



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 07:09 AM EDT

PDB ID : 5SHK
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 10 IN COMPLEX WITH c1(ncc(c2cccnc12)c3cccnc3)Nc4cccc(n4)C, micromolar IC₅₀=0.911105
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Deposited on : 2022-02-01
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

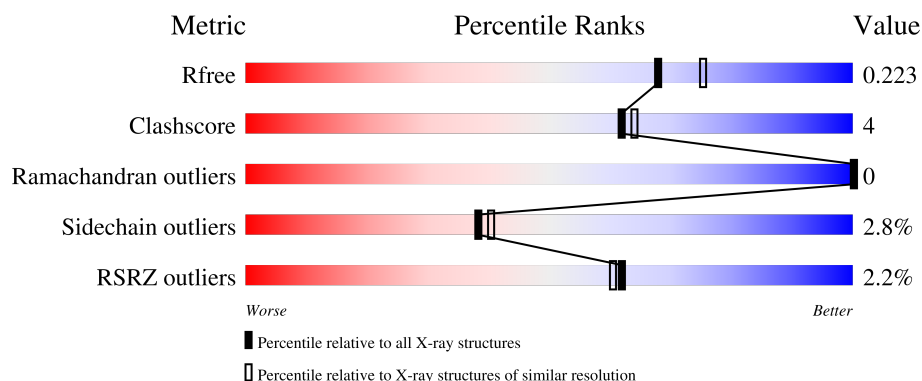
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	<div> <div>0%</div> <div> <div>82%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	343	<div> <div>2%</div> <div> <div>81%</div> <div>9%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	343	<div> <div>0%</div> <div> <div>84%</div> <div>6%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	343	<div> <div>3%</div> <div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>

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
4	JH6	D	803	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2541	1624	432	461	24			
1	B	315	Total	C	N	O	S	0	0	0
			2551	1630	434	463	24			
1	C	313	Total	C	N	O	S	0	0	0
			2541	1624	432	461	24			
1	D	313	Total	C	N	O	S	0	0	0
			2537	1622	433	458	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

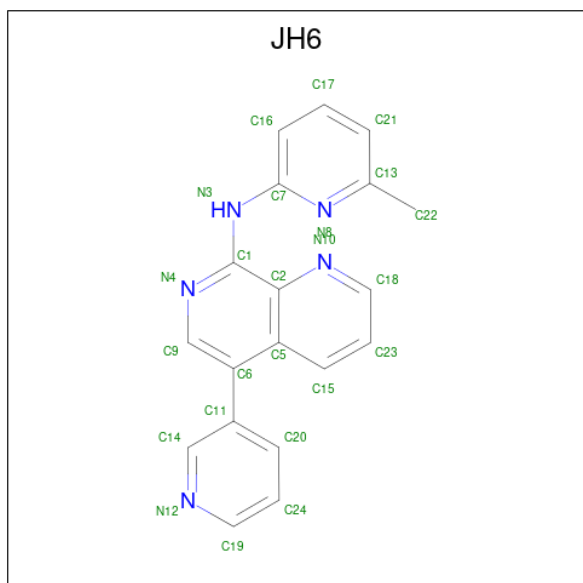
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: 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 N-(6-methylpyridin-2-yl)-5-(pyridin-3-yl)-1,7-naphthyridin-8-amine (three-letter code: JH6) (formula: C₁₉H₁₅N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			24	19	5		
4	B	1	Total	C	N	0	0
			24	19	5		
4	C	1	Total	C	N	0	0
			24	19	5		
4	D	1	Total	C	N	0	0
			24	19	5		

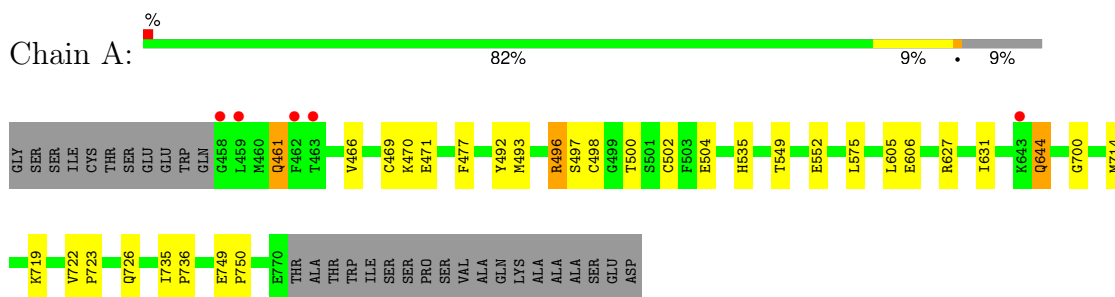
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	129	Total 129	O 129	0	0
5	B	136	Total 136	O 136	0	0
5	C	125	Total 125	O 125	0	0
5	D	76	Total 76	O 76	0	0

