



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 PM UTC

PDB ID : 5FH6 / pdb_00005fh6
Title : Crystal structure of the fifth bromodomain of human PB1 in complex with compound 10
Authors : Tallant, C.; Sutherell, C.L.; Siejka, P.; Krojer, T.; Picaud, S.; Fonseca, M.; Fedorov, O.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Brennan, P.E.; Ley, S.V.; Knapp, S.
Deposited on : 2015-12-21
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](#) ①) were used in the production of this report:

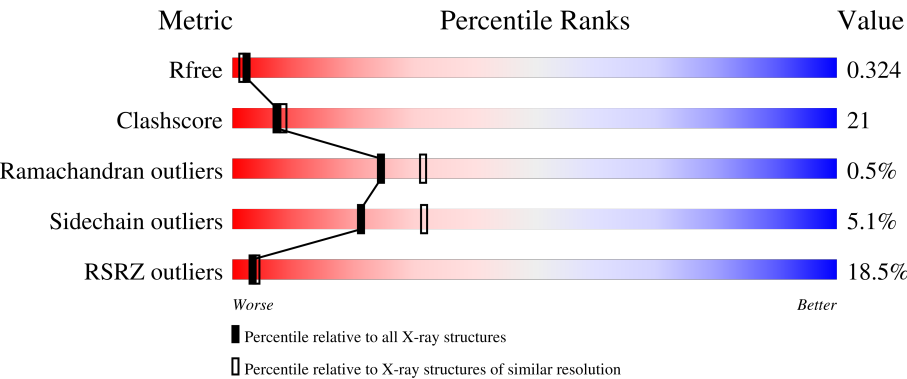
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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	124	8% 63%23%••10%
1	B	124	21% 53%29%5%•10%
1	C	124	17% 52%30%6%12%
1	D	124	19% 56%27%•14%

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
2	5XM	B	801	X	-	-	-
2	5XM	C	801	X	-	-	-
2	5XM	D	801	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3743 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.

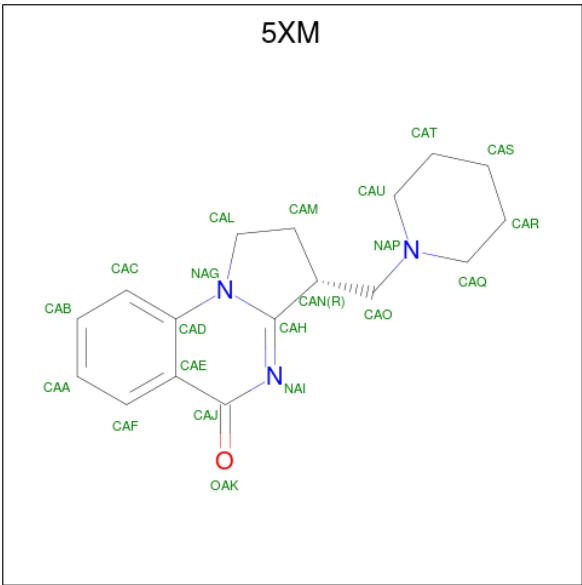
- Molecule 1 is a protein called Protein polybromo-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			929	590	158	171	10			
1	B	111	Total	C	N	O	S	0	0	0
			918	583	156	169	10			
1	C	109	Total	C	N	O	S	0	0	0
			908	575	155	168	10			
1	D	107	Total	C	N	O	S	0	0	0
			893	566	153	165	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	643	SER	-	expression tag	UNP Q86U86
A	644	MET	-	expression tag	UNP Q86U86
B	643	SER	-	expression tag	UNP Q86U86
B	644	MET	-	expression tag	UNP Q86U86
C	643	SER	-	expression tag	UNP Q86U86
C	644	MET	-	expression tag	UNP Q86U86
D	643	SER	-	expression tag	UNP Q86U86
D	644	MET	-	expression tag	UNP Q86U86

- Molecule 2 is (3 {R})-3-(piperidin-1-ylmethyl)-2,3-dihydro-1 {H}-pyrrolo[1,2-a]quinazolin-5-one (CCD ID: 5XM) (formula: C₁₇H₂₁N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	17	3	1		
2	B	1	Total	C	N	O	0	0
			21	17	3	1		
2	C	1	Total	C	N	O	0	0
			21	17	3	1		
2	D	1	Total	C	N	O	0	0
			19	15	3	1		

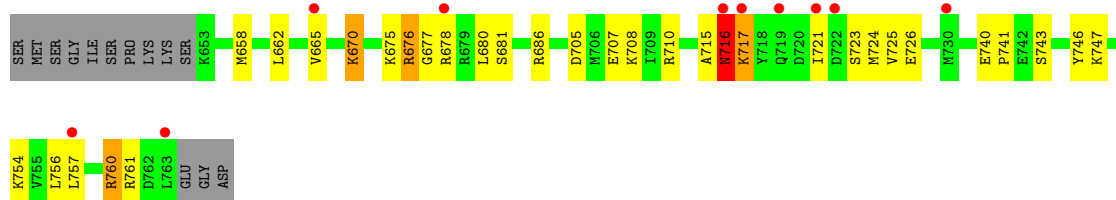
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	4	Total	O	0	0
			4	4		
3	C	3	Total	O	0	0
			3	3		
3	D	3	Total	O	0	0
			3	3		

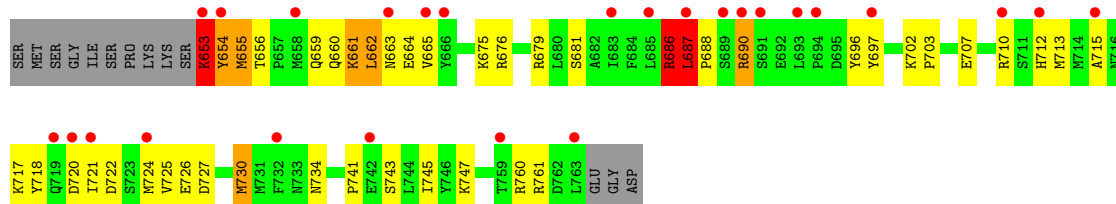
3 Residue-property plots [i](#)

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.

