



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:34 AM UTC

PDB ID : 5SFI / pdb_00005sfi
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH n1(nc(nc1CCc2nn3c(n2)c(ncc3C)C)N4[C@H](CCC4)C)C, micromolar IC₅₀=0.028433
Authors : Joseph, C.; Flohr, A.; Benz, J.; Schlatter, D.; Rudolph, M.G.
Deposited on : 2022-01-21
Resolution : 2.01 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

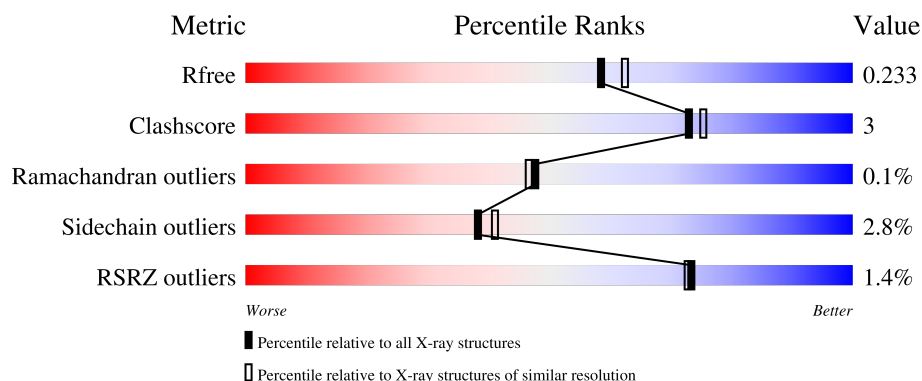
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	343	
1	B	343	
1	C	343	
1	D	343	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10835 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 cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2537	1622	431	460	24			
1	B	316	Total	C	N	O	S	0	1	0
			2559	1634	435	466	24			
1	C	314	Total	C	N	O	S	0	1	0
			2549	1629	433	463	24			
1	D	312	Total	C	N	O	S	0	0	0
			2528	1617	431	456	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	SER	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	SER	-	expression tag	UNP Q9Y233
C	447	GLY	-	expression tag	UNP Q9Y233
C	448	SER	-	expression tag	UNP Q9Y233
D	447	GLY	-	expression tag	UNP Q9Y233
D	448	SER	-	expression tag	UNP Q9Y233

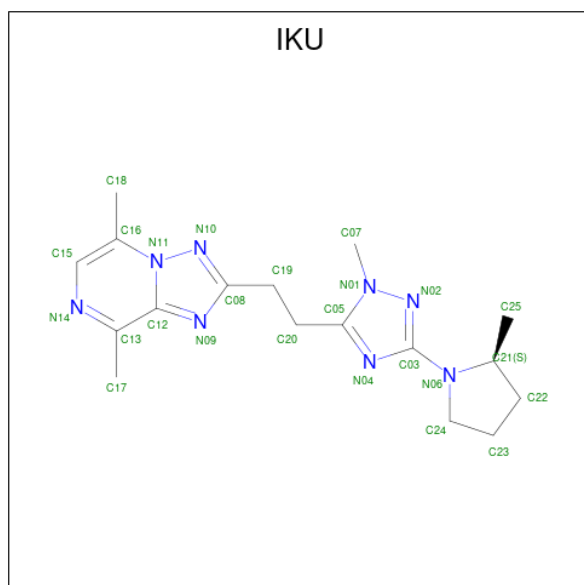
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

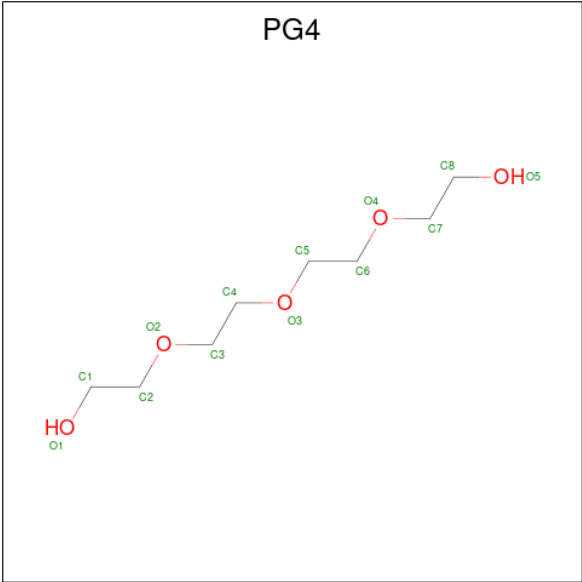
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (4S)-5,8-dimethyl-2-(2-{1-methyl-3-[(2S)-2-methylpyrrolidin-1-yl]-1H-1,2,4-triazol-5-yl}ethyl)[1,2,4]triazolo[1,5-a]pyrazine (CCD ID: IKU) (formula: C₁₇H₂₄N₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			25	17	8		
4	B	1	Total	C	N	0	0
			25	17	8		
4	C	1	Total	C	N	0	0
			25	17	8		
4	D	1	Total	C	N	0	0
			25	17	8		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			13	8	5		

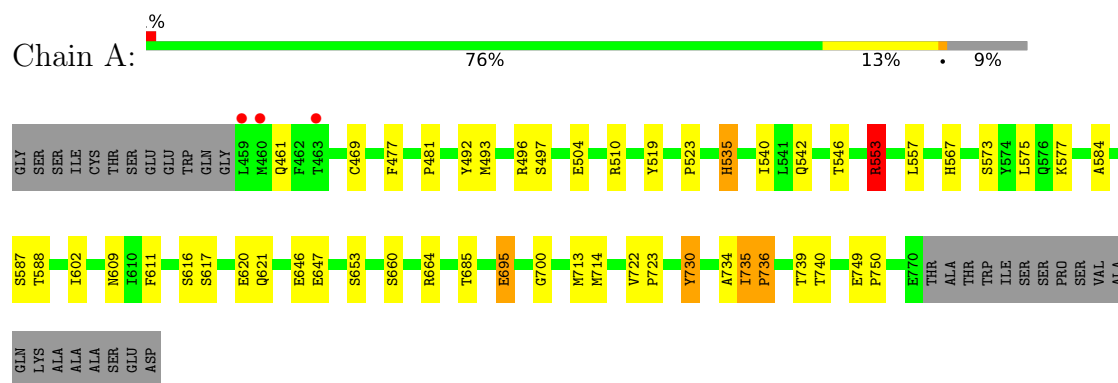
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	136	Total	O	0	0
			136	136		
6	B	174	Total	O	0	0
			174	174		
6	C	147	Total	O	0	0
			147	147		
6	D	84	Total	O	0	0
			84	84		

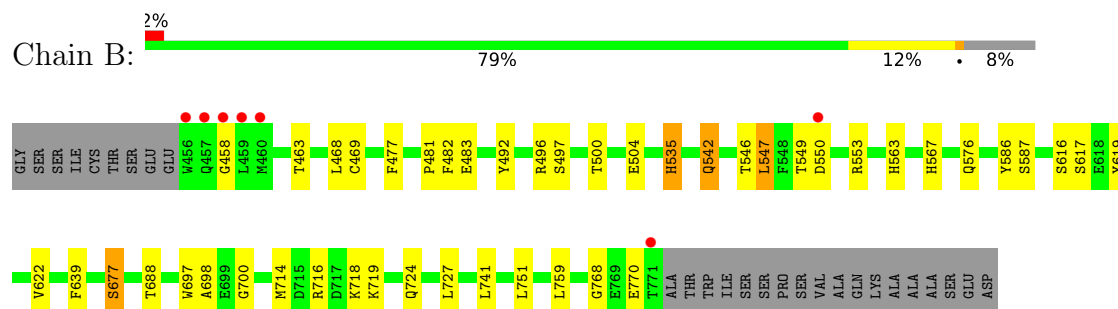
3 Residue-property plots [i](#)

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.