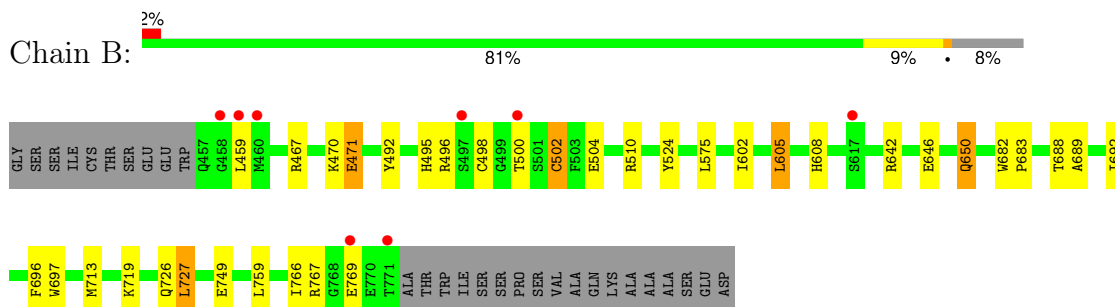
3 Residue-property plots [i](#)

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.

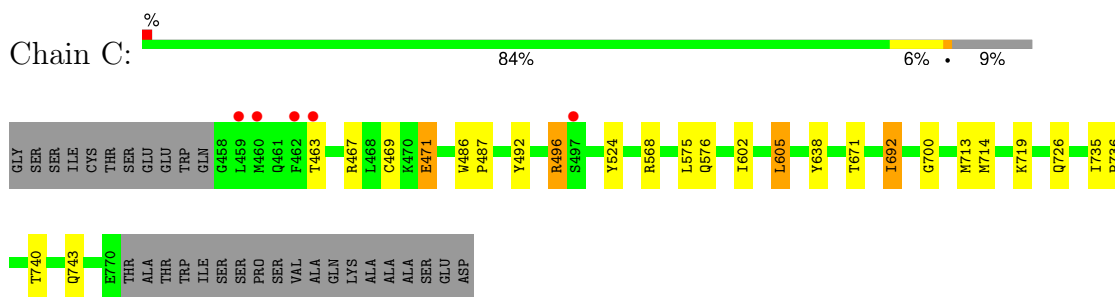
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



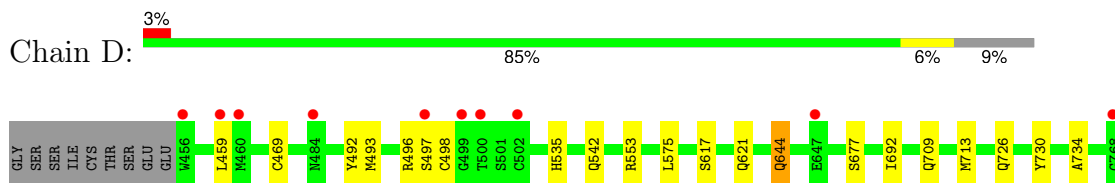
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



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



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



GLU
GLU
THR
ALA
THR
TRP
ILE
SER
SER
PRO
SER
SER
VAL
ALA
GLN
LYS
ALA
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	134.74Å 134.74Å 235.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.84 – 2.00 34.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (34.84-2.00) 91.6 (34.84-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.189 , 0.218 0.195 , 0.223	Depositor DCC
R_{free} test set	5384 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10740	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, ZN, MG, JH6

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	0.64	0/2592	0.70	0/3507
1	B	0.64	0/2602	0.72	0/3521
1	C	0.64	0/2592	0.71	0/3507
1	D	0.67	0/2588	0.70	0/3502
All	All	0.65	0/10374	0.70	0/14037

