



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 12:35 PM EDT

PDB ID : 7MYC  
Title : Structure of proline utilization A with the FAD covalently modified by tetrahydrothiophene  
Authors : Tanner, J.J.; Campbell, A.C.  
Deposited on : 2021-05-20  
Resolution : 1.90 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](mailto: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>.

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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	:	2.29
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)	:	2.29

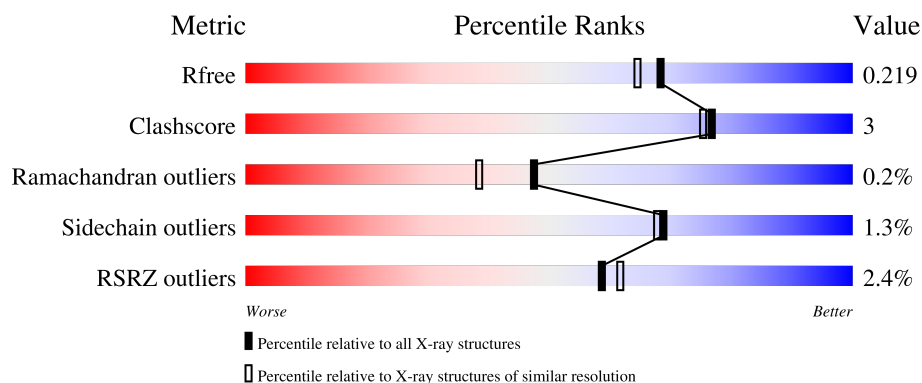
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	1235	
1	B	1235	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19699 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.

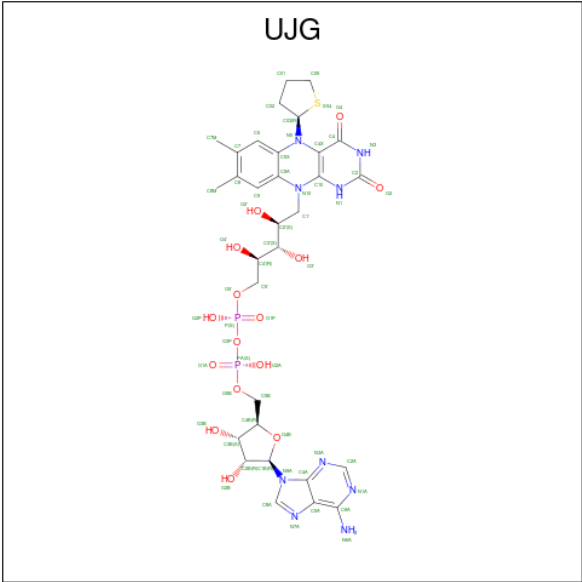
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1216	Total	C	N	O	S	0	4	0
			8947	5634	1600	1680	33			
1	B	1216	Total	C	N	O	S	0	7	0
			8928	5626	1595	1675	32			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl (2R,3S,4S)-5-{7,8-dimethyl-2,4-dioxo-5-[(2R)-tetrahydrothiophen-2-yl]-1,3,4,5-tetrahydrobenzo[g]pteridin-10(2H)-yl}-2,3,4-trihydroxypentyl dihydrogen diphosphate (non-preferred name) (three-letter code: UJG) (formula: C<sub>31</sub>H<sub>41</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



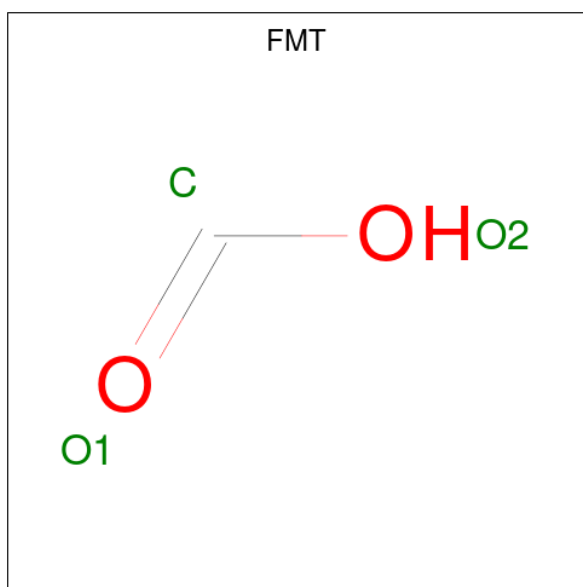
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		

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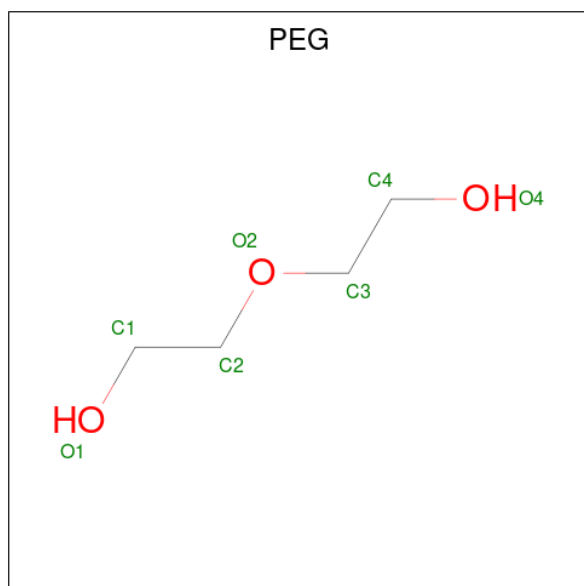
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is water.

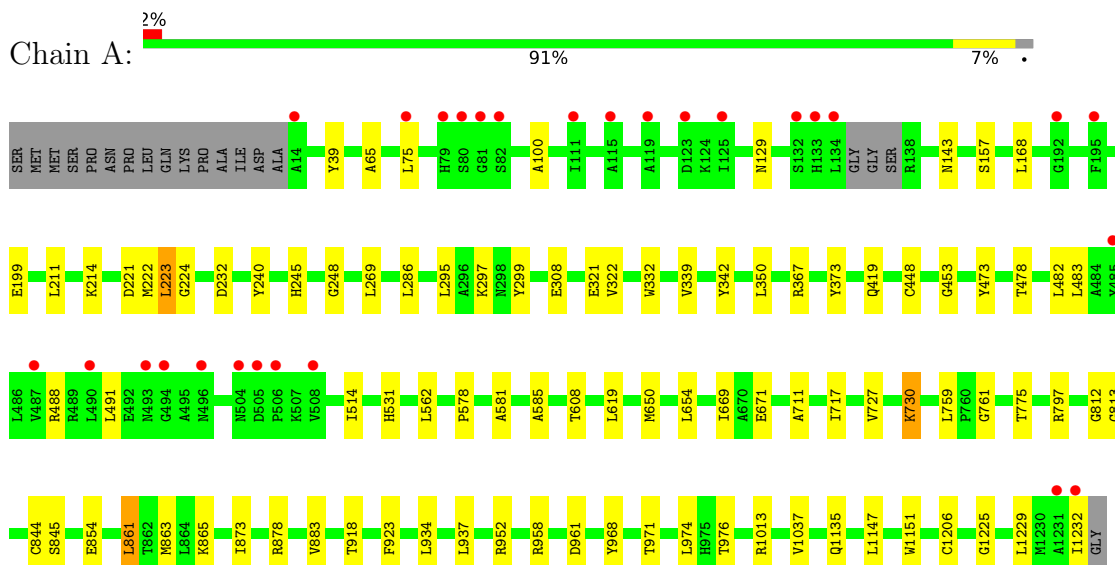
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	777	Total 777	O 777	0	0
9	B	760	Total 760	O 760	0	0