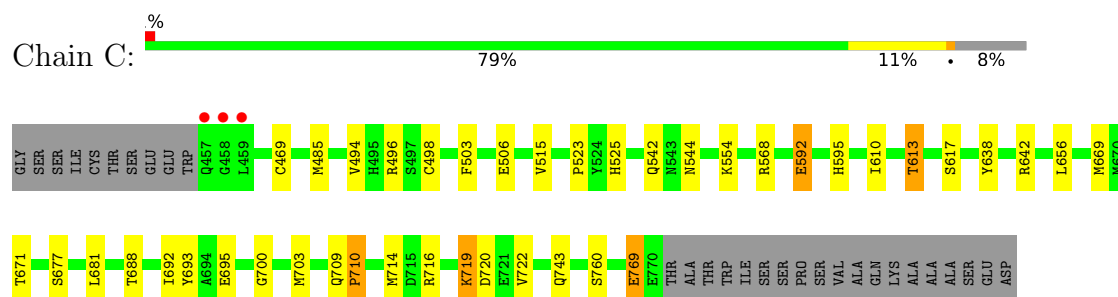
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



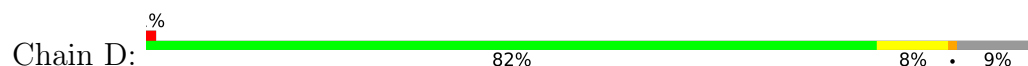
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

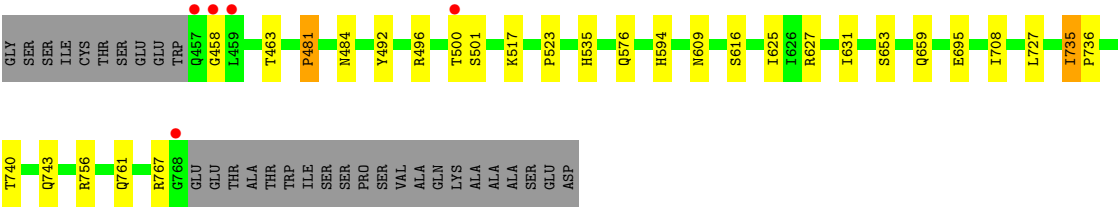


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	135.23Å 135.23Å 235.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.70 – 2.01 43.70 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.5 (43.70-2.01) 95.5 (43.70-2.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.170 , 0.228 0.178 , 0.233	Depositor DCC
R_{free} test set	5297 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10835	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, IKU, CME, PG4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.30	14/2588 (0.5%)	1.43	9/3502 (0.3%)
1	B	1.23	7/2613 (0.3%)	1.50	18/3535 (0.5%)
1	C	1.23	6/2603 (0.2%)	1.47	8/3522 (0.2%)
1	D	1.27	7/2579 (0.3%)	1.51	10/3490 (0.3%)
All	All	1.26	34/10383 (0.3%)	1.48	45/14049 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	535	HIS	CE1-NE2	8.24	1.40	1.32
1	A	481	PRO	C-O	-8.19	1.14	1.24
1	D	481	PRO	C-O	-7.74	1.15	1.23
1	A	730	TYR	C-O	7.10	1.32	1.24
1	C	710	PRO	C-O	-6.55	1.16	1.23
1	C	525	HIS	CE1-NE2	6.19	1.38	1.32
1	D	735	ILE	CA-CB	6.17	1.57	1.54
1	A	695	GLU	C-O	6.10	1.31	1.24
1	A	567	HIS	CE1-NE2	5.96	1.38	1.32
1	C	692	ILE	C-O	5.77	1.30	1.24
1	C	568	ARG	C-O	-5.75	1.16	1.23
1	B	563	HIS	CG-ND1	-5.59	1.32	1.38
1	A	584	ALA	C-O	-5.50	1.17	1.24
1	D	501	SER	C-O	-5.47	1.18	1.23
1	B	542	GLN	C-O	-5.45	1.17	1.24
1	C	669	MET	C-O	-5.43	1.17	1.24
1	A	740	THR	C-O	5.41	1.30	1.24
1	D	708	ILE	C-O	5.37	1.30	1.24
1	B	586	TYR	C-O	5.36	1.30	1.23
1	A	739	THR	C-O	5.35	1.30	1.24
1	B	481	PRO	C-O	-5.32	1.17	1.24
1	C	592	GLU	C-O	-5.32	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	685	THR	C-O	5.25	1.30	1.24
1	A	540	ILE	C-O	5.18	1.29	1.24
1	A	535	HIS	CE1-NE2	5.18	1.37	1.32
1	B	549	THR	C-O	5.14	1.30	1.23
1	B	567	HIS	CE1-NE2	5.14	1.37	1.32
1	B	677	SER	C-O	5.14	1.30	1.24
1	D	594	HIS	CE1-NE2	5.14	1.37	1.32
1	A	736	PRO	C-O	5.12	1.30	1.24
1	A	519	TYR	C-O	-5.12	1.17	1.23
1	A	611	PHE	C-O	5.07	1.30	1.24
1	A	620	GLU	C-O	5.07	1.30	1.24
1	D	625	ILE	C-O	5.01	1.29	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	ASN	CA-CB-CG	-8.66	103.94	112.60
1	C	613	THR	CB-CA-C	-7.43	99.21	110.88
1	B	639	PHE	CA-C-N	6.76	127.48	119.98
1	B	639	PHE	C-N-CA	6.76	127.48	119.98
1	A	553	ARG	CA-C-N	6.64	129.07	120.44
1	A	553	ARG	C-N-CA	6.64	129.07	120.44
1	D	458	GLY	CA-C-N	6.63	131.80	120.72
1	D	458	GLY	C-N-CA	6.63	131.80	120.72
1	B	535	HIS	CA-CB-CG	-6.38	107.42	113.80
1	D	535	HIS	CA-CB-CG	-6.37	107.43	113.80
1	A	602	ILE	N-CA-C	-6.15	104.50	110.72
1	B	616	SER	CA-C-N	6.08	128.67	120.65
1	B	616	SER	C-N-CA	6.08	128.67	120.65
1	B	504	GLU	CB-CA-C	6.03	119.54	109.89
1	A	735	ILE	CA-C-O	5.95	122.67	118.69
1	D	484	ASN	CA-CB-CG	-5.95	106.66	112.60
1	D	609	ASN	N-CA-CB	5.75	118.87	110.58
1	B	468	LEU	N-CA-C	-5.72	104.66	111.69
1	D	767	ARG	CA-C-O	-5.72	116.06	119.55
1	C	722	VAL	N-CA-CB	5.66	114.87	110.45
1	D	727	LEU	CA-C-N	5.65	126.25	119.98
1	D	727	LEU	C-N-CA	5.65	126.25	119.98
1	A	609	ASN	N-CA-CB	5.59	118.39	110.46
1	A	647	GLU	CA-C-O	-5.45	115.09	120.70
1	B	768	GLY	CA-C-N	5.40	128.52	120.31
1	B	768	GLY	C-N-CA	5.40	128.52	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	703	MET	N-CA-C	-5.37	105.42	111.28
1	B	619	TYR	N-CA-C	-5.37	105.34	111.14
1	B	718	LYS	CA-C-N	5.33	127.68	120.38
1	B	718	LYS	C-N-CA	5.33	127.68	120.38
1	B	482	PHE	CA-C-N	5.29	127.68	120.54
1	B	482	PHE	C-N-CA	5.29	127.68	120.54
1	A	546	THR	CA-CB-OG1	-5.26	101.70	109.60
1	C	544	ASN	N-CA-C	-5.22	104.72	111.71
1	C	719	LYS	CB-CA-C	-5.17	100.44	110.46
1	B	741	LEU	N-CA-C	-5.13	105.77	111.36
1	B	698	ALA	N-CA-C	-5.13	105.77	111.36
1	C	769	GLU	CB-CA-C	-5.12	102.73	111.02
1	B	483	GLU	CB-CA-C	-5.11	102.63	110.81
1	D	659	GLN	CA-C-N	5.03	127.02	120.28
1	D	659	GLN	C-N-CA	5.03	127.02	120.28
1	B	751	LEU	N-CA-C	-5.03	105.71	111.14
1	C	494	VAL	CA-C-O	-5.03	115.84	121.17
1	C	515	VAL	CA-C-O	-5.01	115.86	121.17
1	A	588	THR	CA-CB-OG1	-5.00	102.09	109.60