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2541	0	2513	20	0
1	B	2551	0	2515	23	0
1	C	2541	0	2511	13	0
1	D	2537	0	2511	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	0	1	0
4	B	24	0	0	6	0
4	C	24	0	0	4	0
4	D	24	0	0	13	0
5	A	129	0	0	2	1
5	B	136	0	0	3	0
5	C	125	0	0	2	1
5	D	76	0	0	1	1
All	All	10740	0	10050	80	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (80) 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:D:692:ILE:CD1	4:D:803:JH6:C20	2.34	1.05
1:D:692:ILE:HD13	4:D:803:JH6:C20	1.90	1.02
1:C:469:CYS:SG	5:C:1011:HOH:O	2.18	1.00
1:A:461:GLN:HE21	1:A:461:GLN:HA	1.23	1.00
1:A:469:CYS:SG	5:A:1019:HOH:O	2.34	0.83
1:A:498:CYS:HG	1:A:502:CYS:HG	1.12	0.78
1:D:713:MET:SD	4:D:803:JH6:C16	2.76	0.74
1:D:469:CYS:SG	5:D:972:HOH:O	2.50	0.69
1:A:606:GLU:OE2	5:A:901:HOH:O	2.12	0.68
1:A:498:CYS:HG	1:A:502:CYS:CB	2.09	0.65
1:D:692:ILE:CD1	4:D:803:JH6:C24	2.74	0.65
1:B:492:TYR:OH	5:B:901:HOH:O	2.15	0.64
1:B:726:GLN:HE22	4:B:803:JH6:C9	2.13	0.61
1:D:677:SER:HB2	4:D:803:JH6:C24	2.30	0.61
1:C:568:ARG:NH1	5:C:901:HOH:O	2.33	0.61
4:D:803:JH6:C20	4:D:803:JH6:C15	2.78	0.60
1:D:692:ILE:HD11	4:D:803:JH6:C20	2.29	0.60
1:A:461:GLN:HE21	1:A:461:GLN:CA	2.08	0.57
1:A:461:GLN:HA	1:A:461:GLN:NE2	2.05	0.57
1:C:524:TYR:CD2	1:C:692:ILE:HD13	2.41	0.56
1:D:692:ILE:HD13	4:D:803:JH6:C11	2.36	0.56
1:B:727:LEU:HD12	1:B:766:ILE:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:THR:HG22	4:B:803:JH6:C24	2.37	0.54
1:B:767:ARG:NH2	1:B:769:GLU:OE1	2.40	0.54
1:B:498:CYS:O	1:B:502:CYS:SG	2.66	0.53
1:D:677:SER:CB	4:D:803:JH6:C24	2.87	0.53
1:D:644:GLN:HE21	1:D:644:GLN:HA	1.73	0.53
1:A:461:GLN:HE22	1:A:500:THR:HG22	1.74	0.53
4:C:803:JH6:C16	4:C:803:JH6:N4	2.71	0.52
1:B:713:MET:SD	4:B:803:JH6:C16	2.98	0.52
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.45	0.52
1:A:644:GLN:HE21	1:A:644:GLN:HA	1.74	0.51
1:A:549:THR:OG1	1:A:552:GLU:HG3	2.10	0.51
1:D:692:ILE:HD11	4:D:803:JH6:C24	2.40	0.51
1:B:689:ALA:O	1:B:692:ILE:HG22	2.12	0.50
1:B:467:ARG:O	1:B:471:GLU:HB2	2.12	0.50
1:B:642:ARG:NH2	5:B:904:HOH:O	2.45	0.49
1:D:726:GLN:HE22	4:D:803:JH6:C9	2.26	0.49
1:A:726:GLN:HE22	4:A:803:JH6:C9	2.26	0.48
1:C:492:TYR:CZ	1:C:496:ARG:HD2	2.49	0.48
1:B:727:LEU:HD23	1:B:759:LEU:HD11	1.96	0.47
1:C:467:ARG:O	1:C:471:GLU:HB2	2.15	0.47
1:C:700:GLY:HA3	1:C:714:MET:O	2.16	0.46
1:B:697:TRP:CZ2	1:B:719:LYS:HG3	2.51	0.46
1:D:497:SER:HA	1:D:542:GLN:NE2	2.31	0.46
1:A:749:GLU:N	1:A:750:PRO:CD	2.79	0.45
1:D:493:MET:SD	1:D:535:HIS:HA	2.56	0.45
1:B:727:LEU:HD12	1:B:766:ILE:HD13	1.99	0.45
1:B:495:HIS:CD2	1:B:500:THR:HA	2.51	0.45
1:D:498:CYS:HB3	1:D:553:ARG:HB3	1.98	0.45
1:D:713:MET:SD	4:D:803:JH6:C17	3.04	0.45
1:D:713:MET:SD	4:D:803:JH6:C7	3.05	0.45
1:B:713:MET:SD	4:B:803:JH6:C17	3.05	0.45
4:B:803:JH6:C16	4:B:803:JH6:N4	2.81	0.44
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.52	0.44
1:C:602:ILE:HA	1:C:605:LEU:HD22	2.00	0.44
1:A:735:ILE:N	1:A:736:PRO:HD2	2.33	0.43
1:B:467:ARG:HA	1:B:470:LYS:HE3	1.99	0.43
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.53	0.43
1:B:692:ILE:HG13	1:B:696:PHE:CE2	2.54	0.43
1:A:466:VAL:HG13	1:A:470:LYS:HE3	2.00	0.43
1:A:493:MET:O	1:A:497:SER:HB2	2.19	0.43
1:B:510:ARG:HG2	1:B:608:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:HB	1:A:723:PRO:HD3	2.01	0.42
4:B:803:JH6:C14	5:B:905:HOH:O	2.66	0.42
1:C:735:ILE:HB	1:C:736:PRO:HD3	2.01	0.42
1:C:740:THR:HA	1:C:743:GLN:NE2	2.35	0.42
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.55	0.42
1:A:627:ARG:O	1:A:631:ILE:HG12	2.20	0.42
1:B:524:TYR:CD2	1:B:692:ILE:HD13	2.55	0.41
1:D:730:TYR:HA	1:D:734:ALA:HB3	2.02	0.41
1:C:713:MET:SD	4:C:803:JH6:C16	3.09	0.41
1:C:726:GLN:HE22	4:C:803:JH6:C9	2.33	0.41
1:B:602:ILE:O	1:B:605:LEU:HB2	2.21	0.41
1:A:700:GLY:HA3	1:A:714:MET:O	2.21	0.41
1:C:486:TRP:N	1:C:487:PRO:CD	2.84	0.41
4:C:803:JH6:C20	4:C:803:JH6:C15	2.99	0.41
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.56	0.41
1:B:682:TRP:HB3	1:B:683:PRO:HD3	2.02	0.40
1:B:646:GLU:OE2	1:B:650:GLN:OE1	2.38	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:976:HOH:O	5:D:904:HOH:O[7_554]	1.87	0.33
5:C:908:HOH:O	5:C:908:HOH:O[2_655]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/343 (90%)	304 (98%)	6 (2%)	0	100	100
1	B	312/343 (91%)	306 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	310/343 (90%)	304 (98%)	6 (2%)	0	100	100
1	D	310/343 (90%)	299 (96%)	11 (4%)	0	100	100
All	All	1242/1372 (90%)	1213 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	281/305 (92%)	273 (97%)	8 (3%)	38	40
1	B	281/305 (92%)	272 (97%)	9 (3%)	34	35
1	C	281/305 (92%)	273 (97%)	8 (3%)	38	40
1	D	280/305 (92%)	274 (98%)	6 (2%)	48	53
All	All	1123/1220 (92%)	1092 (97%)	31 (3%)	38	40

