



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:15 AM UTC

PDB ID : 5SGJ / pdb_00005sgj
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN
COMPLEX WITH c4c(nc(C(Nc1c(cc2c(c1)nc([nH]2)c3ccccc3)C(NC)=O)=O)c(c4)C)C, micromolar IC50=0.007516
Authors : Joseph, C.; Benz, J.; Flohr, A.; Rudolph, M.G.
Deposited on : 2022-02-01
Resolution : 2.66 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

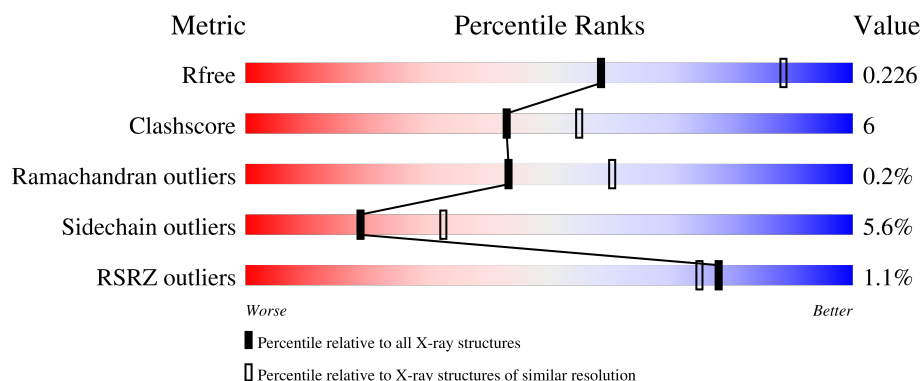
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	71%19%•9%
1	B	343	2% 71%18%•8%
1	C	343	% 70%19%•9%
1	D	343	% 75%15%•10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10601 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	0	0
			2541	1624	432	461	24			
1	B	315	Total	C	N	O	S	0	1	0
			2559	1635	437	463	24			
1	C	313	Total	C	N	O	S	0	1	0
			2549	1629	435	461	24			
1	D	310	Total	C	N	O	S	0	0	0
			2519	1612	429	454	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

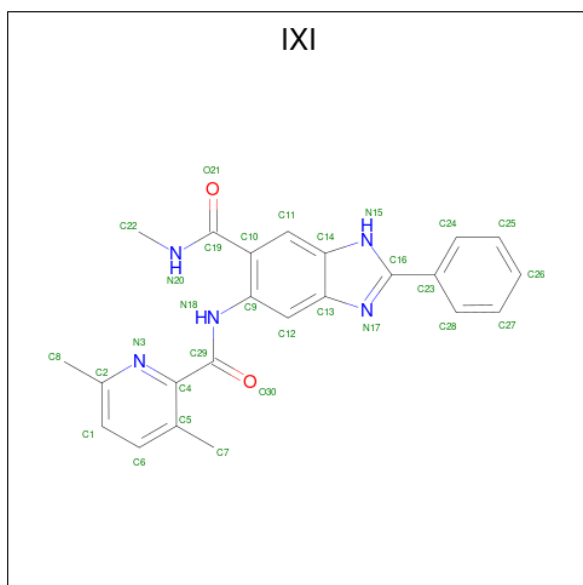
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 5-[(3,6-dimethylpyridine-2-carbonyl)amino]-N-methyl-2-phenyl-1H-benzimidazole-6-carboxamide (CCD ID: IXI) (formula: C₂₃H₂₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			30	23	5	2		
4	B	1	Total	C	N	O	0	0
			30	23	5	2		
4	C	1	Total	C	N	O	0	0
			30	23	5	2		
4	D	1	Total	C	N	O	0	0
			30	23	5	2		

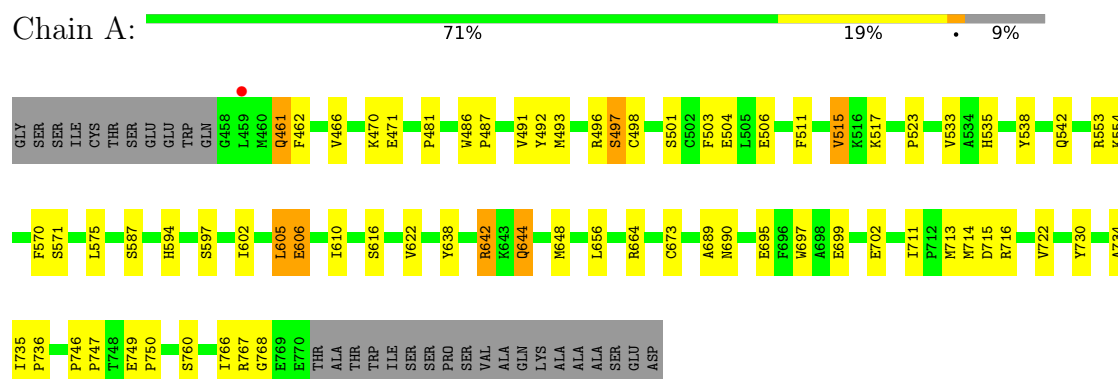
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total 90	O 90	0	0
5	B	85	Total 85	O 85	0	0
5	C	84	Total 84	O 84	0	0
5	D	46	Total 46	O 46	0	0

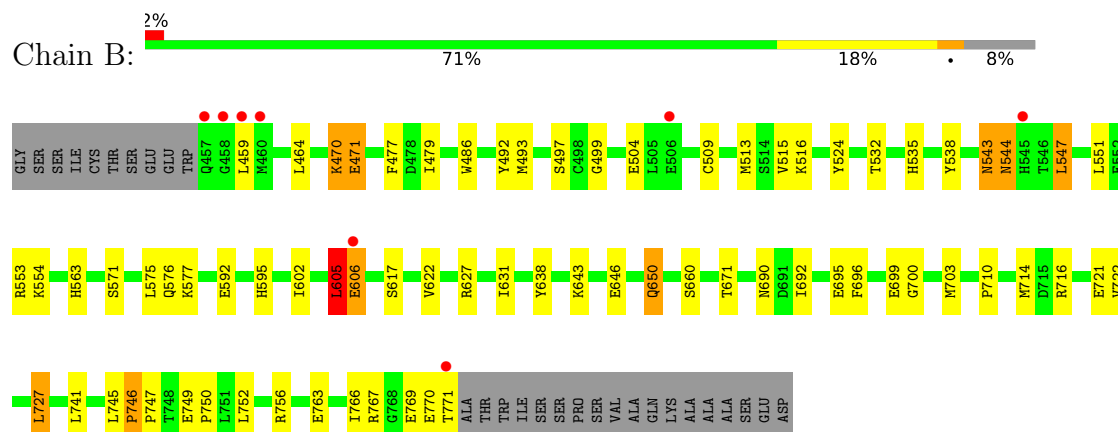
3 Residue-property plots

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.

