



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 04:54 pm BST

PDB ID : 5ZZ4  
Title : Crystal structure of bruton's tyrosine kinase in complex with inhibitor 2e  
Authors : Kawahata, W.; Asami, T.; Irie, T.; Kiyoi, T.; Taniguchi, H.; Asamitsu, Y.;  
Inoue, T.; Miyake, T.; Sawa, M.  
Deposited on : 2018-05-30  
Resolution : 2.90 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](mailto: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.

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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 : 2.11  
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) : 2.11

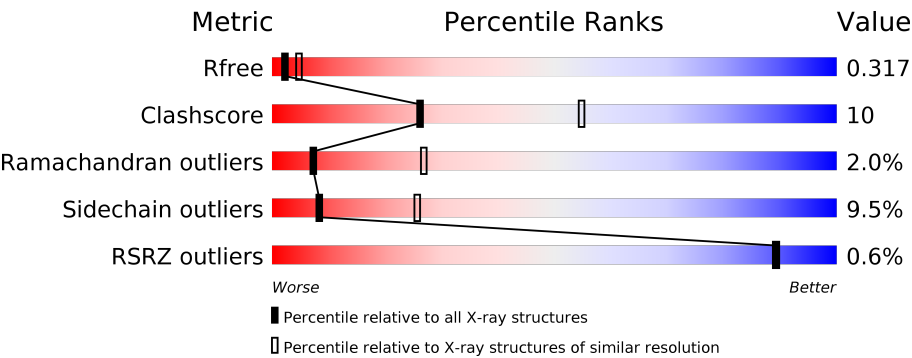
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	268	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>70%23%••</div></div>
1	B	268	<div><div></div><div></div><div></div><div></div><div></div></div> <div>68%26%••</div>
1	C	268	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>66%29%••</div></div>
1	D	268	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>67%26%5%•</div></div>
1	E	268	<div><div></div><div></div><div></div><div></div><div></div></div> <div>68%27%••</div>
1	F	268	<div><div></div><div></div><div></div><div></div><div></div></div> <div>70%26%••</div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12800 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 Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2091	1344	342	387	18			
1	B	263	Total	C	N	O	S	0	0	0
			2090	1338	340	394	18			
1	C	262	Total	C	N	O	S	0	0	0
			2092	1342	341	391	18			
1	D	263	Total	C	N	O	S	0	0	0
			2106	1352	345	390	19			
1	E	262	Total	C	N	O	S	0	0	0
			2089	1338	342	390	19			
1	F	263	Total	C	N	O	S	0	0	0
			2080	1330	343	388	19			

There are 24 discrepancies between the modelled and reference sequences:

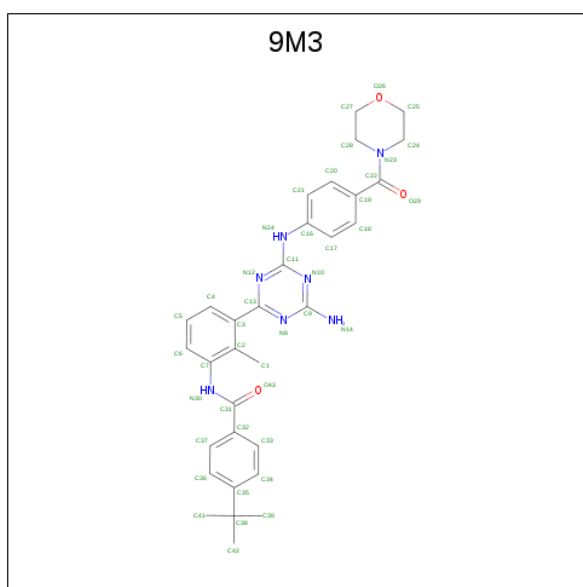
Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLY	-	expression tag	UNP Q06187
A	390	ALA	-	expression tag	UNP Q06187
A	391	MET	-	expression tag	UNP Q06187
A	392	GLY	-	expression tag	UNP Q06187
B	389	GLY	-	expression tag	UNP Q06187
B	390	ALA	-	expression tag	UNP Q06187
B	391	MET	-	expression tag	UNP Q06187
B	392	GLY	-	expression tag	UNP Q06187
C	389	GLY	-	expression tag	UNP Q06187
C	390	ALA	-	expression tag	UNP Q06187
C	391	MET	-	expression tag	UNP Q06187
C	392	GLY	-	expression tag	UNP Q06187
D	389	GLY	-	expression tag	UNP Q06187
D	390	ALA	-	expression tag	UNP Q06187
D	391	MET	-	expression tag	UNP Q06187
D	392	GLY	-	expression tag	UNP Q06187
E	389	GLY	-	expression tag	UNP Q06187

