



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:29 pm BST

PDB ID : 4KQW
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.;
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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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

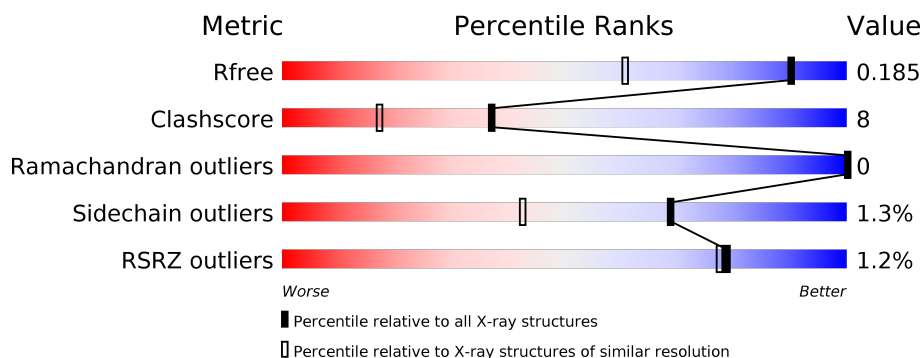
1 Overall quality at a glance

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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (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 on 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	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>
1	B	350	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>

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:

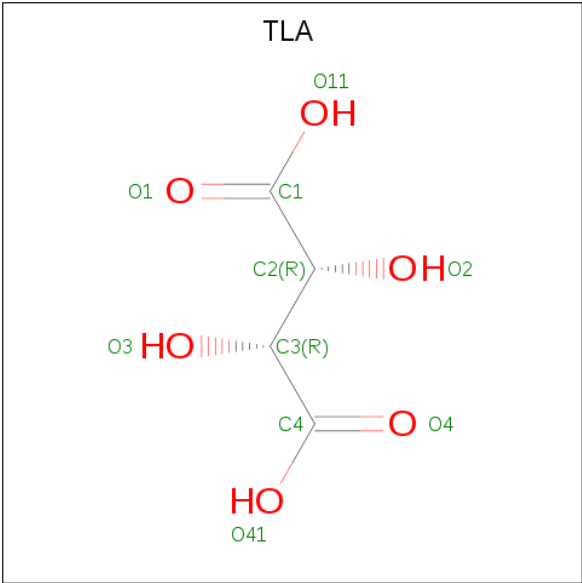
Chain	Residue	Modelled	Actual	Comment	Reference
A	343	LEU	-	EXPRESSION TAG	UNP D0WGK0
A	344	GLU	-	EXPRESSION TAG	UNP D0WGK0
A	345	HIS	-	EXPRESSION TAG	UNP D0WGK0
A	346	HIS	-	EXPRESSION TAG	UNP D0WGK0
A	347	HIS	-	EXPRESSION TAG	UNP D0WGK0
A	348	HIS	-	EXPRESSION TAG	UNP D0WGK0
A	349	HIS	-	EXPRESSION TAG	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 (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



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

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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 (three-letter code: MG) (formula: Mg).

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

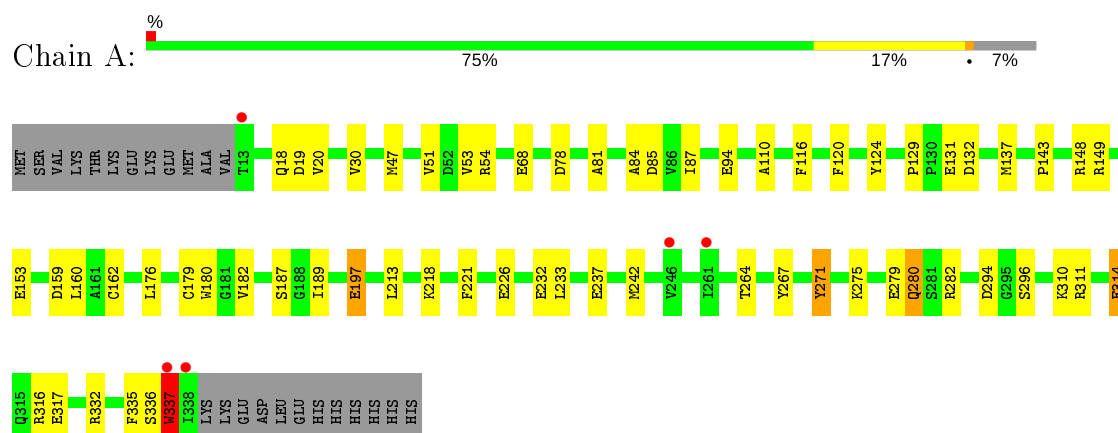
- Molecule 5 is water.