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	471	GLU
1	A	496	ARG
1	A	504	GLU
1	A	575	LEU
1	A	605	LEU
1	A	644	GLN
1	A	719	LYS
1	B	459	LEU
1	B	471	GLU
1	B	502	CYS
1	B	504	GLU
1	B	575	LEU
1	B	605	LEU

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Mol	Chain	Res	Type
1	B	650	GLN
1	B	727	LEU
1	B	749	GLU
1	C	463	THR
1	C	471	GLU
1	C	496	ARG
1	C	575	LEU
1	C	576	GLN
1	C	605	LEU
1	C	692	ILE
1	C	719	LYS
1	D	459	LEU
1	D	575	LEU
1	D	617	SER
1	D	621	GLN
1	D	644	GLN
1	D	709	GLN

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

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	495	HIS
1	A	542	GLN
1	A	604	GLN
1	A	644	GLN
1	A	724	GLN
1	A	726	GLN
1	A	743	GLN
1	B	495	HIS
1	B	604	GLN
1	B	650	GLN
1	B	726	GLN
1	C	542	GLN
1	C	576	GLN
1	C	604	GLN
1	C	726	GLN
1	C	743	GLN
1	D	461	GLN
1	D	484	ASN
1	D	542	GLN

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Mol	Chain	Res	Type
1	D	604	GLN
1	D	644	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	B	509	1	8,9,10	0.35	0	6,9,11	0.57	0
1	CME	C	509	1	8,9,10	0.53	0	6,9,11	0.75	0
1	CME	A	509	1	8,9,10	0.62	0	6,9,11	0.69	0
1	CME	D	509	1	8,9,10	0.48	0	6,9,11	0.49	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JH6	B	803	-	27,27,27	1.40	3 (11%)	33,37,37	1.58	6 (18%)
4	JH6	A	803	-	27,27,27	1.51	3 (11%)	33,37,37	1.69	6 (18%)
4	JH6	D	803	-	27,27,27	1.37	3 (11%)	33,37,37	1.61	7 (21%)
4	JH6	C	803	-	27,27,27	1.33	2 (7%)	33,37,37	1.65	8 (24%)

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	JH6	B	803	-	-	2/8/8/8	0/4/4/4
4	JH6	A	803	-	-	3/8/8/8	0/4/4/4
4	JH6	D	803	-	-	8/8/8/8	0/4/4/4
4	JH6	C	803	-	-	1/8/8/8	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	JH6	C9-C6	5.79	1.40	1.37
4	B	803	JH6	C9-C6	4.79	1.39	1.37
4	D	803	JH6	C9-C6	4.71	1.39	1.37
4	C	803	JH6	C9-C6	4.68	1.39	1.37
4	D	803	JH6	C1-N3	2.79	1.40	1.36
4	C	803	JH6	C1-N3	2.72	1.40	1.36
4	D	803	JH6	C6-C5	2.39	1.48	1.42
4	B	803	JH6	C6-C5	2.39	1.48	1.42
4	B	803	JH6	C1-N3	2.37	1.39	1.36
4	A	803	JH6	C7-N3	2.13	1.42	1.38
4	A	803	JH6	C6-C5	2.07	1.47	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	JH6	C18-N10-C2	4.30	122.38	117.31
4	A	803	JH6	C7-N8-C13	4.17	123.94	118.15
4	D	803	JH6	C9-N4-C1	4.01	124.04	116.20
4	B	803	JH6	C18-N10-C2	3.92	121.93	117.31
4	B	803	JH6	C9-N4-C1	3.61	123.26	116.20
4	C	803	JH6	C9-N4-C1	3.50	123.05	116.20
4	C	803	JH6	C18-N10-C2	3.43	121.35	117.31
4	B	803	JH6	C7-N8-C13	3.25	122.66	118.15
4	A	803	JH6	C9-N4-C1	3.24	122.53	116.20
4	D	803	JH6	C7-N8-C13	3.11	122.47	118.15
4	C	803	JH6	C23-C15-C5	-3.05	116.79	120.91
4	D	803	JH6	C18-N10-C2	3.03	120.88	117.31
4	C	803	JH6	C7-N8-C13	2.85	122.11	118.15
4	D	803	JH6	C19-N12-C14	2.80	121.76	116.85
4	A	803	JH6	C16-C7-N8	-2.78	118.50	123.15
4	D	803	JH6	C23-C15-C5	-2.59	117.41	120.91
4	A	803	JH6	C19-N12-C14	2.56	121.34	116.85
4	B	803	JH6	C19-N12-C14	2.55	121.32	116.85
4	C	803	JH6	C24-C20-C11	-2.47	117.72	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	JH6	C23-C18-N10	-2.45	120.37	123.97
4	D	803	JH6	C16-C7-N8	-2.40	119.14	123.15
4	C	803	JH6	C19-N12-C14	2.32	120.92	116.85
4	D	803	JH6	C22-C13-N8	2.29	120.02	116.56
4	B	803	JH6	C24-C20-C11	-2.23	118.00	120.54
4	C	803	JH6	C16-C7-N8	-2.21	119.46	123.15
4	C	803	JH6	C23-C18-N10	-2.08	120.91	123.97
4	B	803	JH6	C23-C18-N10	-2.04	120.97	123.97

