



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:17 PM UTC

PDB ID : 7BMK / pdb_00007bmk
Title : ATP-Competitive Partial Antagonists-'PAIR's-Rheostatically Modulate IRE1alpha's Kinase Helix-alphaC to Segregate its RNase-Mediated Biological Outputs
Authors : Feldman, H.C.; Ghosh, R.; Auyeung, V.; Mueller, J.L.; Vidadala, V.N.; Olivier, A.; Backes, B.J.; Zikherman, J.; Papa, F.R.; Maly, D.J.
Deposited on : 2021-01-20
Resolution : 1.85 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](#) ①) 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

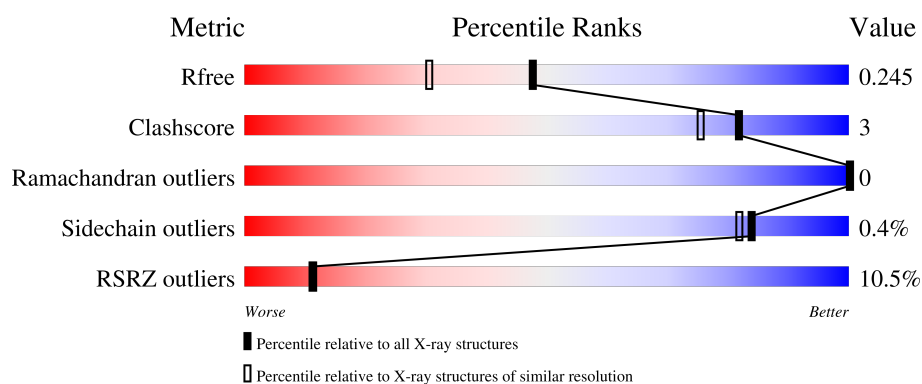
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	434	9% 88% 5% 6%
1	B	434	11% 86% • 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7573 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.

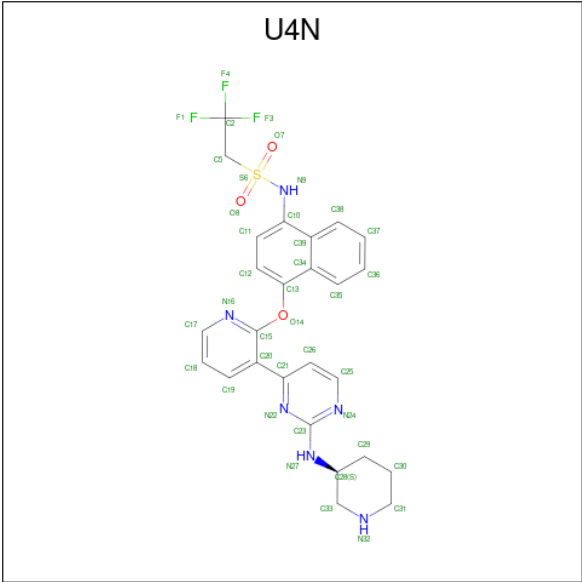
- Molecule 1 is a protein called Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	72	16	0
			3396	2158	599	616	23			
1	B	392	Total	C	N	O	S	87	15	0
			3284	2092	581	589	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLY	-	expression tag	UNP O75460
A	545	ALA	-	expression tag	UNP O75460
A	546	MET	-	expression tag	UNP O75460
B	544	GLY	-	expression tag	UNP O75460
B	545	ALA	-	expression tag	UNP O75460
B	546	MET	-	expression tag	UNP O75460

- Molecule 2 is 2,2,2-tris(fluoranyl)- {N}-[4-[3-[2-[[3 {S}]-piperidin-3-yl]amino]pyrimidin-4-yl]pyridin-2-yl]oxynaphthalen-1-yl]ethanesulfonamide (CCD ID: U4N) (formula: C₂₆H₂₅F₃N₆O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			39	26	3	6	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			39	26	3	6	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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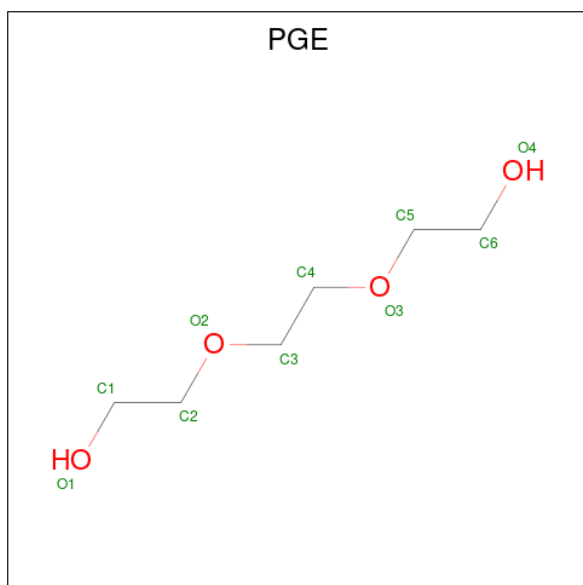
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