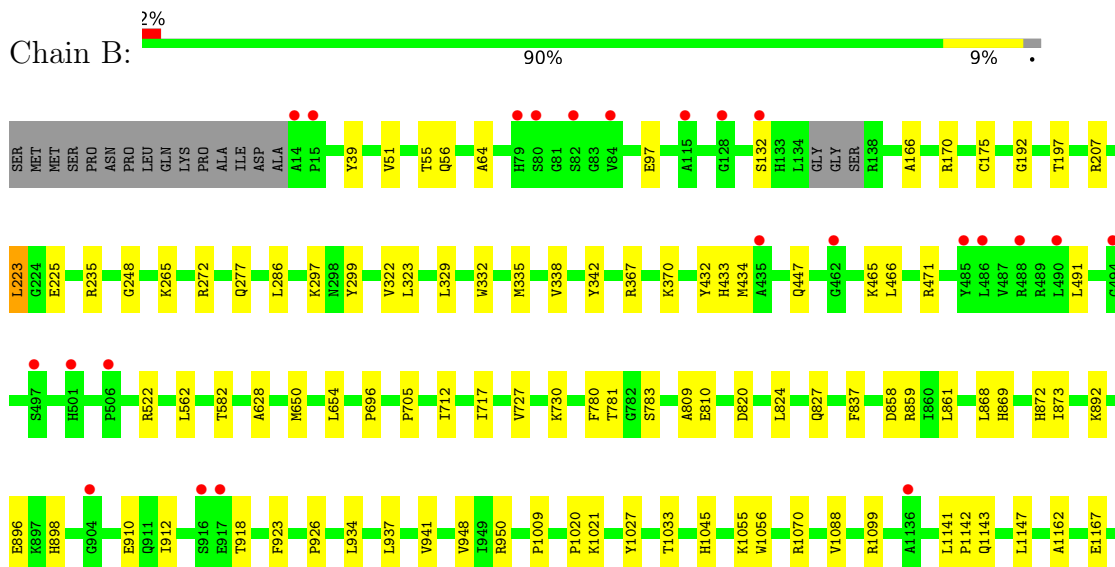
### 3 Residue-property plots [i](#)

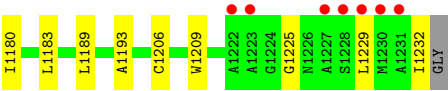
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bifunctional protein PutA



#### • Molecule 1: Bifunctional protein PutA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.93Å 101.50Å 125.74Å 90.00° 106.54° 90.00°	Depositor
Resolution (Å)	45.65 – 1.90 45.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.65-1.90) 99.1 (45.65-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, $R_{free}$	0.176 , 0.219 0.176 , 0.219	Depositor DCC
$R_{free}$ test set	9432 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGE, MG, SO4, UJG, PEG, FMT, NAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.35	0/9117	0.58	0/12419
1	B	0.34	0/9109	0.58	2/12411 (0.0%)
All	All	0.35	0/18226	0.58	2/24830 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	820	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	1141	LEU	CA-CB-CG	5.19	127.24	115.30

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	8947	0	8908	52	0
1	B	8928	0	8895	57	0
2	A	58	0	0	0	0
2	B	58	0	0	1	0
3	A	44	0	27	2	0
3	B	44	0	27	1	0
4	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	0	0	0
5	A	10	0	14	0	0
5	B	20	0	28	3	0
6	A	12	0	4	0	0
6	B	3	0	1	0	0
7	B	1	0	0	0	0
8	B	7	0	10	1	0
9	A	777	0	0	3	0
9	B	760	0	0	5	0
All	All	19699	0	17914	108	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 3.