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	2537	0	2508	20	0
1	B	2559	0	2519	15	0
1	C	2549	0	2518	21	0
1	D	2528	0	2501	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	1	0
4	B	25	0	0	0	0
4	C	25	0	0	1	0
4	D	25	0	0	0	0
5	C	13	0	18	3	0
6	A	136	0	0	3	0
6	B	174	0	0	3	0
6	C	147	0	0	4	0
6	D	84	0	0	3	0
All	All	10835	0	10064	65	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 (65) 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:469:CYS:SG	6:A:1017:HOH:O	2.01	1.16
1:C:720:ASP:HB2	6:C:1006:HOH:O	1.85	0.76
1:B:497:SER:O	1:B:553:ARG:HD2	1.91	0.71
1:B:727:LEU:HD12	1:B:759:LEU:HD11	1.75	0.67
1:A:646:GLU:HG3	6:A:909:HOH:O	1.94	0.67
1:B:469:CYS:SG	6:B:1038:HOH:O	2.53	0.65
1:C:656:LEU:HG	5:C:804:PG4:H51	1.77	0.65
1:C:714:MET:HE2	6:C:987:HOH:O	1.97	0.64
1:B:546:THR:HG23	1:B:547:LEU:HD23	1.79	0.63
1:C:716:ARG:O	1:C:719:LYS:HG3	2.01	0.60
1:C:656:LEU:HG	5:C:804:PG4:C5	2.32	0.59
1:C:714:MET:CE	6:C:987:HOH:O	2.53	0.57
1:C:469:CYS:HB2	6:C:1025:HOH:O	2.07	0.54
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.89	0.54
1:B:727:LEU:HD12	1:B:759:LEU:CD1	2.38	0.54
1:D:627:ARG:O	1:D:631:ILE:HG12	2.08	0.53
1:C:656:LEU:H	5:C:804:PG4:H32	1.74	0.53
1:D:756:ARG:HG2	6:D:972:HOH:O	2.09	0.52
1:B:677:SER:HB2	1:B:688:THR:HG21	1.93	0.51
1:B:576:GLN:HG2	6:B:1037:HOH:O	2.10	0.50
1:A:617:SER:O	1:A:621:GLN:HG3	2.11	0.50
1:C:700:GLY:HA3	1:C:714:MET:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:ARG:HD3	6:D:972:HOH:O	2.11	0.49
1:A:700:GLY:HA3	1:A:714:MET:O	2.13	0.48
1:C:677:SER:HB2	1:C:688:THR:HG21	1.94	0.48
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.48	0.48
1:A:497:SER:O	1:A:553:ARG:HD2	2.13	0.47
1:B:550:ASP:N	1:B:550:ASP:OD1	2.47	0.47
1:C:498:CYS:SG	1:C:554:LYS:HG2	2.55	0.47
1:D:756:ARG:CD	6:D:972:HOH:O	2.62	0.46
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.15	0.46
1:C:523:PRO:HD2	1:C:695:GLU:HG3	1.99	0.45
1:A:497:SER:OG	1:A:557:LEU:HD11	2.17	0.44
1:B:700:GLY:HA3	1:B:714:MET:O	2.18	0.44
1:A:730:TYR:HA	1:A:734:ALA:HB3	2.00	0.44
1:B:724:GLN:NE2	6:B:901:HOH:O	2.36	0.44
1:A:542:GLN:NE2	1:A:542:GLN:HA	2.33	0.44
1:C:693:TYR:OH	4:C:803:IKU:N04	2.51	0.44
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.52	0.44
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.53	0.44
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.33	0.44
1:A:660:SER:O	1:A:664:ARG:HG3	2.17	0.43
1:B:716:ARG:O	1:B:719:LYS:HB2	2.18	0.43
1:D:761:GLN:HE21	1:D:761:GLN:HA	1.84	0.43
1:C:503:PHE:CE1	1:C:610:ILE:HD12	2.53	0.43
1:B:697:TRP:CH2	1:B:719:LYS:HG3	2.52	0.43
1:C:709:GLN:HE21	1:C:710:PRO:HD2	1.84	0.43
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.54	0.43
1:A:735:ILE:N	1:A:736:PRO:HD2	2.34	0.43
1:D:740:THR:HA	1:D:743:GLN:HE21	1.84	0.42
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.54	0.42
1:A:713:MET:HB2	6:A:960:HOH:O	2.19	0.42
1:B:477:PHE:HB3	1:B:535:HIS:CE1	2.54	0.42
1:C:743:GLN:HE21	1:C:743:GLN:HB2	1.57	0.42
1:A:713:MET:HE2	4:A:803:IKU:C07	2.49	0.42
1:A:749:GLU:N	1:A:750:PRO:CD	2.83	0.42
1:C:709:GLN:NE2	1:C:710:PRO:HD2	2.35	0.42
1:A:493:MET:SD	1:A:535:HIS:HA	2.60	0.41
1:A:523:PRO:HD2	1:A:695:GLU:HG2	2.03	0.41
1:B:497:SER:HA	1:B:542:GLN:NE2	2.36	0.41
1:D:523:PRO:HD2	1:D:695:GLU:HG2	2.02	0.41
1:C:592:GLU:HA	1:C:595:HIS:CD2	2.56	0.41
1:D:735:ILE:HB	1:D:736:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:OE1	1:A:461:GLN:HA	2.21	0.41
1:A:722:VAL:HB	1:A:723:PRO:HD3	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	309/343 (90%)	303 (98%)	6 (2%)	0	100	100
1	B	314/343 (92%)	306 (98%)	7 (2%)	1 (0%)	36	35
1	C	312/343 (91%)	305 (98%)	7 (2%)	0	100	100
1	D	309/343 (90%)	302 (98%)	7 (2%)	0	100	100
All	All	1244/1372 (91%)	1216 (98%)	27 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	458	GLY