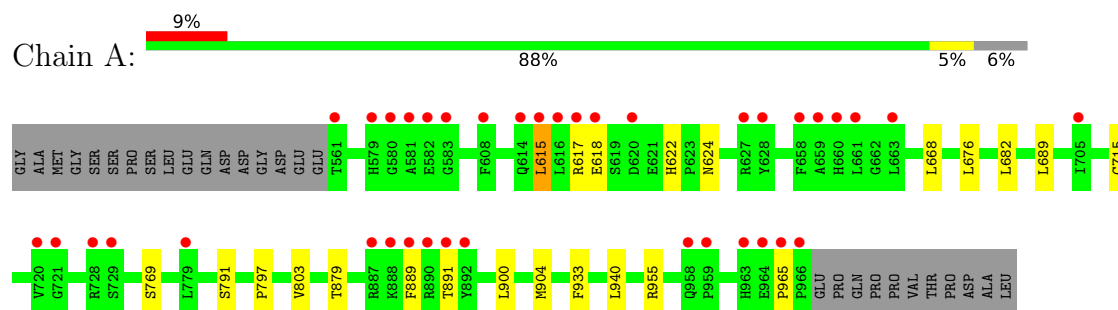
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	376	Total	O	0	7
			383	383		
7	B	253	Total	O	0	5
			258	258		

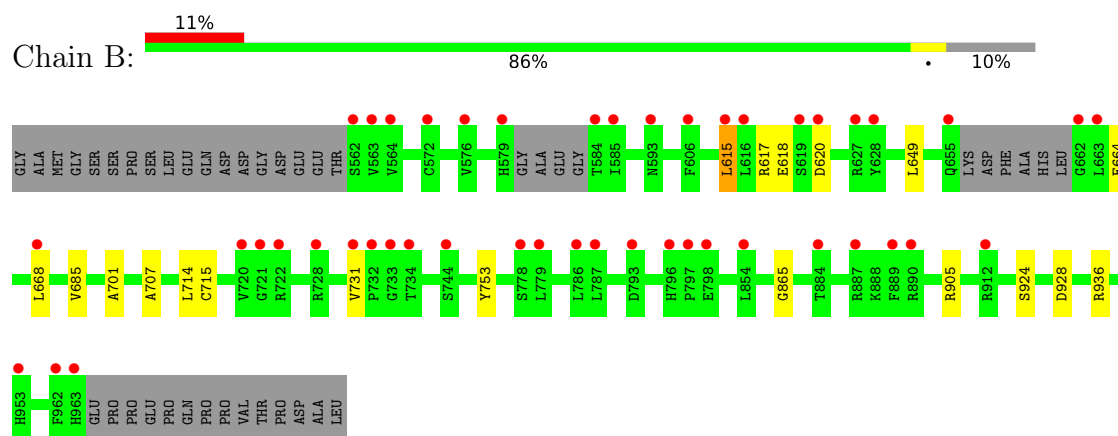
3 Residue-property plots [i](#)

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: Serine/threonine-protein kinase/endoribonuclease IRE1



- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.90Å 72.81Å 119.24Å 90.00° 129.82° 90.00°	Depositor
Resolution (Å)	91.59 – 1.85 91.58 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (91.59-1.85) 98.4 (91.58-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.191 , 0.235 0.199 , 0.245	Depositor DCC
R_{free} test set	2411 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7573	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, EDO, U4N, PEG, GOL

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	0.81	1/3497 (0.0%)	1.00	4/4722 (0.1%)
1	B	0.78	0/3387	0.96	0/4569
All	All	0.80	1/6884 (0.0%)	0.98	4/9291 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	891	THR	CB-OG1	-5.82	1.34	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	965	PRO	N-CA-C	6.66	118.83	110.70
1	A	879	THR	CA-C-N	5.81	123.90	120.24
1	A	879	THR	C-N-CA	5.81	123.90	120.24
1	A	889	PHE	CA-CB-CG	-5.26	108.54	113.80

