



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 5SHR / pdb_00005shr
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN
COMPLEX WITH n1(c(nc(n1)c2cccc2)N(C)Cc4nn3c(cnc(c3n4)C)C)C,
micromolar IC₅₀=1.47052
Authors : Joseph, C.; Benz, J.; Flohr, A.; 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

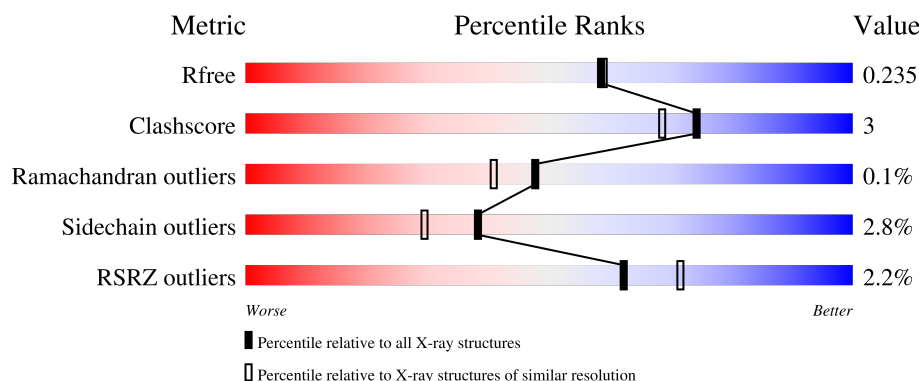
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

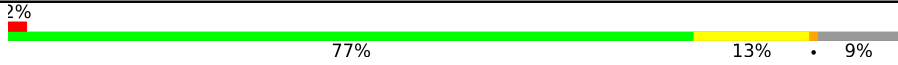
The reported resolution of this entry is 1.98 Å.

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	
2	B	343	
2	C	343	
2	D	343	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10790 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	1	0
			2549	1629	434	461	25			

There are 2 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

- Molecule 2 is a protein called cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	315	Total	C	N	O	S	0	1	0
			2554	1632	434	464	24			
2	C	312	Total	C	N	O	S	0	2	0
			2548	1629	431	464	24			
2	D	312	Total	C	N	O	S	0	0	0
			2528	1617	431	456	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

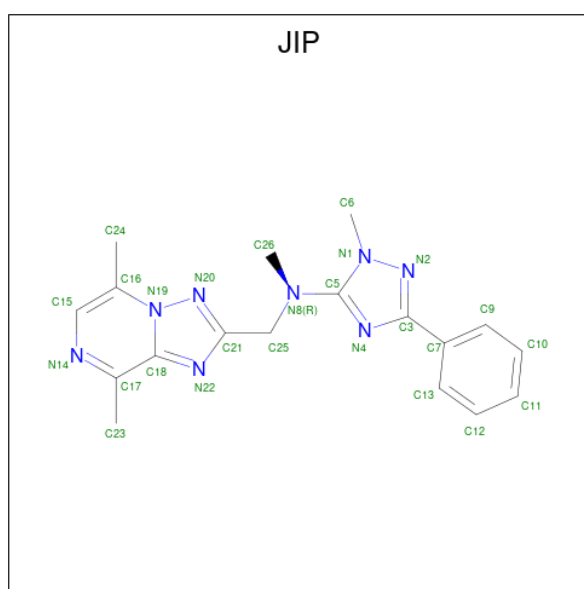
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is N-{[(4R)-5,8-dimethyl[1,2,4]triazolo[1,5-a]pyrazin-2-yl)methyl}-N,1-dimethyl-3-phenyl-1H-1,2,4-triazol-5-amine (CCD ID: JIP) (formula: C₁₈H₂₀N₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			26	18	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			26	18	8		
5	C	1	Total	C	N	0	0
			26	18	8		
5	D	1	Total	C	N	0	0
			26	18	8		

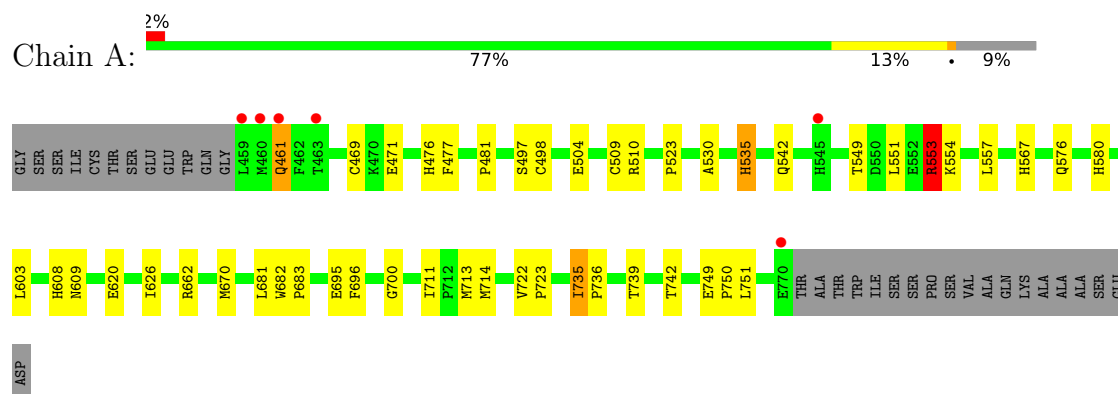
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	152	Total	O	0	0
			152	152		
6	C	131	Total	O	0	0
			131	131		
6	D	88	Total	O	0	0
			88	88		

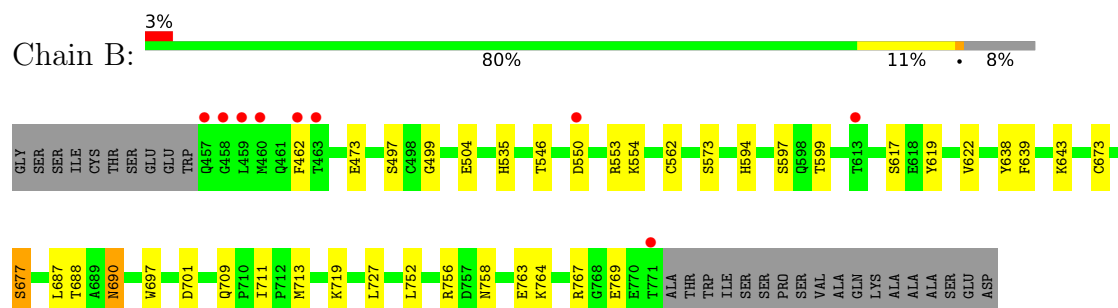
3 Residue-property plots [i](#)