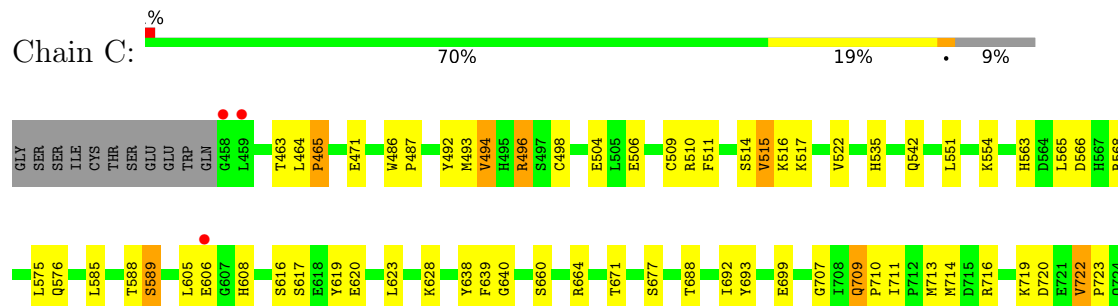
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

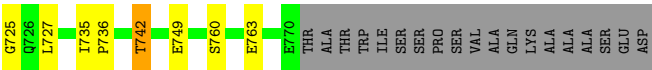


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

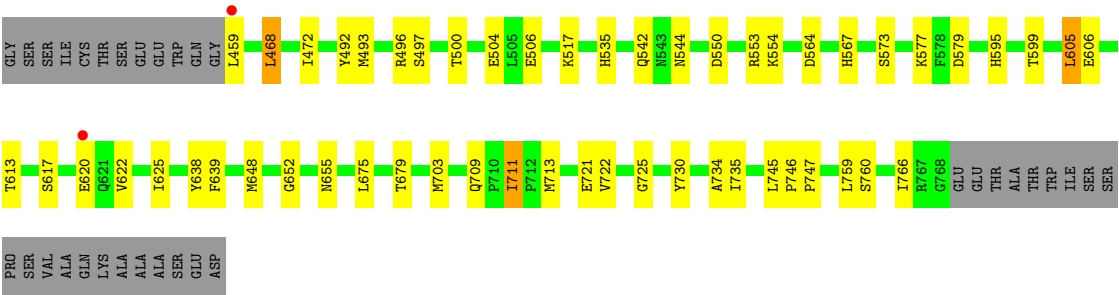
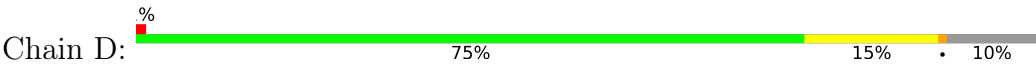


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A





● 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	135.56Å 135.56Å 235.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.75 – 2.66 43.75 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.2 (43.75-2.66) 95.3 (43.75-2.66)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.260 (Not available) , 0.226	Depositor DCC
R_{free} test set	2329 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.7	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	0.94	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: IXI, CME, MG, 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	1.17	3/2592 (0.1%)	1.56	14/3507 (0.4%)
1	B	1.16	3/2613 (0.1%)	1.58	15/3535 (0.4%)
1	C	1.14	2/2603 (0.1%)	1.57	19/3521 (0.5%)
1	D	1.18	0/2570	1.69	17/3478 (0.5%)
All	All	1.16	8/10378 (0.1%)	1.60	65/14041 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	563	HIS	CE1-NE2	6.68	1.39	1.32
1	C	692	ILE	C-O	5.95	1.30	1.24
1	C	563	HIS	CE1-NE2	5.73	1.38	1.32
1	A	481	PRO	C-O	-5.65	1.17	1.24
1	B	710	PRO	C-O	-5.23	1.17	1.23
1	B	606	GLU	N-CA	5.20	1.52	1.46
1	A	570	PHE	C-O	5.17	1.30	1.23
1	A	715	ASP	C-O	5.09	1.30	1.24

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	606	GLU	CB-CG-CD	8.63	127.27	112.60
1	D	606	GLU	CB-CG-CD	8.11	126.39	112.60
1	D	721	GLU	CA-C-N	7.56	126.38	120.33
1	D	721	GLU	C-N-CA	7.56	126.38	120.33
1	A	606	GLU	CB-CG-CD	7.29	124.99	112.60
1	C	606	GLU	CB-CG-CD	7.26	124.94	112.60
1	A	506	GLU	CB-CG-CD	7.25	124.93	112.60
1	D	554	LYS	CA-C-N	7.00	127.75	119.98
1	D	554	LYS	C-N-CA	7.00	127.75	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	639	PHE	CA-C-N	6.99	127.74	119.98
1	D	639	PHE	C-N-CA	6.99	127.74	119.98
1	C	619	TYR	CA-C-N	6.78	129.69	120.54
1	C	619	TYR	C-N-CA	6.78	129.69	120.54
1	B	746	PRO	N-CA-C	6.68	118.85	110.70
1	C	639	PHE	CA-C-N	6.65	127.32	119.94
1	C	639	PHE	C-N-CA	6.65	127.32	119.94
1	C	620	GLU	CB-CG-CD	6.59	123.80	112.60
1	B	493	MET	CA-C-O	-6.45	113.71	120.55
1	C	720	ASP	CA-CB-CG	6.28	118.88	112.60
1	C	640	GLY	CA-C-N	6.15	128.43	120.44
1	C	640	GLY	C-N-CA	6.15	128.43	120.44
1	A	506	GLU	CB-CA-C	6.09	120.55	110.81
1	A	506	GLU	N-CA-C	-5.82	104.13	111.11
1	D	550	ASP	CA-C-N	5.77	128.34	120.54
1	D	550	ASP	C-N-CA	5.77	128.34	120.54
1	A	642	ARG	CA-C-O	-5.71	114.79	120.90
1	B	763	GLU	N-CA-C	-5.70	104.97	111.07
1	B	606	GLU	CB-CA-C	5.64	117.90	110.06
1	A	690	ASN	CB-CA-C	-5.63	102.03	110.88
1	A	689	ALA	CA-C-O	-5.55	114.63	120.63
1	D	620	GLU	N-CA-C	-5.51	105.66	112.38
1	C	742	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	501	SER	CA-C-N	5.45	127.58	120.28
1	A	501	SER	C-N-CA	5.45	127.58	120.28
1	C	620	GLU	CB-CA-C	5.41	119.46	110.81
1	C	606	GLU	N-CA-C	-5.40	102.31	110.24
1	B	605	LEU	CA-C-O	-5.36	115.29	121.19
1	D	468	LEU	CA-C-N	5.31	128.79	120.82
1	D	468	LEU	C-N-CA	5.31	128.79	120.82
1	A	690	ASN	N-CA-CB	5.31	117.71	110.01
1	B	690	ASN	CB-CA-C	-5.26	102.05	110.79
1	C	506	GLU	CB-CG-CD	5.25	121.52	112.60
1	B	532	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	702	GLU	CB-CG-CD	5.21	121.46	112.60
1	C	494	VAL	CA-C-O	-5.21	115.33	120.85
1	B	499	GLY	CA-C-O	-5.21	118.70	122.45
1	C	516	LYS	CA-C-N	5.20	127.97	120.38
1	C	516	LYS	C-N-CA	5.20	127.97	120.38
1	D	648	MET	CA-C-O	-5.20	115.54	121.00
1	C	515	VAL	CA-C-O	-5.19	115.67	121.17
1	B	544	ASN	CA-C-O	-5.17	116.37	121.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	606	GLU	CB-CA-C	5.16	117.58	109.84
1	C	510	ARG	CB-CA-C	5.15	119.89	110.10
1	D	639	PHE	CA-C-O	-5.14	115.40	120.90
1	A	664	ARG	CA-C-N	5.13	127.49	120.46
1	A	664	ARG	C-N-CA	5.13	127.49	120.46
1	B	554	LYS	CA-C-N	5.13	125.63	119.94
1	B	554	LYS	C-N-CA	5.13	125.63	119.94
1	D	605	LEU	CA-C-O	-5.13	115.55	121.19
1	D	506	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	515	VAL	N-CA-C	-5.03	105.59	110.42
1	B	643	LYS	CA-C-O	-5.03	115.52	120.90
1	B	741	LEU	CA-C-N	5.01	126.99	120.28
1	B	741	LEU	C-N-CA	5.01	126.99	120.28
1	D	544	ASN	CA-C-O	-5.01	116.51	121.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2541	0	2511	36	1
1	B	2559	0	2528	37	1
1	C	2549	0	2524	30	0
1	D	2519	0	2496	24	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	30	0	0	3	0
4	B	30	0	0	3	0
4	C	30	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	30	0	0	1	0
5	A	90	0	0	0	1
5	B	85	0	0	3	1
5	C	84	0	0	4	0
5	D	46	0	0	1	0
All	All	10601	0	10059	126	2