All (108) 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:55:THR:HG22	1:B:522:ARG:HH22	1.44	0.83
3:A:2202:NAI:H6N	3:A:2202:NAI:H52N	1.68	0.75
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.74	0.68
1:A:578:PRO:HB2	1:A:585:ALA:HB3	1.77	0.65
1:A:1206:CYS:SG	9:A:3035:HOH:O	2.54	0.65
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.80	0.62
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.82	0.62
1:B:873:ILE:HD11	1:B:912:ILE:HD11	1.82	0.62
1:A:199:GLU:HG2	1:A:478:THR:HA	1.85	0.59
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.87	0.57
1:B:51:VAL:O	1:B:55:THR:HG23	2.03	0.56
1:A:223:LEU:HD23	1:A:482:LEU:HA	1.88	0.55
1:B:338:VAL:HG22	1:B:367:ARG:HB3	1.89	0.54
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.38	0.54
1:A:878:ARG:HD2	9:A:2367:HOH:O	2.09	0.52
1:A:222:MET:O	1:A:224:GLY:N	2.42	0.52
1:A:775:THR:HB	1:A:797:ARG:HH22	1.73	0.52
1:A:65:ALA:HB1	1:A:514:ILE:HD12	1.92	0.52
1:B:197:THR:O	1:B:207:ARG:HD2	2.09	0.51
1:B:869:HIS:CE1	1:B:912:ILE:HG22	2.45	0.51
1:A:211:LEU:HD23	1:A:214:LYS:HD3	1.92	0.51
1:A:813:GLY:HA2	1:A:968:TYR:CD1	2.46	0.51
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.93	0.51
1:B:225:GLU:HB3	1:B:265:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:MET:O	1:B:654:LEU:HG	2.11	0.51
1:B:562:LEU:HD11	1:B:654:LEU:HD12	1.93	0.50
1:B:56:GLN:HE22	1:B:434:MET:HB2	1.75	0.50
1:B:582:THR:HG22	5:B:1308:PGE:H12	1.94	0.49
1:B:858:ASP:OD1	1:B:950:ARG:NH1	2.30	0.49
1:B:175:CYS:SG	9:B:2119:HOH:O	2.60	0.49
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.94	0.49
1:B:370:LYS:NZ	2:B:1301:UJG:O1A	2.45	0.48
1:A:918:THR:HB	1:A:923:PHE:CD1	2.49	0.48
1:B:910:GLU:HB2	9:B:1417:HOH:O	2.12	0.48
1:B:837:PHE:CE2	1:B:868:LEU:HD21	2.48	0.48
1:B:1143:GLN:O	1:B:1147:LEU:HG	2.13	0.48
1:A:143:ASN:ND2	1:A:483:LEU:HD13	2.27	0.48
1:B:56:GLN:NE2	1:B:434:MET:HB2	2.29	0.48
1:B:491:LEU:HD21	1:B:1225:GLY:HA3	1.96	0.47
1:A:654:LEU:HD21	1:A:669:ILE:HA	1.96	0.47
1:A:531:HIS:NE2	1:A:1232:ILE:HG23	2.29	0.47
1:A:1229:LEU:HD12	1:A:1232:ILE:HD12	1.96	0.47
1:A:650:MET:O	1:A:654:LEU:HG	2.16	0.46
1:A:730:LYS:NZ	1:A:761:GLY:O	2.43	0.46
1:A:1147:LEU:HD22	1:B:1147:LEU:HD22	1.98	0.46
1:B:1070:ARG:HD3	9:B:1849:HOH:O	2.15	0.46
1:B:1020:PRO:HG2	1:B:1027:TYR:HA	1.97	0.46
1:A:221:ASP:HB2	1:A:473:TYR:CZ	2.51	0.46
1:B:1206:CYS:SG	9:B:2105:HOH:O	2.61	0.46
1:A:491:LEU:CD2	1:A:1225:GLY:HA3	2.47	0.45
1:B:717:ILE:HG12	1:B:727:VAL:HG11	1.98	0.45
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.51	0.45
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.76	0.45
1:A:608:THR:HG21	1:A:759:LEU:HD12	1.97	0.45
1:B:272:ARG:HB3	1:B:277:GLN:HG3	1.99	0.45
1:A:232:ASP:OD2	9:A:2301:HOH:O	2.21	0.45
1:B:861:LEU:HD21	1:B:948:VAL:HG11	1.98	0.45
1:A:717:ILE:HG12	1:A:727:VAL:HG11	1.99	0.45
1:B:1088:VAL:HG21	1:B:1229:LEU:HD11	1.98	0.45
1:A:844:CYS:HB3	3:A:2202:NAI:O7N	2.17	0.44
1:B:824:LEU:HD23	1:B:827:GLN:HG3	1.99	0.44
1:B:1099:ARG:HB3	1:B:1162:ALA:HB1	2.00	0.44
1:A:491:LEU:HD22	1:A:1225:GLY:HA3	2.00	0.44
1:A:812:GLY:HA2	1:A:844:CYS:HB2	1.99	0.44
1:A:974:LEU:HG	1:A:976:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:TYR:HD2	1:A:269:LEU:HD21	1.83	0.43
1:B:323:LEU:HD13	1:B:335:MET:HE3	1.99	0.43
1:A:448:CYS:HB2	1:A:453:GLY:HA3	2.00	0.43
1:A:958:ARG:O	1:A:961:ASP:HB2	2.19	0.43
1:B:783:SER:HB3	3:B:1303:NAI:O4D	2.18	0.43
1:A:1135:GLN:HA	1:A:1151:TRP:CZ2	2.54	0.42
1:B:780:PHE:O	1:B:809:ALA:HA	2.18	0.42
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.53	0.42
1:B:705:PRO:HD3	1:B:781:THR:HB	2.01	0.42
1:A:297:LYS:HA	1:A:332:TRP:CD1	2.55	0.42
1:B:1009:PRO:HB2	1:B:1021:LYS:HD3	2.01	0.42
1:A:100:ALA:HB1	1:A:168:LEU:HB2	2.02	0.42
1:A:863:MET:HE2	1:A:863:MET:HB3	1.73	0.42
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.55	0.42
1:B:582:THR:HA	5:B:1308:PGE:H2	2.00	0.42
1:B:712:ILE:HD13	1:B:781:THR:HG21	2.01	0.42
1:B:898:HIS:CG	1:B:941:VAL:HG21	2.55	0.42
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.86	0.42
1:A:861:LEU:HD22	1:A:865:LYS:HE3	2.01	0.42
1:A:308:GLU:HA	1:A:373:TYR:CE1	2.55	0.41
1:A:562:LEU:HD11	1:A:654:LEU:HD12	2.01	0.41
1:A:854:GLU:HG2	1:A:952:ARG:HE	1.85	0.41
1:B:1180:ILE:HA	1:B:1183:LEU:HG	2.01	0.41
1:A:581:ALA:HB3	1:A:619:LEU:HD13	2.02	0.41
1:B:1189:LEU:HD13	1:B:1209:TRP:HB3	2.02	0.41
1:A:671:GLU:HG3	1:A:711:ALA:HB2	2.02	0.41
1:B:1045[A]:HIS:ND1	5:B:1306:PGE:H6	2.36	0.41
8:B:1307:PEG:H11	9:B:1540:HOH:O	2.19	0.41
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.56	0.41
1:B:97:GLU:OE2	1:B:170:ARG:HD2	2.21	0.41
1:B:447:GLN:HG2	1:B:471:ARG:HB3	2.02	0.41
1:B:192:GLY:O	1:B:207:ARG:NH1	2.52	0.41
1:B:1167:GLU:HA	1:B:1193:ALA:O	2.21	0.41
1:B:432:TYR:CZ	1:B:466:LEU:HD22	2.56	0.41
1:B:628:ALA:HB2	1:B:696:PRO:HG3	2.02	0.41
1:B:918:THR:HB	1:B:923:PHE:CD1	2.56	0.41
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.03	0.41
1:A:297:LYS:HG3	1:A:332:TRP:HB2	2.03	0.40
1:A:1037:VAL:HG11	1:B:166:ALA:HB1	2.03	0.40
1:A:245:HIS:NE2	1:A:295:LEU:HD21	2.36	0.40
1:A:845:SER:HB2	1:A:971:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:LYS:HE3	1:B:896:GLU:OE2	2.22	0.40
1:B:912:ILE:HD11	1:B:926:PRO:HD2	2.03	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	1216/1235 (98%)	1186 (98%)	28 (2%)	2 (0%)	47 38
1	B	1220/1235 (99%)	1188 (97%)	30 (2%)	2 (0%)	47 38
All	All	2436/2470 (99%)	2374 (98%)	58 (2%)	4 (0%)	47 38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	B	223	LEU
1	A	129	ASN
1	B	465	LYS

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	887/951 (93%)	877 (99%)	10 (1%)	73	73
1	B	885/951 (93%)	872 (98%)	13 (2%)	65	62
All	All	1772/1902 (93%)	1749 (99%)	23 (1%)	69	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	157	SER
1	A	321	GLU
1	A	342	TYR
1	A	488	ARG
1	A	730	LYS
1	A	861	LEU
1	A	934	LEU
1	A	937	LEU
1	A	1013	ARG
1	B	39	TYR
1	B	132	SER
1	B	223	LEU
1	B	235	ARG
1	B	342	TYR
1	B	730	LYS
1	B	810	GLU
1	B	859	ARG
1	B	872	HIS
1	B	934	LEU
1	B	937	LEU
1	B	1033	THR
1	B	1232	ILE

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

Mol	Chain	Res	Type
1	B	56	GLN

### 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 ⓘ

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	UJG	B	1301	-	58,64,64	2.49	23 (39%)	66,98,98	2.30	10 (15%)
5	PGE	B	1306	-	9,9,9	0.33	0	8,8,8	0.24	0
4	SO4	A	2203	-	4,4,4	0.15	0	6,6,6	0.18	0
6	FMT	B	1309	-	2,2,2	0.63	0	1,1,1	0.71	0
4	SO4	A	2205	-	4,4,4	0.15	0	6,6,6	0.20	0
6	FMT	A	2210	-	2,2,2	0.66	0	1,1,1	0.54	0
4	SO4	A	2206	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SO4	B	1305	-	4,4,4	0.20	0	6,6,6	0.25	0
6	FMT	A	2208	-	2,2,2	0.68	0	1,1,1	0.53	0
5	PGE	B	1308	-	9,9,9	0.30	0	8,8,8	0.36	0
3	NAI	A	2202	-	42,48,48	1.44	7 (16%)	47,73,73	1.55	10 (21%)
5	PGE	A	2207	-	9,9,9	0.34	0	8,8,8	0.29	0
6	FMT	A	2211	-	2,2,2	0.49	0	1,1,1	0.58	0
3	NAI	B	1303	7	42,48,48	1.43	4 (9%)	47,73,73	1.49	8 (17%)
2	UJG	A	2201	-	58,64,64	2.53	22 (37%)	66,98,98	2.56	11 (16%)
4	SO4	B	1304	-	4,4,4	0.21	0	6,6,6	0.29	0
4	SO4	A	2204	-	4,4,4	0.12	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FMT	A	2209	-	2,2,2	0.68	0	1,1,1	0.50	0
8	PEG	B	1307	-	6,6,6	0.48	0	5,5,5	0.29	0