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	JH6	C14-C11-C6-C5
4	D	803	JH6	C14-C11-C6-C5
4	D	803	JH6	C20-C11-C6-C9
4	D	803	JH6	C20-C11-C6-C5
4	D	803	JH6	N8-C7-N3-C1
4	D	803	JH6	C16-C7-N3-C1
4	D	803	JH6	C14-C11-C6-C9
4	A	803	JH6	N8-C7-N3-C1
4	A	803	JH6	C16-C7-N3-C1
4	D	803	JH6	C2-C1-N3-C7
4	B	803	JH6	N8-C7-N3-C1
4	B	803	JH6	C16-C7-N3-C1
4	D	803	JH6	N4-C1-N3-C7
4	C	803	JH6	N8-C7-N3-C1

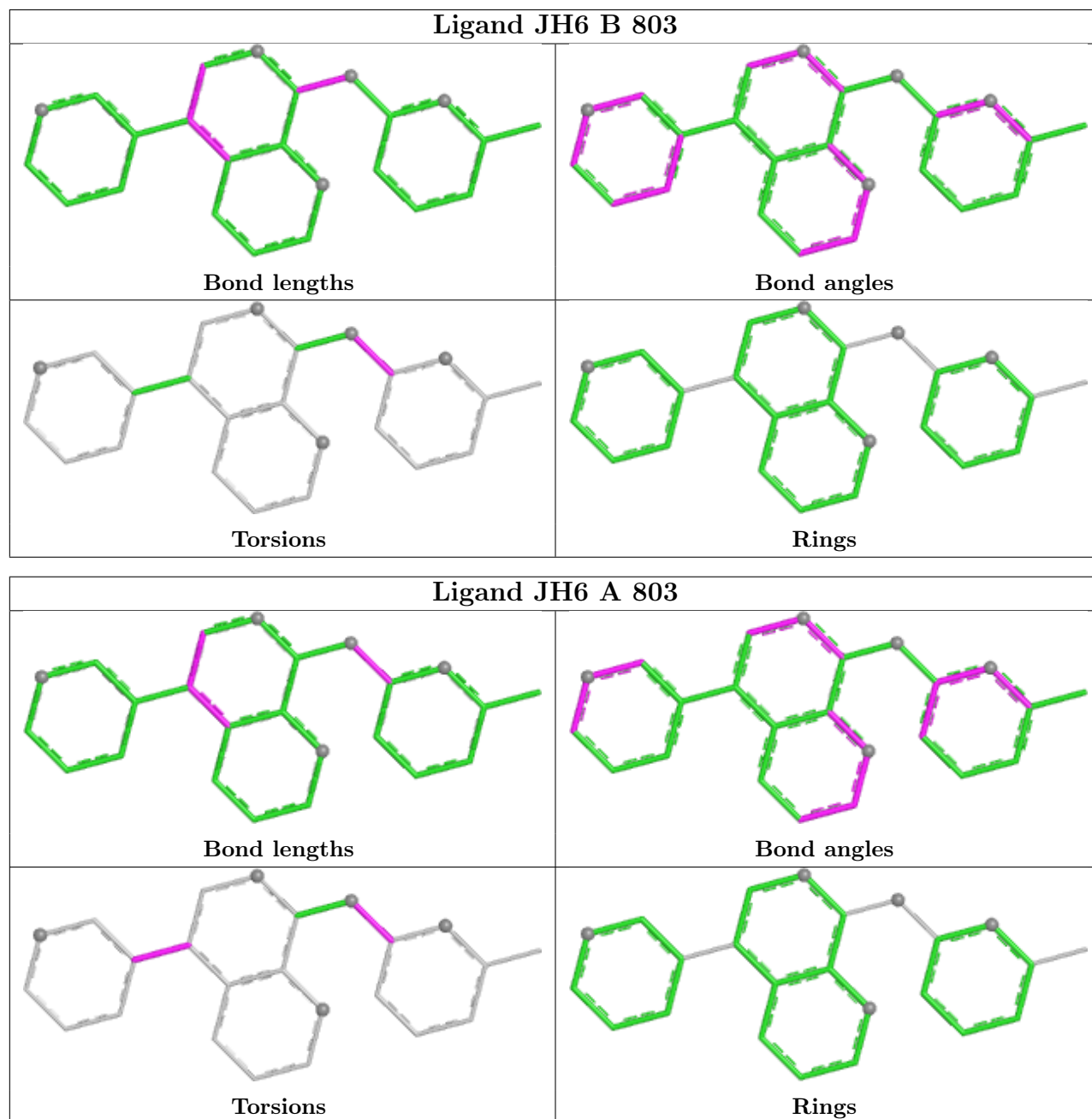
There are no ring outliers.