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 (126) 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:493:MET:O	1:A:497:SER:HB2	1.75	0.86
1:A:461:GLN:HE21	1:A:461:GLN:HA	1.39	0.86
1:C:628:LYS:NZ	5:C:901:HOH:O	2.13	0.81
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.65	0.79
1:A:461:GLN:HA	1:A:461:GLN:NE2	1.96	0.77
1:A:461:GLN:HE21	1:A:461:GLN:CA	2.04	0.70
1:D:497:SER:HA	1:D:542:GLN:HE22	1.58	0.69
1:B:602:ILE:HA	1:B:605:LEU:HD22	1.75	0.68
1:A:644:GLN:HE21	1:A:644:GLN:HA	1.60	0.67
1:C:711:ILE:HD11	1:C:713:MET:HE2	1.79	0.65
1:B:543:ASN:HD22	1:B:543:ASN:N	1.96	0.64
1:A:766:ILE:O	1:A:768:GLY:N	2.30	0.64
1:C:707:GLY:O	1:D:652:GLY:HA3	2.00	0.62
1:C:699:GLU:OE2	1:C:714:MET:HE1	1.99	0.61
1:B:497:SER:O	1:B:553:ARG:HD2	2.01	0.61
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.83	0.61
1:B:571:SER:OG	1:B:699:GLU:OE2	2.14	0.60
1:A:535:HIS:O	1:A:538:TYR:HB3	2.02	0.59
1:B:700:GLY:HA3	1:B:714:MET:O	2.03	0.59
1:A:749:GLU:N	1:A:750:PRO:CD	2.66	0.58
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.84	0.58
1:D:497:SER:HA	1:D:542:GLN:NE2	2.18	0.58
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.40	0.57
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.88	0.56
1:C:709:GLN:NE2	1:C:710:PRO:HD2	2.20	0.56
1:D:766:ILE:HG22	1:D:766:ILE:O	2.05	0.56
1:A:766:ILE:C	1:A:768:GLY:H	2.14	0.56
4:A:803:IXI:O30	4:A:803:IXI:C7	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:LEU:HD12	1:B:766:ILE:HD13	1.89	0.55
1:A:730:TYR:O	1:A:735:ILE:HG12	2.08	0.54
1:B:770:GLU:HG3	1:B:771:THR:N	2.23	0.53
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.90	0.52
1:C:494:VAL:O	1:C:498:CYS:HB3	2.10	0.52
1:B:479:ILE:HD12	1:B:486:TRP:CD1	2.45	0.51
1:B:752:LEU:HD21	1:B:756[B]:ARG:NH2	2.25	0.51
1:B:492:TYR:OH	5:B:901:HOH:O	2.16	0.51
1:B:727:LEU:HD12	1:B:766:ILE:CD1	2.40	0.51
1:D:711:ILE:HD11	1:D:713:MET:HE3	1.92	0.51
1:B:627:ARG:NH1	5:B:902:HOH:O	2.30	0.51
1:B:692:ILE:HG22	1:B:696:PHE:CE2	2.46	0.50
1:C:576:GLN:HB2	5:C:969:HOH:O	2.11	0.50
1:B:577:LYS:HD3	1:B:703:MET:HE1	1.93	0.50
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.47	0.50
1:C:522:VAL:O	5:C:902:HOH:O	2.19	0.50
1:C:725:GLY:HA3	4:C:803:IXI:C23	2.42	0.50
1:A:493:MET:SD	1:A:535:HIS:HA	2.52	0.49
1:B:544:ASN:HB3	1:B:547:LEU:HD22	1.92	0.49
1:A:697:TRP:HA	1:A:714:MET:O	2.12	0.49
1:A:517:LYS:O	1:A:517:LYS:HG2	2.12	0.49
1:B:551:LEU:HD22	1:B:622:VAL:HB	1.95	0.49
1:D:746:PRO:N	1:D:747:PRO:CD	2.75	0.49
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.47	0.49
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.28	0.48
1:A:511:PHE:O	1:A:515:VAL:HG23	2.13	0.48
1:C:492:TYR:CE2	1:C:496:ARG:HD2	2.48	0.48
1:D:766:ILE:O	1:D:766:ILE:CG2	2.61	0.48
1:B:746:PRO:N	1:B:747:PRO:CD	2.76	0.48
1:C:693:TYR:OH	4:C:803:IXI:N17	2.47	0.48
1:B:543:ASN:N	1:B:543:ASN:ND2	2.62	0.47
1:C:509:CME:HB2	5:C:974:HOH:O	2.13	0.47
1:D:493:MET:O	1:D:497:SER:HB3	2.14	0.47
1:A:638:TYR:OH	1:A:642:ARG:HD3	2.14	0.47
1:B:749:GLU:N	1:B:750:PRO:CD	2.78	0.47
1:D:638:TYR:HA	5:D:928:HOH:O	2.15	0.47
1:C:722:VAL:N	1:C:723:PRO:CD	2.78	0.47
1:B:515:VAL:O	1:B:516:LYS:C	2.58	0.47
1:C:735:ILE:HB	1:C:736:PRO:HD3	1.96	0.47
1:C:727:LEU:HD21	1:C:763:GLU:HG3	1.97	0.46
1:D:577:LYS:HD3	1:D:703:MET:HE1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:ARG:O	1:C:719:LYS:HG3	2.15	0.46
1:A:713:MET:HG3	4:A:803:IXI:C13	2.45	0.46
1:C:493:MET:SD	1:C:535:HIS:HA	2.55	0.46
1:B:535:HIS:O	1:B:538:TYR:HB3	2.14	0.46
1:B:745:LEU:C	1:B:747:PRO:HD2	2.41	0.45
1:C:566:ASP:OD2	1:C:568[B]:ARG:NH2	2.49	0.45
1:A:462:PHE:CE1	1:A:491:VAL:HG11	2.52	0.45
1:B:471:GLU:HB3	1:B:477:PHE:CD1	2.51	0.45
1:C:660:SER:O	1:C:664:ARG:HG3	2.17	0.45
1:A:486:TRP:N	1:A:487:PRO:CD	2.80	0.45
1:B:551:LEU:HD23	1:B:551:LEU:HA	1.84	0.45
1:D:493:MET:SD	1:D:535:HIS:HA	2.57	0.44
1:A:503:PHE:HD1	1:A:610:ILE:O	2.00	0.44
1:A:498:CYS:SG	1:A:554:LYS:HG2	2.58	0.44
4:B:803:IXI:O30	4:B:803:IXI:C7	2.66	0.44
1:B:716:ARG:HG2	5:B:920:HOH:O	2.17	0.44
1:A:746:PRO:N	1:A:747:PRO:CD	2.81	0.43
1:A:594:HIS:O	1:A:597:SER:HB3	2.19	0.43
1:C:486:TRP:N	1:C:487:PRO:CD	2.82	0.43
1:B:767:ARG:NH2	1:B:769:GLU:OE1	2.52	0.43
1:B:509:CME:O	1:B:513:MET:HG2	2.18	0.43
1:B:721:GLU:HB3	4:B:803:IXI:C26	2.49	0.43
1:A:571:SER:OG	1:A:699:GLU:OE2	2.24	0.43
1:A:713:MET:HG3	4:A:803:IXI:C14	2.49	0.43
1:A:466:VAL:CG1	1:A:470:LYS:HE3	2.49	0.42
1:B:627:ARG:O	1:B:631:ILE:HG12	2.18	0.42
1:D:497:SER:O	1:D:553:ARG:HD2	2.19	0.42
1:D:730:TYR:O	1:D:735:ILE:HG12	2.19	0.42
1:A:697:TRP:HB3	1:A:716:ARG:HB3	2.01	0.42
1:D:622:VAL:HA	1:D:625:ILE:HD12	2.01	0.42
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.54	0.42
1:D:595:HIS:O	1:D:599:THR:OG1	2.34	0.42
1:D:711:ILE:CD1	1:D:713:MET:HE3	2.49	0.42
1:D:725:GLY:HA3	4:D:803:IXI:C23	2.49	0.42
1:B:592:GLU:HA	1:B:595:HIS:HD2	1.84	0.42
1:D:564:ASP:O	1:D:567:HIS:HB2	2.19	0.42
1:C:677:SER:HB2	1:C:688:THR:HG21	2.01	0.42
1:C:464:LEU:O	1:C:465:PRO:C	2.63	0.41
1:B:524:TYR:HB3	1:B:695:GLU:OE2	2.21	0.41
1:C:511:PHE:O	1:C:515:VAL:HG23	2.21	0.41
1:B:638:TYR:CD1	1:B:671:THR:HG21	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:LEU:C	1:D:747:PRO:HD2	2.45	0.41
1:D:468:LEU:O	1:D:472:ILE:N	2.51	0.41
1:A:542:GLN:HA	1:A:542:GLN:NE2	2.35	0.41
1:A:749:GLU:N	1:A:750:PRO:HD2	2.35	0.41
1:B:464:LEU:HD11	1:B:492:TYR:CD2	2.56	0.41
1:A:523:PRO:HD2	1:A:695:GLU:HG2	2.03	0.41
1:A:533:VAL:HG13	1:A:673:CYS:HB3	2.03	0.41
1:A:735:ILE:N	1:A:736:PRO:CD	2.84	0.41
1:B:470:LYS:HE2	1:D:746:PRO:CG	2.43	0.41
1:B:646:GLU:OE2	1:B:650:GLN:OE1	2.39	0.41
1:B:721:GLU:CB	4:B:803:IXI:C26	2.99	0.41
1:C:498:CYS:SG	1:C:554:LYS:HG3	2.61	0.41
1:C:588:THR:O	1:C:589:SER:C	2.64	0.41
1:A:644:GLN:O	1:A:648:MET:HG3	2.21	0.41
1:C:514:SER:OG	1:C:608:HIS:NE2	2.49	0.41
1:C:551:LEU:HA	1:C:551:LEU:HD23	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:GLU:OE2	1:B:606:GLU:OE2[2_655]	1.97	0.23
5:A:922:HOH:O	5:B:965:HOH:O[3_655]	2.02	0.18