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	281/305 (92%)	272 (97%)	9 (3%)	34	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	282/305 (92%)	275 (98%)	7 (2%)	42	45
1	C	282/305 (92%)	273 (97%)	9 (3%)	34	35
1	D	279/305 (92%)	272 (98%)	7 (2%)	42	45
All	All	1124/1220 (92%)	1092 (97%)	32 (3%)	38	41

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	504	GLU
1	A	510	ARG
1	A	553	ARG
1	A	573	SER
1	A	575	LEU
1	A	577	LYS
1	A	587	SER
1	A	616	SER
1	A	653	SER
1	B	463	THR
1	B	500	THR
1	B	547	LEU
1	B	587	SER
1	B	617	SER
1	B	622	VAL
1	B	770	GLU
1	C	485	MET
1	C	496	ARG
1	C	506	GLU
1	C	613	THR
1	C	617	SER
1	C	681	LEU
1	C	760[A]	SER
1	C	760[B]	SER
1	C	769	GLU
1	D	463	THR
1	D	481	PRO
1	D	500	THR
1	D	517	LYS
1	D	576	GLN
1	D	616	SER
1	D	653	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	542	GLN
1	A	598	GLN
1	A	604	GLN
1	A	726	GLN
1	A	743	GLN
1	A	761	GLN
1	B	484	ASN
1	B	542	GLN
1	B	604	GLN
1	B	644	GLN
1	B	650	GLN
1	B	659	GLN
1	B	724	GLN
1	B	726	GLN
1	C	495	HIS
1	C	542	GLN
1	C	604	GLN
1	C	659	GLN
1	C	709	GLN
1	C	726	GLN
1	C	743	GLN
1	D	484	ASN
1	D	604	GLN
1	D	726	GLN
1	D	743	GLN
1	D	761	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CME	D	509	1	8,9,10	0.63	0	6,9,11	0.60	0
1	CME	C	509	1	8,9,10	0.72	0	6,9,11	0.68	0
1	CME	B	509	1	8,9,10	0.50	0	6,9,11	0.83	0
1	CME	A	509	1	8,9,10	0.40	0	6,9,11	1.09	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
1	CME	D	509	1	-	0/5/8/10	-
1	CME	C	509	1	-	1/5/8/10	-
1	CME	B	509	1	-	2/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	509	CME	SD-CE-CZ-OH
1	C	509	CME	SD-CE-CZ-OH
1	A	509	CME	SD-CE-CZ-OH
1	B	509	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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$
5	PG4	C	804	-	12,12,12	0.36	0	11,11,11	0.47	0
4	IKU	D	803	-	25,28,28	2.55	9 (36%)	23,41,41	2.67	11 (47%)
4	IKU	B	803	-	25,28,28	2.36	8 (32%)	23,41,41	2.76	12 (52%)
4	IKU	C	803	-	25,28,28	2.16	7 (28%)	23,41,41	2.34	9 (39%)
4	IKU	A	803	-	25,28,28	2.19	8 (32%)	23,41,41	2.60	10 (43%)

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	PG4	C	804	-	-	7/10/10/10	-
4	IKU	D	803	-	-	0/6/19/19	0/4/4/4
4	IKU	B	803	-	-	0/6/19/19	0/4/4/4
4	IKU	C	803	-	-	0/6/19/19	0/4/4/4
4	IKU	A	803	-	-	0/6/19/19	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	803	IKU	C13-N14	7.34	1.42	1.32
4	B	803	IKU	C13-N14	7.13	1.42	1.32
4	C	803	IKU	C05-N01	5.72	1.39	1.34
4	A	803	IKU	C13-N14	5.30	1.39	1.32
4	C	803	IKU	C13-N14	5.07	1.39	1.32
4	D	803	IKU	N11-N10	-4.64	1.30	1.38
4	B	803	IKU	C16-N11	4.62	1.45	1.37
4	A	803	IKU	C24-N06	-4.41	1.39	1.47
4	B	803	IKU	C20-C05	4.21	1.54	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	IKU	N11-N10	-4.20	1.30	1.38
4	D	803	IKU	C22-C21	-4.03	1.46	1.53
4	D	803	IKU	C20-C05	3.59	1.54	1.49
4	D	803	IKU	C16-N11	3.50	1.43	1.37
4	C	803	IKU	C08-N10	3.28	1.37	1.32
4	B	803	IKU	C24-N06	-3.19	1.41	1.47
4	C	803	IKU	C20-C05	3.10	1.53	1.49
4	C	803	IKU	C16-N11	3.09	1.42	1.37
4	A	803	IKU	C22-C21	-3.03	1.48	1.53
4	D	803	IKU	C08-N09	-2.95	1.32	1.37
4	A	803	IKU	C12-N11	-2.67	1.34	1.38
4	B	803	IKU	C22-C21	-2.61	1.49	1.53
4	A	803	IKU	C05-N04	2.59	1.37	1.32
4	A	803	IKU	C20-C05	2.57	1.52	1.49
4	D	803	IKU	C05-N04	2.54	1.37	1.32
4	B	803	IKU	C05-N04	2.47	1.36	1.32
4	D	803	IKU	C24-N06	-2.37	1.43	1.47
4	B	803	IKU	C17-C13	-2.31	1.45	1.49
4	B	803	IKU	N11-N10	-2.23	1.34	1.38
4	C	803	IKU	C21-N06	-2.20	1.40	1.48
4	A	803	IKU	C21-N06	-2.09	1.41	1.48
4	D	803	IKU	C18-C16	-2.08	1.46	1.49
4	C	803	IKU	C05-N04	2.03	1.36	1.32