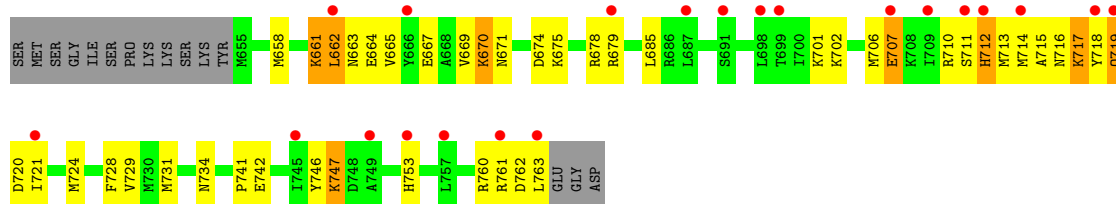
• Molecule 1: Protein polybromo-1



• Molecule 1: Protein polybromo-1

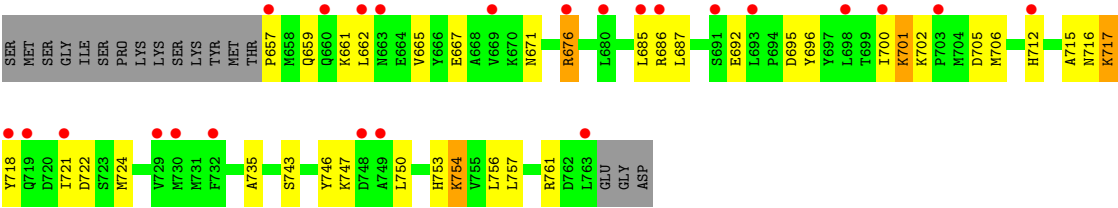


• Molecule 1: Protein polybromo-1



• Molecule 1: Protein polybromo-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.87Å 136.42Å 56.75Å 90.00° 92.33° 90.00°	Depositor
Resolution (Å)	29.73 – 2.30 29.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.73-2.30) 92.5 (29.73-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1682	Depositor
R, R_{free}	0.254 , 0.310 0.267 , 0.324	Depositor DCC
R_{free} test set	1401 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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: 5XM

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	0.62	2/946 (0.2%)	1.18	8/1270 (0.6%)
1	B	0.72	2/935 (0.2%)	1.18	8/1258 (0.6%)
1	C	0.49	0/924	1.17	8/1241 (0.6%)
1	D	0.72	3/909 (0.3%)	1.10	5/1220 (0.4%)
All	All	0.65	7/3714 (0.2%)	1.16	29/4989 (0.6%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	653	LYS	CD-CE	7.68	1.75	1.52
1	D	676	ARG	CG-CD	7.48	1.74	1.52
1	D	676	ARG	CZ-NH1	7.41	1.43	1.32
1	A	686	ARG	CZ-NH1	7.30	1.43	1.32
1	D	676	ARG	CB-CG	6.61	1.72	1.52
1	B	654	TYR	CA-C	6.10	1.60	1.52
1	A	686	ARG	CB-CG	5.04	1.67	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	ARG	NE-CZ-NH1	12.27	133.77	121.50
1	C	662	LEU	N-CA-C	-11.88	98.03	111.82
1	A	686	ARG	NE-CZ-NH2	-9.28	110.85	119.20
1	A	716	ASN	CB-CA-C	-8.75	93.02	110.42
1	B	655	MET	N-CA-C	8.51	122.28	108.41
1	A	717	LYS	N-CA-C	8.08	123.18	113.16
1	D	676	ARG	CD-NE-CZ	7.74	135.24	124.40
1	D	676	ARG	NE-CZ-NH1	7.32	128.82	121.50
1	B	690	ARG	N-CA-C	7.13	119.91	111.71
1	C	712	HIS	N-CA-C	-7.08	104.80	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	676	ARG	CB-CG-CD	6.46	126.17	111.30
1	A	716	ASN	N-CA-C	6.44	124.53	110.80
1	C	762	ASP	N-CA-C	-6.42	105.55	113.19
1	B	686	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	D	717	LYS	CA-CB-CG	6.27	126.64	114.10
1	A	716	ASN	CA-CB-CG	6.12	118.72	112.60
1	B	654	TYR	CA-C-N	-6.12	114.38	123.00
1	B	654	TYR	C-N-CA	-6.12	114.38	123.00
1	A	677	GLY	N-CA-C	5.99	123.53	114.61
1	C	760	ARG	CA-C-N	-5.71	111.44	122.06
1	C	760	ARG	C-N-CA	-5.71	111.44	122.06
1	B	730	MET	CG-SD-CE	-5.67	88.44	100.90
1	C	674	ASP	CA-C-N	5.37	128.22	120.38
1	C	674	ASP	C-N-CA	5.37	128.22	120.38
1	D	701	LYS	N-CA-C	5.34	116.90	111.14
1	C	714	MET	N-CA-C	-5.27	106.11	112.54
1	B	662	LEU	N-CA-C	-5.14	105.86	111.82
1	A	676	ARG	CA-CB-CG	-5.10	103.90	114.10
1	B	687	LEU	CB-CA-C	5.01	115.94	108.87

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	929	0	941	32	0
1	B	918	0	917	51	0
1	C	908	0	919	43	0
1	D	893	0	904	31	0
2	A	21	0	0	0	0
2	B	21	0	0	1	0
2	C	21	0	0	0	0
2	D	19	0	0	1	0
3	A	3	0	0	0	0
3	B	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3	0	0	0	0
3	D	3	0	0	0	0
All	All	3743	0	3681	153	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 21.

