



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:12 AM UTC

PDB ID : 5SGD / pdb_00005sgd
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN
COMPLEX WITH n1(c(c(COC)cn1)C(=O)Nc3cc2nc(nn2cc3)c4ccccc4)
C, micromolar IC50=0.01444
Authors : Joseph, C.; Benz, J.; Flohr, A.; Groebke-Zbinden, K.; Rudolph, M.G.
Deposited on : 2022-02-01
Resolution : 2.54 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

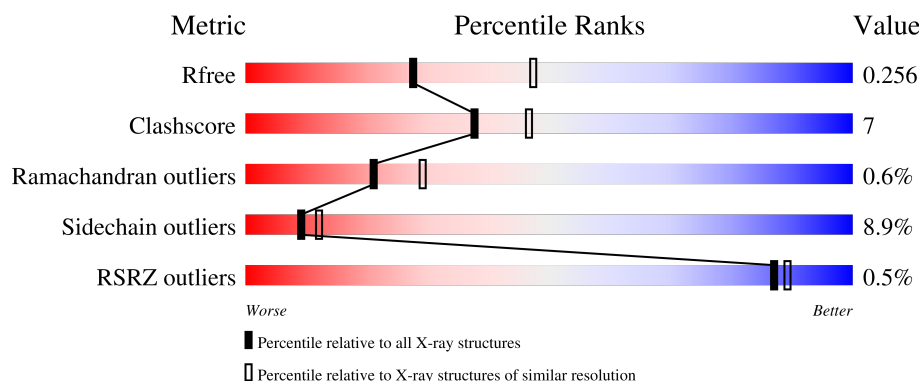
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 5 unique types of molecules in this entry. The entry contains 10465 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	313	Total	C	N	O	S	0	1	0
			2549	1629	435	461	24			
1	B	315	Total	C	N	O	S	0	0	0
			2551	1630	434	463	24			
1	C	313	Total	C	N	O	S	0	1	0
			2549	1629	435	461	24			
1	D	311	Total	C	N	O	S	0	0	0
			2523	1614	430	455	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

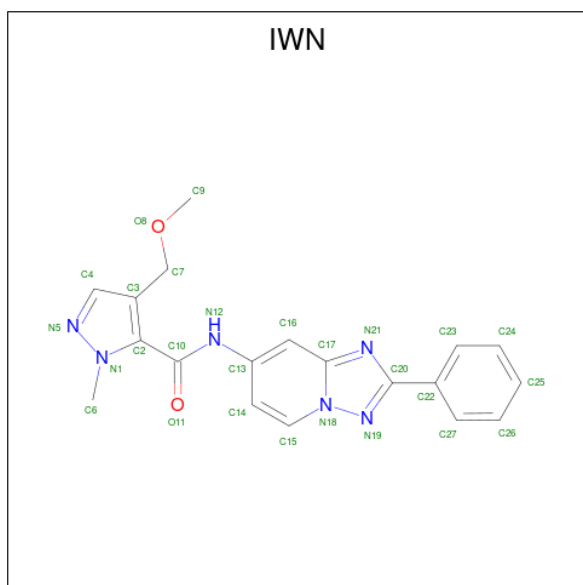
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 4-(methoxymethyl)-1-methyl-N-[(4S)-2-phenyl[1,2,4]triazolo[1,5-a]pyridin-7-yl]-1H-pyrazole-5-carboxamide (CCD ID: IWN) (formula: C₁₉H₁₈N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	19	6	2		
4	B	1	Total	C	N	O	0	0
			27	19	6	2		
4	C	1	Total	C	N	O	0	0
			27	19	6	2		
4	D	1	Total	C	N	O	0	0
			27	19	6	2		

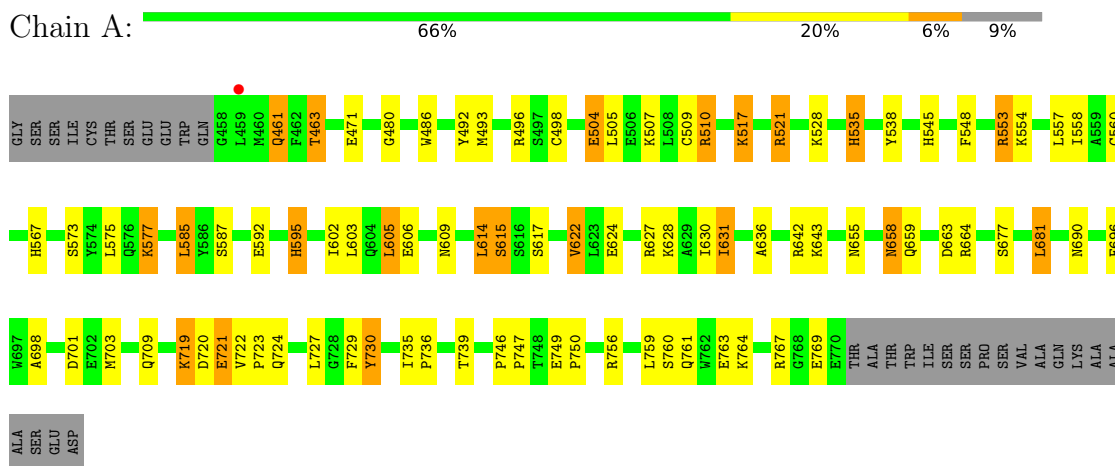
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total 56	O 56	0	0
5	B	61	Total 61	O 61	0	0
5	C	47	Total 47	O 47	0	0
5	D	13	Total 13	O 13	0	0