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

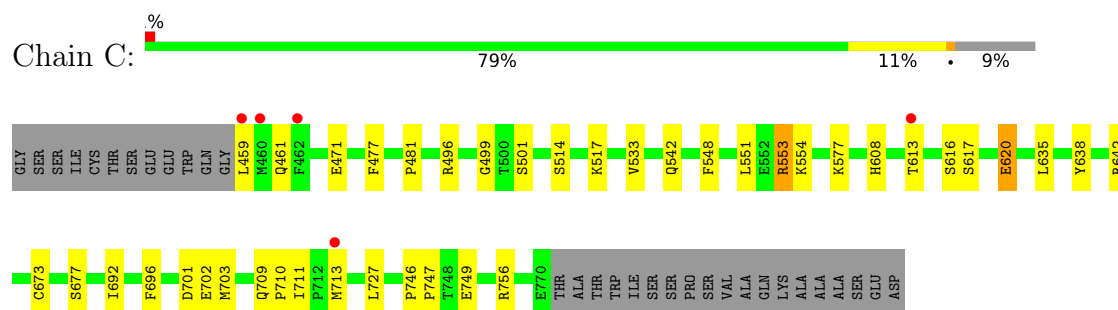
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



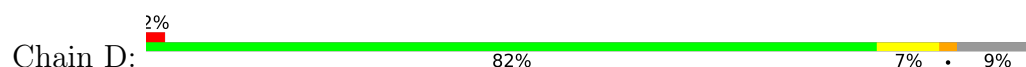
- Molecule 2: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

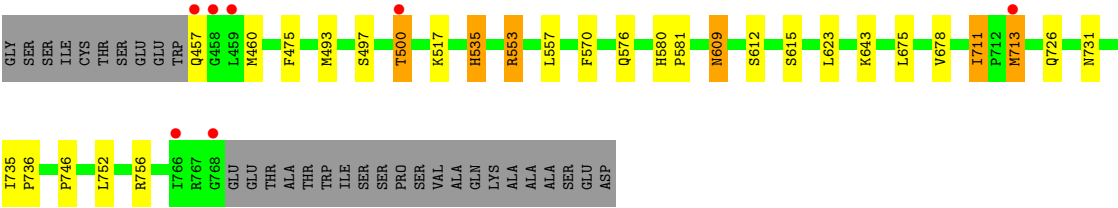


- Molecule 2: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 2: 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	135.12Å 135.12Å 234.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.46 – 1.98 43.46 – 1.98	Depositor EDS
% Data completeness (in resolution range)	87.9 (43.46-1.98) 87.9 (43.46-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.230 0.190 , 0.235	Depositor DCC
R_{free} test set	5102 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.9	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	0.95	EDS
Total number of atoms	10790	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: JIP, ZN, MG, CME

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	1.24	11/2592 (0.4%)	1.46	7/3505 (0.2%)
2	B	1.21	4/2608 (0.2%)	1.46	13/3529 (0.4%)
2	C	1.17	4/2605 (0.2%)	1.44	6/3526 (0.2%)
2	D	1.19	3/2579 (0.1%)	1.49	13/3490 (0.4%)
All	All	1.20	22/10384 (0.2%)	1.46	39/14050 (0.3%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	PRO	C-O	-7.65	1.15	1.23
1	A	567	HIS	CE1-NE2	6.92	1.39	1.32
1	A	739	THR	C-O	6.08	1.31	1.24
1	A	751	LEU	C-O	5.94	1.30	1.24
2	B	673	CYS	C-O	5.80	1.31	1.24
2	B	597	SER	CA-CB	-5.75	1.44	1.53
1	A	476	HIS	CE1-NE2	5.72	1.38	1.32
1	A	580	HIS	CE1-NE2	5.68	1.38	1.32
2	C	554	LYS	C-O	5.59	1.30	1.24
1	A	670	MET	C-O	5.53	1.30	1.24
1	A	530	ALA	C-O	5.50	1.30	1.24
2	B	594	HIS	CE1-NE2	5.44	1.38	1.32
2	C	481	PRO	C-O	-5.37	1.17	1.24
2	D	580	HIS	CE1-NE2	5.24	1.37	1.32
1	A	535	HIS	CE1-NE2	5.22	1.37	1.32
2	C	477	PHE	C-O	5.21	1.29	1.23
2	D	623	LEU	C-O	5.21	1.30	1.24
2	C	499	GLY	C-O	5.21	1.28	1.23
1	A	742	THR	C-O	5.21	1.30	1.24
2	D	726	GLN	C-O	5.17	1.30	1.24
2	B	462	PHE	C-O	-5.07	1.17	1.23
1	A	620	GLU	C-O	5.02	1.30	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	ASN	CA-CB-CG	-8.57	104.03	112.60
2	D	535	HIS	CA-CB-CG	-8.42	105.38	113.80
2	B	701	ASP	CA-CB-CG	7.60	120.20	112.60
1	A	553	ARG	CA-C-N	6.65	131.77	121.19
1	A	553	ARG	C-N-CA	6.65	131.77	121.19
2	B	535	HIS	CA-CB-CG	-6.58	107.22	113.80
2	B	504	GLU	CB-CA-C	6.57	120.12	110.26
1	A	609	ASN	N-CA-CB	6.49	119.68	110.46
2	B	690	ASN	CB-CA-C	-6.41	100.81	110.88
2	D	570	PHE	CA-C-N	6.25	130.01	120.82
2	D	570	PHE	C-N-CA	6.25	130.01	120.82
2	D	609	ASN	CA-CB-CG	-6.00	106.61	112.60
2	B	639	PHE	CA-C-N	5.87	126.49	119.98
2	B	639	PHE	C-N-CA	5.87	126.49	119.98
2	D	553	ARG	CA-C-O	-5.79	114.93	121.00
2	B	499	GLY	CA-C-N	5.71	128.51	120.28
2	B	499	GLY	C-N-CA	5.71	128.51	120.28
2	B	473	GLU	N-CA-C	-5.69	106.30	113.18
2	D	500	THR	CB-CA-C	5.66	122.60	110.21
2	C	701	ASP	N-CA-C	-5.64	105.14	111.28
2	C	554	LYS	CA-C-N	5.61	126.20	119.98
2	C	554	LYS	C-N-CA	5.61	126.20	119.98
2	D	746	PRO	N-CA-C	5.51	117.43	110.70
2	D	475	PHE	CA-C-O	-5.48	114.71	120.63
2	D	643	LYS	CA-C-O	-5.43	115.12	120.82
1	A	626	ILE	CA-C-O	-5.43	115.31	120.95
2	B	619	TYR	N-CA-C	-5.37	105.32	111.07
1	A	735	ILE	CA-C-O	5.37	122.29	118.69
1	A	696	PHE	CA-CB-CG	-5.37	108.43	113.80
2	C	702	GLU	CA-C-O	-5.34	114.76	120.42
2	D	731	ASN	CA-C-O	-5.29	115.26	120.70
2	D	553	ARG	CA-C-N	5.27	127.65	120.54
2	D	553	ARG	C-N-CA	5.27	127.65	120.54
2	C	620	GLU	CB-CG-CD	5.25	121.52	112.60
2	B	554	LYS	CA-C-N	5.23	125.75	119.94
2	B	554	LYS	C-N-CA	5.23	125.75	119.94
2	B	638	TYR	CA-C-O	-5.22	114.88	120.42
2	C	553	ARG	CA-C-O	-5.20	115.54	121.00
2	D	517	LYS	CB-CA-C	5.18	120.25	109.95