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

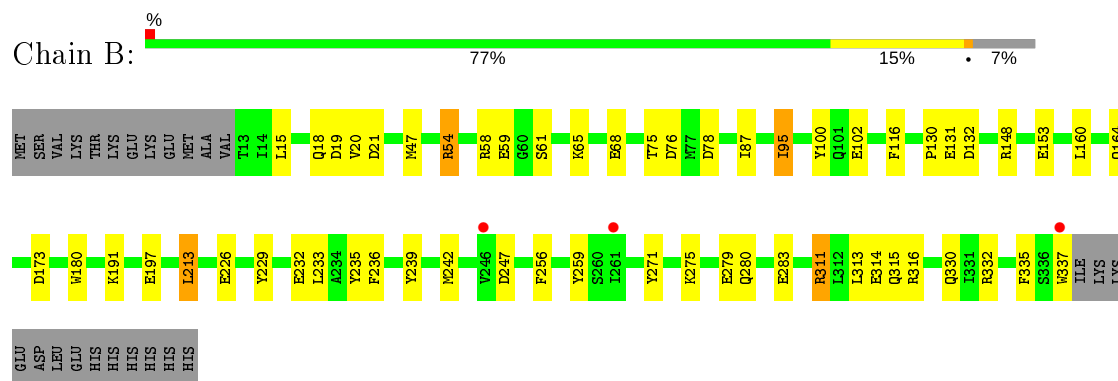
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	52.20 Å 118.93 Å 62.16 Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	60.98 – 1.39 38.81 – 1.39	Depositor EDS
% Data completeness (in resolution range)	92.9 (60.98-1.39) 92.9 (38.81-1.39)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.39 Å)	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 (5.00%)	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 , 42.3	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: MG, NAP, TLA

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	1.50	15/2730 (0.5%)	1.43	22/3698 (0.6%)
1	B	1.48	11/2678 (0.4%)	1.47	26/3627 (0.7%)
All	All	1.49	26/5408 (0.5%)	1.45	48/7325 (0.7%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	TYR	CE1-CZ	7.44	1.48	1.38
1	A	337	TRP	CD2-CE2	7.24	1.50	1.41
1	A	279	GLU	CG-CD	6.80	1.62	1.51
1	A	226	GLU	CD-OE2	6.71	1.33	1.25
1	B	332	ARG	CZ-NH2	6.69	1.41	1.33
1	B	68	GLU	CD-OE1	-6.60	1.18	1.25
1	A	337	TRP	CG-CD2	6.51	1.54	1.43
1	A	94	GLU	CD-OE1	6.43	1.32	1.25
1	A	237	GLU	CD-OE1	6.07	1.32	1.25
1	A	232	GLU	CG-CD	6.00	1.60	1.51
1	B	164	GLN	CG-CD	-5.92	1.37	1.51
1	A	267	TYR	CE1-CZ	-5.87	1.30	1.38
1	A	317	GLU	CD-OE1	5.83	1.32	1.25
1	B	102	GLU	CD-OE1	5.79	1.32	1.25
1	A	124	TYR	CB-CG	-5.68	1.43	1.51
1	B	197	GLU	CD-OE1	-5.66	1.19	1.25
1	A	314[A]	GLU	CG-CD	5.45	1.60	1.51
1	A	314[B]	GLU	CG-CD	5.45	1.60	1.51
1	B	226	GLU	CD-OE2	5.43	1.31	1.25
1	A	337	TRP	CB-CG	5.40	1.59	1.50
1	A	316	ARG	CZ-NH1	5.38	1.40	1.33
1	B	232	GLU	CG-CD	5.33	1.59	1.51
1	A	296	SER	CB-OG	-5.33	1.35	1.42
1	B	259	TYR	CG-CD2	-5.22	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	SER	CA-CB	5.11	1.60	1.52
1	B	95	ILE	CB-CG1	-5.10	1.39	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	ARG	NE-CZ-NH1	14.25	127.42	120.30
1	B	332	ARG	NE-CZ-NH2	-13.15	113.72	120.30
1	A	332	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	B	54	ARG	NE-CZ-NH1	10.97	125.79	120.30
1	B	311	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	A	332	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	A	218	LYS	CD-CE-NZ	10.28	135.35	111.70
1	B	311	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	B	148	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	A	148	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	A	148	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	160	LEU	CB-CG-CD2	8.34	125.18	111.00
1	B	160	LEU	CB-CG-CD2	8.19	124.92	111.00
1	B	316	ARG	NE-CZ-NH1	-8.07	116.26	120.30
1	A	85	ASP	CB-CG-OD2	8.01	125.51	118.30
1	B	78	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	233	LEU	CB-CG-CD1	-7.57	98.13	111.00
1	A	316	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	A	271	TYR	CG-CD1-CE1	-7.01	115.69	121.30
1	B	19	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	58	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	B	233	LEU	CB-CG-CD1	-6.59	99.80	111.00
1	B	116	PHE	CB-CG-CD1	-6.52	116.24	120.80
1	B	316	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	A	294	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	235	TYR	CD1-CE1-CZ	-6.35	114.08	119.80
1	B	213	LEU	CB-CG-CD1	-6.24	100.39	111.00
1	B	335	PHE	CB-CG-CD1	-6.24	116.43	120.80
1	A	78	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	149	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	256	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	120	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	A	335	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	B	100	TYR	CZ-CE2-CD2	-5.71	114.66	119.80
1	B	236	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	B	95	ILE	CB-CG1-CD1	-5.52	98.44	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ALA	CB-CA-C	-5.49	101.86	110.10
1	A	221	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	B	247	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	197	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	B	236	PHE	CB-CG-CD1	5.28	124.50	120.80
1	A	267	TYR	CE1-CZ-CE2	5.19	128.11	119.80
1	A	264	THR	CA-CB-CG2	-5.12	105.23	112.40
1	B	239	TYR	CB-CG-CD2	5.11	124.07	121.00
1	B	54	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	282	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	21	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	337	TRP	CD1-CG-CD2	-5.03	102.28	106.30