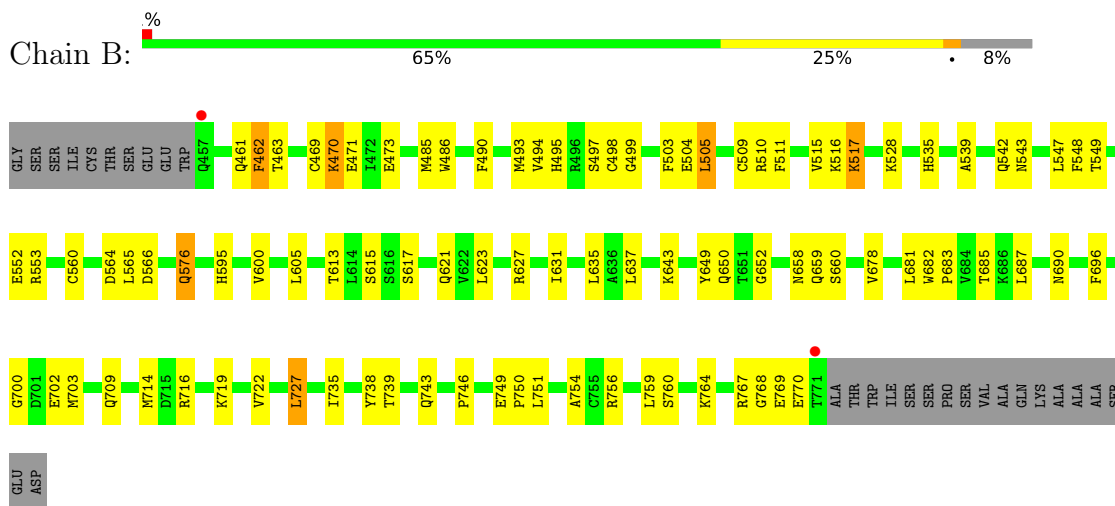
3 Residue-property plots

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

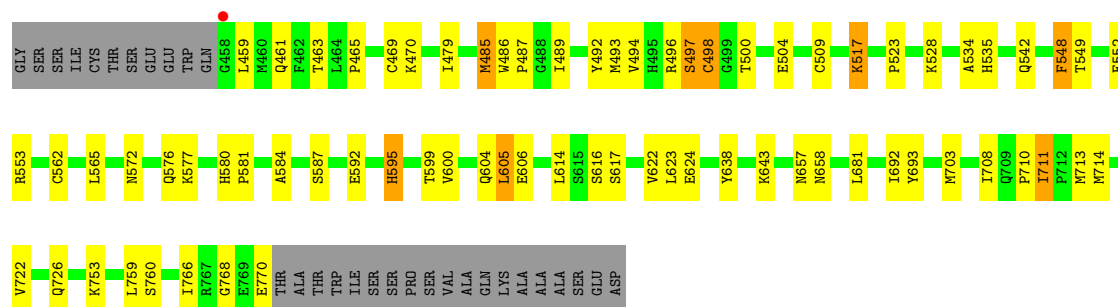


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

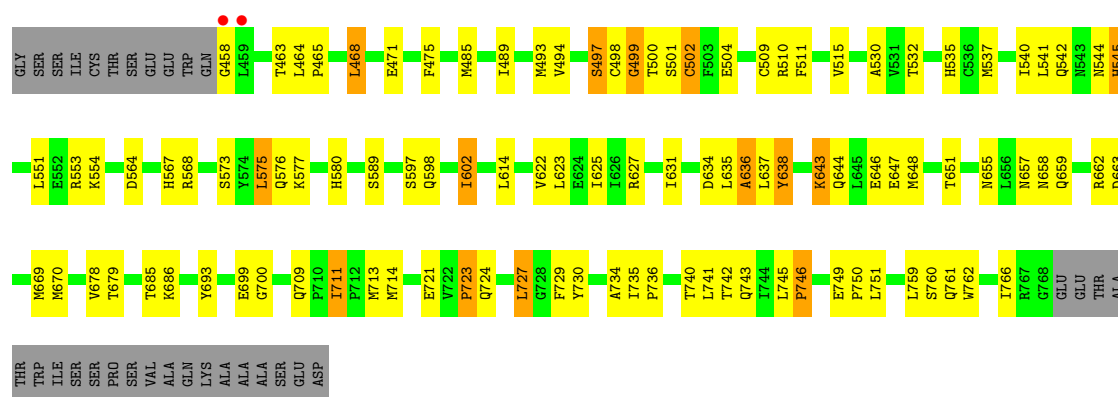


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A





- 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	135.39Å 135.39Å 236.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.56 – 2.54 43.56 – 2.54	Depositor EDS
% Data completeness (in resolution range)	95.2 (43.56-2.54) 95.2 (43.56-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.167 , 0.257 0.174 , 0.256	Depositor DCC
R_{free} test set	2610 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10465	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: ZN, MG, CME, IWN

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	12/2603 (0.5%)	1.61	27/3521 (0.8%)
1	B	1.33	13/2602 (0.5%)	1.61	14/3521 (0.4%)
1	C	1.29	9/2603 (0.3%)	1.64	13/3521 (0.4%)
1	D	1.34	5/2574 (0.2%)	1.74	25/3483 (0.7%)
All	All	1.32	39/10382 (0.4%)	1.65	79/14046 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	703	MET	C-O	7.32	1.32	1.24
1	C	595	HIS	C-O	7.30	1.32	1.24
1	C	572	ASN	C-O	7.23	1.32	1.24
1	B	535	HIS	CE1-NE2	7.20	1.39	1.32
1	B	635	LEU	C-O	-7.00	1.15	1.24
1	A	567	HIS	CE1-NE2	6.94	1.39	1.32
1	A	739	THR	C-O	6.91	1.32	1.24
1	B	702	GLU	C-O	6.89	1.32	1.24
1	B	595	HIS	CE1-NE2	6.79	1.39	1.32
1	B	685	THR	C-O	6.69	1.31	1.24
1	C	710	PRO	C-O	-6.46	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	721	GLU	C-O	6.27	1.32	1.24
1	A	517	LYS	C-O	-6.26	1.15	1.24
1	B	637	LEU	C-O	-6.11	1.16	1.24
1	A	730	TYR	C-O	6.07	1.31	1.24
1	C	479	ILE	C-O	-6.06	1.16	1.24
1	A	631	ILE	C-O	5.87	1.31	1.24
1	A	595	HIS	C-O	5.83	1.30	1.24
1	A	696	PHE	C-O	-5.72	1.17	1.24
1	A	636	ALA	C-O	-5.71	1.16	1.24
1	C	692	ILE	C-O	5.69	1.30	1.24
1	D	589	SER	C-O	5.58	1.30	1.23
1	B	499	GLY	C-O	5.55	1.30	1.23
1	B	495	HIS	CE1-NE2	5.50	1.38	1.32
1	A	703	MET	C-O	5.45	1.30	1.24
1	D	670	MET	C-O	5.38	1.30	1.24
1	C	605	LEU	C-O	5.31	1.30	1.23
1	C	592	GLU	C-O	-5.28	1.17	1.24
1	D	530	ALA	C-O	5.28	1.30	1.24
1	B	660	SER	C-O	-5.16	1.17	1.24
1	A	557	LEU	C-O	5.16	1.30	1.24
1	B	511	PHE	C-O	5.13	1.29	1.24
1	C	534	ALA	C-O	-5.09	1.18	1.24
1	D	458	GLY	N-CA	5.09	1.53	1.45
1	C	523	PRO	C-O	-5.07	1.17	1.24
1	B	754	ALA	C-O	5.05	1.30	1.24
1	D	679	THR	N-CA	5.03	1.51	1.46
1	A	560	CYS	C-O	5.01	1.30	1.24
1	B	560	CYS	C-O	5.00	1.29	1.24