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	NAI	B	1303	7	-	1/25/72/72	0/5/5/5
2	UJG	B	1301	-	-	8/34/61/61	0/6/7/7
5	PGE	A	2207	-	-	1/7/7/7	-
5	PGE	B	1306	-	-	1/7/7/7	-
5	PGE	B	1308	-	-	1/7/7/7	-
3	NAI	A	2202	-	-	7/25/72/72	0/5/5/5
8	PEG	B	1307	-	-	0/4/4/4	-
2	UJG	A	2201	-	-	9/34/61/61	0/6/7/7

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	UJG	O4-C4	7.67	1.38	1.23
2	A	2201	UJG	O4-C4	7.60	1.38	1.23
2	B	1301	UJG	O2-C2	6.71	1.37	1.23
2	A	2201	UJG	C9-C9A	6.16	1.49	1.39
2	A	2201	UJG	O2-C2	6.06	1.36	1.23
2	A	2201	UJG	C6-C5X	6.04	1.49	1.39
2	A	2201	UJG	C4X-N5	5.56	1.46	1.37
2	B	1301	UJG	C9-C9A	5.51	1.48	1.39
2	B	1301	UJG	C6-C5X	5.43	1.48	1.39
2	B	1301	UJG	C4X-N5	4.91	1.45	1.37
2	A	2201	UJG	C10-N1	4.60	1.45	1.37
2	B	1301	UJG	C10-N1	4.47	1.45	1.37
2	B	1301	UJG	C2-N1	4.32	1.44	1.37
3	B	1303	NAI	PN-O5D	3.95	1.75	1.59
3	B	1303	NAI	PA-O5B	3.94	1.75	1.59
3	A	2202	NAI	PA-O5B	3.66	1.74	1.59
2	A	2201	UJG	C2-N1	3.64	1.43	1.37
3	A	2202	NAI	PN-O5D	3.51	1.73	1.59
2	A	2201	UJG	C10-N10	3.40	1.44	1.38
2	B	1301	UJG	C10-N10	3.31	1.44	1.38
3	B	1303	NAI	O4B-C1B	3.27	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	UJG	C2A-N3A	3.27	1.37	1.32
2	A	2201	UJG	C2B-C1B	-3.13	1.49	1.53
2	A	2201	UJG	C2A-N3A	3.07	1.37	1.32
2	A	2201	UJG	C5X-N5	3.02	1.46	1.42
2	A	2201	UJG	C4X-C4	2.97	1.51	1.43
2	A	2201	UJG	C6A-N6A	2.89	1.44	1.34
2	B	1301	UJG	C9A-N10	2.86	1.46	1.41
2	B	1301	UJG	C9A-C5X	-2.80	1.36	1.40
2	A	2201	UJG	C9A-N10	2.79	1.46	1.41
2	B	1301	UJG	C6A-N6A	2.78	1.44	1.34
2	B	1301	UJG	C2B-C1B	-2.76	1.49	1.53
3	A	2202	NAI	C2B-C1B	2.75	1.57	1.53
2	A	2201	UJG	C9A-C5X	-2.63	1.36	1.40
2	A	2201	UJG	O3B-C3B	-2.54	1.37	1.43
2	B	1301	UJG	C2-N3	2.45	1.41	1.37
2	B	1301	UJG	C4X-C4	2.45	1.49	1.43
2	B	1301	UJG	O2'-C2'	-2.43	1.38	1.43
3	A	2202	NAI	C3B-C4B	2.41	1.59	1.53
3	A	2202	NAI	C6N-N1N	2.41	1.43	1.37
2	A	2201	UJG	O2'-C2'	-2.37	1.38	1.43
2	A	2201	UJG	PA-O5B	-2.33	1.49	1.59
2	B	1301	UJG	C5X-N5	2.30	1.45	1.42
2	B	1301	UJG	PA-O2A	-2.27	1.44	1.55
2	B	1301	UJG	PA-O5B	-2.25	1.50	1.59
2	B	1301	UJG	P-O1P	2.25	1.58	1.50
2	B	1301	UJG	O3B-C3B	-2.19	1.37	1.43
2	A	2201	UJG	PA-O2A	-2.15	1.45	1.55
2	A	2201	UJG	C9-C8	2.10	1.42	1.39
2	A	2201	UJG	P-O1P	2.09	1.58	1.50
3	A	2202	NAI	C2A-N3A	2.09	1.35	1.32
2	B	1301	UJG	O2B-C2B	-2.09	1.38	1.43
2	A	2201	UJG	C2B-C3B	-2.08	1.47	1.53
3	B	1303	NAI	C3B-C4B	2.08	1.58	1.53
2	B	1301	UJG	O3'-C3'	-2.07	1.38	1.43
3	A	2202	NAI	O5D-C5D	-2.04	1.36	1.44