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Chain	Residue	Modelled	Actual	Comment	Reference
E	390	ALA	-	expression tag	UNP Q06187
E	391	MET	-	expression tag	UNP Q06187
E	392	GLY	-	expression tag	UNP Q06187
F	389	GLY	-	expression tag	UNP Q06187
F	390	ALA	-	expression tag	UNP Q06187
F	391	MET	-	expression tag	UNP Q06187
F	392	GLY	-	expression tag	UNP Q06187

- Molecule 2 is N-[3-(4-amino-6-{[4-(morpholine-4-carbonyl)phenyl]amino}-1,3,5-triazin-2-yl)-2-methylphenyl]-4-tert-butylbenzamide (three-letter code: 9M3) (formula: C<sub>32</sub>H<sub>35</sub>N<sub>7</sub>O<sub>3</sub>).

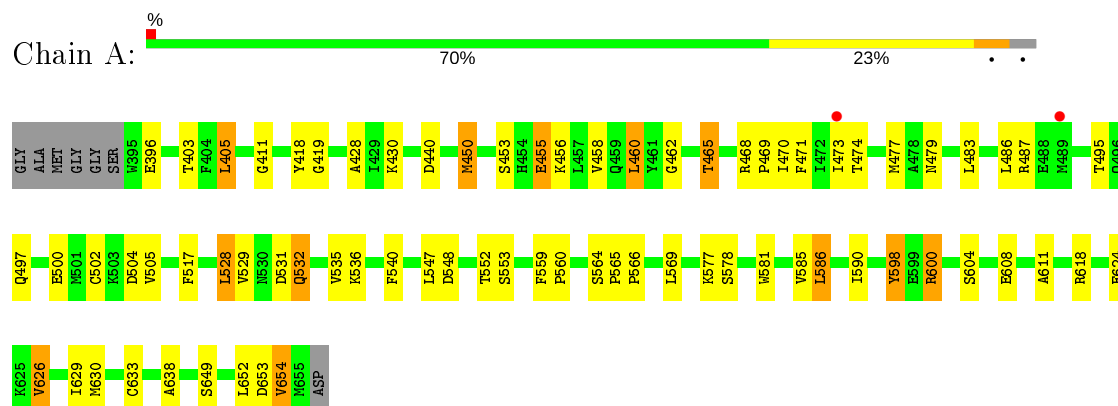


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	32	7	3		
2	B	1	Total	C	N	O	0	0
			42	32	7	3		
2	C	1	Total	C	N	O	0	0
			42	32	7	3		
2	D	1	Total	C	N	O	0	0
			42	32	7	3		
2	E	1	Total	C	N	O	0	0
			42	32	7	3		
2	F	1	Total	C	N	O	0	0
			42	32	7	3		

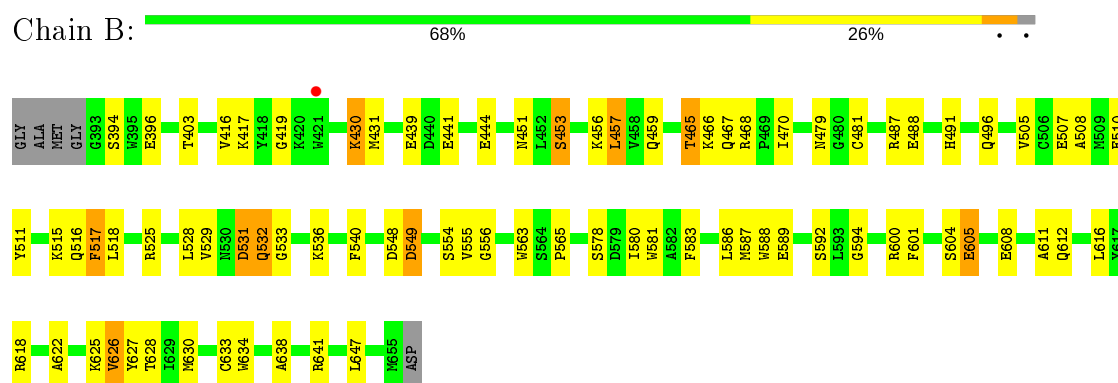
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

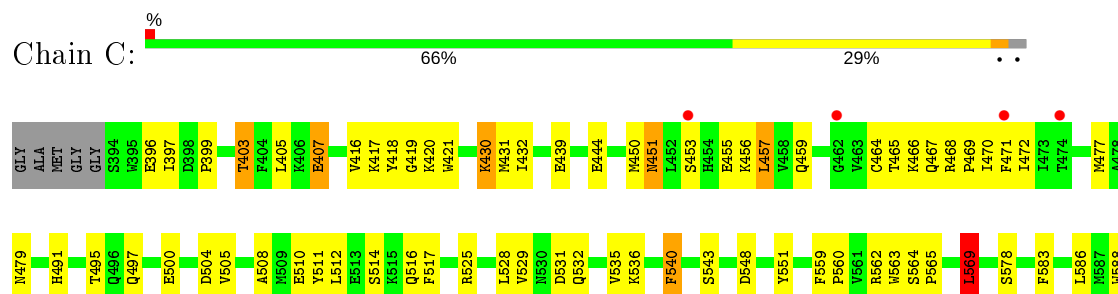
- Molecule 1: Tyrosine-protein kinase BTK



