



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:12 AM UTC

PDB ID : 7MYC / pdb_00007myc
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

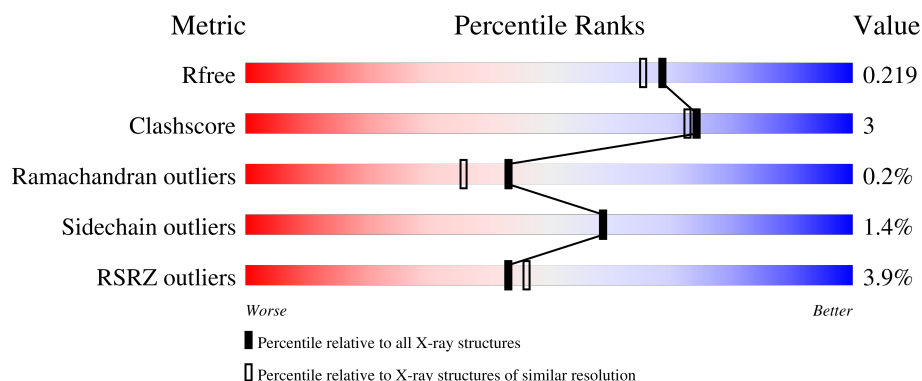
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 ≥ 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	3% 91% 7%
1	B	1235	5% 90% 9%

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.

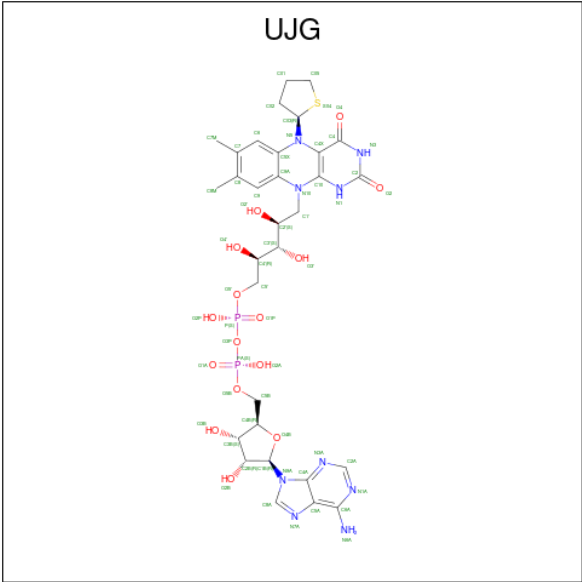
- Molecule 1 is a protein called Bifunctional protein PutA.

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:

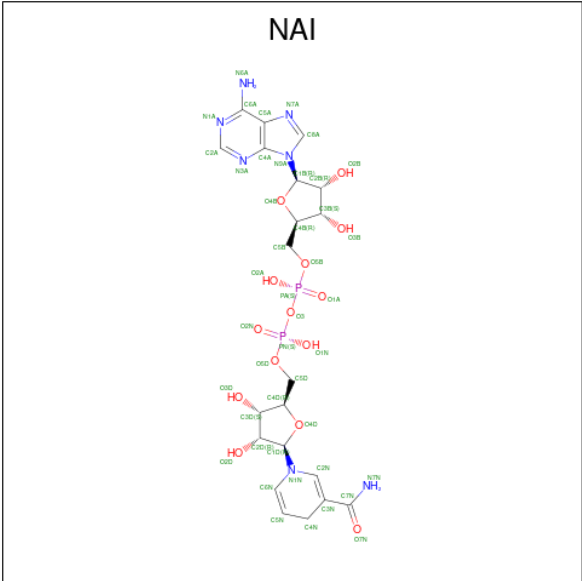
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- 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) (CCD ID: UJG) (formula: C₃₁H₄₁N₉O₁₅P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			58	31	9	15	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			58	31	9	15	2	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

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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 (CCD ID: SO4) (formula: O₄S).



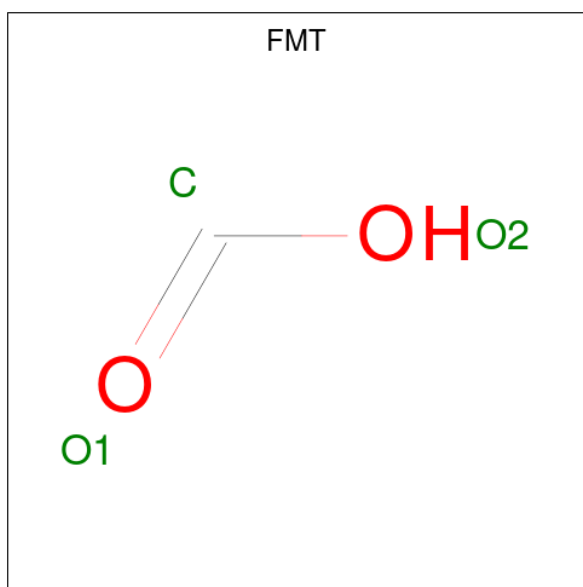
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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 (CCD ID: FMT) (formula: CH_2O_2).



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

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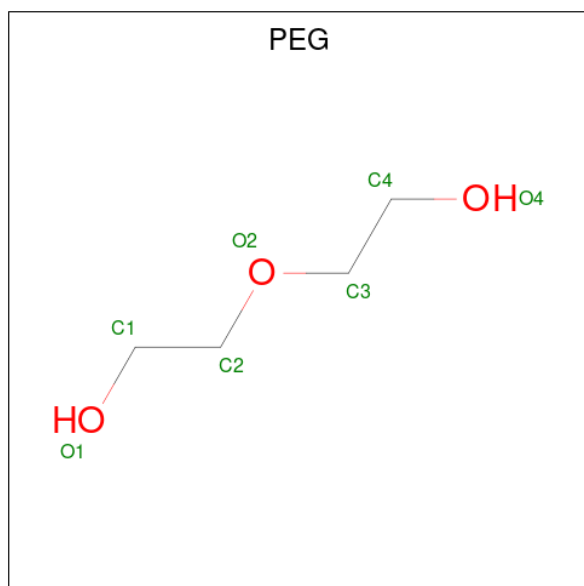
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: 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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

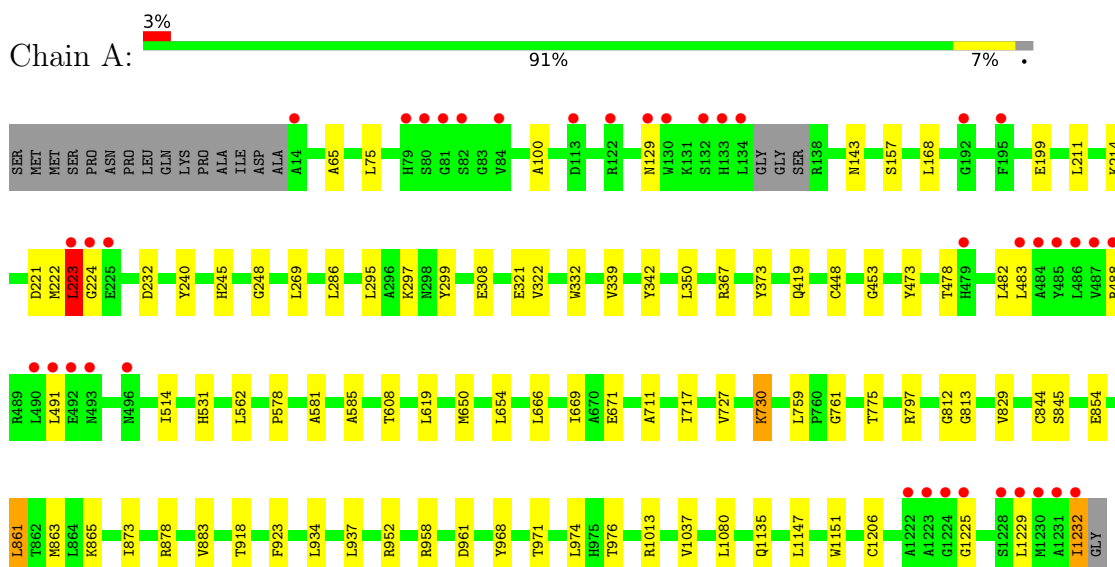
- Molecule 9 is water.