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	657	ASN	N-CA-C	-7.32	104.88	113.88
1	D	746	PRO	N-CA-C	6.80	119.00	110.70
1	C	624	GLU	N-CA-CB	-6.29	100.53	110.28
1	A	558	ILE	N-CA-C	-6.21	104.69	110.53
1	D	638	TYR	CA-C-N	6.10	129.26	120.79
1	D	638	TYR	C-N-CA	6.10	129.26	120.79
1	A	517	LYS	N-CA-C	-6.02	105.90	113.18
1	C	535	HIS	CA-CB-CG	-6.01	107.79	113.80
1	A	609	ASN	N-CA-CB	5.92	119.26	110.49
1	C	638	TYR	CA-C-O	-5.92	114.56	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	622	VAL	CA-C-O	-5.89	114.83	120.95
1	B	690	ASN	N-CA-CB	5.82	118.45	110.01
1	A	521	ARG	N-CA-C	-5.81	103.33	110.65
1	A	720	ASP	CA-C-O	-5.79	114.38	120.63
1	C	657	ASN	N-CA-C	-5.77	106.08	113.23
1	B	621	GLN	CA-C-O	-5.77	114.76	120.82
1	B	548	PHE	CA-C-O	-5.76	114.48	120.70
1	D	646	GLU	O-C-N	5.73	128.22	122.08
1	D	643	LYS	CA-C-N	5.72	128.22	120.44
1	D	643	LYS	C-N-CA	5.72	128.22	120.44
1	C	726	GLN	CA-C-O	-5.71	114.82	120.82
1	A	696	PHE	CA-C-O	-5.70	114.80	120.90
1	B	493	MET	CA-C-O	-5.69	114.39	120.42
1	A	480	GLY	CA-C-N	5.68	126.18	120.04
1	A	480	GLY	C-N-CA	5.68	126.18	120.04
1	C	711	ILE	CA-C-O	5.67	124.75	119.76
1	B	739	THR	CB-CA-C	5.66	119.84	110.90
1	A	664	ARG	CA-C-N	5.62	128.14	120.77
1	A	664	ARG	C-N-CA	5.62	128.14	120.77
1	D	510	ARG	CB-CA-C	5.60	120.75	110.10
1	A	505	LEU	CA-C-O	-5.58	114.96	120.82
1	D	468	LEU	CA-C-N	5.58	128.08	120.54
1	D	468	LEU	C-N-CA	5.58	128.08	120.54
1	C	517	LYS	CB-CA-C	5.53	121.99	110.32
1	B	746	PRO	N-CA-C	5.46	117.36	110.70
1	C	584	ALA	CA-C-N	5.46	127.54	120.44
1	C	584	ALA	C-N-CA	5.46	127.54	120.44
1	D	727	LEU	O-C-N	5.44	127.75	122.09
1	B	517	LYS	N-CA-C	-5.42	105.92	112.54
1	A	642	ARG	CA-C-O	-5.40	114.69	120.42
1	D	576	GLN	CB-CA-C	5.37	119.98	110.85
1	A	553	ARG	CA-C-N	5.36	127.77	120.54
1	A	553	ARG	C-N-CA	5.36	127.77	120.54
1	A	630	ILE	CA-C-O	-5.33	114.71	120.47
1	B	490	PHE	CA-C-O	-5.33	114.77	120.42
1	D	499	GLY	CA-C-O	-5.32	116.97	121.66
1	D	658	ASN	CB-CA-C	5.30	117.43	110.06
1	D	670	MET	CA-C-O	-5.30	115.24	120.70
1	D	544	ASN	CA-C-N	5.30	128.15	120.79
1	D	544	ASN	C-N-CA	5.30	128.15	120.79
1	B	576	GLN	CB-CA-C	5.29	120.38	110.70
1	B	600	VAL	CA-C-O	-5.28	115.58	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	THR	N-CA-CB	5.26	118.60	110.60
1	A	535	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	719	LYS	CB-CA-C	-5.22	102.45	110.81
1	D	723	PRO	CA-C-N	5.22	127.58	120.54
1	D	723	PRO	C-N-CA	5.22	127.58	120.54
1	D	545	HIS	CB-CA-C	5.21	119.21	110.92
1	A	690	ASN	CB-CA-C	-5.20	102.71	110.88
1	A	642	ARG	CA-C-N	5.20	127.56	120.54
1	A	642	ARG	C-N-CA	5.20	127.56	120.54
1	A	617	SER	CA-C-N	5.15	127.49	120.54
1	A	617	SER	C-N-CA	5.15	127.49	120.54
1	D	465	PRO	CA-C-N	5.13	127.49	120.46
1	D	465	PRO	C-N-CA	5.13	127.49	120.46
1	A	504	GLU	CB-CA-C	5.13	117.19	110.06
1	B	462	PHE	CB-CA-C	5.12	118.41	109.65
1	D	761	GLN	CA-C-O	-5.10	115.02	120.42
1	C	548	PHE	CA-C-N	5.09	130.02	120.95
1	C	548	PHE	C-N-CA	5.09	130.02	120.95
1	D	568	ARG	N-CA-C	-5.07	106.51	113.30
1	B	473	GLU	N-CA-C	-5.06	106.61	112.89
1	A	658	ASN	CA-C-N	5.04	127.03	120.28
1	A	658	ASN	C-N-CA	5.04	127.03	120.28
1	D	532	THR	CA-CB-OG1	-5.04	102.05	109.60
1	B	696	PHE	CA-C-O	-5.03	115.52	120.90
1	C	576	GLN	N-CA-C	-5.03	105.71	111.14
1	B	739	THR	N-CA-C	-5.02	105.72	111.14
1	C	517	LYS	N-CA-C	-5.01	106.27	112.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	769	GLU	Peptide
1	C	497	SER	Peptide
1	D	497	SER	Peptide

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	2549	0	2524	47	0
1	B	2551	0	2515	31	0
1	C	2549	0	2524	25	0
1	D	2523	0	2499	39	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	27	0	0	3	0
4	B	27	0	0	0	0
4	C	27	0	0	1	0
4	D	27	0	0	3	0
5	A	56	0	0	3	0
5	B	61	0	0	6	0
5	C	47	0	0	1	0
5	D	13	0	0	0	0
All	All	10465	0	10062	143	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 7.