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	2549	0	2525	22	0
2	B	2554	0	2520	15	0
2	C	2548	0	2518	16	0
2	D	2528	0	2501	11	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	26	0	0	0	0
5	B	26	0	0	1	0
5	C	26	0	0	1	0
5	D	26	0	0	1	0
6	A	128	0	0	0	0
6	B	152	0	0	2	0
6	C	131	0	0	3	0
6	D	88	0	0	0	0
All	All	10790	0	10064	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (64) 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)
2:B:713:MET:SD	5:B:803:JIP:C26	2.69	0.79
2:C:613:THR:HB	6:C:1010:HOH:O	1.87	0.74
1:A:461:GLN:HA	1:A:461:GLN:OE1	1.88	0.73
2:B:497:SER:O	2:B:553:ARG:HD2	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:ILE:HD12	2:B:713:MET:HE3	1.74	0.70
2:D:497:SER:O	2:D:553:ARG:HD2	1.96	0.66
2:C:713:MET:SD	5:C:803:JIP:C26	2.87	0.63
2:D:457:GLN:HA	2:D:460:MET:HE2	1.85	0.58
2:B:719:LYS:NZ	6:B:902:HOH:O	2.35	0.58
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.86	0.56
2:B:677:SER:HB2	2:B:688:THR:HG21	1.89	0.54
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.90	0.54
2:D:711:ILE:HG13	2:D:713:MET:HG3	1.90	0.53
2:D:713:MET:SD	5:D:803:JIP:C26	2.97	0.53
2:B:697:TRP:CZ2	2:B:719:LYS:HG2	2.44	0.52
1:A:662:ARG:HG2	1:A:662:ARG:NH1	2.25	0.52
2:B:687:LEU:O	2:B:690:ASN:HB2	2.10	0.52
2:D:609:ASN:HD22	2:D:612:SER:HB3	1.75	0.51
1:A:549:THR:O	1:A:553:ARG:HG3	2.11	0.51
2:B:697:TRP:CH2	2:B:719:LYS:HE3	2.45	0.51
2:D:497:SER:O	2:D:553:ARG:CD	2.60	0.50
2:B:767:ARG:NH2	2:B:769:GLU:OE2	2.38	0.48
2:B:752:LEU:HD21	2:B:756:ARG:NH2	2.29	0.48
2:C:514:SER:OG	2:C:608:HIS:NE2	2.46	0.47
1:A:498:CYS:SG	1:A:554:LYS:HG3	2.54	0.47
1:A:469:CME:C	1:A:469:CME:SD	3.02	0.47
2:B:550:ASP:N	2:B:550:ASP:OD1	2.49	0.46
1:A:662:ARG:CG	1:A:662:ARG:HH11	2.27	0.46
1:A:735:ILE:N	1:A:736:PRO:HD2	2.31	0.46
2:C:542:GLN:NE2	2:C:542:GLN:HA	2.29	0.46
2:C:548:PHE:O	2:C:553:ARG:NH2	2.49	0.46
2:C:620:GLU:HG3	6:C:927:HOH:O	2.15	0.46
2:C:709:GLN:HE21	2:C:710:PRO:HD2	1.81	0.45
1:A:523:PRO:HD2	1:A:695:GLU:HG2	1.98	0.45
2:D:735:ILE:O	2:D:736:PRO:C	2.58	0.45
2:B:767:ARG:HH21	2:B:769:GLU:CD	2.23	0.45
1:A:542:GLN:NE2	1:A:542:GLN:HA	2.31	0.44
2:D:752:LEU:HD21	2:D:756:ARG:NH2	2.33	0.44
1:A:662:ARG:NH1	1:A:662:ARG:CG	2.80	0.43
1:A:700:GLY:HA3	1:A:714:MET:O	2.18	0.43
2:C:533:VAL:HG13	2:C:673:CYS:HB3	2.00	0.43
2:C:577:LYS:HD3	2:C:703:MET:HE1	2.00	0.43
2:C:746:PRO:N	2:C:747:PRO:CD	2.82	0.43
2:C:692:ILE:HG22	2:C:696:PHE:CE2	2.55	0.42
2:D:457:GLN:HA	2:D:460:MET:CE	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:TRP:N	1:A:683:PRO:CD	2.82	0.42
1:A:711:ILE:HD12	1:A:713:MET:HE3	2.02	0.42
2:B:758:ASN:OD1	6:B:901:HOH:O	2.20	0.42
2:B:727:LEU:HD11	2:B:763:GLU:HG3	2.02	0.42
2:D:675:LEU:O	2:D:678:VAL:HG22	2.20	0.42
2:C:551:LEU:HD23	2:C:551:LEU:HA	1.89	0.42
1:A:749:GLU:N	1:A:750:PRO:CD	2.83	0.41
2:B:562:CYS:HB3	2:B:599:THR:OG1	2.19	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.84	0.41
1:A:735:ILE:HB	1:A:736:PRO:CD	2.50	0.41
1:A:510:ARG:HG2	1:A:608:HIS:CE1	2.56	0.41
2:C:459:LEU:HD12	2:C:459:LEU:HA	1.88	0.41
2:C:635:LEU:HD12	2:C:635:LEU:HA	1.92	0.41
2:D:493:MET:SD	2:D:535:HIS:HA	2.61	0.41
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.57	0.40
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.88	0.40
2:C:756:ARG:HD2	6:C:952:HOH:O	2.21	0.40
1:A:497:SER:OG	1:A:557:LEU:HD11	2.21	0.40
2:C:638:TYR:OH	2:C:642:ARG:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/343 (90%)	298 (96%)	11 (4%)	0	100	100
2	B	313/343 (91%)	306 (98%)	7 (2%)	0	100	100
2	C	311/343 (91%)	307 (99%)	4 (1%)	0	100	100
2	D	309/343 (90%)	298 (96%)	10 (3%)	1 (0%)	36	27
All	All	1242/1372 (90%)	1209 (97%)	32 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	615	SER

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	281/304 (92%)	275 (98%)	6 (2%)	47	40
2	B	282/305 (92%)	274 (97%)	8 (3%)	38	29
2	C	283/305 (93%)	271 (96%)	12 (4%)	26	15
2	D	279/305 (92%)	273 (98%)	6 (2%)	45	38
All	All	1125/1219 (92%)	1093 (97%)	32 (3%)	38	29