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	310/343 (90%)	295 (95%)	14 (4%)	1 (0%)	36	52
1	B	313/343 (91%)	299 (96%)	14 (4%)	0	100	100
1	C	311/343 (91%)	293 (94%)	17 (6%)	1 (0%)	36	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	307/343 (90%)	292 (95%)	14 (5%)	1 (0%)	36	52
All	All	1241/1372 (90%)	1179 (95%)	59 (5%)	3 (0%)	43	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	ARG
1	D	579	ASP
1	C	465	PRO

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%)	266 (95%)	15 (5%)	20	35
1	B	282/305 (92%)	268 (95%)	14 (5%)	22	37
1	C	282/305 (92%)	264 (94%)	18 (6%)	16	28
1	D	279/305 (92%)	263 (94%)	16 (6%)	18	32
All	All	1124/1220 (92%)	1061 (94%)	63 (6%)	19	32

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	471	GLU
1	A	497	SER
1	A	504	GLU
1	A	553	ARG
1	A	575	LEU
1	A	587	SER
1	A	605	LEU
1	A	616	SER
1	A	622	VAL
1	A	644	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	656	LEU
1	A	711	ILE
1	A	722	VAL
1	A	760	SER
1	B	459	LEU
1	B	470	LYS
1	B	471	GLU
1	B	504	GLU
1	B	543	ASN
1	B	547	LEU
1	B	575	LEU
1	B	576	GLN
1	B	605	LEU
1	B	617	SER
1	B	650	GLN
1	B	660	SER
1	B	722	VAL
1	B	727	LEU
1	C	463	THR
1	C	471	GLU
1	C	496	ARG
1	C	504	GLU
1	C	517	LYS
1	C	565	LEU
1	C	575	LEU
1	C	585	LEU
1	C	589	SER
1	C	605	LEU
1	C	616	SER
1	C	617	SER
1	C	623	LEU
1	C	709	GLN
1	C	722	VAL
1	C	742	THR
1	C	749	GLU
1	C	760	SER
1	D	459	LEU
1	D	500	THR
1	D	504	GLU
1	D	517	LYS
1	D	573	SER
1	D	605	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	613	THR
1	D	617	SER
1	D	655	ASN
1	D	675	LEU
1	D	679	THR
1	D	709	GLN
1	D	711	ILE
1	D	722	VAL
1	D	759	LEU
1	D	760	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	542	GLN
1	A	593	GLN
1	A	604	GLN
1	A	644	GLN
1	A	659	GLN
1	A	761	GLN
1	B	542	GLN
1	B	543	ASN
1	B	593	GLN
1	B	598	GLN
1	B	604	GLN
1	B	655	ASN
1	B	658	ASN
1	B	726	GLN
1	C	542	GLN
1	C	593	GLN
1	C	604	GLN
1	C	609	ASN
1	C	621	GLN
1	C	709	GLN
1	C	724	GLN
1	C	743	GLN
1	D	484	ASN
1	D	542	GLN
1	D	576	GLN
1	D	604	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	621	GLN
1	D	644	GLN
1	D	709	GLN
1	D	731	ASN
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	B	509	1	8,9,10	0.49	0	6,9,11	0.78	0
1	CME	C	509	1	8,9,10	0.43	0	6,9,11	0.71	0
1	CME	A	509	1	8,9,10	0.66	0	6,9,11	0.94	0
1	CME	D	509	1	8,9,10	0.38	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	B	509	1	-	1/5/8/10	-
1	CME	C	509	1	-	3/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-
1	CME	D	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	509	CME	1	0
1	C	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	IXI	D	803	-	33,33,33	2.45	12 (36%)	46,47,47	1.54	8 (17%)
4	IXI	C	803	-	33,33,33	2.98	14 (42%)	46,47,47	2.10	17 (36%)
4	IXI	A	803	-	33,33,33	2.43	10 (30%)	46,47,47	2.23	15 (32%)
4	IXI	B	803	-	33,33,33	2.77	13 (39%)	46,47,47	2.01	8 (17%)