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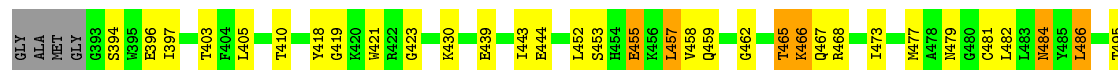


- Molecule 1: Tyrosine-protein kinase BTK

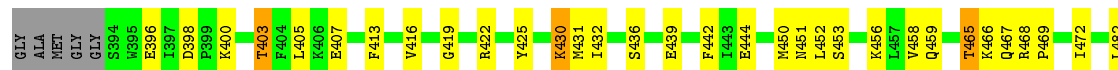




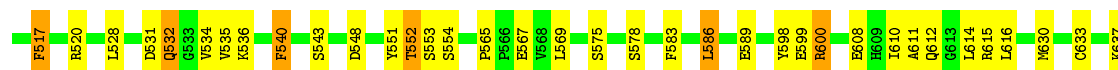
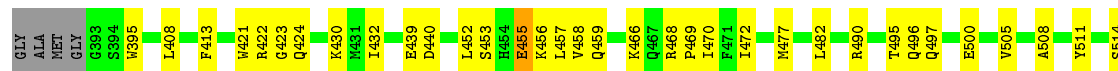
• Molecule 1: Tyrosine-protein kinase BTK



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• Molecule 1: Tyrosine-protein kinase BTK



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.27 Å 41.16 Å 587.94 Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	48.99 – 2.90 35.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.99-2.90) 99.8 (35.64-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.222 , 0.317 0.221 , 0.317	Depositor DCC
$R_{free}$ test set	2042 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.934	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 0.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.429 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.437 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.449 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.448 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.438 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: 9M3

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	0.72	0/2139	0.94	1/2889 (0.0%)
1	B	0.72	0/2139	0.94	2/2892 (0.1%)
1	C	0.72	0/2141	0.96	4/2894 (0.1%)
1	D	0.73	0/2155	0.94	2/2909 (0.1%)
1	E	0.75	0/2138	0.94	2/2888 (0.1%)
1	F	0.71	0/2128	0.94	3/2876 (0.1%)
All	All	0.72	0/12840	0.94	14/17348 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	525	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	B	525	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	525	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	525	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	C	457	LEU	CA-CB-CG	6.19	129.53	115.30
1	E	525	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	F	440	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	569	LEU	CA-CB-CG	5.73	128.47	115.30
1	D	586	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	F	457	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	440	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	457	LEU	CA-CB-CG	5.14	127.12	115.30
1	E	630	MET	CA-CB-CG	5.01	121.81	113.30
1	F	452	LEU	CA-CB-CG	5.01	126.81	115.30

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	2091	0	2029	39	0
1	B	2090	0	1988	41	0
1	C	2092	0	2006	55	0
1	D	2106	0	2046	47	0
1	E	2089	0	2003	44	0
1	F	2080	0	1985	39	0
2	A	42	0	0	1	0
2	B	42	0	0	0	0
2	C	42	0	0	0	0
2	D	42	0	0	0	0
2	E	42	0	0	0	0
2	F	42	0	0	1	0
All	All	12800	0	12057	258	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 10.