All (153) 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:676:ARG:CD	1:D:676:ARG:CG	1.74	1.58
1:B:653:LYS:CE	1:B:653:LYS:CD	1.75	1.58
1:B:712:HIS:HE1	1:B:717:LYS:HD2	1.14	1.06
1:A:716:ASN:HB2	1:A:717:LYS:HD2	1.34	1.04
1:B:712:HIS:CE1	1:B:717:LYS:HD2	1.97	0.99
1:B:686:ARG:HH12	1:C:678:ARG:NE	1.59	0.99
1:A:715:ALA:O	1:A:716:ASN:ND2	2.01	0.93
1:C:729:VAL:HG22	1:C:753:HIS:HE1	1.35	0.92
1:D:712:HIS:CD2	1:D:717:LYS:HG3	2.05	0.90
1:D:667:GLU:OE1	1:D:671:ASN:ND2	2.05	0.90
1:C:661:LYS:HA	1:C:664:GLU:H	1.42	0.85
1:A:757:LEU:HD23	1:A:761:ARG:HH12	1.43	0.83
1:B:662:LEU:HD23	1:B:721:ILE:HD13	1.66	0.77
1:A:757:LEU:HD21	1:A:761:ARG:HH22	1.51	0.75
1:B:702:LYS:HB3	1:B:730:MET:CE	2.16	0.75
1:B:702:LYS:HB3	1:B:730:MET:HE1	1.72	0.71
1:B:687:LEU:HD11	1:B:697:TYR:OH	1.91	0.70
1:B:697:TYR:HD1	1:B:703:PRO:HG2	1.57	0.69
1:B:661:LYS:HE3	1:B:664:GLU:OE1	1.92	0.68
1:C:662:LEU:HD23	1:C:721:ILE:HD13	1.75	0.68
1:C:675:LYS:N	1:C:675:LYS:HD3	2.08	0.68
1:C:675:LYS:HD3	1:C:675:LYS:H	1.60	0.67
1:B:697:TYR:CD1	1:B:703:PRO:HG2	2.32	0.65
1:A:716:ASN:CB	1:A:717:LYS:HD2	2.21	0.65
1:C:761:ARG:NH1	1:C:761:ARG:O	2.31	0.64
1:A:757:LEU:CD2	1:A:761:ARG:HH12	2.10	0.64
1:B:663:ASN:HA	1:B:713:MET:HE1	1.79	0.64
1:B:715:ALA:HB1	1:B:717:LYS:HZ3	1.61	0.64
1:C:715:ALA:HB1	1:C:717:LYS:HE2	1.79	0.63
1:A:715:ALA:O	1:A:716:ASN:CG	2.43	0.62
1:D:685:LEU:HA	1:D:706:MET:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:VAL:HG13	1:B:724:MET:HE1	1.80	0.62
1:D:712:HIS:CG	1:D:717:LYS:HE3	2.35	0.62
1:C:715:ALA:O	1:C:717:LYS:NZ	2.19	0.61
1:C:665:VAL:HG13	1:C:724:MET:HE1	1.81	0.61
1:C:661:LYS:O	1:C:665:VAL:HG12	2.01	0.61
1:A:708:LYS:O	1:A:708:LYS:HD2	2.02	0.59
1:C:712:HIS:CE1	1:C:717:LYS:HB2	2.37	0.59
1:B:702:LYS:HD3	1:B:730:MET:HE1	1.83	0.59
1:D:712:HIS:CG	1:D:717:LYS:HG3	2.36	0.59
1:B:718:TYR:CE2	1:B:724:MET:HA	2.37	0.59
1:A:665:VAL:HG13	1:A:724:MET:HE1	1.85	0.59
1:B:712:HIS:CE1	1:B:717:LYS:CD	2.82	0.59
1:C:658:MET:CE	1:C:720:ASP:HA	2.33	0.59
1:D:662:LEU:HD21	1:D:721:ILE:HA	1.84	0.58
1:B:722:ASP:HA	1:B:725:VAL:HB	1.85	0.58
1:B:686:ARG:HH12	1:C:678:ARG:CD	2.15	0.58
1:B:686:ARG:NH2	1:B:707:GLU:OE2	2.36	0.58
1:B:712:HIS:HE1	1:B:717:LYS:CD	2.04	0.58
1:A:678:ARG:HH22	1:A:680:LEU:HG	1.69	0.57
1:C:715:ALA:HB1	1:C:717:LYS:CE	2.33	0.57
1:C:729:VAL:HG22	1:C:753:HIS:CE1	2.27	0.57
1:B:722:ASP:O	1:B:726:GLU:HG3	2.05	0.57
1:B:653:LYS:HB2	1:B:654:TYR:CD1	2.38	0.57
1:B:712:HIS:CE1	1:B:717:LYS:HB2	2.40	0.56
1:C:718:TYR:CE2	1:C:724:MET:HA	2.40	0.56
1:A:760:ARG:NH1	1:A:761:ARG:HG3	2.21	0.56
1:A:716:ASN:HB2	1:A:717:LYS:CD	2.23	0.56
1:B:712:HIS:NE2	1:B:717:LYS:HB2	2.21	0.56
1:C:670:LYS:NZ	1:C:671:ASN:OD1	2.39	0.56
1:A:675:LYS:O	1:A:676:ARG:HG3	2.06	0.55
1:C:718:TYR:CE2	1:C:724:MET:HG3	2.42	0.55
1:B:687:LEU:C	1:B:687:LEU:HD12	2.32	0.55
1:A:658:MET:O	1:A:662:LEU:HD13	2.07	0.54
1:A:678:ARG:NH1	1:A:680:LEU:HA	2.21	0.54
1:A:757:LEU:HG	1:A:760:ARG:NH1	2.22	0.54
1:B:687:LEU:HD11	1:B:697:TYR:CZ	2.42	0.54
1:B:718:TYR:OH	1:B:727:ASP:OD2	2.16	0.54
1:C:718:TYR:HE2	1:C:724:MET:HG3	1.73	0.54
1:B:718:TYR:HE2	1:B:724:MET:HA	1.73	0.53
1:C:707:GLU:OE2	1:C:710:ARG:NH1	2.41	0.53
1:C:702:LYS:O	1:C:734:ASN:ND2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:VAL:HB	1:D:724:MET:HE1	1.90	0.53
1:D:661:LYS:NZ	1:D:721:ILE:HG21	2.24	0.53
1:D:661:LYS:O	1:D:665:VAL:HG23	2.10	0.52
1:A:662:LEU:HD12	1:A:721:ILE:HD13	1.91	0.52
1:D:661:LYS:HZ3	1:D:721:ILE:HG21	1.75	0.51
1:B:679:ARG:HG2	1:B:681:SER:HB3	1.91	0.51
1:A:707:GLU:HG2	1:A:710:ARG:HD3	1.92	0.51
1:B:655:MET:HG2	1:B:660:GLN:HG3	1.93	0.51
1:D:721:ILE:HG13	1:D:722:ASP:OD1	2.10	0.51
1:A:741:PRO:HA	1:A:746:TYR:CD2	2.46	0.51
1:B:720:ASP:CG	1:B:721:ILE:N	2.69	0.51
1:C:675:LYS:H	1:C:675:LYS:CD	2.21	0.51
1:B:656:THR:HG23	1:B:659:GLN:HB2	1.94	0.49
1:C:761:ARG:C	1:C:763:LEU:N	2.68	0.49
1:C:715:ALA:O	1:C:716:ASN:HB2	2.12	0.49
1:A:662:LEU:CD1	1:A:721:ILE:HD13	2.43	0.49
1:C:741:PRO:HA	1:C:746:TYR:CG	2.47	0.49
1:A:743:SER:O	1:A:747:LYS:HD2	2.13	0.48
1:C:741:PRO:HG2	1:D:702:LYS:HE3	1.95	0.48
1:B:663:ASN:CA	1:B:713:MET:HE1	2.42	0.48
1:B:686:ARG:HH12	1:C:678:ARG:HE	1.53	0.48
1:D:696:TYR:CE2	1:D:700:ILE:HD11	2.49	0.47
1:B:702:LYS:CB	1:B:730:MET:HE1	2.42	0.47
1:D:753:HIS:O	1:D:757:LEU:HD13	2.14	0.47
1:C:663:ASN:CA	1:C:713:MET:HE1	2.45	0.47
1:A:705:ASP:OD1	1:A:708:LYS:HB3	2.14	0.47
1:A:708:LYS:HD2	1:A:708:LYS:C	2.40	0.47
1:C:715:ALA:C	1:C:717:LYS:HD3	2.39	0.47
1:C:663:ASN:HB2	1:C:713:MET:HE1	1.97	0.47
1:B:690:ARG:NH1	3:B:901:HOH:O	2.48	0.46
1:D:712:HIS:CB	1:D:717:LYS:HE3	2.45	0.46
1:B:696:TYR:OH	2:B:801:5XM:OAK	2.26	0.46
1:B:653:LYS:HB2	1:B:654:TYR:CE1	2.51	0.46
1:B:730:MET:HG2	1:B:734:ASN:HD21	1.81	0.46
1:D:715:ALA:O	1:D:716:ASN:HB2	2.15	0.46
1:C:706:MET:HG3	1:C:731:MET:HE1	1.98	0.46
1:C:669:VAL:HG11	1:C:728:PHE:HE2	1.81	0.46
1:A:678:ARG:HH12	1:A:680:LEU:HA	1.81	0.45
1:C:658:MET:HE2	1:C:719:GLN:O	2.16	0.45
1:C:658:MET:HE3	1:C:720:ASP:HA	1.99	0.45
1:B:702:LYS:CG	1:B:730:MET:HE1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:ARG:HG2	1:A:761:ARG:N	2.29	0.45
1:B:687:LEU:HD12	1:B:688:PRO:O	2.16	0.45
1:D:657:PRO:HD2	1:D:659:GLN:HE21	1.82	0.45
1:A:707:GLU:HA	1:A:710:ARG:HB3	1.99	0.45
1:A:670:LYS:HA	1:A:681:SER:HB2	1.99	0.45
1:D:735:ALA:HA	2:D:801:5XM:OAK	2.17	0.45
1:C:742:GLU:OE1	1:C:747:LYS:NZ	2.30	0.44
1:A:754:LYS:NZ	1:A:754:LYS:HB2	2.32	0.44
1:C:761:ARG:C	1:C:763:LEU:H	2.24	0.44
1:D:676:ARG:O	1:D:676:ARG:HG3	2.16	0.44
1:D:743:SER:O	1:D:747:LYS:HG3	2.17	0.44
1:B:745:ILE:H	1:B:745:ILE:HD12	1.81	0.44
1:D:746:TYR:O	1:D:750:LEU:HD13	2.18	0.44
1:C:665:VAL:CG1	1:C:724:MET:HE1	2.46	0.44
1:C:761:ARG:O	1:C:761:ARG:HG3	2.18	0.44
1:D:686:ARG:HA	1:D:705:ASP:OD2	2.17	0.44
1:C:685:LEU:HA	1:C:706:MET:HB2	2.00	0.43
1:C:663:ASN:O	1:C:667:GLU:HB2	2.18	0.43
1:A:723:SER:O	1:A:726:GLU:HG2	2.18	0.43
1:D:667:GLU:OE1	1:D:671:ASN:CG	2.61	0.43
1:D:692:GLU:O	1:D:692:GLU:HG2	2.18	0.42
1:A:675:LYS:C	1:A:676:ARG:HG3	2.44	0.42
1:A:662:LEU:HA	1:A:665:VAL:HG12	2.00	0.42
1:B:702:LYS:CD	1:B:730:MET:HE1	2.49	0.42
1:A:725:VAL:HG13	1:A:756:LEU:HD21	2.02	0.42
1:B:743:SER:O	1:B:747:LYS:HG3	2.19	0.42
1:B:653:LYS:CE	1:B:653:LYS:CG	2.82	0.42
1:B:675:LYS:HG3	1:B:676:ARG:HG3	2.01	0.42
1:D:701:LYS:H	1:D:701:LYS:HG2	1.68	0.41
1:D:686:ARG:HH11	1:D:686:ARG:HD2	1.68	0.41
1:B:718:TYR:HD2	1:B:724:MET:HB2	1.85	0.41
1:C:742:GLU:OE1	1:C:742:GLU:HA	2.20	0.41
1:D:712:HIS:CD2	1:D:718:TYR:CE2	3.09	0.41
1:B:686:ARG:HH11	1:B:686:ARG:HD2	1.54	0.41
1:B:720:ASP:CG	1:B:721:ILE:H	2.29	0.41
1:D:754:LYS:HB2	1:D:754:LYS:HE2	1.88	0.41
1:C:711:SER:O	1:C:715:ALA:HB2	2.22	0.40
1:B:665:VAL:CG1	1:B:724:MET:HE1	2.50	0.40
1:D:753:HIS:O	1:D:756:LEU:HB3	2.21	0.40
1:D:687:LEU:HG	1:D:705:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	109/124 (88%)	106 (97%)	2 (2%)	1 (1%)	14	17
1	B	109/124 (88%)	105 (96%)	3 (3%)	1 (1%)	14	17
1	C	107/124 (86%)	105 (98%)	2 (2%)	0	100	100
1	D	105/124 (85%)	102 (97%)	3 (3%)	0	100	100
All	All	430/496 (87%)	418 (97%)	10 (2%)	2 (0%)	24	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	716	ASN
1	B	741	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	105/116 (90%)	102 (97%)	3 (3%)	37	55
1	B	102/116 (88%)	95 (93%)	7 (7%)	14	20
1	C	103/116 (89%)	95 (92%)	8 (8%)	11	16
1	D	101/116 (87%)	98 (97%)	3 (3%)	36	53
All	All	411/464 (89%)	390 (95%)	21 (5%)	21	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	670	LYS
1	A	740	GLU
1	A	760	ARG
1	B	653	LYS
1	B	661	LYS
1	B	686	ARG
1	B	687	LEU
1	B	710	ARG
1	B	760	ARG
1	B	761	ARG
1	C	661	LYS
1	C	670	LYS
1	C	679	ARG
1	C	701	LYS
1	C	707	GLU
1	C	717	LYS
1	C	719	GLN
1	C	747	LYS
1	D	695	ASP
1	D	754	LYS
1	D	761	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	663	ASN
1	B	660	GLN
1	B	712	HIS
1	B	734	ASN
1	C	753	HIS
1	D	719	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	5XM	B	801	-	23,24,24	3.71	7 (30%)	26,34,34	2.95	4 (15%)
2	5XM	D	801	-	20,21,24	4.47	8 (40%)	21,30,34	3.25	4 (19%)
2	5XM	A	801	-	23,24,24	3.68	7 (30%)	26,34,34	2.88	4 (15%)
2	5XM	C	801	-	23,24,24	4.12	8 (34%)	26,34,34	2.72	4 (15%)

