



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2021 – 08:09 PM JST

PDB ID : 7DN4
Title : The crystal structure of Cpd8 in complex with BPTF bromodomain
Authors : Xiong, L.; Guo, Y.; Yang, S.
Deposited on : 2020-12-08
Resolution : 2.84 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

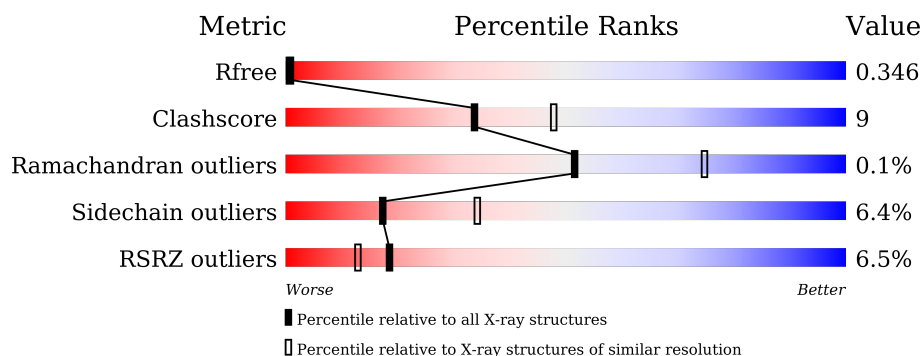
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	123	<div> <div>5%</div> <div>66%</div> <div>26%</div> <div>.</div> <div>.</div> </div>
1	B	123	<div> <div>7%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	C	123	<div> <div>3%</div> <div>72%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	D	123	<div> <div>7%</div> <div>68%</div> <div>26%</div> <div>.</div> <div>.</div> </div>
1	E	123	<div> <div>10%</div> <div>70%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	F	123	<div> <div>6%</div> <div>69%</div> <div>24%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12081 atoms, of which 5976 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.

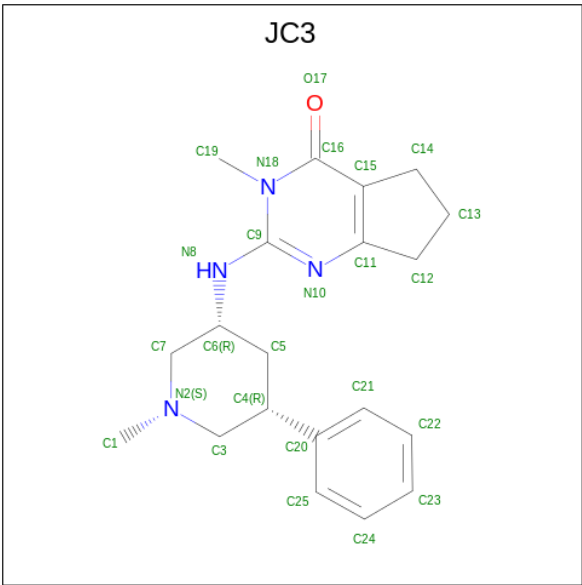
- Molecule 1 is a protein called Nucleosome-remodeling factor subunit BPTF.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	118	Total	C	H	N	O	S	0	7	0
			1952	634	962	159	190	7			
1	B	118	Total	C	H	N	O	S	14	7	0
			1960	636	968	160	189	7			
1	C	118	Total	C	H	N	O	S	0	7	0
			1960	636	968	160	189	7			
1	D	118	Total	C	H	N	O	S	0	6	0
			1954	634	966	160	187	7			
1	E	118	Total	C	H	N	O	S	8	9	0
			1979	641	980	160	190	8			
1	F	118	Total	C	H	N	O	S	0	8	0
			1970	638	976	160	188	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2789	SER	-	expression tag	UNP Q12830
A	2790	MET	-	expression tag	UNP Q12830
B	2789	SER	-	expression tag	UNP Q12830
B	2790	MET	-	expression tag	UNP Q12830
C	2789	SER	-	expression tag	UNP Q12830
C	2790	MET	-	expression tag	UNP Q12830
D	2789	SER	-	expression tag	UNP Q12830
D	2790	MET	-	expression tag	UNP Q12830
E	2789	SER	-	expression tag	UNP Q12830
E	2790	MET	-	expression tag	UNP Q12830
F	2789	SER	-	expression tag	UNP Q12830
F	2790	MET	-	expression tag	UNP Q12830

- Molecule 2 is 3-methyl-2-[[[(3R,5R)-1-methyl-5-phenyl-piperidin-3-yl]amino]-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-one (three-letter code: JC3) (formula: C₂₀H₂₆N₄O) (labeled as "Ligand of Interest" by depositor).

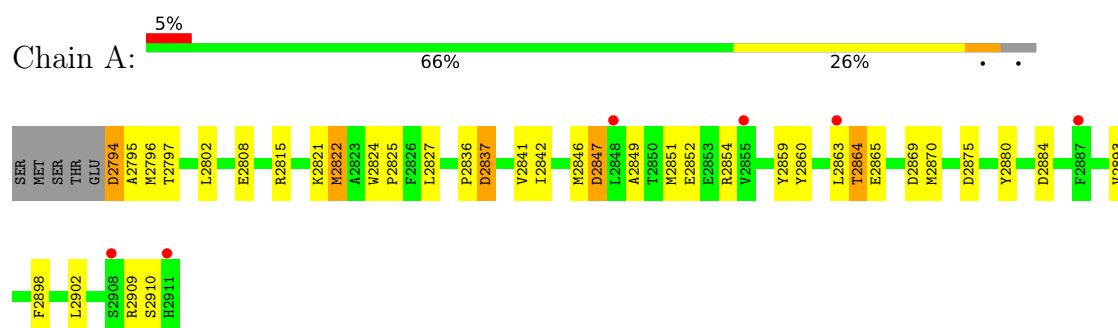


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			51	20	26	4	1		
2	B	1	Total	C	H	N	O	0	0
			51	20	26	4	1		
2	C	1	Total	C	H	N	O	0	0
			51	20	26	4	1		
2	D	1	Total	C	H	N	O	0	0
			51	20	26	4	1		
2	E	1	Total	C	H	N	O	0	0
			51	20	26	4	1		
2	F	1	Total	C	H	N	O	0	0
			51	20	26	4	1		

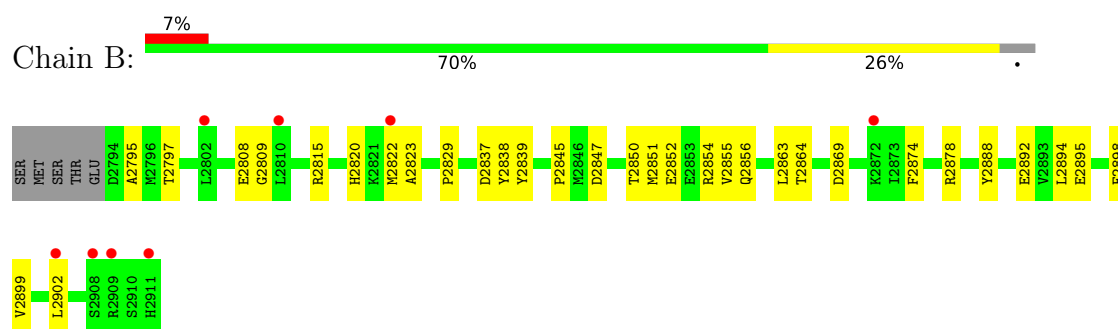
3 Residue-property plots [i](#)

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.

