Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 07:29 PM JST

PDB ID	:	6A3I
Title	:	Levoglucosan dehydrogenase, complex with NADH and levoglucosan
Authors	:	Sugiura, M.; Yamada, C.; Arakawa, T.; Fushinobu, S.
Deposited on	:	2018-06-15
Resolution	:	2.41 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 (i) 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 (i)) were used in the production of this report:

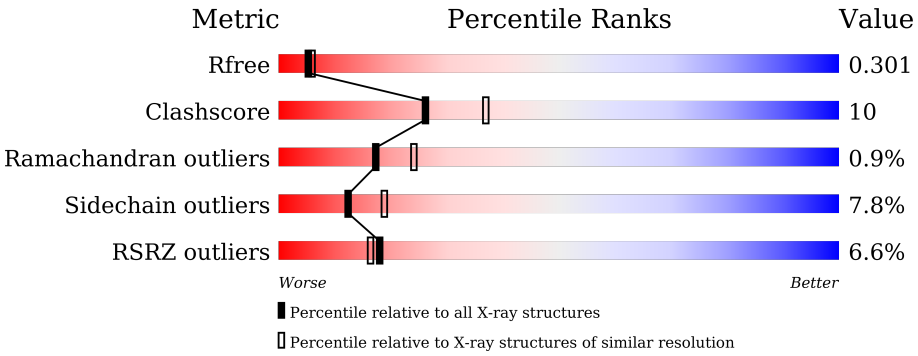
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	410	2% 78% 12% • 9%
1	B	410	5% 75% 14% • 10%
1	C	410	3% 68% 18% • 10%
1	D	410	14% 57% 27% 5% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11518 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 Putative dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2863	1821	497	536	9			
1	B	370	Total	C	N	O	S	0	0	0
			2849	1812	495	533	9			
1	C	367	Total	C	N	O	S	0	0	0
			2829	1800	491	529	9			
1	D	366	Total	C	N	O	S	0	0	0
			2825	1798	490	528	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP F0M433
A	-18	GLY	-	expression tag	UNP F0M433
A	-17	SER	-	expression tag	UNP F0M433
A	-16	SER	-	expression tag	UNP F0M433
A	-15	HIS	-	expression tag	UNP F0M433
A	-14	HIS	-	expression tag	UNP F0M433
A	-13	HIS	-	expression tag	UNP F0M433
A	-12	HIS	-	expression tag	UNP F0M433
A	-11	HIS	-	expression tag	UNP F0M433
A	-10	HIS	-	expression tag	UNP F0M433
A	-9	SER	-	expression tag	UNP F0M433
A	-8	SER	-	expression tag	UNP F0M433
A	-7	GLY	-	expression tag	UNP F0M433
A	-6	LEU	-	expression tag	UNP F0M433
A	-5	VAL	-	expression tag	UNP F0M433
A	-4	PRO	-	expression tag	UNP F0M433
A	-3	ARG	-	expression tag	UNP F0M433
A	-2	GLY	-	expression tag	UNP F0M433
A	-1	SER	-	expression tag	UNP F0M433
A	0	HIS	-	expression tag	UNP F0M433
B	-19	MET	-	expression tag	UNP F0M433

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP F0M433
B	-17	SER	-	expression tag	UNP F0M433
B	-16	SER	-	expression tag	UNP F0M433
B	-15	HIS	-	expression tag	UNP F0M433
B	-14	HIS	-	expression tag	UNP F0M433
B	-13	HIS	-	expression tag	UNP F0M433
B	-12	HIS	-	expression tag	UNP F0M433
B	-11	HIS	-	expression tag	UNP F0M433
B	-10	HIS	-	expression tag	UNP F0M433
B	-9	SER	-	expression tag	UNP F0M433
B	-8	SER	-	expression tag	UNP F0M433
B	-7	GLY	-	expression tag	UNP F0M433
B	-6	LEU	-	expression tag	UNP F0M433
B	-5	VAL	-	expression tag	UNP F0M433
B	-4	PRO	-	expression tag	UNP F0M433
B	-3	ARG	-	expression tag	UNP F0M433
B	-2	GLY	-	expression tag	UNP F0M433
B	-1	SER	-	expression tag	UNP F0M433
B	0	HIS	-	expression tag	UNP F0M433
C	-19	MET	-	expression tag	UNP F0M433
C	-18	GLY	-	expression tag	UNP F0M433
C	-17	SER	-	expression tag	UNP F0M433
C	-16	SER	-	expression tag	UNP F0M433
C	-15	HIS	-	expression tag	UNP F0M433
C	-14	HIS	-	expression tag	UNP F0M433
C	-13	HIS	-	expression tag	UNP F0M433
C	-12	HIS	-	expression tag	UNP F0M433
C	-11	HIS	-	expression tag	UNP F0M433
C	-10	HIS	-	expression tag	UNP F0M433
C	-9	SER	-	expression tag	UNP F0M433
C	-8	SER	-	expression tag	UNP F0M433
C	-7	GLY	-	expression tag	UNP F0M433
C	-6	LEU	-	expression tag	UNP F0M433
C	-5	VAL	-	expression tag	UNP F0M433
C	-4	PRO	-	expression tag	UNP F0M433
C	-3	ARG	-	expression tag	UNP F0M433
C	-2	GLY	-	expression tag	UNP F0M433
C	-1	SER	-	expression tag	UNP F0M433
C	0	HIS	-	expression tag	UNP F0M433
D	-19	MET	-	expression tag	UNP F0M433
D	-18	GLY	-	expression tag	UNP F0M433
D	-17	SER	-	expression tag	UNP F0M433

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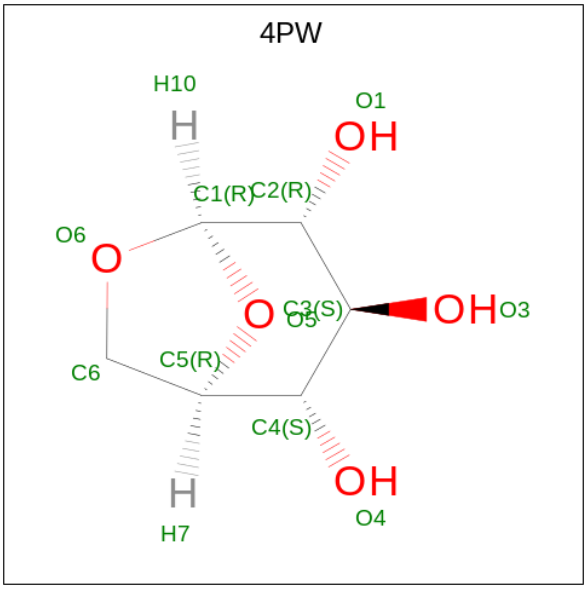
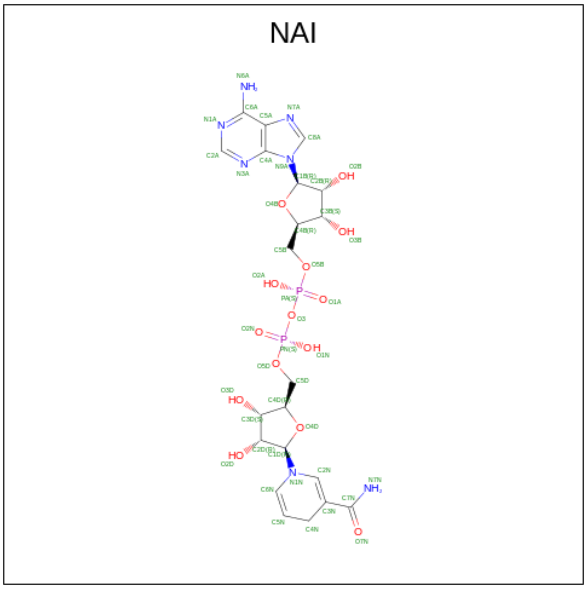
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP F0M433
D	-15	HIS	-	expression tag	UNP F0M433
D	-14	HIS	-	expression tag	UNP F0M433
D	-13	HIS	-	expression tag	UNP F0M433
D	-12	HIS	-	expression tag	UNP F0M433
D	-11	HIS	-	expression tag	UNP F0M433
D	-10	HIS	-	expression tag	UNP F0M433
D	-9	SER	-	expression tag	UNP F0M433
D	-8	SER	-	expression tag	UNP F0M433
D	-7	GLY	-	expression tag	UNP F0M433
D	-6	LEU	-	expression tag	UNP F0M433
D	-5	VAL	-	expression tag	UNP F0M433
D	-4	PRO	-	expression tag	UNP F0M433
D	-3	ARG	-	expression tag	UNP F0M433
D	-2	GLY	-	expression tag	UNP F0M433
D	-1	SER	-	expression tag	UNP F0M433
D	0	HIS	-	expression tag	UNP F0M433

- Molecule 2 is Levoglucosan (three-letter code: 4PW) (formula: $C_6H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 6 5	0	0
2	D	1	Total C O 11 6 5	0	0

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 35 15 5 13 2	0	0
3	B	1	Total C O P 17 5 10 2	0	0
3	C	1	Total C O P 17 5 10 2	0	0

- Molecule 4 is water.

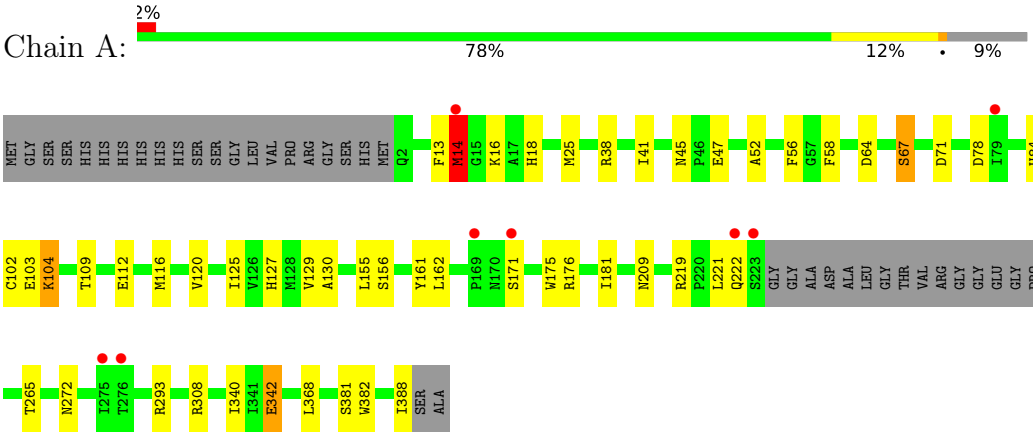
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	17	Total O 17 17	0	0
4	C	10	Total O 10 10	0	0
4	D	4	Total O 4 4	0	0

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.