There are no chirality outliers.

There are no planarity outliers.

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	2631	0	2568	50	0
1	B	2596	0	2504	35	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	20	0
5	B	455	0	0	18	0
All	All	6253	0	5135	82	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 (82) 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: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
1:A:47[B]:MET:HE1	5:A:699:HOH:O	1.55	1.06
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[B]:MET:CE	5:A:699:HOH:O	2.12	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: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:191:LYS:NZ	5:B:921:HOH:O	2.10	0.85
1:A:47[A]:MET:HE2	5:A:839:HOH:O	1.75	0.84
1:B:47[B]:MET:HE3	5:B:532:HOH:O	1.79	0.82
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:B:47[B]:MET:CE	5:B:532:HOH:O	2.28	0.81
1:A:179[B]:CYS:SG	1:A:189:ILE:CD1	2.68	0.81
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:313:LEU:C	1:B:314[B]:GLU:CA	2.50	0.78
1:B:75[A]:THR:HG23	1:B:76:ASP:O	1.86	0.75
1:A:153:GLU:OE2	5:A:704:HOH:O	2.07	0.72
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:47[B]:MET:HE1	5:A:575:HOH:O	1.92	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:47[B]:MET:HE3	5:A:652:HOH:O	2.01	0.59
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:47[B]:MET:HE1	5:B:532:HOH:O	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:47[B]:MET:HE3	5:A:575:HOH:O	2.10	0.48
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:47[A]:MET:CE	5:A:839:HOH:O	2.50	0.46
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:59:GLU:HG2	5:B:757:HOH:O	2.17	0.45
1:B:47[B]:MET:HE3	5:B:687:HOH:O	2.18	0.43
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:B:15:LEU:HD11	1:B:191:LYS:HE3	2.00	0.42
1:A:187[A]:SER:HG	1:B:337:TRP:HH2	1.58	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:B:330[C]:GLN:CD	5:B:852:HOH:O	2.55	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

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	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%)	59	28
1	B	277/288 (96%)	274 (99%)	3 (1%)	73	50
All	All	560/576 (97%)	552 (99%)	8 (1%)	69	40

All (8) 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	54	ARG
1	B	95	ILE
1	B	271	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	TLA	A	402	4	3,9,9	2.06	1 (33%)	6,12,12	3.52	5 (83%)
3	TLA	A	403	-	3,9,9	1.03	0	6,12,12	1.47	1 (16%)
3	TLA	B	401	4	3,9,9	1.93	1 (33%)	6,12,12	1.96	2 (33%)
3	TLA	B	403	-	3,9,9	0.76	0	6,12,12	2.15	3 (50%)
2	NAP	A	401	-	45,52,52	2.13	12 (26%)	56,80,80	2.63	17 (30%)
2	NAP	B	402	-	45,52,52	1.80	11 (24%)	56,80,80	2.34	17 (30%)

