



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:03 AM UTC

PDB ID : 5SGI / pdb_00005sgi
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH n2c(nc1[nH]cnc1c2Oc3cc(ccc3)C)N5CCN(c4ncccc4)CC5, micromolar IC₅₀=0.035
Authors : Joseph, C.; Benz, J.; Flohr, A.; Brunner, M.; Rudolph, M.G.
Deposited on : 2022-02-01
Resolution : 1.97 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

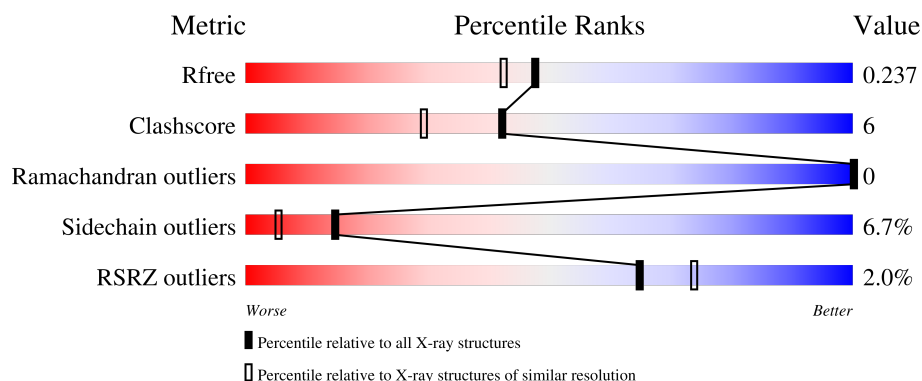
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	0% 77% 13% • 8%
1	B	343	2% 71% 17% • 8%
1	C	343	0% 75% 14% • 9%
1	D	343	2% 73% 16% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	803	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11121 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	314	Total	C	N	O	S	0	6	0
			2578	1648	436	468	26			
1	B	315	Total	C	N	O	S	0	5	0
			2579	1648	437	469	25			
1	C	313	Total	C	N	O	S	0	7	0
			2576	1648	437	466	25			
1	D	313	Total	C	N	O	S	0	5	0
			2566	1641	437	463	25			

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

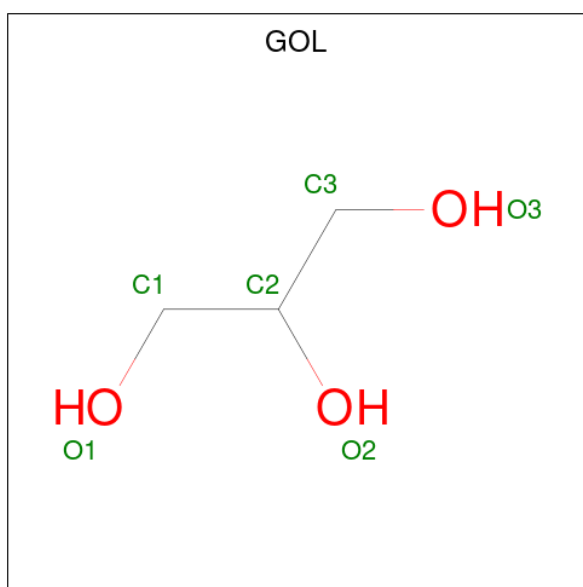
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

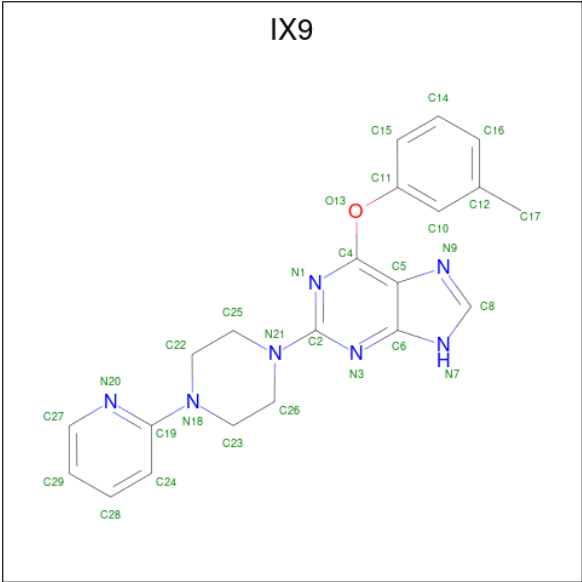
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is 6-(3-methylphenoxy)-2-[4-(pyridin-2-yl)piperazin-1-yl]-9H-purine (CCD ID: IX9) (formula: C₂₁H₂₁N₇O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			29	21	7	1		
5	B	1	Total	C	N	O	0	0
			29	21	7	1		
5	C	1	Total	C	N	O	0	0
			29	21	7	1		
5	D	1	Total	C	N	O	0	0
			29	21	7	1		

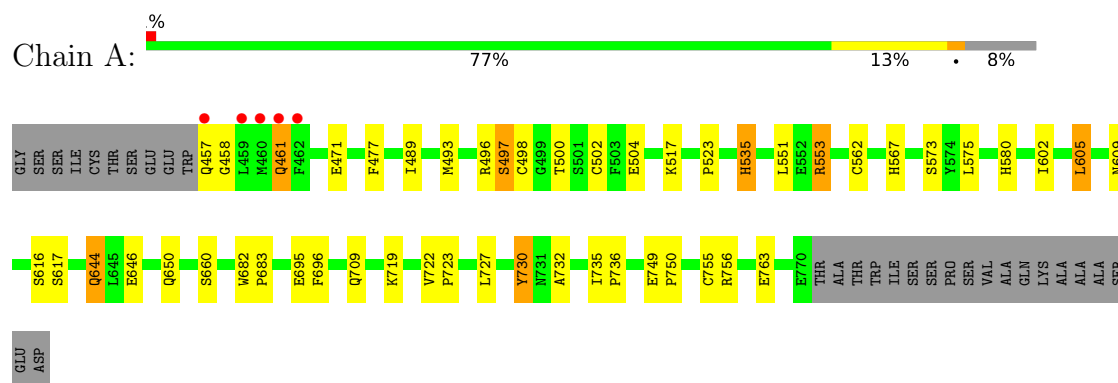
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	167	Total	O	0	0
			167	167		
6	B	190	Total	O	0	0
			190	190		
6	C	187	Total	O	0	0
			187	187		
6	D	142	Total	O	0	0
			142	142		

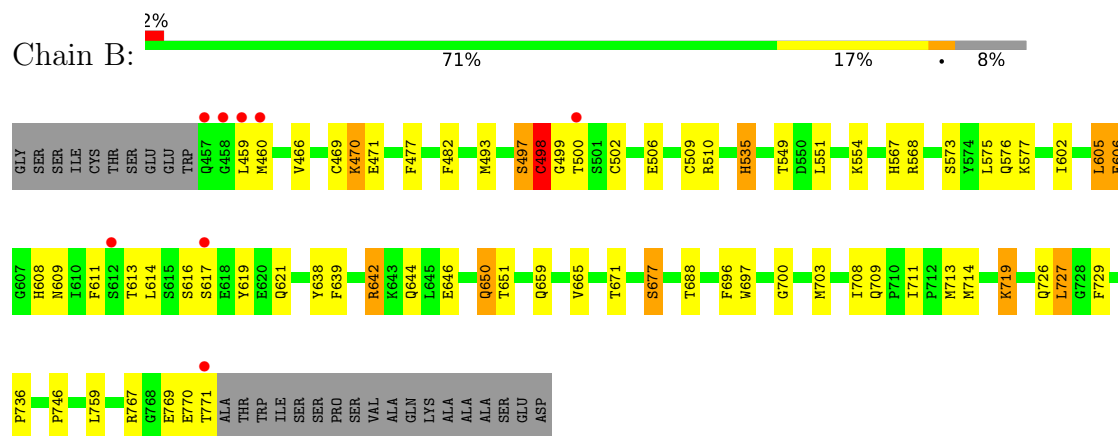
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