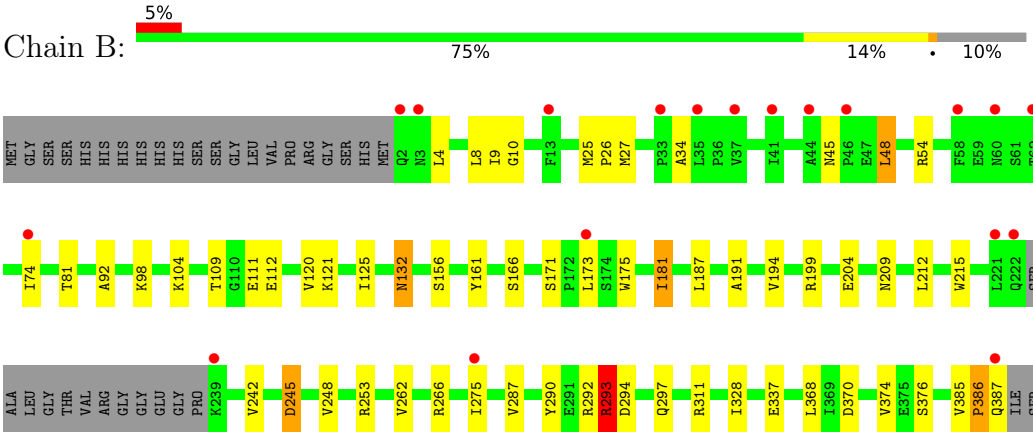
• Molecule 1: Putative dehydrogenase

Chain A:



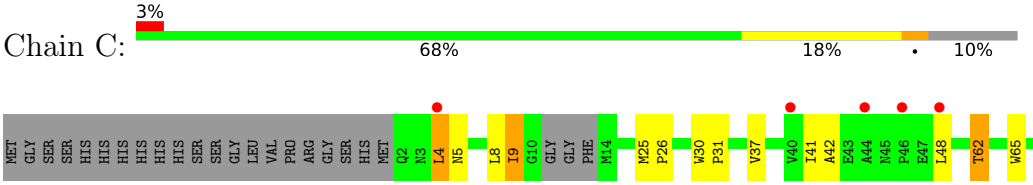
• Molecule 1: Putative dehydrogenase

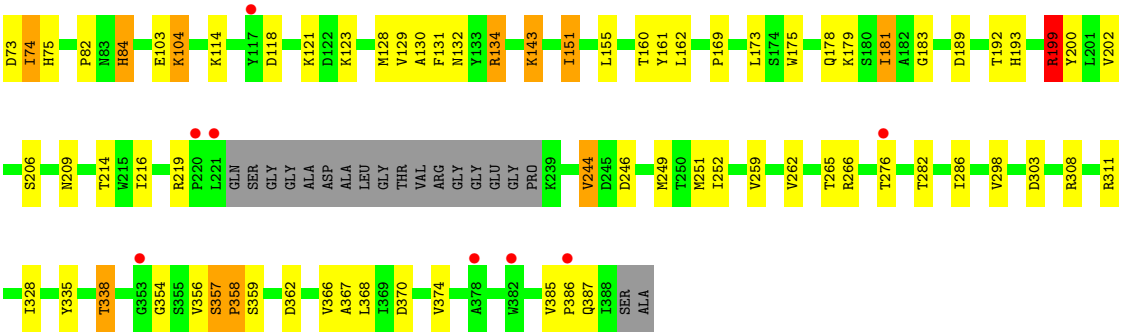
Chain B:



• Molecule 1: Putative dehydrogenase

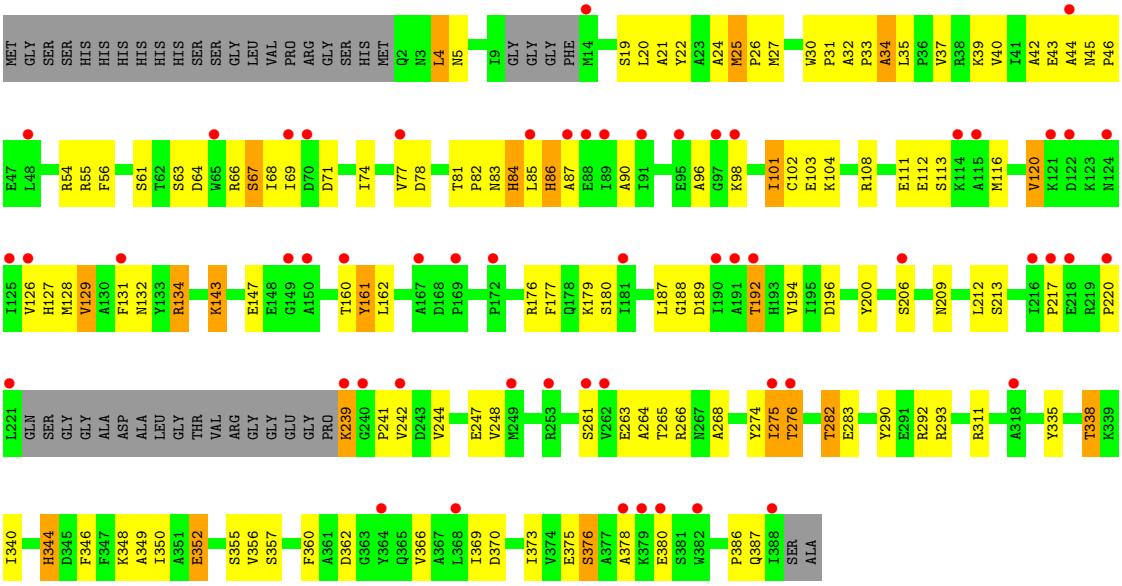
Chain C:





• Molecule 1: Putative dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.72Å 92.35Å 100.56Å 90.00° 104.48° 90.00°	Depositor
Resolution (Å)	34.84 – 2.41 34.82 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.84-2.41) 98.6 (34.82-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.215 , 0.297 0.217 , 0.301	Depositor DCC
R_{free} test set	2618 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11518	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAI, 4PW

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	0.52	0/2935	0.67	0/3989
1	B	0.45	0/2921	0.66	0/3970
1	C	0.43	0/2899	0.64	0/3940
1	D	0.43	0/2895	0.65	0/3935
All	All	0.46	0/11650	0.66	0/15834

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ARG	Sidechain
1	A	308	ARG	Sidechain
1	C	199	ARG	Sidechain
1	D	120	VAL	Peptide
1	D	311	ARG	Sidechain

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	2863	0	2780	33	0
1	B	2849	0	2764	45	0
1	C	2829	0	2751	68	0
1	D	2825	0	2748	106	0
2	A	11	0	10	1	0
2	D	11	0	10	1	0
3	A	35	0	19	3	0
3	B	17	0	7	0	0
3	C	17	0	7	0	0
4	A	30	0	0	0	0
4	B	17	0	0	0	0
4	C	10	0	0	0	0
4	D	4	0	0	0	0
All	All	11518	0	11096	235	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 10.