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	3396	0	3365	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3284	0	3268	15	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
3	A	48	0	64	2	0
3	B	12	0	16	1	0
4	A	44	0	66	5	0
4	B	32	0	48	3	0
5	A	7	0	10	0	0
5	B	21	0	30	2	0
6	B	10	0	14	1	0
7	A	383	0	0	1	0
7	B	258	0	0	2	0
All	All	7573	0	6881	34	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 (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617[A]:ARG:HG2	1:A:618[A]:GLU:N	1.44	1.16
1:A:617[A]:ARG:CG	1:A:618[A]:GLU:H	1.67	1.04
1:A:617[A]:ARG:HG2	1:A:618[A]:GLU:H	0.84	0.99
1:A:617[A]:ARG:CG	1:A:618[A]:GLU:N	2.22	0.98
1:A:622[B]:HIS:HE1	7:A:1283[B]:HOH:O	1.61	0.83
1:B:620[B]:ASP:N	7:B:1321[B]:HOH:O	2.08	0.81
1:B:617[B]:ARG:HG3	1:B:618[B]:GLU:N	1.97	0.80
1:A:904[A]:MET:HE1	1:A:940:LEU:CD2	2.24	0.68
1:A:682:LEU:HA	4:A:1014:EDO:H12	1.76	0.68
1:B:668[A]:LEU:HD12	1:B:707:ALA:HB2	1.84	0.59
1:A:904[A]:MET:HE1	1:A:940:LEU:HD21	1.87	0.56
1:A:803:VAL:HG22	4:A:1018:EDO:H12	1.90	0.54
1:B:685:VAL:HG22	1:B:753[B]:TYR:CD1	2.45	0.52
1:B:865:GLY:H	6:B:1007:PGE:H4	1.75	0.52
1:A:622[A]:HIS:CD2	1:A:624:ASN:H	2.29	0.51
4:A:1014:EDO:H21	1:B:701:ALA:HB1	1.94	0.49
1:A:900:LEU:HG	1:A:904[A]:MET:HE3	1.96	0.47
1:B:905:ARG:HH12	3:B:1002:GOL:H12	1.80	0.46
1:A:797:PRO:HA	4:A:1018:EDO:H11	1.95	0.46
1:B:936:ARG:HH12	4:B:1013:EDO:C1	2.28	0.46
1:A:791:SER:HB3	3:A:1016:GOL:H12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:LEU:HD23	1:B:715[B]:CYS:SG	2.55	0.45
1:B:936:ARG:HH12	4:B:1013:EDO:H12	1.80	0.44
1:A:904[A]:MET:HE2	1:A:933:PHE:CD1	2.53	0.43
1:A:676:LEU:HD13	1:A:689[B]:LEU:HD11	2.01	0.43
1:A:797:PRO:HA	4:A:1018:EDO:C1	2.50	0.42
1:A:615:LEU:HD23	1:A:715[A]:CYS:SG	2.60	0.41
1:A:769:SER:HA	3:A:1010:GOL:O2	2.21	0.41
1:B:649:LEU:HD11	1:B:668[A]:LEU:HD21	2.02	0.41
1:B:664:GLU:HG3	7:B:1281:HOH:O	2.19	0.41
1:B:924:SER:OG	5:B:1006:PEG:H12	2.20	0.41
1:B:714:LEU:HD22	1:B:731:VAL:HG13	2.03	0.41
1:A:955:ARG:HE	5:B:1006:PEG:H41	1.86	0.41
1:B:928:ASP:O	4:B:1012:EDO:H21	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	420/434 (97%)	415 (99%)	5 (1%)	0	100	100
1	B	401/434 (92%)	396 (99%)	5 (1%)	0	100	100
All	All	821/868 (95%)	811 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	376/383 (98%)	374 (100%)	2 (0%)	81	77
1	B	365/383 (95%)	364 (100%)	1 (0%)	86	85
All	All	741/766 (97%)	738 (100%)	3 (0%)	84	82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	615	LEU
1	A	668	LEU
1	B	615	LEU