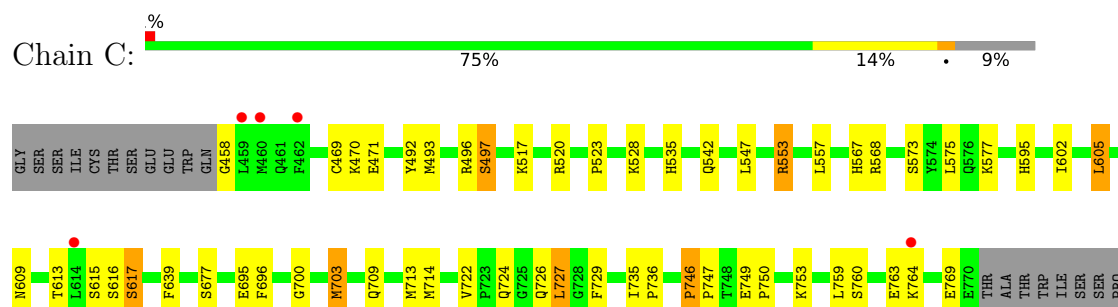
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



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

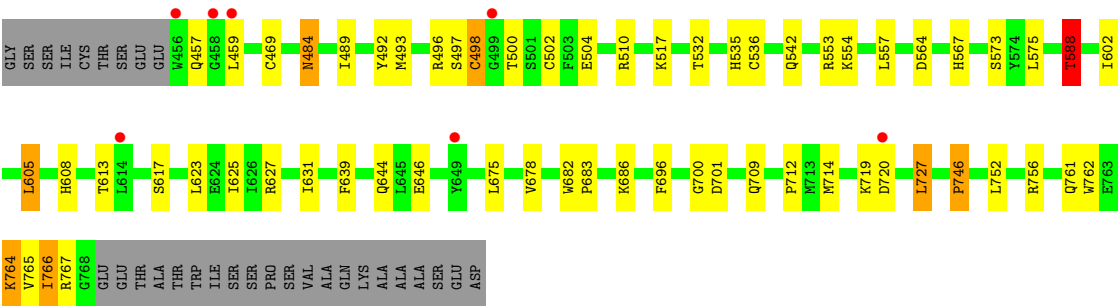


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



SER
VAL
ALA
GLN
LYS
ALA
ALA
ALA
SER
GLU
ASP

● 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	135.86Å 135.86Å 235.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.63 – 1.97 41.63 – 1.97	Depositor EDS
% Data completeness (in resolution range)	85.5 (41.63-1.97) 85.5 (41.63-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.235 0.189 , 0.237	Depositor DCC
R_{free} test set	5440 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11121	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: IX9, CME, MG, GOL, 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	1.19	6/2647 (0.2%)	1.39	4/3580 (0.1%)
1	B	1.17	4/2645 (0.2%)	1.48	20/3578 (0.6%)
1	C	1.17	4/2648 (0.2%)	1.44	15/3581 (0.4%)
1	D	1.15	1/2632 (0.0%)	1.49	15/3560 (0.4%)
All	All	1.17	15/10572 (0.1%)	1.45	54/14299 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	730	TYR	C-O	7.64	1.33	1.24
1	B	567	HIS	CE1-NE2	6.89	1.39	1.32
1	A	567	HIS	CE1-NE2	6.69	1.39	1.32
1	D	625	ILE	C-O	6.48	1.31	1.24
1	C	528	LYS	C-O	6.26	1.31	1.24
1	C	567	HIS	CE1-NE2	6.06	1.38	1.32
1	C	553	ARG	C-O	5.91	1.30	1.24
1	B	549	THR	C-O	5.87	1.31	1.23
1	B	535	HIS	CE1-NE2	5.69	1.38	1.32
1	A	580	HIS	CE1-NE2	5.53	1.38	1.32
1	A	562	CYS	C-O	5.52	1.31	1.24
1	A	535	HIS	CE1-NE2	5.35	1.37	1.32
1	C	595	HIS	CE1-NE2	5.21	1.37	1.32
1	B	736	PRO	C-O	5.17	1.30	1.24
1	A	732	ALA	C-O	5.04	1.30	1.24

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	498	CYS	CB-CA-C	7.81	121.32	109.13
1	D	535	HIS	CA-CB-CG	-7.07	106.73	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	746	PRO	N-CA-C	7.04	119.29	110.70
1	D	588	THR	CA-CB-OG1	-6.57	99.75	109.60
1	A	609	ASN	CA-CB-CG	-6.56	106.04	112.60
1	B	609	ASN	N-CA-CB	6.49	119.68	110.46
1	C	470	LYS	N-CA-CB	-6.15	101.02	110.13
1	D	532	THR	CA-CB-OG1	-6.14	100.39	109.60
1	B	650	GLN	CB-CG-CD	-6.00	102.40	112.60
1	B	651	THR	CA-CB-OG1	-5.96	100.66	109.60
1	D	554	LYS	CA-C-N	5.93	126.56	119.98
1	D	554	LYS	C-N-CA	5.93	126.56	119.98
1	B	609	ASN	CA-CB-CG	-5.83	106.77	112.60
1	C	703	MET	N-CA-C	-5.70	104.97	111.07
1	C	609	ASN	CA-CB-CG	-5.69	106.91	112.60
1	B	535	HIS	CA-CB-CG	-5.68	108.12	113.80
1	D	712	PRO	CA-C-N	5.50	127.66	120.28
1	D	712	PRO	C-N-CA	5.50	127.66	120.28
1	C	617	SER	O-C-N	5.50	128.49	122.11
1	D	746	PRO	N-CA-C	5.49	117.40	110.70
1	D	765	VAL	N-CA-C	-5.46	105.05	110.62
1	C	458	GLY	CA-C-N	5.46	127.60	120.28
1	C	458	GLY	C-N-CA	5.46	127.60	120.28
1	B	619	TYR	N-CA-C	-5.45	105.26	111.14
1	B	466	VAL	CA-C-O	-5.38	115.82	121.41
1	C	617	SER	CA-C-N	5.37	127.47	120.28
1	C	617	SER	C-N-CA	5.37	127.47	120.28
1	C	609	ASN	N-CA-CB	5.36	118.43	110.49
1	B	499	GLY	CA-C-N	5.32	129.11	120.60
1	B	499	GLY	C-N-CA	5.32	129.11	120.60
1	C	639	PHE	CA-C-N	5.32	125.88	119.98
1	C	639	PHE	C-N-CA	5.32	125.88	119.98
1	D	764	LYS	CB-CA-C	-5.30	101.84	110.85
1	B	460	MET	CB-CA-C	-5.29	103.62	111.72
1	B	665	VAL	N-CA-C	-5.28	105.38	110.72
1	B	554	LYS	CA-C-N	5.28	125.81	120.00
1	B	554	LYS	C-N-CA	5.28	125.81	120.00
1	D	484	ASN	CA-CB-CG	-5.27	107.33	112.60
1	A	609	ASN	N-CA-CB	5.23	118.23	110.49
1	D	639	PHE	CA-C-N	5.23	125.89	120.03
1	D	639	PHE	C-N-CA	5.23	125.89	120.03
1	C	535	HIS	CA-CB-CG	-5.19	108.61	113.80
1	B	659	GLN	CA-C-N	5.16	127.45	120.38
1	B	659	GLN	C-N-CA	5.16	127.45	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	722	VAL	O-C-N	-5.13	117.14	120.42
1	B	642	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	C	615	SER	CA-C-O	-5.07	116.30	121.87
1	D	536	CYS	N-CA-C	-5.06	105.84	111.36
1	C	746	PRO	N-CA-C	5.04	116.85	110.70
1	D	701	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	616	SER	CA-C-N	5.01	127.44	120.63
1	A	616	SER	C-N-CA	5.01	127.44	120.63
1	B	639	PHE	CA-C-N	5.00	125.50	120.00
1	B	639	PHE	C-N-CA	5.00	125.50	120.00