All (235) 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:D:86:HIS:CE1	1:D:102:CYS:SG	2.44	1.11
1:C:209:ASN:ND2	1:D:209:ASN:ND2	2.06	1.04
1:C:209:ASN:ND2	1:D:209:ASN:HD22	1.59	0.96
1:C:209:ASN:HD21	1:D:209:ASN:ND2	1.61	0.95
1:C:132:ASN:HD22	1:C:338:THR:CG2	1.80	0.94
1:A:209:ASN:HD21	1:B:209:ASN:HD21	1.18	0.92
1:C:209:ASN:HD21	1:D:209:ASN:HD22	0.92	0.87
1:D:132:ASN:OD1	1:D:338:THR:HG21	1.78	0.82
1:D:87:ALA:HB2	1:D:112:GLU:OE2	1.81	0.81
1:C:132:ASN:HD22	1:C:338:THR:HG21	1.46	0.80
1:B:294:ASP:OD2	1:D:293:ARG:NH2	2.12	0.79
1:C:370:ASP:O	1:C:374:VAL:HG23	1.82	0.79
1:C:357:SER:O	1:C:359:SER:N	2.16	0.78
1:D:116:MET:O	1:D:120:VAL:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:THR:CG2	1:D:276:THR:HB	2.16	0.76
1:B:212:LEU:HD22	1:B:245:ASP:OD2	1.85	0.75
1:D:348:LYS:O	1:D:352:GLU:HG2	1.85	0.75
1:C:84:HIS:CG	1:C:181:ILE:HD12	2.24	0.73
1:D:86:HIS:CE1	1:D:103:GLU:O	2.43	0.71
1:D:187:LEU:HD22	1:D:370:ASP:OD1	1.92	0.69
1:B:290:TYR:CZ	1:B:293:ARG:HD2	2.27	0.69
1:D:177:PHE:HB3	1:D:242:VAL:HG13	1.74	0.69
1:A:130:ALA:HA	1:A:342:GLU:OE2	1.94	0.67
1:D:30:TRP:HA	1:D:31:PRO:C	2.14	0.67
1:D:187:LEU:CD2	1:D:370:ASP:OD1	2.42	0.67
1:A:209:ASN:ND2	1:B:209:ASN:HD21	1.92	0.65
1:D:275:ILE:HG23	1:D:290:TYR:CB	2.26	0.65
1:D:132:ASN:OD1	1:D:338:THR:CG2	2.45	0.65
1:C:216:ILE:HG23	1:C:216:ILE:O	1.97	0.64
1:D:290:TYR:CE1	1:D:293:ARG:HG2	2.32	0.64
1:C:385:VAL:O	1:C:387:GLN:N	2.30	0.64
1:A:18:HIS:NE2	1:A:103:GLU:OE2	2.28	0.63
1:D:22:TYR:OH	1:D:78:ASP:OD1	2.11	0.63
1:C:9:ILE:HD12	1:C:65:TRP:HB2	1.81	0.62
1:D:348:LYS:O	1:D:352:GLU:CG	2.47	0.62
1:A:176:ARG:NH2	3:A:402:NAI:O1N	2.32	0.62
1:D:282:THR:HG22	1:D:283:GLU:HG3	1.80	0.62
1:D:86:HIS:ND1	1:D:102:CYS:SG	2.73	0.62
1:C:132:ASN:ND2	1:C:338:THR:HG21	2.15	0.61
1:C:131:PHE:CE1	1:C:192:THR:HG22	2.35	0.61
1:D:188:GLY:O	1:D:192:THR:HG21	1.99	0.61
1:B:292:ARG:CZ	1:D:292:ARG:NH2	2.64	0.60
1:B:27:MET:HE1	1:D:20:LEU:N	2.17	0.60
1:C:216:ILE:HG21	1:C:219:ARG:NH2	2.16	0.60
1:D:25:MET:HG3	1:D:26:PRO:HD3	1.84	0.60
1:C:128:MET:HB2	1:C:356:VAL:HG11	1.83	0.60
1:C:8:LEU:O	1:C:41:ILE:HA	2.02	0.60
1:B:132:ASN:HD22	1:B:132:ASN:H	1.50	0.59
1:D:86:HIS:HE1	1:D:102:CYS:SG	2.18	0.59
1:D:290:TYR:CD1	1:D:293:ARG:HG2	2.37	0.59
1:C:84:HIS:CD2	1:C:181:ILE:HD12	2.38	0.59
1:D:160:THR:HG22	1:D:276:THR:HB	1.84	0.59
1:A:209:ASN:HD21	1:B:209:ASN:ND2	1.97	0.59
1:D:275:ILE:HG23	1:D:290:TYR:HB3	1.85	0.59
1:C:82:PRO:HB2	1:C:181:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:MET:CE	1:D:346:PHE:HB2	2.33	0.58
1:D:25:MET:HA	1:D:340:ILE:HG23	1.86	0.58
1:A:120:VAL:HG13	1:A:127:HIS:CD2	2.40	0.57
1:C:192:THR:HG23	1:C:366:VAL:HG11	1.84	0.57
1:C:25:MET:HB3	1:C:26:PRO:HD3	1.87	0.56
1:D:101:ILE:HD11	1:D:346:PHE:CD2	2.41	0.56
1:B:385:VAL:O	1:B:387:GLN:N	2.39	0.56
1:D:101:ILE:HD11	1:D:346:PHE:CE2	2.41	0.56
1:B:187:LEU:O	1:B:191:ALA:HB3	2.05	0.55
1:B:98:LYS:O	1:B:125:ILE:HD12	2.06	0.55
1:D:84:HIS:ND1	1:D:85:LEU:N	2.54	0.55
1:A:45:ASN:OD1	1:A:47:GLU:HG2	2.06	0.55
1:D:134:ARG:NH1	1:D:196:ASP:OD1	2.38	0.55
1:B:370:ASP:O	1:B:374:VAL:HG23	2.07	0.55
1:D:86:HIS:NE2	1:D:103:GLU:O	2.40	0.54
1:C:175:TRP:HB2	1:C:181:ILE:HG12	1.89	0.54
1:D:369:ILE:O	1:D:373:ILE:HD12	2.07	0.54
1:B:109:THR:HG23	1:B:112:GLU:H	1.73	0.54
1:D:21:ALA:O	1:D:25:MET:HB3	2.08	0.54
1:C:132:ASN:ND2	1:C:338:THR:CG2	2.62	0.54
1:D:335:TYR:O	1:D:338:THR:HB	2.08	0.54
1:A:109:THR:HG23	1:A:112:GLU:H	1.73	0.54
1:C:155:LEU:HD11	1:C:282:THR:HG23	1.90	0.53
1:C:151:ILE:HD13	1:C:286:ILE:CD1	2.39	0.53
1:D:126:VAL:HG21	1:D:350:ILE:HA	1.91	0.53
1:D:290:TYR:O	1:D:293:ARG:HG3	2.09	0.53
1:B:311:ARG:HA	1:C:311:ARG:HA	1.91	0.53
1:D:220:PRO:HA	1:D:239:LYS:HA	1.91	0.53
1:C:209:ASN:ND2	1:D:209:ASN:HD21	2.00	0.53
1:D:209:ASN:HA	1:D:376:SER:OG	2.09	0.53
1:D:349:ALA:CB	1:D:356:VAL:HG12	2.39	0.53
1:C:131:PHE:HE1	1:C:192:THR:HG22	1.73	0.53
1:D:25:MET:HG3	1:D:26:PRO:CD	2.38	0.53
1:D:160:THR:HA	1:D:263:GLU:O	2.09	0.53
1:D:4:LEU:HD22	1:D:34:ALA:HB1	1.91	0.52
1:D:187:LEU:HD12	1:D:212:LEU:HD21	1.91	0.52
1:D:375:GLU:O	1:D:378:ALA:HB3	2.10	0.52
1:C:362:ASP:O	1:C:366:VAL:HG23	2.09	0.52
1:A:104:LYS:O	3:A:402:NAI:O2D	2.24	0.51
1:B:175:TRP:HB2	1:B:181:ILE:HD11	1.92	0.51
1:A:84:HIS:CD2	1:A:85:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASN:HD22	1:D:209:ASN:ND2	2.00	0.51
1:D:134:ARG:HD2	1:D:196:ASP:OD2	2.10	0.51
1:A:16:LYS:HB2	1:A:56:PHE:CE1	2.46	0.51
1:B:69:ILE:HD13	1:B:92:ALA:HB1	1.93	0.51
1:D:344:HIS:O	1:D:348:LYS:HB2	2.10	0.51
1:C:4:LEU:HD23	1:C:75:HIS:HB3	1.93	0.50
1:C:30:TRP:HA	1:C:31:PRO:C	2.30	0.50
1:D:160:THR:OG1	1:D:162:LEU:HG	2.12	0.50
1:B:173:LEU:CD1	1:B:242:VAL:HG22	2.41	0.50
1:C:74:ILE:HG23	1:C:75:HIS:N	2.26	0.50
1:C:151:ILE:HD13	1:C:286:ILE:HD11	1.94	0.50
1:D:45:ASN:HB2	1:D:46:PRO:HD2	1.93	0.50
1:D:344:HIS:CD2	1:D:344:HIS:C	2.84	0.50
1:B:9:ILE:HG22	1:B:81:THR:CG2	2.42	0.50
1:B:74:ILE:HB	1:B:98:LYS:HE3	1.94	0.50
1:B:120:VAL:O	1:B:121:LYS:C	2.50	0.50
1:B:292:ARG:CZ	1:D:292:ARG:HH21	2.24	0.50
1:B:337:GLU:N	1:B:337:GLU:OE1	2.44	0.49
1:D:64:ASP:O	1:D:67:SER:OG	2.30	0.49
1:D:188:GLY:O	1:D:192:THR:CG2	2.60	0.49
1:D:162:LEU:HD12	1:D:274:TYR:CD2	2.48	0.49
1:D:40:VAL:HG11	1:D:68:ILE:HG12	1.94	0.49
1:A:175:TRP:HB2	1:A:181:ILE:HG21	1.93	0.49
1:B:199:ARG:NH2	1:B:204:GLU:OE1	2.34	0.49
1:C:132:ASN:HD22	1:C:338:THR:HG22	1.73	0.49
1:D:143:LYS:NZ	1:D:200:TYR:O	2.25	0.49
1:C:4:LEU:HD23	1:C:75:HIS:CB	2.43	0.49
1:D:55:ARG:HG2	1:D:56:PHE:CD1	2.48	0.49
1:C:335:TYR:O	1:C:338:THR:HB	2.13	0.48
1:A:171:SER:O	1:A:219:ARG:HD3	2.13	0.48
1:B:290:TYR:CD1	1:B:293:ARG:HG3	2.48	0.48
1:D:161:TYR:O	1:D:264:ALA:HA	2.13	0.48
1:D:77:VAL:HG23	1:D:98:LYS:HB3	1.94	0.48
1:D:349:ALA:HB1	1:D:356:VAL:HG12	1.96	0.48
1:C:214:THR:OG1	1:C:244:VAL:O	2.32	0.47
1:D:176:ARG:NH2	2:D:401:4PW:O4	2.48	0.47
1:D:194:VAL:HG22	1:D:275:ILE:HD12	1.96	0.47
1:A:176:ARG:NH1	2:A:401:4PW:O4	2.47	0.47
1:D:128:MET:HE1	1:D:346:PHE:HB2	1.96	0.47
1:A:120:VAL:HG22	1:A:125:ILE:HD11	1.96	0.47
1:D:375:GLU:O	1:D:378:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:CG1	1:A:127:HIS:CD2	2.98	0.47
1:D:160:THR:HG22	1:D:276:THR:HG22	1.97	0.47
1:D:290:TYR:CZ	1:D:293:ARG:HD3	2.49	0.47
1:C:199:ARG:HG2	1:C:199:ARG:HH11	1.80	0.47
1:A:102:CYS:O	1:A:129:VAL:HA	2.15	0.47
1:D:160:THR:HG22	1:D:276:THR:CG2	2.45	0.46
1:D:346:PHE:CE2	1:D:350:ILE:HD11	2.50	0.46
1:A:71:ASP:C	1:A:71:ASP:OD1	2.53	0.46
1:D:160:THR:HG22	1:D:276:THR:CB	2.46	0.46
1:D:5:ASN:HB2	1:D:74:ILE:HA	1.96	0.46
1:C:5:ASN:HA	1:C:37:VAL:HB	1.97	0.46
1:D:128:MET:HG3	1:D:129:VAL:N	2.31	0.46
1:A:219:ARG:HG3	1:A:242:VAL:CG2	2.46	0.46
1:B:253:ARG:HH11	1:B:253:ARG:HG2	1.82	0.45
1:C:74:ILE:CG2	1:C:75:HIS:N	2.79	0.45
1:C:357:SER:CB	1:C:358:PRO:CD	2.94	0.45
1:D:90:ALA:CB	1:D:116:MET:HE3	2.46	0.45
1:C:162:LEU:HD22	1:C:265:THR:HG22	1.98	0.45
1:A:176:ARG:HH12	3:A:402:NAI:H2D	1.81	0.45
1:B:292:ARG:NE	1:D:292:ARG:HH21	2.15	0.45
1:B:8:LEU:CD2	1:B:10:GLY:O	2.65	0.45
1:B:4:LEU:HD12	1:B:34:ALA:CB	2.47	0.45
1:B:386:PRO:O	1:B:387:GLN:C	2.55	0.45
1:C:216:ILE:O	1:C:216:ILE:CG2	2.64	0.45
1:D:30:TRP:HA	1:D:32:ALA:N	2.32	0.45
1:A:209:ASN:HB2	1:A:382:TRP:CD2	2.52	0.45
1:C:216:ILE:HG22	1:C:246:ASP:OD2	2.17	0.45
1:C:129:VAL:HG13	1:C:131:PHE:CD2	2.52	0.44
1:B:292:ARG:NE	1:D:292:ARG:NH2	2.65	0.44
1:C:251:MET:C	1:C:252:ILE:HG13	2.38	0.44
1:A:18:HIS:ND1	1:A:78:ASP:OD2	2.50	0.44
1:B:166:SER:OG	1:B:266:ARG:HB3	2.17	0.44
1:C:71:ASP:OD1	1:C:73:ASP:N	2.49	0.44
1:D:87:ALA:CB	1:D:112:GLU:OE2	2.61	0.44
1:D:212:LEU:HD23	1:D:248:VAL:HG23	1.99	0.44
1:C:143:LYS:HG3	1:C:200:TYR:CZ	2.53	0.44
1:C:179:LYS:HG3	1:C:183:GLY:O	2.18	0.44
1:C:189:ASP:OD2	1:C:266:ARG:NH2	2.47	0.44
1:C:160:THR:OG1	1:C:276:THR:HB	2.18	0.44
1:D:25:MET:HE1	1:D:33:PRO:HD2	1.99	0.44
1:D:42:ALA:O	1:D:43:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD22	1:B:10:GLY:O	2.18	0.44
1:B:4:LEU:HD12	1:B:34:ALA:HB1	1.99	0.43
1:B:25:MET:HB3	1:B:26:PRO:HD3	2.00	0.43
1:C:298:VAL:O	1:C:311:ARG:HG2	2.18	0.43
1:A:162:LEU:HD22	1:A:265:THR:HG22	2.00	0.43
1:D:5:ASN:HA	1:D:37:VAL:HB	1.99	0.43
1:D:265:THR:HG21	1:D:268:ALA:HB2	2.00	0.43
1:A:38:ARG:O	1:A:58:PHE:HA	2.18	0.43
1:C:199:ARG:NH2	1:C:362:ASP:OD1	2.51	0.43
1:A:13:PHE:CE2	1:A:14:MET:CE	3.02	0.43
1:A:87:ALA:HA	1:A:116:MET:CG	2.49	0.43
1:D:131:PHE:HE1	1:D:192:THR:HG1	1.66	0.42
1:C:173:LEU:CD2	1:C:178:GLN:HE21	2.32	0.42
1:C:249:MET:HA	1:C:262:VAL:O	2.19	0.42
1:B:209:ASN:HA	1:B:376:SER:OG	2.19	0.42
1:B:287:VAL:HB	1:B:297:GLN:HB2	2.00	0.42
1:C:42:ALA:HA	1:C:62:THR:O	2.19	0.42
1:C:151:ILE:CD1	1:C:286:ILE:HD11	2.49	0.42
1:A:221:LEU:HD21	1:A:240:GLY:HA3	2.01	0.42
1:D:127:HIS:HD2	1:D:360:PHE:HB2	1.83	0.42
1:D:247:GLU:HG3	1:D:265:THR:HB	2.01	0.42
1:D:83:ASN:O	1:D:86:HIS:HB2	2.18	0.42
1:C:8:LEU:HD23	1:C:41:ILE:HD12	2.01	0.42
1:D:69:ILE:HG23	1:D:96:ALA:CB	2.49	0.42
1:D:217:PRO:O	1:D:242:VAL:N	2.36	0.42
1:A:64:ASP:O	1:A:67:SER:HB2	2.20	0.42
1:B:187:LEU:HD13	1:B:248:VAL:HG21	2.00	0.42
1:C:134:ARG:NH2	1:C:357:SER:HB3	2.35	0.42
1:B:290:TYR:CZ	1:B:293:ARG:CD	3.00	0.42
1:D:362:ASP:O	1:D:366:VAL:HG23	2.20	0.41
1:B:69:ILE:O	1:B:69:ILE:HG13	2.19	0.41
1:C:84:HIS:ND1	1:C:181:ILE:HD12	2.34	0.41
1:D:282:THR:HG22	1:D:283:GLU:CG	2.47	0.41
1:B:45:ASN:OD1	1:B:48:LEU:HB2	2.21	0.41
1:C:169:PRO:HB3	1:C:216:ILE:CD1	2.50	0.41
1:C:303:ASP:HB2	1:C:308:ARG:HG3	2.02	0.41
1:D:24:ALA:O	1:D:27:MET:HG3	2.20	0.41
1:D:108:ARG:HH21	1:D:112:GLU:CD	2.24	0.41
1:D:25:MET:N	1:D:26:PRO:CD	2.84	0.41
1:D:71:ASP:O	1:D:74:ILE:HG12	2.21	0.41
1:A:221:LEU:O	1:A:222:GLN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:HIS:CE1	1:C:181:ILE:HD12	2.56	0.41
1:C:104:LYS:HE3	1:C:193:HIS:NE2	2.36	0.41
1:D:69:ILE:HG23	1:D:96:ALA:HB2	2.03	0.41
1:D:116:MET:O	1:D:120:VAL:CG2	2.62	0.41
1:B:368:LEU:HD13	1:B:386:PRO:O	2.21	0.41
1:C:104:LYS:NZ	1:C:189:ASP:O	2.52	0.41
1:C:367:ALA:O	1:C:370:ASP:HB2	2.20	0.41
1:D:189:ASP:CB	1:D:266:ARG:HH21	2.34	0.41
1:A:25:MET:HA	1:A:340:ILE:HG23	2.03	0.40
1:D:275:ILE:HG23	1:D:290:TYR:HB2	2.02	0.40
1:B:194:VAL:HG11	1:B:262:VAL:HG13	2.02	0.40
1:B:290:TYR:CE1	1:B:293:ARG:CG	3.04	0.40
1:C:103:GLU:HA	1:C:130:ALA:HB3	2.03	0.40
1:A:41:ILE:HD13	1:A:52:ALA:HB1	2.03	0.40
1:A:155:LEU:HD22	1:B:215:TRP:CE3	2.57	0.40
1:D:24:ALA:O	1:D:27:MET:CG	2.69	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	368/410 (90%)	349 (95%)	18 (5%)	1 (0%)	41	54
1	B	366/410 (89%)	343 (94%)	21 (6%)	2 (0%)	29	40
1	C	361/410 (88%)	333 (92%)	24 (7%)	4 (1%)	14	19
1	D	360/410 (88%)	325 (90%)	29 (8%)	6 (2%)	9	11
All	All	1455/1640 (89%)	1350 (93%)	92 (6%)	13 (1%)	17	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	C	357	SER
1	C	386	PRO
1	D	380	GLU
1	B	386	PRO
1	C	354	GLY
1	C	358	PRO
1	D	34	ALA
1	D	44	ALA
1	B	293	ARG
1	D	82	PRO
1	D	241	PRO
1	D	386	PRO