All (143) 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:461:GLN:HE21	1:A:461:GLN:HA	1.31	0.96
1:C:469:CYS:SG	5:C:941:HOH:O	2.26	0.92
1:A:681:LEU:CG	5:B:950:HOH:O	2.16	0.91
1:A:681:LEU:CB	5:B:950:HOH:O	2.19	0.91
1:A:461:GLN:HA	1:A:461:GLN:NE2	1.89	0.84
1:D:622:VAL:HA	1:D:625:ILE:HD12	1.61	0.83
1:B:767:ARG:NH2	1:B:769:GLU:OE1	2.12	0.81
1:B:769:GLU:O	1:B:769:GLU:HG2	1.78	0.81
1:C:493:MET:O	1:C:497:SER:HB2	1.88	0.74
1:D:627:ARG:O	1:D:631:ILE:HG12	1.88	0.74
1:A:681:LEU:HG	5:B:950:HOH:O	1.84	0.72
1:D:497:SER:O	1:D:553:ARG:HD2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:GLN:O	1:D:602:ILE:HG13	1.93	0.69
1:A:624:GLU:HG2	5:A:949:HOH:O	1.93	0.66
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.78	0.65
1:D:540:ILE:HG21	1:D:669:MET:HE3	1.77	0.65
1:A:681:LEU:HD12	5:B:950:HOH:O	1.97	0.63
1:C:548:PHE:O	1:C:553:ARG:NH2	2.31	0.63
1:A:681:LEU:HB3	5:B:950:HOH:O	1.91	0.62
1:D:475:PHE:CD2	1:D:751:LEU:HD21	2.35	0.62
1:C:486:TRP:CH2	1:C:528:LYS:HG3	2.35	0.61
1:B:497:SER:O	1:B:553:ARG:HD2	2.01	0.61
1:A:507:LYS:NZ	5:A:901:HOH:O	2.34	0.61
1:B:497:SER:HA	1:B:542:GLN:HE22	1.66	0.61
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.83	0.60
1:C:489:ILE:O	1:C:493:MET:HG3	2.03	0.59
1:A:585:LEU:O	1:A:585:LEU:HD12	2.03	0.58
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.18	0.58
1:D:635:LEU:O	1:D:636:ALA:C	2.46	0.58
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.39	0.57
1:A:510:ARG:HH11	1:A:510:ARG:CB	2.17	0.57
1:C:600:VAL:O	1:C:604:GLN:HG3	2.04	0.57
1:A:548:PHE:O	1:A:553:ARG:NH2	2.37	0.57
1:C:486:TRP:CZ2	1:C:528:LYS:HG3	2.40	0.56
1:D:693:TYR:OH	4:D:803:IWN:N21	2.39	0.54
1:B:539:ALA:O	1:B:543:ASN:ND2	2.31	0.54
1:D:742:THR:OG1	1:D:749:GLU:HA	2.08	0.54
1:D:644:GLN:HE22	1:D:648:MET:HE3	1.74	0.53
1:A:735:ILE:N	1:A:736:PRO:CD	2.71	0.53
1:D:475:PHE:HD2	1:D:751:LEU:HD21	1.72	0.53
1:A:719:LYS:O	1:A:722:VAL:HG23	2.09	0.53
1:D:740:THR:HA	1:D:743:GLN:HE21	1.74	0.53
1:A:510:ARG:HH11	1:A:510:ARG:CG	2.22	0.53
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.89	0.53
1:A:761:GLN:HE22	1:A:764:LYS:HE3	1.73	0.53
1:B:515:VAL:HG13	1:B:565:LEU:HD21	1.91	0.52
1:C:497:SER:O	1:C:553:ARG:HD3	2.09	0.52
1:B:716:ARG:O	1:B:719:LYS:HG3	2.09	0.52
1:D:729:PHE:CD1	4:D:803:IWN:C14	2.92	0.52
1:D:659:GLN:NE2	1:D:663:ASP:OD1	2.44	0.51
1:D:723:PRO:HB2	1:D:766:ILE:HG12	1.93	0.51
1:B:470:LYS:HD2	1:D:746:PRO:HA	1.91	0.50
1:B:627:ARG:O	1:B:631:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:635:LEU:O	1:D:637:LEU:N	2.45	0.50
1:A:735:ILE:N	1:A:736:PRO:HD2	2.27	0.50
1:D:493:MET:SD	1:D:535:HIS:HA	2.52	0.50
1:A:746:PRO:N	1:A:747:PRO:CD	2.75	0.50
1:A:486:TRP:CH2	1:A:528:LYS:HB2	2.48	0.49
1:B:564:ASP:O	1:B:565:LEU:C	2.55	0.49
1:C:580:HIS:CG	1:C:581:PRO:HD2	2.47	0.49
1:C:493:MET:O	1:C:497:SER:CB	2.60	0.49
1:B:700:GLY:HA3	1:B:714:MET:O	2.13	0.48
1:B:494:VAL:O	1:B:498:CYS:HB3	2.14	0.48
1:D:711:ILE:HD11	1:D:713:MET:HE2	1.96	0.48
1:B:738:TYR:CD1	1:B:751:LEU:HB3	2.49	0.48
1:B:749:GLU:N	1:B:750:PRO:CD	2.77	0.48
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.49	0.47
1:C:703:MET:HE3	1:C:708:ILE:CG2	2.44	0.47
1:B:486:TRP:CH2	1:B:528:LYS:HG3	2.49	0.47
1:B:549:THR:OG1	1:B:552:GLU:HG3	2.14	0.47
1:A:722:VAL:N	1:A:723:PRO:CD	2.78	0.47
1:A:510:ARG:HH11	1:A:510:ARG:HB2	1.78	0.46
1:C:711:ILE:HD12	1:C:713:MET:HE3	1.98	0.46
1:A:577:LYS:HE3	5:A:937:HOH:O	2.14	0.46
1:B:649:TYR:CE2	1:B:743:GLN:HB3	2.51	0.46
1:A:627:ARG:O	1:A:631:ILE:HG12	2.16	0.46
1:C:549:THR:HG23	1:C:552:GLU:OE1	2.16	0.46
1:D:749:GLU:N	1:D:750:PRO:CD	2.79	0.46
1:C:494:VAL:O	1:C:498:CYS:HB3	2.17	0.45
1:D:489:ILE:HG22	1:D:493:MET:HE2	1.98	0.45
1:D:494:VAL:O	1:D:498:CYS:CB	2.65	0.45
1:D:499:GLY:C	1:D:501:SER:H	2.25	0.45
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.99	0.45
1:C:565:LEU:O	1:C:595:HIS:ND1	2.41	0.45
1:D:678:VAL:HA	1:D:685:THR:HG23	1.99	0.44
1:D:721:GLU:O	1:D:724:GLN:HB3	2.16	0.44
1:D:762:TRP:O	1:D:766:ILE:HG13	2.17	0.44
1:D:537:MET:HG3	1:D:541:LEU:HD12	1.99	0.44
1:A:730:TYR:O	1:A:735:ILE:HG12	2.18	0.44
1:B:727:LEU:HD23	1:B:759:LEU:CD1	2.47	0.44
1:D:485:MET:HE2	1:D:485:MET:HB3	1.86	0.44
1:A:461:GLN:HE21	1:A:461:GLN:CA	2.16	0.44
1:B:497:SER:HA	1:B:542:GLN:NE2	2.31	0.44
1:D:699:GLU:O	1:D:700:GLY:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:ASP:O	1:D:567:HIS:HB2	2.18	0.44
1:A:721:GLU:HB2	4:A:803:IWN:C25	2.48	0.43
1:A:493:MET:HB3	1:A:538:TYR:CD1	2.54	0.43
1:A:498:CYS:SG	1:A:554:LYS:HG3	2.59	0.43
1:C:693:TYR:OH	4:C:803:IWN:N21	2.51	0.43
1:D:575:LEU:HD13	1:D:580:HIS:CG	2.53	0.43
1:C:485:MET:HE2	1:C:485:MET:HB3	1.86	0.43
1:A:493:MET:SD	1:A:535:HIS:HA	2.57	0.43
1:D:635:LEU:O	1:D:638:TYR:N	2.48	0.43
1:A:763:GLU:O	1:A:767:ARG:HG3	2.18	0.43
1:D:735:ILE:O	1:D:736:PRO:C	2.60	0.43
1:A:724:GLN:O	1:A:727:LEU:HB2	2.19	0.43
4:D:803:IWN:O11	4:D:803:IWN:C16	2.67	0.43
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.84	0.43
1:A:756[A]:ARG:HG2	1:A:756[A]:ARG:HH11	1.83	0.43
1:B:658:ASN:OD1	1:B:658:ASN:C	2.61	0.43
1:C:658:ASN:OD1	1:C:658:ASN:C	2.62	0.42
1:B:658:ASN:OD1	1:B:659:GLN:N	2.52	0.42
1:D:700:GLY:HA3	1:D:714:MET:O	2.20	0.42
1:A:727:LEU:HD23	1:A:759:LEU:CD1	2.50	0.42
1:B:566:ASP:O	1:B:566:ASP:CG	2.62	0.42
1:A:698:ALA:O	1:A:701:ASP:HB2	2.19	0.42
1:D:502:CYS:SG	1:D:554:LYS:HE2	2.59	0.42
1:A:614:LEU:O	1:A:615:SER:C	2.63	0.42
1:D:542:GLN:NE2	1:D:542:GLN:HA	2.34	0.42
1:A:655:ASN:O	1:A:658:ASN:HB3	2.19	0.42
1:A:729:PHE:CD1	4:A:803:IWN:C14	3.02	0.42
1:B:727:LEU:CD2	1:B:759:LEU:HD11	2.50	0.42
1:B:462:PHE:CE2	1:B:509:CME:HZ2	2.55	0.42
1:B:503:PHE:HA	5:B:914:HOH:O	2.19	0.41
1:B:547:LEU:HD12	1:B:547:LEU:N	2.36	0.41
1:B:735:ILE:HD12	1:B:756:ARG:HG2	2.02	0.41
1:C:713:MET:HG2	1:C:714:MET:HG2	2.01	0.41
1:B:683:PRO:O	1:B:687:LEU:HD12	2.21	0.41
1:A:624:GLU:HG3	1:A:628:LYS:HE3	2.03	0.41
1:A:592:GLU:HA	1:A:595:HIS:CD2	2.56	0.41
1:A:749:GLU:N	1:A:750:PRO:CD	2.84	0.41
1:A:535:HIS:O	1:A:538:TYR:HB3	2.21	0.41
1:B:505:LEU:HD13	1:B:505:LEU:HA	1.91	0.41
1:B:515:VAL:O	1:B:516:LYS:C	2.63	0.41
1:B:682:TRP:HB3	1:B:683:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:TRP:N	1:C:487:PRO:CD	2.84	0.41
1:D:634:ASP:HB3	1:D:637:LEU:HD12	2.03	0.41
1:C:580:HIS:ND1	1:C:581:PRO:HD2	2.36	0.40
1:D:511:PHE:O	1:D:515:VAL:HG23	2.21	0.40
1:C:562:CYS:HB3	1:C:599:THR:OG1	2.22	0.40
1:A:659:GLN:NE2	1:A:663:ASP:OD1	2.55	0.40
4:A:803:IWN:O11	4:A:803:IWN:C16	2.69	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	311/343 (91%)	295 (95%)	15 (5%)	1 (0%)	36	45
1	B	312/343 (91%)	285 (91%)	25 (8%)	2 (1%)	21	29
1	C	311/343 (91%)	286 (92%)	22 (7%)	3 (1%)	12	17
1	D	308/343 (90%)	272 (88%)	34 (11%)	2 (1%)	21	29
All	All	1242/1372 (90%)	1138 (92%)	96 (8%)	8 (1%)	21	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	636	ALA
1	C	768	GLY
1	C	498	CYS
1	B	652	GLY
1	B	768	GLY
1	D	647	GLU
1	A	615	SER
1	C	465	PRO