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	5XM	A	801	-	-	0/4/21/21	0/4/4/4
2	5XM	D	801	-	1/1/2/2	3/6/15/21	0/3/3/4
2	5XM	B	801	-	1/1/2/2	1/4/21/21	0/4/4/4
2	5XM	C	801	-	1/1/2/2	0/4/21/21	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	5XM	CAO-CAN	-15.55	1.31	1.53
2	D	801	5XM	CAO-CAN	-14.77	1.32	1.53
2	B	801	5XM	CAO-CAN	-12.82	1.35	1.53
2	A	801	5XM	CAO-CAN	-12.75	1.35	1.53
2	C	801	5XM	CAO-NAP	-7.31	1.32	1.47
2	D	801	5XM	CAM-CAN	-6.61	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	5XM	CAO-NAP	-6.28	1.34	1.47
2	A	801	5XM	CAO-NAP	-6.18	1.34	1.47
2	D	801	5XM	CAE-CAJ	-6.15	1.37	1.48
2	D	801	5XM	CAO-NAP	-6.03	1.32	1.47
2	A	801	5XM	CAM-CAN	-5.86	1.37	1.54
2	B	801	5XM	CAM-CAN	-5.78	1.38	1.54
2	C	801	5XM	CAE-CAJ	-5.63	1.38	1.48
2	A	801	5XM	CAE-CAJ	-5.22	1.39	1.48
2	B	801	5XM	CAD-NAG	-5.08	1.32	1.41
2	C	801	5XM	CAM-CAN	-5.05	1.40	1.54
2	B	801	5XM	CAE-CAJ	-5.01	1.39	1.48
2	A	801	5XM	CAD-NAG	-4.78	1.32	1.41
2	D	801	5XM	CAH-NAG	-4.69	1.31	1.37
2	B	801	5XM	CAH-NAI	4.22	1.39	1.31
2	A	801	5XM	CAH-NAI	4.04	1.39	1.31
2	D	801	5XM	CAD-NAG	-3.90	1.34	1.41
2	D	801	5XM	CAM-CAL	-3.34	1.46	1.52
2	C	801	5XM	CAD-NAG	-3.32	1.35	1.41
2	C	801	5XM	CAH-NAG	-2.44	1.34	1.37
2	B	801	5XM	CAM-CAL	-2.41	1.48	1.52
2	C	801	5XM	CAM-CAL	-2.32	1.48	1.52
2	C	801	5XM	CAH-NAI	2.29	1.35	1.31
2	A	801	5XM	CAM-CAL	-2.21	1.48	1.52
2	D	801	5XM	CAC-CAD	2.16	1.43	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	5XM	CAM-CAL-NAG	-11.98	89.73	102.90
2	B	801	5XM	CAM-CAL-NAG	-9.85	92.07	102.90
2	A	801	5XM	CAM-CAL-NAG	-9.43	92.53	102.90
2	C	801	5XM	CAM-CAL-NAG	-8.69	93.34	102.90
2	B	801	5XM	CAN-CAO-NAP	8.10	125.21	113.17
2	A	801	5XM	CAN-CAO-NAP	7.71	124.64	113.17
2	C	801	5XM	CAL-CAM-CAN	-7.65	94.82	105.80
2	A	801	5XM	CAL-CAM-CAN	-7.11	95.59	105.80
2	B	801	5XM	CAL-CAM-CAN	-6.71	96.16	105.80
2	D	801	5XM	CAL-CAM-CAN	-6.40	96.60	105.80
2	C	801	5XM	CAN-CAO-NAP	5.87	121.89	113.17
2	C	801	5XM	CAL-NAG-CAD	2.72	133.60	123.68
2	D	801	5XM	CAA-CAB-CAC	-2.65	116.97	120.24
2	B	801	5XM	CAL-NAG-CAD	2.40	132.43	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	5XM	CAL-NAG-CAD	2.32	132.13	123.68
2	D	801	5XM	CAL-NAG-CAD	2.10	131.31	123.68