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	290/316 (92%)	279 (96%)	11 (4%)	33 50
1	B	288/316 (91%)	273 (95%)	15 (5%)	23 37
1	C	287/316 (91%)	263 (92%)	24 (8%)	11 16
1	D	287/316 (91%)	247 (86%)	40 (14%)	3 4
All	All	1152/1264 (91%)	1062 (92%)	90 (8%)	12 19

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	67	SER
1	A	85	LEU
1	A	104	LYS
1	A	156	SER
1	A	161	TYR
1	A	272	ASN
1	A	342	GLU
1	A	368	LEU

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Mol	Chain	Res	Type
1	A	381	SER
1	A	388	ILE
1	B	48	LEU
1	B	54	ARG
1	B	63	SER
1	B	69	ILE
1	B	104	LYS
1	B	111	GLU
1	B	132	ASN
1	B	156	SER
1	B	161	TYR
1	B	171	SER
1	B	181	ILE
1	B	245	ASP
1	B	275	ILE
1	B	293	ARG
1	B	328	ILE
1	C	4	LEU
1	C	9	ILE
1	C	48	LEU
1	C	62	THR
1	C	74	ILE
1	C	84	HIS
1	C	104	LYS
1	C	114	LYS
1	C	118	ASP
1	C	121	LYS
1	C	123	LYS
1	C	134	ARG
1	C	143	LYS
1	C	151	ILE
1	C	161	TYR
1	C	181	ILE
1	C	199	ARG
1	C	202	VAL
1	C	206	SER
1	C	244	VAL
1	C	259	VAL
1	C	328	ILE
1	C	338	THR
1	C	368	LEU
1	D	4	LEU

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Mol	Chain	Res	Type
1	D	19	SER
1	D	25	MET
1	D	35	LEU
1	D	39	LYS
1	D	54	ARG
1	D	61	SER
1	D	63	SER
1	D	66	ARG
1	D	67	SER
1	D	81	THR
1	D	84	HIS
1	D	86	HIS
1	D	101	ILE
1	D	104	LYS
1	D	111	GLU
1	D	113	SER
1	D	129	VAL
1	D	134	ARG
1	D	143	LYS
1	D	147	GLU
1	D	161	TYR
1	D	179	LYS
1	D	180	SER
1	D	192	THR
1	D	206	SER
1	D	213	SER
1	D	239	LYS
1	D	244	VAL
1	D	261	SER
1	D	275	ILE
1	D	276	THR
1	D	282	THR
1	D	338	THR
1	D	344	HIS
1	D	352	GLU
1	D	355	SER
1	D	357	SER
1	D	376	SER
1	D	387	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	B	209	ASN
1	B	344	HIS
1	C	83	ASN
1	C	132	ASN
1	C	170	ASN
1	C	209	ASN
1	C	297	GLN
1	C	319	HIS
1	D	2	GLN
1	D	83	ASN
1	D	86	HIS
1	D	99	HIS
1	D	267	ASN
1	D	344	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 monosaccharides in this entry.