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	2578	0	2554	32	0
1	B	2579	0	2549	36	0
1	C	2576	0	2566	27	0
1	D	2566	0	2547	35	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
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	4	0
4	B	6	0	8	3	0
5	A	29	0	0	1	0
5	B	29	0	0	4	0
5	C	29	0	0	4	0
5	D	29	0	0	2	0
6	A	167	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	190	0	0	3	0
6	C	187	0	0	5	0
6	D	142	0	0	5	0
All	All	11121	0	10232	129	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 6.

All (129) 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:457:GLN:CB	1:A:458:GLY:HA2	1.93	0.99
1:D:469:CYS:SG	6:D:1028:HOH:O	2.27	0.92
1:A:461:GLN:NE2	1:A:461:GLN:HA	1.92	0.84
1:D:493:MET:O	1:D:497:SER:HB2	1.79	0.83
1:B:606:GLU:HG2	6:B:1067:HOH:O	1.82	0.78
1:D:756[A]:ARG:HG2	1:D:756[A]:ARG:HH11	1.47	0.77
1:C:493:MET:O	1:C:497:SER:HB2	1.86	0.76
1:B:696:PHE:HE2	5:B:804:IX9:C15	2.00	0.74
1:D:756[A]:ARG:HG2	1:D:756[A]:ARG:NH1	2.04	0.72
1:C:764[B]:LYS:HG3	1:C:769:GLU:HB2	1.75	0.69
1:A:493:MET:O	1:A:497:SER:HB2	1.93	0.68
1:A:457:GLN:CB	1:A:458:GLY:CA	2.71	0.67
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.76	0.67
1:D:727:LEU:CD1	1:D:766:ILE:HD12	2.25	0.67
1:A:646[A]:GLU:OE2	1:A:650:GLN:NE2	2.29	0.66
1:C:714:MET:HE2	6:C:960:HOH:O	1.95	0.65
4:A:803:GOL:H12	1:B:568:ARG:HH11	1.62	0.64
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.80	0.63
1:D:696:PHE:HE2	5:D:803:IX9:C15	2.13	0.62
1:C:696:PHE:HE2	5:C:803:IX9:C15	2.13	0.61
1:B:506[B]:GLU:HG2	1:B:510:ARG:NH1	2.16	0.60
1:A:553:ARG:HD3	6:A:1006:HOH:O	2.05	0.57
1:D:727:LEU:HD13	1:D:766:ILE:HD12	1.86	0.57
1:B:696:PHE:CE2	5:B:804:IX9:C15	2.85	0.57
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.18	0.57
1:A:644:GLN:HE21	1:A:644:GLN:HA	1.68	0.56
1:A:461:GLN:NE2	1:A:461:GLN:CA	2.67	0.56
1:D:714:MET:HE2	6:D:1013:HOH:O	2.05	0.55
1:C:700:GLY:HA3	1:C:714:MET:O	2.06	0.55
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:LYS:HD3	1:C:703:MET:HE1	1.89	0.55
1:B:770:GLU:HG3	1:B:771:THR:N	2.21	0.54
1:D:752:LEU:HD21	1:D:756[B]:ARG:NH2	2.23	0.54
1:B:677:SER:HB2	1:B:688:THR:HG21	1.89	0.54
1:D:588:THR:CG2	6:D:968:HOH:O	2.54	0.53
4:A:803:GOL:H12	1:B:568:ARG:NH1	2.23	0.53
1:B:482:PHE:HA	4:B:803:GOL:H2	1.91	0.53
1:B:727:LEU:HD23	1:B:759:LEU:CD1	2.39	0.53
1:A:461:GLN:NE2	1:A:500:THR:HG21	2.24	0.53
1:B:719:LYS:NZ	6:B:902:HOH:O	2.37	0.53
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.91	0.52
1:D:727:LEU:CD1	1:D:766:ILE:CD1	2.88	0.52
1:C:727:LEU:HD22	1:C:759:LEU:HD11	1.91	0.52
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.45	0.52
1:B:602:ILE:HA	1:B:605:LEU:HD22	1.91	0.52
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.45	0.51
1:D:498:CYS:SG	1:D:502[A]:CYS:CB	2.95	0.51
1:D:675:LEU:O	1:D:678:VAL:HG22	2.11	0.51
1:C:677:SER:HB3	6:C:932:HOH:O	2.12	0.50
1:D:696:PHE:CE2	5:D:803:IX9:C15	2.94	0.50
1:D:602:ILE:O	1:D:605:LEU:HB2	2.12	0.49
1:B:477:PHE:HB3	1:B:535:HIS:CE1	2.48	0.49
1:A:523:PRO:HD2	1:A:695:GLU:HG2	1.95	0.49
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.28	0.49
1:B:509:CME:HB2	6:B:1047:HOH:O	2.11	0.49
1:D:714:MET:CE	6:D:1013:HOH:O	2.59	0.49
1:B:767:ARG:NH1	1:B:769:GLU:OE2	2.46	0.48
1:A:696:PHE:HE2	5:A:804:IX9:C15	2.26	0.48
1:C:696:PHE:CE2	5:C:803:IX9:C15	2.96	0.48
1:A:735:ILE:HD13	1:A:755:CYS:SG	2.53	0.48
1:B:493:MET:O	1:B:497:SER:HB2	2.13	0.48
1:C:492:TYR:CE2	1:C:496:ARG:HD2	2.49	0.48
1:D:700:GLY:HA3	1:D:714:MET:O	2.13	0.48
1:D:498:CYS:C	1:D:502[B]:CYS:SG	2.97	0.48
4:A:803:GOL:O2	1:B:568:ARG:HB3	2.14	0.47
1:B:697:TRP:CZ2	1:B:719:LYS:HG2	2.49	0.47
1:B:726:GLN:HE22	5:B:804:IX9:C16	2.27	0.47
1:C:602:ILE:O	1:C:605:LEU:HB2	2.14	0.47
1:C:553:ARG:NH1	6:C:907:HOH:O	2.47	0.47
1:D:627:ARG:O	1:D:631:ILE:HG12	2.15	0.47
1:C:727:LEU:CD2	1:C:759:LEU:CD1	2.93	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:HE22	1:A:500:THR:HG22	1.79	0.46
1:D:762:TRP:O	1:D:766:ILE:HG13	2.14	0.46
1:C:523:PRO:HD2	1:C:695:GLU:HG3	1.98	0.46
1:C:727:LEU:HD21	1:C:763:GLU:HG3	1.97	0.46
4:B:803:GOL:H11	1:C:520:ARG:NH1	2.31	0.46
1:A:498:CYS:SG	1:A:502[A]:CYS:CB	3.03	0.46
1:B:644:GLN:NE2	1:B:644:GLN:HA	2.31	0.46
1:C:714:MET:CE	6:C:960:HOH:O	2.61	0.46
1:A:749:GLU:N	1:A:750:PRO:CD	2.79	0.46
1:B:727:LEU:CD2	1:B:759:LEU:HD11	2.46	0.46
1:B:729:PHE:HB2	5:B:804:IX9:N21	2.31	0.45
1:D:493:MET:O	1:D:497:SER:CB	2.58	0.45
1:A:756[A]:ARG:HD3	6:A:922:HOH:O	2.17	0.45
1:B:700:GLY:HA3	1:B:714:MET:O	2.16	0.45
1:D:542:GLN:NE2	6:D:906:HOH:O	2.49	0.45
1:B:638:TYR:CD1	1:B:671:THR:HG21	2.52	0.45
1:C:729:PHE:HB2	5:C:803:IX9:N21	2.31	0.45
1:C:749[B]:GLU:HB3	1:C:750:PRO:HD3	1.99	0.45
1:A:553:ARG:CD	6:A:1006:HOH:O	2.64	0.44
1:B:727:LEU:HD23	1:B:759:LEU:HD11	1.98	0.44
1:A:461:GLN:HE22	1:A:500:THR:HG21	1.82	0.44
1:A:489:ILE:O	1:A:493:MET:HG3	2.18	0.44
1:D:761:GLN:HE22	1:D:764:LYS:NZ	2.16	0.44
1:C:602:ILE:HA	1:C:605:LEU:HD22	1.98	0.43
1:D:564:ASP:O	1:D:567:HIS:HB2	2.17	0.43
1:B:498:CYS:C	1:B:502:CYS:SG	3.02	0.43
1:A:719:LYS:O	1:A:722:VAL:HG23	2.19	0.43
1:B:577:LYS:HD3	1:B:703:MET:HE1	2.00	0.43
1:D:766:ILE:HG22	1:D:766:ILE:O	2.18	0.43
1:A:727:LEU:HD21	1:A:763:GLU:HG3	2.01	0.43
1:C:727:LEU:CD2	1:C:759:LEU:HD11	2.49	0.43
1:D:484:ASN:HD22	1:D:484:ASN:HA	1.67	0.43
1:A:682:TRP:HB3	1:A:683:PRO:HD3	2.01	0.43
1:C:726:GLN:HE22	5:C:803:IX9:C16	2.32	0.43
1:C:735:ILE:HB	1:C:736:PRO:HD3	2.01	0.42
1:B:703:MET:HE3	1:B:708:ILE:CG2	2.49	0.42
1:A:730:TYR:O	1:A:735:ILE:HG12	2.19	0.42
1:B:711:ILE:HD11	1:B:713:MET:HE2	2.01	0.42
1:A:497:SER:O	1:A:553:ARG:HD2	2.20	0.42
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.87	0.42
1:D:510:ARG:HD3	1:D:608:HIS:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:NE2	1:A:500:THR:CG2	2.82	0.42
1:D:727:LEU:HD13	1:D:766:ILE:CD1	2.49	0.42
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.89	0.42
1:B:506[B]:GLU:HG2	1:B:510:ARG:HH12	1.84	0.42
1:B:611:PHE:HB3	1:B:614:LEU:HD22	2.01	0.42
1:C:724:GLN:HB2	6:C:1007:HOH:O	2.19	0.41
1:D:682:TRP:N	1:D:683:PRO:CD	2.83	0.41
1:D:498:CYS:HB2	1:D:553:ARG:HB3	2.02	0.41
1:B:605:LEU:HB3	1:B:608:HIS:ND1	2.36	0.41
1:A:498:CYS:C	1:A:502[B]:CYS:SG	3.04	0.41
4:B:803:GOL:H12	1:C:568:ARG:HH11	1.86	0.41
1:C:746:PRO:N	1:C:747:PRO:CD	2.84	0.41
4:A:803:GOL:C1	1:B:568:ARG:HH11	2.32	0.40
1:D:682:TRP:CZ2	1:D:686:LYS:HD3	2.56	0.40
1:D:727:LEU:HD12	1:D:766:ILE:CD1	2.51	0.40
1:B:646:GLU:OE1	1:B:646:GLU:HA	2.21	0.40
1:D:489:ILE:O	1:D:493:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	317/343 (92%)	308 (97%)	9 (3%)	0	100	100
1	B	317/343 (92%)	308 (97%)	9 (3%)	0	100	100
1	C	317/343 (92%)	311 (98%)	6 (2%)	0	100	100
1	D	315/343 (92%)	304 (96%)	11 (4%)	0	100	100
All	All	1266/1372 (92%)	1231 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	287/305 (94%)	272 (95%)	15 (5%)	21	9
1	B	286/305 (94%)	263 (92%)	23 (8%)	11	3
1	C	288/305 (94%)	269 (93%)	19 (7%)	15	6
1	D	285/305 (93%)	263 (92%)	22 (8%)	12	4
All	All	1146/1220 (94%)	1067 (93%)	79 (7%)	15	5