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	UJG	S04-C03-N5	15.51	131.13	112.30
2	B	1301	UJG	S04-C03-N5	9.27	123.56	112.30
2	B	1301	UJG	C02-C03-N5	9.08	123.40	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	UJG	N3A-C2A-N1A	-5.85	119.53	128.68
3	A	2202	NAI	PN-O3-PA	-5.58	113.68	132.83
2	A	2201	UJG	N3A-C2A-N1A	-5.55	120.00	128.68
2	A	2201	UJG	C02-C03-N5	-5.53	107.05	113.24
3	B	1303	NAI	PN-O3-PA	-5.17	115.10	132.83
2	A	2201	UJG	C4X-C4-N3	5.06	119.90	110.99
2	B	1301	UJG	C4X-C4-N3	4.97	119.75	110.99
2	B	1301	UJG	C4-N3-C2	-4.80	119.42	126.34
2	A	2201	UJG	C4-N3-C2	-4.48	119.88	126.34
2	B	1301	UJG	C01-C02-C03	4.13	111.39	104.15
2	A	2201	UJG	C01-C02-C03	3.71	110.66	104.15
3	B	1303	NAI	C3N-C2N-N1N	-3.48	118.13	123.10
2	B	1301	UJG	N3-C2-N1	3.44	121.33	115.80
2	A	2201	UJG	N3-C2-N1	3.29	121.10	115.80
2	B	1301	UJG	O4-C4-C4X	-3.29	119.47	127.54
3	B	1303	NAI	O5D-PN-O2N	-3.06	97.10	109.07
3	A	2202	NAI	PN-O5D-C5D	-3.05	103.80	121.68
3	A	2202	NAI	O2A-PA-O1A	2.97	126.94	112.24
3	A	2202	NAI	O1N-PN-O2N	2.95	126.82	112.24
3	A	2202	NAI	O5D-PN-O2N	-2.68	98.59	109.07
3	B	1303	NAI	O2A-PA-O1A	2.48	124.50	112.24
3	B	1303	NAI	C2D-C3D-C4D	-2.47	97.85	102.64
3	B	1303	NAI	O1N-PN-O2N	2.42	124.21	112.24
3	A	2202	NAI	C5D-C4D-C3D	-2.37	106.30	115.18
2	A	2201	UJG	O2A-PA-O5B	-2.37	96.75	107.75
3	A	2202	NAI	C1B-N9A-C4A	-2.35	122.52	126.64
3	B	1303	NAI	PN-O5D-C5D	-2.32	108.09	121.68
3	A	2202	NAI	PA-O5B-C5B	-2.22	108.66	121.68
2	A	2201	UJG	O4-C4-C4X	-2.22	122.11	127.54
3	A	2202	NAI	O7N-C7N-N7N	-2.21	117.72	122.88
3	A	2202	NAI	C3N-C2N-N1N	-2.17	120.00	123.10
3	B	1303	NAI	O7N-C7N-N7N	-2.16	117.82	122.88
2	A	2201	UJG	C1B-N9A-C4A	-2.16	122.85	126.64
2	A	2201	UJG	O2P-P-O5'	-2.05	98.23	107.75
2	B	1301	UJG	C1B-N9A-C4A	-2.04	123.06	126.64
2	B	1301	UJG	C4A-C5A-N7A	-2.03	107.28	109.40

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	UJG	C02-C03-N5-C5X

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Mol	Chain	Res	Type	Atoms
2	B	1301	UJG	S04-C03-N5-C4X
2	B	1301	UJG	C02-C03-N5-C5X
3	A	2202	NAI	C5B-O5B-PA-O1A
3	A	2202	NAI	C3D-C4D-C5D-O5D
3	A	2202	NAI	O4D-C1D-N1N-C2N
3	A	2202	NAI	C2N-C3N-C7N-N7N
3	B	1303	NAI	O4D-C1D-N1N-C2N
5	B	1308	PGE	O2-C3-C4-O3
3	A	2202	NAI	O4D-C4D-C5D-O5D
2	A	2201	UJG	C2'-C3'-C4'-O4'
5	A	2207	PGE	O1-C1-C2-O2
2	A	2201	UJG	O3'-C3'-C4'-O4'
2	A	2201	UJG	PA-O3P-P-O1P
2	B	1301	UJG	PA-O3P-P-O1P
2	A	2201	UJG	O3'-C3'-C4'-C5'
2	A	2201	UJG	C2'-C3'-C4'-C5'
2	A	2201	UJG	S04-C03-N5-C5X
2	B	1301	UJG	S04-C03-N5-C5X
5	B	1306	PGE	C6-C5-O3-C4
3	A	2202	NAI	C5B-O5B-PA-O3
2	B	1301	UJG	C2'-C3'-C4'-O4'
3	A	2202	NAI	C5B-O5B-PA-O2A
2	A	2201	UJG	PA-O3P-P-O2P
2	B	1301	UJG	PA-O3P-P-O2P
2	B	1301	UJG	O3'-C3'-C4'-O4'
2	A	2201	UJG	S04-C03-N5-C4X
2	B	1301	UJG	O3'-C3'-C4'-C5'

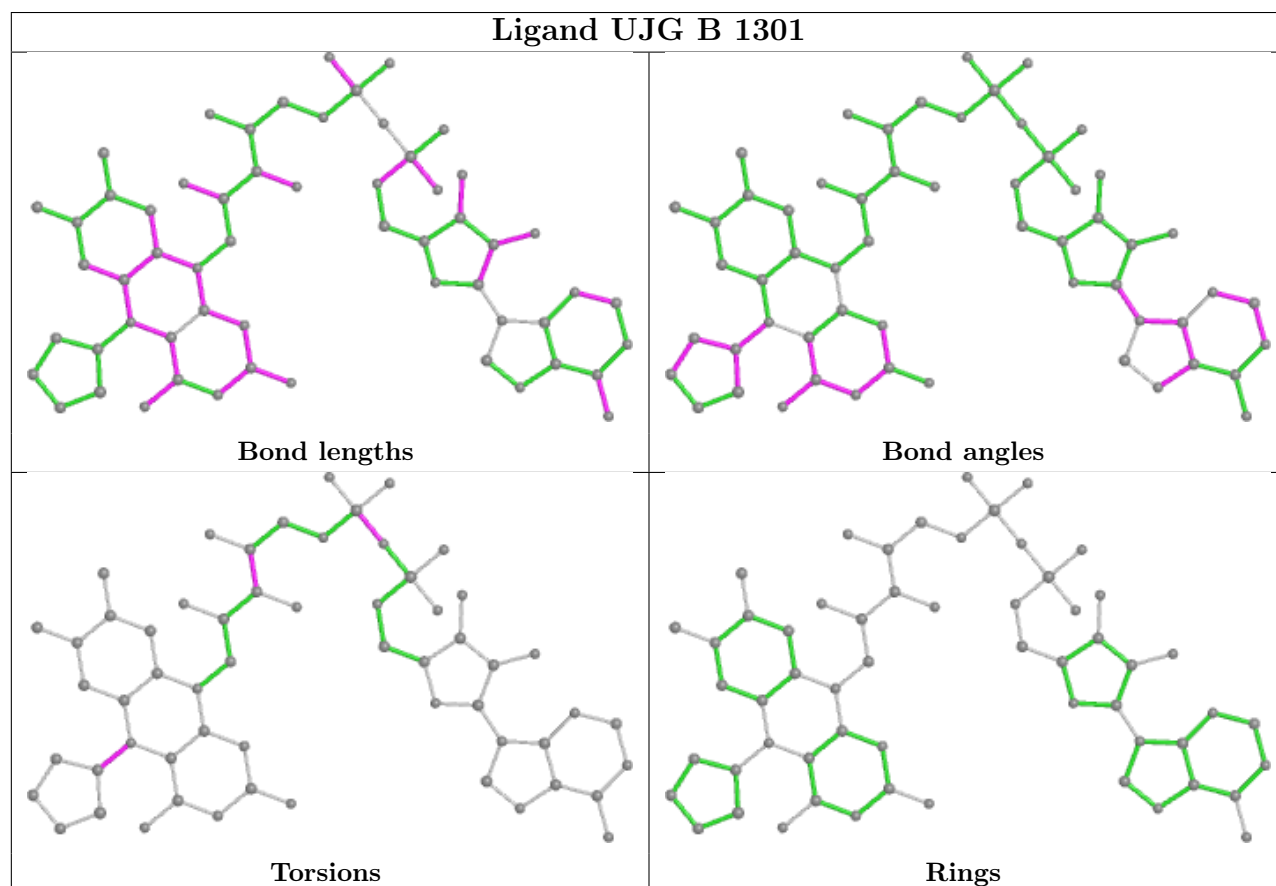
There are no ring outliers.