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

Mol	Chain	Res	Type
1	A	461	GLN
1	A	471	GLU
1	A	504	GLU
1	A	553	ARG
1	A	576	GLN
1	A	681	LEU
2	B	546	THR
2	B	573	SER
2	B	617	SER
2	B	622	VAL
2	B	643	LYS
2	B	677	SER
2	B	709	GLN
2	B	764	LYS
2	C	461	GLN
2	C	471	GLU
2	C	496	ARG
2	C	501	SER
2	C	517	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	616	SER
2	C	617	SER
2	C	677	SER
2	C	711	ILE
2	C	727	LEU
2	C	749[A]	GLU
2	C	749[B]	GLU
2	D	500	THR
2	D	557	LEU
2	D	576	GLN
2	D	581	PRO
2	D	711	ILE
2	D	713	MET

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

Mol	Chain	Res	Type
1	A	542	GLN
1	A	544	ASN
1	A	576	GLN
1	A	604	GLN
1	A	644	GLN
1	A	709	GLN
1	A	726	GLN
1	A	743	GLN
1	A	761	GLN
2	B	484	ASN
2	B	545	HIS
2	B	604	GLN
2	B	650	GLN
2	B	761	GLN
2	C	461	GLN
2	C	542	GLN
2	C	604	GLN
2	C	621	GLN
2	C	709	GLN
2	C	726	GLN
2	C	743	GLN
2	D	484	ASN
2	D	604	GLN
2	D	609	ASN
2	D	659	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	743	GLN
2	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 ⓘ

5 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	$\# Z > 2$
2	CME	B	509	2	8,9,10	0.55	0	6,9,11	0.82	0
2	CME	C	509	2	8,9,10	0.47	0	6,9,11	0.75	0
2	CME	D	509	2	8,9,10	0.66	0	6,9,11	0.82	0
1	CME	A	509	1	8,9,10	0.52	0	6,9,11	1.14	1 (16%)
1	CME	A	469	1	8,9,10	0.65	0	6,9,11	1.18	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
2	CME	B	509	2	-	0/5/8/10	-
2	CME	C	509	2	-	1/5/8/10	-
2	CME	D	509	2	-	1/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-
1	CME	A	469	1	-	2/5/8/10	-

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	-2.02	106.63	113.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	469	CME	SD-CE-CZ-OH
1	A	509	CME	SD-CE-CZ-OH
2	C	509	CME	SD-CE-CZ-OH
2	D	509	CME	CZ-CE-SD-SG
1	A	469	CME	CE-SD-SG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	469	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	$\# Z > 2$
5	JIP	C	803	-	27,29,29	4.37	14 (51%)	27,42,42	2.40	11 (40%)
5	JIP	D	803	-	27,29,29	3.00	14 (51%)	27,42,42	2.64	11 (40%)
5	JIP	B	803	-	27,29,29	3.81	12 (44%)	27,42,42	2.62	11 (40%)
5	JIP	A	803	-	27,29,29	3.63	15 (55%)	27,42,42	1.99	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JIP	C	803	-	-	5/12/12/12	0/4/4/4
5	JIP	D	803	-	-	2/12/12/12	0/4/4/4
5	JIP	B	803	-	-	2/12/12/12	0/4/4/4
5	JIP	A	803	-	-	2/12/12/12	0/4/4/4

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	JIP	C5-N1	11.97	1.51	1.35
5	C	803	JIP	C5-N1	11.45	1.50	1.35
5	A	803	JIP	C5-N1	11.03	1.50	1.35
5	D	803	JIP	C5-N1	9.56	1.48	1.35
5	C	803	JIP	C3-N2	8.82	1.45	1.33
5	C	803	JIP	C21-N20	8.61	1.45	1.32
5	C	803	JIP	C13-C7	7.82	1.51	1.39
5	B	803	JIP	C3-N2	7.15	1.43	1.33
5	B	803	JIP	C25-C21	-6.69	1.46	1.49
5	A	803	JIP	C3-N2	6.34	1.42	1.33
5	A	803	JIP	C21-N20	6.05	1.41	1.32
5	D	803	JIP	C3-N2	5.69	1.41	1.33
5	C	803	JIP	C25-N8	5.40	1.55	1.46
5	B	803	JIP	C6-N1	4.78	1.54	1.46
5	B	803	JIP	C13-C7	4.72	1.46	1.39
5	C	803	JIP	C25-C21	-4.71	1.47	1.49
5	A	803	JIP	N19-N20	-4.69	1.29	1.38
5	B	803	JIP	C21-N20	4.34	1.39	1.32
5	C	803	JIP	C3-N4	4.34	1.46	1.37
5	D	803	JIP	C21-N20	4.27	1.39	1.32
5	C	803	JIP	C12-C11	4.21	1.47	1.38
5	A	803	JIP	C17-N14	-4.17	1.27	1.32
5	A	803	JIP	C5-N8	4.06	1.49	1.39
5	A	803	JIP	C3-N4	4.04	1.45	1.37
5	B	803	JIP	C17-N14	3.90	1.37	1.32
5	B	803	JIP	C21-N22	-3.83	1.30	1.37
5	C	803	JIP	C9-C7	3.71	1.45	1.39
5	C	803	JIP	C6-N1	3.70	1.52	1.46
5	D	803	JIP	N1-N2	3.69	1.44	1.36
5	A	803	JIP	C18-N22	3.46	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	803	JIP	C3-N4	3.43	1.44	1.37
5	B	803	JIP	N19-N20	-3.41	1.32	1.38
5	A	803	JIP	C13-C7	3.39	1.44	1.39
5	C	803	JIP	C10-C9	3.21	1.44	1.38
5	A	803	JIP	C21-N22	-3.19	1.31	1.37
5	D	803	JIP	C11-C10	3.10	1.45	1.38
5	B	803	JIP	C18-N19	2.95	1.43	1.38
5	C	803	JIP	C18-N22	2.93	1.39	1.33
5	D	803	JIP	C26-N8	2.88	1.55	1.45
5	C	803	JIP	N1-N2	2.82	1.42	1.36
5	B	803	JIP	C3-N4	2.81	1.43	1.37
5	D	803	JIP	C5-N4	2.77	1.37	1.33
5	D	803	JIP	C23-C17	-2.72	1.44	1.49
5	A	803	JIP	C25-C21	2.68	1.51	1.49
5	D	803	JIP	C18-N22	2.52	1.38	1.33
5	A	803	JIP	N1-N2	2.47	1.41	1.36
5	B	803	JIP	C12-C11	2.40	1.43	1.38
5	A	803	JIP	C5-N4	2.40	1.37	1.33
5	D	803	JIP	C7-C3	-2.28	1.43	1.47
5	D	803	JIP	C5-N8	2.22	1.44	1.39
5	C	803	JIP	C5-N8	2.16	1.44	1.39
5	A	803	JIP	C16-N19	2.14	1.41	1.37
5	D	803	JIP	C12-C13	-2.12	1.35	1.38
5	A	803	JIP	C10-C9	2.11	1.42	1.38
5	D	803	JIP	C13-C7	2.10	1.42	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	803	JIP	C23-C17-N14	7.43	126.64	116.83
5	D	803	JIP	C23-C17-C18	-6.32	109.60	117.55
5	D	803	JIP	C23-C17-N14	6.06	124.82	116.83
5	B	803	JIP	C25-C21-N22	-5.66	116.76	122.73
5	C	803	JIP	C23-C17-N14	5.31	123.84	116.83
5	C	803	JIP	C25-C21-N22	-4.93	117.52	122.73
5	A	803	JIP	C24-C16-N19	4.69	123.68	118.00
5	B	803	JIP	C18-N19-N20	-4.57	106.46	112.80
5	A	803	JIP	C5-N4-C3	4.56	105.50	102.22
5	D	803	JIP	C9-C7-C13	4.37	124.12	118.57
5	D	803	JIP	C10-C9-C7	-4.31	116.13	120.36
5	A	803	JIP	C25-C21-N22	-4.11	118.39	122.73
5	C	803	JIP	C26-N8-C25	3.80	122.49	116.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	803	JIP	C23-C17-C18	-3.78	112.79	117.55
5	C	803	JIP	C6-N1-N2	3.62	124.70	119.29
5	C	803	JIP	C10-C9-C7	-3.37	117.05	120.36
5	D	803	JIP	C16-N19-N20	3.33	130.90	125.74
5	D	803	JIP	C25-C21-N22	-3.31	119.24	122.73
5	B	803	JIP	C16-N19-N20	3.23	130.75	125.74
5	D	803	JIP	C18-N19-N20	-3.14	108.45	112.80
5	C	803	JIP	C9-C7-C13	3.06	122.45	118.57
5	A	803	JIP	C18-N19-N20	-3.05	108.58	112.80
5	D	803	JIP	C13-C7-C3	-2.98	117.02	120.78
5	C	803	JIP	C23-C17-C18	-2.96	113.83	117.55
5	C	803	JIP	C7-C3-N4	-2.82	117.98	122.92
5	B	803	JIP	C9-C7-C13	2.70	122.00	118.57
5	B	803	JIP	C10-C9-C7	-2.68	117.73	120.36
5	D	803	JIP	C5-N4-C3	2.61	104.10	102.22
5	A	803	JIP	C16-N19-N20	2.57	129.72	125.74
5	B	803	JIP	C6-N1-N2	2.38	122.84	119.29
5	A	803	JIP	C10-C9-C7	-2.32	118.08	120.36
5	B	803	JIP	C7-C3-N4	-2.30	118.90	122.92
5	D	803	JIP	C6-N1-N2	2.23	122.63	119.29
5	C	803	JIP	C16-N19-N20	2.23	129.19	125.74
5	B	803	JIP	C26-N8-C25	2.10	119.98	116.89
5	C	803	JIP	C12-C11-C10	2.09	122.73	119.87
5	C	803	JIP	C12-C13-C7	-2.08	118.33	120.36
5	D	803	JIP	C7-C3-N4	-2.07	119.30	122.92
5	B	803	JIP	C24-C16-N19	2.01	120.43	118.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