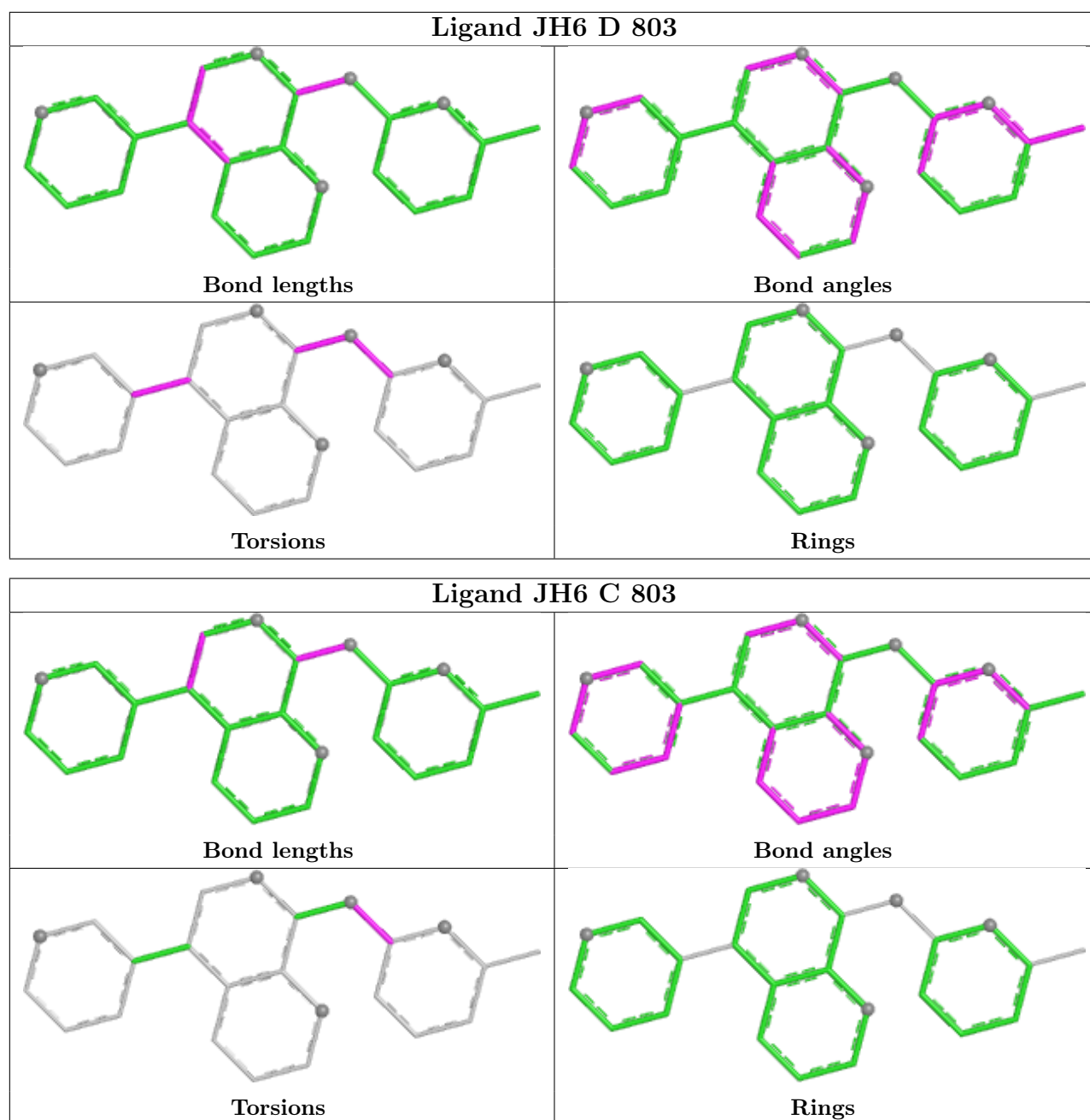
4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	JH6	6	0
4	A	803	JH6	1	0
4	D	803	JH6	13	0
4	C	803	JH6	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	312/343 (90%)	-0.02	5 (1%) 70 69	25, 36, 63, 87	0
1	B	314/343 (91%)	0.05	8 (2%) 58 57	25, 37, 63, 90	0
1	C	312/343 (90%)	-0.03	5 (1%) 70 69	25, 38, 63, 88	0
1	D	312/343 (90%)	0.40	10 (3%) 50 48	32, 48, 72, 109	0
All	All	1250/1372 (91%)	0.10	28 (2%) 62 60	25, 40, 67, 109	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	456	TRP	5.5
1	D	459	LEU	5.1
1	B	459	LEU	3.9
1	D	502	CYS	3.7
1	B	460	MET	3.6
1	D	768	GLY	3.4
1	D	460	MET	2.9
1	B	458	GLY	2.9
1	A	462	PHE	2.8
1	A	459	LEU	2.5
1	D	499	GLY	2.5
1	A	643	LYS	2.4
1	C	460	MET	2.4
1	B	771	THR	2.4
1	C	463	THR	2.4
1	C	459	LEU	2.4
1	C	497	SER	2.3
1	B	617	SER	2.3
1	B	500	THR	2.3
1	B	497	SER	2.3
1	A	458	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	500	THR	2.2
1	D	647	GLU	2.1
1	A	463	THR	2.1
1	D	484	ASN	2.1
1	B	769	GLU	2.1
1	D	497	SER	2.0
1	C	462	PHE	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
1	CME	B	509	10/11	0.86	0.15	39,50,79,80	0
1	CME	D	509	10/11	0.86	0.15	49,62,90,93	0
1	CME	C	509	10/11	0.90	0.13	38,48,75,77	0
1	CME	A	509	10/11	0.92	0.12	41,50,79,81	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	JH6	D	803	24/24	0.75	0.18	62,72,86,90	0
4	JH6	B	803	24/24	0.80	0.16	55,62,68,69	0
4	JH6	A	803	24/24	0.82	0.14	49,52,63,67	0
4	JH6	C	803	24/24	0.83	0.14	50,56,70,73	0
3	MG	D	802	1/1	0.98	0.06	36,36,36,36	0
3	MG	C	802	1/1	0.99	0.02	26,26,26,26	0
2	ZN	D	801	1/1	0.99	0.03	40,40,40,40	0