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

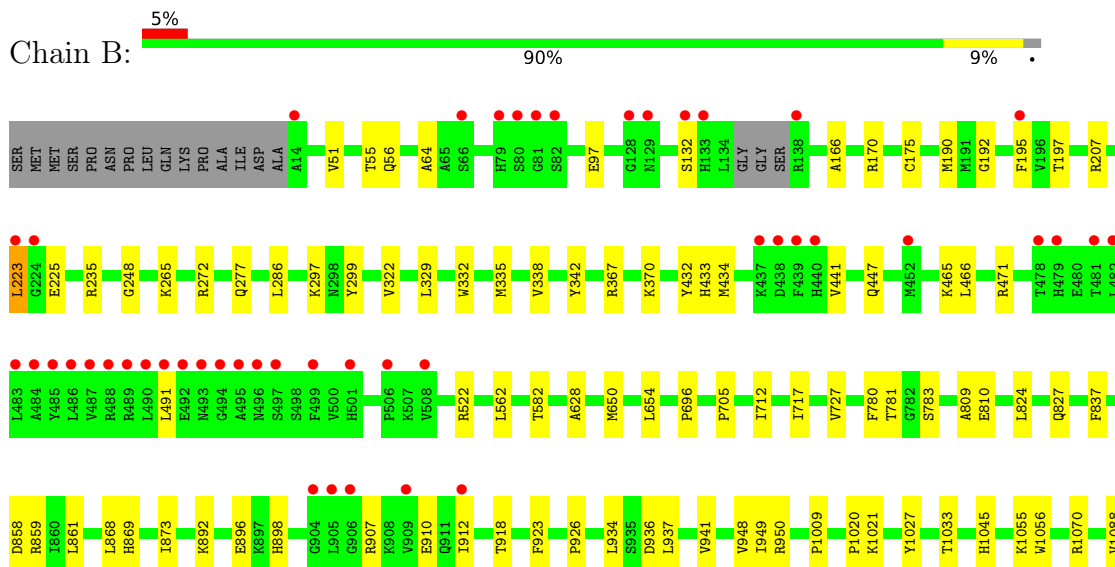
3 Residue-property plots [i](#)

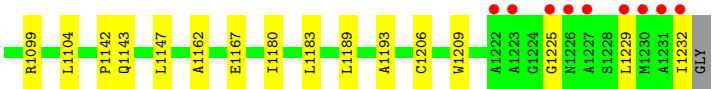
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UJG, FMT, SO4, PEG, NAI, PGE

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	0.28	0/9117	0.46	0/12419
1	B	0.27	0/9109	0.45	0/12411
All	All	0.27	0/18226	0.45	0/24830

There are no bond length outliers.

There are no bond angle outliers.

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	8947	0	8908	53	0
1	B	8928	0	8895	60	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	112	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 (112) 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:332:TRP:HZ3	1:B:335:MET:HE2	1.64	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:B:332:TRP:CZ3	1:B:335:MET:HE2	2.39	0.58
1:A:829:VAL:HG21	1:A:863:MET:HE2	1.84	0.58
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
1:B:650:MET:O	1:B:654:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:370:LYS:NZ	2:B:1301:UJG:O1A	2.45	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
1:A:240:TYR:HD2	1:A:269:LEU:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:MET:HE2	1:B:195:PHE:CZ	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: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:A:1080:LEU:C	1:A:1080:LEU:HD23	2.45	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:B:907:ARG:HH21	1:B:936:ASP:CG	2.29	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%)	43	36
1	B	1220/1235 (99%)	1188 (97%)	30 (2%)	2 (0%)	43	36
All	All	2436/2470 (99%)	2374 (98%)	58 (2%)	4 (0%)	43	36

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%)	875 (99%)	12 (1%)	59	59
1	B	885/951 (93%)	872 (98%)	13 (2%)	57	56
All	All	1772/1902 (93%)	1747 (99%)	25 (1%)	59	59

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	SER
1	A	223	LEU
1	A	321	GLU
1	A	342	TYR
1	A	488	ARG
1	A	666	LEU
1	A	730	LYS
1	A	861	LEU
1	A	934	LEU
1	A	937	LEU
1	A	1013	ARG
1	A	1232	ILE
1	B	132	SER
1	B	223	LEU
1	B	235	ARG
1	B	342	TYR
1	B	441	VAL
1	B	810	GLU
1	B	859	ARG
1	B	934	LEU
1	B	937	LEU
1	B	949	ILE
1	B	1033	THR
1	B	1104	LEU
1	B	1232	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	419	GLN

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Mol	Chain	Res	Type
1	A	716	GLN
1	B	56	GLN
1	B	440	HIS
1	B	667	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	$\# Z > 2$
3	NAI	A	2202	-	47,48,48	1.58	8 (17%)	64,73,73	1.51	12 (18%)
2	UJG	A	2201	-	63,64,64	2.79	24 (38%)	84,98,98	2.84	21 (25%)
5	PGE	B	1308	-	9,9,9	0.30	0	8,8,8	0.36	0
4	SO4	B	1305	-	4,4,4	0.29	0	6,6,6	0.26	0
3	NAI	B	1303	7	47,48,48	1.50	6 (12%)	64,73,73	1.56	11 (17%)
6	FMT	A	2211	-	2,2,2	0.49	0	1,1,1	0.58	0
6	FMT	A	2208	-	2,2,2	0.66	0	1,1,1	0.53	0
2	UJG	B	1301	-	63,64,64	2.69	23 (36%)	84,98,98	2.52	22 (26%)
5	PGE	A	2207	-	9,9,9	0.35	0	8,8,8	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	2203	-	4,4,4	0.25	0	6,6,6	0.12	0
4	SO4	A	2204	-	4,4,4	0.23	0	6,6,6	0.10	0
6	FMT	A	2210	-	2,2,2	0.65	0	1,1,1	0.54	0
6	FMT	A	2209	-	2,2,2	0.67	0	1,1,1	0.50	0
6	FMT	B	1309	-	2,2,2	0.63	0	1,1,1	0.71	0
4	SO4	B	1304	-	4,4,4	0.24	0	6,6,6	0.28	0
4	SO4	A	2206	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	A	2205	-	4,4,4	0.24	0	6,6,6	0.22	0
8	PEG	B	1307	-	6,6,6	0.49	0	5,5,5	0.29	0
5	PGE	B	1306	-	9,9,9	0.34	0	8,8,8	0.24	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
5	PGE	B	1308	-	-	1/7/7/7	-
3	NAI	A	2202	-	-	9/29/72/72	0/5/5/5
2	UJG	A	2201	-	-	9/38/61/61	0/6/7/7
2	UJG	B	1301	-	-	8/38/61/61	0/6/7/7
5	PGE	A	2207	-	-	1/7/7/7	-
8	PEG	B	1307	-	-	0/4/4/4	-
5	PGE	B	1306	-	-	1/7/7/7	-
3	NAI	B	1303	7	-	4/29/72/72	0/5/5/5