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	471[A]	GLU
1	A	471[B]	GLU
1	A	496	ARG
1	A	497	SER
1	A	504	GLU
1	A	517	LYS
1	A	553	ARG
1	A	573	SER
1	A	575	LEU
1	A	605	LEU
1	A	617	SER
1	A	644	GLN
1	A	660	SER
1	A	709	GLN
1	B	459	LEU
1	B	469[A]	CYS
1	B	469[B]	CYS
1	B	470	LYS
1	B	471	GLU
1	B	497	SER
1	B	498	CYS
1	B	500	THR
1	B	573	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	575	LEU
1	B	576	GLN
1	B	605	LEU
1	B	606	GLU
1	B	613	THR
1	B	616	SER
1	B	617	SER
1	B	621	GLN
1	B	642	ARG
1	B	650	GLN
1	B	677	SER
1	B	709	GLN
1	B	719	LYS
1	B	727	LEU
1	C	469[A]	CYS
1	C	469[B]	CYS
1	C	471	GLU
1	C	497	SER
1	C	517	LYS
1	C	547	LEU
1	C	557	LEU
1	C	573[A]	SER
1	C	573[B]	SER
1	C	575	LEU
1	C	605	LEU
1	C	613	THR
1	C	616	SER
1	C	617	SER
1	C	709	GLN
1	C	713	MET
1	C	727	LEU
1	C	753	LYS
1	C	760	SER
1	D	457	GLN
1	D	459	LEU
1	D	498	CYS
1	D	500	THR
1	D	504	GLU
1	D	517	LYS
1	D	557	LEU
1	D	573	SER
1	D	575	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	588	THR
1	D	605	LEU
1	D	613	THR
1	D	617	SER
1	D	623	LEU
1	D	644	GLN
1	D	646	GLU
1	D	709	GLN
1	D	719	LYS
1	D	720	ASP
1	D	727	LEU
1	D	766	ILE
1	D	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	495	HIS
1	A	542	GLN
1	A	544	ASN
1	A	604	GLN
1	A	609	ASN
1	A	644	GLN
1	A	650	GLN
1	A	724	GLN
1	A	726	GLN
1	A	761	GLN
1	B	484	ASN
1	B	545	HIS
1	B	604	GLN
1	B	621	GLN
1	B	644	GLN
1	B	726	GLN
1	B	743	GLN
1	C	484	ASN
1	C	542	GLN
1	C	604	GLN
1	C	659	GLN
1	C	709	GLN
1	C	726	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	743	GLN
1	D	484	ASN
1	D	542	GLN
1	D	604	GLN
1	D	609	ASN
1	D	621	GLN
1	D	644	GLN
1	D	731	ASN
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	0.30	0	6,9,11	0.85	0
1	CME	B	509	1	8,9,10	0.59	0	6,9,11	1.23	0
1	CME	C	509	1	8,9,10	0.70	0	6,9,11	1.02	0
1	CME	A	509	1	8,9,10	0.45	0	6,9,11	0.77	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	-	2/5/8/10	-
1	CME	B	509	1	-	1/5/8/10	-
1	CME	C	509	1	-	1/5/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	509	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	IX9	C	803	-	33,33,33	1.46	6 (18%)	43,46,46	2.78	21 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IX9	D	803	-	33,33,33	1.17	2 (6%)	43,46,46	2.67	18 (41%)
4	GOL	A	803	-	5,5,5	0.19	0	5,5,5	0.93	0
4	GOL	B	803	-	5,5,5	0.30	0	5,5,5	0.68	0
5	IX9	B	804	-	33,33,33	1.32	6 (18%)	43,46,46	3.24	26 (60%)
5	IX9	A	804	-	33,33,33	1.32	5 (15%)	43,46,46	3.30	20 (46%)