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

Mol	Chain	Res	Type
1	A	702	HIS
1	A	953	HIS
1	B	840	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 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	U4N	A	1001	-	42,43,43	1.12	5 (11%)	52,62,62	2.15	9 (17%)
3	GOL	A	1010	-	5,5,5	0.31	0	5,5,5	0.39	0
3	GOL	A	1002	-	5,5,5	0.24	0	5,5,5	0.24	0
4	EDO	A	1013	-	3,3,3	0.41	0	2,2,2	0.21	0
4	EDO	A	1012	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	B	1013	-	3,3,3	0.30	0	2,2,2	0.30	0
4	EDO	B	1014	-	3,3,3	0.41	0	2,2,2	0.10	0
5	PEG	B	1009	-	6,6,6	0.40	0	5,5,5	0.38	0
4	EDO	B	1003	-	3,3,3	0.41	0	2,2,2	0.30	0
3	GOL	B	1005	-	5,5,5	0.28	0	5,5,5	0.59	0
4	EDO	B	1012	-	3,3,3	0.40	0	2,2,2	0.32	0
5	PEG	B	1006	-	6,6,6	0.35	0	5,5,5	0.25	0
5	PEG	B	1004	-	6,6,6	0.48	0	5,5,5	0.35	0
4	EDO	B	1010	-	3,3,3	0.47	0	2,2,2	0.16	0
3	GOL	A	1017	-	5,5,5	0.27	0	5,5,5	0.31	0
4	EDO	A	1020	-	3,3,3	0.16	0	2,2,2	0.17	0
5	PEG	A	1021	-	6,6,6	0.42	0	5,5,5	0.20	0
3	GOL	B	1002	-	5,5,5	0.25	0	5,5,5	0.25	0
2	U4N	B	1001	-	42,43,43	1.12	2 (4%)	52,62,62	2.38	10 (19%)
3	GOL	A	1004	-	5,5,5	0.23	0	5,5,5	0.25	0
4	EDO	B	1011	-	3,3,3	0.39	0	2,2,2	0.28	0
3	GOL	A	1016	-	5,5,5	0.20	0	5,5,5	0.40	0
4	EDO	A	1015	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	A	1005	-	3,3,3	0.30	0	2,2,2	0.23	0
4	EDO	A	1008	-	3,3,3	0.45	0	2,2,2	0.27	0
3	GOL	A	1003	-	5,5,5	0.23	0	5,5,5	0.22	0
4	EDO	A	1011	-	3,3,3	0.48	0	2,2,2	0.13	0
4	EDO	B	1015	-	3,3,3	0.44	0	2,2,2	0.21	0
4	EDO	A	1014	-	3,3,3	0.39	0	2,2,2	0.09	0
6	PGE	B	1007	-	9,9,9	0.48	0	8,8,8	0.45	0
3	GOL	A	1007	-	5,5,5	0.26	0	5,5,5	0.42	0
4	EDO	B	1008	-	3,3,3	0.43	0	2,2,2	0.23	0
4	EDO	A	1019	-	3,3,3	0.39	0	2,2,2	0.25	0
4	EDO	A	1006	-	3,3,3	0.40	0	2,2,2	0.32	0
4	EDO	A	1018	-	3,3,3	0.23	0	2,2,2	0.14	0
3	GOL	A	1009	-	5,5,5	0.30	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
2	U4N	A	1001	-	-	2/23/31/31	0/5/5/5
3	GOL	A	1010	-	-	0/4/4/4	-
3	GOL	A	1002	-	-	0/4/4/4	-
4	EDO	A	1013	-	-	0/1/1/1	-
4	EDO	A	1012	-	-	1/1/1/1	-
4	EDO	B	1013	-	-	1/1/1/1	-
4	EDO	B	1014	-	-	0/1/1/1	-
5	PEG	B	1009	-	-	1/4/4/4	-
4	EDO	B	1003	-	-	0/1/1/1	-
3	GOL	B	1005	-	-	0/4/4/4	-
4	EDO	B	1012	-	-	0/1/1/1	-
5	PEG	B	1006	-	-	2/4/4/4	-
5	PEG	B	1004	-	-	1/4/4/4	-
4	EDO	B	1010	-	-	0/1/1/1	-
3	GOL	A	1017	-	-	0/4/4/4	-
4	EDO	A	1020	-	-	0/1/1/1	-
5	PEG	A	1021	-	-	0/4/4/4	-
3	GOL	B	1002	-	-	0/4/4/4	-
2	U4N	B	1001	-	-	3/23/31/31	0/5/5/5
3	GOL	A	1004	-	-	0/4/4/4	-
4	EDO	B	1011	-	-	0/1/1/1	-
3	GOL	A	1016	-	-	1/4/4/4	-
4	EDO	A	1015	-	-	0/1/1/1	-
4	EDO	A	1005	-	-	0/1/1/1	-
4	EDO	A	1008	-	-	1/1/1/1	-
3	GOL	A	1003	-	-	0/4/4/4	-
4	EDO	A	1011	-	-	0/1/1/1	-
4	EDO	B	1015	-	-	0/1/1/1	-
4	EDO	A	1014	-	-	0/1/1/1	-
6	PGE	B	1007	-	-	4/7/7/7	-
3	GOL	A	1007	-	-	0/4/4/4	-
4	EDO	B	1008	-	-	0/1/1/1	-
4	EDO	A	1019	-	-	0/1/1/1	-
4	EDO	A	1006	-	-	1/1/1/1	-
4	EDO	A	1018	-	-	0/1/1/1	-
3	GOL	A	1009	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	U4N	C5-C2	3.16	1.55	1.48
2	B	1001	U4N	C23-N27	3.12	1.38	1.34
2	B	1001	U4N	C5-C2	2.44	1.53	1.48
2	A	1001	U4N	C5-S6	2.23	1.82	1.78
2	A	1001	U4N	O14-C13	-2.15	1.34	1.39
2	A	1001	U4N	C23-N27	2.07	1.37	1.34
2	A	1001	U4N	C10-N9	-2.00	1.38	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	U4N	C21-N22-C23	9.74	124.31	116.81
2	A	1001	U4N	C21-N22-C23	8.27	123.18	116.81
2	A	1001	U4N	C25-N24-C23	6.00	120.43	115.42
2	B	1001	U4N	N24-C23-N22	-5.92	120.70	126.42
2	A	1001	U4N	N24-C23-N22	-5.83	120.78	126.42
2	B	1001	U4N	C13-O14-C15	5.79	130.12	117.47
2	B	1001	U4N	C26-C21-N22	-5.57	114.64	121.97
2	B	1001	U4N	C25-N24-C23	5.39	119.92	115.42
2	A	1001	U4N	C13-O14-C15	4.75	127.85	117.47
2	A	1001	U4N	C26-C21-N22	-4.63	115.86	121.97
2	B	1001	U4N	C25-C26-C21	3.12	120.21	117.20
2	B	1001	U4N	C26-C25-N24	-3.06	120.23	123.97
2	A	1001	U4N	C26-C25-N24	-2.89	120.43	123.97
2	A	1001	U4N	N27-C23-N22	2.88	121.61	117.09
2	B	1001	U4N	N27-C23-N22	2.23	120.59	117.09
2	A	1001	U4N	C25-C26-C21	2.16	119.29	117.20
2	A	1001	U4N	C18-C17-N16	-2.13	120.05	123.42
2	B	1001	U4N	C39-C10-N9	2.11	122.47	119.85
2	B	1001	U4N	O7-S6-C5	-2.02	104.36	108.06