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	UJG	PA-O3P	-8.64	1.50	1.59
2	A	2201	UJG	PA-O3P	-8.59	1.50	1.59
2	B	1301	UJG	O4-C4	7.70	1.38	1.23
2	A	2201	UJG	O4-C4	7.63	1.38	1.23
2	B	1301	UJG	O2-C2	6.64	1.37	1.23
2	A	2201	UJG	C9-C9A	6.20	1.49	1.39
2	A	2201	UJG	C6-C5X	6.07	1.49	1.39
2	A	2201	UJG	O2-C2	5.99	1.36	1.23
2	A	2201	UJG	P-O3P	5.88	1.65	1.59
2	B	1301	UJG	C9-C9A	5.54	1.48	1.39
2	B	1301	UJG	C6-C5X	5.46	1.48	1.39
2	A	2201	UJG	C4X-N5	5.45	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	UJG	C4X-N5	4.81	1.45	1.37
2	A	2201	UJG	C10-N1	4.76	1.45	1.37
2	B	1301	UJG	C10-N1	4.62	1.45	1.37
2	B	1301	UJG	C2-N1	4.51	1.44	1.37
3	A	2202	NAI	PN-O3	4.43	1.64	1.59
2	A	2201	UJG	C6A-N6A	4.06	1.44	1.34
3	B	1303	NAI	PN-O5D	4.06	1.75	1.59
3	B	1303	NAI	PA-O5B	4.05	1.75	1.59
2	B	1301	UJG	C6A-N6A	3.90	1.44	1.34
2	A	2201	UJG	C2-N1	3.80	1.43	1.37
3	A	2202	NAI	PA-O5B	3.76	1.74	1.59
3	A	2202	NAI	PN-O5D	3.61	1.73	1.59
2	A	2201	UJG	C10-N10	3.53	1.44	1.38
2	B	1301	UJG	C10-N10	3.44	1.44	1.38
2	B	1301	UJG	P-O3P	3.40	1.63	1.59
3	B	1303	NAI	PN-O3	3.28	1.63	1.59
2	A	2201	UJG	C4X-C4	3.08	1.51	1.43
2	A	2201	UJG	C5X-N5	3.06	1.46	1.42
2	B	1301	UJG	C9A-N10	2.90	1.46	1.41
2	A	2201	UJG	C9A-N10	2.83	1.46	1.41
3	A	2202	NAI	C8A-N9A	2.78	1.42	1.37
3	B	1303	NAI	C8A-N9A	2.76	1.42	1.37
2	B	1301	UJG	C9A-C5X	-2.72	1.36	1.41
2	B	1301	UJG	C2-N3	2.57	1.41	1.37
2	A	2201	UJG	C9A-C5X	-2.56	1.36	1.41
2	B	1301	UJG	C4X-C4	2.53	1.49	1.43
3	A	2202	NAI	C6N-N1N	2.49	1.43	1.37
2	B	1301	UJG	O2'-C2'	-2.45	1.38	1.43
2	A	2201	UJG	PA-O5B	-2.43	1.49	1.59
3	A	2202	NAI	C3B-C4B	2.43	1.59	1.53
2	A	2201	UJG	O3B-C3B	-2.41	1.37	1.43
2	A	2201	UJG	O2'-C2'	-2.39	1.38	1.43
2	B	1301	UJG	PA-O5B	-2.35	1.50	1.59
2	B	1301	UJG	C5X-N5	2.34	1.45	1.42
2	B	1301	UJG	P-O1P	2.32	1.58	1.50
2	B	1301	UJG	PA-O2A	-2.30	1.44	1.55
3	A	2202	NAI	PA-O3	2.27	1.61	1.59
2	A	2201	UJG	C9-C8	2.23	1.42	1.39
2	B	1301	UJG	C4A-N9A	2.20	1.42	1.37
2	A	2201	UJG	C5A-C4A	2.19	1.43	1.39
2	A	2201	UJG	PA-O2A	-2.19	1.45	1.55
2	A	2201	UJG	P-O1P	2.17	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2201	UJG	C2B-C3B	-2.11	1.47	1.53
3	B	1303	NAI	C3B-C4B	2.10	1.58	1.53
2	B	1301	UJG	O3B-C3B	-2.08	1.37	1.43
2	A	2201	UJG	C2-N3	2.04	1.40	1.37
3	A	2202	NAI	O5D-C5D	-2.03	1.36	1.44
3	B	1303	NAI	C4A-N3A	2.02	1.38	1.34
2	B	1301	UJG	C5A-C4A	2.01	1.42	1.39