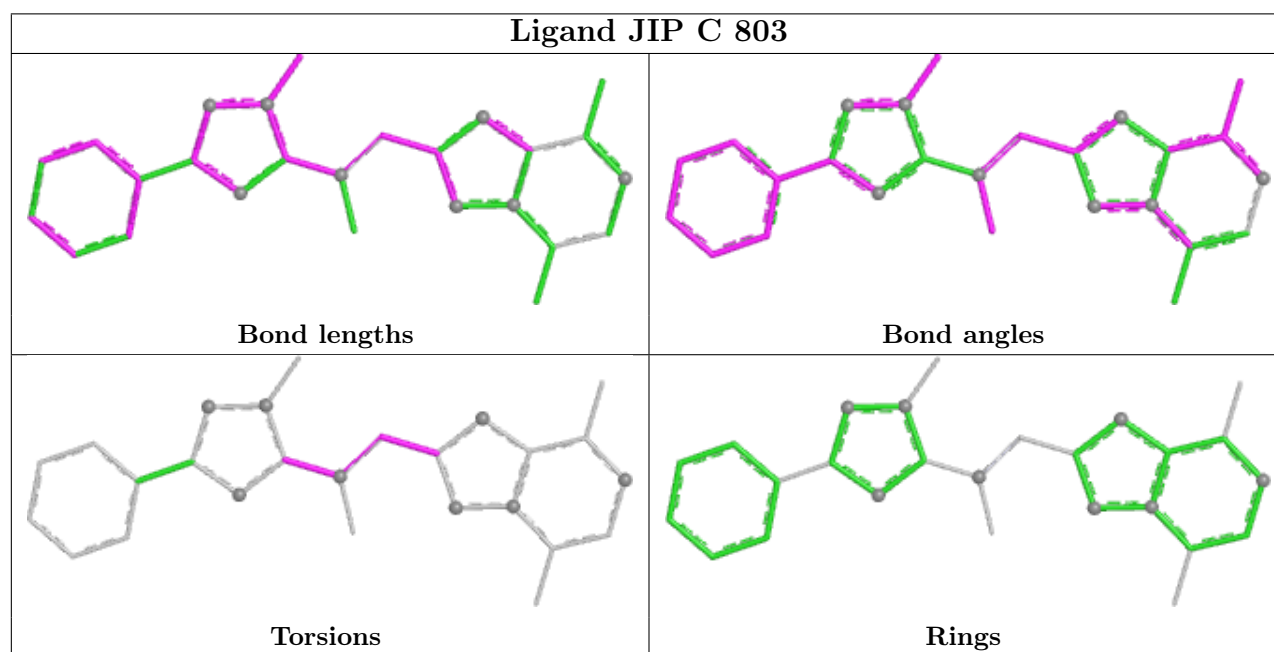
Mol	Chain	Res	Type	Atoms
5	A	803	JIP	N1-C5-N8-C25
5	A	803	JIP	N4-C5-N8-C25
5	B	803	JIP	N1-C5-N8-C25
5	B	803	JIP	N4-C5-N8-C25
5	C	803	JIP	N4-C5-N8-C25
5	D	803	JIP	N4-C5-N8-C25
5	C	803	JIP	N22-C21-C25-N8
5	C	803	JIP	N1-C5-N8-C25
5	D	803	JIP	N1-C5-N8-C25
5	C	803	JIP	C21-C25-N8-C26
5	C	803	JIP	N4-C5-N8-C26

There are no ring outliers.

