



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:17 AM UTC

PDB ID : 5SH3 / pdb_00005sh3
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH c1(cc(nn2c1nc(c2C)C)CCc3nc(nn3C)N4CCCC4)[S](C)(=O)=O, micromolar IC₅₀=0.041332
Authors : Joseph, C.; Benz, J.; Flohr, A.; Groebke-Zbinden, K.; Rudolph, M.G.
Deposited on : 2022-02-01
Resolution : 1.98 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

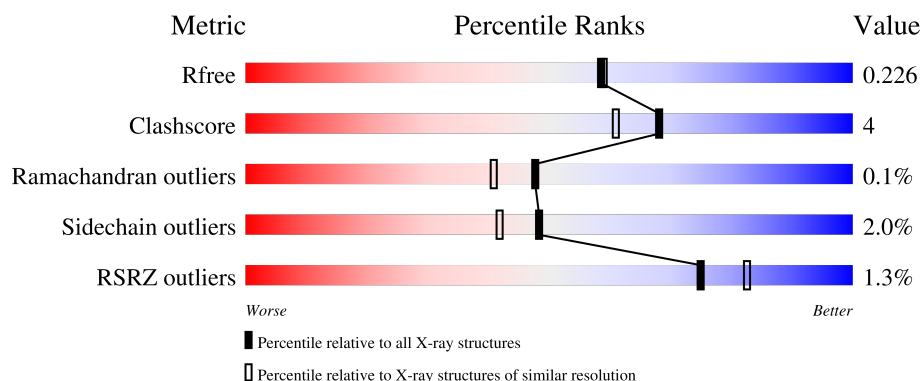
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	% 73% 16% • 9%
1	B	343	2% 73% 17% • 8%
1	C	343	% 74% 14% • 9%
1	D	343	% 77% 12% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10949 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	3	0
			2554	1633	434	463	24			
1	B	315	Total	C	N	O	S	0	2	0
			2559	1635	434	466	24			
1	C	312	Total	C	N	O	S	0	2	0
			2548	1629	434	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

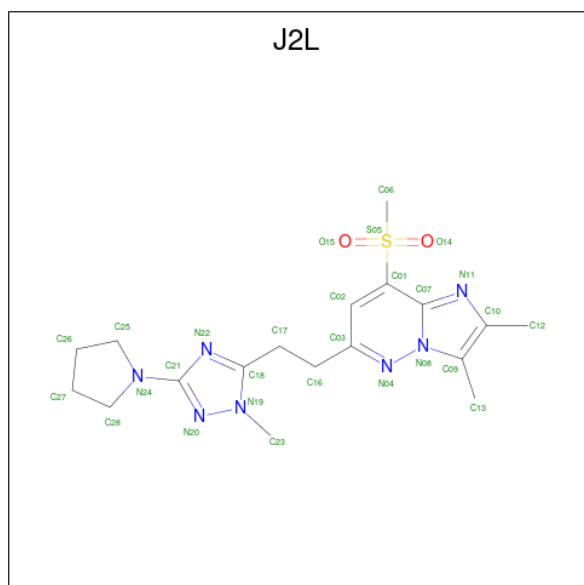
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (4S)-8-(methanesulfonyl)-2,3-dimethyl-6-{2-[1-methyl-3-(pyrrolidin-1-yl)-1H-1,2,4-triazol-5-yl]ethyl}imidazo[1,2-b]pyridazine (CCD ID: J2L) (formula: C₁₈H₂₅N₇O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			56	36	14	4	2		
4	B	1	Total	C	N	O	S	0	0
			28	18	7	2	1		
4	C	1	Total	C	N	O	S	0	0
			28	18	7	2	1		
4	D	1	Total	C	N	O	S	0	0
			28	18	7	2	1		

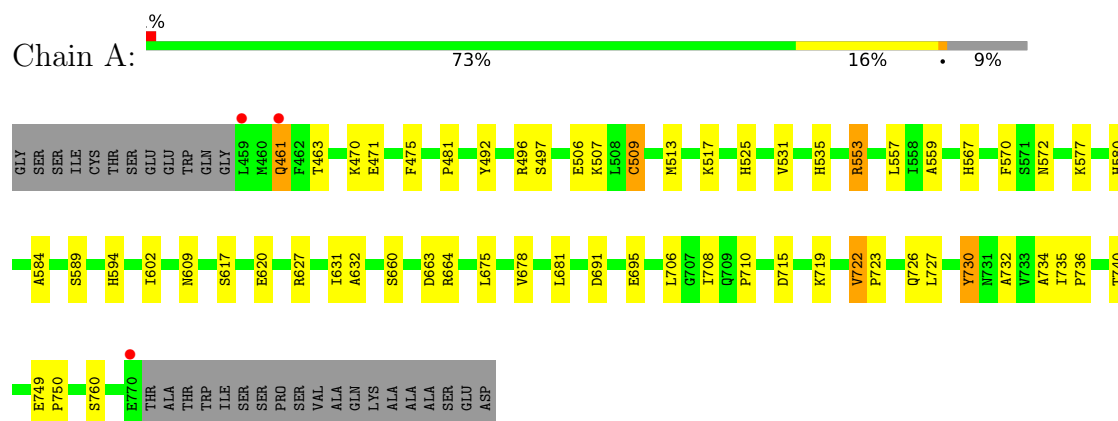
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	151	Total 152	O 152	0	1
5	B	184	Total 184	O 184	0	0
5	C	174	Total 174	O 174	0	0
5	D	111	Total 111	O 111	0	0

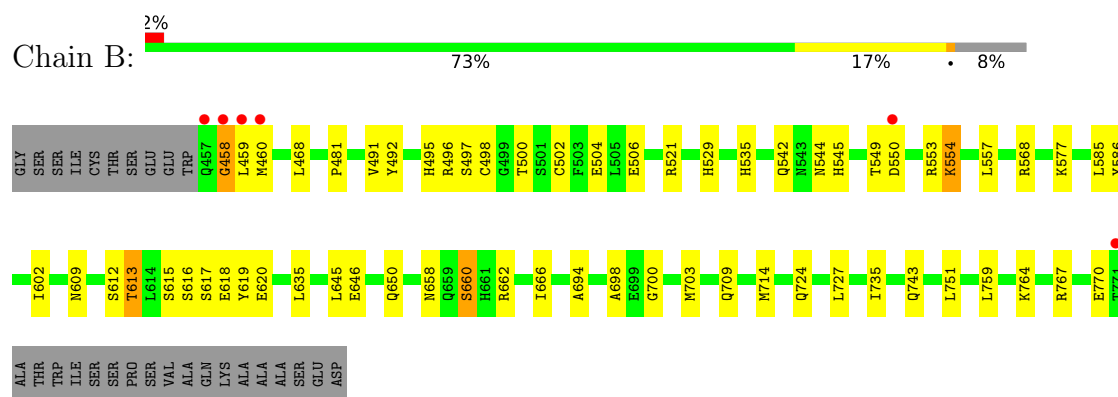
3 Residue-property plots [i](#)

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

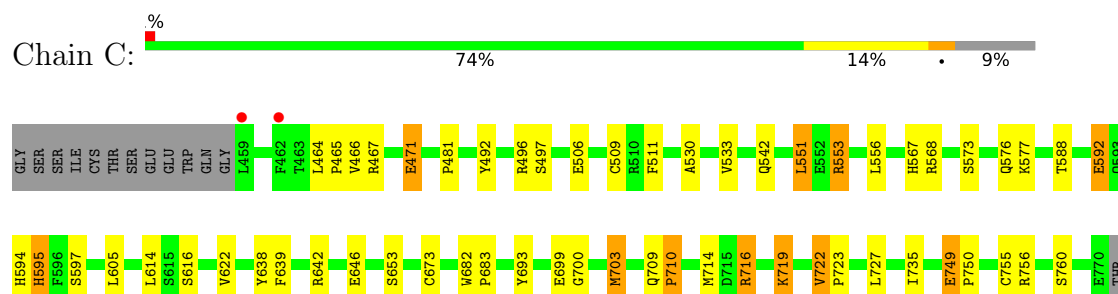
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