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
3	TLA	A	402	4	-	2/4/12/12	-
3	TLA	A	403	-	-	0/4/12/12	-
3	TLA	B	401	4	-	1/4/12/12	-
3	TLA	B	403	-	-	0/4/12/12	-
2	NAP	A	401	-	-	6/31/67/67	0/5/5/5
2	NAP	B	402	-	-	5/31/67/67	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O4D-C1D	5.56	1.48	1.41
2	B	402	NAP	O4D-C1D	5.01	1.48	1.41
2	A	401	NAP	C4A-N3A	-4.97	1.28	1.35
2	B	402	NAP	C4N-C3N	4.31	1.46	1.39
2	A	401	NAP	C2A-N3A	4.28	1.39	1.32
2	A	401	NAP	C2D-C1D	-3.94	1.47	1.53
2	A	401	NAP	P2B-O2B	3.66	1.66	1.59
2	A	401	NAP	C3N-C7N	-3.54	1.45	1.50
2	A	401	NAP	C2N-C3N	-3.38	1.33	1.39
3	A	402	TLA	C3-C2	-3.37	1.41	1.53
2	B	402	NAP	C2N-C3N	-3.28	1.33	1.39
2	A	401	NAP	O4B-C1B	3.27	1.45	1.41
3	B	401	TLA	C3-C2	-2.98	1.42	1.53
2	A	401	NAP	C6A-C5A	2.98	1.54	1.43
2	B	402	NAP	C2A-N3A	2.96	1.36	1.32
2	A	401	NAP	C4N-C3N	2.85	1.44	1.39
2	B	402	NAP	C2A-N1A	2.82	1.39	1.33
2	B	402	NAP	C2N-N1N	2.80	1.38	1.35
2	A	401	NAP	C5A-C4A	2.71	1.48	1.40
2	B	402	NAP	P2B-O2B	2.50	1.64	1.59
2	B	402	NAP	C2D-C1D	-2.33	1.50	1.53
2	B	402	NAP	C4A-N3A	-2.30	1.32	1.35
2	B	402	NAP	C7N-N7N	-2.29	1.28	1.33
2	B	402	NAP	C5N-C4N	2.12	1.43	1.38
2	A	401	NAP	O2D-C2D	2.09	1.47	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C2A-N1A-C6A	8.31	132.97	118.75
2	A	401	NAP	N3A-C2A-N1A	-8.20	115.86	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C3N-C7N-N7N	7.71	127.01	117.75
2	B	402	NAP	C6N-N1N-C2N	-7.08	115.52	121.97
2	B	402	NAP	C3N-C7N-N7N	5.24	124.03	117.75
2	B	402	NAP	C5N-C4N-C3N	-5.19	114.20	120.34
2	B	402	NAP	N3A-C2A-N1A	-5.11	120.68	128.68
2	B	402	NAP	N6A-C6A-N1A	5.00	128.94	118.57
2	B	402	NAP	C2A-N1A-C6A	4.98	127.28	118.75
3	A	402	TLA	C4-C3-C2	4.77	123.36	113.11
3	A	402	TLA	C1-C2-C3	-4.77	102.85	113.11
2	A	401	NAP	O7N-C7N-N7N	-4.39	116.33	122.58
2	A	401	NAP	C6N-N1N-C2N	-4.20	118.14	121.97
2	A	401	NAP	C5N-C4N-C3N	-3.87	115.77	120.34
2	A	401	NAP	O4B-C1B-C2B	-3.80	100.00	106.59
2	B	402	NAP	O4B-C1B-C2B	-3.70	100.16	106.59
2	A	401	NAP	N6A-C6A-N1A	3.63	126.11	118.57
3	B	403	TLA	C4-C3-C2	-3.41	105.77	113.11
2	B	402	NAP	C5A-C6A-N6A	-3.35	115.27	120.35
2	B	402	NAP	O4D-C1D-C2D	-3.30	102.10	106.93
2	A	401	NAP	C5B-C4B-C3B	-3.23	103.09	115.18
2	B	402	NAP	C3N-C2N-N1N	3.21	123.57	120.43
3	A	402	TLA	O2-C2-C1	3.19	118.79	111.10
3	A	402	TLA	O3-C3-C4	3.08	118.52	111.10
3	A	402	TLA	O2-C2-C3	3.04	119.05	108.90
2	A	401	NAP	O4D-C1D-C2D	-3.04	102.49	106.93
2	B	402	NAP	C5N-C6N-N1N	3.02	124.73	120.40
2	A	401	NAP	C5A-C6A-N1A	-2.94	113.70	120.35
2	B	402	NAP	O7N-C7N-C3N	-2.89	116.17	119.63
3	A	403	TLA	C1-C2-C3	-2.89	106.89	113.11
3	B	401	TLA	O2-C2-C1	2.73	117.67	111.10
2	A	401	NAP	C1B-N9A-C4A	-2.73	121.85	126.64
2	A	401	NAP	O7N-C7N-C3N	-2.70	116.40	119.63
2	B	402	NAP	O3X-P2B-O2X	2.53	117.31	107.64
2	B	402	NAP	C5B-C4B-C3B	-2.46	105.96	115.18
3	B	401	TLA	O2-C2-C3	2.41	116.95	108.90
2	A	401	NAP	C2D-C3D-C4D	-2.38	98.01	102.64
3	B	403	TLA	O2-C2-C1	2.37	116.80	111.10
2	B	402	NAP	PN-O3-PA	-2.30	124.92	132.83
3	B	403	TLA	O3-C3-C4	-2.25	105.68	111.10
2	A	401	NAP	C2N-N1N-C1D	2.09	123.80	119.14
2	A	401	NAP	O5B-C5B-C4B	-2.05	101.92	108.99
2	B	402	NAP	C5A-C6A-N1A	-2.03	115.75	120.35
2	B	402	NAP	O7N-C7N-N7N	-2.02	119.71	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	O4D-C4D-C5D	2.02	116.01	109.37