5.6 Ligand geometry

5 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	4PW	D	401	-	12,12,12	1.66	2 (16%)	18,18,18	2.39	5 (27%)
3	NAI	C	401	-	15,17,48	0.78	0	21,26,73	1.59	4 (19%)
3	NAI	B	401	-	15,17,48	1.20	1 (6%)	21,26,73	1.48	4 (19%)
3	NAI	A	402	-	33,38,48	0.95	2 (6%)	37,58,73	1.97	10 (27%)
2	4PW	A	401	-	12,12,12	1.86	6 (50%)	18,18,18	2.43	6 (33%)

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	4PW	D	401	-	-	-	0/3/2/2
3	NAI	C	401	-	-	3/12/25/72	0/1/1/5
3	NAI	B	401	-	-	3/12/25/72	0/1/1/5
3	NAI	A	402	-	-	5/18/51/72	0/4/4/5
2	4PW	A	401	-	-	-	0/3/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAI	PA-O1A	4.15	1.63	1.50
2	D	401	4PW	O6-C1	3.10	1.48	1.41
2	A	401	4PW	O6-C1	3.08	1.48	1.41
2	D	401	4PW	C4-C5	2.68	1.58	1.53
2	A	401	4PW	C4-C5	2.63	1.58	1.53
2	A	401	4PW	O3-C3	2.58	1.49	1.43
3	A	402	NAI	C5A-C4A	2.26	1.46	1.40
2	A	401	4PW	C6-C5	-2.13	1.48	1.52
2	A	401	4PW	O5-C1	2.12	1.45	1.41
3	A	402	NAI	C2A-N3A	2.08	1.35	1.32
2	A	401	4PW	O1-C2	2.01	1.47	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	4PW	O5-C1-O6	-7.10	100.67	105.98
3	A	402	NAI	C1D-C2D-C3D	6.24	111.14	101.63
2	A	401	4PW	O5-C1-O6	-5.80	101.64	105.98
2	A	401	4PW	O5-C5-C6	-5.26	96.56	101.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	NAI	N3A-C2A-N1A	-4.58	121.51	128.68
2	D	401	4PW	O5-C5-C6	-4.48	97.29	101.55
3	A	402	NAI	O4D-C4D-C3D	4.00	108.25	104.70
3	C	401	NAI	O5B-PA-O3	-3.94	91.42	104.64
2	A	401	4PW	O5-C5-C4	3.93	112.75	108.54
3	B	401	NAI	C1D-C2D-C3D	3.44	106.86	101.63
2	A	401	4PW	C6-C5-C4	-3.30	109.89	113.69
3	B	401	NAI	O5B-PA-O2A	2.96	118.96	107.64
3	B	401	NAI	C1D-O4D-C4D	2.88	114.88	108.16
2	D	401	4PW	O5-C1-C2	2.71	111.79	109.49
3	A	402	NAI	C1D-O4D-C4D	2.58	114.18	108.16
3	A	402	NAI	O4B-C4B-C3B	2.57	110.19	105.11
3	B	401	NAI	O5B-PA-O3	2.54	113.15	104.64
3	C	401	NAI	PN-O3-PA	-2.50	124.24	132.83
3	A	402	NAI	O2D-C2D-C3D	-2.43	106.67	111.27
3	C	401	NAI	O1N-PN-O2N	2.34	123.82	112.24
3	A	402	NAI	N6A-C6A-N1A	2.33	123.40	118.57
3	A	402	NAI	O2A-PA-O1A	2.31	123.64	112.24
2	D	401	4PW	C4-C3-C2	-2.30	106.81	110.82
3	A	402	NAI	C1B-N9A-C4A	-2.25	122.69	126.64
2	A	401	4PW	C4-C3-C2	-2.24	106.92	110.82
2	D	401	4PW	O6-C6-C5	-2.16	100.66	104.52
3	C	401	NAI	C1D-C2D-C3D	2.14	104.89	101.63
2	A	401	4PW	O6-C6-C5	-2.08	100.81	104.52
3	A	402	NAI	C5A-C6A-N6A	-2.06	117.22	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAI	O4B-C4B-C5B-O5B
3	A	402	NAI	C5D-O5D-PN-O2N
3	B	401	NAI	PN-O3-PA-O5B
3	A	402	NAI	C3B-C4B-C5B-O5B
3	B	401	NAI	PN-O3-PA-O2A
3	C	401	NAI	C5D-O5D-PN-O3
3	A	402	NAI	C5D-O5D-PN-O1N
3	C	401	NAI	PN-O3-PA-O2A
3	A	402	NAI	C5D-O5D-PN-O3
3	C	401	NAI	C5D-O5D-PN-O1N
3	B	401	NAI	PN-O3-PA-O1A

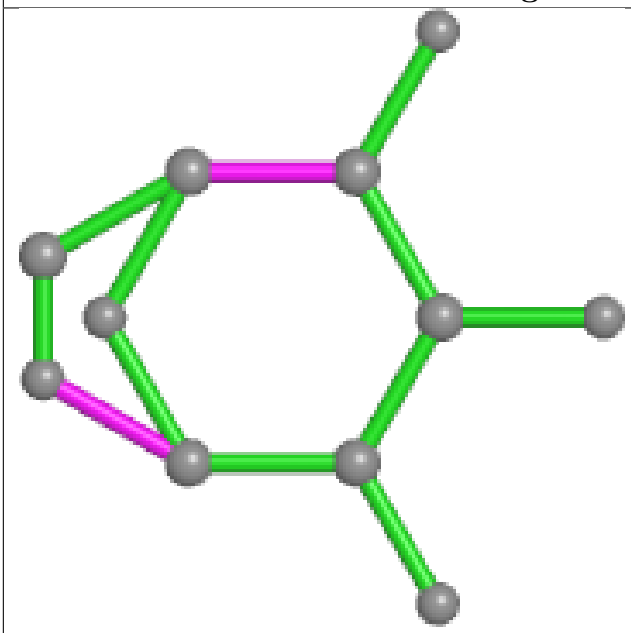
There are no ring outliers.

3 monomers are involved in 5 short contacts:

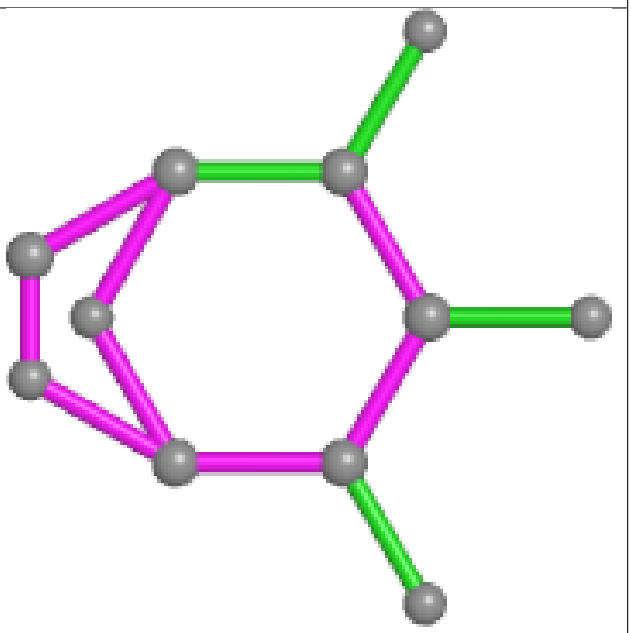
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	4PW	1	0
3	A	402	NAI	3	0
2	A	401	4PW	1	0

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 then 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.