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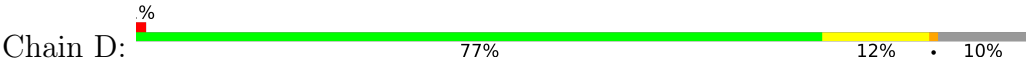


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



ALA
THR
TRP
ILE
SER
SER
PRO
SER
VAL
ALA
GLN
LYS
ALA
ALA
SER
GLU
ASP

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



GLY
SER
SER
ILE
CYS
THR
SER
GLU
TRP
GLN
GLY
L459
T463
V466
C469
I472
P481
Y492
M493
R496
T500
S501
R510
K516
H535
C536
M537
Y538
A539
H563
S571
L575
Q576
K577
S589
F596
H608
N609
S612
S616

Q621
R627
I631
E646
Y649
Q659
H669
W697
M703
R716
K719
V722
P723
Q726
L727
T739
T740
Q743
P746
S760
T766
R767
G768
GLU
GLU
THR
ALA
THR
TRP
ILE
SER
SER
PRO
SER
VAL
ALA
ALA
GLN
LYS
ALA
ALA
SER

GLU
ASP

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	135.34Å 135.34Å 235.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.64 – 1.98 43.64 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.6 (43.64-1.98) 96.6 (43.64-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.171 , 0.222 0.178 , 0.226	Depositor DCC
R_{free} test set	5570 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10949	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: CME, J2L, ZN, MG

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	1.47	25/2614 (1.0%)	1.51	14/3536 (0.4%)
1	B	1.37	13/2616 (0.5%)	1.59	28/3540 (0.8%)
1	C	1.38	15/2605 (0.6%)	1.51	12/3524 (0.3%)
1	D	1.38	15/2570 (0.6%)	1.54	15/3478 (0.4%)
All	All	1.40	68/10405 (0.7%)	1.53	69/14078 (0.5%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	580	HIS	CE1-NE2	9.12	1.41	1.32
1	A	695	GLU	C-O	8.38	1.33	1.24
1	D	589	SER	C-O	8.04	1.33	1.23
1	A	727	LEU	C-O	7.84	1.33	1.24
1	D	516	LYS	C-O	7.68	1.32	1.24
1	B	502	CYS	C-O	7.42	1.32	1.24
1	A	470	LYS	C-O	-7.08	1.15	1.24
1	A	620	GLU	C-O	7.00	1.32	1.24
1	A	481	PRO	C-O	-6.87	1.15	1.24
1	A	584	ALA	C-O	-6.78	1.15	1.24
1	D	726	GLN	C-O	6.71	1.31	1.24
1	D	539	ALA	C-O	-6.69	1.16	1.24
1	B	549	THR	C-O	6.69	1.32	1.23
1	A	715	ASP	C-O	6.65	1.31	1.24
1	D	535	HIS	CE1-NE2	6.63	1.39	1.32
1	C	530	ALA	C-O	6.62	1.31	1.24
1	B	495	HIS	CE1-NE2	6.52	1.39	1.32
1	C	568	ARG	C-O	-6.51	1.15	1.23
1	A	594	HIS	CE1-NE2	6.42	1.39	1.32
1	D	501	SER	C-O	-6.41	1.17	1.24
1	A	525	HIS	C-O	-6.36	1.15	1.23
1	A	559	ALA	C-O	-6.31	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	568	ARG	C-O	-6.28	1.15	1.24
1	A	475	PHE	C-O	-6.28	1.16	1.24
1	C	605	LEU	C-O	6.21	1.31	1.23
1	A	506	GLU	C-O	6.18	1.31	1.24
1	A	535	HIS	CE1-NE2	6.03	1.38	1.32
1	C	710	PRO	C-O	-5.98	1.16	1.23
1	A	706	LEU	C-O	-5.95	1.16	1.24
1	A	567	HIS	CE1-NE2	5.93	1.38	1.32
1	D	571	SER	C-O	5.83	1.31	1.23
1	C	481	PRO	C-O	-5.81	1.17	1.23
1	B	544	ASN	C-O	5.78	1.29	1.23
1	A	678	VAL	C-O	-5.74	1.17	1.24
1	C	595	HIS	CE1-NE2	5.74	1.38	1.32
1	C	594	HIS	CE1-NE2	5.74	1.38	1.32
1	C	466	VAL	C-O	5.68	1.30	1.24
1	C	553	ARG	C-O	5.63	1.30	1.24
1	C	588	THR	N-CA	5.63	1.52	1.45
1	B	481	PRO	C-O	-5.63	1.17	1.24
1	B	491	VAL	C-O	-5.63	1.17	1.24
1	A	732	ALA	C-O	5.61	1.31	1.24
1	C	511	PHE	C-O	-5.57	1.17	1.24
1	C	639	PHE	C-O	5.56	1.30	1.24
1	A	710	PRO	C-O	-5.54	1.16	1.23
1	B	586	TYR	C-O	5.51	1.30	1.23
1	B	666	ILE	C-O	5.46	1.30	1.24
1	D	649	TYR	C-O	-5.45	1.17	1.24
1	A	632	ALA	C-O	5.43	1.30	1.24
1	D	739	THR	N-CA	5.42	1.52	1.46
1	D	743	GLN	C-O	-5.38	1.17	1.24
1	B	529	HIS	CE1-NE2	-5.35	1.27	1.32
1	C	592	GLU	C-O	-5.27	1.17	1.24
1	A	726	GLN	C-O	5.25	1.30	1.24
1	D	669	MET	C-O	5.25	1.30	1.24
1	A	691	ASP	CG-OD1	-5.23	1.15	1.25
1	D	481	PRO	C-O	-5.23	1.17	1.24
1	B	609	ASN	C-O	5.22	1.29	1.23
1	C	567	HIS	CE1-NE2	5.22	1.37	1.32
1	A	570	PHE	C-O	5.19	1.30	1.23
1	D	575	LEU	C-O	5.16	1.30	1.24
1	B	521	ARG	C-O	-5.12	1.16	1.23
1	D	563	HIS	CE1-NE2	5.10	1.37	1.32
1	C	755	CYS	C-O	5.10	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	730	TYR	C-O	5.09	1.30	1.24
1	B	620	GLU	C-O	5.07	1.30	1.24
1	D	472	ILE	C-O	5.01	1.30	1.24
1	A	740	THR	C-O	5.01	1.29	1.24