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	801	5XM	CAN
2	C	801	5XM	CAN
2	D	801	5XM	CAN

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	5XM	CAR-CAQ-NAP-CAU
2	D	801	5XM	CAM-CAN-CAO-NAP
2	D	801	5XM	CAN-CAO-NAP-CAU
2	B	801	5XM	CAM-CAN-CAO-NAP

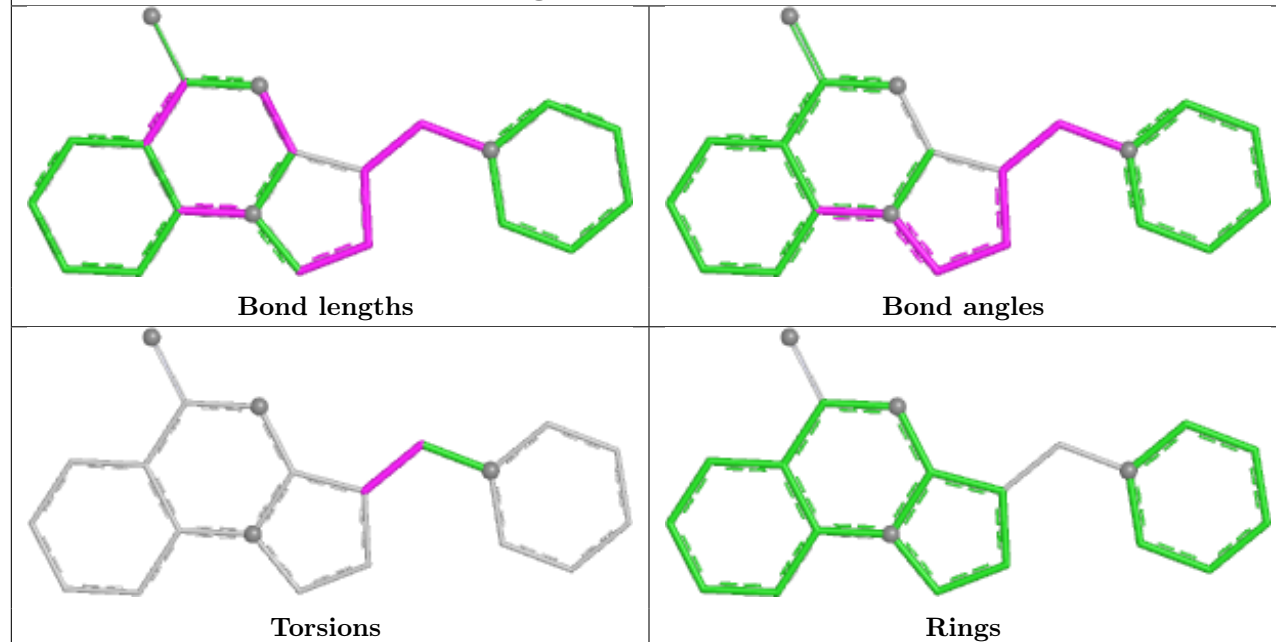
There are no ring outliers.