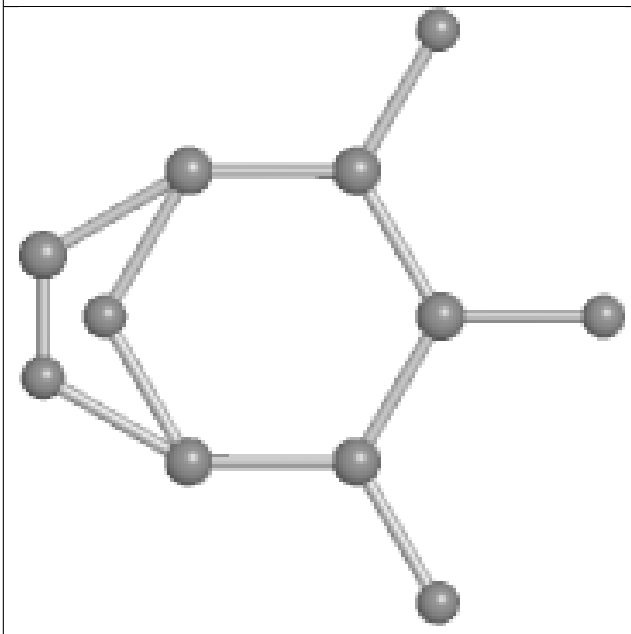
Ligand 4PW D 401



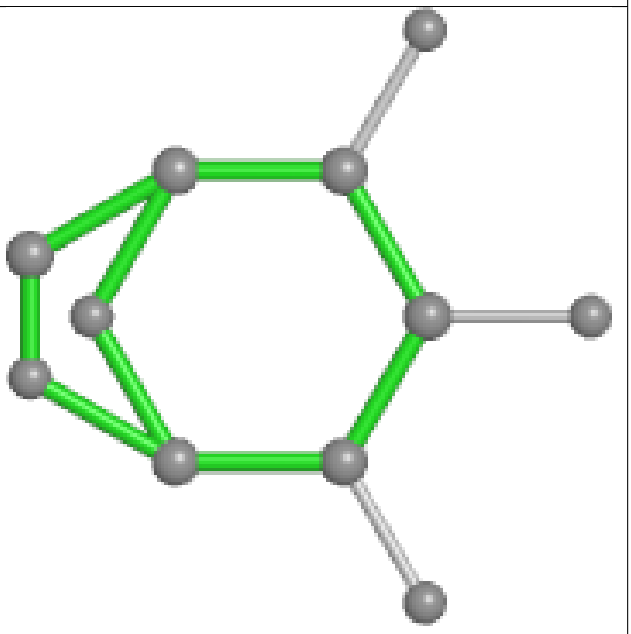
Bond lengths



Bond angles

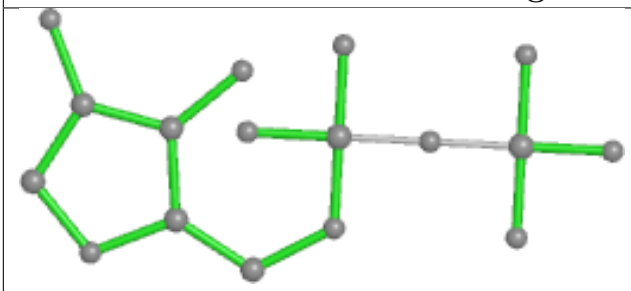


Torsions

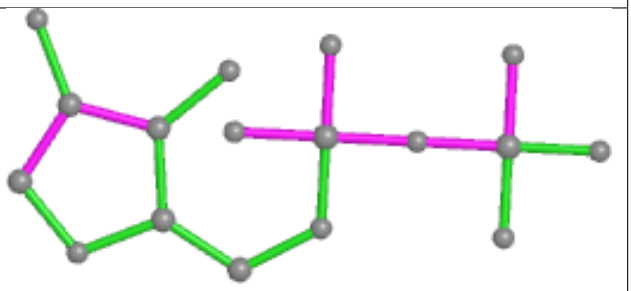


Rings

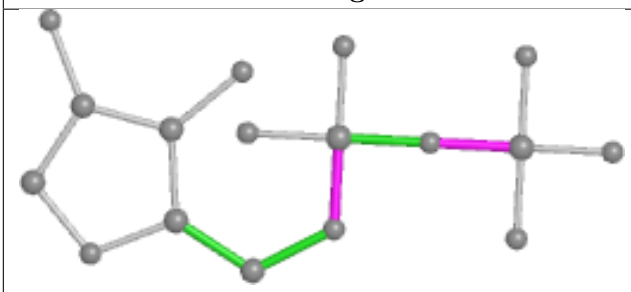
Ligand NAI C 401



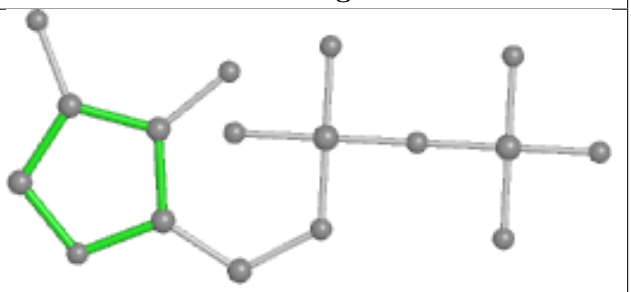
Bond lengths



Bond angles

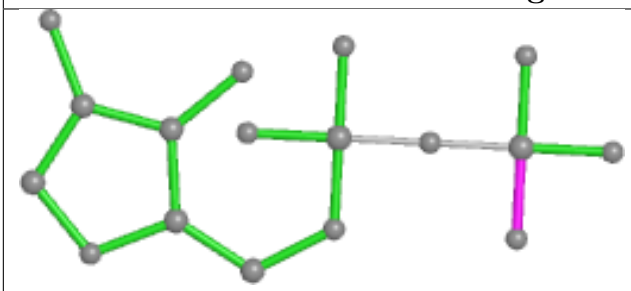


Torsions

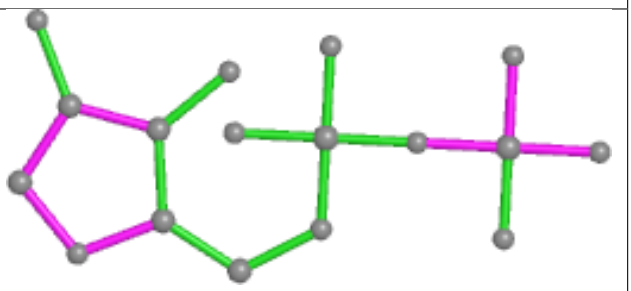


Rings

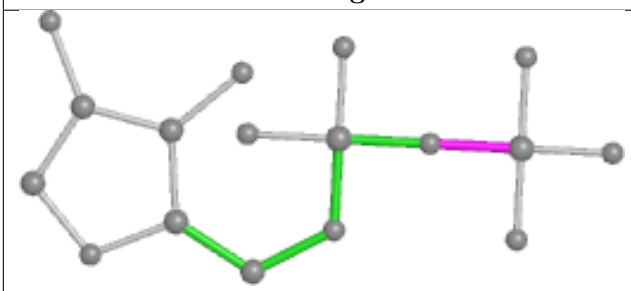
Ligand NAI B 401



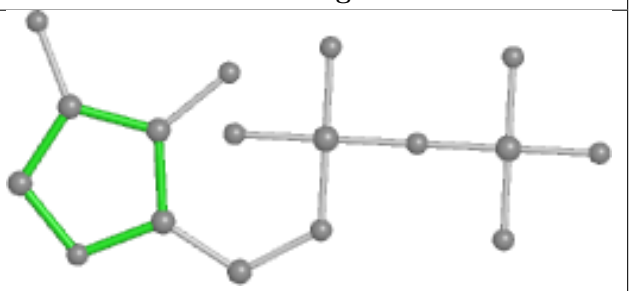
Bond lengths



Bond angles

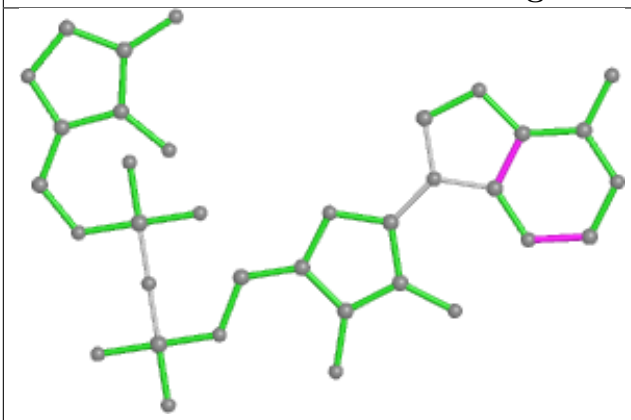


Torsions

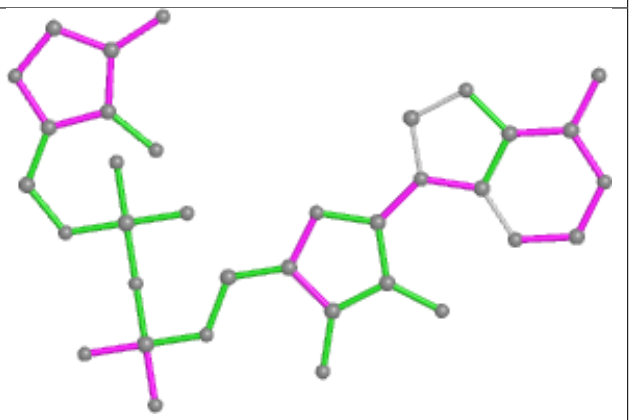


Rings

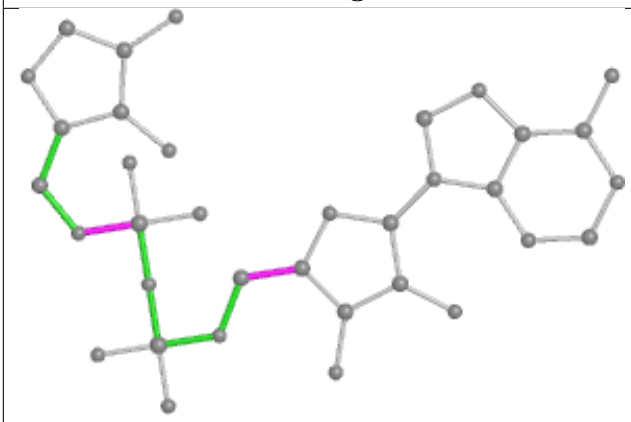
Ligand NAI A 402



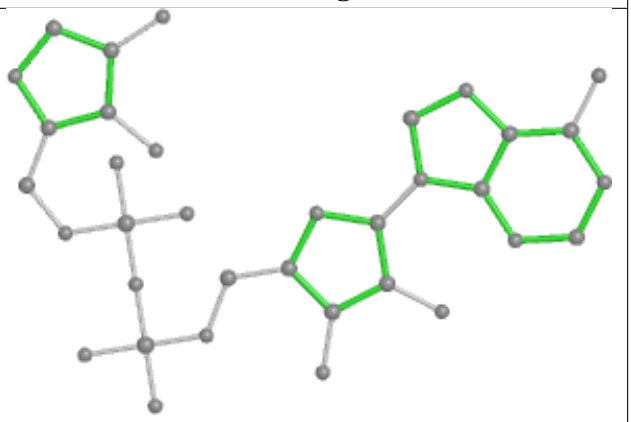
Bond lengths



Bond angles

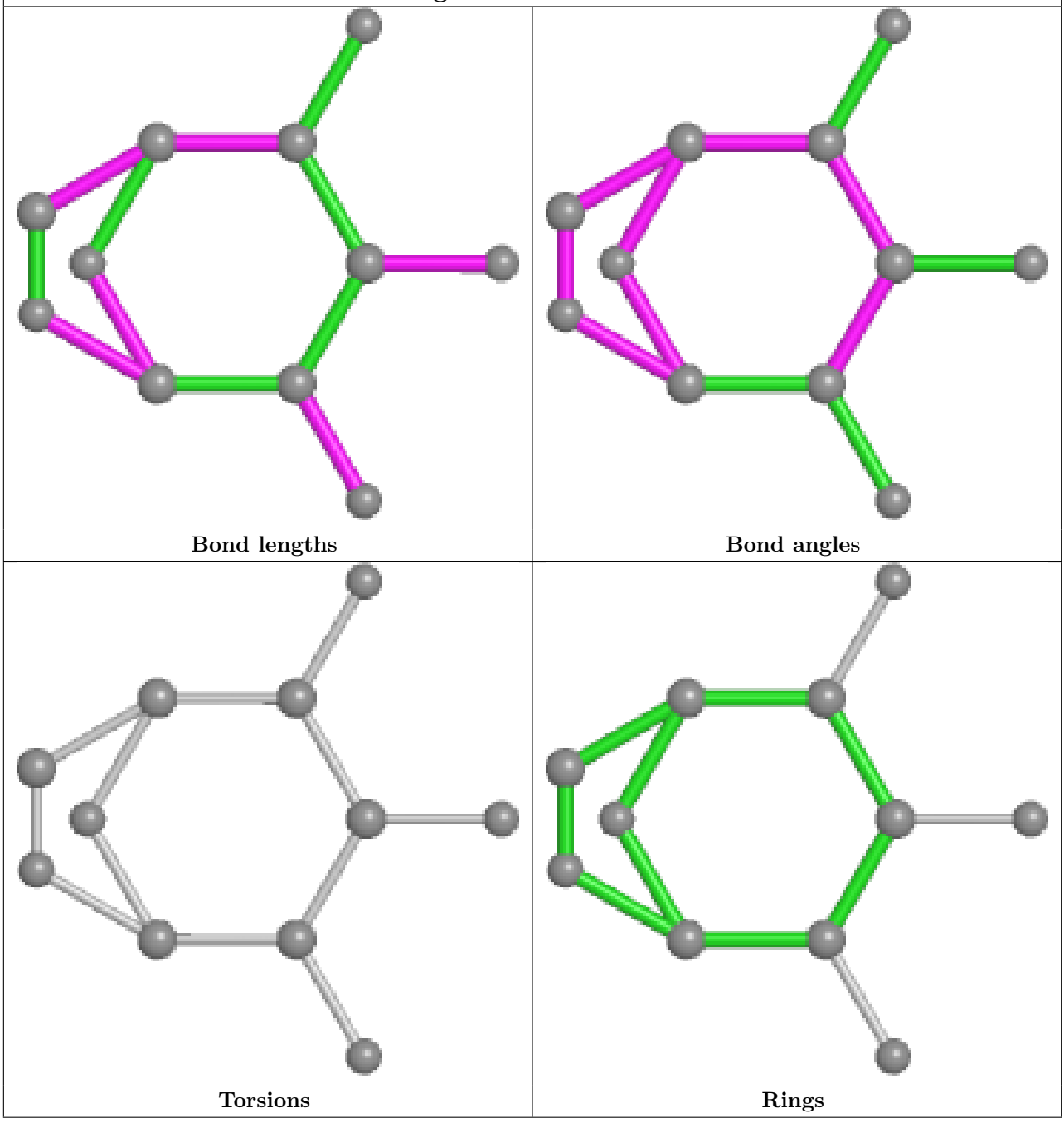


Torsions



Rings

Ligand 4PW 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, 95^{th} 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	372/410 (90%)	0.03	8 (2%) 62 59	37, 51, 71, 106	0
1	B	370/410 (90%)	0.28	20 (5%) 25 23	41, 60, 87, 100	0
1	C	367/410 (89%)	0.48	14 (3%) 40 38	44, 72, 95, 112	0
1	D	366/410 (89%)	0.88	56 (15%) 2 1	45, 77, 106, 134	0
All	All	1475/1640 (89%)	0.42	98 (6%) 18 16	37, 64, 96, 134	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	388	ILE	6.5
1	D	44	ALA	6.3
1	D	216	ILE	6.2
1	D	87	ALA	5.7
1	D	221	LEU	5.4
1	D	91	ILE	4.7
1	D	125	ILE	4.6
1	D	124	ASN	4.4
1	A	223	SER	4.4
1	D	217	PRO	4.3
1	B	221	LEU	4.2
1	A	222	GLN	3.9
1	D	220	PRO	3.8
1	D	115	ALA	3.5
1	D	14	MET	3.5
1	C	378	ALA	3.4
1	D	382	TRP	3.4
1	D	122	ASP	3.4
1	B	387	GLN	3.3
1	D	121	LYS	3.3