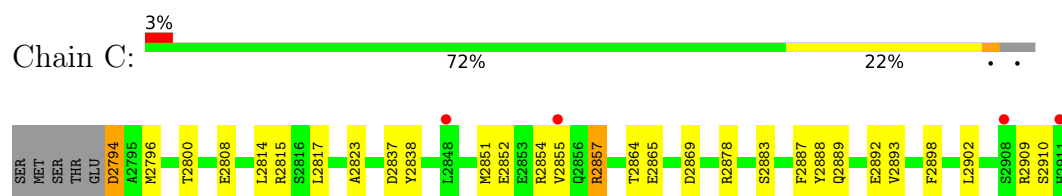
- Molecule 1: Nucleosome-remodeling factor subunit BPTF



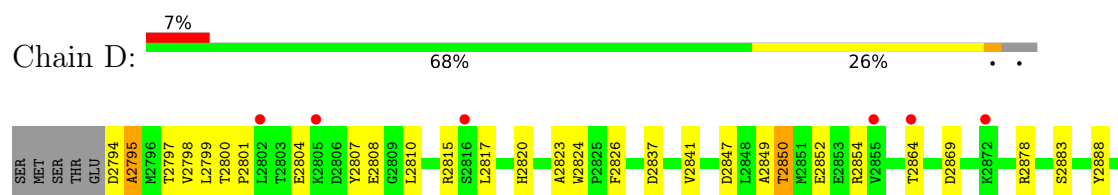
- Molecule 1: Nucleosome-remodeling factor subunit BPTF

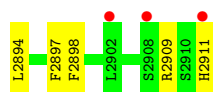


- Molecule 1: Nucleosome-remodeling factor subunit BPTF

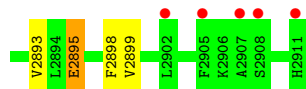
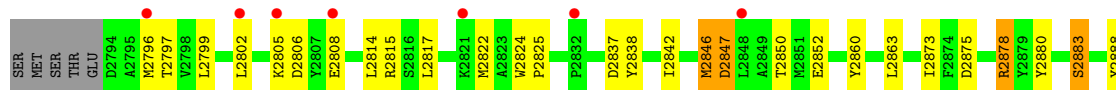


- Molecule 1: Nucleosome-remodeling factor subunit BPTF

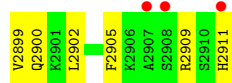
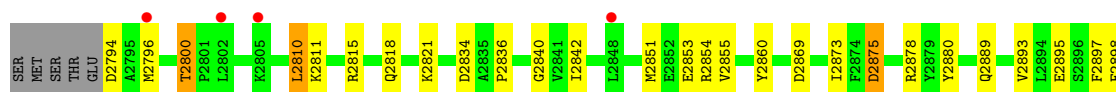




- Molecule 1: Nucleosome-remodeling factor subunit BPTF



- Molecule 1: Nucleosome-remodeling factor subunit BPTF



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.75Å 166.75Å 161.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.82 – 2.84 53.82 – 2.84	Depositor EDS
% Data completeness (in resolution range)	98.6 (53.82-2.84) 98.6 (53.82-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.267 , 0.346 0.267 , 0.346	Depositor DCC
R_{free} test set	1627 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12081	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2068e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: JC3

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	0.74	0/1051	0.79	2/1422 (0.1%)
1	B	0.73	0/1053	0.76	0/1423
1	C	0.81	0/1053	0.89	1/1423 (0.1%)
1	D	0.70	0/1045	0.78	0/1412
1	E	0.74	1/1068 (0.1%)	0.87	2/1443 (0.1%)
1	F	0.91	1/1059 (0.1%)	0.95	3/1431 (0.2%)
All	All	0.78	2/6329 (0.0%)	0.84	8/8554 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2895	GLU	CB-CG	5.53	1.62	1.52
1	F	2821	LYS	CB-CG	5.06	1.66	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2794	ASP	CB-CG-OD1	6.08	123.77	118.30
1	E	2875	ASP	CB-CG-OD1	5.51	123.26	118.30
1	F	2810	LEU	CA-CB-CG	5.46	127.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2875	ASP	CB-CG-OD1	5.31	123.08	118.30
1	E	2878	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	2875	ASP	CB-CG-OD1	5.24	123.01	118.30
1	F	2834	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	C	2794	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2809	GLY	Peptide
1	D	2795	ALA	Peptide

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	990	962	935	23	0
1	B	992	968	941	16	0
1	C	992	968	941	14	0
1	D	988	966	941	16	0
1	E	999	980	949	19	0
1	F	994	976	947	16	0
2	A	25	26	0	0	0
2	B	25	26	0	0	0
2	C	25	26	0	0	0
2	D	25	26	0	0	0
2	E	25	26	0	0	0
2	F	25	26	0	0	0
All	All	6105	5976	5654	101	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 9.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2854:ARG:NH1	1:B:2869:ASP:OD2	1.99	0.95
1:D:2854:ARG:NH1	1:D:2869:ASP:OD2	2.09	0.86
1:D:2847:ASP:OD1	1:D:2850:THR:N	2.19	0.75
1:C:2800:THR:O	1:C:2909:ARG:NH2	2.22	0.73
1:D:2800:THR:O	1:D:2909:ARG:NH2	2.26	0.68
1:C:2854:ARG:NH1	1:C:2869:ASP:OD2	2.26	0.67
1:E:2815:ARG:NH1	1:E:2852[A]:GLU:OE2	2.28	0.65
1:D:2795:ALA:HB1	1:D:2798:VAL:HG23	1.82	0.62
1:E:2895:GLU:O	1:E:2899:VAL:HG23	1.99	0.62
1:E:2802:LEU:HD12	1:E:2860:TYR:O	2.02	0.60
1:D:2795:ALA:HA	1:D:2797:THR:H	1.69	0.58
1:F:2800:THR:HG22	1:F:2800:THR:O	2.04	0.58
1:D:2815:ARG:NH1	1:D:2852:GLU:OE1	2.37	0.57
1:B:2847:ASP:N	1:B:2847:ASP:OD1	2.34	0.57
1:E:2878:ARG:NH2	1:E:2895:GLU:OE1	2.34	0.56
1:F:2842:ILE:HD11	1:F:2880:TYR:HB2	1.88	0.56
1:C:2815:ARG:CZ	1:C:2852[A]:GLU:OE2	2.53	0.56
1:A:2815:ARG:NH1	1:A:2852[A]:GLU:OE2	2.39	0.55
1:C:2814:LEU:HD23	1:C:2852[A]:GLU:HG3	1.89	0.54
1:B:2851:MET:O	1:B:2855:VAL:HG23	2.08	0.53
1:A:2847:ASP:N	1:A:2847:ASP:OD1	2.42	0.53
1:A:2836:PRO:O	1:A:2837:ASP:OD1	2.26	0.53
1:C:2889:GLN:O	1:C:2893:VAL:HG23	2.09	0.52
1:B:2829:PRO:HG3	1:B:2847:ASP:OD2	2.10	0.52
1:B:2823:ALA:HA	1:B:2894:LEU:HD22	1.91	0.52
1:B:2878:ARG:HD3	1:B:2892:GLU:OE1	2.10	0.52
1:C:2898:PHE:CZ	1:C:2902:LEU:HD22	2.46	0.51
1:A:2797:THR:HG23	1:A:2863:LEU:HD23	1.92	0.51
1:A:2854:ARG:NH1	1:A:2869:ASP:OD2	2.45	0.50
1:E:2846:MET:HB3	1:E:2873:ILE:HG13	1.93	0.50
1:E:2842:ILE:HD11	1:E:2880:TYR:HB2	1.93	0.50
1:E:2814:LEU:HD23	1:E:2852[A]:GLU:HG3	1.92	0.50
1:F:2895:GLU:O	1:F:2899:VAL:HG23	2.11	0.49
1:C:2796:MET:SD	1:C:2910:SER:HA	2.52	0.49
1:D:2799:LEU:O	1:D:2801:PRO:HD3	2.12	0.49
1:A:2824:TRP:N	1:A:2825:PRO:CD	2.76	0.49
1:B:2878:ARG:HA	1:B:2888:TYR:CD2	2.48	0.48
1:B:2898:PHE:CZ	1:B:2902:LEU:HD22	2.48	0.48
1:C:2837:ASP:O	1:C:2838:TYR:C	2.51	0.47
1:C:2817:LEU:O	1:C:2823:ALA:HB2	2.13	0.47
1:C:2878:ARG:HA	1:C:2888:TYR:CD2	2.50	0.47
1:E:2817:LEU:HD21	1:E:2898:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2797:THR:HG23	1:E:2863:LEU:HD23	1.97	0.47
1:D:2817:LEU:O	1:D:2823:ALA:HB2	2.15	0.47
1:F:2898:PHE:CZ	1:F:2902:LEU:HD22	2.50	0.47
1:E:2822:MET:HG3	1:E:2893:VAL:HG11	1.96	0.46
1:B:2797:THR:HG23	1:B:2863:LEU:HD23	1.98	0.46
1:A:2822:MET:HG2	1:A:2893:VAL:HG11	1.98	0.46
1:D:2817:LEU:O	1:D:2823:ALA:CB	2.64	0.45
1:A:2842:ILE:HD11	1:A:2880:TYR:HB2	1.97	0.45
1:B:2837:ASP:O	1:B:2838:TYR:C	2.54	0.45
1:A:2837:ASP:O	1:A:2841:VAL:HG22	2.16	0.45
1:F:2796[B]:MET:SD	1:F:2800:THR:HG21	2.56	0.45
1:A:2824:TRP:N	1:A:2825:PRO:HD3	2.32	0.45
1:A:2847:ASP:O	1:A:2851:MET:HG3	2.17	0.45
1:D:2878:ARG:HA	1:D:2888:TYR:CD2	2.51	0.45
1:E:2883:SER:HA	1:E:2888:TYR:CD2	2.52	0.45
1:C:2878:ARG:HD3	1:C:2892:GLU:OE1	2.17	0.45
1:C:2851:MET:O	1:C:2855:VAL:HG23	2.16	0.45
1:B:2874:PHE:CD2	1:B:2895:GLU:HB2	2.52	0.45
1:A:2796:MET:SD	1:A:2910:SER:HB3	2.58	0.44
1:E:2824:TRP:N	1:E:2825:PRO:HD3	2.32	0.44
1:B:2795:ALA:HB2	1:D:2824:TRP:CZ2	2.52	0.44
1:D:2837:ASP:O	1:D:2841:VAL:HG13	2.18	0.44
1:F:2854:ARG:NH1	1:F:2869:ASP:OD2	2.50	0.44
1:F:2889:GLN:O	1:F:2893:VAL:HG23	2.17	0.44
1:D:2894:LEU:HD12	1:D:2894:LEU:HA	1.90	0.43
1:A:2851:MET:HE3	1:A:2860:TYR:OH	2.18	0.43
1:E:2838:TYR:CZ	1:E:2842:ILE:HG13	2.54	0.43
1:E:2805:LYS:O	1:E:2806:ASP:C	2.56	0.43
1:A:2794:ASP:HB3	1:A:2797:THR:OG1	2.19	0.43
1:F:2851:MET:O	1:F:2855:VAL:HG23	2.19	0.42
1:A:2898:PHE:O	1:A:2902:LEU:N	2.51	0.42
1:B:2847:ASP:OD1	1:B:2850:THR:HB	2.18	0.42
1:E:2805:LYS:O	1:E:2808:GLU:N	2.48	0.42
1:F:2875:ASP:OD1	1:F:2878:ARG:NH2	2.49	0.42
1:E:2837:ASP:HB2	1:F:2840:GLY:HA2	2.00	0.42
1:B:2839:TYR:CE2	1:B:2845:PRO:HG2	2.55	0.42
1:C:2883:SER:HA	1:C:2888:TYR:CD2	2.53	0.42
1:B:2815:ARG:NH1	1:B:2852[A]:GLU:OE2	2.53	0.42
1:A:2795:ALA:HB2	1:E:2824:TRP:CE2	2.55	0.41
1:A:2870:MET:HG2	1:A:2898:PHE:CZ	2.55	0.41
1:E:2824:TRP:N	1:E:2825:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2800:THR:O	1:F:2800:THR:CG2	2.68	0.41
1:A:2864[A]:THR:CG2	1:A:2865:GLU:N	2.83	0.41
1:A:2851:MET:HE3	1:A:2869:ASP:HB3	2.03	0.41
1:A:2851:MET:CE	1:A:2860:TYR:OH	2.68	0.41
1:D:2847:ASP:OD1	1:D:2849:ALA:N	2.53	0.41
1:D:2897:PHE:O	1:D:2898:PHE:C	2.59	0.41
1:E:2847:ASP:OD2	1:E:2850:THR:N	2.44	0.41
1:A:2846:MET:HG2	1:A:2869:ASP:O	2.21	0.41
1:F:2815:ARG:O	1:F:2818:GLN:N	2.53	0.41
1:A:2802:LEU:HD12	1:A:2860:TYR:O	2.21	0.41
1:B:2820:HIS:HD2	1:B:2822:MET:H	1.68	0.41
1:F:2810:LEU:HD23	1:F:2905:PHE:CZ	2.55	0.40
1:C:2883:SER:HA	1:C:2888:TYR:CG	2.56	0.40
1:F:2897:PHE:HA	1:F:2900:GLN:OE1	2.21	0.40
1:A:2827:LEU:O	1:A:2849:ALA:HB2	2.22	0.40
1:F:2851:MET:HE3	1:F:2860:TYR:OH	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/123 (100%)	116 (94%)	7 (6%)	0	100	100
1	B	123/123 (100%)	116 (94%)	7 (6%)	0	100	100
1	C	123/123 (100%)	114 (93%)	8 (6%)	1 (1%)	19	38
1	D	122/123 (99%)	103 (84%)	19 (16%)	0	100	100
1	E	125/123 (102%)	113 (90%)	12 (10%)	0	100	100
1	F	124/123 (101%)	116 (94%)	8 (6%)	0	100	100
All	All	740/738 (100%)	678 (92%)	61 (8%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2857	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	113/112 (101%)	103 (91%)	10 (9%)	10	21
1	B	113/112 (101%)	109 (96%)	4 (4%)	36	61
1	C	113/112 (101%)	107 (95%)	6 (5%)	22	43
1	D	112/112 (100%)	101 (90%)	11 (10%)	8	16
1	E	115/112 (103%)	109 (95%)	6 (5%)	23	44
1	F	114/112 (102%)	107 (94%)	7 (6%)	18	36
All	All	680/672 (101%)	636 (94%)	44 (6%)	17	33

