



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:58 AM UTC

PDB ID : 5SHS / pdb_00005shs
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH c34c(n(Cc1cccc2c1cccc2)nn3)ncnc4N5CCCCC5, micromolar IC₅₀=0.183
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Deposited on : 2022-02-01
Resolution : 2.30 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

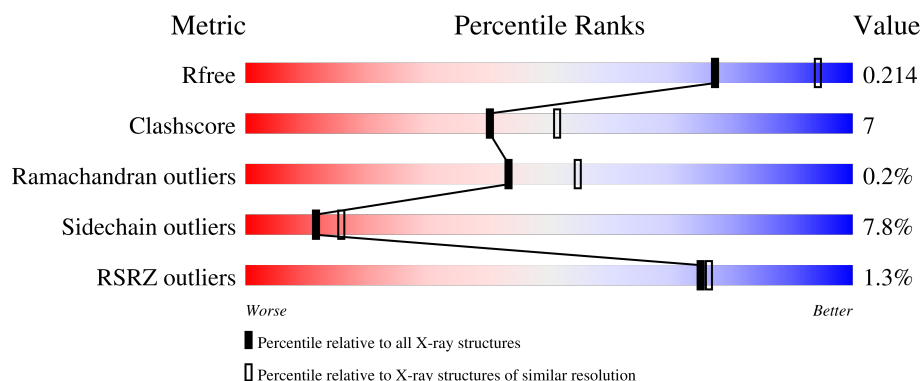
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	% 68% 21% • 8%
1	B	343	% 66% 21% • 8%
1	C	343	% 63% 23% • 9%
1	D	343	% 66% 22% • 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	JIS	B	803	-	X	-	-
5	JIS	C	803	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	6	0
			2578	1648	436	468	26			
1	B	315	Total	C	N	O	S	0	5	0
			2579	1648	437	469	25			
1	C	313	Total	C	N	O	S	0	7	0
			2576	1648	437	466	25			
1	D	313	Total	C	N	O	S	0	4	0
			2560	1637	436	462	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	SER	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	SER	-	expression tag	UNP Q9Y233
C	447	GLY	-	expression tag	UNP Q9Y233
C	448	SER	-	expression tag	UNP Q9Y233
D	447	GLY	-	expression tag	UNP Q9Y233
D	448	SER	-	expression tag	UNP Q9Y233

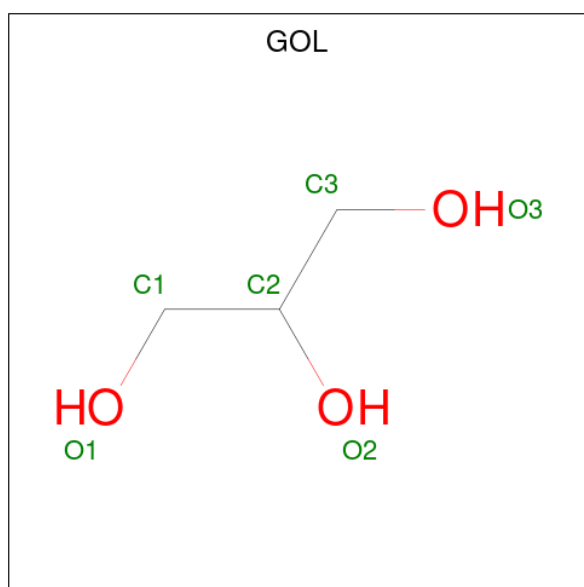
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

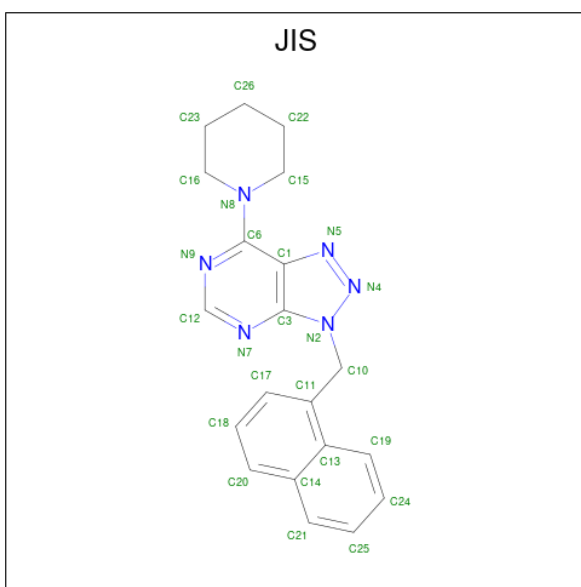
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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



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

- Molecule 5 is 3-[(naphthalen-1-yl)methyl]-7-(piperidin-1-yl)-3H-[1,2,3]triazolo[4,5-d]pyrimidine (CCD ID: JIS) (formula: C₂₀H₂₀N₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 26	C 20	N 6	0	0
5	B	1	Total 26	C 20	N 6	0	0
5	C	1	Total 26	C 20	N 6	0	0
5	D	1	Total 26	C 20	N 6	0	0

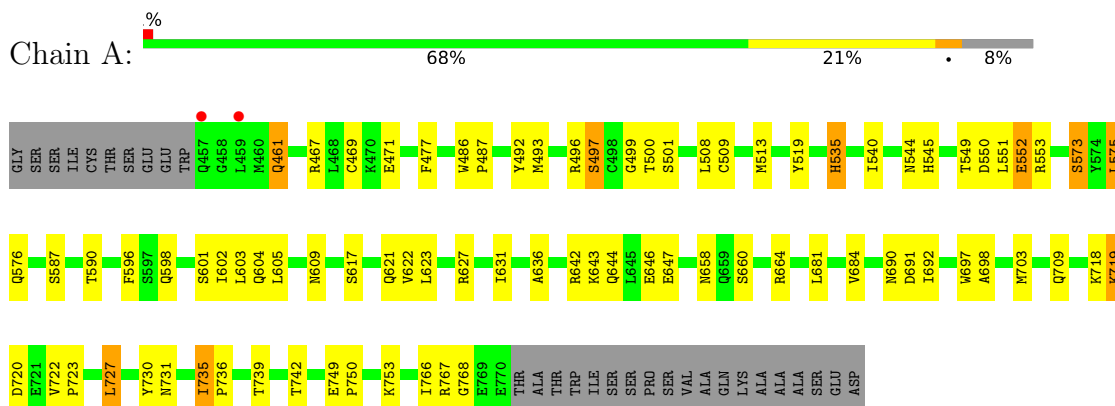
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	137	Total O 137 137	0	0
6	B	154	Total O 154 154	0	0
6	C	156	Total O 156 156	0	0
6	D	85	Total O 85 85	0	0

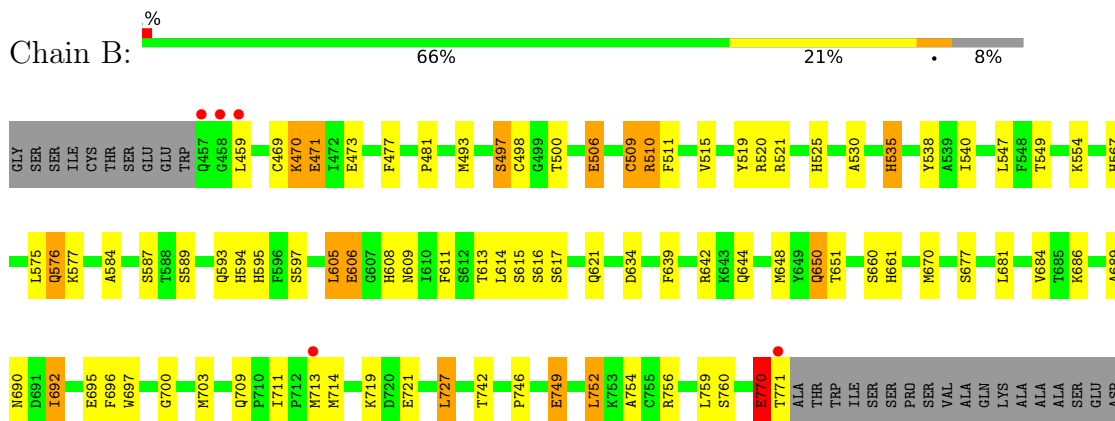
3 Residue-property plots

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.