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	IKU	C18-C16-N11	6.45	125.83	118.00
4	D	803	IKU	C12-N11-N10	-5.24	105.53	112.80
4	A	803	IKU	N10-C08-N09	-5.13	108.45	115.26
4	A	803	IKU	C07-N01-N02	5.08	126.89	119.29
4	D	803	IKU	C17-C13-N14	5.06	123.51	116.83
4	B	803	IKU	C17-C13-C12	5.05	123.89	117.55
4	D	803	IKU	C16-N11-N10	4.84	133.23	125.74
4	C	803	IKU	C17-C13-N14	4.77	123.12	116.83
4	A	803	IKU	C12-N11-N10	-4.58	106.45	112.80
4	C	803	IKU	C19-C20-C05	-4.42	107.44	111.62
4	A	803	IKU	C19-C20-C05	-4.13	107.72	111.62
4	B	803	IKU	N10-C08-N09	-4.08	109.84	115.26
4	B	803	IKU	C12-N11-N10	-3.97	107.29	112.80
4	B	803	IKU	C07-N01-N02	3.92	125.16	119.29
4	B	803	IKU	C19-C20-C05	-3.89	107.94	111.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	IKU	N06-C03-N04	3.88	130.10	119.34
4	C	803	IKU	C18-C16-N11	3.69	122.47	118.00
4	D	803	IKU	N10-C08-N09	-3.66	110.40	115.26
4	C	803	IKU	C19-C08-N09	3.59	128.38	120.27
4	A	803	IKU	C18-C16-N11	3.57	122.33	118.00
4	A	803	IKU	N06-C03-N04	3.53	129.13	119.34
4	B	803	IKU	N06-C03-N04	3.42	128.84	119.34
4	D	803	IKU	C07-N01-N02	3.37	124.33	119.29
4	A	803	IKU	C17-C13-N14	3.18	121.03	116.83
4	D	803	IKU	C15-C16-N11	3.15	119.82	115.22
4	A	803	IKU	C19-C08-N09	3.12	127.31	120.27
4	D	803	IKU	C22-C21-N06	3.11	106.54	102.41
4	D	803	IKU	C24-N06-C03	-2.92	112.01	122.76
4	D	803	IKU	N06-C03-N04	2.65	126.70	119.34
4	B	803	IKU	C18-C16-C15	-2.61	118.36	123.06
4	C	803	IKU	C12-N11-N10	-2.59	109.21	112.80
4	C	803	IKU	C07-N01-N02	2.58	123.15	119.29
4	D	803	IKU	C18-C16-N11	2.52	121.05	118.00
4	C	803	IKU	N10-C08-N09	-2.46	112.00	115.26
4	A	803	IKU	C24-N06-C03	-2.45	113.75	122.76
4	C	803	IKU	C24-N06-C03	-2.25	114.49	122.76
4	B	803	IKU	C16-N11-N10	2.24	129.21	125.74
4	A	803	IKU	C16-N11-N10	2.23	129.20	125.74
4	D	803	IKU	C18-C16-C15	-2.20	119.11	123.06
4	B	803	IKU	C19-C08-N09	2.14	125.10	120.27
4	B	803	IKU	C22-C21-N06	2.08	105.17	102.41
4	B	803	IKU	C24-N06-C03	-2.05	115.22	122.76

There are no chirality outliers.

All (7) torsion outliers are listed below:

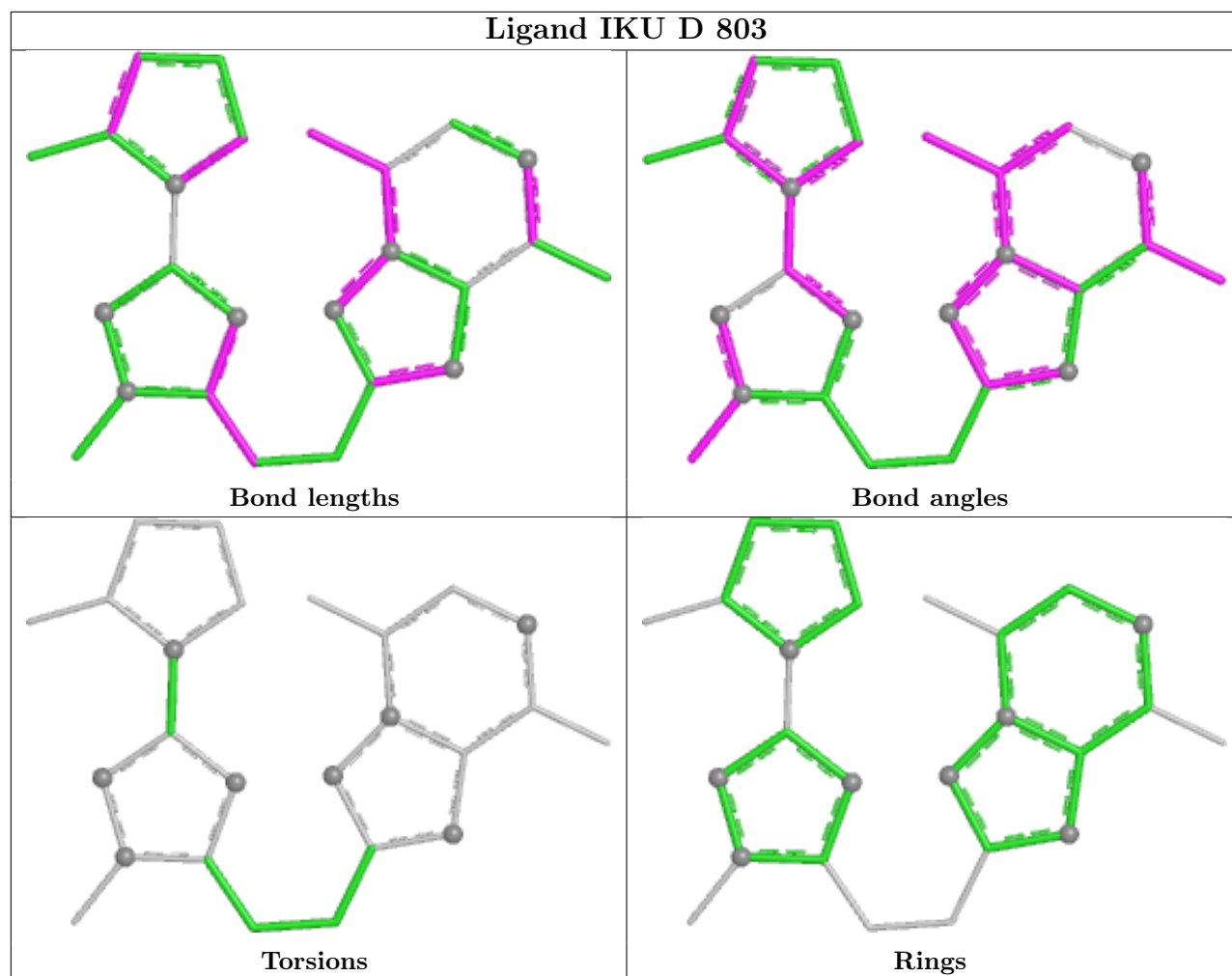
Mol	Chain	Res	Type	Atoms
5	C	804	PG4	O2-C3-C4-O3
5	C	804	PG4	C8-C7-O4-C6
5	C	804	PG4	O3-C5-C6-O4
5	C	804	PG4	O4-C7-C8-O5
5	C	804	PG4	C5-C6-O4-C7
5	C	804	PG4	C4-C3-O2-C2
5	C	804	PG4	C6-C5-O3-C4

There are no ring outliers.