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2808	GLU
1	A	2821	LYS
1	A	2822	MET
1	A	2837	ASP
1	A	2847	ASP
1	A	2859	TYR
1	A	2864[A]	THR
1	A	2864[B]	THR
1	A	2884	ASP
1	A	2909	ARG
1	B	2808	GLU
1	B	2856	GLN
1	B	2864	THR
1	B	2899	VAL
1	C	2794	ASP
1	C	2808	GLU

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Mol	Chain	Res	Type
1	C	2857	ARG
1	C	2864	THR
1	C	2865	GLU
1	C	2887	PHE
1	D	2794	ASP
1	D	2804	GLU
1	D	2808	GLU
1	D	2810	LEU
1	D	2820	HIS
1	D	2826	PHE
1	D	2850	THR
1	D	2864[A]	THR
1	D	2864[B]	THR
1	D	2883	SER
1	D	2911	HIS
1	E	2796[A]	MET
1	E	2796[B]	MET
1	E	2799	LEU
1	E	2846	MET
1	E	2847	ASP
1	E	2883	SER
1	F	2794	ASP
1	F	2800	THR
1	F	2811	LYS
1	F	2836	PRO
1	F	2853	GLU
1	F	2909	ARG
1	F	2911	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	2833	ASN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	JC3	C	3001	-	26,28,28	4.40	10 (38%)	26,40,40	3.03	17 (65%)
2	JC3	E	3001	-	26,28,28	4.45	12 (46%)	26,40,40	2.86	12 (46%)
2	JC3	A	3001	-	26,28,28	4.33	13 (50%)	26,40,40	2.57	9 (34%)
2	JC3	D	3001	-	26,28,28	4.63	12 (46%)	26,40,40	2.86	14 (53%)
2	JC3	F	3001	-	26,28,28	4.47	11 (42%)	26,40,40	2.92	13 (50%)
2	JC3	B	3001	-	26,28,28	4.56	12 (46%)	26,40,40	2.20	9 (34%)

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	JC3	C	3001	-	-	0/8/26/26	0/4/4/4
2	JC3	E	3001	-	-	0/8/26/26	0/4/4/4
2	JC3	A	3001	-	-	0/8/26/26	0/4/4/4
2	JC3	D	3001	-	-	0/8/26/26	0/4/4/4
2	JC3	F	3001	-	-	0/8/26/26	0/4/4/4
2	JC3	B	3001	-	-	0/8/26/26	0/4/4/4