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	282/305 (92%)	260 (92%)	22 (8%)	11	16
1	B	281/305 (92%)	255 (91%)	26 (9%)	8	10
1	C	282/305 (92%)	258 (92%)	24 (8%)	10	13
1	D	279/305 (92%)	251 (90%)	28 (10%)	7	9
All	All	1124/1220 (92%)	1024 (91%)	100 (9%)	9	12

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	463	THR
1	A	471	GLU
1	A	504	GLU
1	A	510	ARG
1	A	517	LYS
1	A	521	ARG
1	A	545	HIS
1	A	573	SER
1	A	575	LEU
1	A	577	LYS
1	A	585	LEU
1	A	587	SER
1	A	605	LEU
1	A	606	GLU
1	A	614	LEU
1	A	622	VAL
1	A	643	LYS
1	A	677	SER
1	A	681	LEU
1	A	709	GLN
1	A	760	SER
1	B	461	GLN
1	B	463	THR

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Mol	Chain	Res	Type
1	B	469	CYS
1	B	470	LYS
1	B	471	GLU
1	B	485	MET
1	B	504	GLU
1	B	505	LEU
1	B	510	ARG
1	B	517	LYS
1	B	576	GLN
1	B	605	LEU
1	B	613	THR
1	B	615	SER
1	B	617	SER
1	B	623	LEU
1	B	643	LYS
1	B	650	GLN
1	B	678	VAL
1	B	681	LEU
1	B	709	GLN
1	B	722	VAL
1	B	727	LEU
1	B	760	SER
1	B	764	LYS
1	B	770	GLU
1	C	459	LEU
1	C	461	GLN
1	C	463	THR
1	C	470	LYS
1	C	485	MET
1	C	500	THR
1	C	504	GLU
1	C	517	LYS
1	C	577	LYS
1	C	587	SER
1	C	605	LEU
1	C	606	GLU
1	C	614	LEU
1	C	616	SER
1	C	617	SER
1	C	622	VAL
1	C	623	LEU
1	C	643	LYS

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Mol	Chain	Res	Type
1	C	681	LEU
1	C	722	VAL
1	C	753	LYS
1	C	760	SER
1	C	766	ILE
1	C	770	GLU
1	D	463	THR
1	D	464	LEU
1	D	468	LEU
1	D	471	GLU
1	D	500	THR
1	D	502	CYS
1	D	504	GLU
1	D	545	HIS
1	D	551	LEU
1	D	573	SER
1	D	575	LEU
1	D	577	LYS
1	D	597	SER
1	D	602	ILE
1	D	614	LEU
1	D	623	LEU
1	D	643	LYS
1	D	651	THR
1	D	655	ASN
1	D	662	ARG
1	D	686	LYS
1	D	709	GLN
1	D	711	ILE
1	D	727	LEU
1	D	741	LEU
1	D	745	LEU
1	D	759	LEU
1	D	760	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	495	HIS
1	A	542	GLN
1	A	644	GLN

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Mol	Chain	Res	Type
1	A	761	GLN
1	B	484	ASN
1	B	495	HIS
1	B	542	GLN
1	B	604	GLN
1	B	644	GLN
1	B	650	GLN
1	B	709	GLN
1	C	484	ASN
1	C	495	HIS
1	C	542	GLN
1	C	545	HIS
1	C	576	GLN
1	C	593	GLN
1	C	709	GLN
1	D	484	ASN
1	D	542	GLN
1	D	593	GLN
1	D	604	GLN
1	D	644	GLN
1	D	659	GLN
1	D	743	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	A	509	1	8,9,10	0.60	0	6,9,11	1.17	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	B	509	1	8,9,10	0.65	0	6,9,11	0.78	0
1	CME	D	509	1	8,9,10	0.88	1 (12%)	6,9,11	1.31	1 (16%)
1	CME	C	509	1	8,9,10	0.77	0	6,9,11	1.38	1 (16%)

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	A	509	1	-	1/5/8/10	-
1	CME	B	509	1	-	1/5/8/10	-
1	CME	D	509	1	-	3/5/8/10	-
1	CME	C	509	1	-	2/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	509	CME	O-C	2.15	1.28	1.20

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	509	CME	CB-SG-SD	2.76	111.02	103.86
1	D	509	CME	CB-SG-SD	2.70	110.86	103.86
1	A	509	CME	CB-CA-C	2.30	117.05	110.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	509	CME	CZ-CE-SD-SG
1	D	509	CME	N-CA-CB-SG
1	D	509	CME	CE-SD-SG-CB
1	B	509	CME	SD-CE-CZ-OH
1	A	509	CME	CZ-CE-SD-SG
1	C	509	CME	SD-CE-CZ-OH
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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
4	IWN	B	803	-	28,30,30	3.06	13 (46%)	32,42,42	3.77	15 (46%)
4	IWN	D	803	-	28,30,30	3.55	14 (50%)	32,42,42	3.64	15 (46%)
4	IWN	C	803	-	28,30,30	3.35	15 (53%)	32,42,42	2.90	9 (28%)
4	IWN	A	803	-	28,30,30	3.38	14 (50%)	32,42,42	2.57	12 (37%)