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	IXI	D	803	-	-	1/18/18/18	0/4/4/4
4	IXI	C	803	-	-	0/18/18/18	0/4/4/4
4	IXI	A	803	-	-	0/18/18/18	0/4/4/4
4	IXI	B	803	-	-	1/18/18/18	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	IXI	C19-N20	9.36	1.46	1.33
4	B	803	IXI	C19-N20	7.97	1.44	1.33
4	A	803	IXI	C19-N20	7.72	1.43	1.33
4	D	803	IXI	C4-C5	6.37	1.47	1.40
4	A	803	IXI	C14-C13	5.84	1.48	1.40
4	C	803	IXI	C14-C13	5.81	1.48	1.40
4	D	803	IXI	C19-N20	5.65	1.41	1.33
4	B	803	IXI	C4-C5	5.61	1.46	1.40
4	C	803	IXI	C10-C9	5.51	1.49	1.41
4	B	803	IXI	C14-C13	5.08	1.47	1.40
4	B	803	IXI	C10-C9	5.03	1.48	1.41
4	A	803	IXI	C10-C9	5.02	1.48	1.41
4	D	803	IXI	C14-C13	4.66	1.46	1.40
4	C	803	IXI	C4-C5	4.08	1.44	1.40
4	C	803	IXI	C16-N15	4.02	1.44	1.36
4	C	803	IXI	C4-C29	3.93	1.56	1.50
4	D	803	IXI	C16-N15	3.87	1.44	1.36
4	B	803	IXI	C1-C2	3.69	1.47	1.39
4	B	803	IXI	C16-N15	3.54	1.43	1.36
4	D	803	IXI	C10-C9	3.45	1.46	1.41
4	C	803	IXI	C10-C19	3.40	1.57	1.50
4	B	803	IXI	C1-C6	3.39	1.44	1.38
4	C	803	IXI	C1-C2	3.17	1.46	1.39
4	D	803	IXI	C1-C2	3.17	1.46	1.39
4	A	803	IXI	C16-N15	3.03	1.42	1.36
4	C	803	IXI	C6-C5	3.02	1.45	1.39
4	A	803	IXI	C4-C29	3.01	1.54	1.50
4	C	803	IXI	C16-N17	3.01	1.39	1.33
4	B	803	IXI	C10-C19	2.96	1.56	1.50
4	D	803	IXI	C4-C29	2.81	1.54	1.50
4	D	803	IXI	C4-N3	2.76	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	IXI	C24-C23	2.75	1.43	1.39
4	D	803	IXI	O21-C19	2.62	1.29	1.23
4	B	803	IXI	C16-N17	2.59	1.38	1.33
4	A	803	IXI	C4-N3	2.53	1.39	1.34
4	B	803	IXI	C4-N3	2.51	1.39	1.34
4	A	803	IXI	O21-C19	2.50	1.29	1.23
4	A	803	IXI	C24-C23	2.50	1.43	1.39
4	B	803	IXI	C13-N17	2.44	1.44	1.39
4	A	803	IXI	C10-C19	2.37	1.54	1.50
4	B	803	IXI	C4-C29	2.37	1.54	1.50
4	D	803	IXI	C10-C19	2.33	1.54	1.50
4	D	803	IXI	C14-N15	2.30	1.42	1.38
4	A	803	IXI	C2-N3	2.16	1.38	1.34
4	B	803	IXI	C12-C9	2.12	1.42	1.39
4	C	803	IXI	C4-N3	2.12	1.39	1.34
4	C	803	IXI	O21-C19	2.10	1.28	1.23
4	C	803	IXI	C12-C9	2.05	1.42	1.39
4	D	803	IXI	C24-C23	2.05	1.42	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	IXI	C10-C19-N20	6.00	125.75	116.98
4	A	803	IXI	C27-C28-C23	-5.94	114.52	120.36
4	A	803	IXI	C29-C4-N3	5.89	121.79	116.02
4	A	803	IXI	C10-C19-N20	5.54	125.08	116.98
4	C	803	IXI	C22-N20-C19	5.02	131.35	121.80
4	B	803	IXI	C6-C1-C2	4.91	124.73	119.90
4	C	803	IXI	C10-C19-N20	4.53	123.61	116.98
4	B	803	IXI	O21-C19-N20	-4.36	116.22	122.67
4	D	803	IXI	C6-C1-C2	4.20	124.03	119.90
4	A	803	IXI	C28-C23-C24	4.08	123.76	118.57
4	B	803	IXI	C9-C10-C19	3.94	126.01	120.96
4	A	803	IXI	C8-C2-N3	3.78	122.28	116.56
4	C	803	IXI	C9-C10-C19	3.75	125.76	120.96
4	B	803	IXI	C1-C2-N3	-3.71	116.77	121.59
4	C	803	IXI	C12-C9-N18	-3.58	112.56	121.95
4	C	803	IXI	C11-C10-C9	-3.49	115.95	119.09
4	A	803	IXI	O21-C19-N20	-3.49	117.50	122.67
4	D	803	IXI	C1-C6-C5	-3.27	117.09	121.98
4	B	803	IXI	C1-C6-C5	-3.27	117.10	121.98
4	D	803	IXI	O21-C19-N20	-3.14	118.02	122.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	IXI	C26-C25-C24	-3.06	116.47	120.24
4	C	803	IXI	C12-C9-C10	3.04	123.56	118.86
4	C	803	IXI	C7-C5-C4	-2.99	119.08	123.34
4	A	803	IXI	C14-N15-C16	-2.88	104.17	107.06
4	D	803	IXI	C29-C4-N3	-2.88	113.20	116.02
4	C	803	IXI	C10-C9-N18	2.88	123.88	118.70
4	A	803	IXI	C24-C23-C16	-2.86	115.75	120.83
4	C	803	IXI	C8-C2-C1	2.80	127.00	121.61
4	C	803	IXI	C23-C16-N15	-2.79	118.68	123.23
4	A	803	IXI	O21-C19-C10	-2.59	116.28	121.03
4	C	803	IXI	C4-N3-C2	2.55	120.64	118.28
4	C	803	IXI	O21-C19-N20	-2.52	118.93	122.67
4	C	803	IXI	C7-C5-C6	2.51	125.10	120.28
4	A	803	IXI	C4-N3-C2	2.48	120.58	118.28
4	C	803	IXI	C23-C16-N17	2.46	128.48	124.20
4	B	803	IXI	C5-C4-N3	2.42	126.64	120.56
4	C	803	IXI	O21-C19-C10	-2.23	116.94	121.03
4	A	803	IXI	C27-C26-C25	2.23	122.93	119.87
4	A	803	IXI	C7-C5-C4	-2.22	120.18	123.34
4	D	803	IXI	C24-C23-C16	-2.21	116.90	120.83
4	A	803	IXI	C11-C10-C9	2.19	121.06	119.09
4	D	803	IXI	C10-C19-N20	2.16	120.14	116.98
4	C	803	IXI	C8-C2-N3	-2.16	113.30	116.56
4	D	803	IXI	C12-C9-N18	-2.14	116.33	121.95
4	C	803	IXI	C12-C13-C14	-2.08	117.59	120.50
4	D	803	IXI	C12-C9-C10	2.07	122.05	118.86
4	A	803	IXI	C9-N18-C29	2.03	132.54	126.90
4	B	803	IXI	C12-C9-N18	-2.02	116.66	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	IXI	C10-C19-N20-C22
4	D	803	IXI	C10-C19-N20-C22

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	803	IXI	1	0

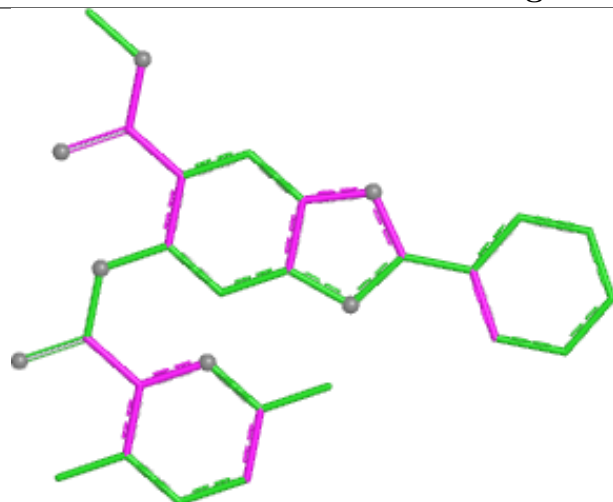
Continued on next page...

Continued from previous page...