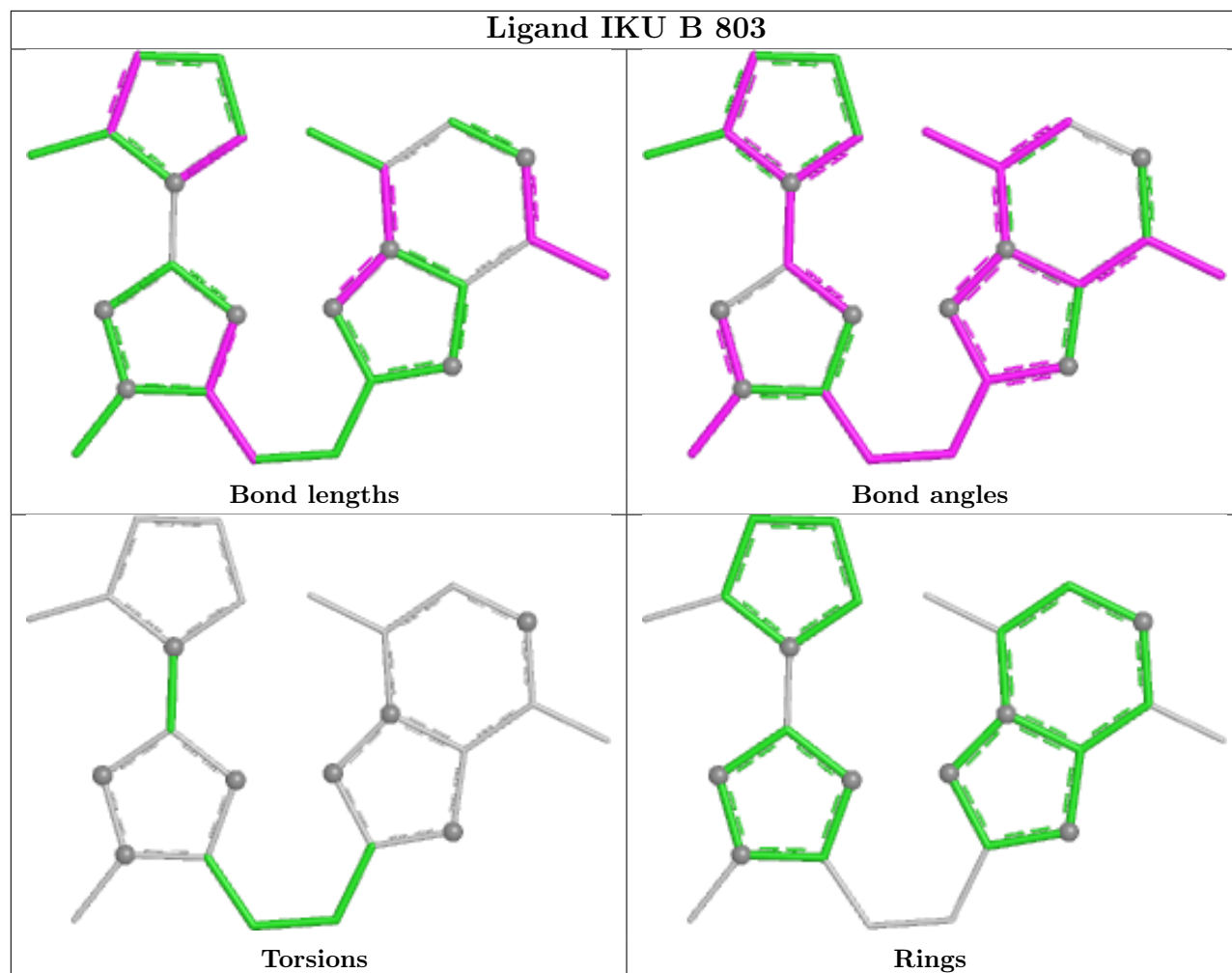
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	804	PG4	3	0
4	C	803	IKU	1	0
4	A	803	IKU	1	0

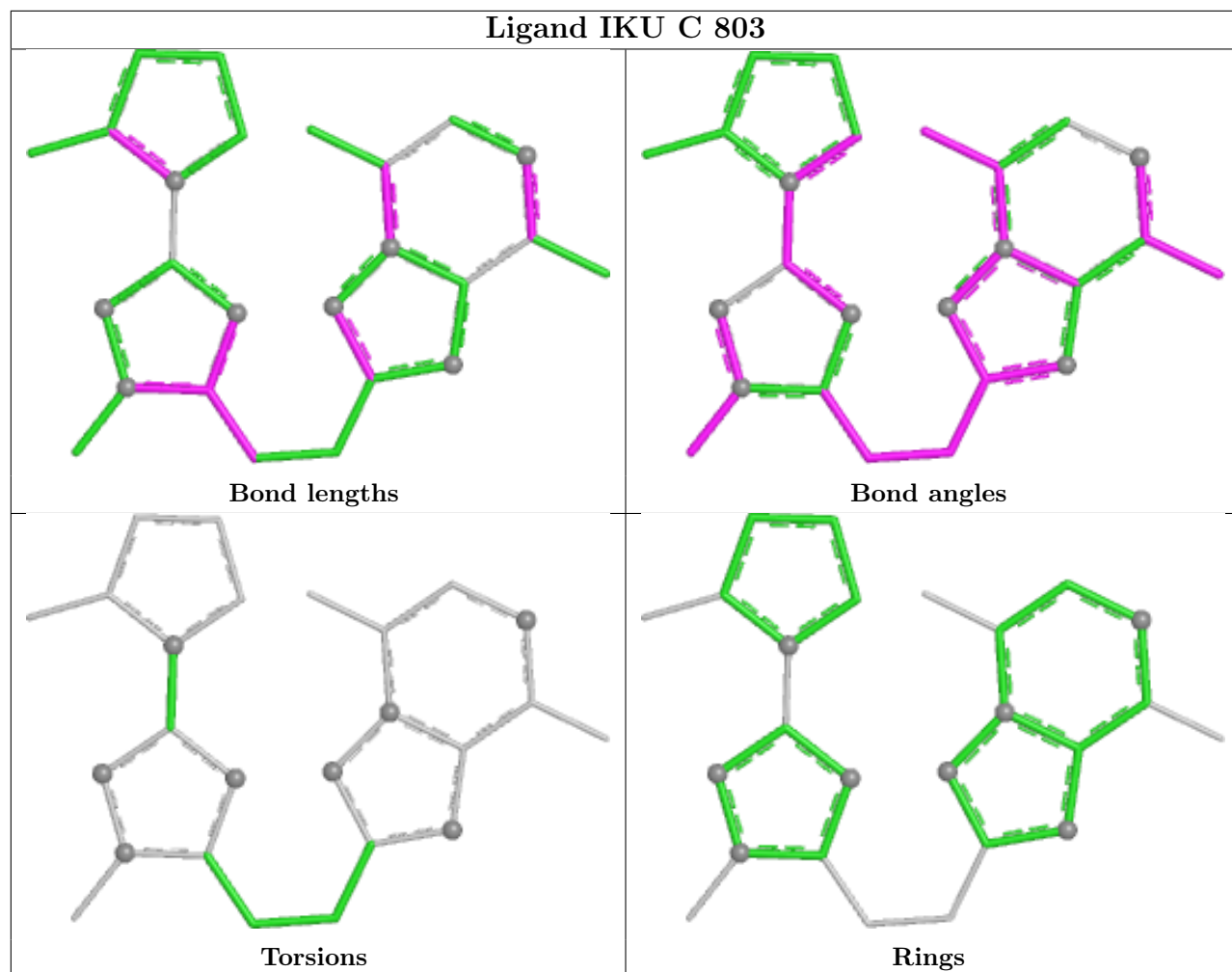
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