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	ASN	CA-CB-CG	-7.98	104.62	112.60
1	B	504	GLU	CB-CA-C	7.86	122.47	109.89
1	C	719	LYS	CB-CA-C	-7.56	97.83	110.68
1	B	735	ILE	N-CA-CB	7.55	116.34	110.45
1	A	609	ASN	N-CA-CB	7.44	121.51	110.49
1	D	535	HIS	CA-CB-CG	-6.76	107.04	113.80
1	D	746	PRO	N-CA-C	6.51	118.65	110.70
1	A	663	ASP	N-CA-C	-6.51	104.19	111.28
1	B	535	HIS	CA-CB-CG	-6.46	107.34	113.80
1	B	554	LYS	CA-C-N	6.32	127.00	119.98
1	B	554	LYS	C-N-CA	6.32	127.00	119.98
1	C	703	MET	N-CA-C	-6.29	104.50	111.36
1	A	602	ILE	N-CA-C	-6.22	104.44	110.72
1	C	722	VAL	N-CA-CB	6.13	115.23	110.45
1	A	531	VAL	N-CA-C	-6.09	104.57	110.72
1	D	537	MET	N-CA-C	-6.05	104.77	111.36
1	D	649	TYR	CA-C-N	6.00	128.33	120.28
1	D	649	TYR	C-N-CA	6.00	128.33	120.28
1	A	722	VAL	CA-C-O	5.99	122.70	118.69
1	B	613	THR	CA-CB-OG1	-5.97	100.65	109.60
1	C	622	VAL	N-CA-C	-5.90	104.76	110.72
1	D	466	VAL	CA-C-O	-5.79	115.38	121.41
1	D	743	GLN	N-CA-C	-5.78	104.98	111.28
1	A	589	SER	CA-C-O	-5.68	115.25	121.84
1	A	507	LYS	N-CA-C	-5.64	105.21	111.36
1	B	612	SER	CA-C-N	5.62	128.08	120.38
1	B	612	SER	C-N-CA	5.62	128.08	120.38
1	B	458	GLY	CA-C-N	5.61	132.25	121.54
1	B	458	GLY	C-N-CA	5.61	132.25	121.54
1	D	760	SER	N-CA-C	-5.55	105.23	112.23
1	B	616	SER	CA-C-N	5.53	127.95	120.65
1	B	616	SER	C-N-CA	5.53	127.95	120.65
1	D	469	CYS	N-CA-C	-5.50	105.28	111.28
1	B	500	THR	CA-CB-OG1	-5.50	101.36	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	698	ALA	N-CA-C	-5.48	105.38	111.36
1	A	463	THR	CA-CB-OG1	-5.47	101.39	109.60
1	B	751	LEU	N-CA-C	-5.45	105.25	111.14
1	C	551	LEU	N-CA-C	-5.40	105.47	111.36
1	D	609	ASN	N-CA-CB	5.36	118.07	110.46
1	A	617	SER	CA-C-N	5.34	127.88	120.29
1	A	617	SER	C-N-CA	5.34	127.88	120.29
1	C	576	GLN	CB-CG-CD	5.32	121.65	112.60
1	B	662	ARG	N-CA-C	-5.32	105.48	111.28
1	A	553	ARG	CA-C-N	5.29	127.31	120.44
1	A	553	ARG	C-N-CA	5.29	127.31	120.44
1	D	596	PHE	CA-C-O	-5.27	114.96	120.55
1	B	545	HIS	CA-C-N	5.27	128.32	120.31
1	B	545	HIS	C-N-CA	5.27	128.32	120.31
1	B	694	ALA	N-CA-C	-5.26	105.44	111.07
1	B	585	LEU	N-CA-CB	-5.22	102.43	110.16
1	C	719	LYS	N-CA-CB	5.21	117.87	110.06
1	B	619	TYR	N-CA-C	-5.19	105.52	111.07
1	C	735	ILE	N-CA-CB	5.17	114.49	110.45
1	B	602	ILE	CA-C-O	-5.15	115.39	120.85
1	B	660[A]	SER	O-C-N	5.15	127.37	122.07
1	B	660[B]	SER	O-C-N	5.15	127.37	122.07
1	B	468	LEU	N-CA-C	-5.14	105.13	111.40
1	C	556	LEU	N-CA-C	-5.13	105.77	112.23
1	C	576	GLN	CB-CA-C	5.12	118.99	110.90
1	B	506	GLU	CA-C-O	-5.11	115.45	120.82
1	B	645	LEU	CA-C-N	5.10	127.37	120.38
1	B	645	LEU	C-N-CA	5.10	127.37	120.38
1	C	614	LEU	CA-C-O	-5.08	115.97	121.87
1	D	646	GLU	N-CA-C	-5.08	105.64	111.07
1	A	572	ASN	N-CA-C	-5.07	105.75	111.28
1	D	659	GLN	CA-C-N	5.03	127.02	120.28
1	D	659	GLN	C-N-CA	5.03	127.02	120.28
1	C	716	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	D	609	ASN	CA-CB-CG	-5.01	107.59	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2554	0	2532	14	0
1	B	2559	0	2524	24	0
1	C	2548	0	2526	25	0
1	D	2519	0	2496	11	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	56	0	0	1	0
4	B	28	0	0	1	0
4	C	28	0	0	1	0
4	D	28	0	0	0	0
5	A	152	0	0	1	0
5	B	184	0	0	1	0
5	C	174	0	0	6	0
5	D	111	0	0	0	0
All	All	10949	0	10078	74	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 4.

All (74) 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:B:497:SER:O	1:B:553:ARG:HD2	1.75	0.85
1:B:650:GLN:NE2	1:B:650:GLN:HA	2.05	0.72
1:A:497:SER:O	1:A:553:ARG:HD2	1.91	0.70
1:B:727:LEU:CD1	1:B:759:LEU:HD11	2.27	0.64
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.34	0.63
1:A:461:GLN:HA	1:A:461:GLN:OE1	1.99	0.62
1:A:497:SER:OG	1:A:557:LEU:HD11	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:LEU:HD22	4:B:803:J2L:C06	2.30	0.61
1:B:650:GLN:HE21	1:B:650:GLN:CA	2.14	0.59
1:C:653:SER:O	5:C:902:HOH:O	2.17	0.58
1:B:650:GLN:NE2	1:B:650:GLN:CA	2.66	0.58
1:B:727:LEU:HD12	1:B:759:LEU:HD11	1.86	0.58
1:A:722:VAL:N	1:A:723:PRO:CD	2.68	0.57
1:C:553:ARG:NH1	5:C:903:HOH:O	2.38	0.55
1:B:727:LEU:HD12	1:B:759:LEU:CD1	2.38	0.54
1:B:650:GLN:HA	1:B:650:GLN:HE21	1.69	0.53
1:D:627:ARG:O	1:D:631:ILE:HG12	2.11	0.50
1:D:510:ARG:HG2	1:D:608:HIS:CE1	2.47	0.50
1:C:497:SER:O	1:C:553:ARG:HD3	2.11	0.50
1:B:646:GLU:O	1:B:650:GLN:HG2	2.12	0.49
1:C:577:LYS:HD3	1:C:703:MET:HE1	1.94	0.48
1:D:609:ASN:ND2	1:D:612:SER:N	2.62	0.48
1:A:719:LYS:HE3	5:A:986:HOH:O	2.14	0.48
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.49	0.47
1:D:493:MET:SD	1:D:535:HIS:HA	2.55	0.47
1:B:724:GLN:NE2	5:B:901:HOH:O	2.23	0.46
1:C:467:ARG:O	1:C:471:GLU:HB2	2.15	0.46
1:C:699:GLU:OE2	1:C:714:MET:HE1	2.15	0.46
1:C:716:ARG:O	1:C:719:LYS:HG3	2.14	0.46
1:B:550:ASP:N	1:B:550:ASP:OD1	2.46	0.46
1:C:542:GLN:NE2	1:C:542:GLN:HA	2.31	0.46
1:A:577:LYS:HD3	1:A:708:ILE:HD13	1.98	0.45
1:B:727:LEU:CD1	1:B:759:LEU:CD1	2.93	0.45
1:A:509:CME:O	1:A:513:MET:HG2	2.16	0.45
1:C:709:GLN:NE2	1:C:710:PRO:HD2	2.32	0.45
1:B:577:LYS:HD3	1:B:703:MET:HE1	1.99	0.45
1:A:660:SER:O	1:A:664:ARG:HG3	2.17	0.45
1:C:700:GLY:HA3	1:C:714:MET:O	2.17	0.45
1:B:458:GLY:C	1:B:460:MET:H	2.24	0.44
1:B:498:CYS:SG	1:B:554:LYS:HG3	2.58	0.44
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.53	0.44
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.00	0.44
1:D:722:VAL:N	1:D:723:PRO:CD	2.81	0.44
1:A:749:GLU:N	1:A:750:PRO:CD	2.81	0.44
1:C:722:VAL:N	1:C:723:PRO:CD	2.81	0.43
1:D:740:THR:HA	1:D:743:GLN:HE21	1.83	0.43
1:B:497:SER:HA	1:B:542:GLN:NE2	2.34	0.43
1:A:675:LEU:HD21	4:A:803[A]:J2L:C06	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:TYR:OH	1:C:642:ARG:HD3	2.18	0.43
1:B:497:SER:HA	1:B:542:GLN:HE22	1.84	0.42
1:C:592:GLU:HA	1:C:595:HIS:CD2	2.55	0.42
1:C:646:GLU:HG2	5:C:1046:HOH:O	2.18	0.42
1:C:749:GLU:HB3	1:C:750:PRO:HD3	2.00	0.42
1:B:497:SER:OG	1:B:557:LEU:HD11	2.20	0.42
1:C:682:TRP:N	1:C:683:PRO:CD	2.82	0.42
1:D:727:LEU:C	1:D:727:LEU:HD23	2.44	0.42
1:C:464:LEU:O	1:C:465:PRO:C	2.61	0.42
1:D:719:LYS:O	1:D:722:VAL:HG23	2.20	0.42
1:C:693:TYR:OH	4:C:803:J2L:N22	2.53	0.42
1:C:727:LEU:C	1:C:727:LEU:HD23	2.45	0.42
1:A:730:TYR:HA	1:A:734:ALA:HB3	2.02	0.41
1:D:577:LYS:HD3	1:D:703:MET:HE1	2.01	0.41
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.91	0.41
1:C:756[A]:ARG:HD2	5:C:1038:HOH:O	2.19	0.41
1:A:627:ARG:O	1:A:631:ILE:HG12	2.21	0.41
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.55	0.41
1:B:615:SER:OG	1:B:618:GLU:HG3	2.20	0.41
1:B:646:GLU:OE1	1:B:743:GLN:NE2	2.53	0.41
1:B:658:ASN:OD1	1:B:660[B]:SER:HB2	2.21	0.41
1:C:533:VAL:HG13	1:C:673:CYS:HB3	2.03	0.41
1:B:700:GLY:HA3	1:B:714:MET:O	2.21	0.41
1:C:509:CME:HB2	5:C:1044:HOH:O	2.21	0.40
1:D:697:TRP:HB3	1:D:716:ARG:HB3	2.02	0.40
1:C:714:MET:HE2	5:C:1024:HOH:O	2.20	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	312/343 (91%)	306 (98%)	6 (2%)	0	100	100
1	B	314/343 (92%)	306 (98%)	7 (2%)	1 (0%)	36	27
1	C	311/343 (91%)	305 (98%)	6 (2%)	0	100	100
1	D	307/343 (90%)	298 (97%)	9 (3%)	0	100	100
All	All	1244/1372 (91%)	1215 (98%)	28 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	LEU