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	JC3	C1-N2	-11.71	1.19	1.46
2	F	3001	JC3	C1-N2	-11.59	1.19	1.46
2	B	3001	JC3	C1-N2	-11.18	1.20	1.46
2	A	3001	JC3	C1-N2	-11.14	1.21	1.46
2	E	3001	JC3	C1-N2	-11.08	1.21	1.46
2	E	3001	JC3	C9-N10	10.86	1.48	1.33
2	D	3001	JC3	C1-N2	-10.77	1.21	1.46
2	F	3001	JC3	C9-N10	10.55	1.48	1.33
2	D	3001	JC3	C9-N10	10.45	1.48	1.33
2	C	3001	JC3	C9-N10	10.17	1.47	1.33
2	A	3001	JC3	C9-N10	10.10	1.47	1.33
2	B	3001	JC3	C9-N10	9.87	1.47	1.33
2	B	3001	JC3	C5-C4	-9.46	1.41	1.53
2	F	3001	JC3	C5-C4	-8.95	1.42	1.53
2	D	3001	JC3	C15-C11	8.52	1.51	1.39
2	C	3001	JC3	C5-C4	-8.49	1.42	1.53
2	B	3001	JC3	C15-C11	8.06	1.51	1.39
2	D	3001	JC3	C5-C4	-8.03	1.43	1.53
2	F	3001	JC3	C15-C11	7.79	1.50	1.39
2	A	3001	JC3	C15-C11	7.58	1.50	1.39
2	E	3001	JC3	C15-C11	7.56	1.50	1.39
2	A	3001	JC3	C5-C4	-7.49	1.43	1.53
2	E	3001	JC3	C5-C4	-7.43	1.44	1.53
2	D	3001	JC3	C16-N18	7.42	1.49	1.38
2	E	3001	JC3	C16-N18	7.11	1.48	1.38
2	F	3001	JC3	C11-N10	6.47	1.45	1.34
2	C	3001	JC3	C11-N10	6.34	1.45	1.34
2	D	3001	JC3	C11-N10	6.27	1.45	1.34
2	C	3001	JC3	C15-C11	6.17	1.48	1.39
2	B	3001	JC3	C11-N10	6.15	1.45	1.34
2	D	3001	JC3	C5-C6	-5.87	1.43	1.52
2	B	3001	JC3	C16-N18	5.86	1.46	1.38
2	C	3001	JC3	C16-N18	5.79	1.46	1.38
2	A	3001	JC3	C11-N10	5.52	1.44	1.34
2	C	3001	JC3	C5-C6	-4.98	1.45	1.52
2	B	3001	JC3	C5-C6	-4.95	1.45	1.52
2	A	3001	JC3	C5-C6	-4.92	1.45	1.52
2	D	3001	JC3	C16-C15	4.78	1.51	1.41
2	E	3001	JC3	C11-N10	4.77	1.42	1.34
2	E	3001	JC3	C5-C6	-4.69	1.45	1.52
2	A	3001	JC3	C16-N18	4.66	1.45	1.38
2	F	3001	JC3	C5-C6	-4.64	1.45	1.52
2	F	3001	JC3	C16-N18	4.45	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3001	JC3	C16-C15	4.18	1.50	1.41
2	B	3001	JC3	C16-C15	4.08	1.50	1.41
2	C	3001	JC3	C14-C15	-3.96	1.46	1.51
2	A	3001	JC3	C20-C4	3.96	1.60	1.52
2	F	3001	JC3	C14-C15	-3.90	1.46	1.51
2	B	3001	JC3	C12-C11	-3.77	1.47	1.50
2	A	3001	JC3	C3-C4	3.58	1.57	1.53
2	E	3001	JC3	C12-C11	-3.57	1.47	1.50
2	C	3001	JC3	C7-C6	3.45	1.57	1.51
2	F	3001	JC3	C16-C15	3.44	1.48	1.41
2	A	3001	JC3	C12-C11	-3.41	1.48	1.50
2	A	3001	JC3	C16-C15	3.17	1.48	1.41
2	D	3001	JC3	C12-C11	-3.16	1.48	1.50
2	E	3001	JC3	C20-C4	3.15	1.58	1.52
2	E	3001	JC3	C14-C15	-3.07	1.47	1.51
2	C	3001	JC3	C16-C15	2.91	1.47	1.41
2	D	3001	JC3	C7-C6	2.88	1.56	1.51
2	B	3001	JC3	C20-C4	2.87	1.58	1.52
2	A	3001	JC3	C14-C15	-2.71	1.48	1.51
2	F	3001	JC3	C20-C4	2.60	1.57	1.52
2	D	3001	JC3	C20-C4	2.59	1.57	1.52
2	B	3001	JC3	C14-C15	-2.49	1.48	1.51
2	E	3001	JC3	C7-C6	2.47	1.56	1.51
2	D	3001	JC3	C3-C4	2.39	1.56	1.53
2	A	3001	JC3	O17-C16	-2.39	1.18	1.24
2	B	3001	JC3	C7-N2	-2.23	1.43	1.46
2	F	3001	JC3	O17-C16	-2.02	1.19	1.24

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	JC3	C4-C5-C6	-6.69	104.73	110.83
2	F	3001	JC3	C12-C11-N10	6.45	132.44	123.41
2	E	3001	JC3	C7-N2-C3	5.81	120.31	111.20
2	D	3001	JC3	C15-C11-N10	-5.77	119.48	125.80
2	C	3001	JC3	C12-C11-N10	5.66	131.32	123.41
2	D	3001	JC3	C12-C11-N10	5.54	131.16	123.41
2	F	3001	JC3	C15-C11-N10	-5.47	119.80	125.80
2	D	3001	JC3	C9-N10-C11	5.47	122.22	116.33
2	F	3001	JC3	C5-C6-N8	-5.42	102.33	110.60
2	E	3001	JC3	C4-C3-N2	5.33	113.85	110.56
2	E	3001	JC3	C4-C5-C6	-5.10	106.18	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3001	JC3	C7-C6-N8	4.92	116.01	109.71
2	C	3001	JC3	C5-C6-N8	-4.89	103.13	110.60
2	C	3001	JC3	C15-C11-N10	-4.68	120.67	125.80
2	F	3001	JC3	C12-C11-C15	-4.62	107.76	111.09
2	A	3001	JC3	C15-C11-N10	-4.51	120.86	125.80
2	A	3001	JC3	C7-N2-C3	4.50	118.26	111.20
2	E	3001	JC3	C15-C11-N10	-4.46	120.91	125.80
2	B	3001	JC3	C15-C11-N10	-4.33	121.05	125.80
2	C	3001	JC3	C7-N2-C3	4.31	117.96	111.20
2	C	3001	JC3	C12-C11-C15	-4.29	108.00	111.09
2	D	3001	JC3	C5-C4-C3	4.25	113.93	109.76
2	E	3001	JC3	C12-C11-N10	4.14	129.20	123.41
2	B	3001	JC3	C12-C11-N10	4.05	129.07	123.41
2	A	3001	JC3	C12-C11-N10	4.01	129.02	123.41
2	A	3001	JC3	C5-C6-N8	-3.99	104.51	110.60
2	C	3001	JC3	C25-C20-C21	3.90	123.15	118.29
2	D	3001	JC3	C5-C6-N8	-3.88	104.68	110.60
2	F	3001	JC3	C7-C6-N8	3.86	114.67	109.71
2	A	3001	JC3	C1-N2-C7	3.71	114.80	110.57
2	C	3001	JC3	C5-C4-C20	-3.65	105.80	112.56
2	F	3001	JC3	C4-C5-C6	-3.64	107.51	110.83
2	D	3001	JC3	C13-C12-C11	3.58	106.54	103.93
2	C	3001	JC3	C14-C13-C12	-3.56	99.86	107.08
2	B	3001	JC3	C14-C15-C11	-3.52	106.80	110.96
2	F	3001	JC3	C13-C12-C11	3.48	106.46	103.93
2	C	3001	JC3	C9-N10-C11	3.47	120.07	116.33
2	E	3001	JC3	C14-C15-C11	-3.46	106.87	110.96
2	D	3001	JC3	C7-N2-C3	3.44	116.60	111.20
2	D	3001	JC3	C7-C6-N8	3.40	114.07	109.71
2	A	3001	JC3	C7-C6-N8	3.40	114.06	109.71
2	C	3001	JC3	C13-C12-C11	3.35	106.37	103.93
2	C	3001	JC3	C7-C6-N8	3.34	114.00	109.71
2	B	3001	JC3	C13-C12-C11	3.34	106.36	103.93
2	F	3001	JC3	C7-N2-C3	3.33	116.43	111.20
2	B	3001	JC3	C5-C6-N8	-3.29	105.57	110.60
2	D	3001	JC3	C5-C4-C20	-3.19	106.64	112.56
2	B	3001	JC3	C7-C6-N8	3.18	113.79	109.71
2	C	3001	JC3	C14-C15-C11	-3.14	107.25	110.96
2	E	3001	JC3	C9-N10-C11	3.12	119.69	116.33
2	C	3001	JC3	C4-C3-N2	-3.08	108.65	110.56
2	F	3001	JC3	C14-C15-C11	-3.06	107.34	110.96
2	C	3001	JC3	C4-C5-C6	-3.00	108.10	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3001	JC3	C5-C6-N8	-2.93	106.13	110.60
2	D	3001	JC3	C4-C5-C6	-2.92	108.16	110.83
2	F	3001	JC3	C14-C13-C12	-2.82	101.37	107.08
2	B	3001	JC3	C9-N10-C11	2.80	119.35	116.33
2	B	3001	JC3	C1-N2-C3	-2.77	107.41	110.57
2	B	3001	JC3	C25-C20-C21	2.62	121.56	118.29
2	E	3001	JC3	C1-N2-C3	-2.61	107.60	110.57
2	A	3001	JC3	C9-N10-C11	2.58	119.11	116.33
2	D	3001	JC3	C14-C15-C11	-2.51	108.00	110.96
2	D	3001	JC3	C1-N2-C3	-2.50	107.72	110.57
2	F	3001	JC3	C1-N2-C3	-2.46	107.77	110.57
2	F	3001	JC3	C25-C20-C21	2.43	121.32	118.29
2	D	3001	JC3	C12-C11-C15	-2.39	109.37	111.09
2	E	3001	JC3	C25-C20-C21	2.31	121.17	118.29
2	F	3001	JC3	C5-C4-C3	-2.26	107.54	109.76
2	C	3001	JC3	C25-C20-C4	-2.23	115.31	121.11
2	C	3001	JC3	C24-C25-C20	-2.23	117.89	120.65
2	D	3001	JC3	C25-C20-C21	2.22	121.07	118.29
2	A	3001	JC3	C1-N2-C3	2.08	112.94	110.57
2	C	3001	JC3	C1-N2-C7	2.04	112.90	110.57
2	E	3001	JC3	C14-C13-C12	-2.03	102.97	107.08