All (258) 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:E:396:GLU:OE2	1:E:465:THR:HG23	1.66	0.94
1:D:505:VAL:HG11	1:D:586:LEU:HD21	1.65	0.79
1:D:569:LEU:HD22	1:D:610:ILE:HD11	1.63	0.79
1:B:601:PHE:HB3	1:B:605:GLU:HB3	1.65	0.78
1:B:453:SER:HA	1:B:459:GLN:HE22	1.50	0.76
1:E:416:VAL:HG22	1:E:430:LYS:HB3	1.66	0.76
1:A:505:VAL:HG11	1:A:586:LEU:HD21	1.69	0.75
1:B:396:GLU:OE2	1:B:465:THR:HG23	1.86	0.74
1:E:505:VAL:HG11	1:E:586:LEU:HD21	1.70	0.73
1:C:564:SER:HB2	1:C:569:LEU:HD13	1.71	0.72
1:D:564:SER:HB2	1:D:569:LEU:HD11	1.71	0.72
1:D:396:GLU:OE2	1:D:465:THR:HG23	1.89	0.72
1:F:608:GLU:O	1:F:611:ALA:HB3	1.90	0.71
1:E:505:VAL:HG11	1:E:586:LEU:CD2	2.21	0.71
1:C:583:PHE:CD2	1:C:647:LEU:HD13	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:SER:HA	1:F:459:GLN:HE22	1.57	0.68
1:C:479:ASN:HB2	1:C:529:VAL:HG12	1.75	0.67
1:C:397:ILE:HG23	1:C:421:TRP:HE1	1.59	0.67
1:B:630:MET:O	1:B:633:CYS:HB2	1.94	0.67
1:B:456:LYS:HA	1:B:536:LYS:HG2	1.76	0.66
1:B:439:GLU:OE1	1:B:468:ARG:NH1	2.28	0.66
1:C:505:VAL:HG11	1:C:586:LEU:HD21	1.76	0.66
1:C:416:VAL:HG22	1:C:430:LYS:HB3	1.78	0.65
1:D:453:SER:HA	1:D:459:GLN:HE22	1.61	0.65
1:C:497:GLN:O	1:C:500:GLU:HB3	1.97	0.65
1:F:643:THR:OG1	1:F:646:ILE:HD12	1.97	0.65
1:C:615:ARG:NH1	1:C:634:TRP:O	2.30	0.64
1:E:609:HIS:HA	1:E:612:GLN:HG3	1.78	0.64
1:B:416:VAL:HG22	1:B:430:LYS:HB3	1.78	0.64
1:D:405:LEU:HD12	1:D:418:TYR:CE2	2.31	0.64
1:B:608:GLU:O	1:B:611:ALA:HB3	1.97	0.64
1:E:453:SER:HA	1:E:459:GLN:HE22	1.63	0.64
1:A:505:VAL:HG11	1:A:586:LEU:CD2	2.28	0.63
1:E:548:ASP:OD1	1:E:550:GLU:HB2	1.98	0.63
1:C:467:GLN:O	1:C:468:ARG:HD3	2.00	0.62
1:D:569:LEU:CD2	1:D:610:ILE:HD11	2.30	0.62
1:F:630:MET:O	1:F:633:CYS:HB2	1.99	0.62
1:B:517:PHE:C	1:B:517:PHE:CD1	2.74	0.61
1:C:396:GLU:OE2	1:C:465:THR:HG23	2.01	0.60
1:C:540:PHE:HD1	1:C:540:PHE:H	1.48	0.60
1:F:548:ASP:O	1:F:552:THR:HB	2.01	0.60
1:D:564:SER:HB2	1:D:569:LEU:CD1	2.32	0.60
1:D:550:GLU:O	1:D:558:LYS:HB2	2.02	0.60
1:D:608:GLU:O	1:D:611:ALA:HB3	2.01	0.60
1:B:417:LYS:HE3	1:B:431:MET:HE3	1.84	0.59
1:E:561:VAL:HG21	1:E:603:ASN:HB3	1.84	0.59
1:D:479:ASN:HB2	1:D:529:VAL:HG12	1.84	0.59
1:E:456:LYS:NZ	1:E:507:GLU:OE2	2.35	0.58
1:C:618:ARG:HG3	1:C:627:TYR:HB2	1.86	0.58
1:D:457:LEU:HD23	1:D:508:ALA:HB1	1.86	0.58
1:D:405:LEU:HG	1:D:419:GLY:HA2	1.86	0.58
1:A:477:MET:HE1	1:A:536:LYS:HD2	1.86	0.57
1:A:396:GLU:OE1	1:A:465:THR:HG23	2.05	0.57
1:B:618:ARG:HG3	1:B:627:TYR:HB2	1.86	0.57
1:A:608:GLU:O	1:A:611:ALA:HB3	2.04	0.56
1:E:511:TYR:O	1:E:514:SER:OG	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:THR:C	1:B:467:GLN:H	2.08	0.56
1:C:505:VAL:HG11	1:C:586:LEU:CD2	2.36	0.56
1:D:439:GLU:OE1	1:D:468:ARG:NH1	2.39	0.56
1:A:600:ARG:HD3	1:B:601:PHE:CZ	2.41	0.56
1:D:600:ARG:HD2	1:D:601:PHE:CE2	2.41	0.56
1:F:543:SER:HB2	1:F:551:TYR:OH	2.06	0.55
1:C:464:CYS:HB2	1:C:471:PHE:HB2	1.87	0.55
1:B:505:VAL:HG11	1:B:586:LEU:CD2	2.36	0.55