There are no chirality outliers.

All (14) torsion outliers are listed below:

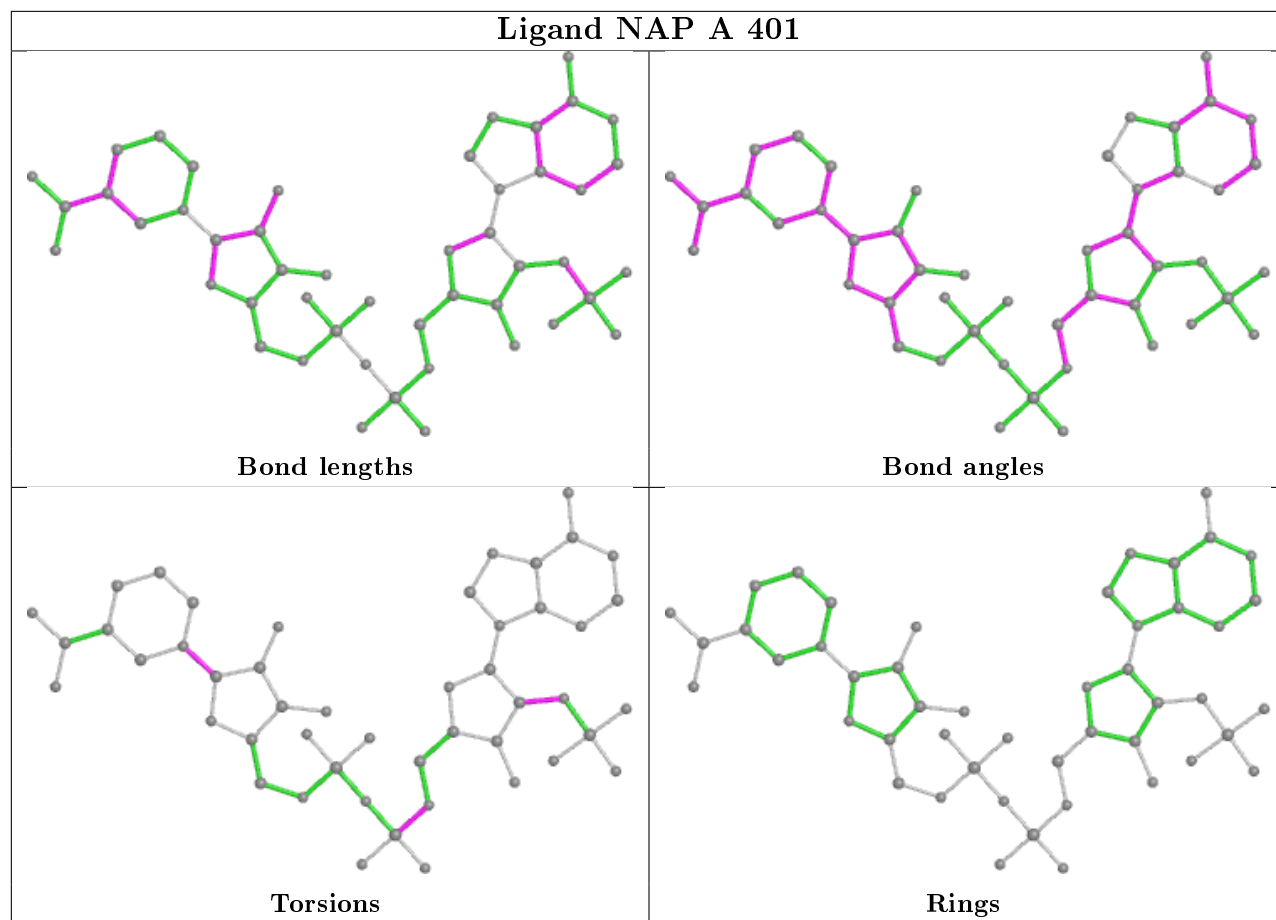
Mol	Chain	Res	Type	Atoms
3	A	402	TLA	O2-C2-C3-O3
3	B	401	TLA	O2-C2-C3-O3
2	A	401	NAP	C3B-C2B-O2B-P2B
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	C2D-C1D-N1N-C6N
2	B	402	NAP	O4D-C1D-N1N-C2N
2	B	402	NAP	O4D-C1D-N1N-C6N
2	B	402	NAP	C2D-C1D-N1N-C6N
2	B	402	NAP	C3B-C2B-O2B-P2B
2	A	401	NAP	C1B-C2B-O2B-P2B
2	B	402	NAP	C1B-C2B-O2B-P2B
3	A	402	TLA	C1-C2-C3-O3
2	A	401	NAP	C5B-O5B-PA-O2A