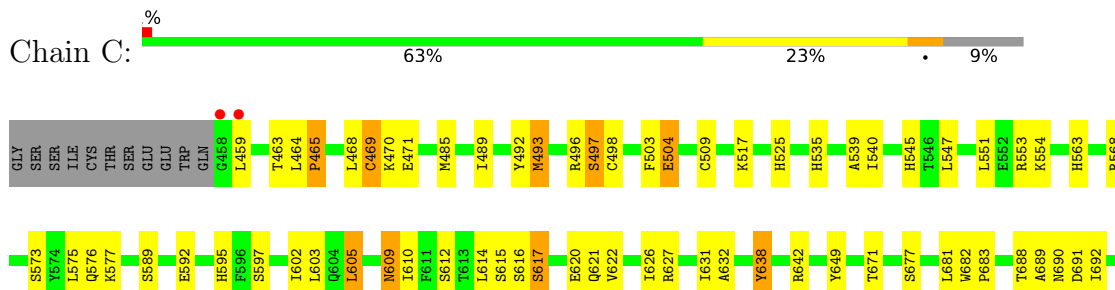
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

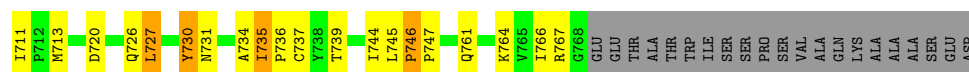
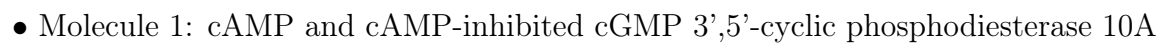


- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



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





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	135.35Å 135.35Å 235.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.77 – 2.30 43.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.3 (43.77-2.30) 89.3 (43.77-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.163 , 0.233 (Not available) , 0.214	Depositor DCC
R_{free} test set	3539 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10943	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MG, CME, JIS

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	1.41	21/2647 (0.8%)	1.58	21/3580 (0.6%)
1	B	1.36	12/2645 (0.5%)	1.67	39/3578 (1.1%)
1	C	1.35	16/2648 (0.6%)	1.63	32/3581 (0.9%)
1	D	1.31	11/2623 (0.4%)	1.63	20/3548 (0.6%)
All	All	1.36	60/10563 (0.6%)	1.63	112/14287 (0.8%)

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	465	PRO	C-O	-9.42	1.11	1.24
1	B	567	HIS	CE1-NE2	8.47	1.41	1.32
1	B	593	GLN	C-O	8.34	1.34	1.24
1	A	739	THR	C-O	8.02	1.33	1.24
1	C	695	GLU	C-O	7.64	1.32	1.24
1	B	584	ALA	C-O	-7.61	1.14	1.24
1	B	481	PRO	C-O	-7.27	1.15	1.24
1	C	632	ALA	C-O	7.27	1.33	1.24
1	A	727	LEU	C-O	7.08	1.32	1.24
1	A	698	ALA	C-O	-6.96	1.16	1.24
1	B	595	HIS	CE1-NE2	6.87	1.39	1.32
1	A	731	ASN	C-O	6.75	1.32	1.24
1	A	596	PHE	C-O	6.56	1.31	1.24
1	A	519	TYR	C-O	-6.46	1.16	1.23
1	D	493	MET	C-O	6.27	1.31	1.24
1	A	535	HIS	C-O	-6.26	1.16	1.24
1	D	735	ILE	CA-CB	6.26	1.57	1.54
1	A	590	THR	C-O	6.26	1.31	1.24
1	B	597	SER	C-O	-6.22	1.17	1.24
1	A	604	GLN	C-O	-6.13	1.16	1.24
1	D	730	TYR	C-O	6.04	1.31	1.24
1	C	485	MET	C-O	-6.00	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	554	LYS	C-O	6.00	1.31	1.24
1	D	605	LEU	C-O	5.98	1.31	1.23
1	A	730	TYR	C-O	5.96	1.31	1.24
1	A	643	LYS	C-O	-5.93	1.17	1.24
1	C	577	LYS	C-O	5.81	1.31	1.24
1	A	540	ILE	C-O	-5.80	1.17	1.24
1	C	568	ARG	C-O	-5.75	1.16	1.24
1	D	601	SER	CA-CB	-5.64	1.44	1.53
1	A	576	GLN	C-O	-5.63	1.17	1.24
1	D	670	MET	C-O	5.59	1.30	1.24
1	C	489	ILE	C-O	5.57	1.30	1.24
1	C	545	HIS	C-O	5.54	1.31	1.24
1	C	698	ALA	C-O	-5.53	1.17	1.24
1	D	589	SER	C-O	5.52	1.30	1.23
1	C	755	CYS	C-O	5.45	1.30	1.24
1	C	563	HIS	CE1-NE2	5.40	1.38	1.32
1	D	629	ALA	C-O	-5.36	1.18	1.24
1	C	539	ALA	C-O	-5.32	1.17	1.24
1	B	594	HIS	CE1-NE2	5.29	1.37	1.32
1	A	691	ASP	C-O	5.28	1.30	1.24
1	D	685	THR	C-O	5.27	1.30	1.24
1	C	493	MET	C-O	-5.25	1.17	1.24
1	D	559	ALA	C-O	-5.25	1.18	1.24
1	C	525	HIS	C-O	5.22	1.29	1.23
1	A	647	GLU	C-O	-5.22	1.18	1.24
1	C	589	SER	C-O	5.21	1.30	1.24
1	B	754	ALA	C-O	5.20	1.30	1.24
1	B	692	ILE	C-O	-5.14	1.18	1.24
1	A	598	GLN	C-O	-5.13	1.18	1.24
1	A	684	VAL	C-O	-5.12	1.18	1.24
1	A	742	THR	C-O	5.12	1.30	1.24
1	A	545	HIS	C-O	5.11	1.30	1.24
1	B	595	HIS	C-O	5.11	1.29	1.24
1	A	499	GLY	C-O	5.09	1.29	1.23
1	B	525	HIS	C-O	5.06	1.29	1.23
1	A	602	ILE	C-O	5.03	1.30	1.24
1	D	726	GLN	C-O	5.02	1.29	1.24
1	B	677	SER	C-O	5.01	1.30	1.24