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	IX9	C	803	-	-	2/12/22/22	0/5/5/5
5	IX9	D	803	-	-	3/12/22/22	0/5/5/5
4	GOL	A	803	-	-	3/4/4/4	-
4	GOL	B	803	-	-	2/4/4/4	-
5	IX9	B	804	-	-	1/12/22/22	0/5/5/5
5	IX9	A	804	-	-	2/12/22/22	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	803	IX9	C5-C4	-3.24	1.35	1.41
5	D	803	IX9	O13-C11	-2.87	1.33	1.39
5	C	803	IX9	C15-C11	2.82	1.44	1.38
5	B	804	IX9	O13-C11	-2.66	1.33	1.39
5	C	803	IX9	C2-N21	2.61	1.41	1.35
5	C	803	IX9	O13-C11	-2.60	1.34	1.39
5	B	804	IX9	C5-N9	-2.53	1.34	1.39
5	A	804	IX9	C16-C12	2.51	1.44	1.38
5	A	804	IX9	C14-C16	2.43	1.43	1.38
5	B	804	IX9	C16-C12	2.39	1.44	1.38
5	B	804	IX9	C10-C11	-2.37	1.35	1.39
5	C	803	IX9	C26-N21	2.32	1.50	1.46
5	D	803	IX9	C26-N21	2.32	1.50	1.46
5	A	804	IX9	C5-C6	2.28	1.42	1.39
5	B	804	IX9	C6-N3	-2.26	1.30	1.34
5	C	803	IX9	C22-N18	2.13	1.50	1.46
5	A	804	IX9	C5-N9	-2.05	1.35	1.39
5	B	804	IX9	C25-N21	2.04	1.50	1.46
5	A	804	IX9	C15-C11	2.02	1.42	1.38

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	IX9	C26-N21-C2	-9.59	102.72	121.67
5	B	804	IX9	C5-C6-N3	-9.47	117.26	126.55
5	D	803	IX9	C5-C6-N3	-8.87	117.85	126.55
5	B	804	IX9	C5-N9-C8	6.97	111.34	103.48
5	B	804	IX9	C26-N21-C2	-6.74	108.34	121.67
5	A	804	IX9	C5-C6-N3	-6.72	119.96	126.55
5	A	804	IX9	C25-N21-C2	-6.71	108.40	121.67
5	A	804	IX9	C23-N18-C22	6.38	125.93	111.57
5	D	803	IX9	C26-N21-C2	-6.18	109.46	121.67
5	C	803	IX9	C5-C6-N3	-5.95	120.72	126.55
5	A	804	IX9	C25-N21-C26	5.80	124.62	111.57
5	C	803	IX9	C26-N21-C2	-5.65	110.50	121.67
5	C	803	IX9	C5-N9-C8	5.57	109.77	103.48
5	A	804	IX9	C5-N9-C8	5.52	109.71	103.48
5	D	803	IX9	N7-C6-N3	5.32	135.99	127.45
5	C	803	IX9	N7-C6-N3	5.30	135.97	127.45
5	D	803	IX9	C5-N9-C8	5.15	109.29	103.48
5	B	804	IX9	C6-C5-C4	4.86	120.17	115.38
5	C	803	IX9	C25-N21-C26	4.84	122.45	111.57
5	B	804	IX9	N7-C6-N3	4.83	135.21	127.45
5	A	804	IX9	C6-C5-C4	4.75	120.07	115.38
5	A	804	IX9	N7-C6-N3	4.74	135.07	127.45
5	B	804	IX9	C17-C12-C10	-4.73	114.52	120.92
5	A	804	IX9	C16-C14-C15	-4.47	114.49	120.24
5	B	804	IX9	C25-N21-C26	4.46	121.61	111.57
5	C	803	IX9	N7-C8-N9	-4.46	107.08	113.87
5	C	803	IX9	C6-N7-C8	4.23	110.38	106.43
5	B	804	IX9	N7-C8-N9	-3.99	107.79	113.87
5	B	804	IX9	C27-N20-C19	3.94	122.54	116.81
5	C	803	IX9	C25-N21-C2	-3.85	114.06	121.67
5	B	804	IX9	C16-C14-C15	-3.84	115.31	120.24
5	A	804	IX9	C11-C10-C12	-3.63	115.79	119.67
5	A	804	IX9	C15-C11-C10	3.53	125.26	120.50
5	D	803	IX9	C16-C14-C15	-3.52	115.72	120.24
5	A	804	IX9	C5-C4-N1	-3.51	118.80	123.49
5	B	804	IX9	C6-C5-N9	-3.48	105.84	110.67
5	A	804	IX9	C22-C25-N21	3.46	118.06	110.78
5	C	803	IX9	C23-N18-C19	-3.41	111.32	120.41
5	B	804	IX9	C23-N18-C22	3.39	119.18	111.57
5	B	804	IX9	C23-N18-C19	-3.36	111.46	120.41
5	D	803	IX9	C25-N21-C26	3.27	118.93	111.57
5	C	803	IX9	C23-N18-C22	3.27	118.92	111.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	803	IX9	C5-C4-N1	-3.24	119.15	123.49
5	D	803	IX9	C23-N18-C22	3.22	118.80	111.57
5	B	804	IX9	C11-C10-C12	-3.18	116.27	119.67
5	C	803	IX9	C6-C5-C4	3.12	118.45	115.38
5	D	803	IX9	N7-C8-N9	-3.03	109.26	113.87
5	C	803	IX9	C11-C10-C12	-2.97	116.49	119.67
5	A	804	IX9	C29-C28-C24	-2.90	116.67	120.24
5	C	803	IX9	C15-C11-C10	2.89	124.39	120.50
5	A	804	IX9	C23-C26-N21	2.87	116.82	110.78
5	B	804	IX9	C16-C12-C10	2.86	122.18	117.96
5	B	804	IX9	N1-C2-N21	2.85	121.18	117.12
5	D	803	IX9	C6-C5-C4	2.80	118.14	115.38
5	B	804	IX9	C25-C22-N18	2.78	116.63	110.78
5	C	803	IX9	O13-C4-N1	2.77	124.25	119.61
5	D	803	IX9	C25-C22-N18	2.75	116.58	110.78
5	C	803	IX9	C29-C28-C24	-2.71	116.90	120.24
5	D	803	IX9	C29-C28-C24	-2.69	116.92	120.24
5	A	804	IX9	C28-C24-C19	2.58	121.16	117.61
5	A	804	IX9	C6-C5-N9	-2.52	107.17	110.67
5	B	804	IX9	C25-N21-C2	-2.49	116.75	121.67
5	D	803	IX9	C27-N20-C19	2.48	120.42	116.81
5	A	804	IX9	C23-N18-C19	-2.47	113.83	120.41
5	C	803	IX9	C22-N18-C19	-2.41	113.98	120.41
5	B	804	IX9	C22-N18-C19	-2.41	114.00	120.41
5	D	803	IX9	C23-N18-C19	-2.40	114.02	120.41
5	B	804	IX9	C15-C11-C10	2.40	123.73	120.50
5	A	804	IX9	C22-N18-C19	-2.37	114.09	120.41
5	D	803	IX9	C23-C26-N21	2.35	115.73	110.78
5	C	803	IX9	C23-C26-N21	2.33	115.69	110.78
5	D	803	IX9	C11-C10-C12	-2.32	117.18	119.67
5	A	804	IX9	N7-C8-N9	-2.32	110.34	113.87
5	C	803	IX9	C27-N20-C19	2.31	120.17	116.81
5	D	803	IX9	C6-C5-N9	-2.27	107.52	110.67
5	B	804	IX9	C26-C23-N18	2.21	115.44	110.78
5	B	804	IX9	C11-O13-C4	-2.18	113.55	118.27
5	D	803	IX9	C15-C11-C10	2.16	123.41	120.50
5	B	804	IX9	C14-C15-C11	2.14	122.21	118.98
5	D	803	IX9	C5-C4-N1	-2.12	120.66	123.49
5	C	803	IX9	N3-C2-N1	-2.09	122.56	126.27
5	B	804	IX9	C22-C25-N21	2.06	115.11	110.78
5	B	804	IX9	C5-C4-N1	-2.03	120.77	123.49
5	C	803	IX9	C25-C22-N18	2.03	115.05	110.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	IX9	C23-C26-N21	2.01	115.01	110.78