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
4	IWN	B	803	-	-	0/15/15/15	0/4/4/4
4	IWN	D	803	-	-	1/15/15/15	0/4/4/4
4	IWN	C	803	-	-	1/15/15/15	0/4/4/4
4	IWN	A	803	-	-	1/15/15/15	0/4/4/4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	IWN	C2-C10	7.12	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	IWN	C15-C14	7.08	1.51	1.35
4	D	803	IWN	C23-C22	6.94	1.49	1.39
4	B	803	IWN	C23-C22	6.90	1.49	1.39
4	D	803	IWN	C15-C14	6.35	1.49	1.35
4	C	803	IWN	C20-N21	6.22	1.49	1.37
4	A	803	IWN	C23-C22	6.14	1.48	1.39
4	A	803	IWN	C15-C14	6.13	1.49	1.35
4	A	803	IWN	C20-N21	6.11	1.49	1.37
4	C	803	IWN	C2-C10	5.85	1.59	1.46
4	D	803	IWN	C7-C3	5.71	1.57	1.50
4	C	803	IWN	C15-C14	5.69	1.48	1.35
4	D	803	IWN	C4-N5	5.63	1.41	1.32
4	D	803	IWN	C2-C10	5.25	1.58	1.46
4	B	803	IWN	C2-C10	5.22	1.58	1.46
4	D	803	IWN	C20-N21	5.14	1.47	1.37
4	C	803	IWN	N18-N19	5.11	1.43	1.37
4	D	803	IWN	C17-N18	5.07	1.47	1.38
4	C	803	IWN	C17-N18	5.04	1.47	1.38
4	C	803	IWN	C4-N5	5.00	1.40	1.32
4	A	803	IWN	C17-N18	4.93	1.47	1.38
4	C	803	IWN	C7-C3	4.90	1.56	1.50
4	D	803	IWN	C15-N18	4.87	1.47	1.37
4	B	803	IWN	C20-N21	4.80	1.47	1.37
4	D	803	IWN	C26-C25	4.76	1.48	1.38
4	A	803	IWN	C7-C3	4.72	1.56	1.50
4	A	803	IWN	N18-N19	4.66	1.42	1.37
4	B	803	IWN	C26-C25	4.48	1.48	1.38
4	D	803	IWN	N18-N19	4.35	1.42	1.37
4	A	803	IWN	C26-C25	4.34	1.47	1.38
4	C	803	IWN	C15-N18	4.28	1.45	1.37
4	A	803	IWN	C10-N12	3.91	1.45	1.37
4	C	803	IWN	N1-N5	3.90	1.42	1.36
4	C	803	IWN	C23-C22	3.86	1.45	1.39
4	C	803	IWN	C16-C17	3.84	1.50	1.41
4	B	803	IWN	C17-N18	3.73	1.45	1.38
4	B	803	IWN	C10-N12	3.69	1.44	1.37
4	D	803	IWN	C2-N1	3.67	1.41	1.36
4	B	803	IWN	C15-N18	3.46	1.44	1.37
4	B	803	IWN	C7-C3	3.34	1.54	1.50
4	D	803	IWN	C10-N12	3.29	1.43	1.37
4	B	803	IWN	C4-N5	3.23	1.37	1.32
4	A	803	IWN	C4-N5	3.19	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	IWN	C2-N1	3.18	1.40	1.36
4	D	803	IWN	C16-C17	3.12	1.48	1.41
4	A	803	IWN	C2-N1	3.06	1.40	1.36
4	C	803	IWN	C26-C25	2.86	1.44	1.38
4	A	803	IWN	C4-C3	-2.75	1.37	1.40
4	B	803	IWN	C16-C17	2.71	1.48	1.41
4	D	803	IWN	C20-N19	2.67	1.37	1.33
4	C	803	IWN	C10-N12	2.67	1.42	1.37
4	C	803	IWN	C22-C20	2.64	1.51	1.47
4	A	803	IWN	C25-C24	2.58	1.43	1.38
4	A	803	IWN	C16-C17	2.47	1.47	1.41
4	B	803	IWN	N18-N19	2.40	1.40	1.37
4	B	803	IWN	C25-C24	2.01	1.42	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	IWN	C20-N19-N18	13.91	109.92	101.98
4	D	803	IWN	C20-N19-N18	12.35	109.03	101.98
4	C	803	IWN	C20-N19-N18	9.88	107.62	101.98
4	A	803	IWN	C20-N19-N18	7.24	106.11	101.98
4	C	803	IWN	N19-C20-N21	-6.95	107.82	114.71
4	B	803	IWN	N19-C20-N21	-6.90	107.87	114.71
4	D	803	IWN	N19-C20-N21	-6.76	108.01	114.71
4	D	803	IWN	C3-C4-N5	-6.45	107.23	112.33
4	D	803	IWN	O8-C7-C3	6.17	124.89	110.31
4	B	803	IWN	C3-C4-N5	-5.62	107.88	112.33
4	D	803	IWN	C4-N5-N1	5.59	110.39	105.06
4	A	803	IWN	C24-C23-C22	-5.33	115.12	120.36
4	C	803	IWN	C6-N1-C2	-5.09	122.36	129.21
4	B	803	IWN	C22-C20-N21	5.07	131.79	122.92
4	C	803	IWN	C6-N1-N5	5.03	129.25	119.22
4	B	803	IWN	C24-C23-C22	-4.54	115.90	120.36
4	A	803	IWN	N19-C20-N21	-4.47	110.28	114.71
4	A	803	IWN	C6-N1-C2	-4.25	123.50	129.21
4	D	803	IWN	C17-N18-N19	-4.14	105.82	111.33
4	B	803	IWN	C17-N18-N19	-4.13	105.83	111.33
4	A	803	IWN	C6-N1-N5	3.88	126.96	119.22
4	B	803	IWN	C6-N1-N5	3.83	126.85	119.22
4	B	803	IWN	C27-C22-C23	3.70	123.28	118.57
4	B	803	IWN	C4-N5-N1	3.69	108.58	105.06
4	D	803	IWN	C15-N18-N19	3.65	131.71	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	803	IWN	C2-C10-N12	-3.60	110.96	116.31
4	D	803	IWN	C6-N1-N5	3.58	126.35	119.22
4	A	803	IWN	C27-C22-C23	3.56	123.10	118.57
4	A	803	IWN	C9-O8-C7	3.56	125.98	112.53
4	B	803	IWN	C16-C13-N12	-3.51	118.03	126.42
4	B	803	IWN	C23-C22-C20	-3.50	116.37	120.78
4	C	803	IWN	C22-C20-N21	3.47	129.00	122.92
4	D	803	IWN	O11-C10-C2	3.33	128.46	121.96
4	C	803	IWN	C9-O8-C7	3.33	125.11	112.53
4	B	803	IWN	C15-N18-N19	3.31	131.07	124.70
4	B	803	IWN	C15-C14-C13	-3.26	115.44	120.33
4	A	803	IWN	C25-C24-C23	2.88	123.79	120.24
4	D	803	IWN	C16-C13-N12	-2.84	119.62	126.42
4	D	803	IWN	C23-C22-C20	-2.78	117.27	120.78
4	D	803	IWN	C27-C22-C23	2.54	121.80	118.57
4	C	803	IWN	C15-N18-N19	2.53	129.57	124.70
4	A	803	IWN	C23-C22-C20	-2.44	117.71	120.78
4	A	803	IWN	C22-C20-N21	2.41	127.13	122.92
4	B	803	IWN	C6-N1-C2	-2.39	125.99	129.21
4	A	803	IWN	C15-N18-N19	2.32	129.15	124.70
4	D	803	IWN	C26-C27-C22	-2.31	118.09	120.36
4	C	803	IWN	C3-C4-N5	-2.31	110.50	112.33
4	D	803	IWN	C10-C2-C3	-2.24	123.22	129.00
4	B	803	IWN	O8-C7-C3	2.08	115.24	110.31
4	A	803	IWN	C16-C13-N12	-2.07	121.47	126.42
4	C	803	IWN	C17-N18-N19	-2.06	108.59	111.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	803	IWN	C4-C3-C7-O8
4	D	803	IWN	C3-C7-O8-C9
4	A	803	IWN	C4-C3-C7-O8

There are no ring outliers.