All (66) 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	A	2201	UJG	C5X-N5-C03	-9.84	97.98	119.90
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
2	B	1301	UJG	N3A-C2A-N1A	-5.98	119.53	128.58
2	B	1301	UJG	C5X-N5-C03	-5.74	107.13	119.90
2	A	2201	UJG	N3A-C2A-N1A	-5.67	120.00	128.58
2	A	2201	UJG	C02-C03-N5	-5.53	107.05	113.24
2	B	1301	UJG	C5A-C4A-N3A	-5.21	119.54	126.72
3	B	1303	NAI	O1N-PN-O3	5.16	121.21	107.27
2	A	2201	UJG	C5A-C4A-N3A	-5.11	119.68	126.72
2	A	2201	UJG	C4X-C4-N3	5.09	119.90	110.94
2	B	1301	UJG	C4-N3-C2	-5.04	119.42	126.37
2	B	1301	UJG	C4X-C4-N3	5.01	119.75	110.94
2	A	2201	UJG	C4-N3-C2	-4.71	119.88	126.37
2	B	1301	UJG	O2A-PA-O3P	-4.53	95.03	107.27
3	A	2202	NAI	O1N-PN-O3	4.45	119.30	107.27
2	B	1301	UJG	N3A-C4A-N9A	4.39	134.63	127.17
2	A	2201	UJG	O2A-PA-O3P	-4.31	95.62	107.27
2	A	2201	UJG	N3A-C4A-N9A	4.30	134.48	127.17
2	B	1301	UJG	C01-C02-C03	4.23	111.39	104.15
3	B	1303	NAI	O2A-PA-O3	4.01	118.10	107.27
2	A	2201	UJG	O3P-PA-O1A	3.94	122.57	110.70
2	B	1301	UJG	C5A-N7A-C8A	3.92	109.61	103.45
2	A	2201	UJG	C01-C02-C03	3.80	110.66	104.15
2	A	2201	UJG	C5A-N7A-C8A	3.76	109.37	103.45
2	B	1301	UJG	C2A-N3A-C4A	3.71	120.89	111.83
2	A	2201	UJG	C2A-N3A-C4A	3.58	120.57	111.83
2	B	1301	UJG	N3-C2-N1	3.56	121.33	115.74
3	B	1303	NAI	O3-PN-O2N	-3.50	100.17	110.70
3	B	1303	NAI	C3N-C2N-N1N	-3.46	118.13	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	UJG	N3-C2-N1	3.41	121.10	115.74
3	A	2202	NAI	O3-PN-O2N	-3.41	100.46	110.70
2	B	1301	UJG	O3P-PA-O1A	3.40	120.92	110.70
2	B	1301	UJG	N9A-C8A-N7A	-3.39	109.12	113.94
3	A	2202	NAI	O2A-PA-O3	3.33	116.28	107.27
2	B	1301	UJG	O4-C4-C4X	-3.32	119.47	127.62
3	A	2202	NAI	O3-PA-O1A	-3.25	100.92	110.70
2	A	2201	UJG	N9A-C8A-N7A	-3.20	109.39	113.94
3	A	2202	NAI	O2A-PA-O1A	3.12	126.94	112.44
3	A	2202	NAI	O1N-PN-O2N	3.09	126.82	112.44
3	A	2202	NAI	PN-O5D-C5D	-3.06	103.80	121.35
3	B	1303	NAI	O5D-PN-O2N	-2.99	97.10	108.94
3	B	1303	NAI	O3-PA-O1A	-2.91	101.95	110.70
2	B	1301	UJG	C4A-C5A-N7A	-2.89	107.28	110.58
2	A	2201	UJG	C4A-C5A-N7A	-2.73	107.46	110.58
2	B	1301	UJG	O3P-P-O1P	2.62	118.58	110.70
3	A	2202	NAI	O5D-PN-O2N	-2.61	98.59	108.94
3	B	1303	NAI	O2A-PA-O1A	2.59	124.50	112.44
3	B	1303	NAI	O1N-PN-O2N	2.53	124.21	112.44
2	A	2201	UJG	O3P-P-O1P	2.50	118.21	110.70
3	A	2202	NAI	C5D-C4D-C3D	-2.48	106.30	115.21
3	B	1303	NAI	C2D-C3D-C4D	-2.47	97.85	102.61
2	A	2201	UJG	O2A-PA-O5B	-2.39	96.75	107.57
3	B	1303	NAI	PN-O5D-C5D	-2.31	108.09	121.35
3	A	2202	NAI	O7N-C7N-N7N	-2.31	117.72	122.89
2	B	1301	UJG	C4A-N9A-C8A	2.30	108.15	105.74
3	B	1303	NAI	O7N-C7N-N7N	-2.26	117.82	122.89
2	A	2201	UJG	O4-C4-C4X	-2.25	122.11	127.62
3	A	2202	NAI	PA-O5B-C5B	-2.22	108.66	121.35
3	A	2202	NAI	C3N-C2N-N1N	-2.18	120.00	123.20
2	B	1301	UJG	C6-C5X-N5	-2.15	118.41	121.89
2	B	1301	UJG	O2-C2-N1	-2.14	118.05	121.86
2	A	2201	UJG	C4A-N9A-C8A	2.10	107.94	105.74
2	A	2201	UJG	O2P-P-O5'	-2.06	98.23	107.57
2	B	1301	UJG	C2A-N1A-C6A	2.00	122.02	118.73

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	UJG	C02-C03-N5-C5X
2	B	1301	UJG	S04-C03-N5-C4X

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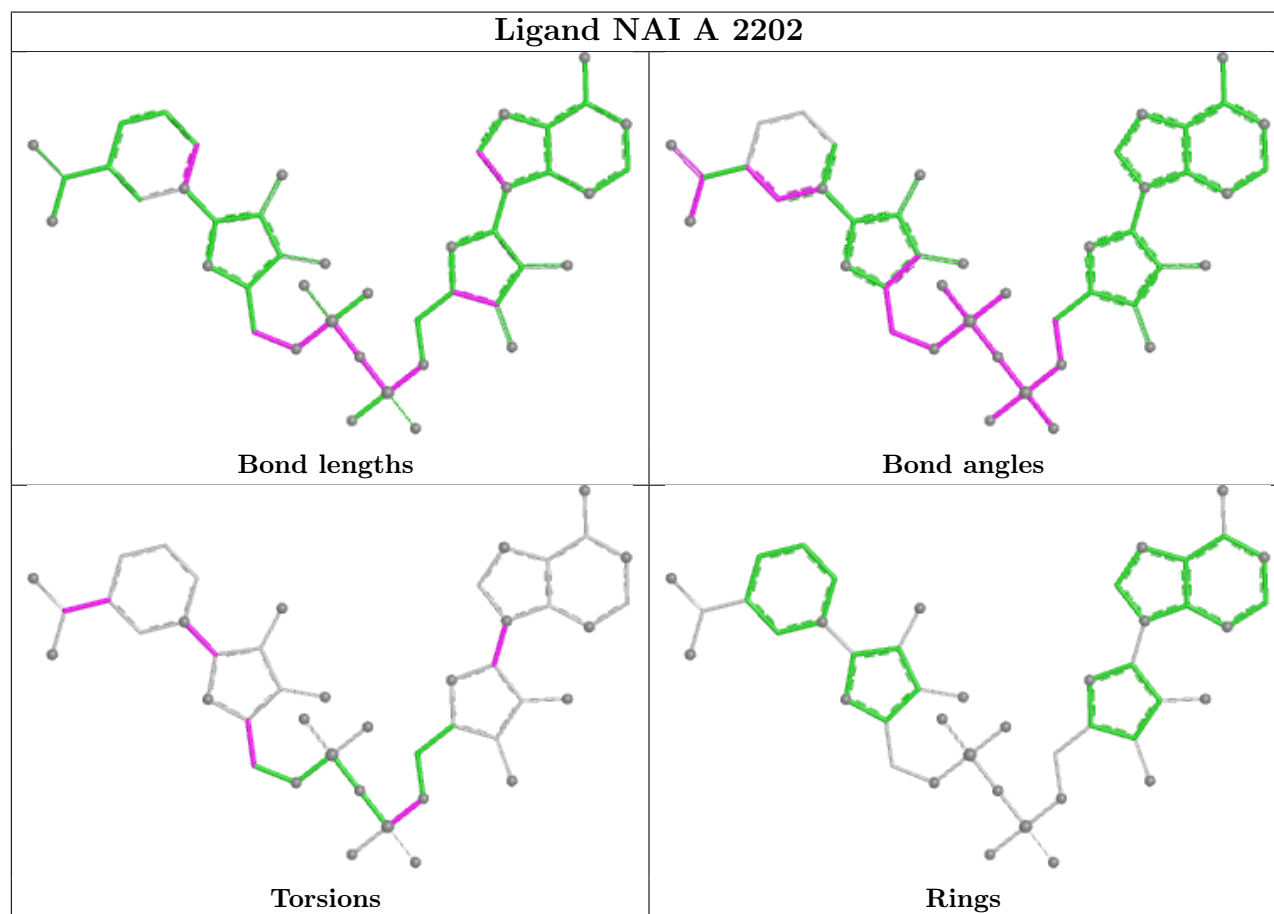
Mol	Chain	Res	Type	Atoms
2	B	1301	UJG	C02-C03-N5-C5X
3	A	2202	NAI	C5B-O5B-PA-O1A
3	A	2202	NAI	C5B-O5B-PA-O3
3	A	2202	NAI	O4D-C1D-N1N-C2N
3	A	2202	NAI	C2N-C3N-C7N-N7N
3	B	1303	NAI	O4D-C1D-N1N-C2N
3	A	2202	NAI	C3D-C4D-C5D-O5D
2	A	2201	UJG	C2'-C3'-C4'-O4'
5	B	1308	PGE	O2-C3-C4-O3
3	A	2202	NAI	O4D-C4D-C5D-O5D
5	A	2207	PGE	O1-C1-C2-O2
2	A	2201	UJG	O3'-C3'-C4'-O4'
2	A	2201	UJG	O3'-C3'-C4'-C5'
2	A	2201	UJG	PA-O3P-P-O1P
2	B	1301	UJG	PA-O3P-P-O1P
2	A	2201	UJG	C2'-C3'-C4'-C5'
2	B	1301	UJG	C2'-C3'-C4'-O4'
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	C2B-C1B-N9A-C8A
3	B	1303	NAI	C2B-C1B-N9A-C8A
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	B	1301	UJG	O3'-C3'-C4'-C5'
2	A	2201	UJG	S04-C03-N5-C4X
3	A	2202	NAI	O4B-C1B-N9A-C8A
3	B	1303	NAI	O4B-C1B-N9A-C8A
3	B	1303	NAI	PA-O3-PN-O2N