1	D	65	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	GLN	3.2
1	D	192	THR	3.2
1	D	276	THR	3.2
1	D	97	GLY	3.2
1	D	149	GLY	3.1
1	D	239	LYS	3.1
1	D	95	GLU	3.0
1	D	191	ALA	3.0
1	B	60	ASN	2.9
1	D	172	PRO	2.8
1	D	167	ALA	2.8
1	C	46	PRO	2.8
1	C	117	TYR	2.7
1	C	276	THR	2.7
1	C	48	LEU	2.7
1	B	222	GLN	2.7
1	D	69	ILE	2.7
1	B	3	ASN	2.7
1	B	44	ALA	2.7
1	D	89	ILE	2.7
1	D	114	LYS	2.6
1	D	364	TYR	2.6
1	D	218	GLU	2.6
1	D	70	ASP	2.6
1	C	69	ILE	2.6
1	A	276	THR	2.5
1	B	33	PRO	2.5
1	B	74	ILE	2.5
1	D	181	ILE	2.5
1	D	275	ILE	2.5
1	B	58	PHE	2.5
1	D	190	ILE	2.5
1	C	220	PRO	2.5
1	C	353	GLY	2.5
1	B	62	THR	2.5
1	A	14	MET	2.5
1	D	85	LEU	2.4
1	B	68	ILE	2.4
1	D	380	GLU	2.4
1	D	262	VAL	2.4
1	B	35	LEU	2.4
1	B	173	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	368	LEU	2.3
1	D	48	LEU	2.3
1	A	169	PRO	2.3
1	D	242	VAL	2.3
1	D	150	ALA	2.3
1	B	275	ILE	2.3
1	D	240	GLY	2.3
1	C	4	LEU	2.3
1	D	77	VAL	2.3
1	D	160	THR	2.3
1	D	253	ARG	2.2
1	D	261	SER	2.2
1	B	239	LYS	2.2
1	B	41	ILE	2.2
1	D	378	ALA	2.2
1	D	169	PRO	2.2
1	D	379	LYS	2.2
1	D	206	SER	2.2
1	C	40	VAL	2.2
1	D	98	LYS	2.2
1	C	382	TRP	2.1
1	A	275	ILE	2.1
1	D	126	VAL	2.1
1	A	79	ILE	2.1
1	C	221	LEU	2.1
1	B	37	VAL	2.1
1	C	386	PRO	2.1
1	B	13	PHE	2.1
1	D	249	MET	2.1
1	C	44	ALA	2.1
1	D	88	GLU	2.1
1	B	46	PRO	2.0
1	D	318	ALA	2.0
1	A	171	SER	2.0
1	D	131	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

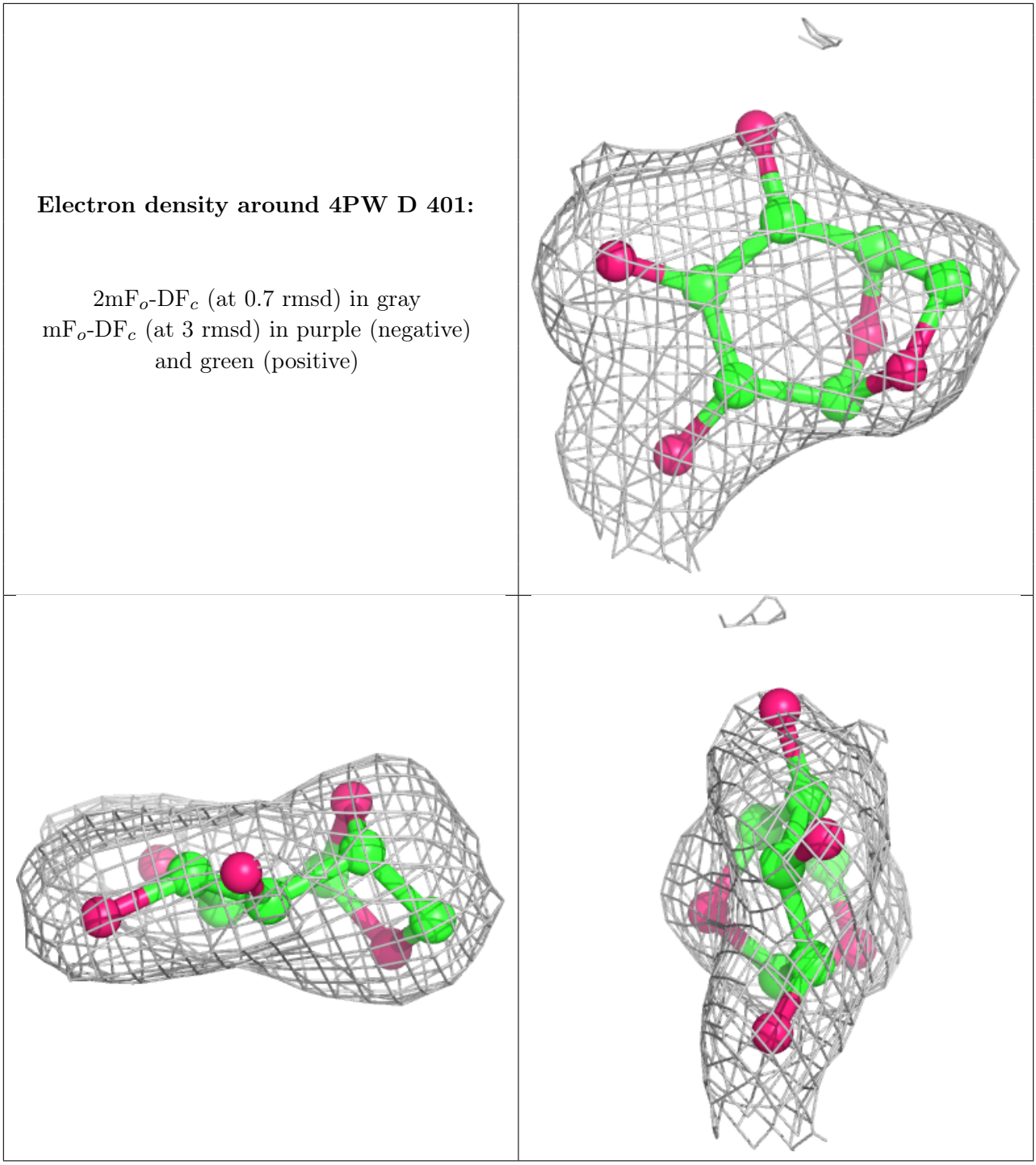
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	4PW	D	401	11/11	0.91	0.17	52,65,72,73	0
2	4PW	A	401	11/11	0.94	0.18	56,63,65,66	0
3	NAI	A	402	35/44	0.94	0.15	35,48,54,57	0
3	NAI	B	401	17/44	0.95	0.13	46,55,68,69	0
3	NAI	C	401	17/44	0.95	0.11	55,65,71,71	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.