3 monomers are involved in 7 short contacts:

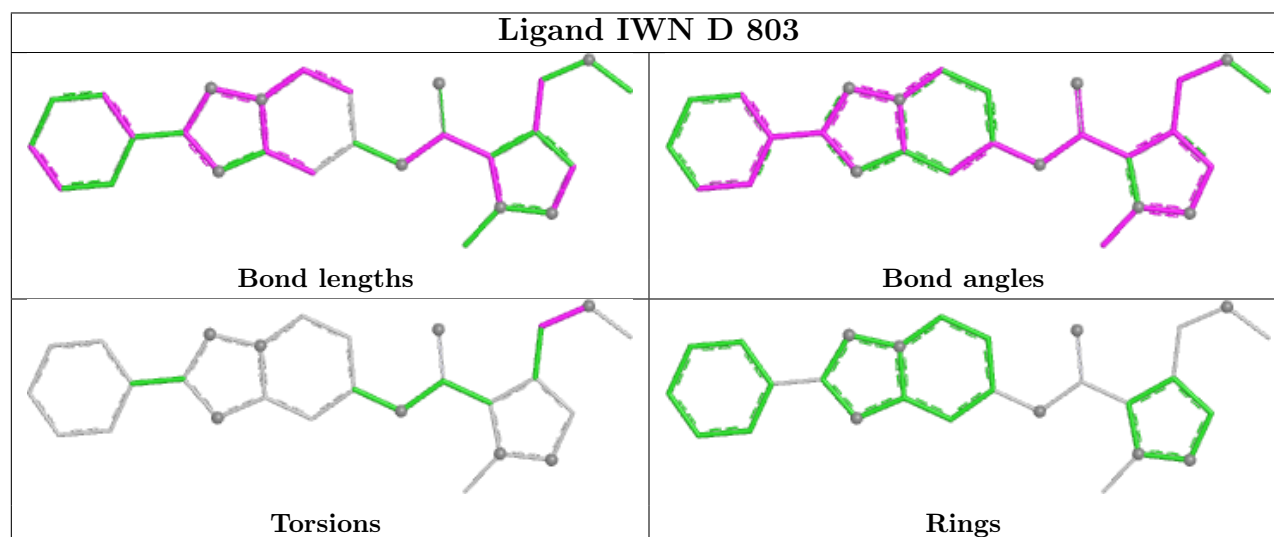
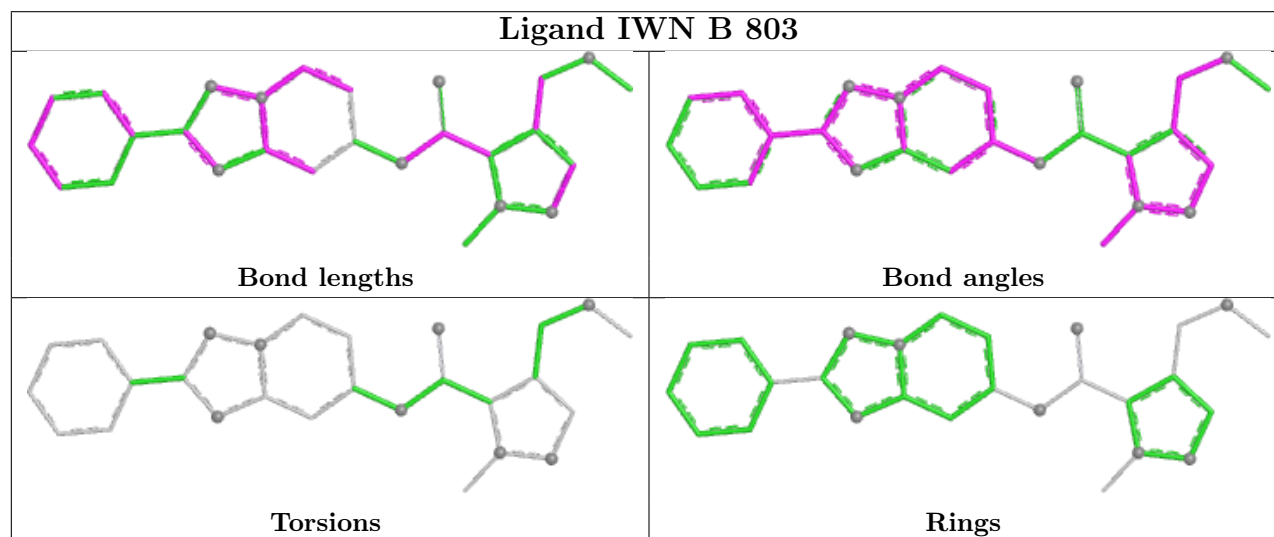
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	803	IWN	3	0
4	C	803	IWN	1	0

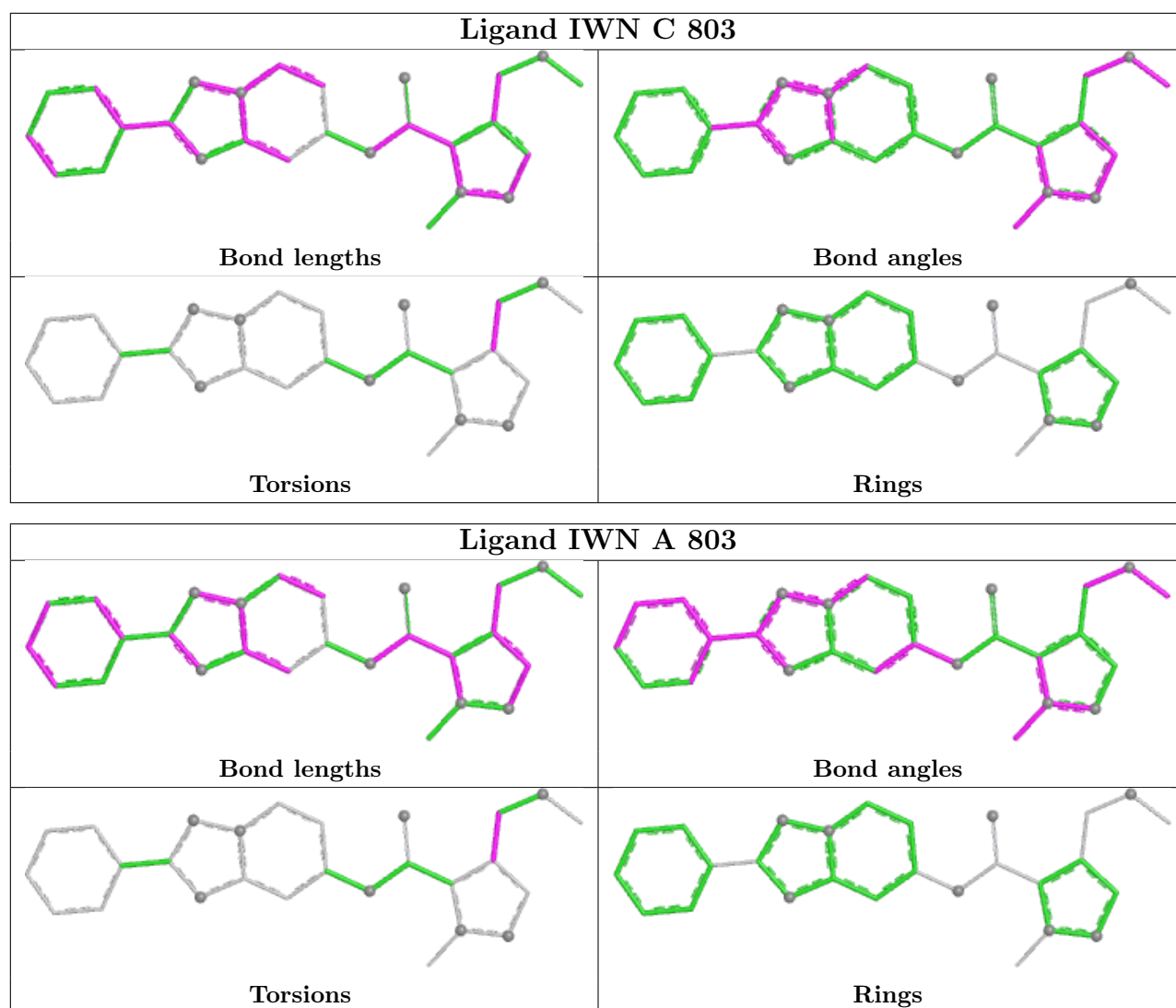
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	IWN	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	312/343 (90%)	-0.41	1 (0%) 90 92	33, 57, 86, 121	1 (0%)
1	B	314/343 (91%)	-0.39	2 (0%) 85 88	40, 56, 83, 113	0
1	C	312/343 (90%)	-0.47	1 (0%) 90 92	38, 55, 82, 101	1 (0%)
1	D	310/343 (90%)	0.04	2 (0%) 85 88	60, 82, 104, 115	0
All	All	1248/1372 (90%)	-0.31	6 (0%) 87 89	33, 62, 95, 121	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	458	GLY	2.9
1	D	459	LEU	2.5
1	D	458	GLY	2.4
1	B	771	THR	2.4
1	B	457	GLN	2.3
1	A	459	LEU	2.2