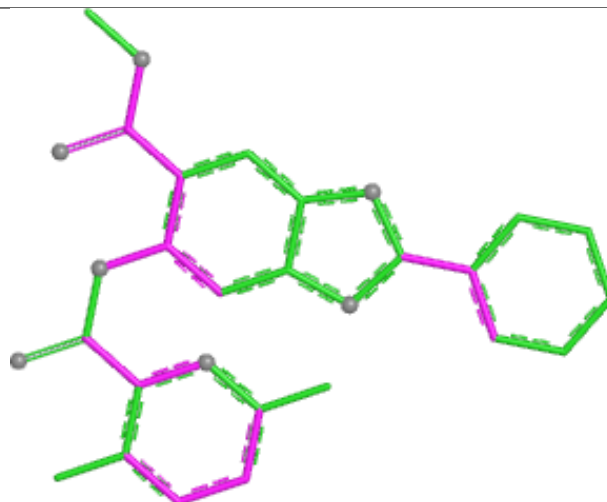
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	803	IXI	2	0
4	A	803	IXI	3	0
4	B	803	IXI	3	0

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.

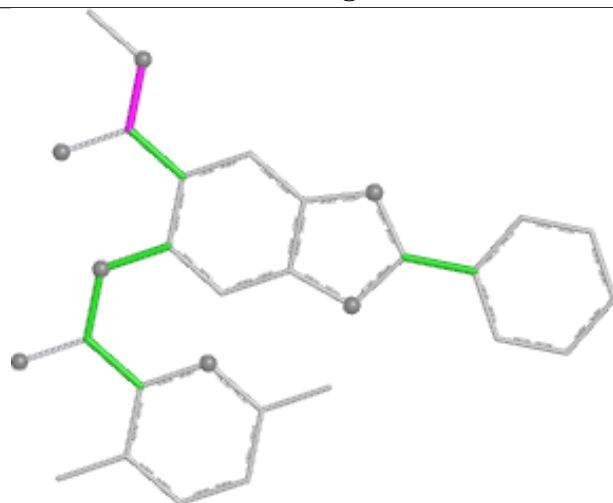
Ligand IXI D 803



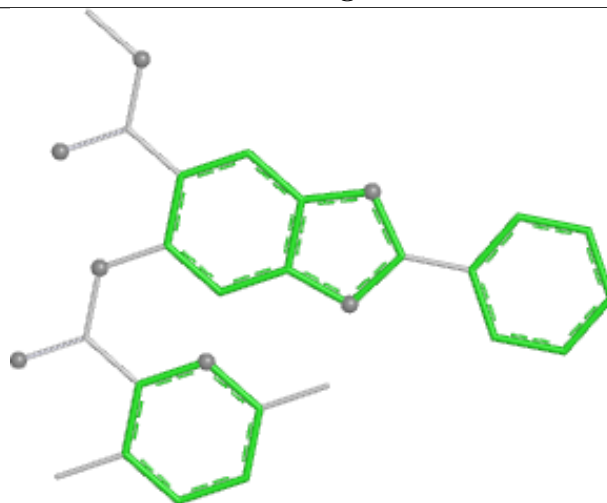
Bond lengths



Bond angles

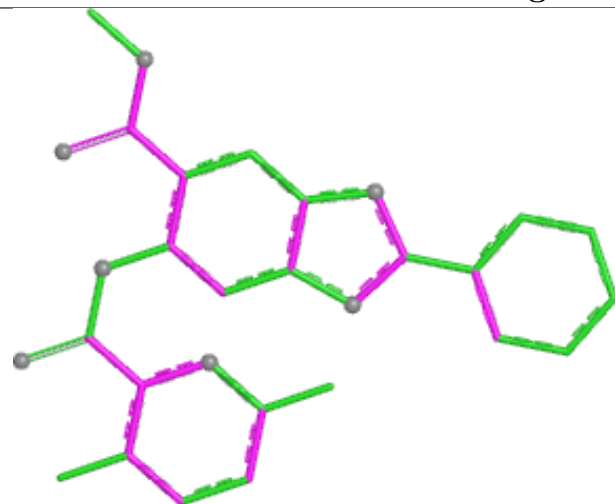


Torsions

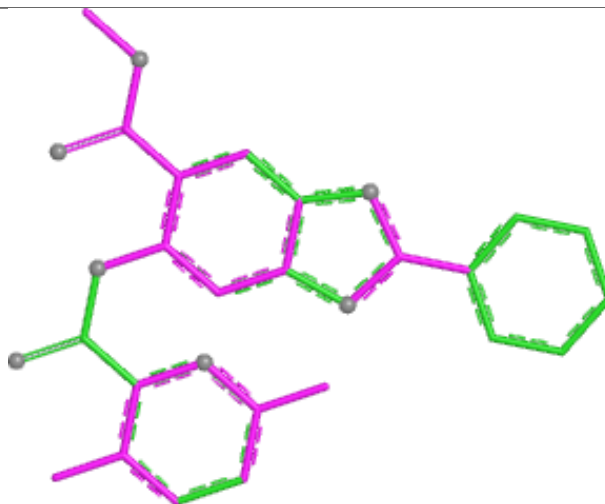


Rings

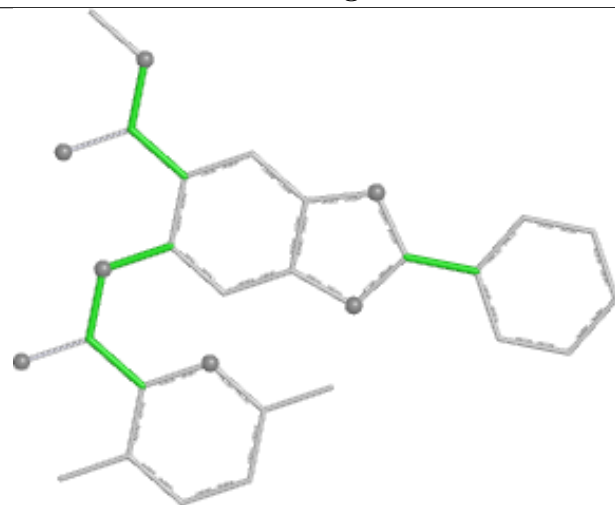
Ligand IXI C 803



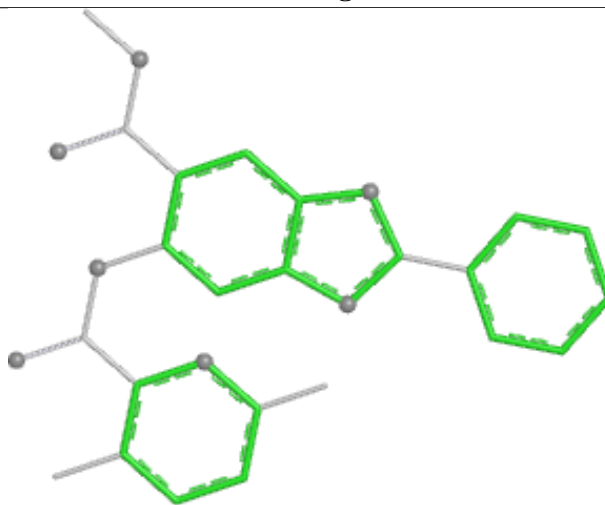
Bond lengths



Bond angles

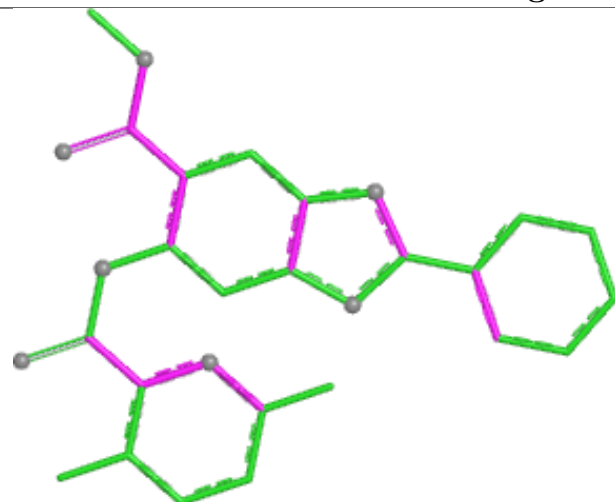


Torsions

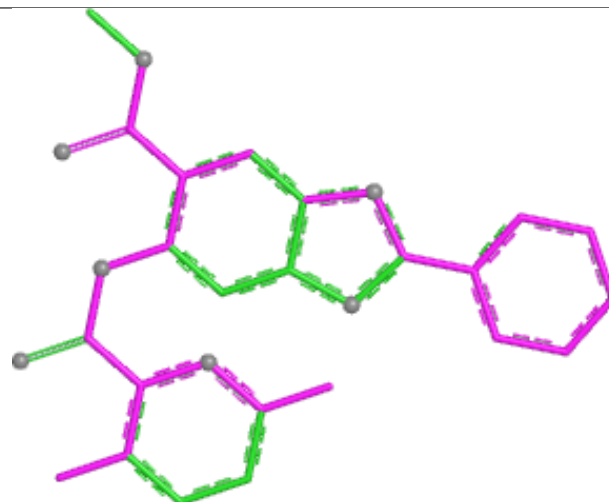


Rings

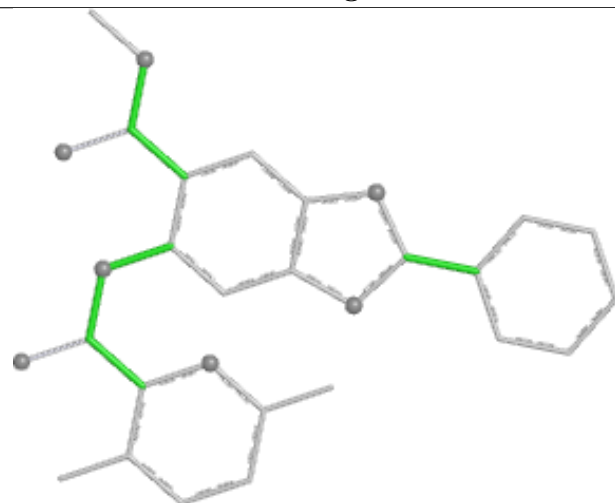
Ligand IXI A 803



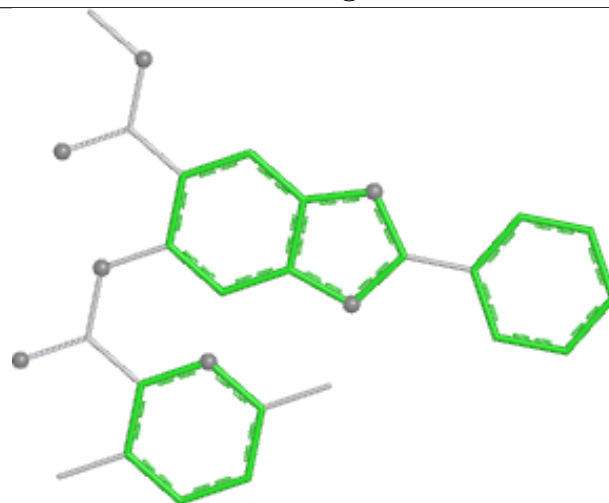
Bond lengths



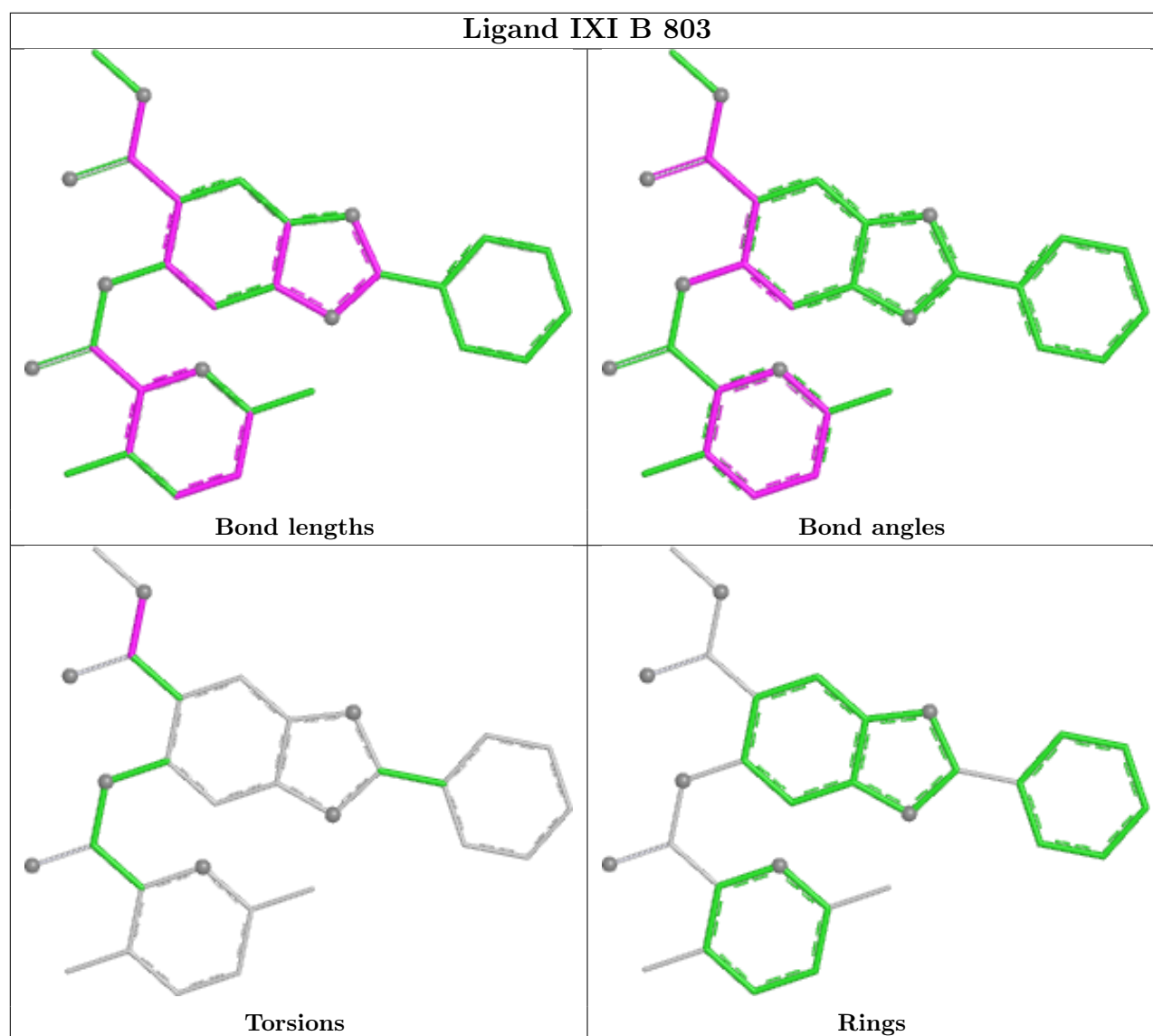
Bond angles



Torsions



Rings