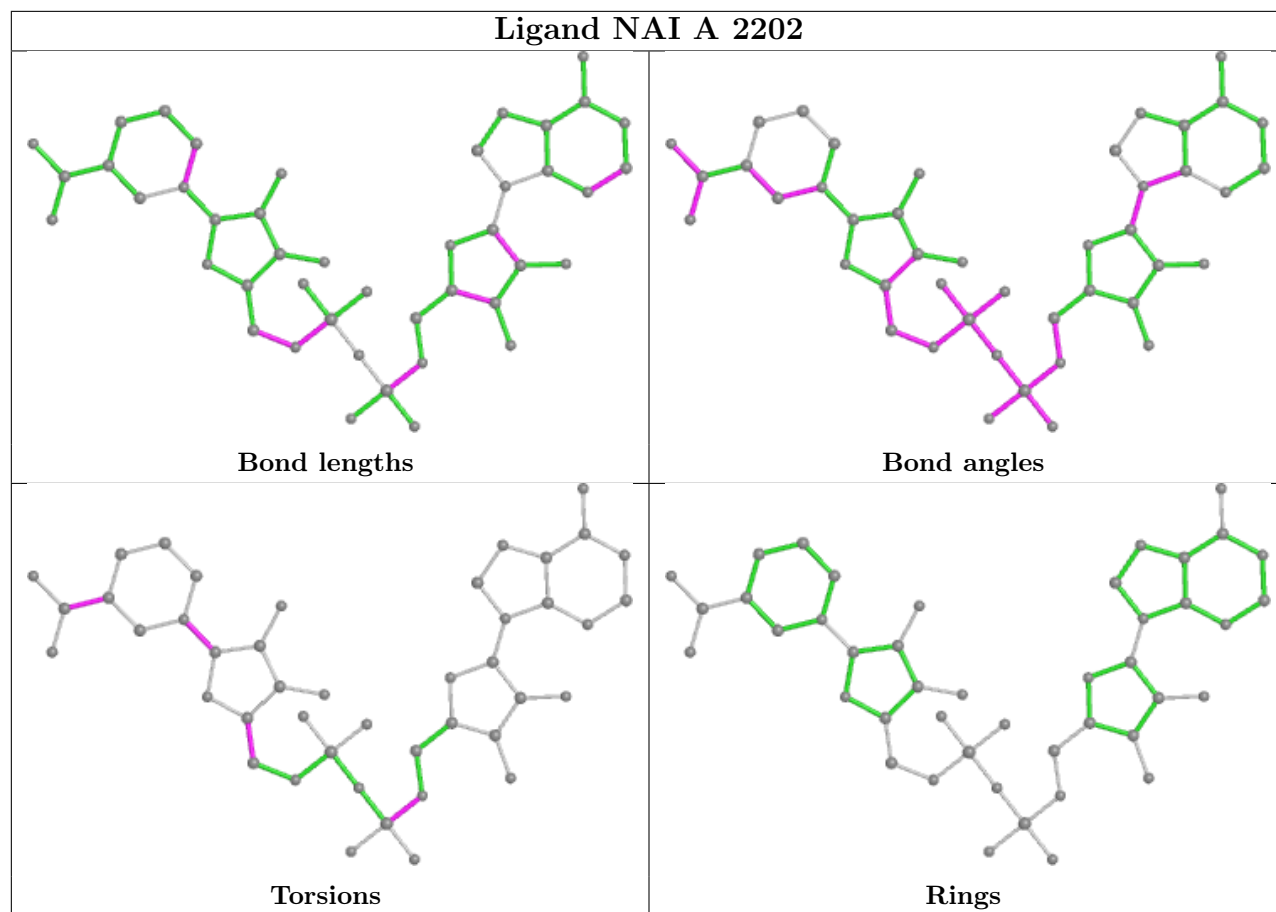
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	UJG	1	0
5	B	1306	PGE	1	0
5	B	1308	PGE	2	0
3	A	2202	NAI	2	0
3	B	1303	NAI	1	0
8	B	1307	PEG	1	0

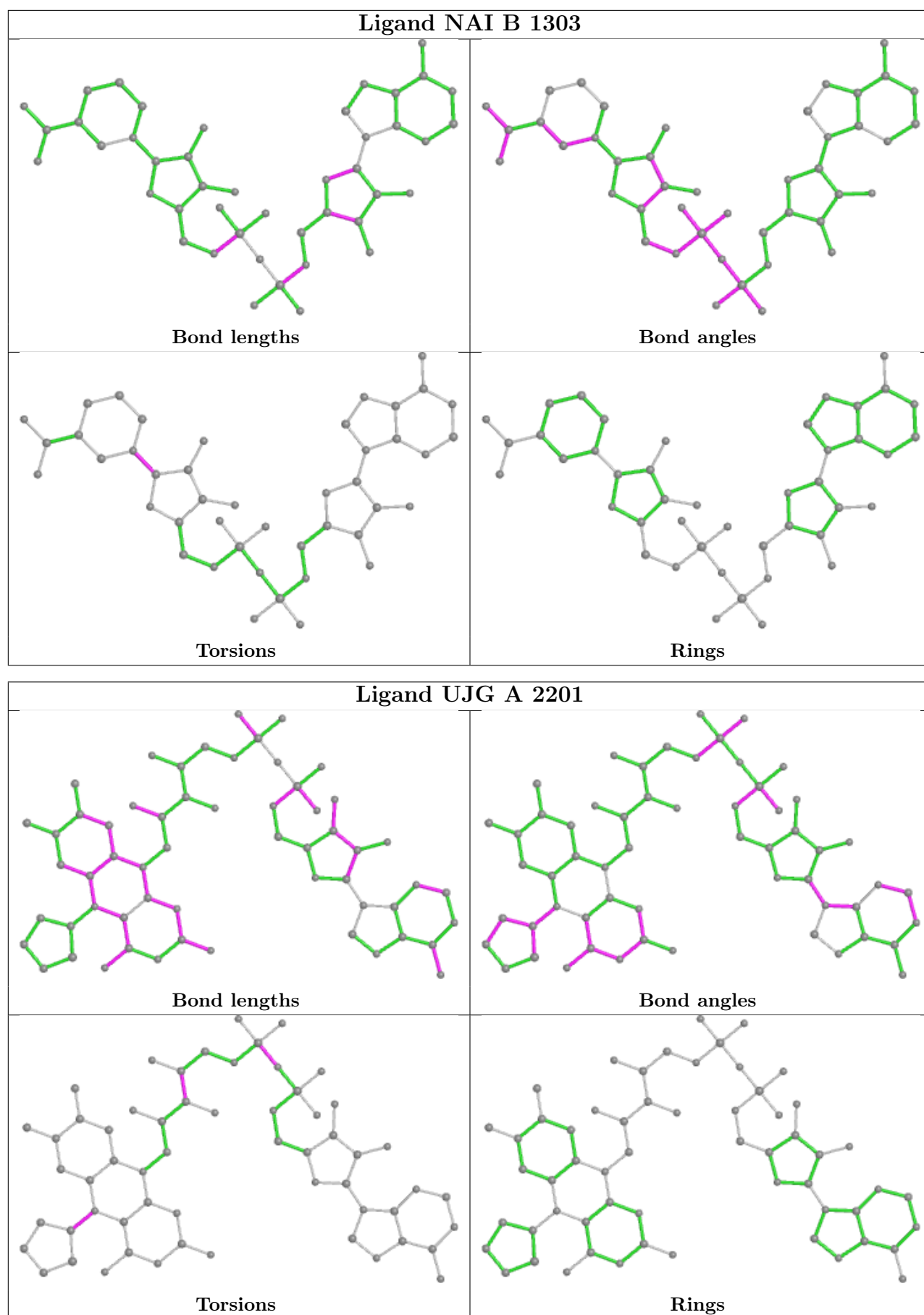
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1216/1235 (98%)	-0.35	28 (2%) 60 63	15, 25, 54, 95	0
1	B	1216/1235 (98%)	-0.25	30 (2%) 57 60	14, 26, 58, 93	0
All	All	2432/2470 (98%)	-0.30	58 (2%) 59 62	14, 26, 56, 95	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1227	ALA	6.0
1	A	81	GLY	5.9
1	A	79	HIS	5.7
1	A	485	TYR	5.0
1	B	128	GLY	4.9
1	B	506	PRO	4.8
1	A	493	ASN	4.7
1	B	1231	ALA	4.4
1	A	506	PRO	4.4
1	A	80	SER	4.3
1	A	490	LEU	4.0
1	B	1230	MET	3.9
1	B	485	TYR	3.9
1	A	119	ALA	3.8
1	A	111	ILE	3.8
1	A	134	LEU	3.7
1	B	14	ALA	3.6
1	B	82	SER	3.5
1	A	1231	ALA	3.3
1	A	195	PHE	3.2
1	B	494	GLY	3.2
1	B	1223	ALA	3.1
1	B	1229	LEU	2.9
1	B	490	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	133	HIS	2.8
1	B	1228	SER	2.8
1	A	82	SER	2.8
1	B	15	PRO	2.7
1	B	488	ARG	2.7
1	B	486	LEU	2.7
1	B	916	SER	2.7
1	B	462	GLY	2.7
1	A	125	ILE	2.6
1	B	132	SER	2.6
1	B	1222	ALA	2.6
1	B	1136	ALA	2.6
1	A	75	LEU	2.4
1	A	505	ASP	2.4
1	A	123	ASP	2.3
1	B	84	VAL	2.3
1	A	192	GLY	2.3
1	A	1232	ILE	2.3
1	B	80	SER	2.3
1	B	79	HIS	2.3
1	B	115	ALA	2.2
1	B	917	GLU	2.2
1	B	501	HIS	2.2
1	A	494	GLY	2.2
1	A	14	ALA	2.1
1	B	904	GLY	2.1
1	A	132	SER	2.1
1	A	487	VAL	2.1
1	B	435	ALA	2.1
1	A	115	ALA	2.1
1	A	504	ASN	2.1
1	A	508	VAL	2.0
1	A	496	ASN	2.0
1	B	497	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