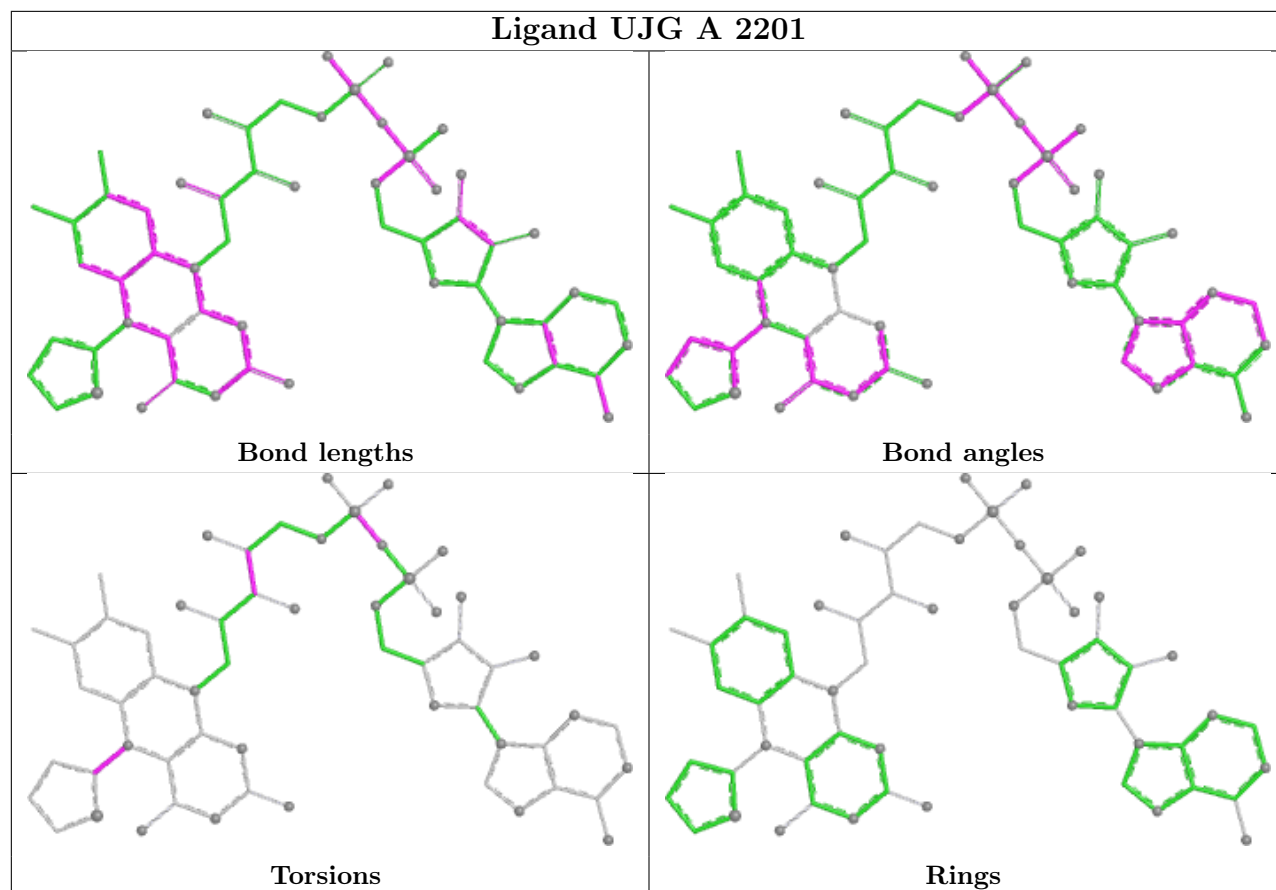
There are no ring outliers.

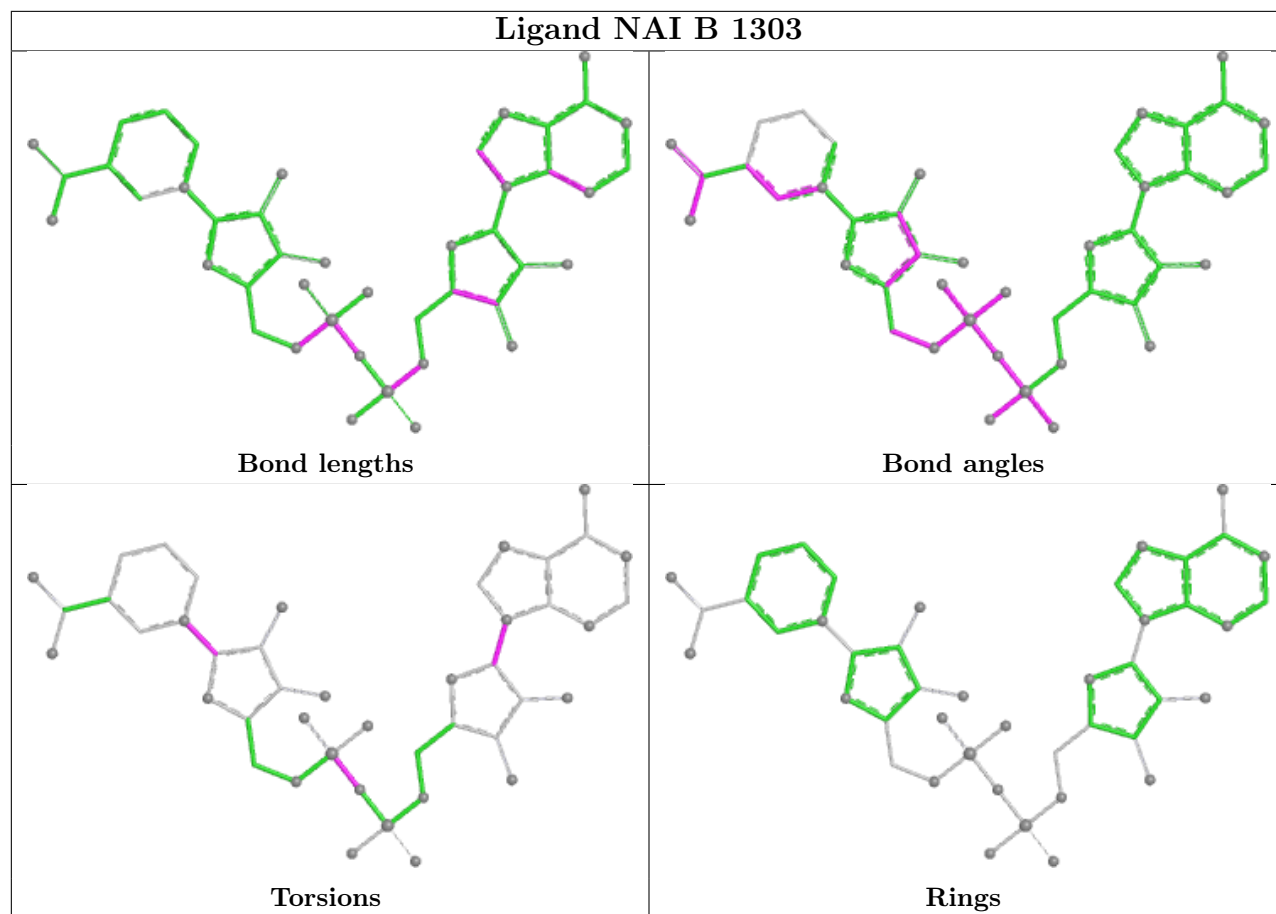
6 monomers are involved in 8 short contacts:

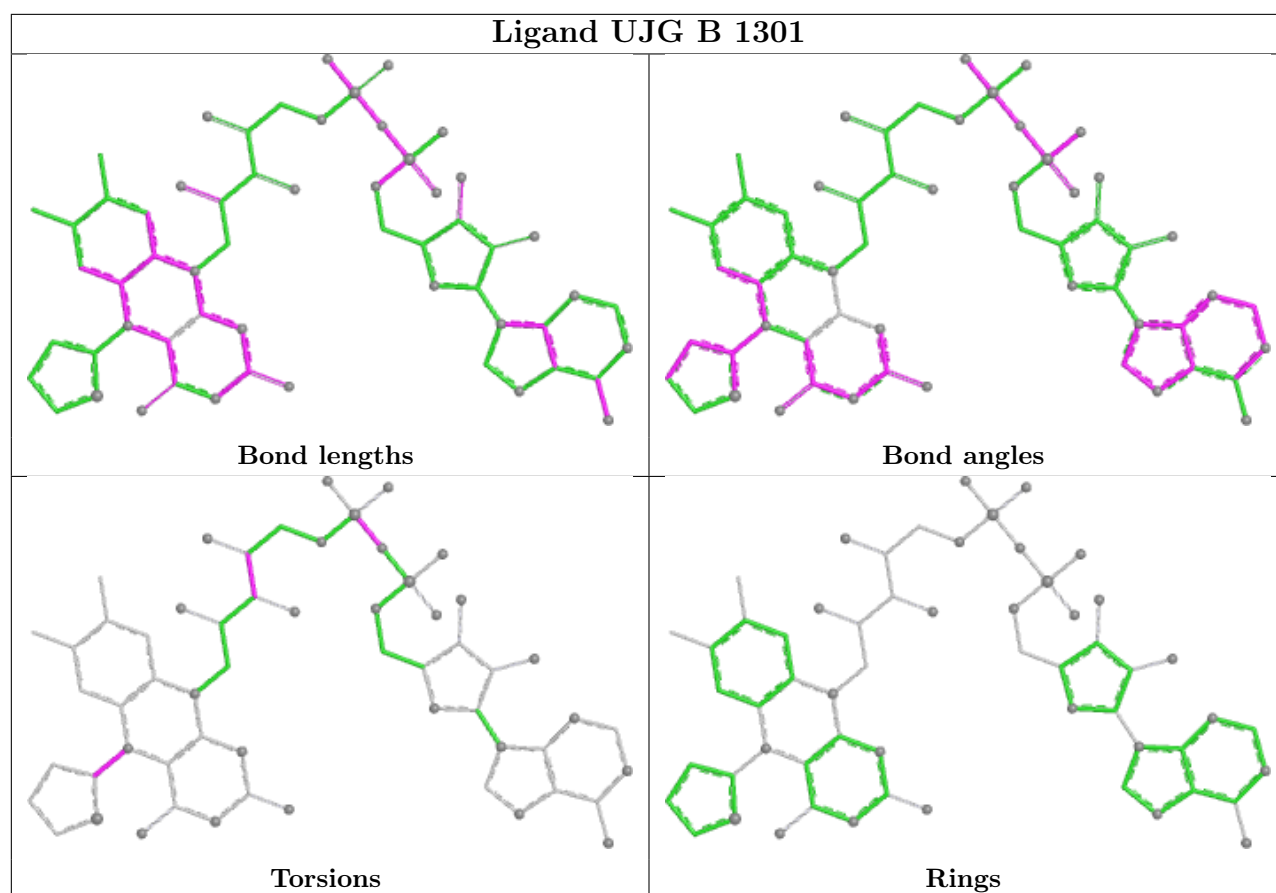
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2202	NAI	2	0
5	B	1308	PGE	2	0
3	B	1303	NAI	1	0
2	B	1301	UJG	1	0
8	B	1307	PEG	1	0
5	B	1306	PGE	1	0

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, 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	1216/1235 (98%)	-0.12	39 (3%)	50 54	12, 25, 54, 95	4 (0%)
1	B	1216/1235 (98%)	0.04	56 (4%)	37 40	12, 26, 58, 93	7 (0%)
All	All	2432/2470 (98%)	-0.04	95 (3%)	43 46	12, 26, 56, 95	11 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	6.5
1	A	490	LEU	5.5
1	B	486	LEU	5.4
1	B	485	TYR	5.3
1	B	483	LEU	5.2
1	B	1227	ALA	5.2
1	B	484	ALA	4.6
1	B	490	LEU	4.6
1	A	486	LEU	4.6
1	B	1222	ALA	4.2
1	B	487	VAL	4.2
1	A	134	LEU	4.2
1	A	484	ALA	4.1
1	A	223	LEU	4.1
1	B	82	SER	4.0
1	B	1223	ALA	3.9
1	A	493	ASN	3.8
1	B	488	ARG	3.8
1	B	1229	LEU	3.8
1	B	482	LEU	3.7
1	A	132	SER	3.7
1	A	1232	ILE	3.6
1	A	1222	ALA	3.5
1	A	491	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	905	LEU	3.5
1	B	1231	ALA	3.5
1	B	1230	MET	3.5
1	B	492	GLU	3.4
1	B	79	HIS	3.4
1	A	195	PHE	3.4
1	B	481	THR	3.4
1	B	129	ASN	3.4
1	B	497	SER	3.3
1	B	495	ALA	3.3
1	B	491	LEU	3.3
1	B	1232	ILE	3.2
1	B	1226	ASN	3.1
1	B	128	GLY	3.1
1	B	912	ILE	3.1
1	A	1230	MET	3.1
1	B	506	PRO	3.0
1	B	223	LEU	3.0
1	A	79	HIS	3.0
1	B	224	GLY	3.0
1	A	483	LEU	2.9
1	A	81	GLY	2.9
1	A	80	SER	2.9
1	B	133	HIS	2.9
1	B	501	HIS	2.9
1	B	80	SER	2.9
1	A	1229	LEU	2.8
1	B	493	ASN	2.8
1	B	496	ASN	2.8
1	A	1224	GLY	2.8
1	B	494	GLY	2.8
1	A	492	GLU	2.8
1	A	487	VAL	2.8
1	A	224	GLY	2.8
1	B	195	PHE	2.7
1	A	129	ASN	2.7
1	A	192	GLY	2.7
1	B	14	ALA	2.6
1	B	479	HIS	2.6
1	B	452	MET	2.6
1	A	113	ASP	2.6
1	B	909	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	439	PHE	2.6
1	A	496	ASN	2.6
1	A	1228	SER	2.5
1	A	488	ARG	2.5
1	B	489	ARG	2.4
1	A	14	ALA	2.4
1	B	499	PHE	2.4
1	B	438	ASP	2.4
1	B	437	LYS	2.4
1	B	138	ARG	2.3
1	A	1231	ALA	2.3
1	A	82	SER	2.3
1	A	479	HIS	2.3
1	B	478	THR	2.3
1	B	66	SER	2.3
1	B	906	GLY	2.2
1	B	904	GLY	2.2
1	B	81	GLY	2.2
1	A	130	TRP	2.1
1	A	1225	GLY	2.1
1	B	1225	GLY	2.1
1	B	440	HIS	2.1
1	A	1223	ALA	2.1
1	B	132	SER	2.1
1	A	84	VAL	2.1
1	A	225	GLU	2.0
1	A	122	ARG	2.0
1	A	133	HIS	2.0
1	B	508	VAL	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 oligosaccharides in this entry.