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	284/305 (93%)	278 (98%)	6 (2%)	47	40
1	B	283/305 (93%)	277 (98%)	6 (2%)	47	40
1	C	283/305 (93%)	275 (97%)	8 (3%)	38	29
1	D	279/305 (92%)	274 (98%)	5 (2%)	51	46
All	All	1129/1220 (92%)	1104 (98%)	25 (2%)	48	38

All (25) 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	517	LYS
1	A	681	LEU
1	A	760	SER
1	B	613	THR
1	B	617	SER
1	B	709	GLN
1	B	764	LYS

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Mol	Chain	Res	Type
1	B	767	ARG
1	B	770	GLU
1	C	471	GLU
1	C	506	GLU
1	C	573	SER
1	C	597	SER
1	C	616	SER
1	C	749	GLU
1	C	760[A]	SER
1	C	760[B]	SER
1	D	463	THR
1	D	576	GLN
1	D	616	SER
1	D	621	GLN
1	D	719	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	GLN
1	A	544	ASN
1	A	604	GLN
1	A	644	GLN
1	A	659	GLN
1	A	726	GLN
1	A	743	GLN
1	A	761	GLN
1	B	484	ASN
1	B	542	GLN
1	B	545	HIS
1	B	604	GLN
1	B	650	GLN
1	B	761	GLN
1	C	495	HIS
1	C	542	GLN
1	C	604	GLN
1	C	659	GLN
1	C	709	GLN
1	C	726	GLN
1	C	743	GLN
1	D	484	ASN
1	D	576	GLN

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Mol	Chain	Res	Type
1	D	621	GLN
1	D	650	GLN
1	D	659	GLN
1	D	724	GLN
1	D	726	GLN
1	D	743	GLN
1	D	761	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CME	D	509	1	8,9,10	0.73	0	6,9,11	0.65	0
1	CME	B	509	1	8,9,10	0.64	0	6,9,11	0.63	0
1	CME	A	509	1	8,9,10	0.65	0	6,9,11	1.53	1 (16%)
1	CME	C	509	1	8,9,10	0.80	0	6,9,11	1.02	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	-	1/5/8/10	-
1	CME	B	509	1	-	0/5/8/10	-
1	CME	A	509	1	-	0/5/8/10	-
1	CME	C	509	1	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	CME	CZ-CE-SD	-3.14	102.88	113.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	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 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	J2L	A	803[A]	-	29,31,31	3.04	10 (34%)	31,47,47	3.25	8 (25%)
4	J2L	B	803	-	29,31,31	2.95	11 (37%)	31,47,47	2.84	10 (32%)
4	J2L	D	803	-	29,31,31	2.70	7 (24%)	31,47,47	2.57	12 (38%)
4	J2L	A	803[B]	-	29,31,31	2.95	10 (34%)	31,47,47	2.81	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	J2L	C	803	-	29,31,31	4.03	11 (37%)	31,47,47	3.39	13 (41%)

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	J2L	A	803[A]	-	-	2/13/22/22	0/4/4/4
4	J2L	B	803	-	-	1/13/22/22	0/4/4/4
4	J2L	D	803	-	-	2/13/22/22	0/4/4/4
4	J2L	A	803[B]	-	-	6/13/22/22	0/4/4/4
4	J2L	C	803	-	-	3/13/22/22	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	J2L	C03-N04	12.60	1.43	1.31
4	C	803	J2L	O15-S05	10.79	1.55	1.43
4	B	803	J2L	O14-S05	9.85	1.54	1.43
4	A	803[A]	J2L	C03-N04	9.74	1.40	1.31
4	A	803[B]	J2L	C03-N04	8.95	1.40	1.31
4	D	803	J2L	C06-S05	8.45	1.86	1.75
4	C	803	J2L	O14-S05	7.67	1.52	1.43
4	A	803[A]	J2L	O15-S05	7.56	1.51	1.43
4	B	803	J2L	C03-N04	7.42	1.38	1.31
4	A	803[B]	J2L	C06-S05	7.31	1.84	1.75
4	A	803[A]	J2L	O14-S05	6.73	1.51	1.43
4	C	803	J2L	C18-N19	6.65	1.40	1.34
4	D	803	J2L	O15-S05	6.33	1.50	1.43
4	A	803[B]	J2L	O14-S05	6.13	1.50	1.43
4	B	803	J2L	O15-S05	5.57	1.49	1.43
4	D	803	J2L	C03-N04	5.57	1.36	1.31
4	C	803	J2L	C09-N08	-4.19	1.30	1.38
4	A	803[A]	J2L	C06-S05	4.16	1.80	1.75
4	A	803[B]	J2L	O15-S05	4.08	1.48	1.43
4	D	803	J2L	O14-S05	4.07	1.48	1.43
4	B	803	J2L	C18-N19	3.95	1.37	1.34
4	C	803	J2L	C21-N24	3.76	1.42	1.35
4	C	803	J2L	C21-N20	3.41	1.37	1.32
4	A	803[A]	J2L	C25-N24	-3.40	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	J2L	C07-N11	3.36	1.40	1.33
4	C	803	J2L	C17-C18	3.25	1.53	1.49
4	D	803	J2L	C17-C18	3.23	1.53	1.49
4	A	803[B]	J2L	C21-N24	3.21	1.41	1.35
4	B	803	J2L	C02-C03	-3.20	1.37	1.44
4	A	803[B]	J2L	C18-N19	3.10	1.37	1.34
4	A	803[B]	J2L	C25-N24	-2.91	1.41	1.47
4	C	803	J2L	C13-C09	2.86	1.53	1.49
4	A	803[A]	J2L	C21-N24	2.77	1.40	1.35
4	D	803	J2L	C02-C03	-2.64	1.38	1.44
4	B	803	J2L	C09-N08	-2.61	1.33	1.38
4	D	803	J2L	C18-N19	2.53	1.36	1.34
4	A	803[B]	J2L	C07-N11	2.50	1.38	1.33
4	B	803	J2L	C21-N24	2.42	1.39	1.35
4	A	803[A]	J2L	C18-N19	2.41	1.36	1.34
4	A	803[A]	J2L	N08-N04	2.41	1.44	1.38
4	A	803[B]	J2L	C13-C09	2.37	1.53	1.49
4	B	803	J2L	C18-N22	2.37	1.36	1.32
4	B	803	J2L	C09-C10	2.32	1.41	1.37
4	A	803[A]	J2L	C13-C09	2.20	1.52	1.49
4	A	803[A]	J2L	C17-C18	2.20	1.52	1.49
4	B	803	J2L	C07-C01	-2.16	1.40	1.44
4	A	803[B]	J2L	C09-N08	-2.09	1.34	1.38
4	C	803	J2L	C12-C10	-2.07	1.45	1.49
4	B	803	J2L	C25-N24	-2.02	1.43	1.47