All (112) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	690	ASN	CB-CA-C	-9.10	96.25	110.81
1	B	690	ASN	CB-CA-C	-8.03	97.46	110.79
1	C	735	ILE	O-C-N	-7.88	115.38	120.42
1	B	609	ASN	CA-CB-CG	-7.34	105.26	112.60
1	B	535	HIS	CA-CB-CG	-7.27	106.53	113.80
1	B	746	PRO	N-CA-C	6.97	119.21	110.70
1	C	718	LYS	CA-C-N	6.70	129.80	120.29
1	C	718	LYS	C-N-CA	6.70	129.80	120.29
1	A	575	LEU	N-CA-C	-6.64	104.04	111.28
1	B	651	THR	CA-CB-OG1	-6.60	99.70	109.60
1	A	735	ILE	CA-C-O	6.56	123.08	118.69
1	D	588	THR	CA-CB-OG1	-6.55	99.78	109.60
1	C	735	ILE	CA-C-O	6.46	123.02	118.69
1	C	470	LYS	N-CA-CB	-6.33	100.38	110.19
1	B	515	VAL	N-CA-C	-6.32	104.59	110.53
1	C	617	SER	O-C-N	6.15	128.67	122.03
1	B	540	ILE	N-CA-C	-6.11	104.55	110.42
1	A	703	MET	N-CA-C	-6.06	104.59	111.07
1	D	554	LYS	CA-C-N	6.05	126.80	120.03
1	D	554	LYS	C-N-CA	6.05	126.80	120.03
1	D	639	PHE	O-C-N	6.01	128.28	122.03
1	B	498	CYS	CB-CA-C	6.00	119.11	109.27
1	B	510	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	D	535	HIS	CA-CB-CG	-5.95	107.85	113.80
1	D	739	THR	N-CA-C	-5.89	104.50	111.03
1	C	649	TYR	CA-C-N	5.87	128.73	120.28
1	C	649	TYR	C-N-CA	5.87	128.73	120.28
1	B	609	ASN	N-CA-CB	5.84	118.99	110.58
1	C	540	ILE	N-CA-C	-5.81	105.06	110.53
1	A	621	GLN	CA-C-O	-5.81	114.72	120.82
1	C	742	THR	CA-CB-OG1	-5.78	100.93	109.60
1	D	700	GLY	N-CA-C	-5.77	105.81	112.50
1	B	721	GLU	CA-C-N	5.75	124.93	120.33
1	B	721	GLU	C-N-CA	5.75	124.93	120.33
1	D	552	GLU	O-C-N	5.75	128.21	122.12
1	C	535	HIS	CA-CB-CG	-5.71	108.09	113.80
1	B	606	GLU	CB-CG-CD	5.70	122.29	112.60
1	B	500	THR	CA-CB-OG1	-5.69	101.07	109.60
1	B	616	SER	CA-C-N	5.69	128.37	120.63
1	B	616	SER	C-N-CA	5.69	128.37	120.63
1	A	573	SER	O-C-N	5.68	127.92	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	609	ASN	N-CA-CB	5.62	118.44	110.46
1	B	650	GLN	CA-C-O	-5.62	112.69	119.49
1	C	713	MET	N-CA-C	-5.62	105.25	111.71
1	D	746	PRO	N-CA-C	5.61	117.54	110.70
1	C	642	ARG	N-CA-C	-5.60	105.26	111.36
1	A	550	ASP	N-CA-C	-5.59	105.27	111.36
1	C	712	PRO	CB-CA-C	-5.59	103.49	112.21
1	D	574	TYR	N-CA-C	-5.59	105.11	111.14
1	A	642	ARG	CA-C-O	-5.58	114.51	120.42
1	D	537	MET	N-CA-C	-5.57	105.21	111.28
1	C	617	SER	CA-C-N	5.53	127.69	120.28
1	C	617	SER	C-N-CA	5.53	127.69	120.28
1	B	615	SER	CA-C-O	-5.52	115.80	121.87
1	B	473	GLU	N-CA-C	-5.52	106.55	113.28
1	C	712	PRO	N-CA-C	5.50	121.07	113.65
1	C	746	PRO	N-CA-C	5.48	117.38	110.70
1	C	498	CYS	N-CA-C	-5.47	104.79	112.12
1	C	763	GLU	N-CA-C	-5.45	105.24	111.07
1	B	584	ALA	CA-C-N	5.45	128.59	120.31
1	B	584	ALA	C-N-CA	5.45	128.59	120.31
1	B	506[A]	GLU	CA-C-N	5.44	127.89	120.54
1	B	506[A]	GLU	C-N-CA	5.44	127.89	120.54
1	B	506[B]	GLU	CA-C-N	5.44	127.89	120.54
1	B	506[B]	GLU	C-N-CA	5.44	127.89	120.54
1	C	468	LEU	O-C-N	5.43	128.34	122.15
1	C	554	LYS	CA-C-N	5.38	126.05	120.03
1	C	554	LYS	C-N-CA	5.38	126.05	120.03
1	B	639	PHE	CA-C-N	5.37	125.90	119.94
1	B	639	PHE	C-N-CA	5.37	125.90	119.94
1	C	691	ASP	CA-C-O	-5.34	115.21	120.82
1	B	752	LEU	N-CA-C	-5.33	105.55	111.36
1	C	504	GLU	CB-CA-C	5.33	118.25	110.26
1	B	770	GLU	CA-C-N	5.32	131.27	121.70
1	B	770	GLU	C-N-CA	5.32	131.27	121.70
1	C	735	ILE	N-CA-CB	5.31	114.59	110.45
1	D	494	VAL	N-CA-C	-5.26	105.25	110.62
1	B	589	SER	CA-C-O	-5.26	115.62	122.14
1	B	642	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	B	670	MET	CA-C-O	-5.24	115.31	120.70
1	D	735	ILE	CA-C-O	5.23	122.20	118.69
1	A	552	GLU	N-CA-C	-5.23	105.66	111.36
1	B	644	GLN	CB-CA-C	-5.21	102.14	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	690	ASN	N-CA-CB	5.20	117.69	109.94
1	A	535	HIS	CA-C-O	-5.19	115.37	120.82
1	D	649	TYR	CA-C-N	5.19	127.18	120.44
1	D	649	TYR	C-N-CA	5.19	127.18	120.44
1	D	552	GLU	CA-C-N	5.18	127.48	120.65
1	D	552	GLU	C-N-CA	5.18	127.48	120.65
1	B	511	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	554	LYS	CA-C-N	5.17	125.83	119.99
1	B	554	LYS	C-N-CA	5.17	125.83	119.99
1	C	757	ASP	CA-CB-CG	-5.16	107.44	112.60
1	A	718	LYS	CA-C-N	5.14	127.13	120.44
1	A	718	LYS	C-N-CA	5.14	127.13	120.44
1	D	504	GLU	CB-CA-C	5.13	118.70	110.29
1	A	636	ALA	N-CA-C	-5.12	105.82	111.71
1	B	617	SER	CA-C-O	-5.10	115.65	120.90
1	A	647	GLU	N-CA-CB	5.10	117.71	110.16
1	C	459	LEU	N-CA-CB	-5.09	102.62	110.20
1	A	544	ASN	CA-C-N	5.08	129.27	121.19
1	A	544	ASN	C-N-CA	5.08	129.27	121.19
1	C	690	ASN	CB-CA-C	-5.07	102.92	110.88
1	A	609	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	646[A]	GLU	N-CA-C	-5.06	104.84	111.02
1	A	646[B]	GLU	N-CA-C	-5.06	104.84	111.02
1	C	724	GLN	CA-C-N	5.06	125.46	119.94
1	C	724	GLN	C-N-CA	5.06	125.46	119.94
1	D	536	CYS	N-CA-C	-5.04	105.70	111.14
1	B	634	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	553	ARG	CA-C-O	-5.02	115.73	121.00
1	A	601	SER	CA-C-O	-5.02	115.53	120.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2578	0	2554	27	0
1	B	2579	0	2549	28	0
1	C	2576	0	2566	38	0
1	D	2560	0	2539	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	1	0
5	A	26	0	0	1	0
5	B	26	0	0	2	0
5	C	26	0	0	2	0
5	D	26	0	0	2	0
6	A	137	0	0	2	0
6	B	154	0	0	2	0
6	C	156	0	0	7	0
6	D	85	0	0	6	0
All	All	10943	0	10216	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (135) 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:C:469[B]:CYS:SG	6:C:1042:HOH:O	2.00	1.15
5:B:803:JIS:N5	5:B:803:JIS:C16	2.35	0.90
1:A:469[A]:CYS:SG	6:A:1006:HOH:O	2.32	0.86
1:A:461:GLN:NE2	1:A:461:GLN:HA	1.89	0.85
1:B:770:GLU:HG3	1:B:771:THR:N	1.90	0.85
1:D:713:MET:SD	5:D:803:JIS:C10	2.65	0.85
5:C:803:JIS:C16	5:C:803:JIS:N5	2.41	0.84
1:C:724:GLN:HB2	6:C:1005:HOH:O	1.85	0.76
1:B:576:GLN:HB2	6:B:1010:HOH:O	1.89	0.73
1:A:627:ARG:O	1:A:631:ILE:HG12	1.88	0.73
1:A:461:GLN:NE2	1:A:500:THR:HG21	2.05	0.72
1:A:461:GLN:NE2	1:A:461:GLN:CA	2.55	0.70
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:MET:O	1:C:497:SER:HB2	1.92	0.69