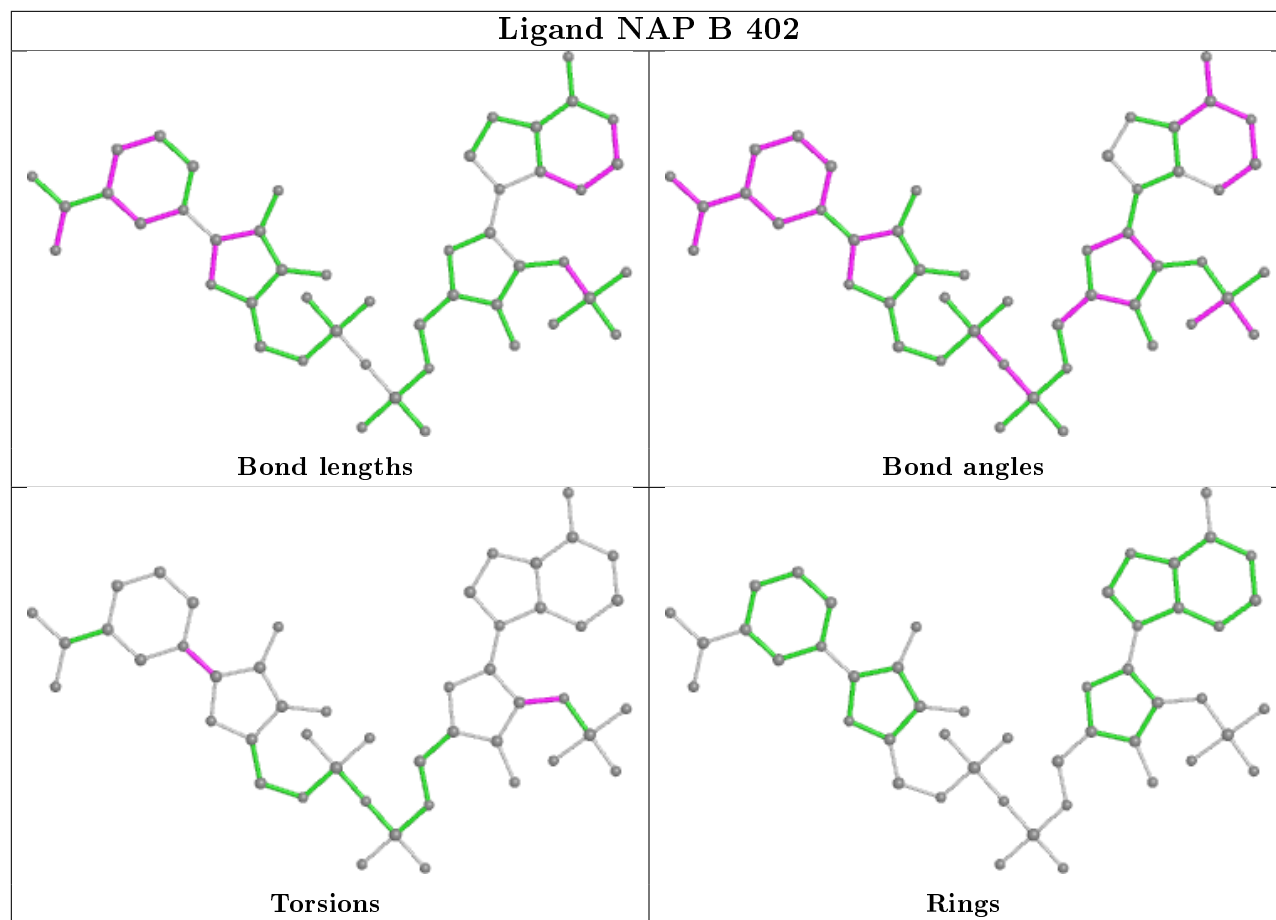
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	TLA	1	0
3	B	401	TLA	3	0
2	A	401	NAP	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%)	0.04	5 (1%) 73 72	8, 13, 24, 48	0
1	B	325/350 (92%)	-0.04	3 (0%) 84 82	8, 13, 23, 40	2 (0%)
All	All	651/700 (93%)	-0.00	8 (1%) 79 77	8, 13, 24, 48	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	ILE	6.9
1	A	337	TRP	5.0
1	B	337	TRP	3.0
1	A	13	THR	2.7
1	A	261	ILE	2.3
1	B	261	ILE	2.2
1	B	246	VAL	2.2
1	A	246	VAL	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 carbohydrates in this entry.