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803[A]	J2L	O15-S05-C06	-14.81	92.76	108.47
4	C	803	J2L	O15-S05-C06	-10.53	97.30	108.47
4	A	803[B]	J2L	O15-S05-O14	-9.01	107.89	118.26
4	B	803	J2L	O15-S05-C01	-8.34	97.37	108.11
4	C	803	J2L	O14-S05-C06	7.62	116.56	108.47
4	B	803	J2L	O15-S05-C06	-7.26	100.77	108.47
4	B	803	J2L	O14-S05-C06	7.10	116.00	108.47
4	C	803	J2L	O15-S05-C01	-6.37	99.91	108.11
4	C	803	J2L	N24-C21-N20	-5.97	117.36	123.51
4	A	803[B]	J2L	C23-N19-N20	5.66	127.75	119.29
4	A	803[B]	J2L	C28-N24-C25	-5.62	103.92	111.37
4	A	803[A]	J2L	C23-N19-N20	5.61	127.68	119.29
4	D	803	J2L	C07-N11-C10	-5.29	103.41	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	803	J2L	O14-S05-C06	-5.24	102.91	108.47
4	A	803[B]	J2L	C16-C17-C18	-5.19	106.71	111.62
4	A	803[A]	J2L	C16-C17-C18	-5.07	106.83	111.62
4	D	803	J2L	C02-C03-N04	-4.95	118.47	121.44
4	D	803	J2L	N24-C21-N20	-4.84	118.52	123.51
4	D	803	J2L	C13-C09-N08	-4.75	115.20	123.44
4	A	803[B]	J2L	C07-N11-C10	4.50	107.72	105.74
4	C	803	J2L	C13-C09-N08	-4.31	115.96	123.44
4	B	803	J2L	C23-N19-N20	3.74	124.89	119.29
4	C	803	J2L	O15-S05-O14	-3.64	114.07	118.26
4	C	803	J2L	N24-C21-N22	3.53	129.12	119.34
4	C	803	J2L	C23-N19-N20	3.49	124.50	119.29
4	D	803	J2L	C13-C09-C10	3.33	137.96	131.23
4	D	803	J2L	C23-N19-N20	3.16	124.02	119.29
4	D	803	J2L	C03-N04-N08	3.15	118.62	114.54
4	C	803	J2L	C16-C17-C18	-3.14	108.65	111.62
4	D	803	J2L	N24-C21-N22	3.14	128.05	119.34
4	A	803[A]	J2L	N24-C21-N22	2.96	127.55	119.34
4	C	803	J2L	C02-C03-N04	2.94	123.20	121.44
4	A	803[B]	J2L	C01-C07-N11	2.91	134.35	127.80
4	B	803	J2L	C02-C03-N04	-2.82	119.74	121.44
4	B	803	J2L	N24-C21-N20	-2.80	120.63	123.51
4	B	803	J2L	C03-N04-N08	2.69	118.03	114.54
4	B	803	J2L	N24-C21-N22	2.68	126.77	119.34
4	D	803	J2L	O15-S05-O14	-2.60	115.28	118.26
4	C	803	J2L	C28-N24-C25	2.46	114.63	111.37
4	C	803	J2L	C01-C07-N11	2.42	133.23	127.80
4	C	803	J2L	C03-N04-N08	-2.39	111.44	114.54
4	B	803	J2L	C16-C17-C18	-2.29	109.45	111.62
4	A	803[A]	J2L	N24-C21-N20	-2.26	121.18	123.51
4	A	803[A]	J2L	N08-C07-N11	2.26	112.20	110.13
4	A	803[B]	J2L	C02-C03-N04	-2.20	120.12	121.44
4	D	803	J2L	C01-C07-N11	2.11	132.55	127.80
4	A	803[B]	J2L	C12-C10-N11	2.11	123.55	119.32
4	A	803[A]	J2L	O15-S05-O14	-2.10	115.85	118.26
4	A	803[B]	J2L	C13-C09-N08	-2.09	119.81	123.44
4	D	803	J2L	N08-C07-N11	2.08	112.03	110.13
4	A	803[B]	J2L	C26-C27-C28	-2.05	99.42	105.10
4	B	803	J2L	C07-N11-C10	2.01	106.63	105.74
4	A	803[A]	J2L	C26-C25-N24	-2.01	100.05	103.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803[B]	J2L	C02-C01-S05-O14
4	A	803[B]	J2L	C07-C01-S05-O14
4	A	803[B]	J2L	N20-C21-N24-C25
4	C	803	J2L	C02-C01-S05-O15
4	A	803[B]	J2L	C03-C16-C17-C18
4	D	803	J2L	C16-C17-C18-N22
4	A	803[A]	J2L	C16-C17-C18-N19
4	A	803[B]	J2L	C16-C17-C18-N19
4	C	803	J2L	C16-C17-C18-N19
4	D	803	J2L	C16-C17-C18-N19
4	A	803[A]	J2L	C16-C17-C18-N22
4	A	803[B]	J2L	C16-C17-C18-N22
4	C	803	J2L	C07-C01-S05-O15
4	B	803	J2L	C16-C17-C18-N19

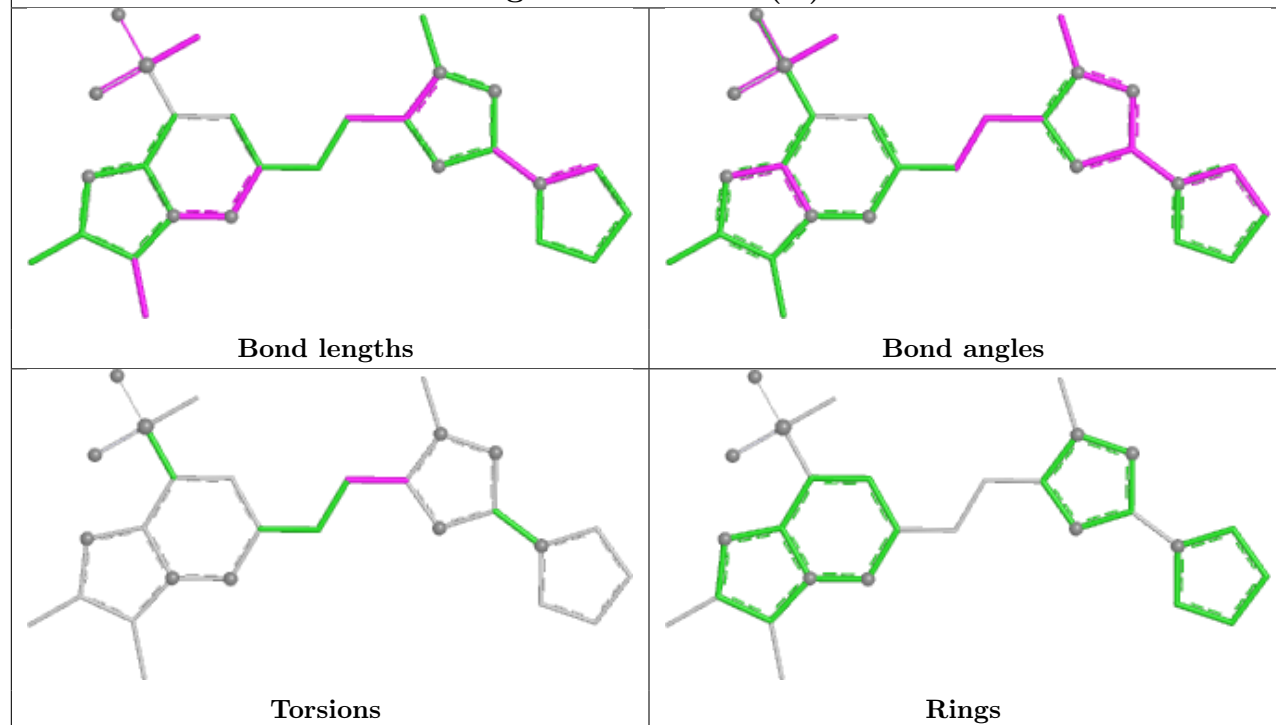
There are no ring outliers.