5:A:804:JIS:N5	5:A:804:JIS:C16	2.55	0.69
1:A:461:GLN:HE22	1:A:500:THR:HG21	1.56	0.68
1:B:509:CME:HB2	6:B:1013:HOH:O	1.94	0.67
1:D:509:CME:HB2	6:D:981:HOH:O	1.93	0.66
1:A:493:MET:O	1:A:497:SER:HB2	1.96	0.66
1:D:648:MET:HE1	6:D:973:HOH:O	1.96	0.66
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.78	0.66
1:D:627:ARG:O	1:D:631:ILE:HG12	1.96	0.65
1:B:697:TRP:CZ2	1:B:719:LYS:HG2	2.33	0.63
1:A:753:LYS:HG3	6:A:1002:HOH:O	2.01	0.60
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.15	0.60
1:B:727:LEU:CD2	1:B:759:LEU:HD11	2.32	0.59
1:B:742:THR:HG21	1:B:749:GLU:HG2	1.85	0.58
1:D:644:GLN:NE2	1:D:648:MET:HE3	2.19	0.58
1:B:713:MET:SD	5:B:803:JIS:C10	2.93	0.57
1:B:711:ILE:HD11	1:B:713:MET:HE2	1.86	0.57
1:A:658:ASN:OD1	1:A:660:SER:HB3	2.06	0.56
1:D:677:SER:OG	1:D:688:THR:HG21	2.07	0.55
1:C:753:LYS:HE2	6:C:1021:HOH:O	2.06	0.55
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.43	0.54
1:B:506[B]:GLU:CD	1:B:510:ARG:HH12	2.15	0.53
1:D:493:MET:O	1:D:497:SER:CB	2.57	0.53
5:D:803:JIS:C16	5:D:803:JIS:N5	2.71	0.53
1:C:689:ALA:HA	1:C:692:ILE:HG22	1.90	0.53
1:D:493:MET:O	1:D:497:SER:HB2	2.07	0.53
1:D:727:LEU:CD1	1:D:766:ILE:HD12	2.39	0.53
4:A:803:GOL:H2	1:B:520:ARG:NH1	2.23	0.53
1:B:700:GLY:HA3	1:B:714:MET:O	2.09	0.53
1:D:761:GLN:HE22	1:D:764:LYS:NZ	2.06	0.52
1:B:648:MET:HE2	1:B:661:HIS:NE2	2.25	0.52
1:C:553:ARG:NH1	6:C:908:HOH:O	2.41	0.52
1:D:700:GLY:O	1:D:703:MET:HB2	2.09	0.52
1:C:492:TYR:CE2	1:C:496:ARG:HD2	2.45	0.52
1:A:749:GLU:N	1:A:750:PRO:CD	2.73	0.51
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.91	0.51
1:B:611:PHE:HB3	1:B:614:LEU:HD22	1.94	0.50
1:D:744:ILE:HG22	1:D:744:ILE:O	2.11	0.50
1:B:684:VAL:HG22	1:C:705:LYS:HG2	1.94	0.50
1:D:628:LYS:NZ	6:D:906:HOH:O	2.45	0.50
1:A:697:TRP:CZ2	1:A:719:LYS:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ARG:O	1:D:471:GLU:HB2	2.12	0.49
1:D:766:ILE:O	1:D:766:ILE:HG22	2.11	0.49
1:B:493:MET:O	1:B:497:SER:HB2	2.13	0.49
1:D:727:LEU:HD23	1:D:731:ASN:ND2	2.28	0.48
1:C:711:ILE:HD11	1:C:713:MET:HE2	1.95	0.48
1:C:620:GLU:HG3	6:C:990:HOH:O	2.14	0.48
1:A:486:TRP:N	1:A:487:PRO:CD	2.77	0.48
1:C:767:ARG:HH21	1:C:769:GLU:CD	2.22	0.47
1:D:535:HIS:O	1:D:538:TYR:HB3	2.14	0.47
1:C:681:LEU:HD23	6:C:1041:HOH:O	2.13	0.47
1:D:542:GLN:NE2	1:D:542:GLN:HA	2.29	0.47
1:D:727:LEU:CD1	1:D:766:ILE:CD1	2.93	0.47
1:D:766:ILE:O	1:D:766:ILE:CG2	2.63	0.47
1:C:764[B]:LYS:HG3	1:C:769:GLU:HB2	1.97	0.47
1:D:489:ILE:O	1:D:493:MET:HG3	2.14	0.47
1:A:735:ILE:N	1:A:736:PRO:HD2	2.30	0.47
1:D:624:GLU:OE2	1:D:627:ARG:NH1	2.34	0.46
1:B:506[B]:GLU:HG2	1:B:510:ARG:NH1	2.31	0.46
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.51	0.46
1:C:700:GLY:HA3	1:C:714:MET:O	2.15	0.46
1:D:510:ARG:HD2	1:D:607:GLY:O	2.15	0.46
1:C:503:PHE:CE2	1:C:610:ILE:HD12	2.51	0.45
1:B:742:THR:CG2	1:B:749:GLU:HG2	2.45	0.45
1:C:622:VAL:O	1:C:626:ILE:HG13	2.17	0.45
1:C:713:MET:SD	5:C:803:JIS:C10	3.05	0.45
1:D:745:LEU:C	1:D:747:PRO:CD	2.89	0.45
1:A:766:ILE:C	1:A:768:GLY:H	2.24	0.44
1:B:727:LEU:HD22	1:B:759:LEU:HD11	1.98	0.44
1:C:609:ASN:O	1:C:612:SER:HB3	2.17	0.44
1:B:471:GLU:HB3	1:B:477:PHE:CD1	2.52	0.44
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.00	0.44
1:D:598:GLN:O	1:D:602:ILE:HG13	2.17	0.44
1:A:549:THR:OG1	1:A:552:GLU:HG3	2.18	0.44
1:C:746:PRO:N	1:C:747:PRO:CD	2.81	0.43
1:B:695:GLU:O	1:B:696:PHE:C	2.59	0.43
1:C:553:ARG:HD3	6:C:970:HOH:O	2.18	0.43
1:B:493:MET:SD	1:B:535:HIS:HA	2.59	0.43
1:A:497:SER:O	1:A:553:ARG:HD2	2.19	0.43
1:D:564:ASP:O	1:D:567:HIS:HB2	2.18	0.43
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.87	0.43
1:C:682:TRP:N	1:C:683:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:LEU:HD13	1:D:766:ILE:HD12	2.01	0.43
1:D:735:ILE:HB	1:D:736:PRO:HD3	1.99	0.43
1:C:713:MET:HG2	1:C:714:MET:HG2	2.01	0.43
1:D:576:GLN:HB2	6:D:957:HOH:O	2.18	0.43
1:C:677:SER:OG	1:C:688:THR:HG21	2.19	0.42
1:C:689:ALA:O	1:C:692:ILE:HG22	2.20	0.42
1:C:711:ILE:HA	1:C:712:PRO:HD3	1.92	0.42
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.82	0.42
1:C:464:LEU:O	1:C:465:PRO:C	2.62	0.42
1:D:458:GLY:C	1:D:460:MET:H	2.27	0.42
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.85	0.42
1:B:689:ALA:O	1:B:692:ILE:HG22	2.19	0.42
1:C:592:GLU:HA	1:C:595:HIS:CD2	2.54	0.42
1:D:645:LEU:HD21	1:D:664:ARG:HB3	2.01	0.42
1:C:603:LEU:HD23	1:C:603:LEU:HA	1.88	0.42
1:A:467:ARG:O	1:A:467:ARG:HG2	2.20	0.42
1:A:508:LEU:HD12	1:A:508:LEU:HA	1.87	0.42
1:C:503:PHE:CD2	1:C:610:ILE:HB	2.55	0.42
1:C:592:GLU:HA	1:C:595:HIS:HD2	1.85	0.42
1:D:734:ALA:O	1:D:737:CYS:HB3	2.20	0.42
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.54	0.42
1:C:602:ILE:HA	1:C:605:LEU:HD22	2.01	0.41
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.55	0.41
1:B:535:HIS:O	1:B:538:TYR:HB3	2.19	0.41
1:C:749[B]:GLU:HB3	1:C:750:PRO:HD3	2.02	0.41
1:D:761:GLN:HE22	1:D:764:LYS:HZ2	1.68	0.41
1:B:605:LEU:HB3	1:B:608:HIS:ND1	2.35	0.41
1:D:462:PHE:CE1	1:D:491:VAL:HG11	2.55	0.41
1:B:577:LYS:HD3	1:B:703:MET:HE1	2.03	0.41
1:C:627:ARG:O	1:C:631:ILE:HG12	2.21	0.41
1:C:706:LEU:HD23	1:C:706:LEU:HA	1.88	0.41
1:D:542:GLN:NE2	6:D:911:HOH:O	2.53	0.41
1:A:660:SER:O	1:A:664:ARG:HG3	2.20	0.41
1:D:546:THR:HG23	6:D:948:HOH:O	2.21	0.41
1:B:752:LEU:HD21	1:B:756[B]:ARG:NH2	2.36	0.40
1:B:519:TYR:CZ	1:B:530:ALA:HB2	2.56	0.40
1:A:509:CME:O	1:A:513:MET:HG2	2.21	0.40
1:D:727:LEU:HD13	1:D:766:ILE:CD1	2.51	0.40
1:C:602:ILE:O	1:C:605:LEU:HB2	2.22	0.40
1:C:727:LEU:HD21	1:C:763:GLU:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/343 (92%)	305 (96%)	10 (3%)	2 (1%)	21	27
1	B	317/343 (92%)	305 (96%)	12 (4%)	0	100	100
1	C	317/343 (92%)	302 (95%)	15 (5%)	0	100	100
1	D	314/343 (92%)	295 (94%)	18 (6%)	1 (0%)	36	46
All	All	1265/1372 (92%)	1207 (95%)	55 (4%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	615	SER
1	A	720	ASP
1	A	767	ARG