1:A:479:ASN:HB2	1:A:529:VAL:HB	1.89	0.55
1:A:456:LYS:HA	1:A:536:LYS:HG2	1.89	0.55
1:B:622:ALA:HB1	1:B:626:VAL:HG12	1.89	0.55
1:D:405:LEU:HD12	1:D:418:TYR:HE2	1.72	0.54
1:E:622:ALA:HB1	1:E:626:VAL:HG12	1.90	0.54
1:A:405:LEU:HD12	1:A:418:TYR:CE2	2.43	0.54
1:A:626:VAL:O	1:A:629:ILE:HB	2.08	0.54
1:B:517:PHE:CD1	1:B:518:LEU:N	2.76	0.54
1:F:598:TYR:CE1	1:F:616:LEU:HG	2.43	0.54
1:F:413:PHE:HB3	1:F:432:ILE:HG23	1.90	0.54
1:C:638:ALA:HA	1:C:641:ARG:HD2	1.88	0.53
1:D:477:MET:HE1	1:D:536:LYS:HD2	1.90	0.53
1:E:547:LEU:O	1:E:548:ASP:HB2	2.09	0.53
1:A:405:LEU:HG	1:A:419:GLY:HA2	1.90	0.53
1:A:630:MET:O	1:A:633:CYS:HB2	2.08	0.53
1:C:504:ASP:HB3	1:C:535:VAL:O	2.09	0.53
1:C:564:SER:HB2	1:C:569:LEU:CD1	2.37	0.53
1:D:627:TYR:O	1:D:628:THR:C	2.45	0.53
1:E:559:PHE:CG	1:E:560:PRO:HD2	2.44	0.53
1:F:477:MET:HE1	1:F:536:LYS:HD2	1.91	0.52
1:F:497:GLN:O	1:F:500:GLU:HB3	2.09	0.52
1:C:600:ARG:HG3	1:D:600:ARG:HB3	1.90	0.52
1:C:517:PHE:CD1	1:C:517:PHE:C	2.83	0.52
1:C:455:GLU:O	1:C:536:LYS:HE2	2.09	0.52
1:C:559:PHE:CG	1:C:560:PRO:HD2	2.45	0.52
1:A:468:ARG:HA	1:A:469:PRO:C	2.29	0.52
1:A:497:GLN:O	1:A:500:GLU:HB3	2.09	0.52
1:D:517:PHE:C	1:D:517:PHE:CD1	2.82	0.52
1:E:453:SER:HB3	1:E:459:GLN:OE1	2.10	0.52
1:D:565:PRO:HG3	1:D:578:SER:HA	1.92	0.52
1:E:600:ARG:HB3	1:F:600:ARG:HB3	1.91	0.52
1:B:583:PHE:CD2	1:B:647:LEU:HD13	2.45	0.52
1:D:462:GLY:O	1:D:473:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:LEU:C	1:D:654:VAL:H	2.13	0.51
1:A:598:TYR:HA	1:A:600:ARG:HE	1.75	0.51
1:B:616:LEU:HB2	1:B:634:TRP:CH2	2.45	0.51
1:F:468:ARG:HA	1:F:469:PRO:C	2.30	0.51
1:C:511:TYR:O	1:C:514:SER:OG	2.26	0.51
1:D:505:VAL:HG11	1:D:586:LEU:CD2	2.39	0.51
1:B:638:ALA:HA	1:B:641:ARG:HD2	1.91	0.51
1:D:553:SER:C	1:D:555:VAL:H	2.14	0.51
1:A:577:LYS:HD2	1:A:638:ALA:O	2.11	0.51
1:C:588:TRP:CE2	1:C:616:LEU:HD22	2.45	0.51
1:A:504:ASP:HB3	1:A:535:VAL:O	2.11	0.51
1:D:443:ILE:HG23	1:D:465:THR:HG21	1.93	0.50
1:D:602:THR:OG1	1:D:605:GLU:HG3	2.11	0.50
1:E:566:PRO:HA	1:E:569:LEU:HD12	1.92	0.50
1:E:609:HIS:ND1	1:E:612:GLN:NE2	2.59	0.50
1:C:464:CYS:HB3	1:C:467:GLN:HE21	1.76	0.50
1:F:517:PHE:C	1:F:517:PHE:CD1	2.83	0.50
1:C:457:LEU:HD23	1:C:508:ALA:HB1	1.93	0.50
1:E:608:GLU:O	1:E:611:ALA:HB3	2.12	0.50
1:A:477:MET:HE2	1:A:536:LYS:HB2	1.94	0.49
1:E:598:TYR:HA	1:E:600:ARG:HE	1.77	0.49
1:C:405:LEU:HD12	1:C:418:TYR:CE2	2.47	0.49
1:F:505:VAL:HG11	1:F:586:LEU:CD2	2.43	0.49
1:E:601:PHE:HB3	1:E:605:GLU:HB2	1.94	0.49
1:D:596:MET:O	1:D:599:GLU:HG3	2.11	0.49
1:C:399:PRO:HG3	1:C:467:GLN:NE2	2.28	0.49
1:C:407:GLU:HA	1:C:417:LYS:HG2	1.94	0.49
1:C:643:THR:H	1:C:646:ILE:HD12	1.78	0.49
1:C:630:MET:O	1:C:633:CYS:HB2	2.13	0.48
1:A:462:GLY:O	1:A:473:ILE:HB	2.12	0.48
1:A:455:GLU:O	1:A:536:LYS:HE2	2.14	0.48
1:E:565:PRO:HG3	1:E:578:SER:HA	1.95	0.48
1:A:531:ASP:HB2	1:A:532:GLN:HE21	1.78	0.48
1:A:458:VAL:HG21	1:A:528:LEU:HD12	1.96	0.48
1:B:517:PHE:C	1:B:517:PHE:HD1	2.15	0.48