2 monomers are involved in 2 short contacts:

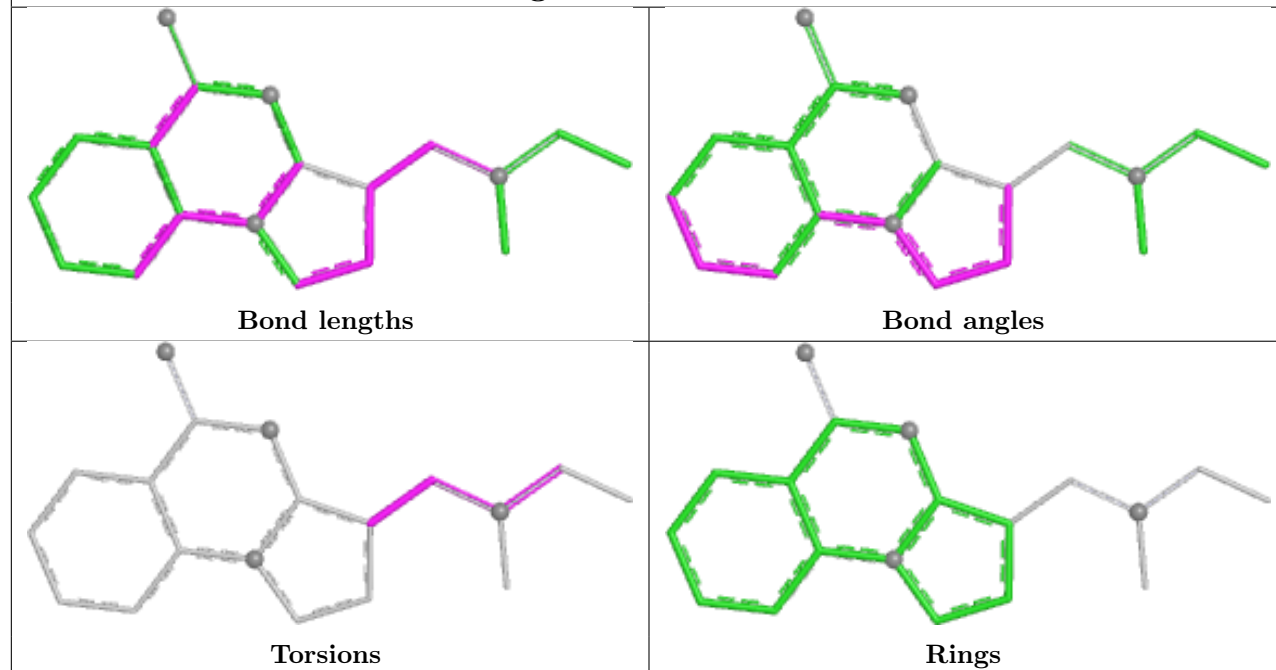
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	5XM	1	0
2	D	801	5XM	1	0

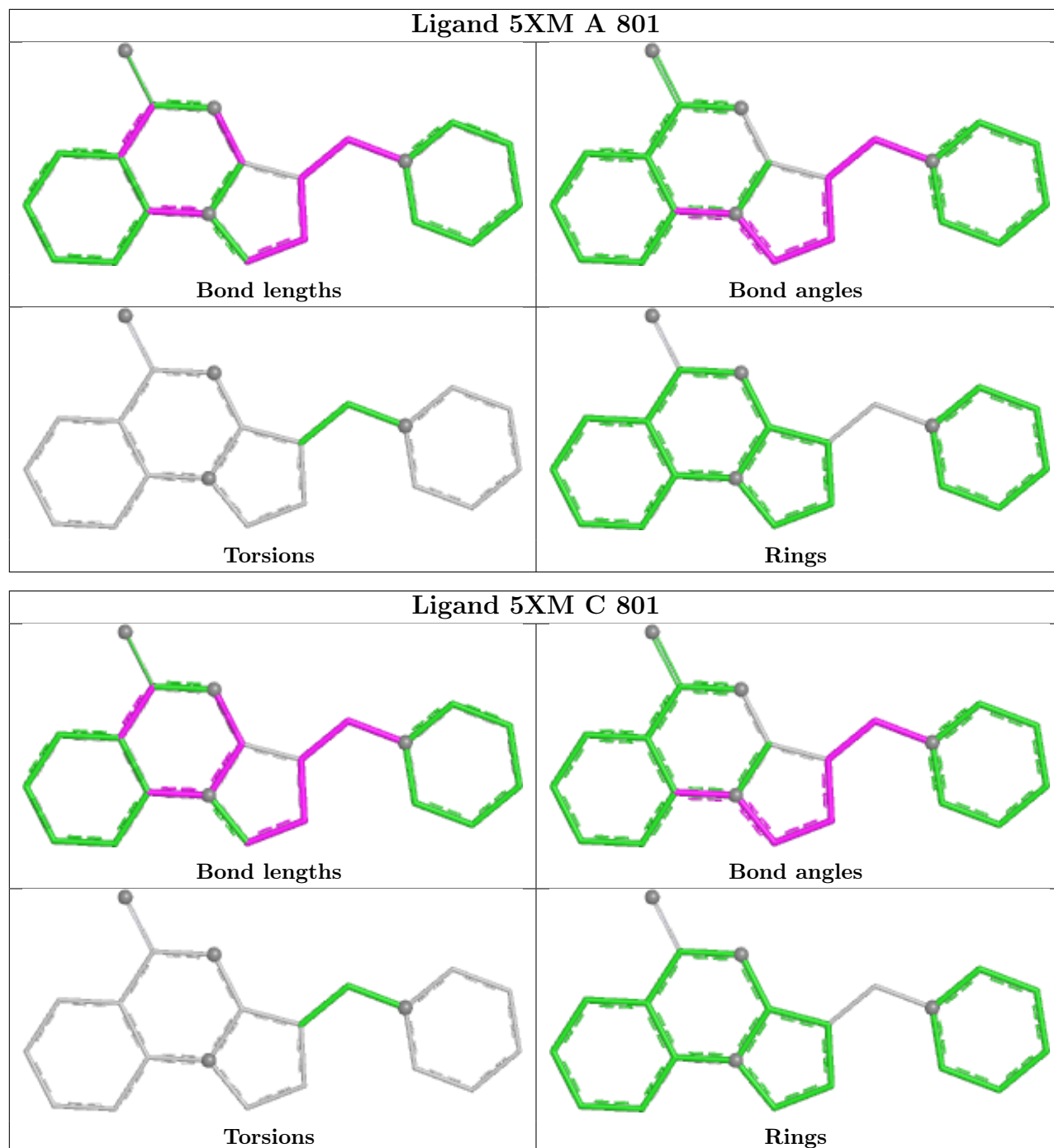
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 5XM B 801