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/305 (94%)	269 (94%)	18 (6%)	16	23
1	B	286/305 (94%)	261 (91%)	25 (9%)	9	12
1	C	288/305 (94%)	260 (90%)	28 (10%)	8	10
1	D	284/305 (93%)	261 (92%)	23 (8%)	11	14
All	All	1145/1220 (94%)	1051 (92%)	94 (8%)	11	14

All (94) 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	497	SER
1	A	501	SER
1	A	573	SER
1	A	575	LEU
1	A	587	SER
1	A	605	LEU
1	A	617	SER
1	A	622	VAL
1	A	623	LEU
1	A	644	GLN
1	A	681	LEU
1	A	692	ILE
1	A	709	GLN
1	A	719	LYS
1	A	727	LEU
1	B	459	LEU
1	B	469[A]	CYS
1	B	469[B]	CYS
1	B	470	LYS
1	B	471	GLU
1	B	497	SER
1	B	521	ARG
1	B	547	LEU
1	B	549	THR
1	B	575	LEU
1	B	576	GLN
1	B	587	SER
1	B	605	LEU
1	B	606	GLU
1	B	613	THR
1	B	621	GLN
1	B	650	GLN
1	B	660	SER
1	B	681	LEU
1	B	686	LYS
1	B	709	GLN
1	B	727	LEU
1	B	749	GLU
1	B	760	SER
1	B	770	GLU

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Mol	Chain	Res	Type
1	C	463	THR
1	C	469[A]	CYS
1	C	469[B]	CYS
1	C	471	GLU
1	C	497	SER
1	C	504	GLU
1	C	517	LYS
1	C	547	LEU
1	C	573[A]	SER
1	C	573[B]	SER
1	C	575	LEU
1	C	576[A]	GLN
1	C	576[B]	GLN
1	C	597	SER
1	C	605	LEU
1	C	614	LEU
1	C	615	SER
1	C	616	SER
1	C	617	SER
1	C	621	GLN
1	C	638	TYR
1	C	709	GLN
1	C	711	ILE
1	C	713	MET
1	C	749[A]	GLU
1	C	749[B]	GLU
1	C	760	SER
1	C	765	VAL
1	D	457	GLN
1	D	459	LEU
1	D	471	GLU
1	D	494	VAL
1	D	500	THR
1	D	504	GLU
1	D	517	LYS
1	D	573	SER
1	D	575	LEU
1	D	576	GLN
1	D	588	THR
1	D	605	LEU
1	D	613	THR
1	D	616	SER

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Mol	Chain	Res	Type
1	D	617	SER
1	D	651	THR
1	D	656	LEU
1	D	692	ILE
1	D	709	GLN
1	D	711	ILE
1	D	720	ASP
1	D	727	LEU
1	D	767	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	542	GLN
1	A	644	GLN
1	A	659	GLN
1	A	726	GLN
1	A	743	GLN
1	B	484	ASN
1	B	495	HIS
1	B	644	GLN
1	B	761	GLN
1	C	484	ASN
1	C	542	GLN
1	C	604	GLN
1	C	709	GLN
1	C	743	GLN
1	D	484	ASN
1	D	542	GLN
1	D	576	GLN
1	D	604	GLN
1	D	609	ASN
1	D	621	GLN
1	D	644	GLN
1	D	709	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	A	509	1	8,9,10	0.67	0	6,9,11	0.76	0
1	CME	D	509	1	8,9,10	0.64	0	6,9,11	1.00	0
1	CME	B	509	1	8,9,10	0.68	0	6,9,11	0.96	1 (16%)
1	CME	C	509	1	8,9,10	0.66	0	6,9,11	1.24	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	509	1	-	0/5/8/10	-
1	CME	D	509	1	-	2/5/8/10	-
1	CME	B	509	1	-	1/5/8/10	-
1	CME	C	509	1	-	2/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	509	CME	CB-CA-C	2.42	117.36	110.80
1	B	509	CME	CE-SD-SG	2.08	112.58	103.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	509	CME	1	0
1	D	509	CME	1	0
1	B	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	GOL	A	803	-	5,5,5	0.25	0	5,5,5	0.89	0
5	JIS	A	804	-	30,30,30	2.74	13 (43%)	41,42,42	3.39	20 (48%)
5	JIS	B	803	-	30,30,30	2.33	11 (36%)	41,42,42	3.65	25 (60%)
5	JIS	C	803	-	30,30,30	2.28	14 (46%)	41,42,42	3.22	26 (63%)
5	JIS	D	803	-	30,30,30	2.11	8 (26%)	41,42,42	2.93	19 (46%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	803	-	-	4/4/4/4	-
5	JIS	A	804	-	-	3/8/16/16	0/5/5/5
5	JIS	B	803	-	-	3/8/16/16	0/5/5/5
5	JIS	C	803	-	-	2/8/16/16	0/5/5/5
5	JIS	D	803	-	-	2/8/16/16	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804	JIS	N2-N4	7.03	1.43	1.36
5	A	804	JIS	C10-N2	6.67	1.54	1.46
5	D	803	JIS	N2-N4	6.55	1.43	1.36
5	B	803	JIS	C18-C17	5.53	1.48	1.38
5	C	803	JIS	N2-N4	5.31	1.41	1.36
5	B	803	JIS	N2-N4	5.30	1.41	1.36
5	A	804	JIS	C3-N2	5.19	1.40	1.35
5	B	803	JIS	C17-C11	4.72	1.46	1.37
5	B	803	JIS	C3-N7	4.63	1.43	1.34
5	C	803	JIS	C18-C17	4.56	1.46	1.38
5	D	803	JIS	C3-N2	4.31	1.39	1.35
5	A	804	JIS	C18-C17	4.11	1.45	1.38
5	A	804	JIS	C1-C3	3.81	1.45	1.39
5	C	803	JIS	C16-N8	3.55	1.52	1.46
5	B	803	JIS	C1-C3	3.47	1.45	1.39
5	D	803	JIS	C1-C3	3.37	1.45	1.39
5	D	803	JIS	C17-C11	3.14	1.43	1.37
5	C	803	JIS	C13-C14	2.99	1.48	1.43
5	A	804	JIS	C6-N9	2.92	1.39	1.34
5	C	803	JIS	C19-C13	2.84	1.47	1.42
5	B	803	JIS	C20-C14	2.80	1.48	1.42
5	A	804	JIS	C3-N7	2.79	1.39	1.34
5	C	803	JIS	C1-C3	2.79	1.44	1.39
5	A	804	JIS	C13-C14	2.78	1.48	1.43
5	C	803	JIS	C18-C20	2.72	1.42	1.36
5	A	804	JIS	C25-C21	2.69	1.42	1.36
5	C	803	JIS	C20-C14	2.68	1.47	1.42
5	C	803	JIS	C10-N2	2.66	1.49	1.46
5	B	803	JIS	C3-N2	2.55	1.38	1.35
5	A	804	JIS	C24-C19	2.54	1.42	1.36
5	C	803	JIS	C3-N2	2.50	1.37	1.35
5	B	803	JIS	C6-N9	2.44	1.39	1.34
5	C	803	JIS	C25-C24	2.42	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	803	JIS	C18-C17	2.36	1.42	1.38
5	C	803	JIS	C17-C11	2.34	1.41	1.37
5	A	804	JIS	C25-C24	2.30	1.43	1.38
5	C	803	JIS	C25-C21	2.30	1.41	1.36
5	B	803	JIS	C10-C11	2.29	1.57	1.52
5	D	803	JIS	C25-C21	2.23	1.41	1.36
5	B	803	JIS	C12-N9	2.20	1.37	1.33
5	D	803	JIS	C13-C14	2.17	1.47	1.43
5	A	804	JIS	C16-N8	2.16	1.50	1.46
5	D	803	JIS	C3-N7	2.07	1.38	1.34
5	B	803	JIS	C10-N2	2.04	1.49	1.46
5	A	804	JIS	C12-N7	2.03	1.37	1.33
5	C	803	JIS	C6-N8	2.02	1.42	1.37