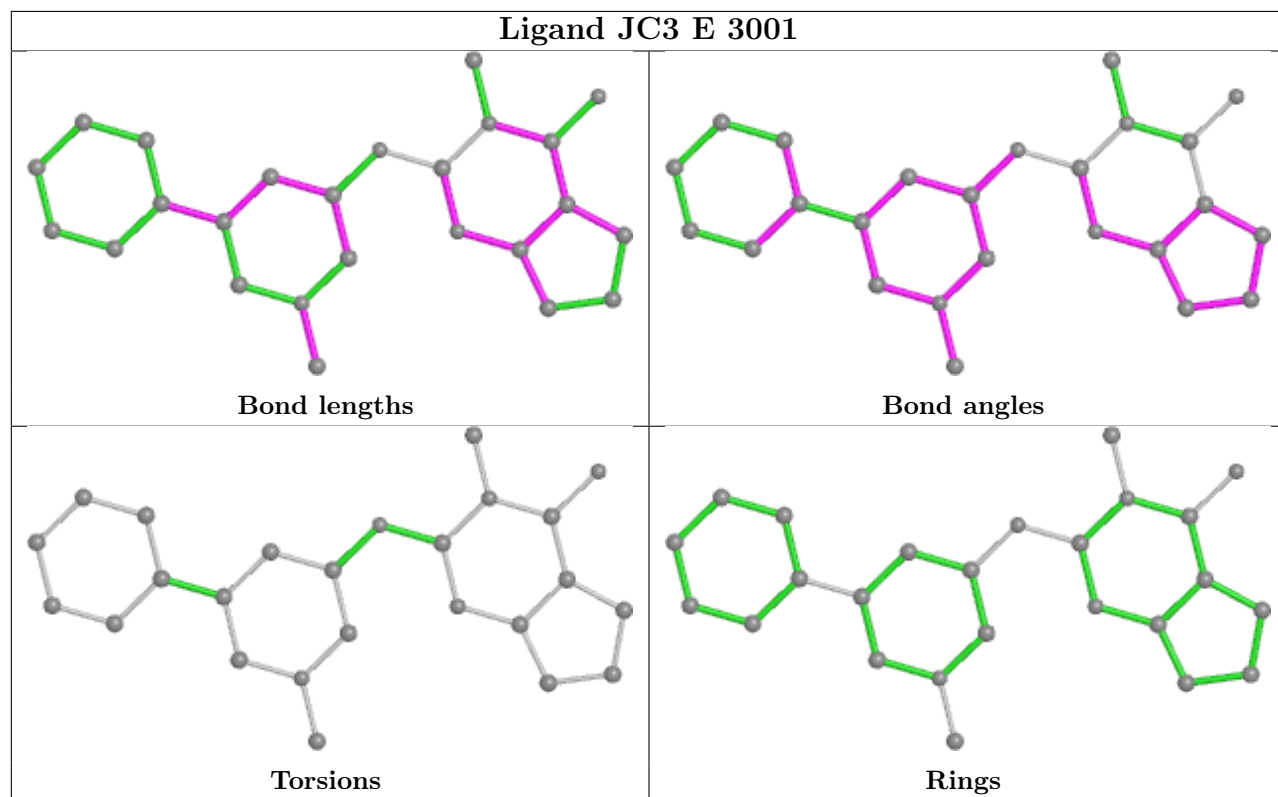
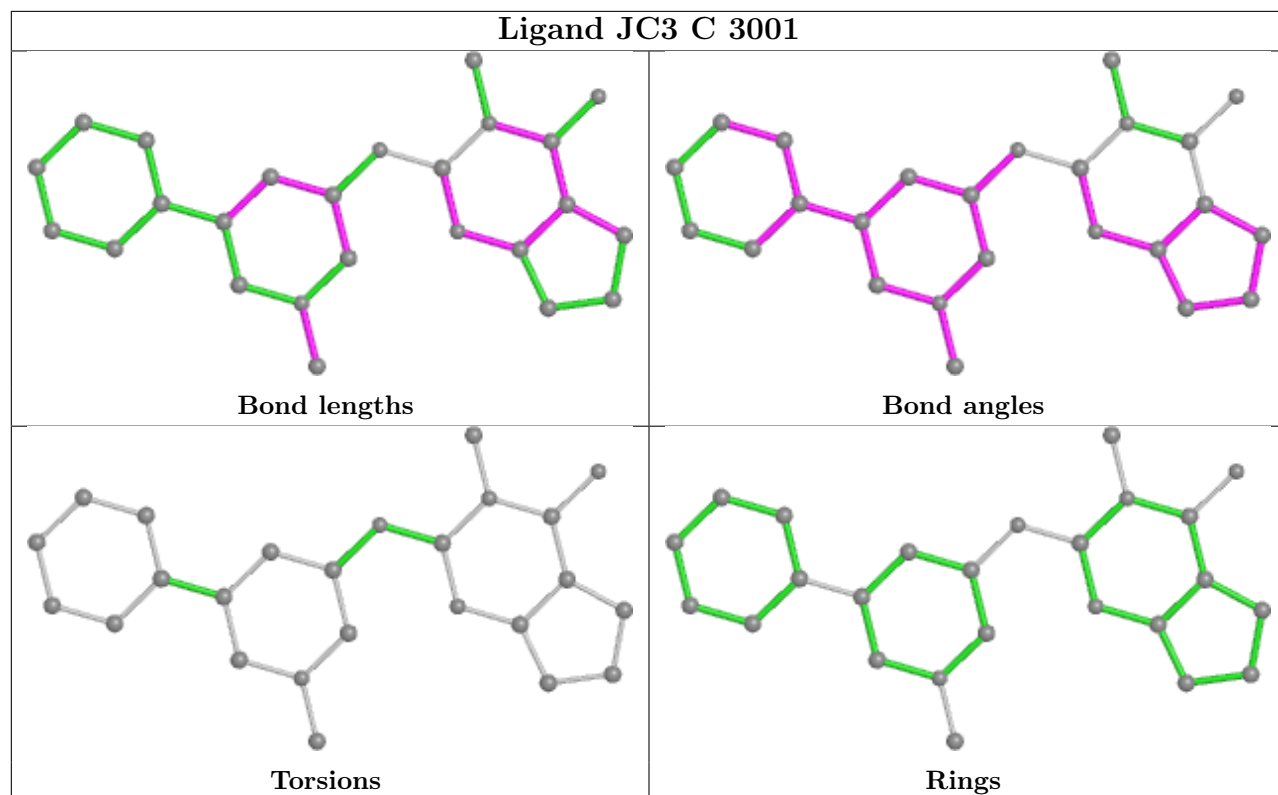
There are no chirality outliers.