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	0.85	0.15	51,62,98,102	0
1	CME	D	509	10/11	0.88	0.13	84,101,124,131	0
1	CME	A	509	10/11	0.89	0.12	52,70,109,116	0
1	CME	B	509	10/11	0.89	0.12	53,77,97,106	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

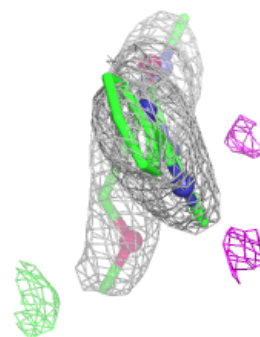
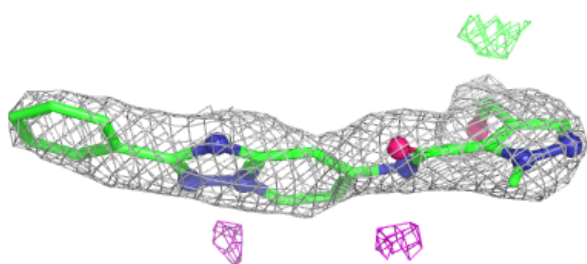
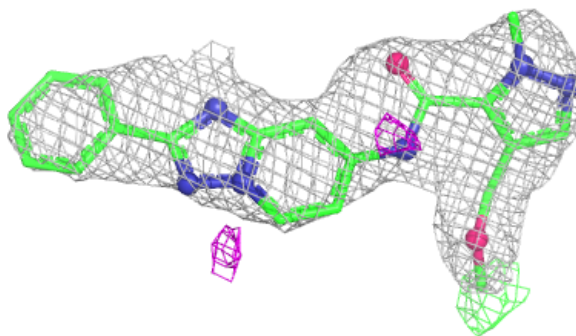
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IWN	D	803	27/27	0.88	0.12	72,85,97,104	0
4	IWN	C	803	27/27	0.92	0.11	55,71,80,84	0
4	IWN	A	803	27/27	0.94	0.09	47,59,68,72	0
4	IWN	B	803	27/27	0.95	0.09	43,60,74,84	0
3	MG	A	802	1/1	1.00	0.01	52,52,52,52	0
3	MG	B	802	1/1	1.00	0.01	44,44,44,44	0
3	MG	C	802	1/1	1.00	0.01	43,43,43,43	0
3	MG	D	802	1/1	1.00	0.04	55,55,55,55	0
2	ZN	A	801	1/1	1.00	0.01	53,53,53,53	0
2	ZN	B	801	1/1	1.00	0.01	50,50,50,50	0
2	ZN	C	801	1/1	1.00	0.01	53,53,53,53	0
2	ZN	D	801	1/1	1.00	0.02	72,72,72,72	0

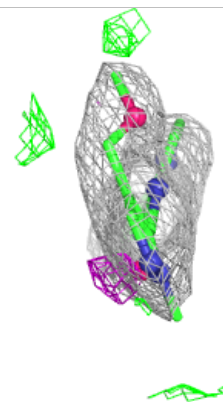
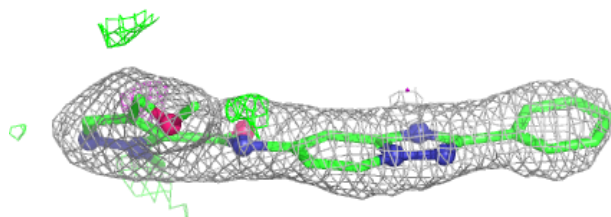
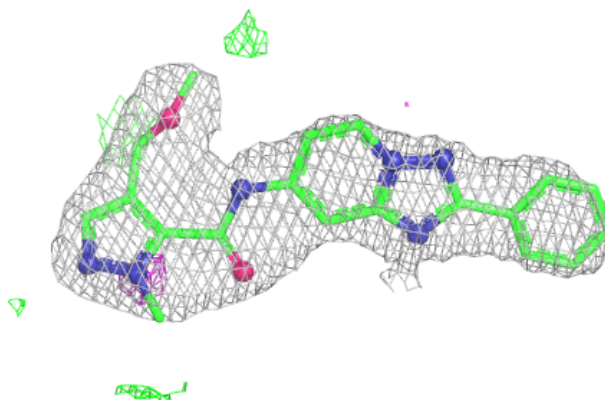
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IWN 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)

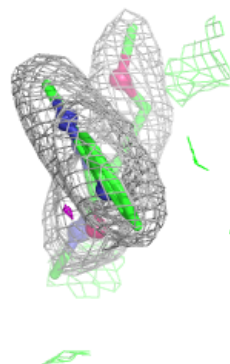
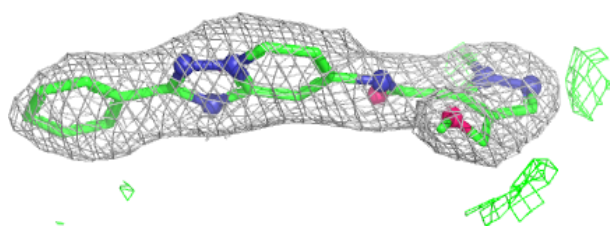
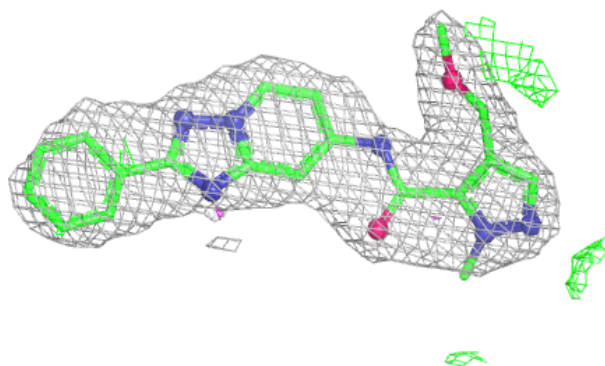
**Electron density around IWN C 803:**

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

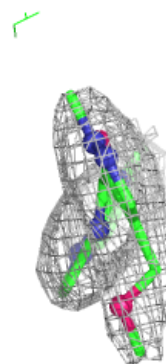
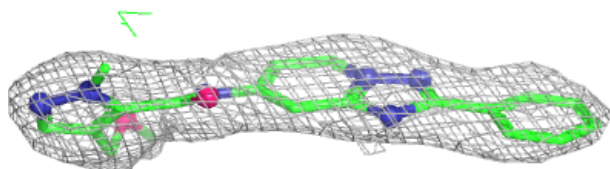
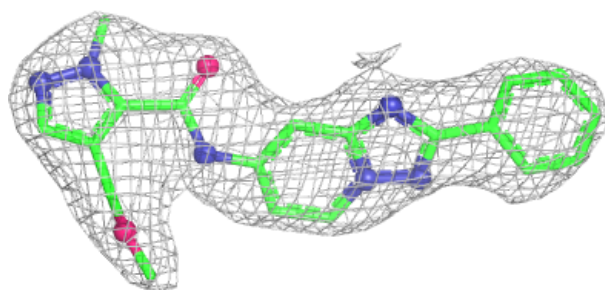


Electron density around IWN A 803:

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

**Electron density around IWN 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.