Ligand 5XM D 801





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	111/124 (89%)	1.10	10 (9%) 15 16	47, 70, 113, 153	0
1	B	111/124 (89%)	1.38	26 (23%) 2 2	46, 74, 129, 162	0
1	C	109/124 (87%)	1.31	21 (19%) 3 3	47, 75, 106, 153	0
1	D	107/124 (86%)	1.33	24 (22%) 2 2	45, 75, 116, 141	0
All	All	438/496 (88%)	1.28	81 (18%) 3 4	45, 74, 120, 162	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	763	LEU	5.8
1	B	763	LEU	4.9
1	C	763	LEU	3.9
1	C	719	GLN	3.8
1	A	716	ASN	3.6
1	B	690	ARG	3.6
1	B	654	TYR	3.6
1	B	697	TYR	3.5
1	D	686	ARG	3.3
1	B	694	PRO	3.3
1	B	693	LEU	3.1
1	D	698	LEU	3.0
1	A	721	ILE	3.0
1	B	653	LYS	3.0
1	D	685	LEU	2.9
1	B	691	SER	2.9
1	C	711	SER	2.9
1	D	691	SER	2.9
1	B	666	TYR	2.9
1	C	712	HIS	2.9
1	B	720	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	712	HIS	2.8
1	D	662	LEU	2.8
1	B	710	ARG	2.8
1	A	763	LEU	2.7
1	C	718	TYR	2.7
1	B	724	MET	2.7
1	D	669	VAL	2.7
1	B	683	ILE	2.7
1	B	742	GLU	2.6
1	C	761	ARG	2.6
1	A	730	MET	2.6
1	B	719	GLN	2.6
1	B	721	ILE	2.6
1	C	721	ILE	2.6
1	B	732	PHE	2.6
1	D	700	ILE	2.6
1	D	660	GLN	2.5
1	C	691	SER	2.5
1	D	693	LEU	2.5
1	C	757	LEU	2.5
1	B	665	VAL	2.4
1	D	721	ILE	2.4
1	B	687	LEU	2.4
1	A	722	ASP	2.4
1	D	676	ARG	2.4
1	A	719	GLN	2.4
1	B	689	SER	2.3
1	C	666	TYR	2.3
1	B	715	ALA	2.3
1	C	749	ALA	2.3
1	B	712	HIS	2.3
1	A	757	LEU	2.3
1	B	658	MET	2.3
1	D	719	GLN	2.3
1	C	753	HIS	2.2
1	A	665	VAL	2.2
1	C	662	LEU	2.2
1	D	663	ASN	2.2
1	C	714	MET	2.2
1	D	703	PRO	2.2
1	A	717	LYS	2.2
1	C	687	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	759	THR	2.2
1	B	685	LEU	2.2
1	B	663	ASN	2.2
1	D	729	VAL	2.2
1	D	732	PHE	2.2
1	D	718	TYR	2.1
1	C	745	ILE	2.1
1	D	680	LEU	2.1
1	D	748	ASP	2.1
1	C	699	THR	2.1
1	D	730	MET	2.1
1	C	709	ILE	2.1
1	C	679	ARG	2.1
1	C	707	GLU	2.0
1	A	678	ARG	2.0
1	D	749	ALA	2.0
1	C	698	LEU	2.0
1	D	657	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

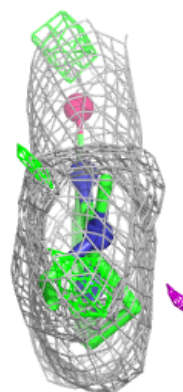
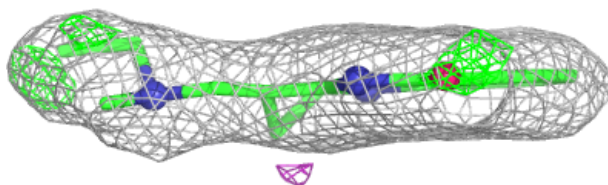
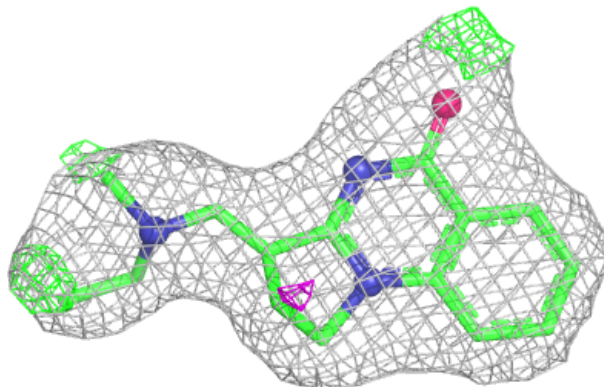
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5XM	D	801	19/21	0.86	0.16	45,61,83,84	0
2	5XM	A	801	21/21	0.88	0.15	46,57,80,87	0
2	5XM	C	801	21/21	0.89	0.15	53,79,90,92	0
2	5XM	B	801	21/21	0.89	0.13	45,68,88,92	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.