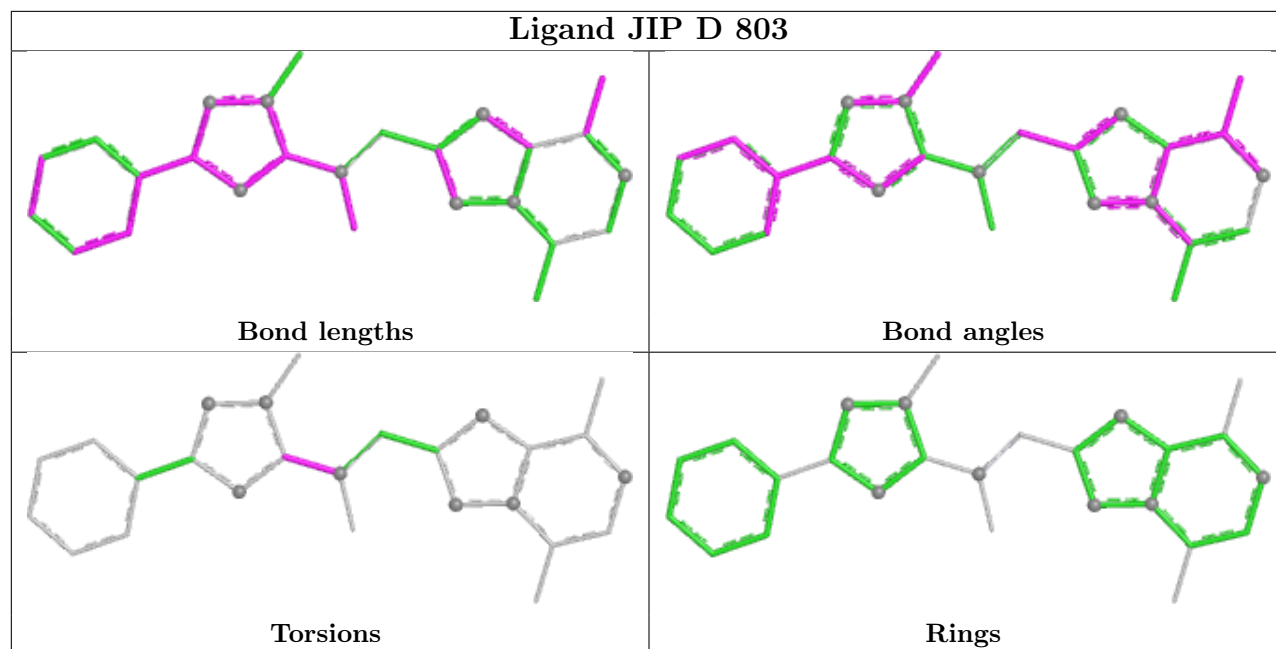
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	803	JIP	1	0
5	D	803	JIP	1	0
5	B	803	JIP	1	0

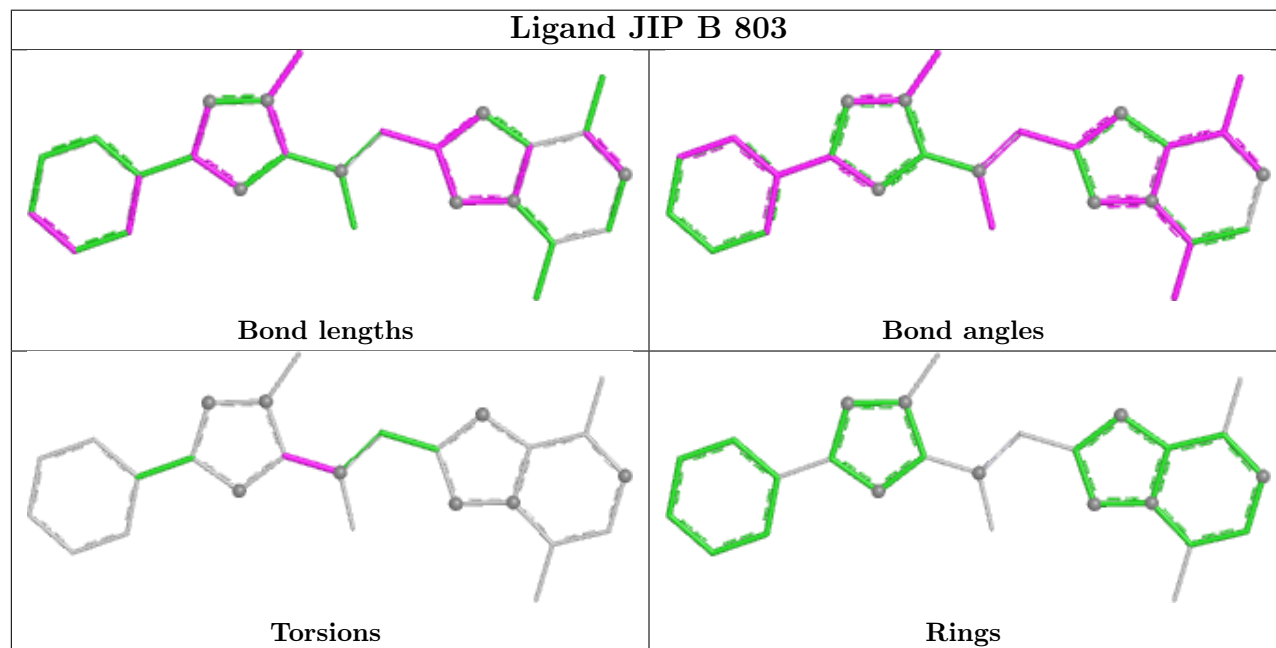
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