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1007	PGE	O1-C1-C2-O2
3	A	1016	GOL	O1-C1-C2-C3
4	A	1008	EDO	O1-C1-C2-O2
5	B	1009	PEG	O1-C1-C2-O2
5	B	1006	PEG	O1-C1-C2-O2
6	B	1007	PGE	O3-C5-C6-O4
6	B	1007	PGE	O2-C3-C4-O3

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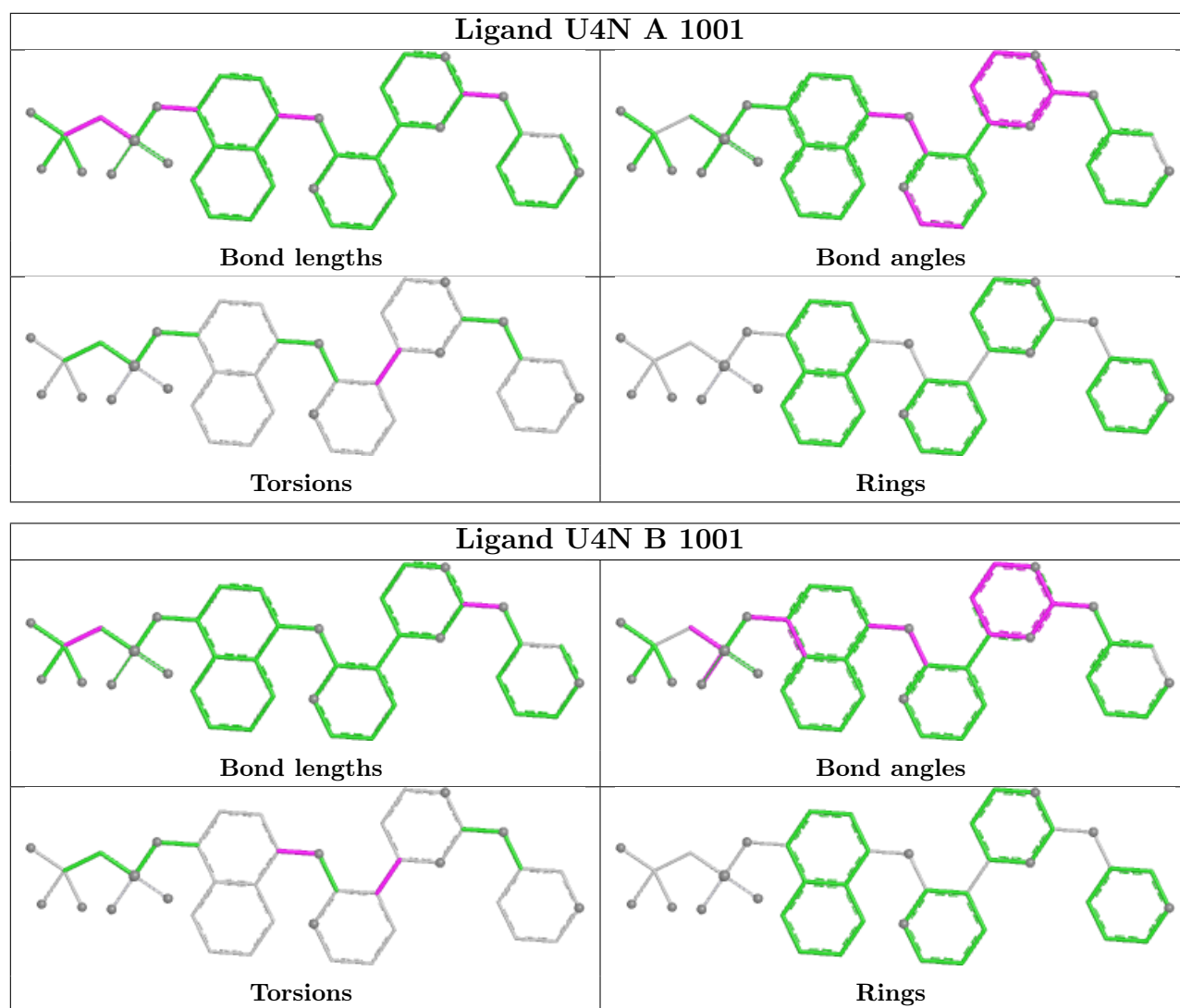
Mol	Chain	Res	Type	Atoms
5	B	1004	PEG	O2-C3-C4-O4
4	A	1012	EDO	O1-C1-C2-O2
2	B	1001	U4N	C19-C20-C21-C26
2	B	1001	U4N	C19-C20-C21-N22
6	B	1007	PGE	C6-C5-O3-C4
4	B	1013	EDO	O1-C1-C2-O2
2	A	1001	U4N	C19-C20-C21-C26
5	B	1006	PEG	C1-C2-O2-C3
2	A	1001	U4N	C19-C20-C21-N22
2	B	1001	U4N	C34-C13-O14-C15
4	A	1006	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1010	GOL	1	0
4	B	1013	EDO	2	0
4	B	1012	EDO	1	0
5	B	1006	PEG	2	0
3	B	1002	GOL	1	0
3	A	1016	GOL	1	0
4	A	1014	EDO	2	0
6	B	1007	PGE	1	0
4	A	1018	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	406/434 (93%)	0.31	38 (9%) 14 14	10, 32, 61, 129	35 (8%)
1	B	392/434 (90%)	0.68	46 (11%) 9 8	15, 39, 69, 110	39 (9%)
All	All	798/868 (91%)	0.49	84 (10%) 11 11	10, 36, 66, 129	74 (9%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	889	PHE	5.9
1	B	962	PHE	5.8
1	B	889	PHE	5.3
1	A	965	PRO	5.1
1	B	579	HIS	4.8
1	B	731	VAL	4.7
1	A	966	PRO	4.5
1	B	797	PRO	4.3
1	A	891	THR	4.3
1	B	615	LEU	4.2
1	B	721	GLY	4.1
1	A	615	LEU	4.1
1	B	663	LEU	4.0
1	B	662	GLY	3.9
1	A	658	PHE	3.8
1	A	579	HIS	3.8
1	B	796	HIS	3.7
1	A	581	ALA	3.6