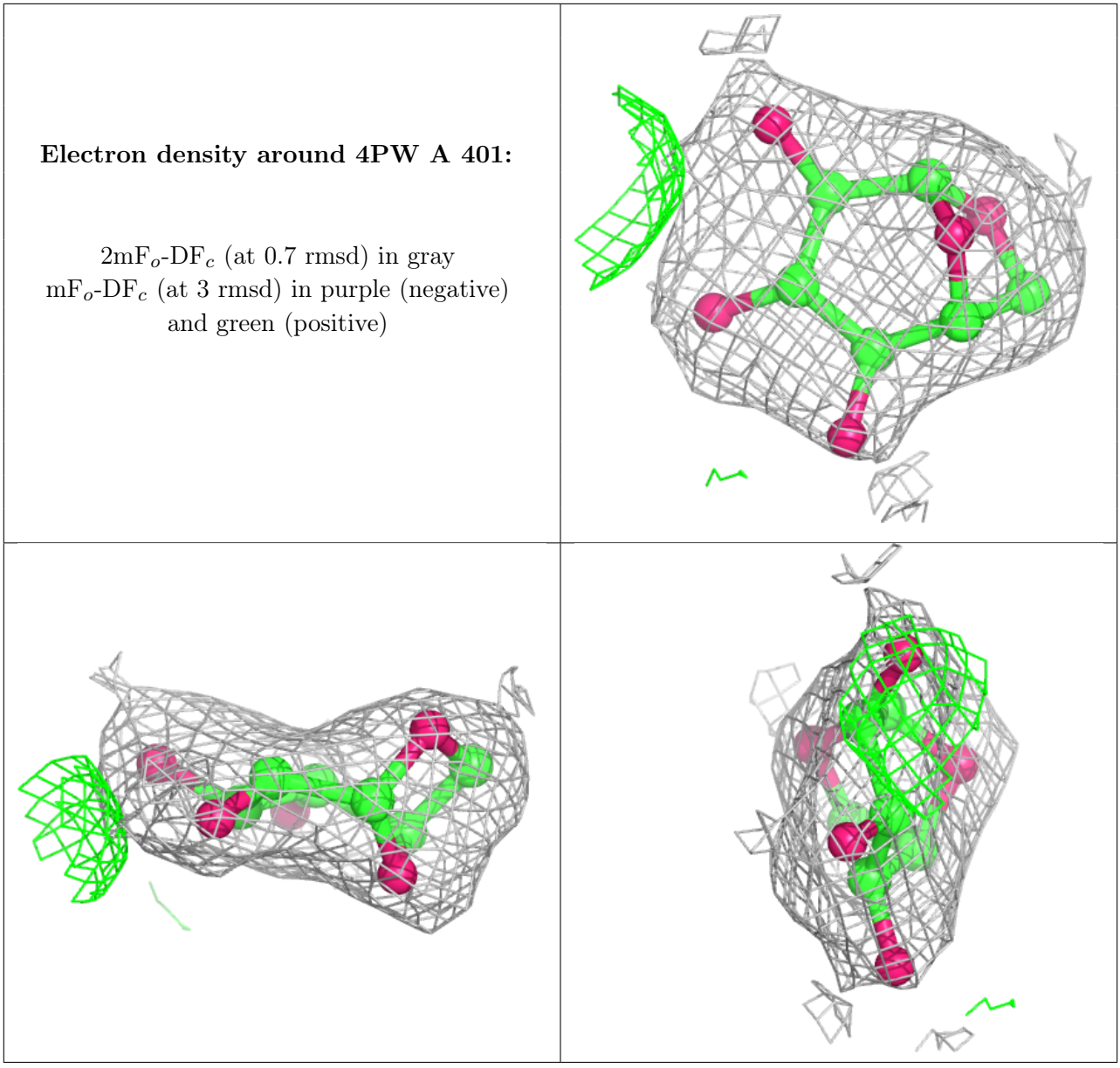
Electron density around 4PW D 401:

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



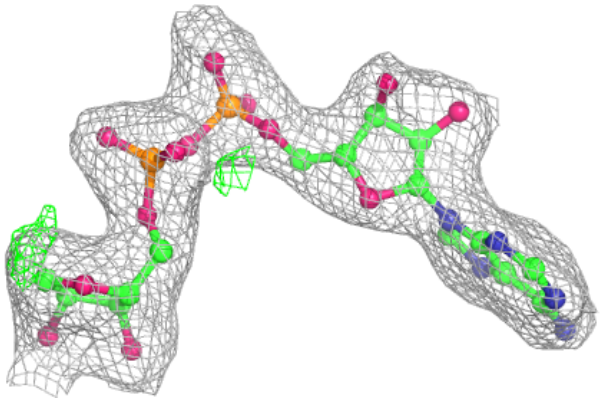
Electron density around 4PW A 401:

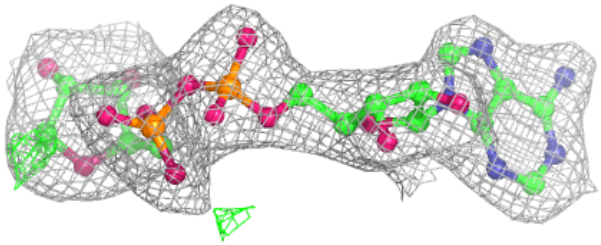
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

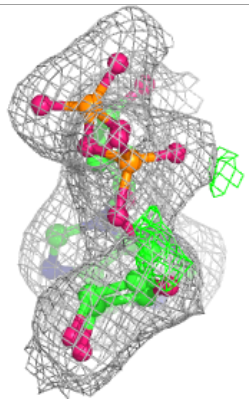


Electron density around NAI A 402:

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

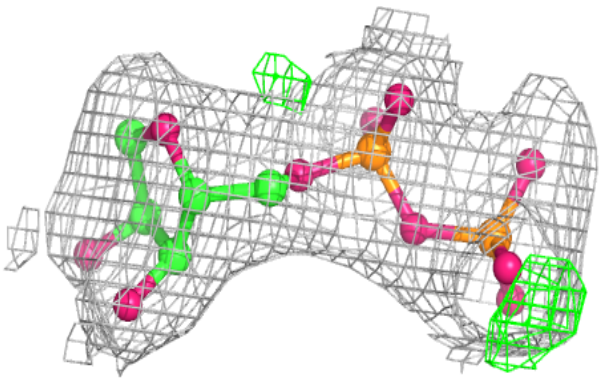


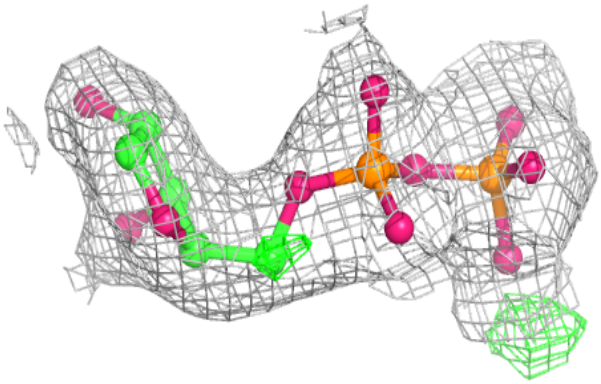


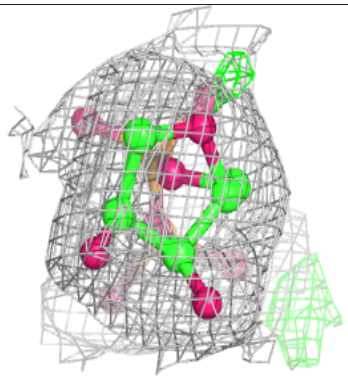


Electron density around NAI B 401:

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

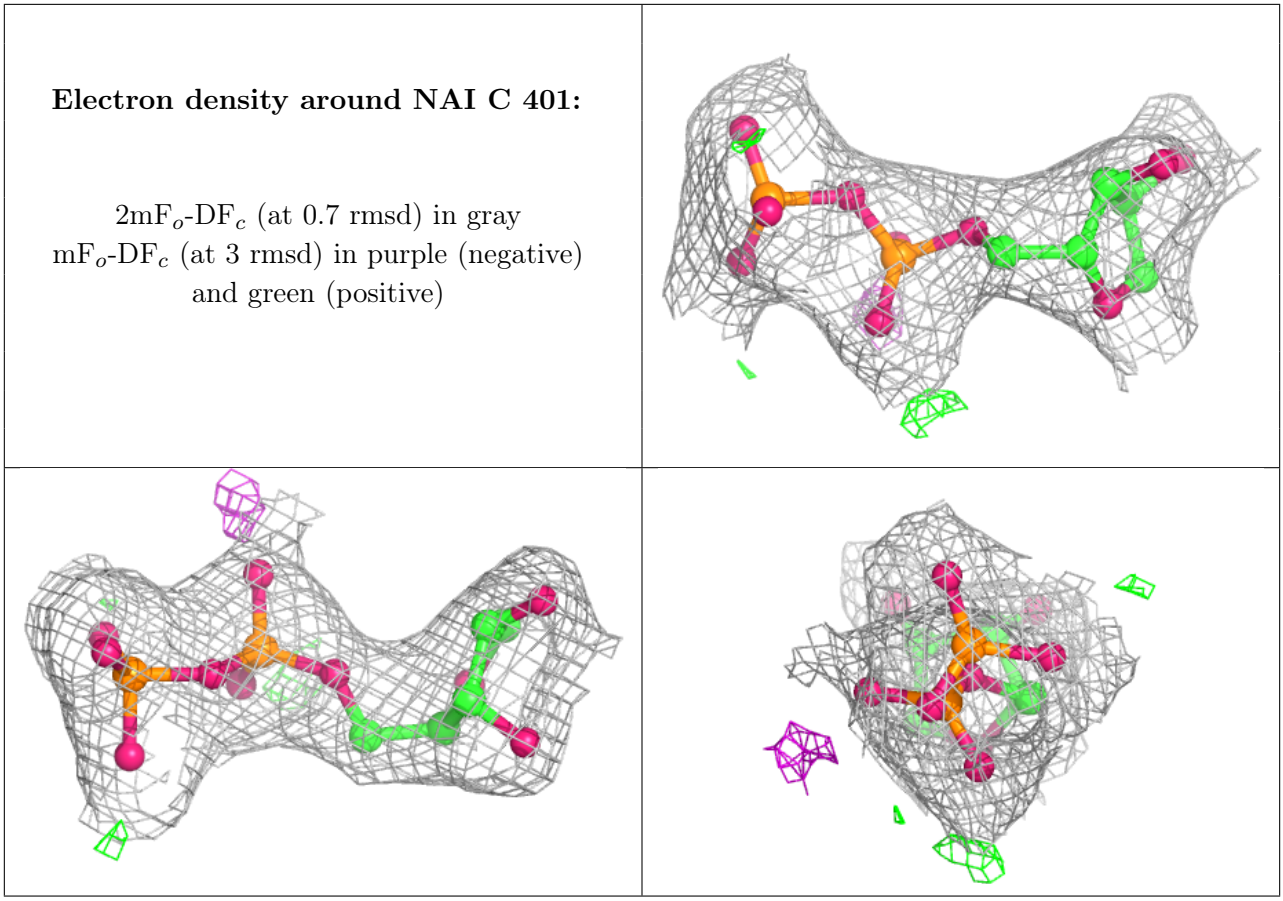






Electron density around NAI C 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.