6.4 Ligands

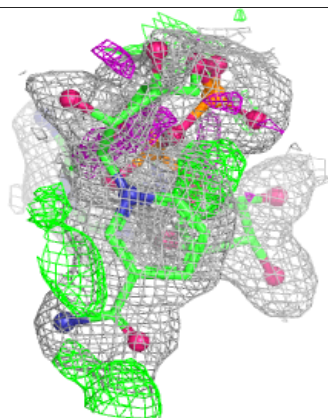
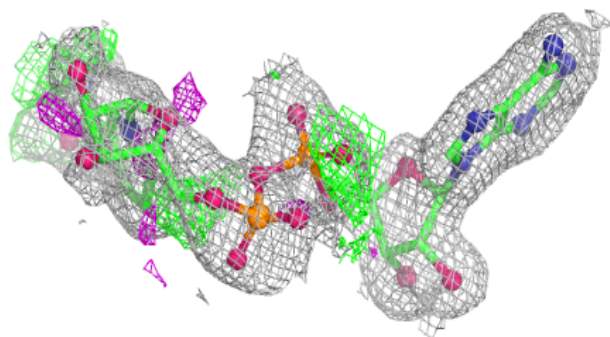
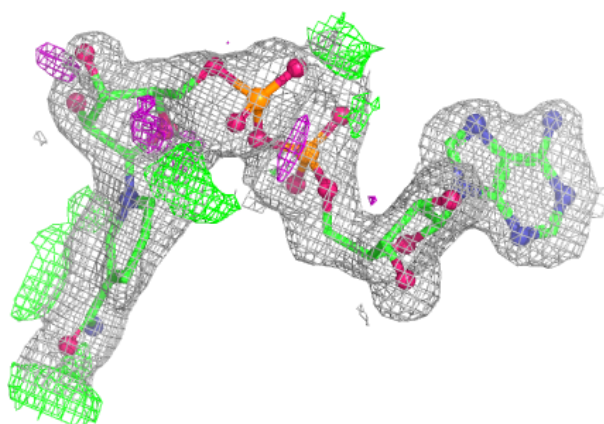
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	2206	5/5	0.79	0.11	78,78,79,87	0
4	SO4	A	2205	5/5	0.83	0.15	63,69,73,75	0
5	PGE	B	1308	10/10	0.85	0.16	52,54,61,63	0
6	FMT	A	2208	3/3	0.86	0.13	51,51,54,55	0
8	PEG	B	1307	7/7	0.86	0.13	43,45,49,51	0
4	SO4	A	2204	5/5	0.87	0.11	65,69,75,82	0
6	FMT	A	2210	3/3	0.88	0.12	46,46,47,50	0
6	FMT	A	2209	3/3	0.88	0.11	40,40,42,44	0
3	NAI	A	2202	44/44	0.89	0.11	25,36,64,66	0
4	SO4	A	2203	5/5	0.90	0.09	37,43,48,60	5
6	FMT	B	1309	3/3	0.93	0.08	27,27,35,36	0
5	PGE	A	2207	10/10	0.93	0.10	28,45,53,54	0
5	PGE	B	1306	10/10	0.94	0.09	23,40,47,47	0
2	UJG	B	1301	58/58	0.95	0.08	18,27,42,52	5
6	FMT	A	2211	3/3	0.96	0.07	18,18,27,33	0
2	UJG	A	2201	58/58	0.96	0.07	18,28,40,42	5
3	NAI	B	1303	44/44	0.96	0.07	18,24,31,33	0
4	SO4	B	1305	5/5	0.99	0.03	22,24,27,27	0
4	SO4	B	1304	5/5	0.99	0.04	21,21,24,25	0
7	MG	B	1302	1/1	1.00	0.03	28,28,28,28	0

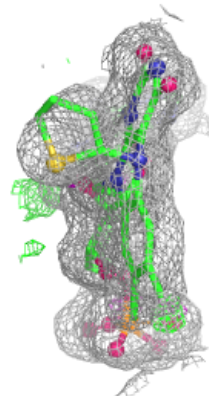
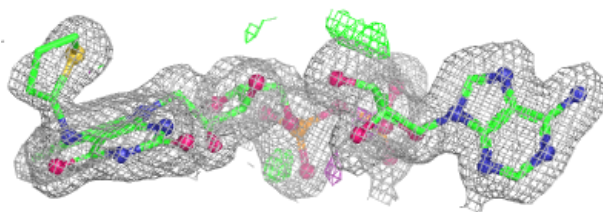
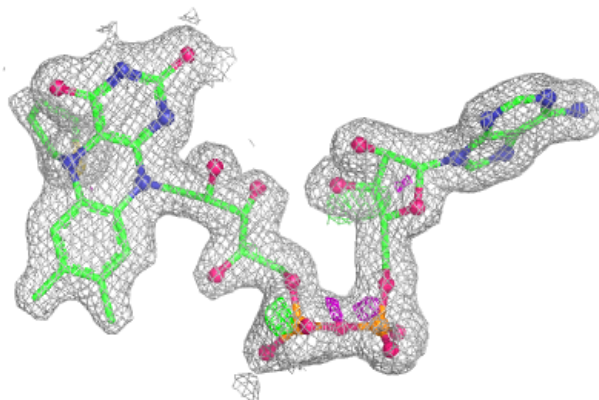
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

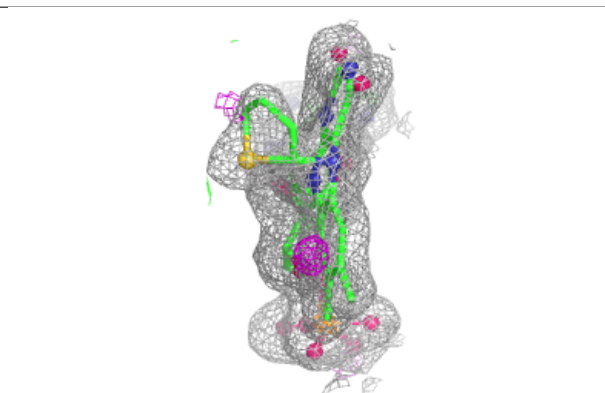
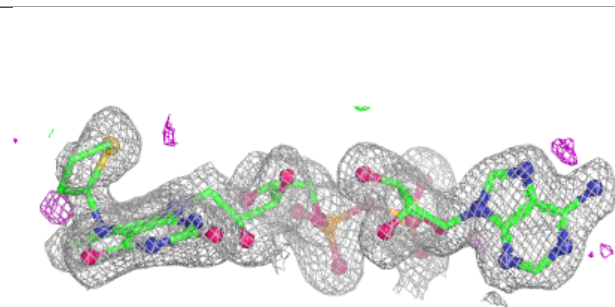
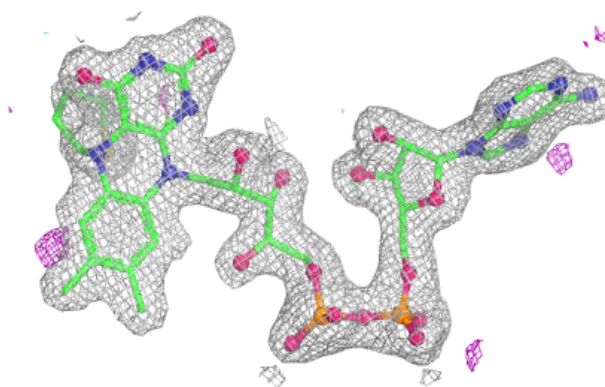
**Electron density around UJG B 1301:**