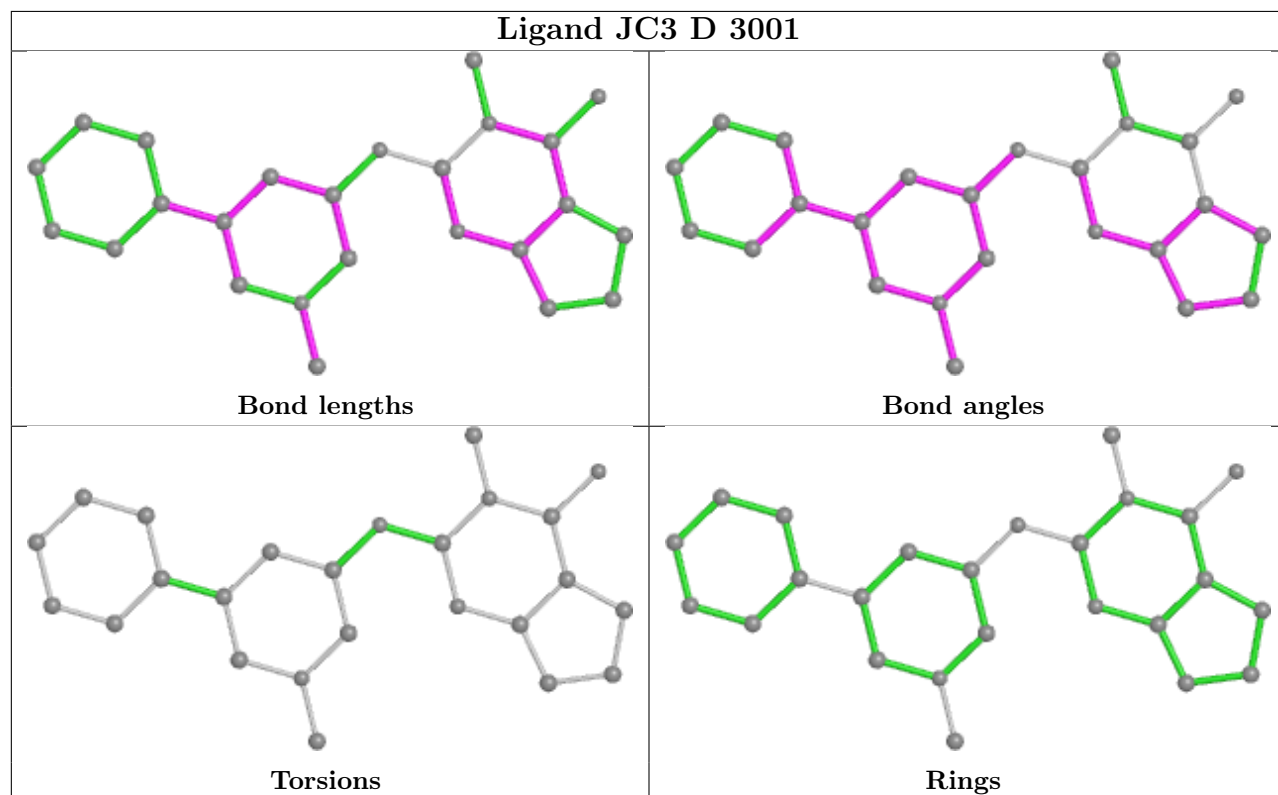
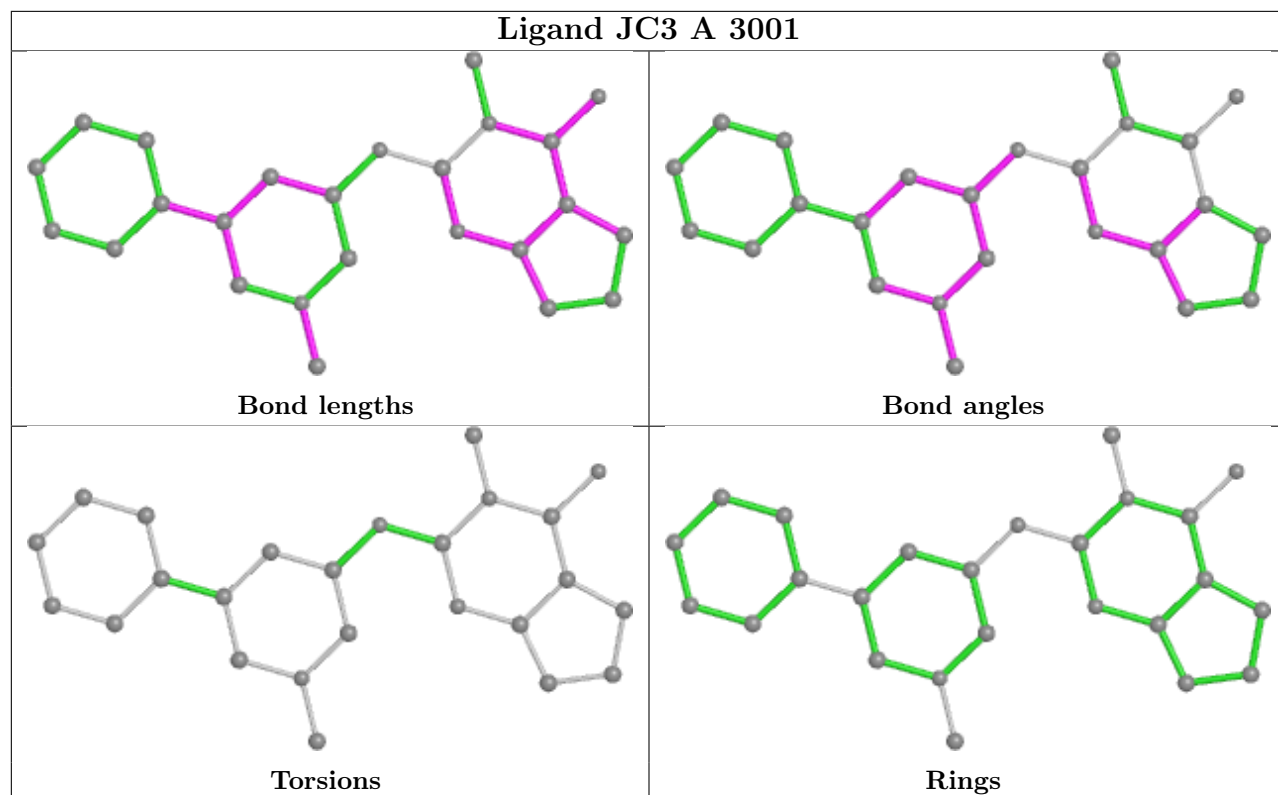
There are no torsion outliers.