1:C:456:LYS:HA	1:C:536:LYS:HG2	1.95	0.48
1:E:465:THR:C	1:E:467:GLN:H	2.17	0.48
1:F:456:LYS:HE2	1:F:534:VAL:HG11	1.96	0.48
1:F:540:PHE:CD1	1:F:540:PHE:N	2.71	0.48
1:A:477:MET:CE	1:A:536:LYS:HD2	2.42	0.48
1:B:417:LYS:HE3	1:B:431:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:ARG:NE	1:B:594:GLY:O	2.44	0.48
1:E:430:LYS:HG3	1:E:472:ILE:HB	1.95	0.48
1:E:580:ILE:HD13	1:E:642:PRO:O	2.14	0.48
1:B:457:LEU:HD23	1:B:508:ALA:HB1	1.96	0.48
1:A:560:PRO:O	1:A:564:SER:OG	2.25	0.47
1:D:553:SER:O	1:D:555:VAL:N	2.48	0.47
1:D:559:PHE:CG	1:D:560:PRO:HD2	2.49	0.47
1:B:488:GLU:HB3	1:B:491:HIS:HD2	1.79	0.47
1:B:456:LYS:NZ	1:B:507:GLU:OE2	2.47	0.47
1:C:468:ARG:HA	1:C:469:PRO:C	2.34	0.47
1:E:600:ARG:HD3	1:F:600:ARG:HD3	1.96	0.47
1:F:477:MET:HE2	1:F:536:LYS:HB2	1.96	0.47
1:B:531:ASP:C	1:B:533:GLY:H	2.18	0.47
1:C:403:THR:O	1:C:419:GLY:HA3	2.14	0.47
1:F:508:ALA:O	1:F:511:TYR:HB3	2.15	0.47
1:A:565:PRO:HG3	1:A:578:SER:HA	1.97	0.47
1:D:482:LEU:HG	1:D:486:LEU:HD22	1.97	0.47
1:A:581:TRP:O	1:A:585:VAL:HG23	2.15	0.47
1:C:405:LEU:HD11	1:C:420:LYS:HG2	1.97	0.47
1:B:505:VAL:HG11	1:B:586:LEU:HD21	1.97	0.46
1:F:600:ARG:HG3	1:F:600:ARG:H	1.45	0.46
1:C:405:LEU:HG	1:C:419:GLY:HA2	1.97	0.46
1:C:465:THR:C	1:C:467:GLN:H	2.19	0.46
1:A:405:LEU:HD12	1:A:418:TYR:HE2	1.79	0.46
1:D:477:MET:HE2	1:D:536:LYS:HB2	1.97	0.46
1:C:467:GLN:O	1:C:468:ARG:CD	2.64	0.46
1:C:479:ASN:HB2	1:C:529:VAL:CG1	2.45	0.46
1:D:549:ASP:O	1:D:553:SER:HB2	2.16	0.46
1:E:398:ASP:OD1	1:E:400:LYS:HG3	2.16	0.46
1:B:479:ASN:HB2	1:B:529:VAL:HG12	1.97	0.46
1:E:618:ARG:O	1:F:612:GLN:NE2	2.49	0.46
1:E:468:ARG:HA	1:E:469:PRO:C	2.36	0.46
1:E:598:TYR:CE1	1:E:610:ILE:HD11	2.51	0.46
1:E:605:GLU:O	1:E:608:GLU:HB3	2.15	0.46
1:A:411:GLY:HA3	2:A:701:9M3:C31	2.46	0.45
1:C:477:MET:HE1	1:C:536:LYS:HD2	1.98	0.45
1:A:566:PRO:HA	1:A:569:LEU:HD12	1.98	0.45
1:A:652:LEU:C	1:A:654:VAL:H	2.20	0.45
1:B:554:SER:O	1:B:556:GLY:N	2.49	0.45
1:E:458:VAL:HG21	1:E:528:LEU:HD12	1.99	0.45
1:C:399:PRO:HG3	1:C:467:GLN:HE22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:GLU:O	1:D:536:LYS:HE2	2.15	0.45
1:F:458:VAL:HG21	1:F:528:LEU:HD12	1.98	0.45
1:F:583:PHE:CD2	1:F:647:LEU:HD13	2.52	0.45
1:A:559:PHE:CG	1:A:560:PRO:HD2	2.50	0.45
1:B:549:ASP:N	1:B:549:ASP:OD1	2.50	0.45
1:F:511:TYR:O	1:F:514:SER:OG	2.32	0.45
1:A:618:ARG:O	1:B:612:GLN:NE2	2.48	0.44
1:F:455:GLU:O	1:F:536:LYS:HE2	2.17	0.44
1:F:586:LEU:O	1:F:589:GLU:HB2	2.17	0.44
1:A:428:ALA:HB3	1:A:474:THR:OG1	2.17	0.44
1:C:477:MET:HE2	1:C:536:LYS:HB2	1.99	0.44
1:F:453:SER:HA	1:F:459:GLN:NE2	2.30	0.44
1:C:416:VAL:HA	1:C:430:LYS:HA	2.00	0.44
1:D:452:LEU:CD2	1:D:515:LYS:HG3	2.47	0.44
1:E:442:PHE:CZ	1:E:472:ILE:HD11	2.52	0.44
1:E:614:LEU:O	1:E:615:ARG:HD3	2.18	0.44
1:F:456:LYS:HE2	1:F:534:VAL:CG1	2.47	0.44
1:F:408:LEU:HD22	2:F:701:9M3:C17	2.49	0.43
1:B:563:TRP:O	1:B:581:TRP:HD1	2.02	0.43
1:B:625:LYS:O	1:B:628:THR:HB	2.17	0.43
1:C:543:SER:CB	1:C:551:TYR:OH	2.66	0.43