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	GOL	O1-C1-C2-O2
4	A	803	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
4	B	803	GOL	O2-C2-C3-O3
5	A	804	IX9	N1-C2-N21-C25
5	D	803	IX9	N20-C19-N18-C23
5	C	803	IX9	N20-C19-N18-C23
5	A	804	IX9	N3-C2-N21-C25
4	A	803	GOL	O2-C2-C3-O3
5	C	803	IX9	C24-C19-N18-C23
5	D	803	IX9	C24-C19-N18-C23
5	B	804	IX9	N20-C19-N18-C23
5	D	803	IX9	N3-C2-N21-C25

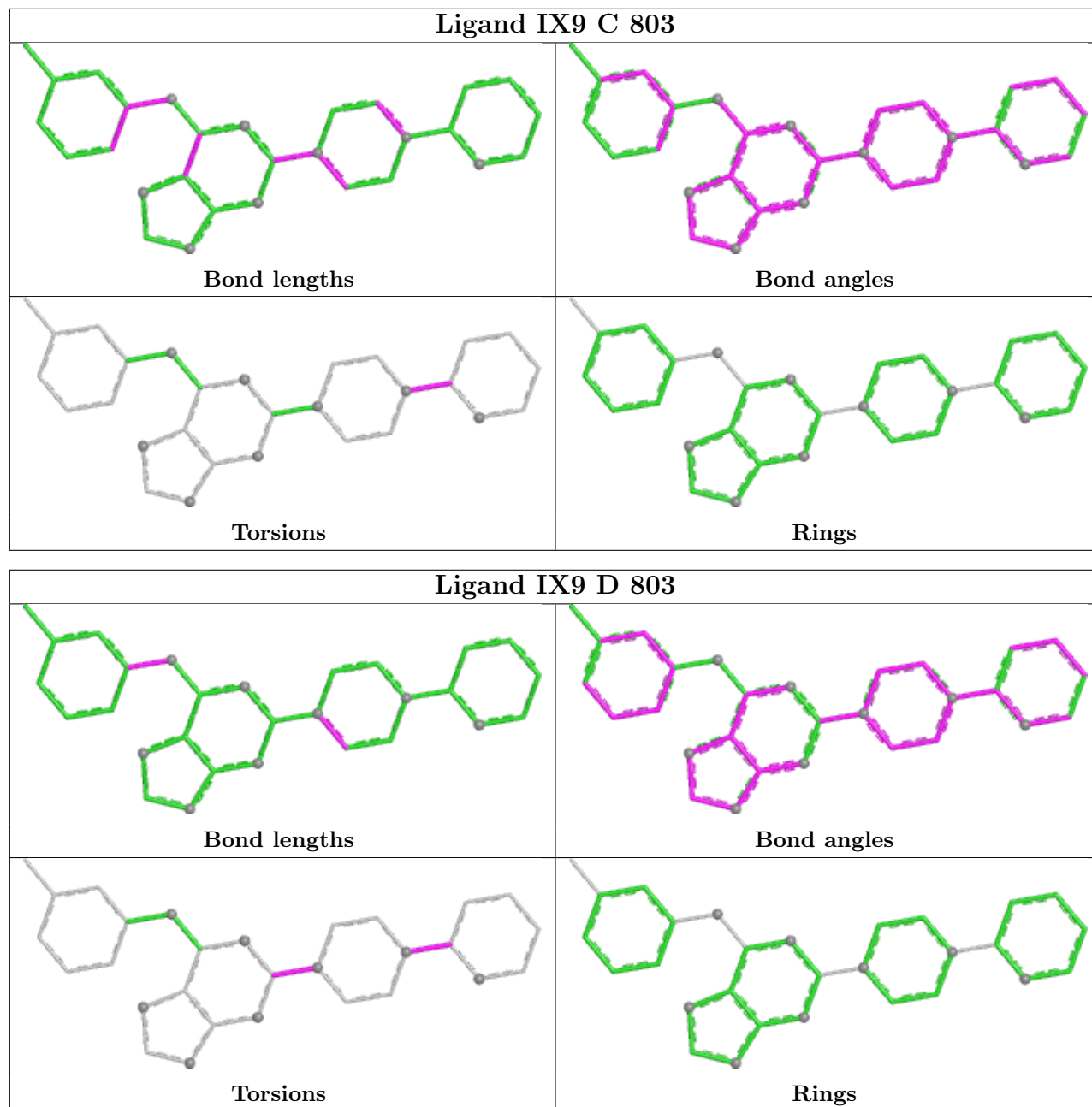
There are no ring outliers.