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	JIS	C22-C15-N8	-10.58	91.07	111.06
5	A	804	JIS	C11-C10-N2	9.18	122.35	113.14
5	C	803	JIS	N7-C3-N2	7.13	136.47	125.34
5	B	803	JIS	C10-C11-C13	-7.02	107.77	119.95
5	D	803	JIS	C11-C10-N2	6.84	120.01	113.14
5	B	803	JIS	N7-C3-N2	6.57	135.60	125.34
5	A	804	JIS	N7-C3-N2	6.41	135.34	125.34
5	D	803	JIS	C10-N2-C3	-6.33	123.80	127.81
5	B	803	JIS	C11-C10-N2	6.26	119.42	113.14
5	B	803	JIS	C19-C13-C14	6.16	125.88	117.92
5	B	803	JIS	C21-C14-C13	-6.05	111.32	119.12
5	D	803	JIS	N7-C3-N2	5.98	134.67	125.34
5	A	804	JIS	C3-N2-N4	-5.91	105.61	109.93
5	D	803	JIS	C22-C15-N8	-5.70	100.29	111.06
5	D	803	JIS	C23-C16-N8	-5.65	100.38	111.06
5	B	803	JIS	C22-C15-N8	-5.63	100.41	111.06
5	B	803	JIS	N9-C12-N7	-5.61	120.09	128.58
5	B	803	JIS	C10-N2-C3	-5.48	124.34	127.81
5	C	803	JIS	C10-N2-C3	-5.47	124.34	127.81
5	C	803	JIS	C11-C10-N2	5.28	118.44	113.14
5	C	803	JIS	C26-C22-C15	5.05	120.54	111.19
5	B	803	JIS	C10-C11-C17	4.98	133.97	119.81
5	A	804	JIS	C1-C3-N7	-4.60	120.38	126.72
5	B	803	JIS	N9-C6-N8	4.57	126.74	117.01
5	C	803	JIS	N2-N4-N5	4.51	113.20	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	JIS	C10-N2-N4	4.44	128.37	120.27
5	D	803	JIS	C10-N2-N4	4.43	128.34	120.27
5	C	803	JIS	C21-C14-C13	-4.41	113.44	119.12
5	B	803	JIS	C12-N9-C6	4.33	122.41	111.83
5	A	804	JIS	N9-C6-N8	4.28	126.11	117.01
5	C	803	JIS	C10-C11-C13	-4.24	112.58	119.95
5	C	803	JIS	N9-C6-N8	4.23	126.01	117.01
5	B	803	JIS	N2-N4-N5	4.14	112.84	108.82
5	C	803	JIS	C1-C3-N7	-4.13	121.03	126.72
5	A	804	JIS	N2-N4-N5	4.08	112.79	108.82
5	C	803	JIS	C24-C25-C21	4.07	125.85	120.40
5	B	803	JIS	C10-N2-N4	4.05	127.65	120.27
5	C	803	JIS	C19-C13-C14	4.04	123.15	117.92
5	C	803	JIS	C10-N2-N4	3.90	127.37	120.27
5	D	803	JIS	N9-C12-N7	-3.84	122.76	128.58
5	A	804	JIS	C10-C11-C13	-3.80	113.35	119.95
5	B	803	JIS	C3-C1-N5	3.78	112.22	109.31
5	D	803	JIS	C1-C3-N7	-3.75	121.56	126.72
5	A	804	JIS	C19-C13-C14	3.71	122.72	117.92
5	D	803	JIS	C12-N9-C6	3.71	120.88	111.83
5	C	803	JIS	N9-C12-N7	-3.70	122.99	128.58
5	D	803	JIS	C19-C13-C14	3.62	122.60	117.92
5	B	803	JIS	C19-C13-C11	-3.60	116.53	122.55
5	B	803	JIS	C1-C3-N7	-3.57	121.80	126.72
5	C	803	JIS	C12-N9-C6	3.53	120.46	111.83
5	B	803	JIS	C23-C16-N8	-3.52	104.40	111.06
5	C	803	JIS	C16-N8-C15	3.47	119.38	111.57
5	B	803	JIS	C20-C18-C17	-3.47	115.67	121.00
5	C	803	JIS	C22-C15-N8	-3.46	104.53	111.06
5	C	803	JIS	C25-C24-C19	-3.37	115.89	120.40
5	B	803	JIS	C26-C22-C15	-3.37	104.95	111.19
5	C	803	JIS	C3-C1-N5	3.33	111.88	109.31
5	B	803	JIS	C1-N5-N4	-3.29	104.34	108.07
5	D	803	JIS	C23-C26-C22	3.25	120.84	111.19
5	C	803	JIS	C1-N5-N4	-3.24	104.39	108.07
5	D	803	JIS	C10-C11-C13	-3.20	114.40	119.95
5	B	803	JIS	C20-C14-C13	3.17	123.21	119.12
5	D	803	JIS	C3-N2-N4	-3.09	107.67	109.93
5	B	803	JIS	C12-N7-C3	3.04	119.26	111.83
5	A	804	JIS	C26-C22-C15	2.98	116.70	111.19
5	A	804	JIS	C12-N9-C6	2.97	119.08	111.83
5	D	803	JIS	C21-C14-C13	-2.94	115.33	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	JIS	C21-C14-C13	-2.94	115.34	119.12
5	C	803	JIS	C18-C20-C14	-2.86	116.51	120.48
5	C	803	JIS	C12-N7-C3	2.83	118.75	111.83
5	A	804	JIS	C10-N2-C3	-2.83	126.02	127.81
5	D	803	JIS	N9-C6-N8	2.82	123.00	117.01
5	A	804	JIS	C16-N8-C15	-2.78	105.32	111.57
5	D	803	JIS	C12-N7-C3	2.74	118.52	111.83
5	B	803	JIS	C3-N2-N4	-2.72	107.95	109.93
5	D	803	JIS	C26-C23-C16	-2.71	106.18	111.19
5	A	804	JIS	C12-N7-C3	2.61	118.20	111.83
5	B	803	JIS	C24-C25-C21	2.49	123.73	120.40
5	C	803	JIS	C1-C3-N2	-2.45	102.30	104.25
5	C	803	JIS	C3-N2-N4	-2.38	108.19	109.93
5	C	803	JIS	C23-C26-C22	2.37	118.22	111.19
5	D	803	JIS	C24-C25-C21	2.36	123.56	120.40
5	A	804	JIS	N9-C12-N7	-2.34	125.04	128.58
5	D	803	JIS	C10-C11-C17	2.21	126.11	119.81
5	C	803	JIS	C19-C13-C11	-2.19	118.89	122.55
5	A	804	JIS	C19-C13-C11	-2.18	118.91	122.55
5	A	804	JIS	C17-C11-C13	2.14	122.25	119.06
5	A	804	JIS	C18-C17-C11	-2.10	117.78	121.50
5	B	803	JIS	C1-C3-N2	-2.09	102.58	104.25
5	C	803	JIS	C10-C11-C17	2.03	125.59	119.81

There are no chirality outliers.

All (14) torsion outliers are listed below:

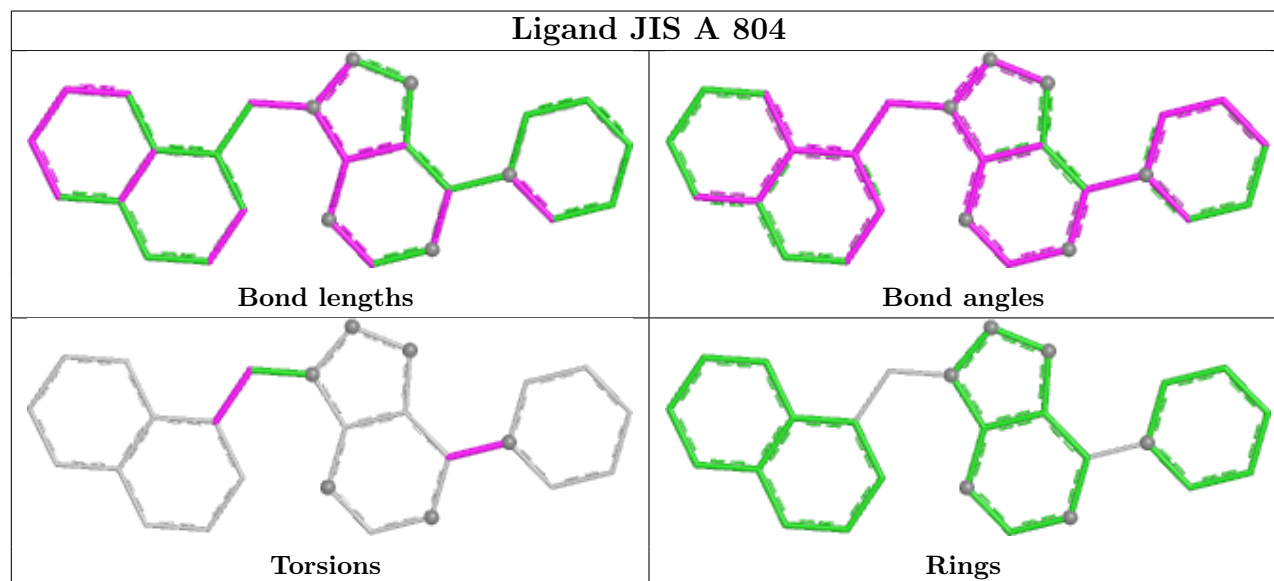
Mol	Chain	Res	Type	Atoms
4	A	803	GOL	O1-C1-C2-C3
4	A	803	GOL	C1-C2-C3-O3
4	A	803	GOL	O1-C1-C2-O2
5	B	803	JIS	N2-C10-C11-C13
5	D	803	JIS	N2-C10-C11-C13
5	A	804	JIS	N9-C6-N8-C15
5	B	803	JIS	N9-C6-N8-C15
4	A	803	GOL	O2-C2-C3-O3
5	C	803	JIS	N2-C10-C11-C13
5	C	803	JIS	N2-C10-C11-C17
5	B	803	JIS	N2-C10-C11-C17
5	D	803	JIS	N2-C10-C11-C17
5	A	804	JIS	N2-C10-C11-C17
5	A	804	JIS	N2-C10-C11-C13

There are no ring outliers.