3 monomers are involved in 3 short contacts:

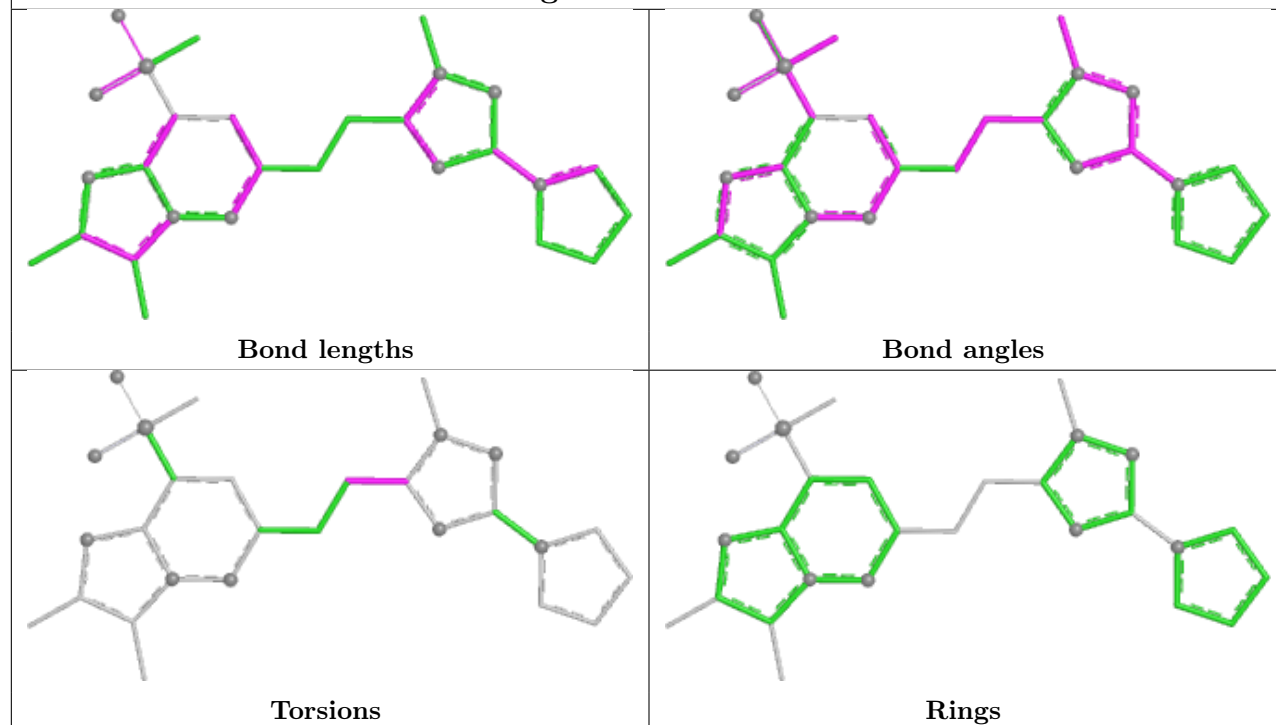
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803[A]	J2L	1	0
4	B	803	J2L	1	0
4	C	803	J2L	1	0

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

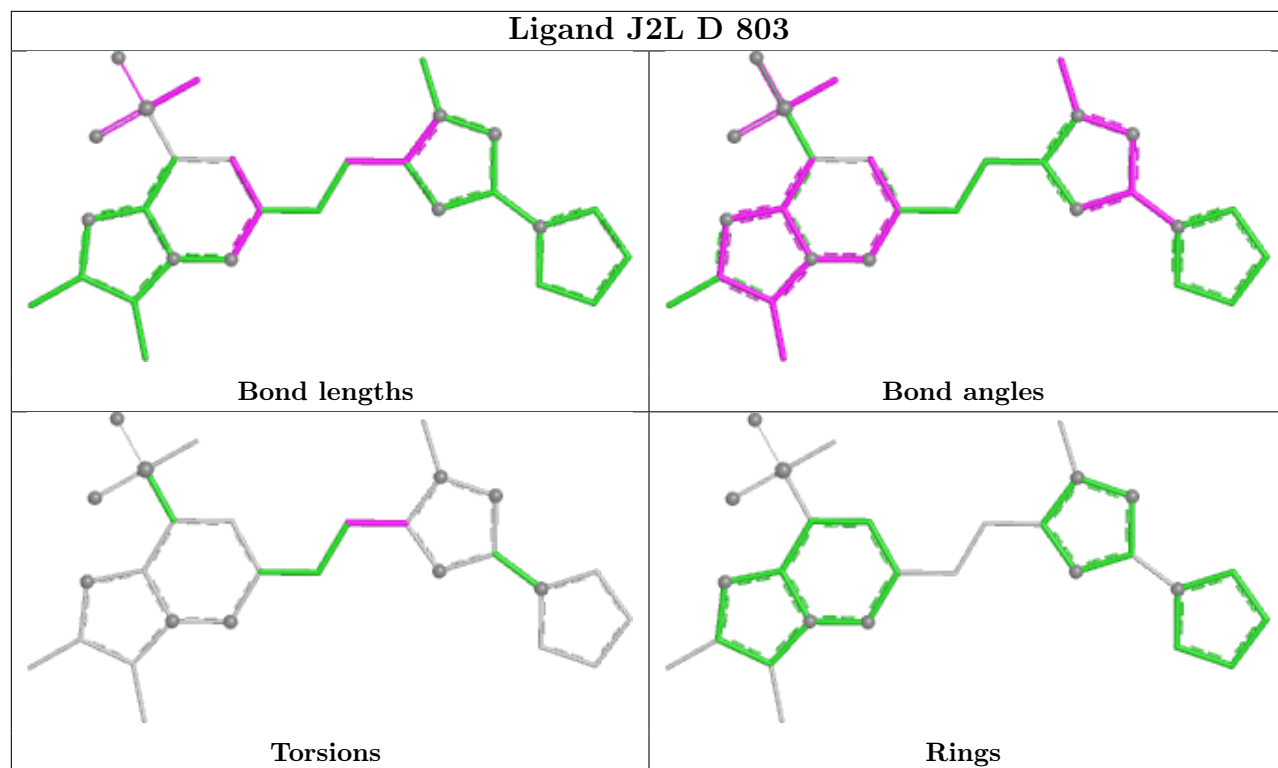
Ligand J2L A 803 (A)