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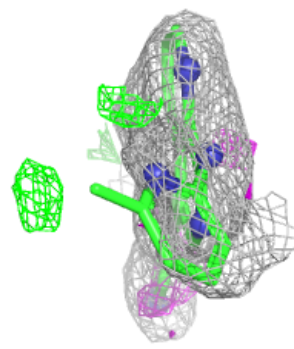
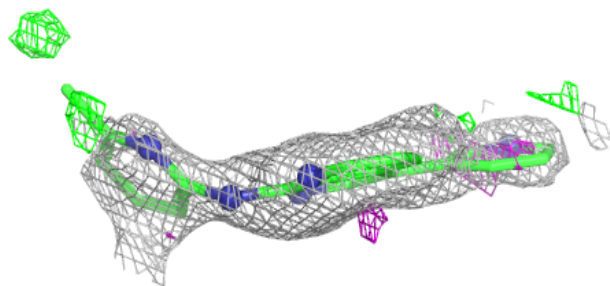
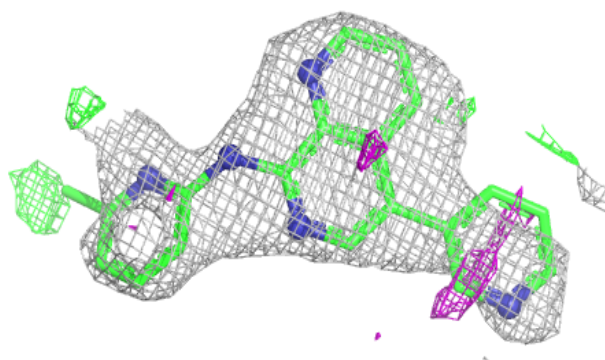
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	802	1/1	0.99	0.03	24,24,24,24	0
2	ZN	B	801	1/1	1.00	0.02	28,28,28,28	0
3	MG	B	802	1/1	1.00	0.01	20,20,20,20	0
2	ZN	C	801	1/1	1.00	0.01	31,31,31,31	0
2	ZN	A	801	1/1	1.00	0.01	29,29,29,29	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.