1	A	620[A]	ASP	3.5
1	B	563	VAL	3.5
1	B	728	ARG	3.5
1	A	580	GLY	3.4
1	B	953[A]	HIS	3.4
1	B	620[A]	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	618[A]	GLU	3.3
1	B	619[A]	SER	3.2
1	B	890	ARG	3.1
1	A	720	VAL	3.1
1	A	888	LYS	3.1
1	A	561	THR	3.0
1	B	963	HIS	3.0
1	A	617[A]	ARG	3.0
1	B	585	ILE	2.9
1	B	744	SER	2.8
1	A	721	GLY	2.8
1	B	616	LEU	2.8
1	B	734	THR	2.8
1	B	572	CYS	2.8
1	A	616	LEU	2.8
1	A	959	PRO	2.8
1	B	779	LEU	2.7
1	A	892	TYR	2.7
1	B	668[A]	LEU	2.7
1	B	584	THR	2.7
1	B	722	ARG	2.7
1	A	729	SER	2.7
1	B	732	PRO	2.7
1	A	582	GLU	2.7
1	B	912	ARG	2.6
1	B	576	VAL	2.6
1	B	562	SER	2.6
1	A	608	PHE	2.6
1	A	660	HIS	2.5
1	B	733	GLY	2.5
1	A	963	HIS	2.5
1	B	787	LEU	2.5
1	B	628	TYR	2.4
1	A	614	GLN	2.4
1	B	655	GLN	2.4
1	B	564	VAL	2.4
1	B	720	VAL	2.4
1	A	887	ARG	2.3
1	B	778	SER	2.3
1	B	887	ARG	2.3
1	A	705	ILE	2.3
1	A	958	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	2.2
1	A	659	ALA	2.2
1	A	663	LEU	2.2
1	A	779	LEU	2.2
1	B	593	ASN	2.2
1	A	627	ARG	2.2
1	B	627	ARG	2.2
1	A	661	LEU	2.2
1	B	793[A]	ASP	2.1
1	B	798	GLU	2.1
1	B	606	PHE	2.1
1	B	786	LEU	2.1
1	A	728	ARG	2.1
1	B	854	LEU	2.1
1	A	890	ARG	2.1
1	A	628	TYR	2.0
1	B	884	THR	2.0
1	A	964	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	1015	4/4	0.53	0.26	85,86,102,103	0
4	EDO	B	1013	4/4	0.65	0.20	72,73,76,83	0
3	GOL	A	1017	6/6	0.67	0.21	54,71,73,81	0
4	EDO	A	1012	4/4	0.68	0.22	50,57,67,69	0
4	EDO	B	1008	4/4	0.68	0.20	67,69,74,79	0