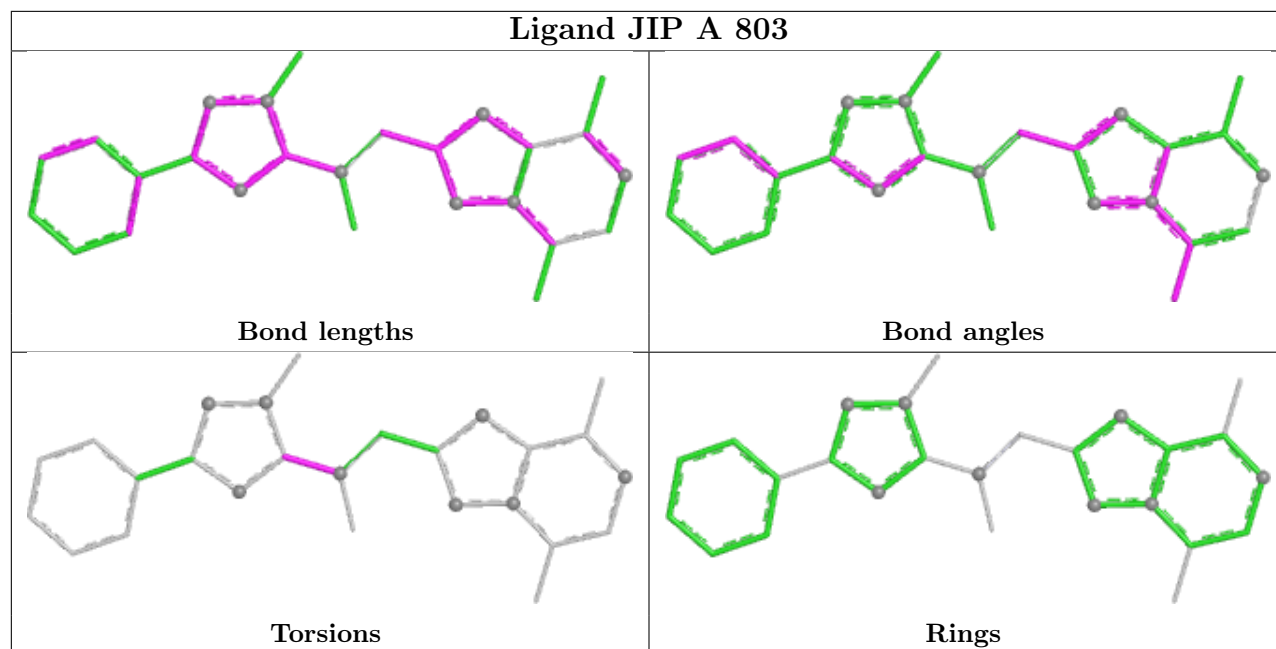


Ligand JIP D 803



Ligand JIP B 803





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	310/343 (90%)	0.14	6 (1%) 66 75	18, 36, 61, 97	1 (0%)
2	B	314/343 (91%)	0.14	9 (2%) 53 63	24, 34, 61, 88	1 (0%)
2	C	311/343 (90%)	0.09	5 (1%) 70 79	23, 36, 58, 90	2 (0%)
2	D	311/343 (90%)	0.36	7 (2%) 61 70	29, 42, 65, 81	0
All	All	1246/1372 (90%)	0.18	27 (2%) 62 71	18, 37, 62, 97	4 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	LEU	7.3
2	B	771	THR	6.2
2	C	459	LEU	5.3
2	B	459	LEU	4.9
2	D	459	LEU	4.8
2	D	457	GLN	4.1
2	D	768	GLY	4.1
2	B	458	GLY	3.3
2	D	458	GLY	3.1
2	C	460	MET	3.0
1	A	545	HIS	2.9
2	B	457	GLN	2.8
1	A	460	MET	2.7
1	A	461	GLN	2.6
2	D	766	ILE	2.6
2	D	500	THR	2.6
2	C	613	THR	2.5
2	B	462	PHE	2.5
2	B	460	MET	2.4
2	C	713	MET	2.3
2	B	550	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	463	THR	2.2
2	C	462	PHE	2.1
2	B	613	THR	2.1
1	A	770	GLU	2.1
2	D	713	MET	2.1
2	B	463	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CME	D	509	10/11	0.86	0.15	40,53,100,101	0
1	CME	A	509	10/11	0.88	0.14	39,52,92,94	0
1	CME	A	469	10/11	0.90	0.14	34,40,69,80	0
2	CME	C	509	10/11	0.91	0.12	35,46,73,76	0
2	CME	B	509	10/11	0.91	0.13	30,47,77,81	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	JIP	C	803	26/26	0.88	0.13	34,53,63,69	0
5	JIP	D	803	26/26	0.91	0.12	39,55,69,79	0
5	JIP	B	803	26/26	0.93	0.10	38,48,60,62	0
5	JIP	A	803	26/26	0.94	0.09	33,50,58,62	0
4	MG	B	802	1/1	0.98	0.02	25,25,25,25	0
4	MG	C	802	1/1	0.99	0.02	27,27,27,27	0
4	MG	D	802	1/1	0.99	0.02	35,35,35,35	0

Continued on next page...

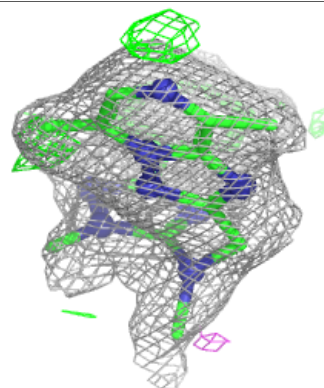
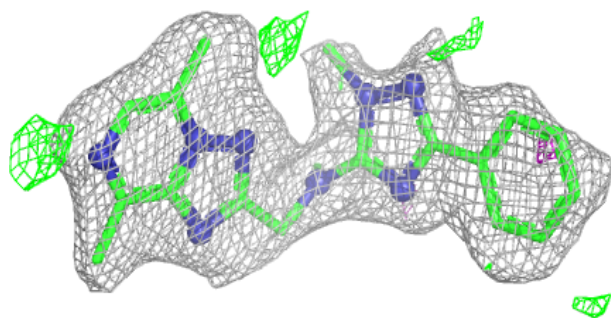
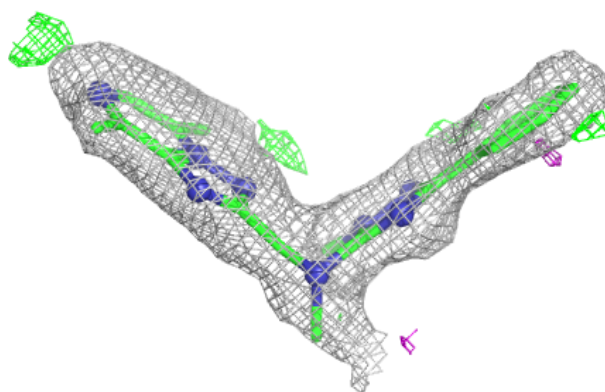
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	802	1/1	0.99	0.03	28,28,28,28	0
3	ZN	A	801	1/1	1.00	0.01	30,30,30,30	0
3	ZN	B	801	1/1	1.00	0.01	30,30,30,30	0
3	ZN	C	801	1/1	1.00	0.01	32,32,32,32	0
3	ZN	D	801	1/1	1.00	0.01	35,35,35,35	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.