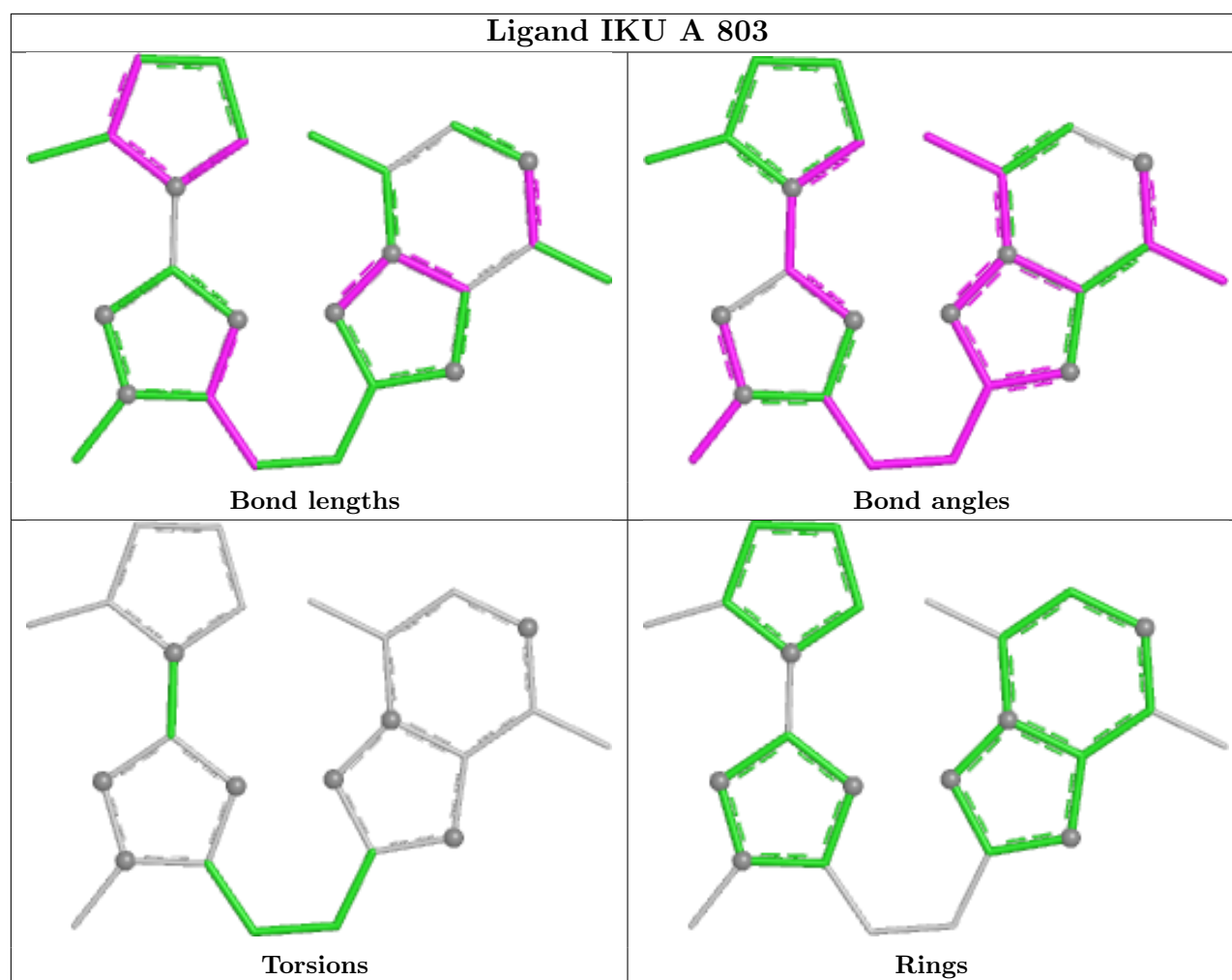


Ligand IKU B 803



Ligand IKU C 803





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	311/343 (90%)	-0.21	3 (0%) 79 79	24, 35, 63, 90	0
1	B	315/343 (91%)	-0.20	7 (2%) 62 61	24, 34, 64, 102	1 (0%)
1	C	313/343 (91%)	-0.18	3 (0%) 79 79	25, 36, 60, 93	1 (0%)
1	D	311/343 (90%)	0.08	5 (1%) 70 70	32, 43, 69, 89	0
All	All	1250/1372 (91%)	-0.13	18 (1%) 73 73	24, 38, 64, 102	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	LEU	5.2
1	D	457	GLN	4.3
1	B	771	THR	4.3
1	D	768	GLY	4.2
1	B	456	TRP	3.9
1	D	459	LEU	3.7
1	C	459	LEU	3.6
1	B	459	LEU	3.4
1	C	458	GLY	2.7
1	B	458	GLY	2.5
1	A	460	MET	2.4
1	B	460	MET	2.4
1	C	457	GLN	2.3
1	D	458	GLY	2.2
1	B	457	GLN	2.2
1	A	463	THR	2.2
1	B	550	ASP	2.2
1	D	500	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CME	D	509	10/11	0.85	0.15	41,59,99,99	0
1	CME	C	509	10/11	0.88	0.14	38,44,82,87	0
1	CME	A	509	10/11	0.88	0.15	37,48,87,97	0
1	CME	B	509	10/11	0.90	0.13	33,42,84,90	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