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%)	-0.28	1 (0%) 90 89	28, 42, 73, 102	0
1	B	314/343 (91%)	-0.18	8 (2%) 58 52	25, 42, 74, 103	1 (0%)
1	C	312/343 (90%)	-0.29	3 (0%) 79 76	19, 44, 68, 96	1 (0%)
1	D	309/343 (90%)	0.00	2 (0%) 85 83	37, 55, 79, 100	0
All	All	1247/1372 (90%)	-0.19	14 (1%) 78 75	19, 47, 77, 103	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	459	LEU	4.7
1	C	606	GLU	3.1
1	B	606	GLU	2.9
1	B	458	GLY	2.7
1	B	771	THR	2.6
1	C	458	GLY	2.5
1	C	459	LEU	2.5
1	B	545	HIS	2.5
1	B	459	LEU	2.3
1	A	459	LEU	2.2
1	B	457	GLN	2.1
1	B	460	MET	2.1
1	D	620	GLU	2.1
1	B	506	GLU	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($\text{\AA}^2$)	Q<0.9
1	CME	B	509	10/11	0.83	0.20	52,66,98,103	0
1	CME	D	509	10/11	0.86	0.15	58,75,106,106	0
1	CME	C	509	10/11	0.90	0.12	51,60,92,95	0
1	CME	A	509	10/11	0.91	0.11	53,62,91,92	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