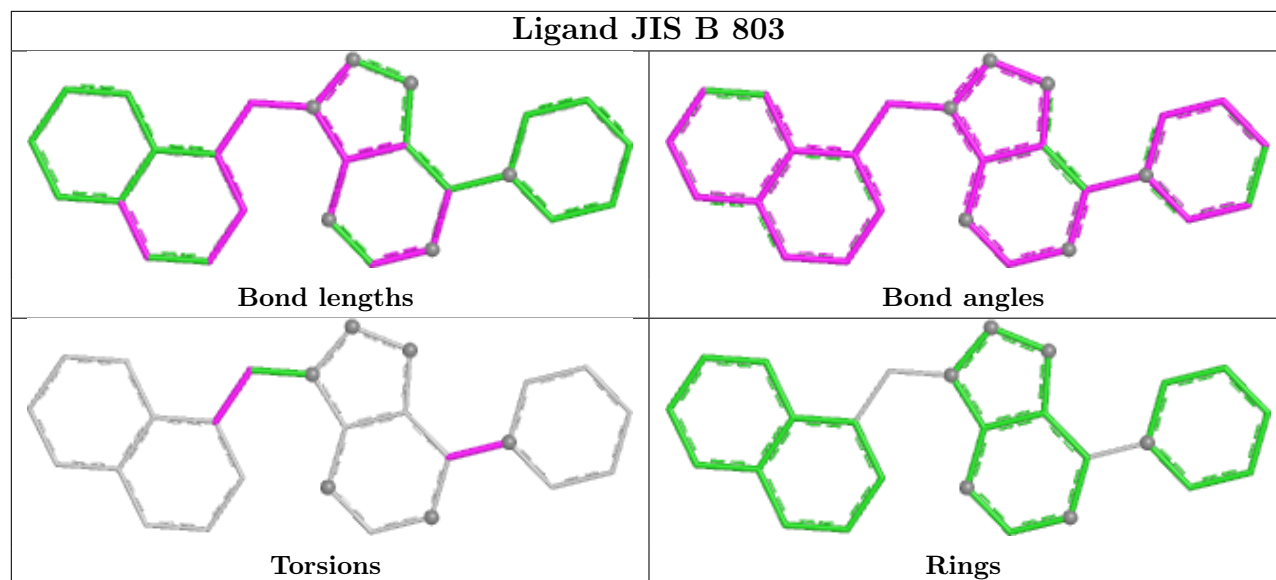
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	GOL	1	0
5	A	804	JIS	1	0
5	B	803	JIS	2	0
5	C	803	JIS	2	0
5	D	803	JIS	2	0

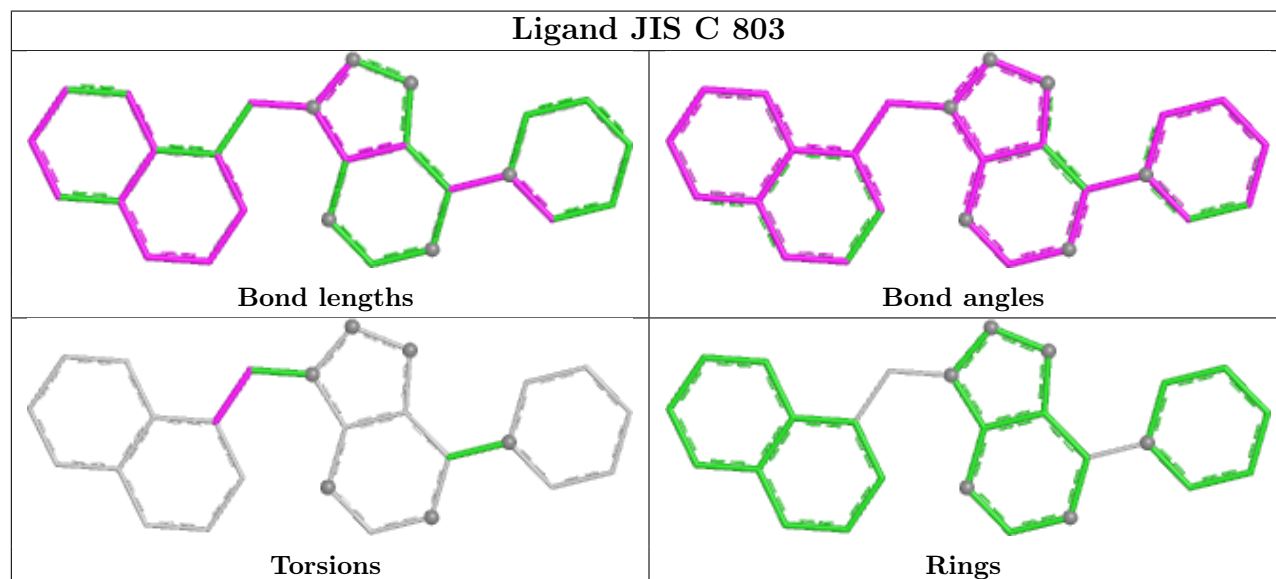
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



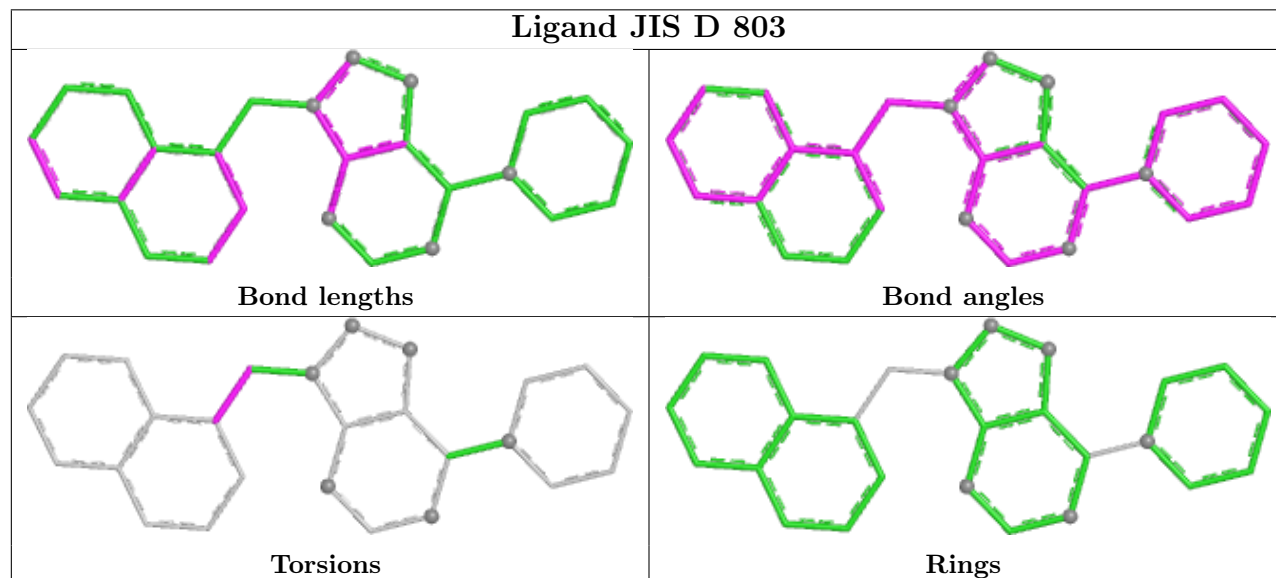
Ligand JIS B 803



Ligand JIS C 803



Ligand JIS D 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	313/343 (91%)	-0.39	2 (0%) 85 86	20, 38, 71, 107	6 (1%)
1	B	314/343 (91%)	-0.33	5 (1%) 70 72	21, 38, 65, 94	5 (1%)
1	C	312/343 (90%)	-0.37	4 (1%) 75 76	20, 38, 67, 90	7 (2%)
1	D	312/343 (90%)	-0.01	5 (1%) 70 72	30, 52, 80, 109	4 (1%)
All	All	1251/1372 (91%)	-0.28	16 (1%) 75 76	20, 42, 75, 109	22 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	771	THR	4.2
1	C	459	LEU	3.3
1	D	456	TRP	3.1
1	B	458	GLY	3.0
1	B	457	GLN	3.0
1	A	457	GLN	2.9
1	C	713	MET	2.7
1	D	649	TYR	2.5
1	C	458	GLY	2.5
1	D	458	GLY	2.5
1	D	457	GLN	2.4
1	A	459	LEU	2.3
1	B	459	LEU	2.2
1	D	459	LEU	2.2
1	C	711	ILE	2.1
1	B	713	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	0.89	0.13	43,56,100,103	0
1	CME	B	509	10/11	0.90	0.13	34,54,85,98	0
1	CME	A	509	10/11	0.90	0.12	39,55,83,104	0
1	CME	C	509	10/11	0.91	0.11	38,47,75,84	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