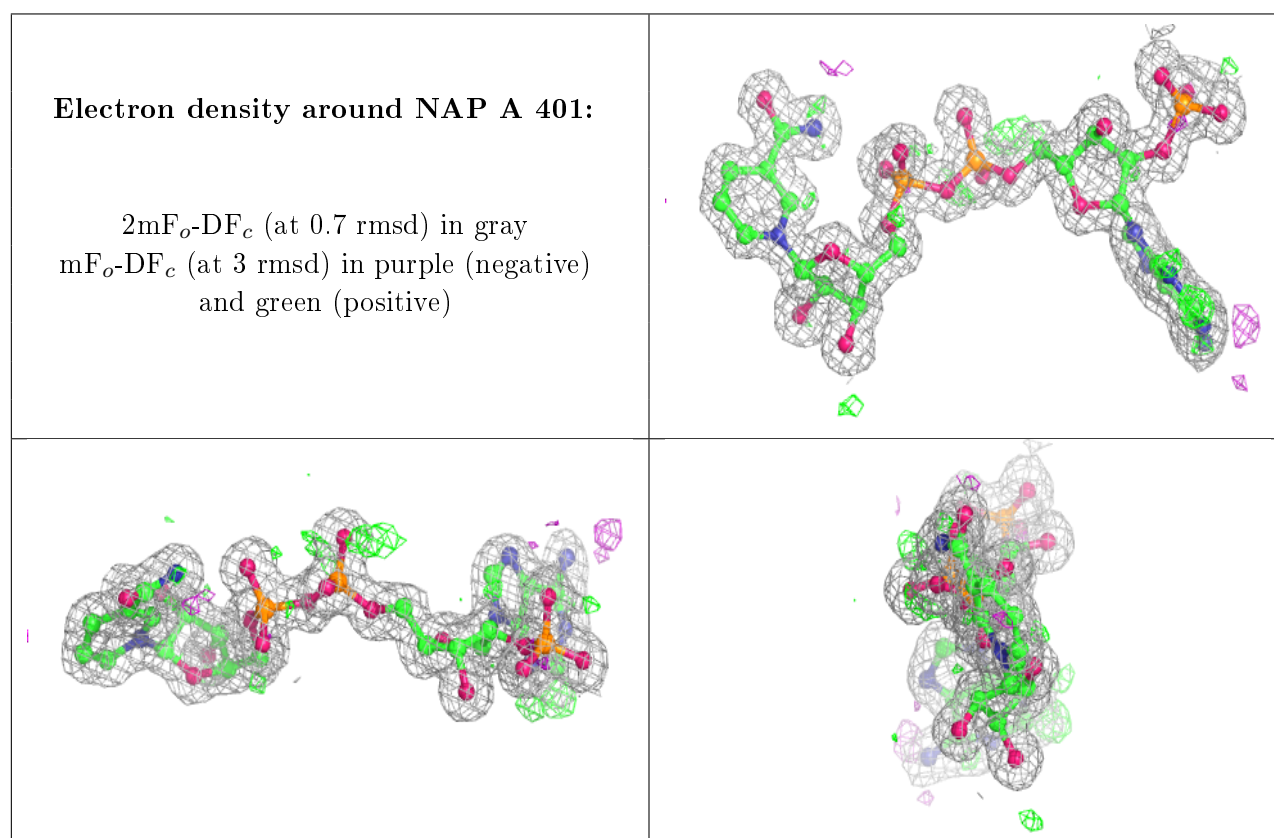
6.4 Ligands [i](#)

