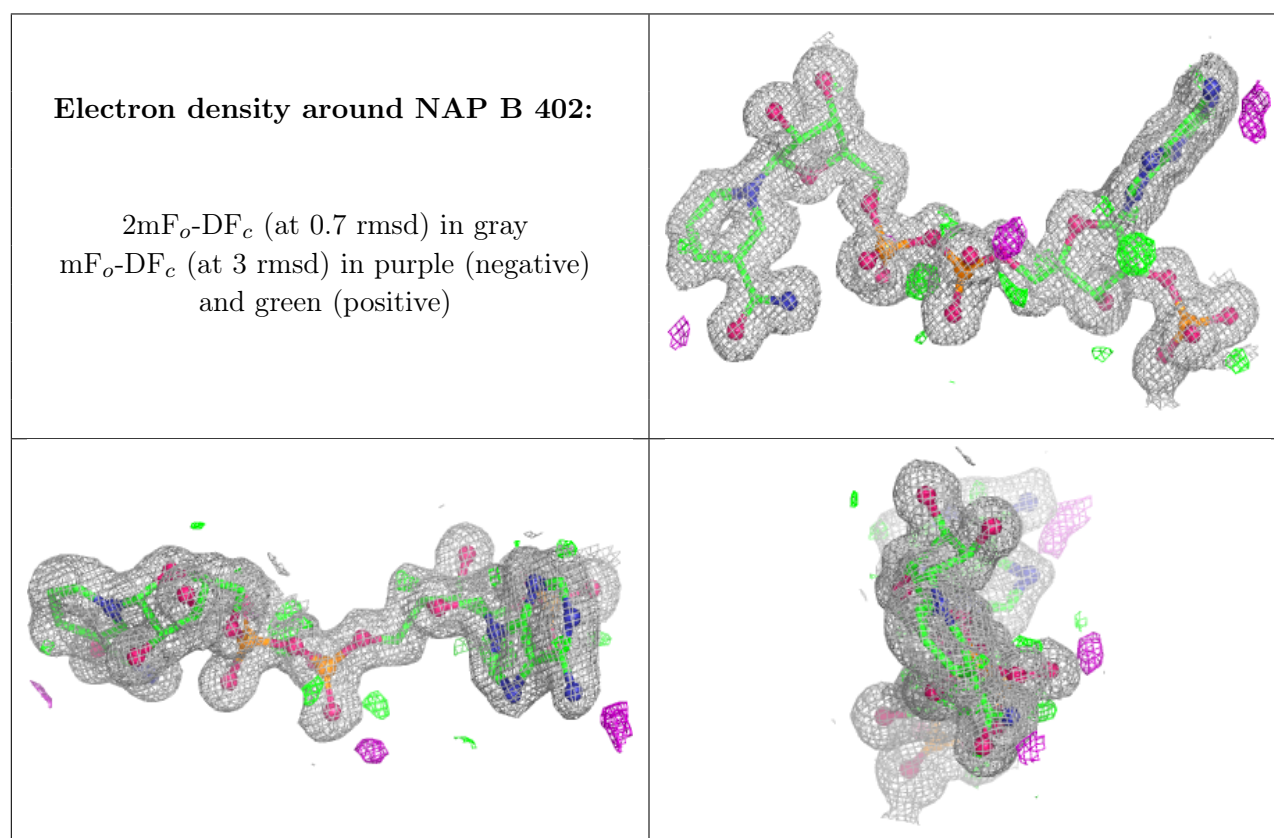
6.4 Ligands [i](#)

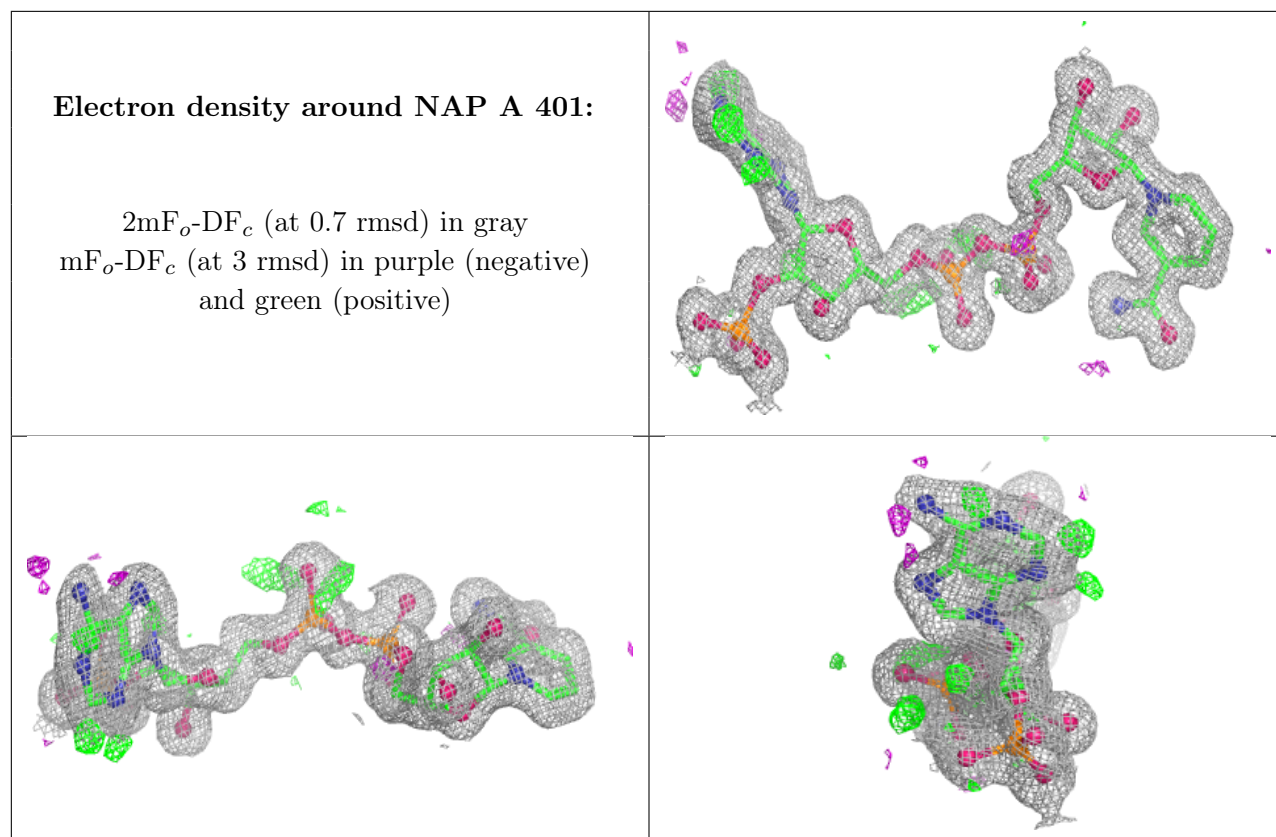
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TLA	A	403	10/10	0.87	0.12	22,36,52,54	0
3	TLA	B	403	10/10	0.87	0.14	24,40,67,72	0
3	TLA	B	401	10/10	0.96	0.11	10,24,40,50	0
3	TLA	A	402	10/10	0.96	0.10	11,22,42,45	0
4	MG	A	405	1/1	0.96	0.23	20,20,20,20	0
2	NAP	B	402	48/48	0.98	0.05	7,12,19,23	0
2	NAP	A	401	48/48	0.98	0.05	8,12,19,25	0
4	MG	B	405	1/1	0.98	0.25	19,19,19,19	0
4	MG	B	404	1/1	1.00	0.02	9,9,9,9	0
4	MG	A	404	1/1	1.00	0.03	9,9,9,9	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.