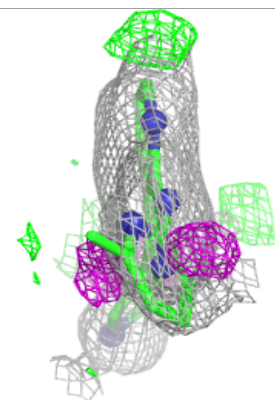
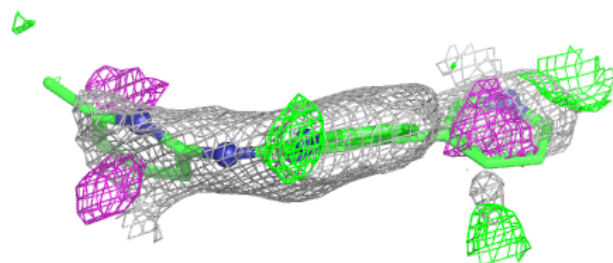
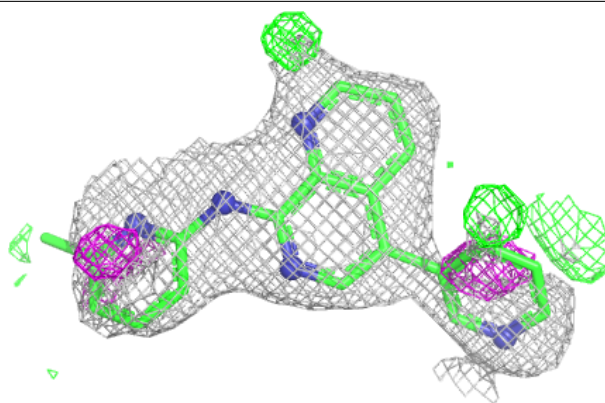
Electron density around JH6 D 803:

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

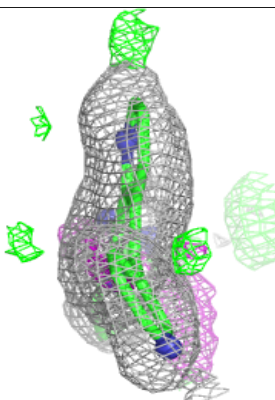
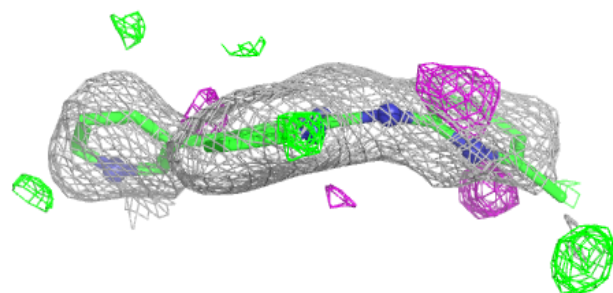
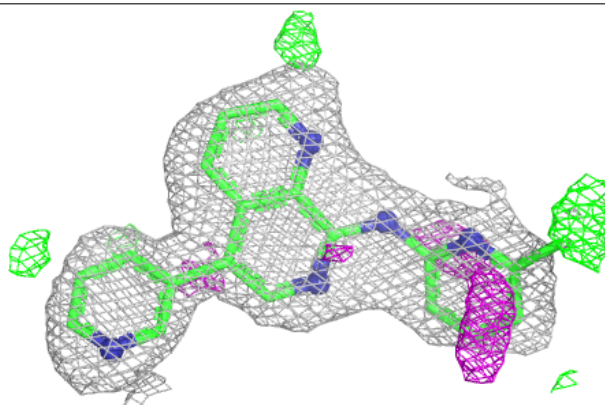


Electron density around JH6 B 803:

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

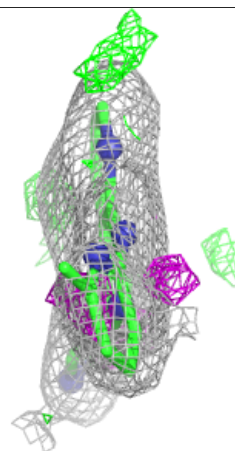
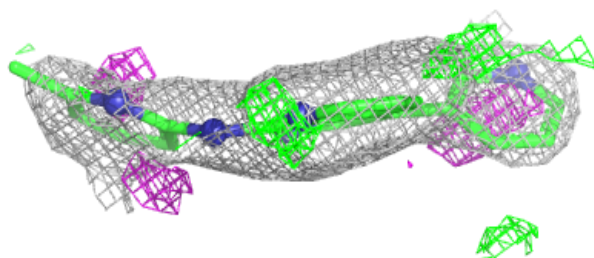
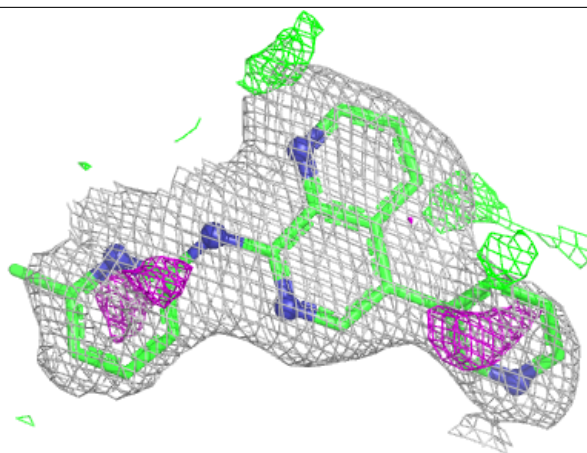
**Electron density around JH6 A 803:**

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



Electron density around JH6 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.