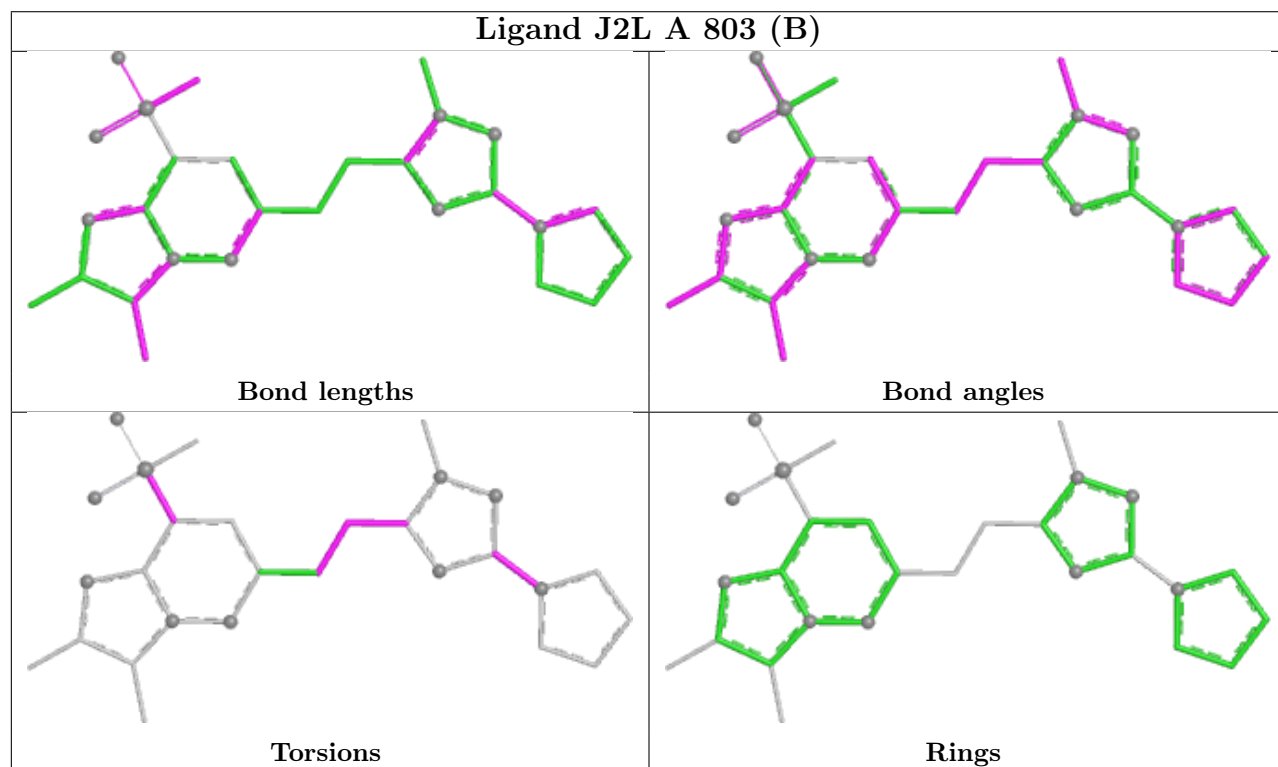
Ligand J2L B 803

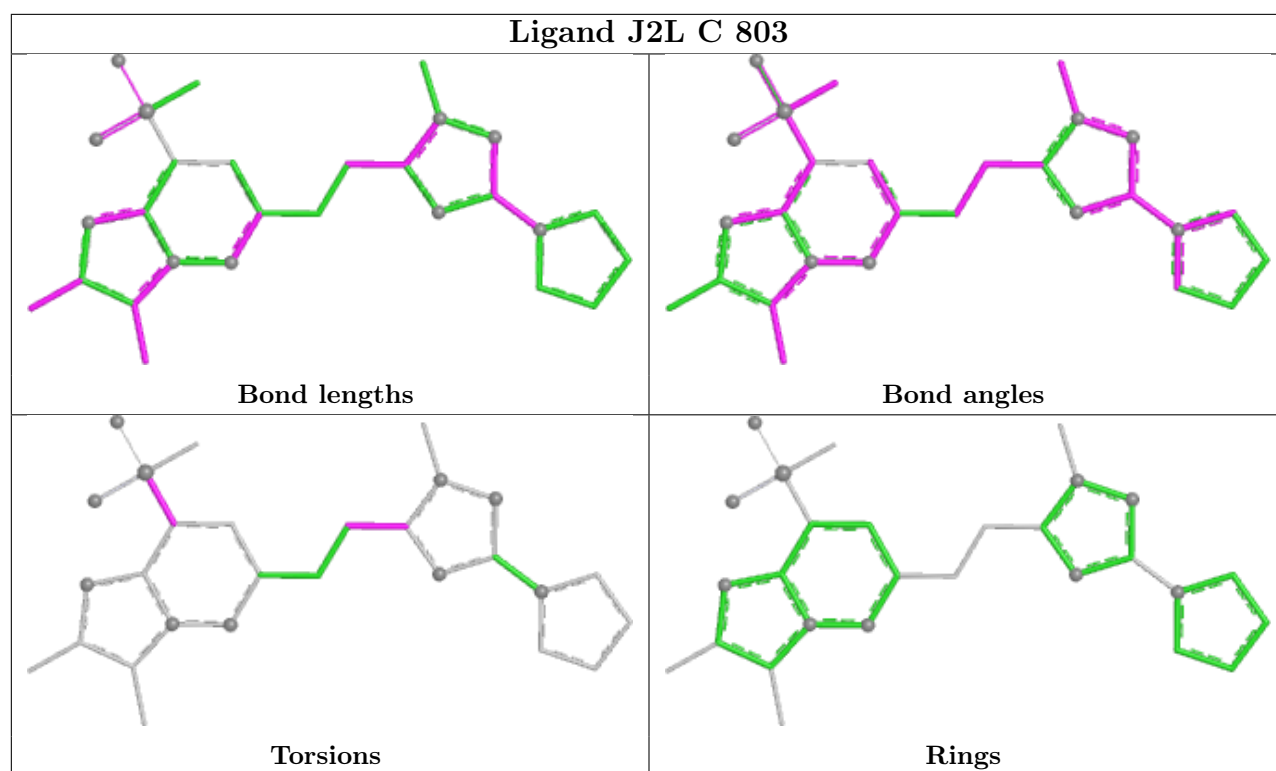


Ligand J2L D 803



Ligand J2L A 803 (B)





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	311/343 (90%)	-0.07	3 (0%) 79 86	18, 34, 61, 96	3 (0%)
1	B	314/343 (91%)	-0.07	6 (1%) 66 75	22, 33, 58, 90	2 (0%)
1	C	311/343 (90%)	-0.15	2 (0%) 85 90	20, 34, 58, 100	2 (0%)
1	D	309/343 (90%)	0.15	5 (1%) 70 79	29, 41, 63, 77	0
All	All	1245/1372 (90%)	-0.03	16 (1%) 75 82	18, 36, 61, 100	7 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	LEU	7.0
1	C	459	LEU	6.0
1	D	459	LEU	5.5
1	B	771	THR	4.5
1	D	768	GLY	4.5
1	B	459	LEU	4.3
1	B	458	GLY	3.9
1	B	457	GLN	3.1
1	B	550	ASP	2.5
1	A	461	GLN	2.5
1	D	727	LEU	2.3
1	A	770	GLU	2.1
1	C	462	PHE	2.1
1	D	500	THR	2.1
1	D	766	ILE	2.1
1	B	460	MET	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CME	D	509	10/11	0.84	0.17	38,51,99,104	0
1	CME	B	509	10/11	0.90	0.15	34,43,92,97	0
1	CME	A	509	10/11	0.90	0.13	37,47,73,79	0
1	CME	C	509	10/11	0.92	0.12	33,41,69,76	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

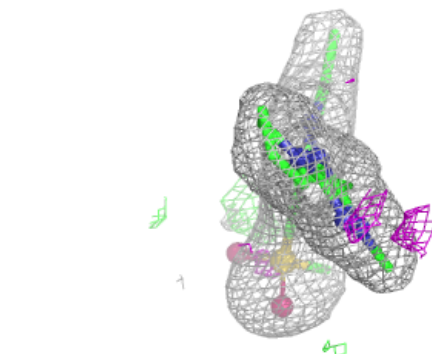
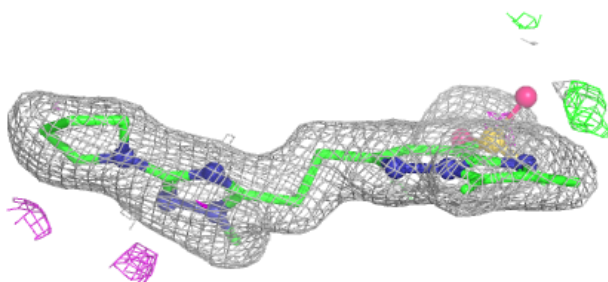
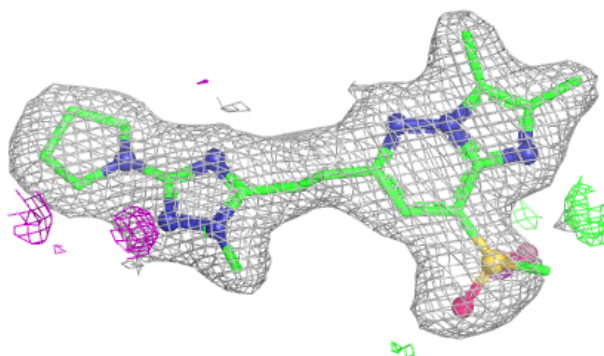
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	J2L	A	803[A]	28/28	0.95	0.08	22,28,43,48	28
4	J2L	A	803[B]	28/28	0.95	0.08	24,31,47,54	28
4	J2L	D	803	28/28	0.96	0.07	30,36,56,72	0
4	J2L	C	803	28/28	0.97	0.06	24,34,50,73	0
4	J2L	B	803	28/28	0.97	0.07	25,31,50,63	0
2	ZN	D	801	1/1	0.99	0.02	35,35,35,35	0
3	MG	A	802	1/1	0.99	0.03	25,25,25,25	0
3	MG	B	802	1/1	0.99	0.02	23,23,23,23	0
3	MG	C	802	1/1	0.99	0.02	25,25,25,25	0
3	MG	D	802	1/1	0.99	0.03	35,35,35,35	0
2	ZN	B	801	1/1	1.00	0.01	28,28,28,28	0
2	ZN	C	801	1/1	1.00	0.02	29,29,29,29	0
2	ZN	A	801	1/1	1.00	0.01	29,29,29,29	0