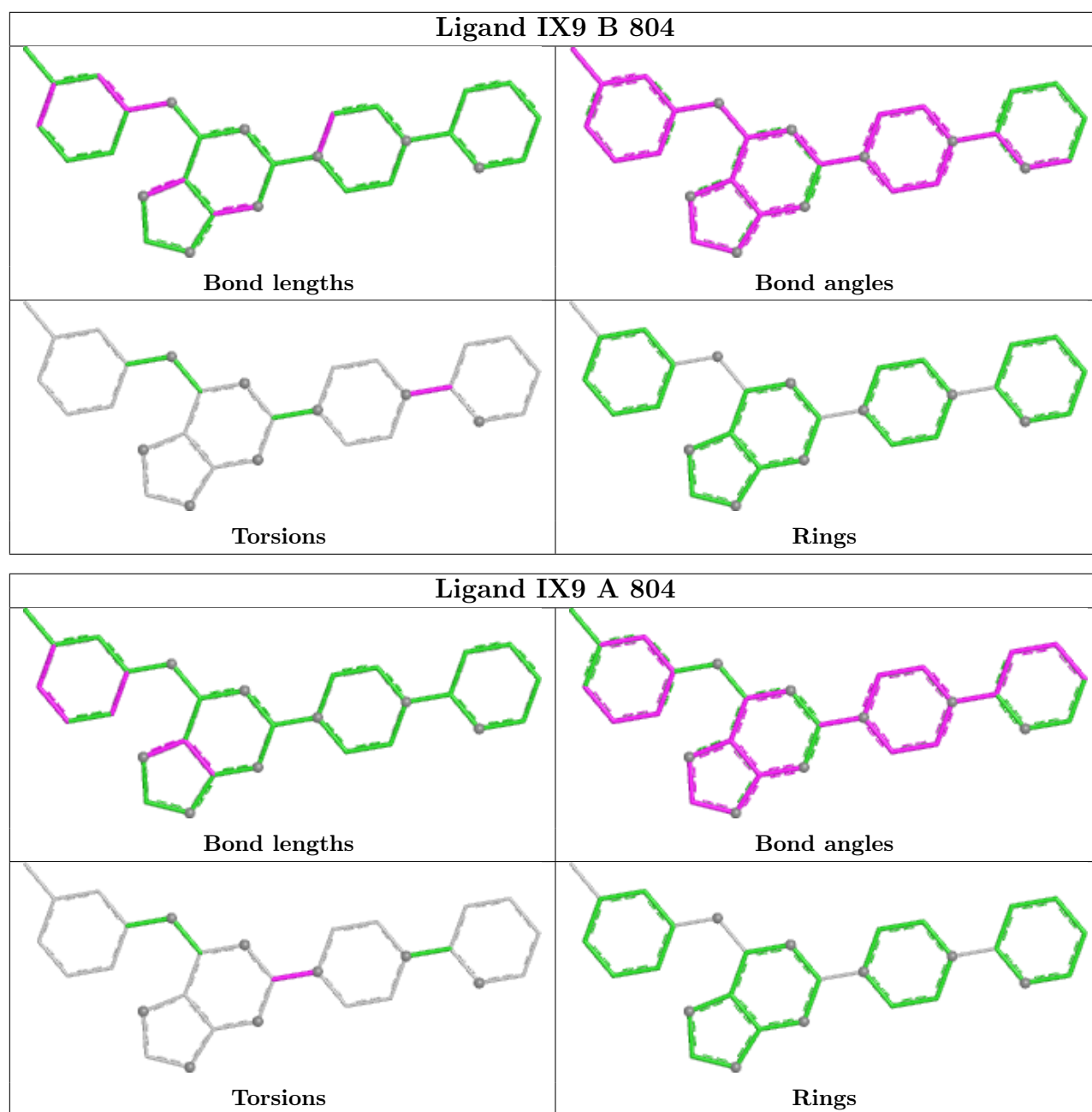
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	803	IX9	4	0
5	D	803	IX9	2	0
4	A	803	GOL	4	0
4	B	803	GOL	3	0
5	B	804	IX9	4	0
5	A	804	IX9	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	313/343 (91%)	-0.03	5 (1%) 70 79	16, 31, 57, 92	6 (1%)
1	B	314/343 (91%)	-0.02	8 (2%) 58 68	17, 30, 53, 89	5 (1%)
1	C	312/343 (90%)	-0.08	5 (1%) 70 79	17, 31, 53, 93	7 (2%)
1	D	312/343 (90%)	0.29	7 (2%) 62 71	21, 38, 63, 104	5 (1%)
All	All	1251/1372 (91%)	0.04	25 (1%) 65 74	16, 33, 58, 104	23 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	456	TRP	6.2
1	D	459	LEU	3.7
1	D	649	TYR	3.7
1	B	771	THR	3.6
1	B	460	MET	3.5
1	A	459	LEU	3.4
1	B	459	LEU	3.3
1	C	459	LEU	3.2
1	A	461	GLN	3.1
1	D	458	GLY	2.8
1	B	458	GLY	2.6
1	D	614	LEU	2.6
1	B	617	SER	2.6
1	B	612	SER	2.4
1	B	500	THR	2.4
1	C	614	LEU	2.4
1	A	457	GLN	2.3
1	B	457	GLN	2.3
1	A	462	PHE	2.3
1	A	460	MET	2.2
1	D	720	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	499	GLY	2.1
1	C	764[A]	LYS	2.1
1	C	460	MET	2.1
1	C	462	PHE	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	C	509	10/11	0.89	0.13	33,36,80,87	0
1	CME	D	509	10/11	0.89	0.13	37,48,89,99	0
1	CME	A	509	10/11	0.91	0.12	34,42,77,82	0
1	CME	B	509	10/11	0.91	0.14	33,41,71,72	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
4	GOL	B	803	6/6	0.81	0.15	43,49,51,53	0
3	MG	D	802	1/1	0.84	0.32	46,46,46,46	0
3	MG	A	802	1/1	0.87	0.23	32,32,32,32	0
4	GOL	A	803	6/6	0.88	0.16	47,53,61,61	0
3	MG	C	802	1/1	0.89	0.26	34,34,34,34	0
3	MG	B	802	1/1	0.92	0.19	26,26,26,26	0
5	IX9	A	804	29/29	0.92	0.08	27,37,40,47	0
5	IX9	D	803	29/29	0.92	0.09	41,46,51,58	0
5	IX9	C	803	29/29	0.94	0.08	31,40,49,50	0
5	IX9	B	804	29/29	0.94	0.08	28,33,38,39	0

Continued on next page...

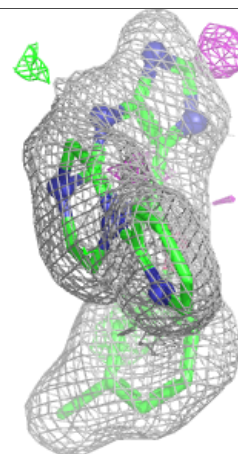
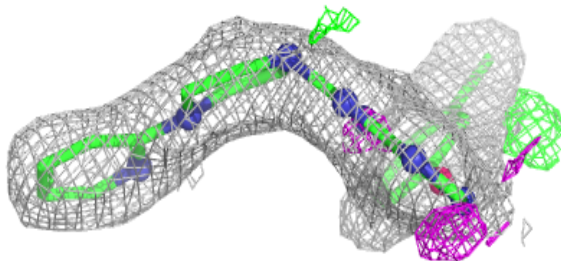
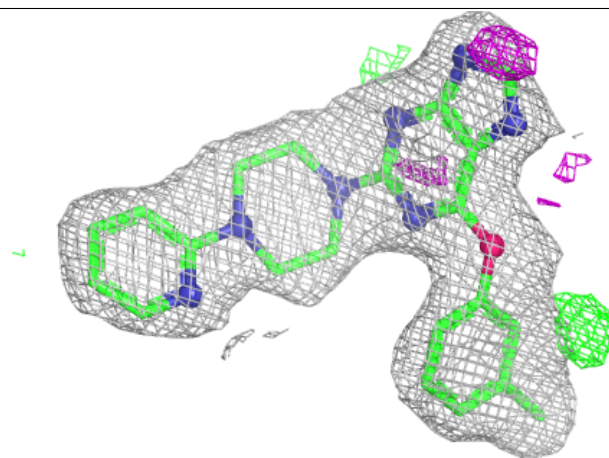
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	801	1/1	0.99	0.03	29,29,29,29	0
2	ZN	D	801	1/1	0.99	0.03	33,33,33,33	0
2	ZN	A	801	1/1	0.99	0.02	27,27,27,27	0
2	ZN	B	801	1/1	0.99	0.03	26,26,26,26	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.