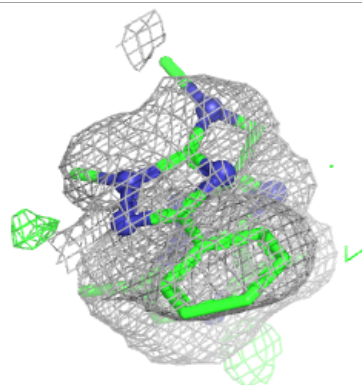
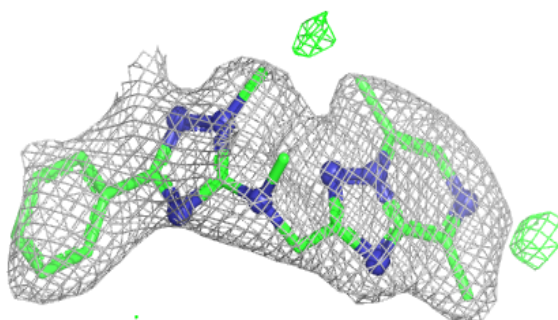
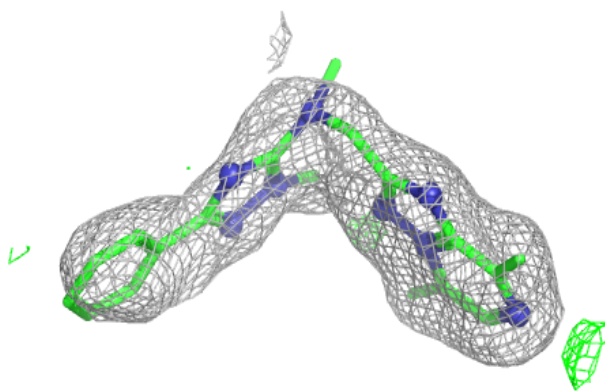
Electron density around JIP C 803:

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

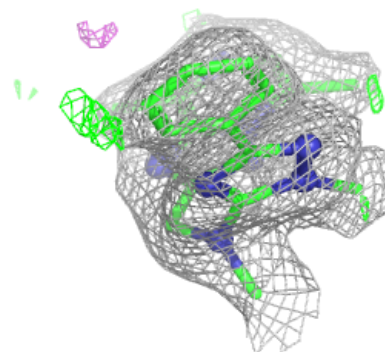
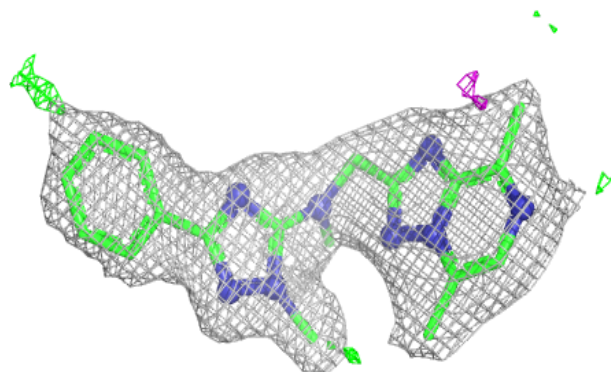
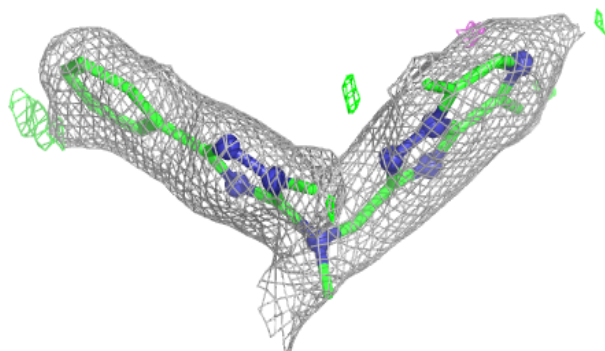


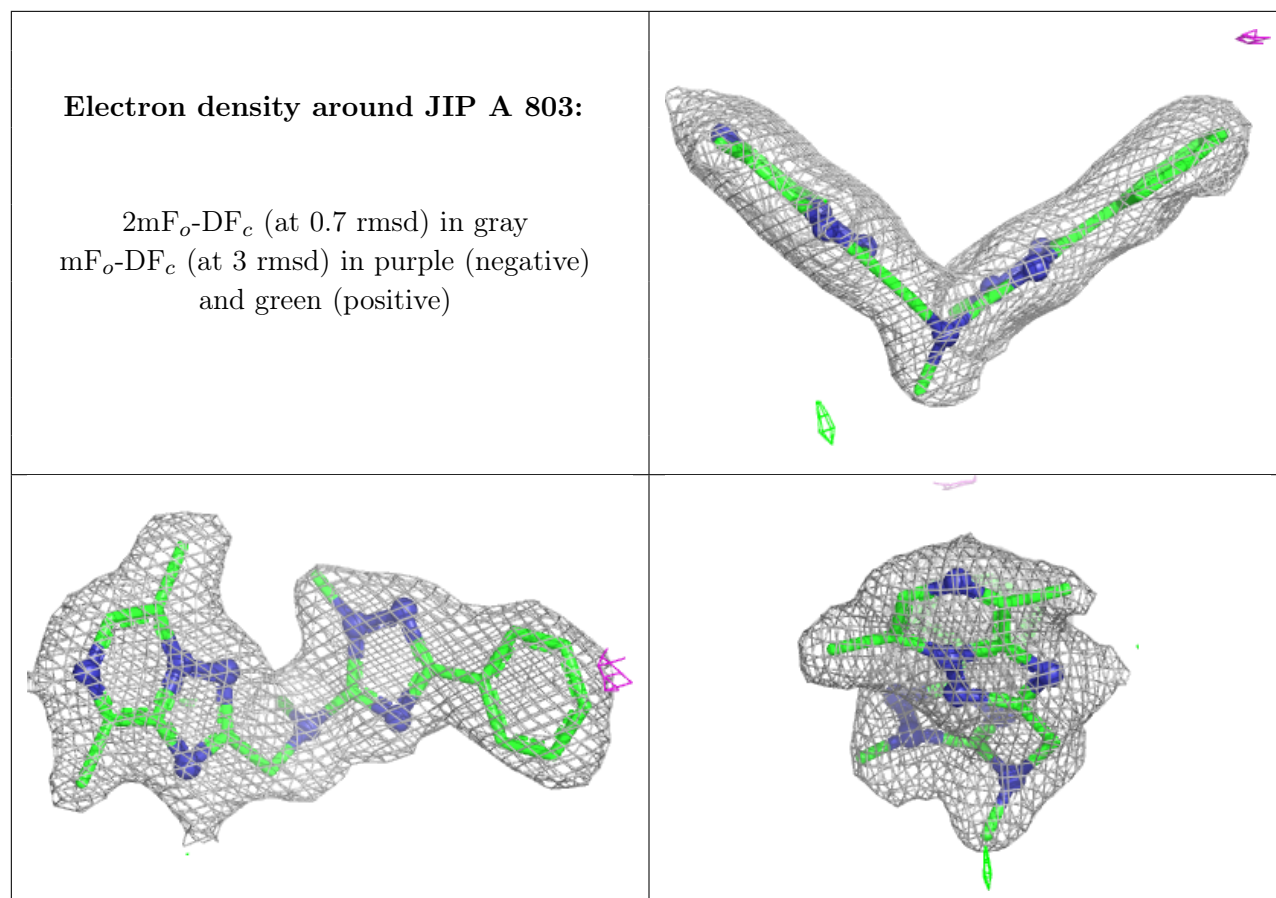
Electron density around JIP D 803:

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

**Electron density around JIP 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 ⓘ

There are no such residues in this entry.