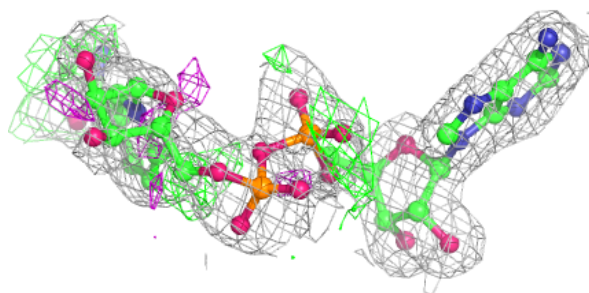
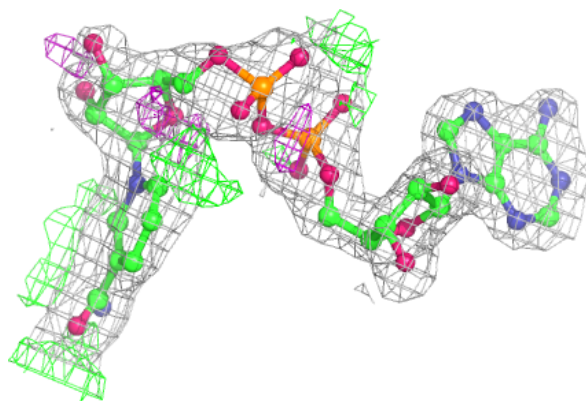
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	FMT	A	2208	3/3	0.74	0.13	51,51,54,55	0
5	PGE	B	1308	10/10	0.89	0.15	52,54,61,63	0
3	NAI	A	2202	44/44	0.92	0.12	25,36,64,66	0
4	SO4	A	2205	5/5	0.92	0.16	63,69,73,75	0
6	FMT	A	2209	3/3	0.92	0.12	40,40,42,44	0
6	FMT	A	2210	3/3	0.92	0.10	46,46,47,50	0
4	SO4	A	2206	5/5	0.93	0.21	78,78,79,87	0
5	PGE	B	1306	10/10	0.93	0.10	23,40,47,47	0
4	SO4	A	2204	5/5	0.93	0.11	65,69,75,82	0
8	PEG	B	1307	7/7	0.93	0.10	43,45,49,51	0
4	SO4	A	2203	5/5	0.94	0.15	37,43,48,60	5
5	PGE	A	2207	10/10	0.94	0.11	28,45,53,54	0
2	UJG	B	1301	58/58	0.95	0.09	18,27,42,52	5
3	NAI	B	1303	44/44	0.96	0.09	18,24,31,33	0
6	FMT	A	2211	3/3	0.96	0.09	18,18,27,33	0
6	FMT	B	1309	3/3	0.96	0.13	27,27,35,36	0
2	UJG	A	2201	58/58	0.96	0.08	18,28,40,42	5
7	MG	B	1302	1/1	0.99	0.05	28,28,28,28	0
4	SO4	B	1304	5/5	0.99	0.06	21,21,24,25	0
4	SO4	B	1305	5/5	1.00	0.06	22,24,27,27	0

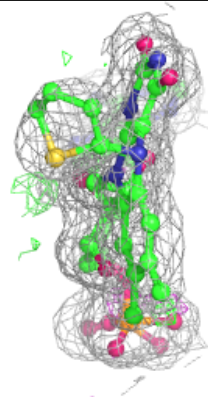
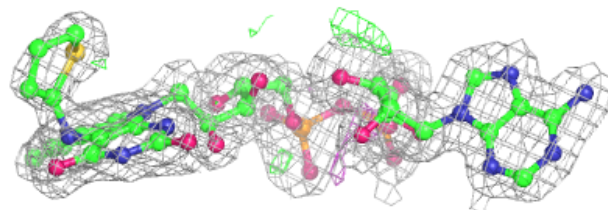
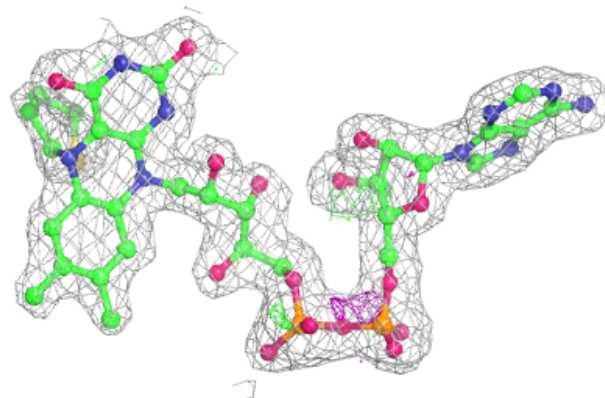
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAI A 2202:**