1:B:416:VAL:HA	1:B:430:LYS:HA	1.99	0.43
1:D:397:ILE:HG23	1:D:421:TRP:HE1	1.83	0.43
1:D:532:GLN:N	1:D:532:GLN:CD	2.71	0.43
1:A:600:ARG:H	1:A:600:ARG:HG3	1.35	0.43
1:B:453:SER:HA	1:B:459:GLN:NE2	2.25	0.43
1:B:403:THR:O	1:B:419:GLY:HA3	2.18	0.43
1:F:565:PRO:HG3	1:F:578:SER:HA	2.00	0.43
1:D:609:HIS:HA	1:D:612:GLN:HG3	2.00	0.43
1:E:520:ARG:HD2	1:E:543:SER:OG	2.19	0.43
1:E:600:ARG:HG3	1:E:600:ARG:H	1.32	0.43
1:B:586:LEU:O	1:B:589:GLU:HB2	2.18	0.43
1:C:512:LEU:HB3	1:C:517:PHE:O	2.19	0.43
1:C:583:PHE:CE2	1:C:647:LEU:HD13	2.53	0.43
1:E:439:GLU:OE1	1:E:468:ARG:NE	2.50	0.43
1:F:439:GLU:OE1	1:F:468:ARG:NH1	2.52	0.43
1:C:562:ARG:HB2	1:C:563:TRP:CE3	2.54	0.43
1:C:612:GLN:NE2	1:D:618:ARG:O	2.52	0.43
1:E:416:VAL:HA	1:E:430:LYS:HA	1.99	0.43
1:C:562:ARG:HB2	1:C:563:TRP:CZ3	2.54	0.42
1:D:598:TYR:CE1	1:D:616:LEU:HG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:LEU:HD22	1:F:535:VAL:HG11	2.01	0.42
1:F:637:LYS:HE2	1:F:640:GLU:OE2	2.19	0.42
1:E:598:TYR:CZ	1:E:610:ILE:HD11	2.55	0.42
1:F:477:MET:CE	1:F:536:LYS:HB2	2.48	0.42
1:B:587:MET:O	1:B:588:TRP:C	2.58	0.42
1:F:543:SER:CB	1:F:551:TYR:OH	2.67	0.42
1:C:453:SER:CB	1:C:459:GLN:HE22	2.32	0.42
1:C:540:PHE:CD1	1:C:540:PHE:N	2.68	0.42
1:C:432:ILE:HD11	1:C:472:ILE:HG13	2.01	0.42
1:E:622:ALA:HB1	1:E:626:VAL:CG1	2.48	0.42
1:D:465:THR:C	1:D:467:GLN:H	2.23	0.42
1:E:482:LEU:HD22	1:E:535:VAL:HG11	2.01	0.41
1:C:565:PRO:HG3	1:C:578:SER:HA	2.02	0.41
1:A:430:LYS:O	1:A:471:PHE:HA	2.20	0.41
1:E:413:PHE:HB3	1:E:432:ILE:HG23	2.03	0.41
1:F:430:LYS:HG3	1:F:472:ILE:HB	2.02	0.41
1:B:600:ARG:HA	1:B:600:ARG:HD3	1.63	0.41
1:E:452:LEU:HA	1:E:511:TYR:OH	2.21	0.41
1:A:450:MET:HG2	1:A:460:LEU:HD23	2.03	0.41
1:B:457:LEU:HD11	1:B:511:TYR:CE2	2.55	0.41
1:A:502:CYS:SG	1:A:590:ILE:HD13	2.61	0.41
1:F:569:LEU:HD12	1:F:610:ILE:HD11	2.03	0.41
1:D:486:LEU:HD12	1:D:486:LEU:HA	1.95	0.41
1:E:403:THR:O	1:E:419:GLY:HA3	2.21	0.41
1:C:543:SER:HB2	1:C:551:TYR:OH	2.21	0.40
1:D:484:ASN:H	1:D:484:ASN:ND2	2.20	0.40
1:F:421:TRP:C	1:F:423:GLY:H	2.25	0.40
1:A:483:LEU:HD21	1:A:487:ARG:NH2	2.36	0.40
1:D:484:ASN:H	1:D:484:ASN:HD22	1.67	0.40
1:D:562:ARG:HB2	1:D:563:TRP:CZ3	2.57	0.40
1:E:597:PRO:CB	1:E:616:LEU:HD21	2.52	0.40
1:C:477:MET:CE	1:C:536:LYS:HB2	2.52	0.40
1:C:638:ALA:HA	1:C:641:ARG:CD	2.52	0.40
1:D:559:PHE:CD1	1:D:560:PRO:HD2	2.56	0.40
1:D:646:ILE:HG22	1:D:650:ASN:ND2	2.37	0.40
1:A:517:PHE:C	1:A:517:PHE:CD1	2.95	0.40
1:B:565:PRO:HG3	1:B:578:SER:HA	2.03	0.40
1:F:614:LEU:O	1:F:615:ARG:HD3	2.21	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	259/268 (97%)	225 (87%)	30 (12%)	4 (2%)	10	34
1	B	261/268 (97%)	227 (87%)	28 (11%)	6 (2%)	6	23
1	C	260/268 (97%)	233 (90%)	23 (9%)	4 (2%)	10	34
1	D	261/268 (97%)	215 (82%)	38 (15%)	8 (3%)	4	16
1	E	260/268 (97%)	230 (88%)	26 (10%)	4 (2%)	10	34
1	F	261/268 (97%)	231 (88%)	25 (10%)	5 (2%)	8	28
All	All	1562/1608 (97%)	1361 (87%)	170 (11%)	31 (2%)	7	27