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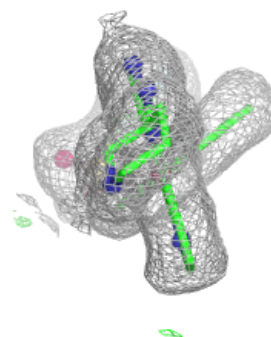
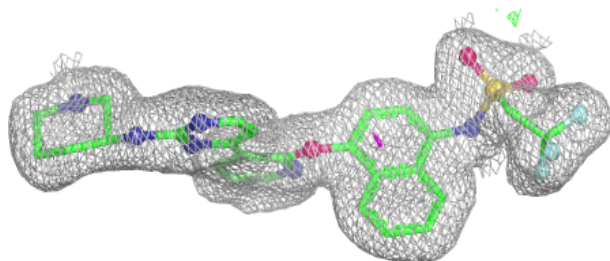
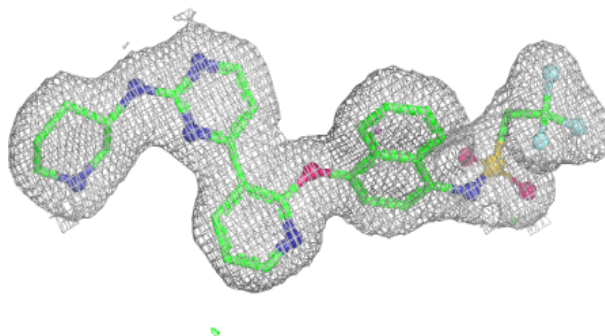
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1004	6/6	0.71	0.17	54,57,60,63	0
5	PEG	B	1004	7/7	0.71	0.24	68,81,85,87	0
6	PGE	B	1007	10/10	0.71	0.21	63,75,85,86	0
5	PEG	B	1009	7/7	0.72	0.25	62,72,81,103	0
3	GOL	A	1003	6/6	0.77	0.20	55,76,77,86	0
5	PEG	A	1021	7/7	0.78	0.20	50,68,79,85	0
4	EDO	B	1010	4/4	0.78	0.17	43,51,60,60	0
4	EDO	A	1015	4/4	0.78	0.23	51,71,72,75	0
3	GOL	A	1009	6/6	0.78	0.23	51,58,62,73	0
4	EDO	A	1013	4/4	0.79	0.14	73,74,76,79	0
4	EDO	A	1014	4/4	0.80	0.16	62,64,65,72	0
5	PEG	B	1006	7/7	0.80	0.21	57,74,87,95	0
4	EDO	A	1005	4/4	0.80	0.28	34,35,36,40	4
4	EDO	B	1011	4/4	0.80	0.17	50,55,56,59	0
4	EDO	A	1006	4/4	0.81	0.18	65,72,73,74	0
4	EDO	A	1019	4/4	0.81	0.22	58,58,65,73	0
4	EDO	B	1003	4/4	0.81	0.20	64,70,71,77	0
4	EDO	B	1014	4/4	0.81	0.24	57,61,62,67	0
3	GOL	A	1007	6/6	0.81	0.21	60,65,66,82	0
3	GOL	A	1002	6/6	0.83	0.21	58,59,73,74	0
3	GOL	B	1005	6/6	0.83	0.21	71,90,96,105	0
3	GOL	A	1016	6/6	0.83	0.18	56,61,67,71	0
4	EDO	A	1008	4/4	0.84	0.20	26,42,51,71	0
3	GOL	A	1010	6/6	0.86	0.18	43,56,70,71	0
4	EDO	A	1020	4/4	0.86	0.18	60,64,65,75	0
3	GOL	B	1002	6/6	0.87	0.15	55,68,75,81	0
4	EDO	A	1011	4/4	0.88	0.15	47,61,61,63	0
4	EDO	A	1018	4/4	0.89	0.17	42,52,53,60	0
4	EDO	B	1012	4/4	0.89	0.15	58,59,64,64	0
2	U4N	B	1001	39/39	0.97	0.06	27,34,45,58	0
2	U4N	A	1001	39/39	0.98	0.06	20,27,34,37	0