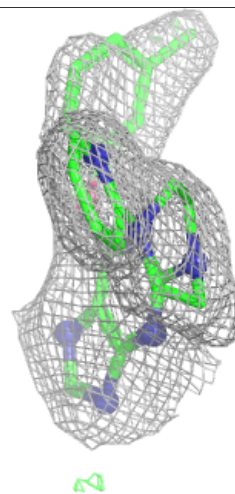
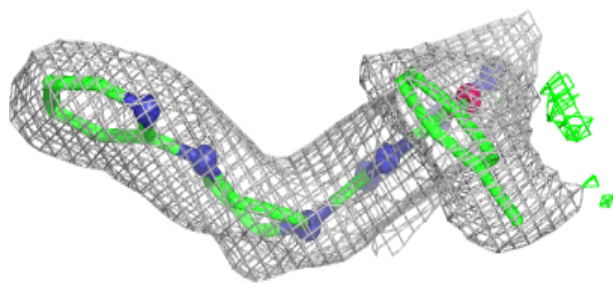
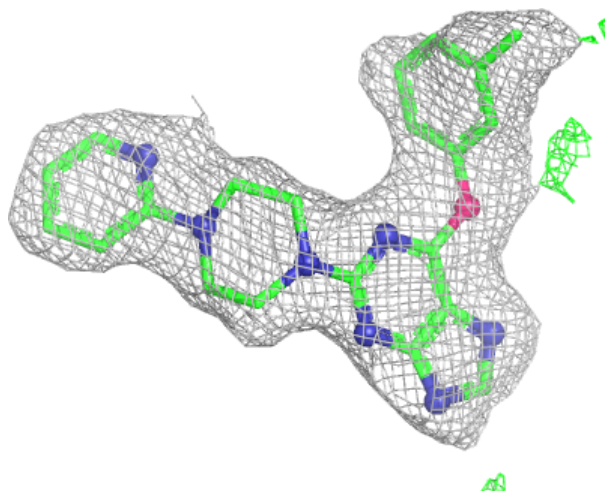
Electron density around IX9 A 804:

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



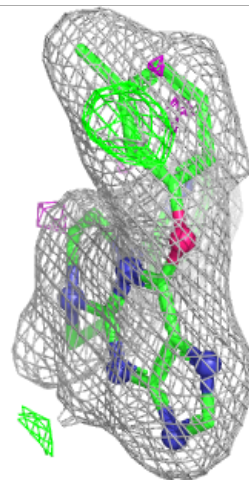
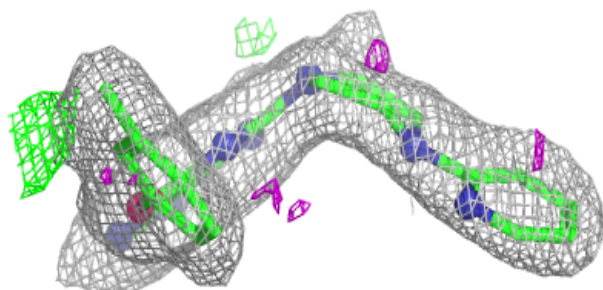
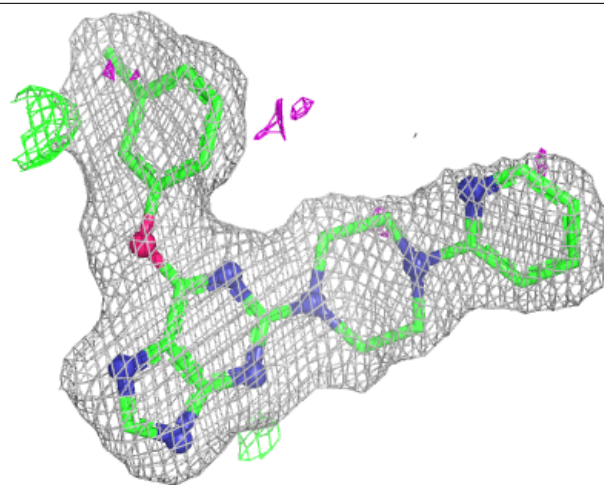
Electron density around IX9 D 803:

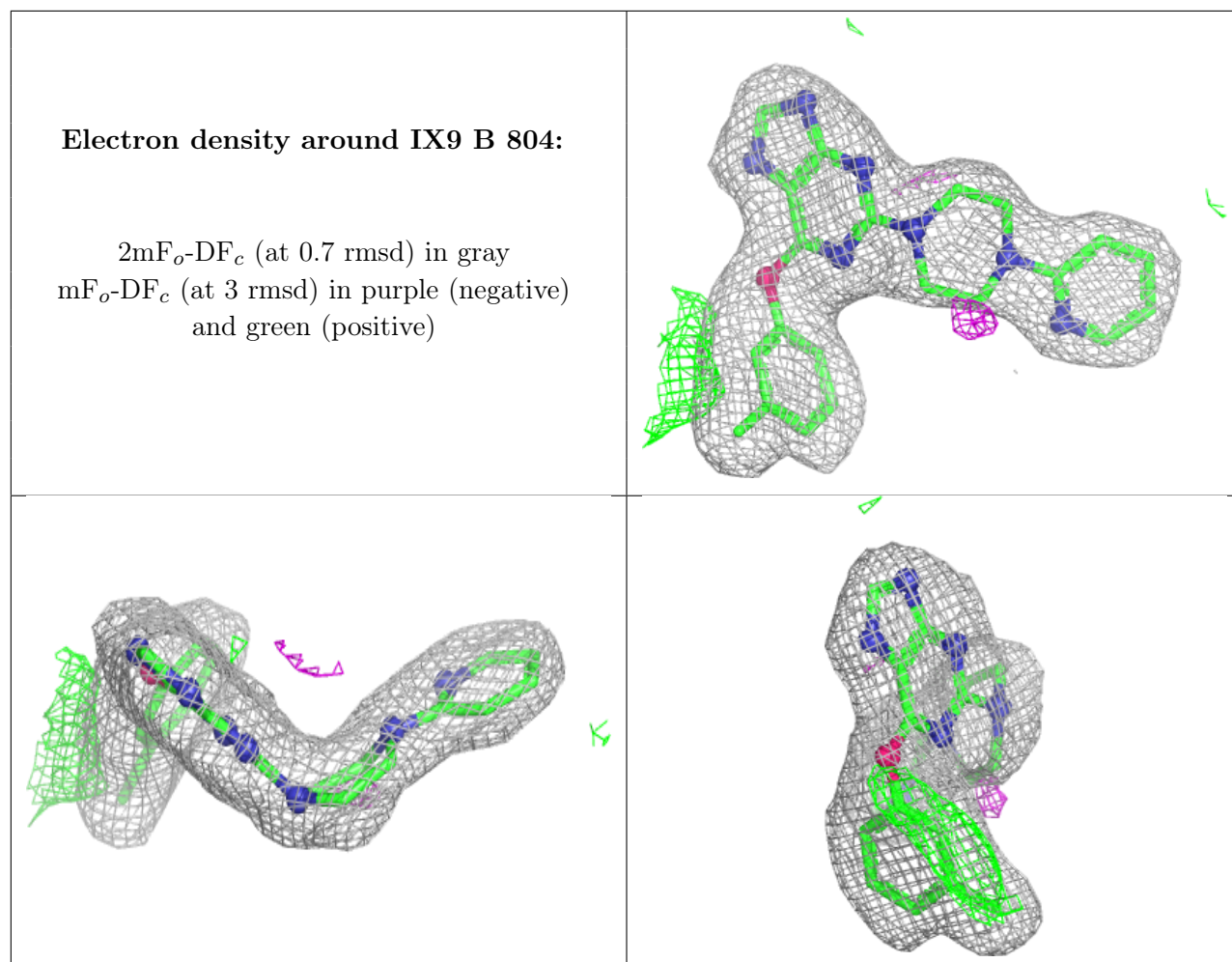
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IX9 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.