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

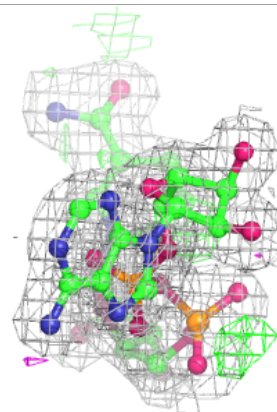
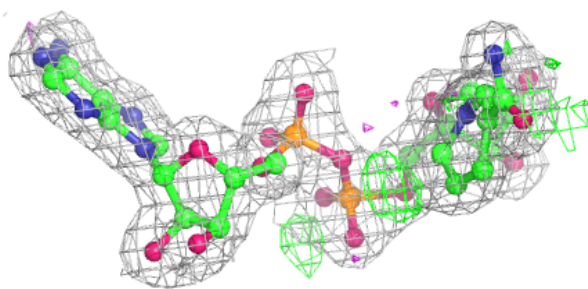
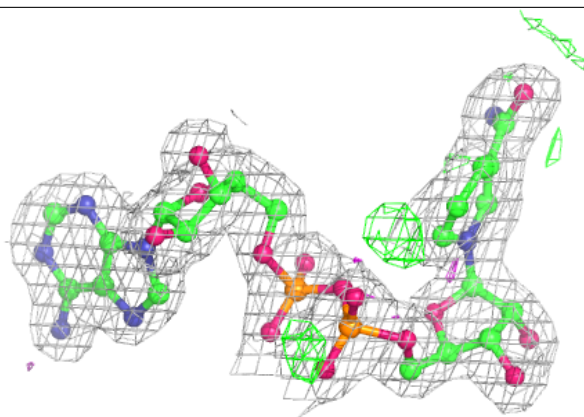
**Electron density around UJG B 1301:**

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

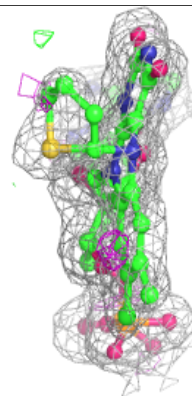
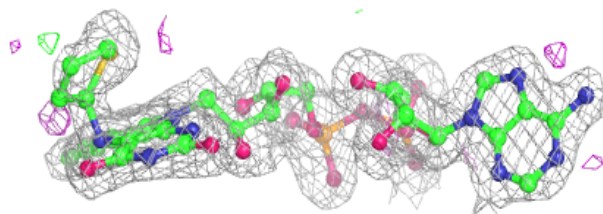
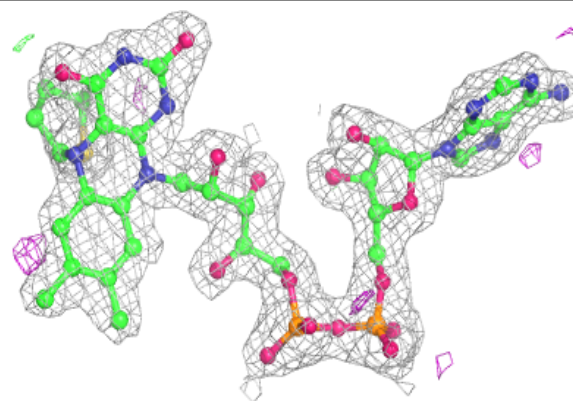


**Electron density around NAI B 1303:**

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

**Electron density around UJG A 2201:**

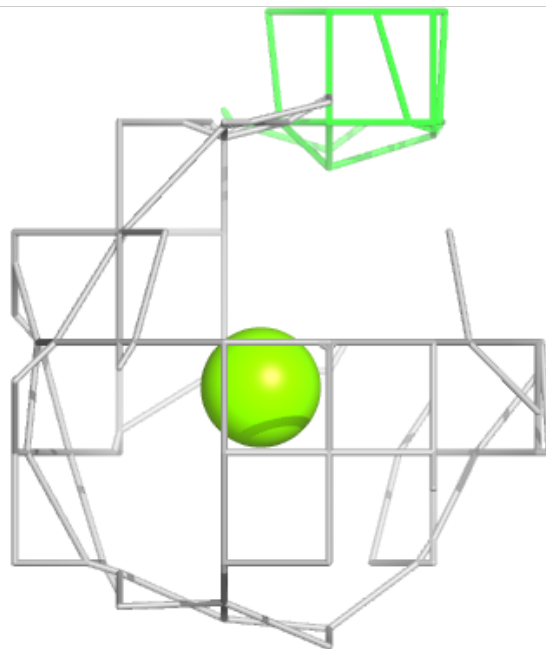
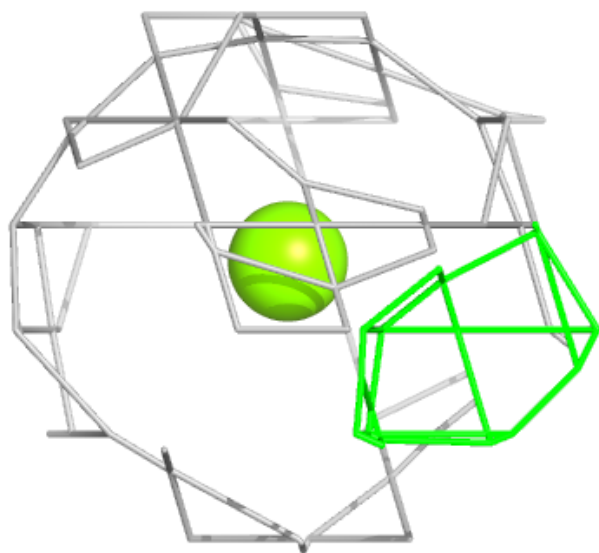
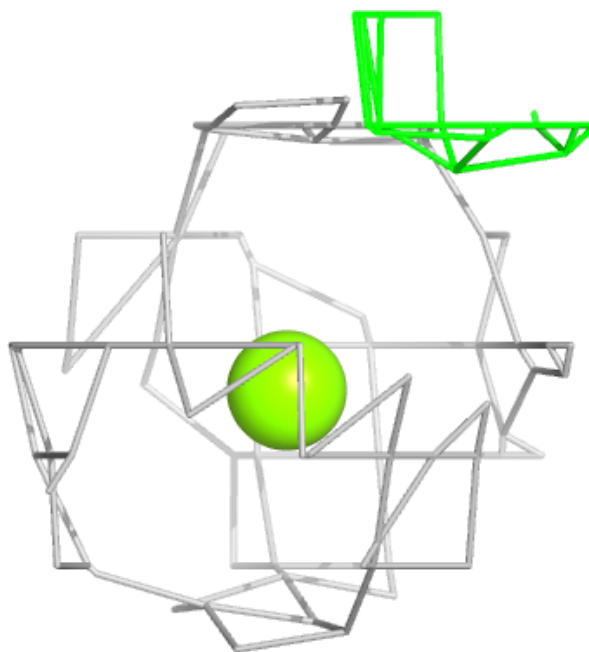
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG B 1302:**

$2mF_o-DF_c$  (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.