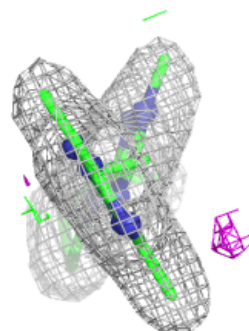
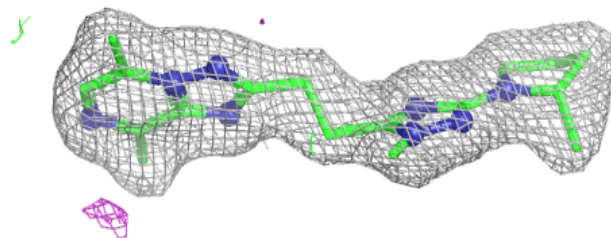
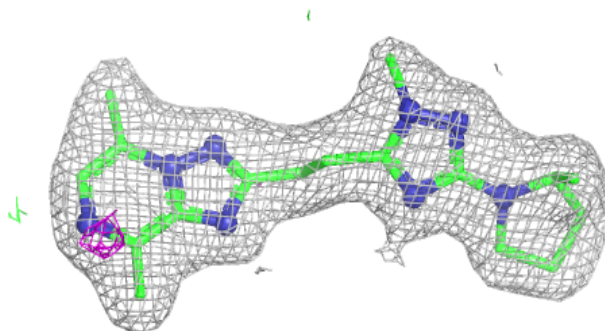
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PG4	C	804	13/13	0.88	0.12	51,58,68,70	0
4	IKU	B	803	25/25	0.97	0.06	23,29,39,40	0
4	IKU	C	803	25/25	0.97	0.06	26,33,39,41	0
4	IKU	D	803	25/25	0.97	0.06	30,37,46,49	0
4	IKU	A	803	25/25	0.97	0.06	27,29,39,46	0
3	MG	D	802	1/1	0.99	0.02	37,37,37,37	0
3	MG	B	802	1/1	0.99	0.01	24,24,24,24	0
3	MG	C	802	1/1	0.99	0.03	27,27,27,27	0
2	ZN	D	801	1/1	1.00	0.02	36,36,36,36	0
3	MG	A	802	1/1	1.00	0.02	27,27,27,27	0
2	ZN	A	801	1/1	1.00	0.01	31,31,31,31	0
2	ZN	B	801	1/1	1.00	0.01	29,29,29,29	0
2	ZN	C	801	1/1	1.00	0.01	31,31,31,31	0

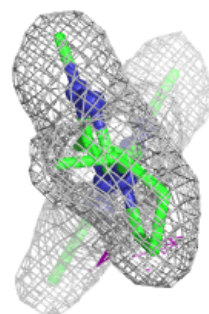
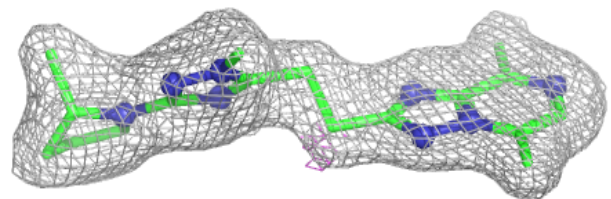
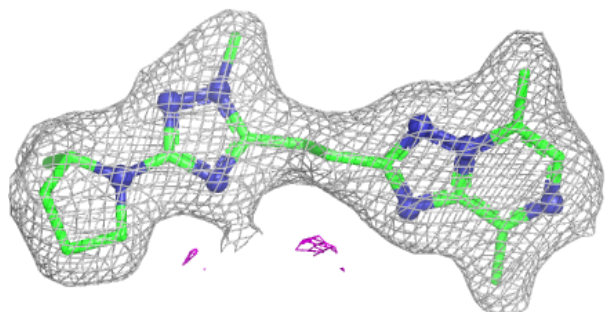
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IKU B 803:

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

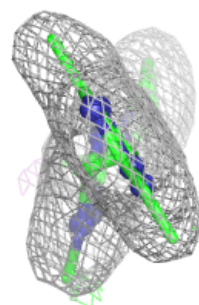
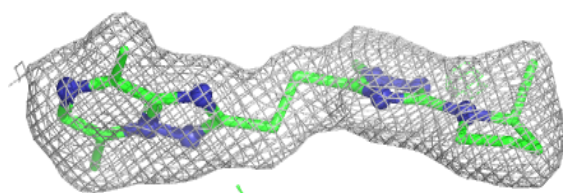
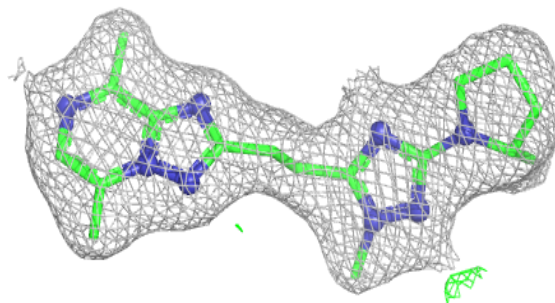
**Electron density around IKU C 803:**

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

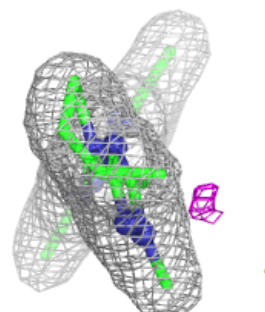
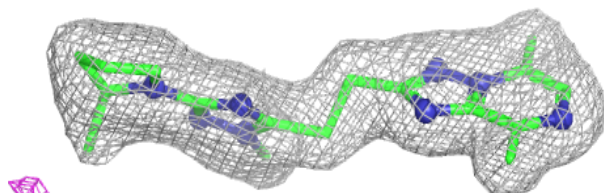
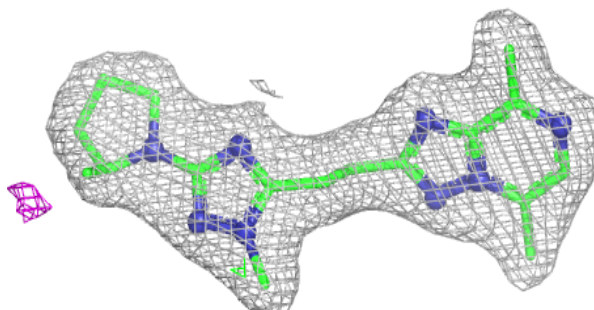


Electron density around IKU D 803:

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

**Electron density around IKU A 803:**

$2mF_o-DF_c$ (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.