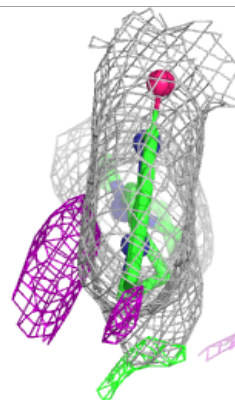
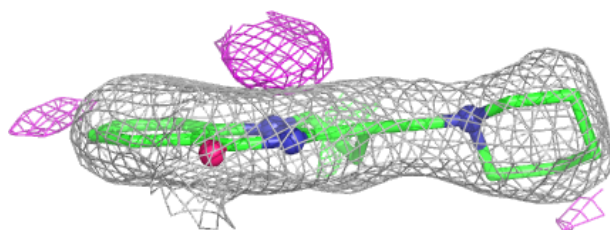
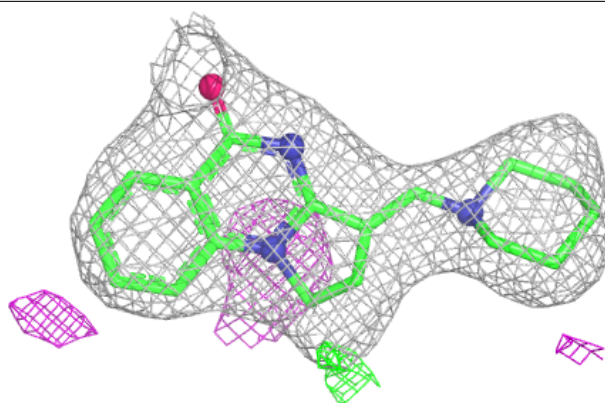
Electron density around 5XM D 801:

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

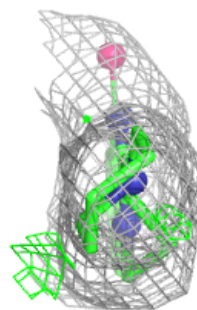
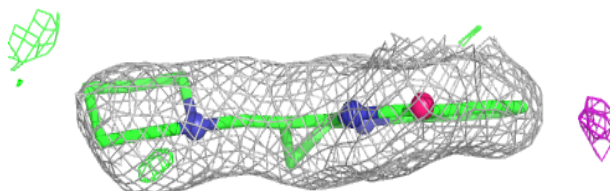
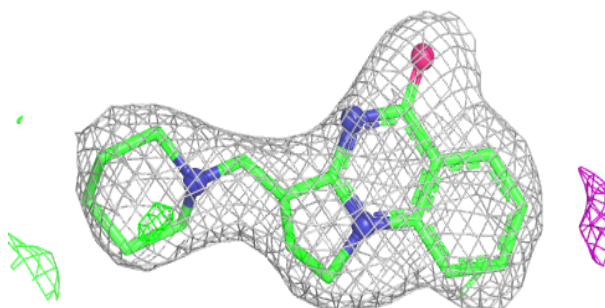


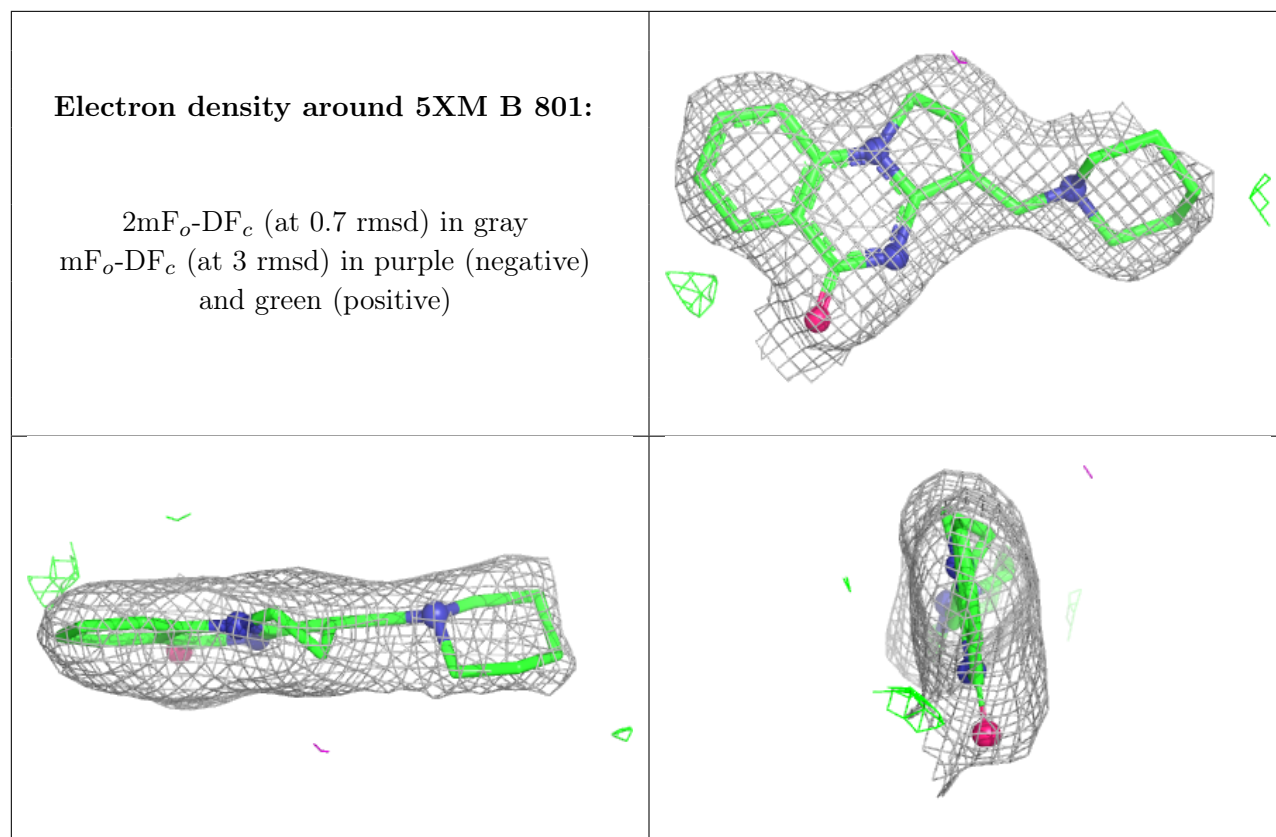
Electron density around 5XM A 801:

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

**Electron density around 5XM C 801:**

$2mF_o-DF_c$ (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.