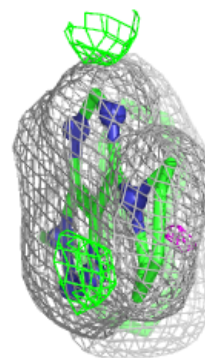
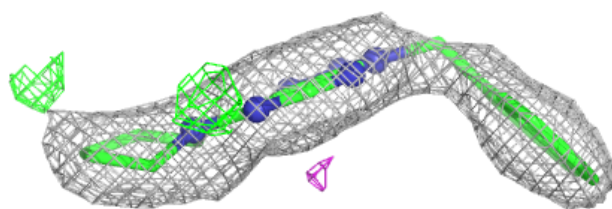
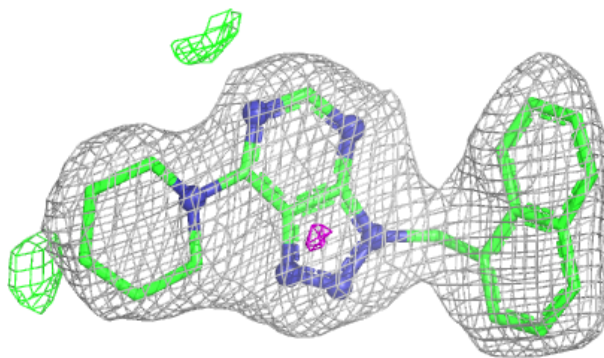
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	803	6/6	0.91	0.12	47,54,56,60	0
5	JIS	C	803	26/26	0.93	0.09	35,46,57,61	0
5	JIS	A	804	26/26	0.94	0.08	34,45,55,72	0
5	JIS	D	803	26/26	0.94	0.09	38,53,70,81	0
5	JIS	B	803	26/26	0.95	0.09	39,50,63,64	0
3	MG	D	802	1/1	0.99	0.03	37,37,37,37	0
3	MG	C	802	1/1	1.00	0.01	26,26,26,26	0
2	ZN	A	801	1/1	1.00	0.01	35,35,35,35	0
2	ZN	B	801	1/1	1.00	0.02	32,32,32,32	0
2	ZN	C	801	1/1	1.00	0.01	33,33,33,33	0
2	ZN	D	801	1/1	1.00	0.01	43,43,43,43	0
3	MG	A	802	1/1	1.00	0.03	27,27,27,27	0
3	MG	B	802	1/1	1.00	0.01	19,19,19,19	0

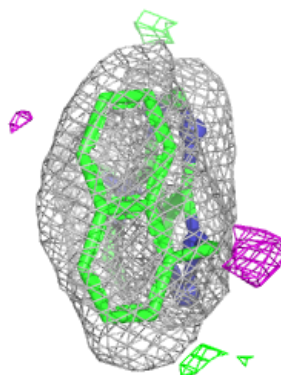
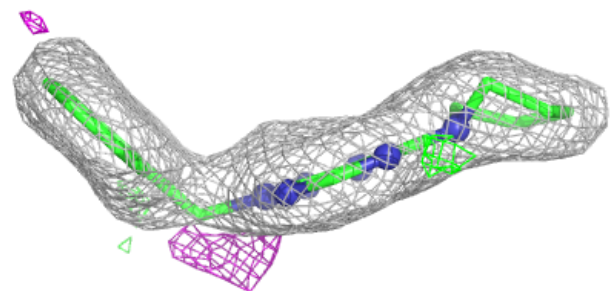
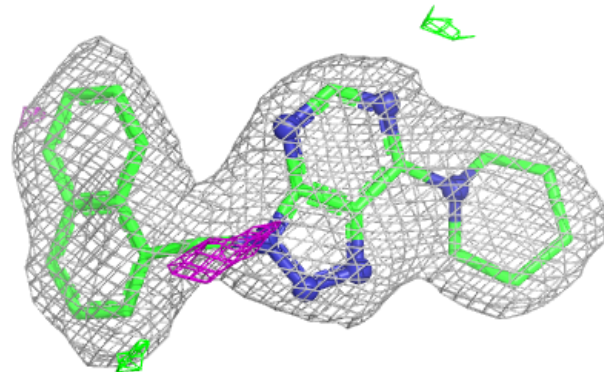
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JIS 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)

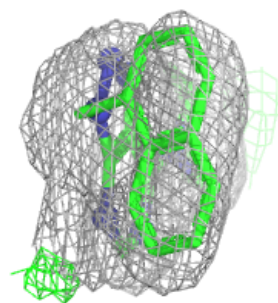
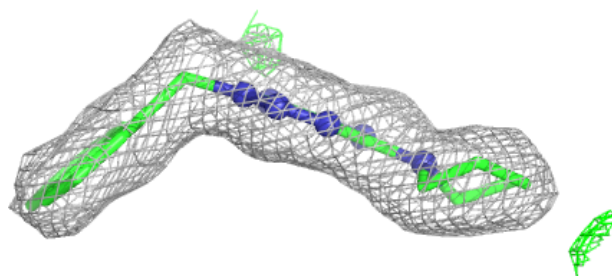
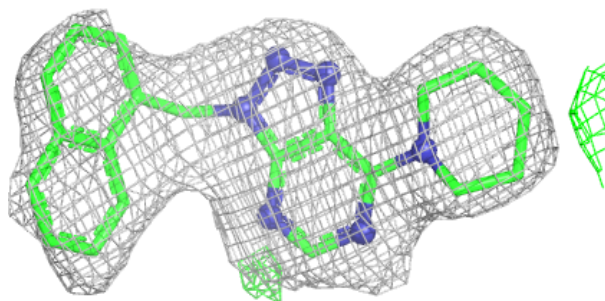
**Electron density around JIS A 804:**

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

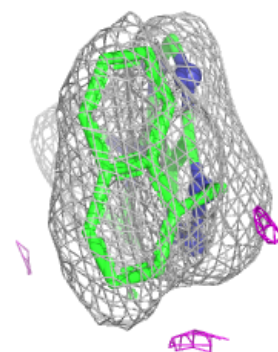
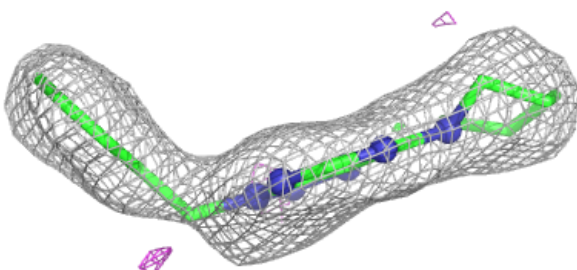
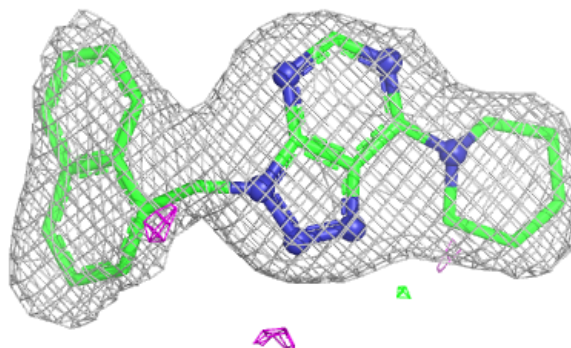


Electron density around JIS D 803:

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

**Electron density around JIS 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.