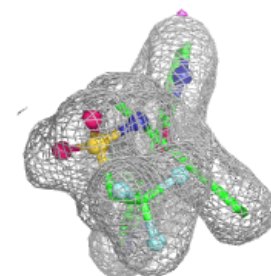
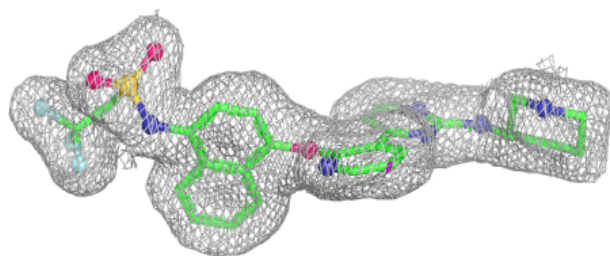
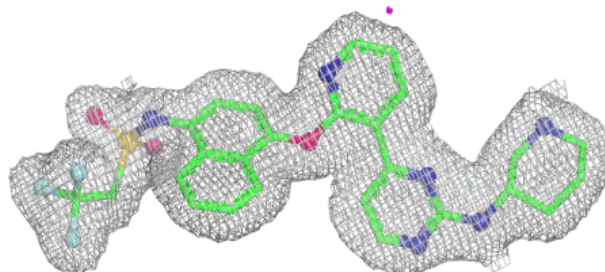
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U4N B 1001:

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

**Electron density around U4N A 1001:**

$2mF_o-DF_c$ (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.