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

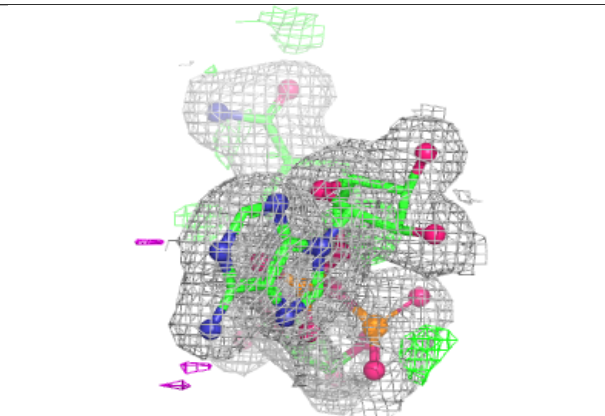
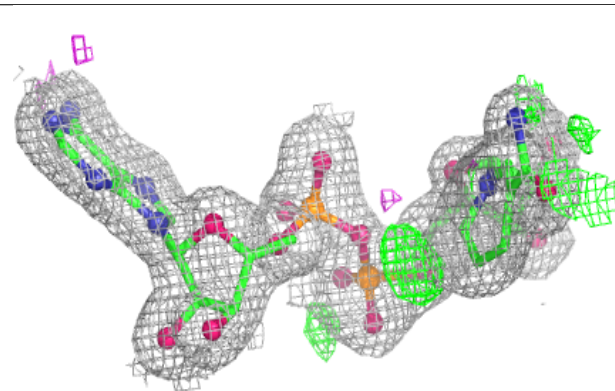
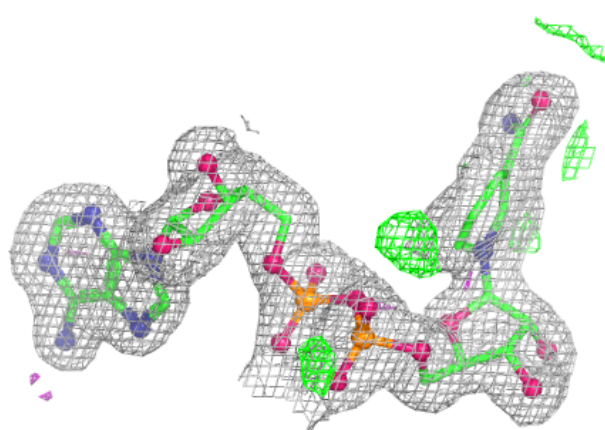


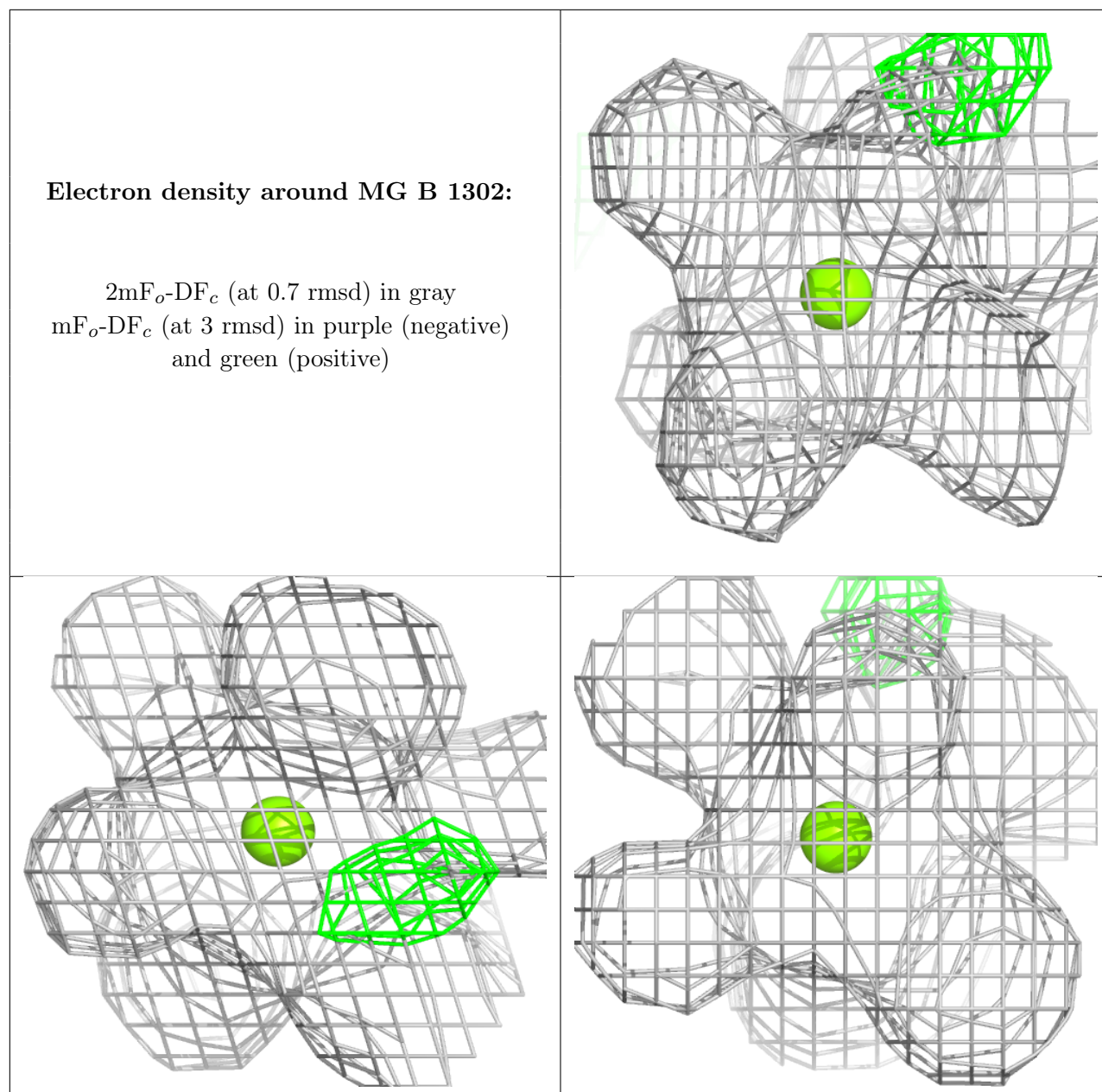
Electron density around UJG A 2201:

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

**Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.