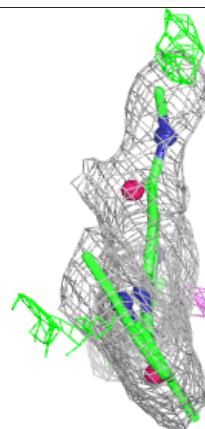
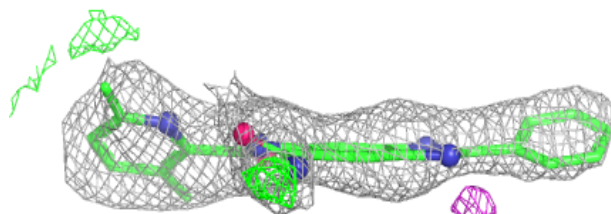
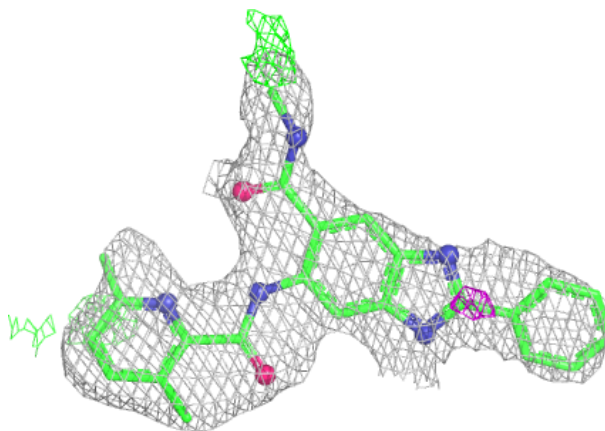
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	D	802	1/1	0.84	0.09	50,50,50,50	0
4	IXI	C	803	30/30	0.87	0.13	43,64,85,89	0
4	IXI	D	803	30/30	0.88	0.12	49,65,72,76	0
4	IXI	B	803	30/30	0.89	0.12	35,56,64,68	0
4	IXI	A	803	30/30	0.94	0.09	40,52,61,66	0
2	ZN	D	801	1/1	0.99	0.02	49,49,49,49	0
2	ZN	C	801	1/1	0.99	0.02	39,39,39,39	0
2	ZN	A	801	1/1	1.00	0.01	38,38,38,38	0
2	ZN	B	801	1/1	1.00	0.02	39,39,39,39	0
3	MG	A	802	1/1	1.00	0.02	31,31,31,31	0
3	MG	B	802	1/1	1.00	0.02	25,25,25,25	0
3	MG	C	802	1/1	1.00	0.01	24,24,24,24	0

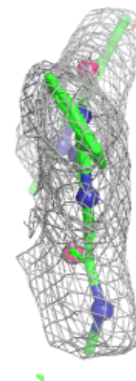
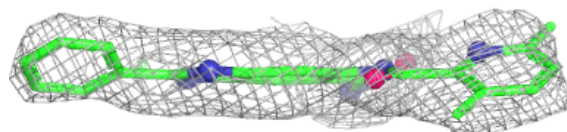
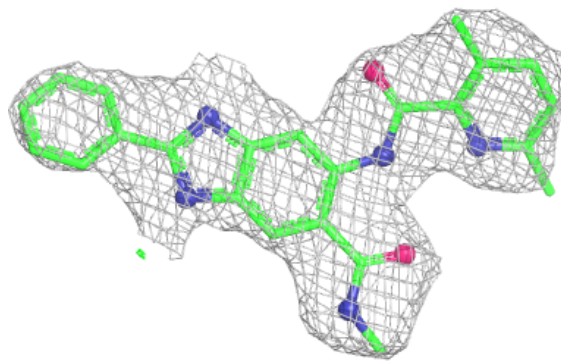
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IXI 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)

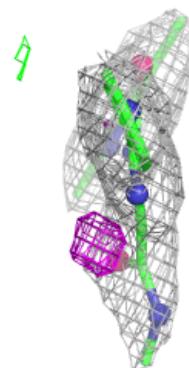
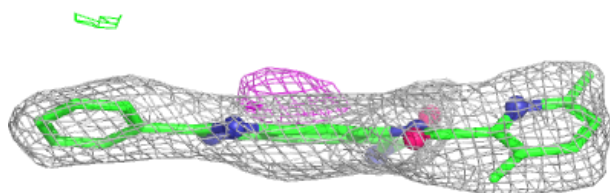
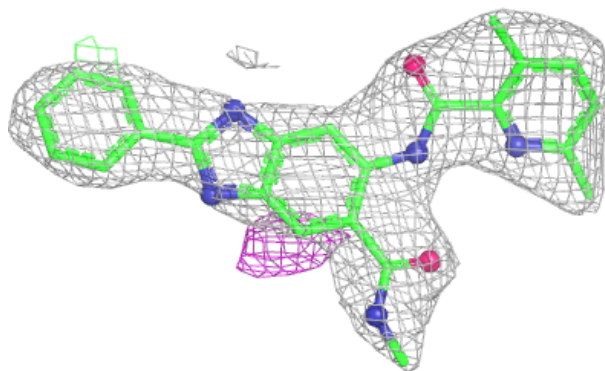
**Electron density around IXI D 803:**

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

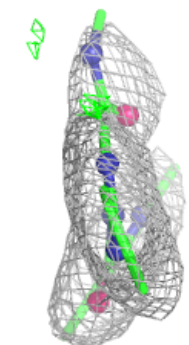
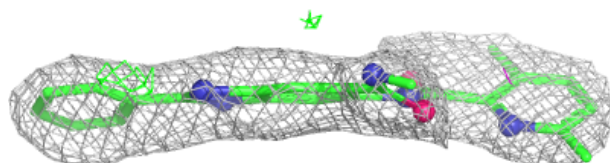
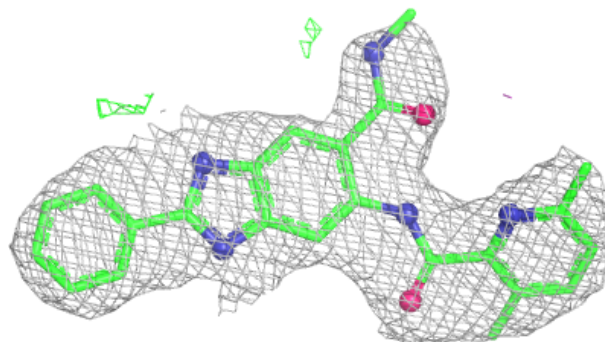


Electron density around IXI B 803:

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

**Electron density around IXI 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 [i](#)

There are no such residues in this entry.