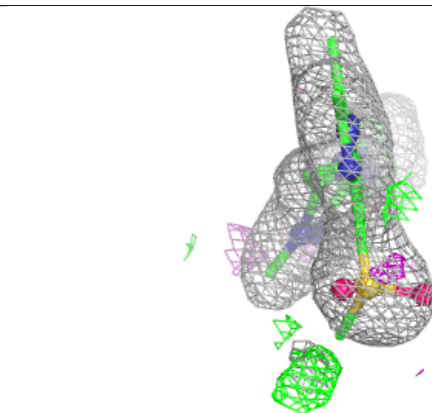
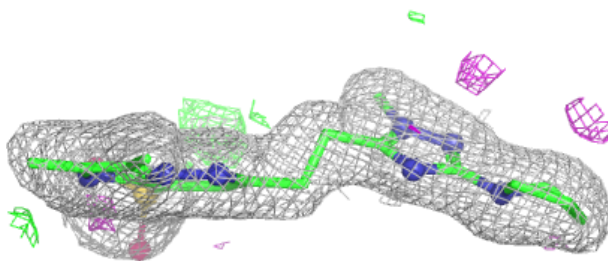
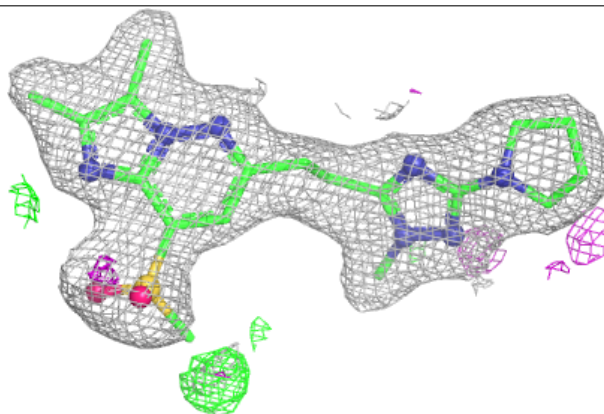
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J2L A 803 (A):

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

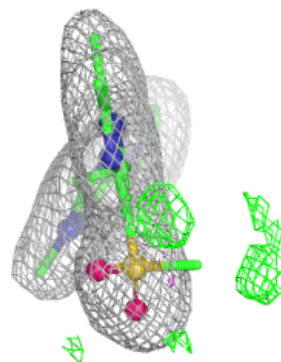
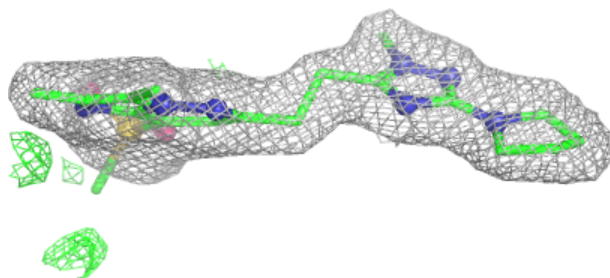
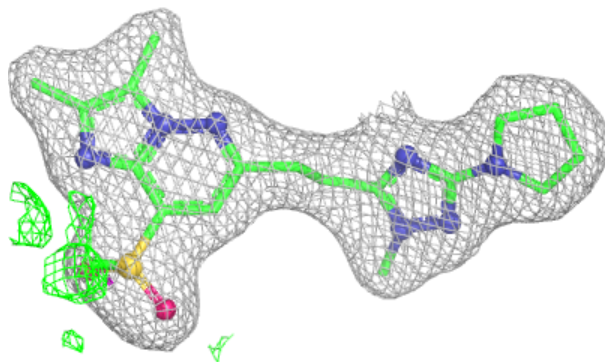
**Electron density around J2L A 803 (B):**

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

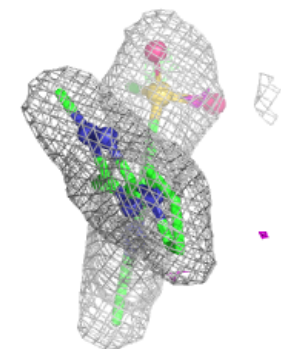
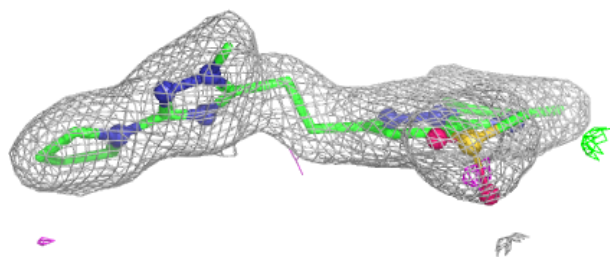
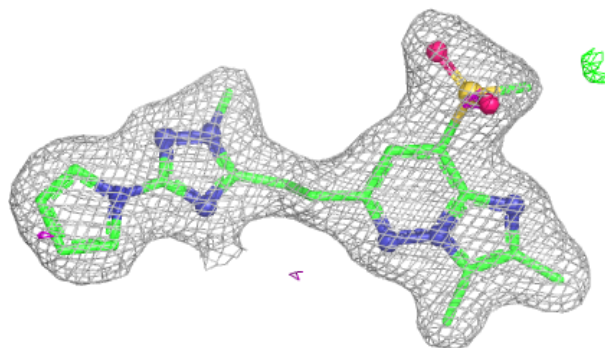


Electron density around J2L D 803:

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

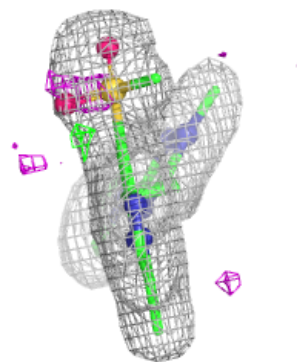
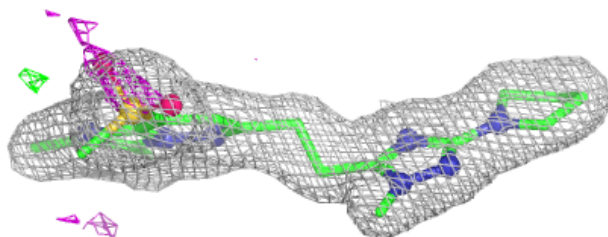
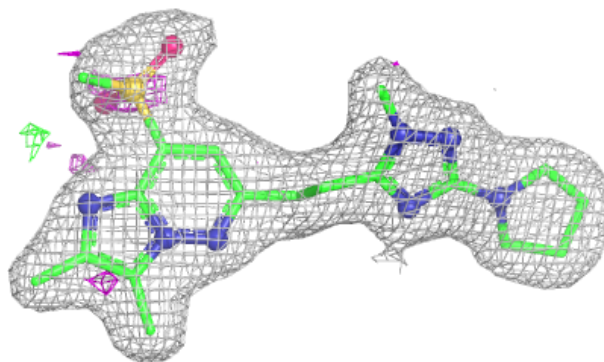
**Electron density around J2L C 803:**

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



Electron density around J2L 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.