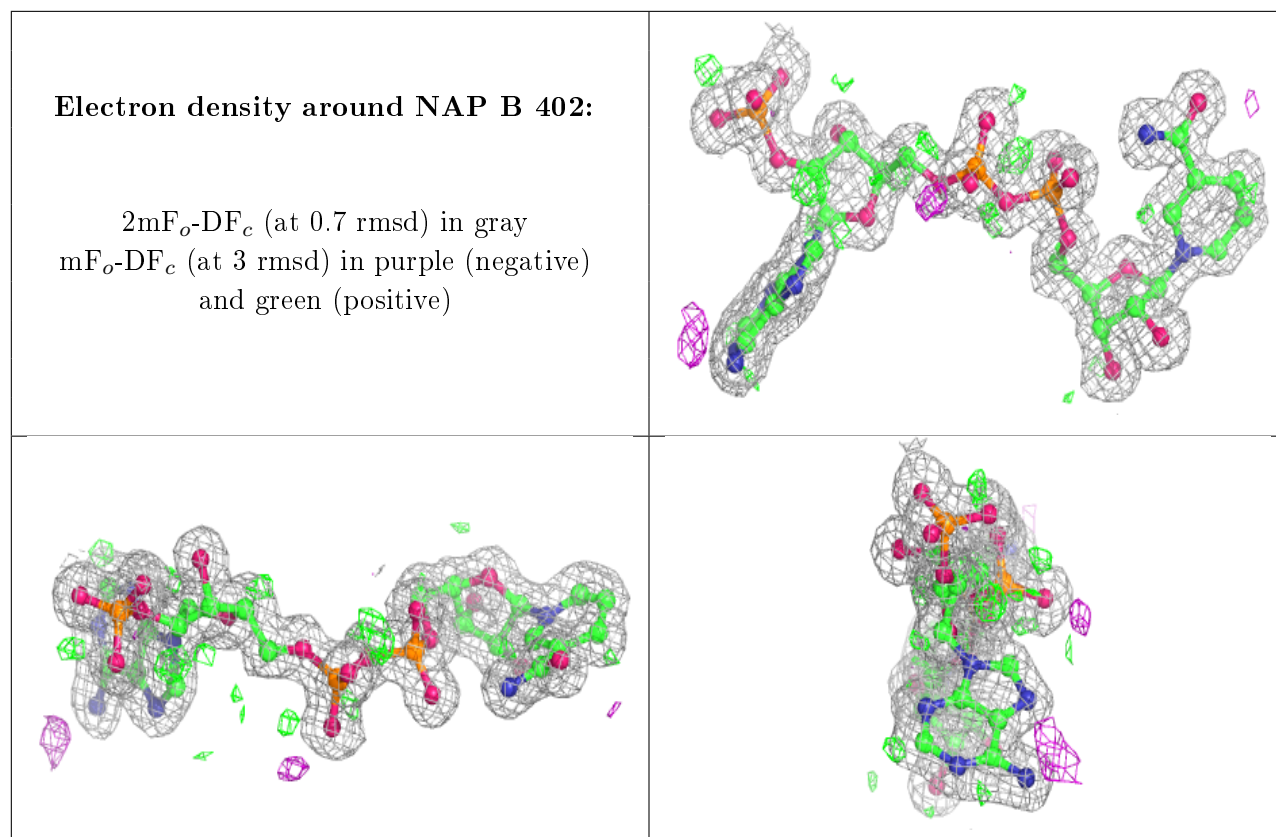
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	0.88	0.17	22,36,52,54	0
3	TLA	B	403	10/10	0.90	0.20	24,40,67,72	0
3	TLA	B	401	10/10	0.97	0.12	10,24,40,50	0
3	TLA	A	402	10/10	0.97	0.14	11,22,42,45	0
4	MG	A	405	1/1	0.98	0.17	20,20,20,20	0
2	NAP	A	401	48/48	0.98	0.07	8,12,19,25	0
2	NAP	B	402	48/48	0.98	0.06	7,12,19,23	0
4	MG	B	405	1/1	0.99	0.19	19,19,19,19	0
4	MG	B	404	1/1	1.00	0.06	9,9,9,9	0
4	MG	A	404	1/1	1.00	0.06	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.