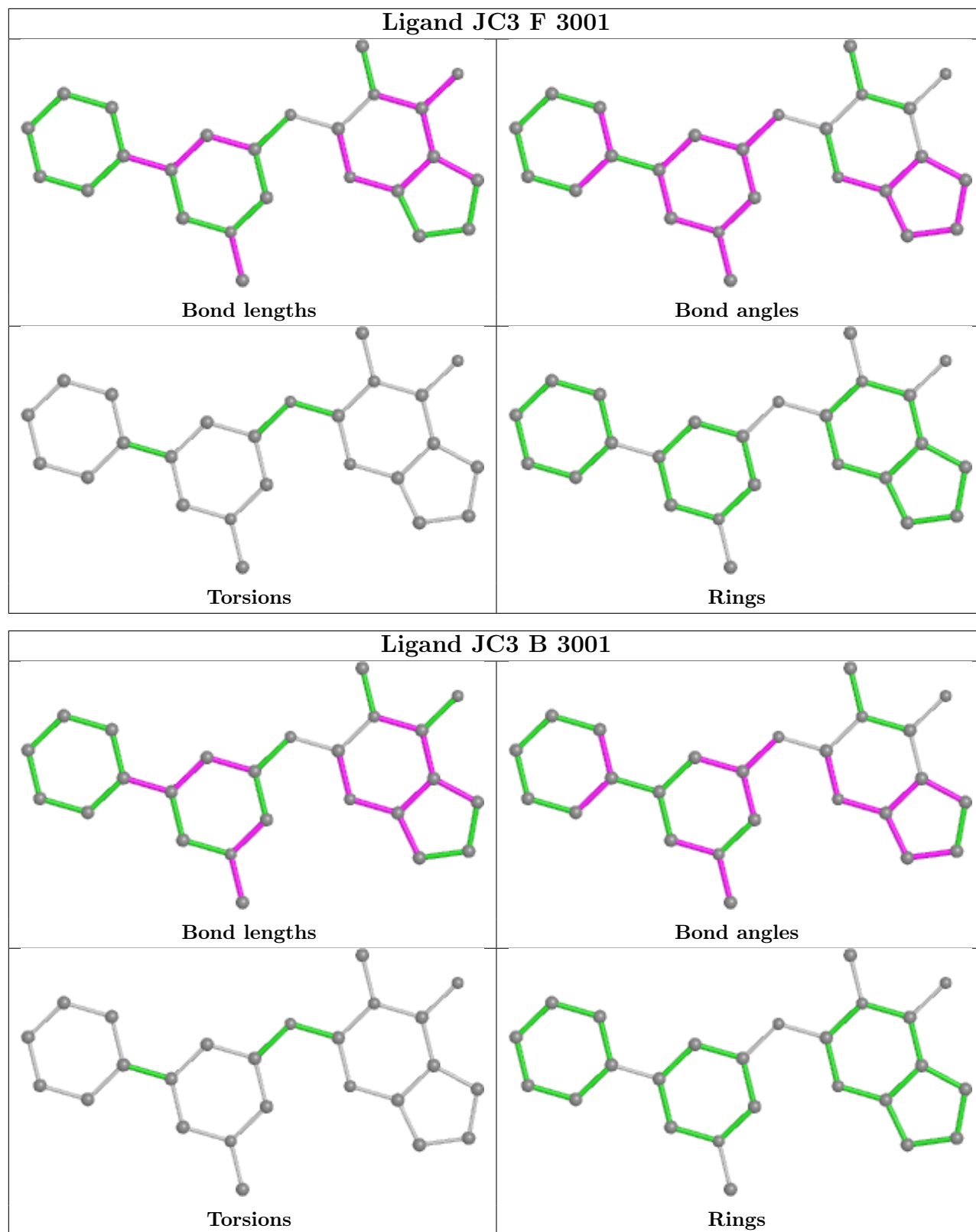
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	118/123 (95%)	0.78	6 (5%)	28 21	58, 78, 113, 151	0
1	B	118/123 (95%)	0.76	8 (6%)	17 11	49, 75, 102, 132	0
1	C	118/123 (95%)	0.75	4 (3%)	45 37	39, 59, 92, 117	0
1	D	118/123 (95%)	0.86	9 (7%)	13 8	60, 78, 105, 140	0
1	E	118/123 (95%)	0.86	12 (10%)	6 4	49, 77, 112, 131	0
1	F	118/123 (95%)	0.82	7 (5%)	22 16	39, 59, 96, 126	0
All	All	708/738 (95%)	0.81	46 (6%)	18 13	39, 73, 106, 151	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2911	HIS	7.8
1	A	2908[A]	SER	7.0
1	F	2908[A]	SER	6.5
1	B	2911	HIS	5.5
1	E	2908[A]	SER	4.7
1	E	2911	HIS	4.3
1	C	2911	HIS	4.1
1	E	2808	GLU	4.0
1	D	2805	LYS	3.9
1	A	2911	HIS	3.8
1	E	2848	LEU	3.4
1	C	2908[A]	SER	3.3
1	D	2855	VAL	3.3
1	E	2805	LYS	3.2
1	B	2802	LEU	2.9
1	A	2855	VAL	2.8
1	E	2796[A]	MET	2.8
1	E	2907	ALA	2.8
1	D	2908[A]	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	2796[A]	MET	2.6
1	F	2911	HIS	2.6
1	B	2908[A]	SER	2.6
1	B	2810	LEU	2.5
1	B	2902	LEU	2.5
1	F	2907	ALA	2.4
1	E	2821	LYS	2.4
1	A	2887	PHE	2.4
1	E	2802	LEU	2.4
1	B	2872[A]	LYS	2.3
1	F	2805	LYS	2.2
1	F	2802	LEU	2.2
1	D	2816[A]	SER	2.2
1	D	2902	LEU	2.2
1	E	2832	PRO	2.2
1	C	2855	VAL	2.2
1	A	2863	LEU	2.2
1	E	2905	PHE	2.2
1	B	2909	ARG	2.1
1	B	2822	MET	2.1
1	D	2864[A]	THR	2.1
1	C	2848	LEU	2.1
1	A	2848	LEU	2.0
1	D	2802	LEU	2.0
1	F	2848	LEU	2.0
1	D	2872[A]	LYS	2.0
1	E	2902	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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,

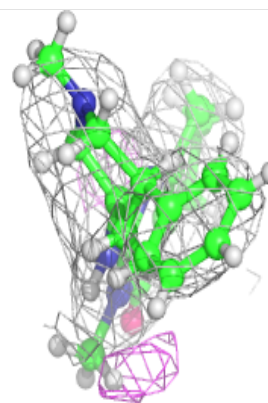
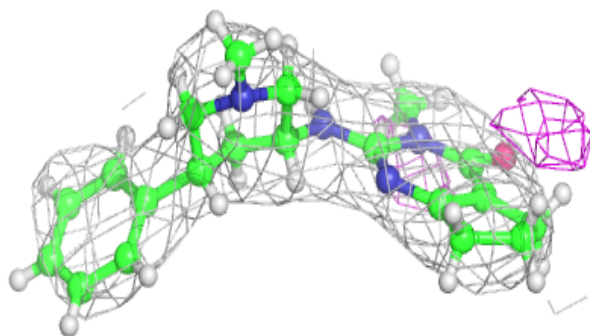
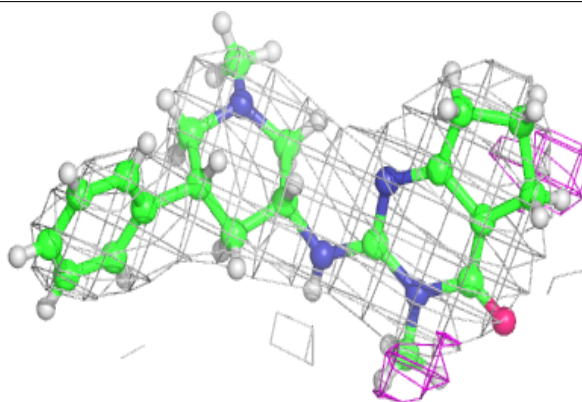
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	JC3	A	3001	25/25	0.92	0.29	48,73,104,113	0
2	JC3	E	3001	25/25	0.93	0.29	44,72,98,109	0
2	JC3	C	3001	25/25	0.94	0.28	29,52,91,109	0
2	JC3	D	3001	25/25	0.94	0.31	51,78,97,111	0
2	JC3	B	3001	25/25	0.94	0.33	36,69,85,89	0
2	JC3	F	3001	25/25	0.94	0.31	41,64,92,98	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.

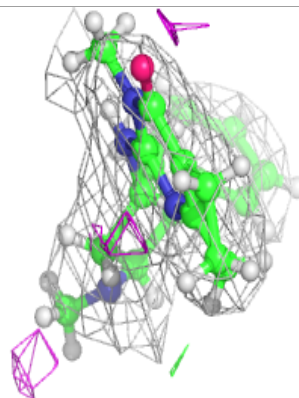
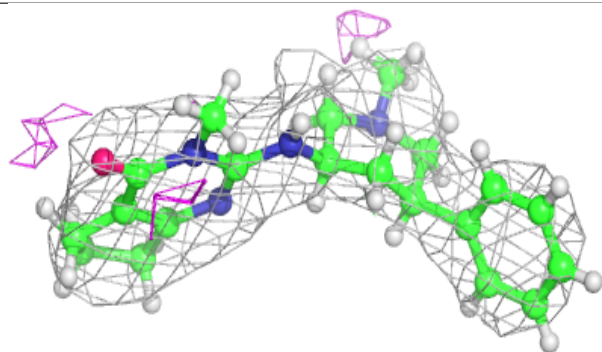
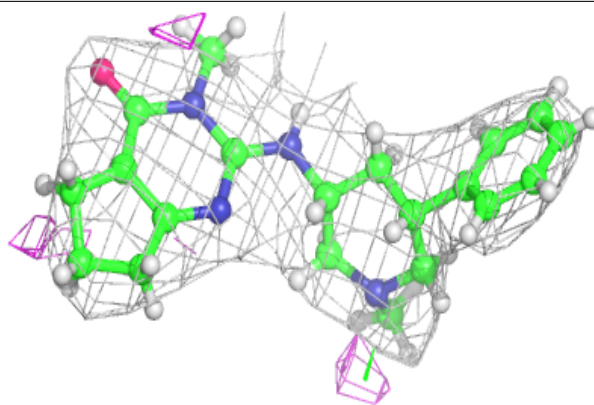
Electron density around JC3 A 3001:

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

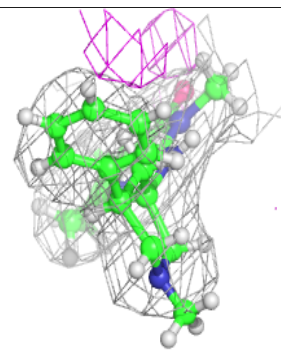
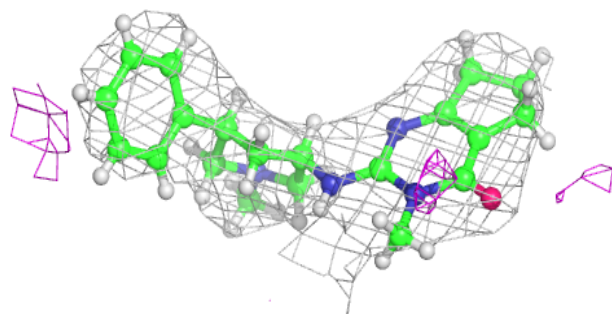
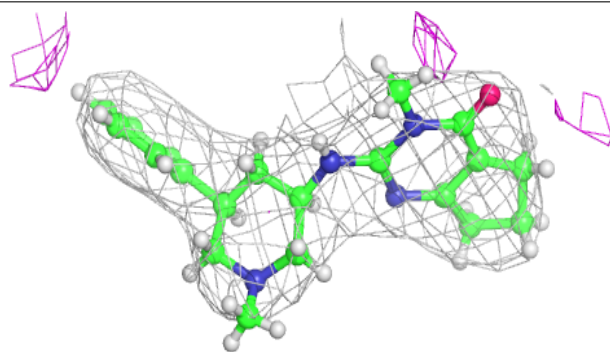


Electron density around JC3 E 3001:

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

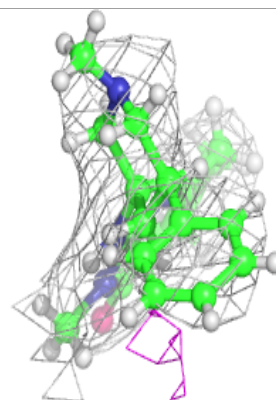
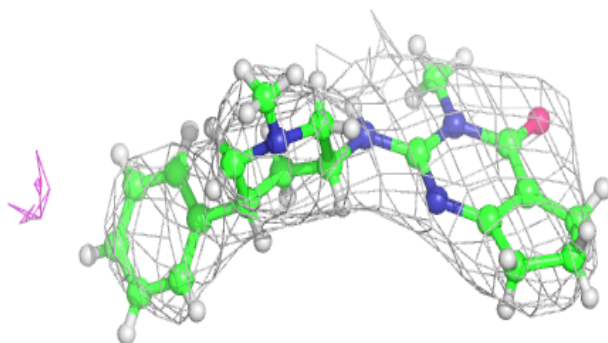
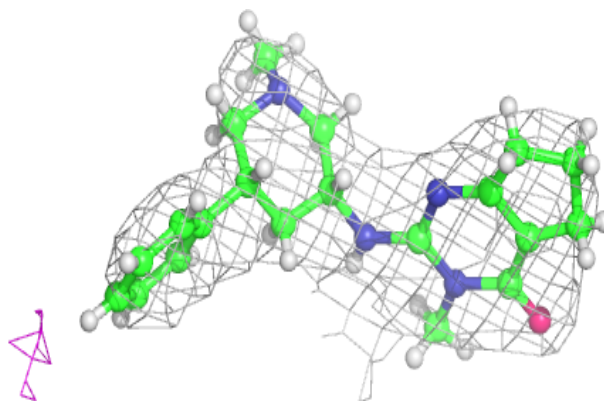
**Electron density around JC3 C 3001:**

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

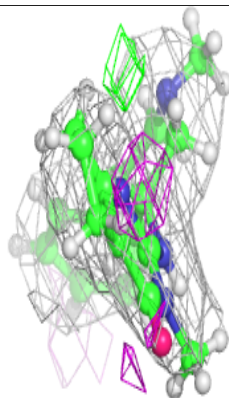
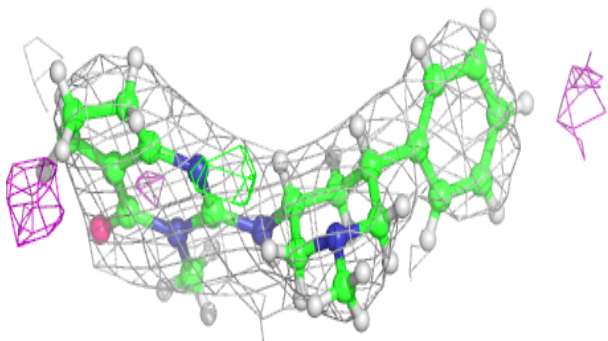
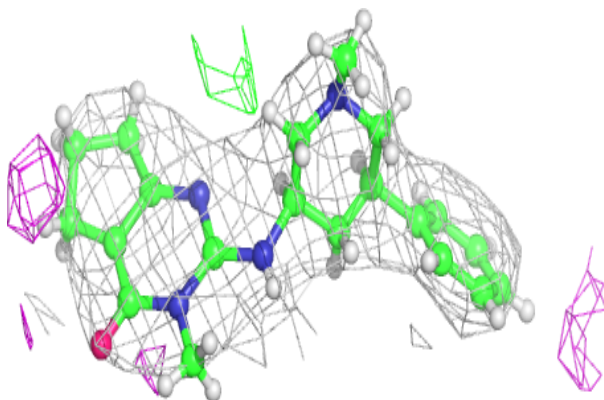


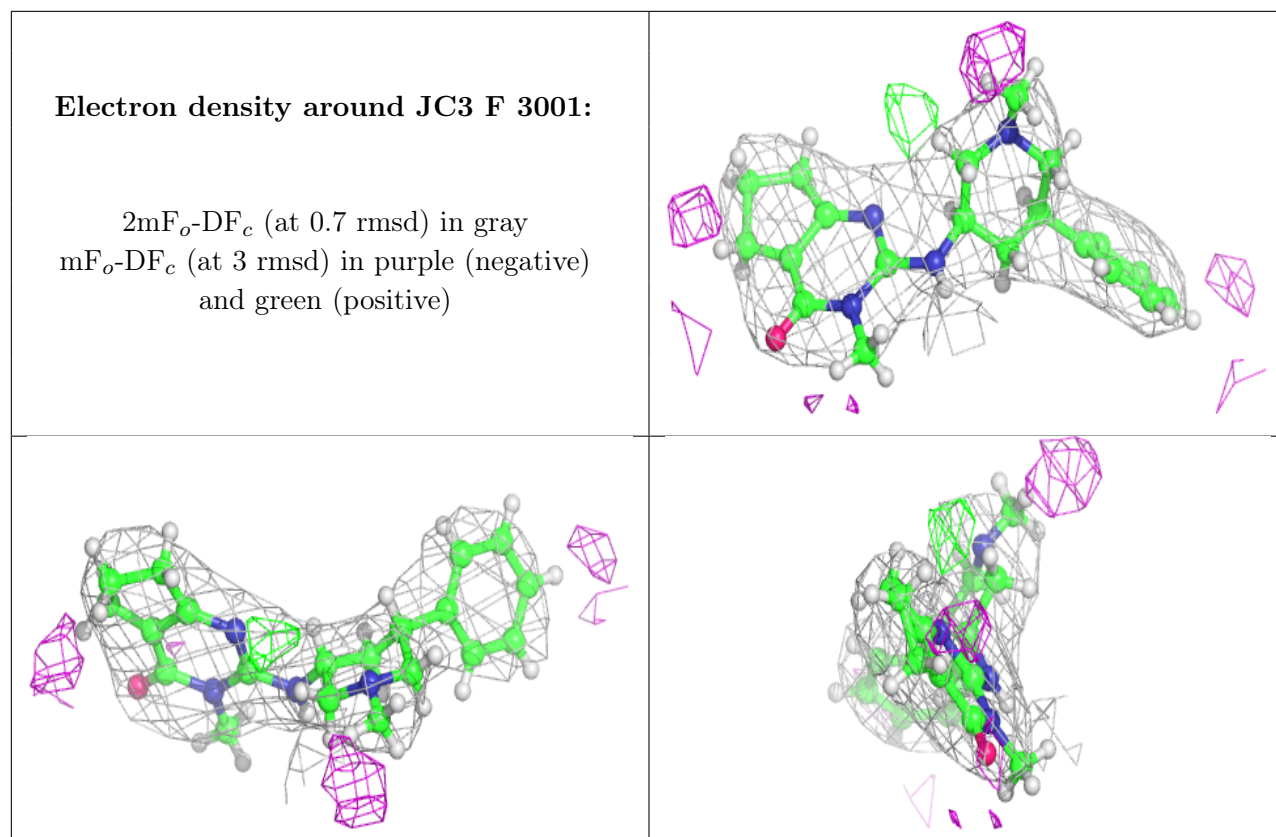
Electron density around JC3 D 3001:

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

**Electron density around JC3 B 3001:**

$2mF_o-DF_c$ (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.