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	653	ASP
1	C	548	ASP
1	D	557	SER
1	D	653	ASP
1	E	548	ASP
1	F	395	TRP
1	A	548	ASP
1	B	548	ASP
1	B	555	VAL
1	D	423	GLY
1	D	554	SER
1	F	490	ARG
1	F	532	GLN
1	B	444	GLU
1	B	580	ILE
1	F	422	ARG
1	A	532	GLN
1	D	532	GLN
1	E	422	ARG
1	B	466	LYS

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Mol	Chain	Res	Type
1	B	532	GLN
1	C	439	GLU
1	C	451	ASN
1	D	466	LYS
1	D	548	ASP
1	E	532	GLN
1	A	624	GLU
1	C	444	GLU
1	D	458	VAL
1	E	444	GLU
1	F	653	ASP

### 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	224/239 (94%)	202 (90%)	22 (10%)	8	24
1	B	222/239 (93%)	199 (90%)	23 (10%)	7	21
1	C	223/239 (93%)	205 (92%)	18 (8%)	11	33
1	D	227/239 (95%)	205 (90%)	22 (10%)	8	25
1	E	223/239 (93%)	201 (90%)	22 (10%)	8	24
1	F	220/239 (92%)	200 (91%)	20 (9%)	9	28
All	All	1339/1434 (93%)	1212 (90%)	127 (10%)	8	26

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	THR
1	A	405	LEU
1	A	450	MET
1	A	453	SER
1	A	455	GLU
1	A	460	LEU
1	A	465	THR

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Mol	Chain	Res	Type
1	A	470	ILE
1	A	486	LEU
1	A	495	THR
1	A	528	LEU
1	A	540	PHE
1	A	547	LEU
1	A	552	THR
1	A	553	SER
1	A	586	LEU
1	A	598	TYR
1	A	600	ARG
1	A	604	SER
1	A	626	VAL
1	A	649	SER
1	A	654	VAL
1	B	394	SER
1	B	430	LYS
1	B	441	GLU
1	B	451	ASN
1	B	453	SER
1	B	457	LEU
1	B	465	THR
1	B	470	ILE
1	B	481	CYS
1	B	496	GLN
1	B	510	GLU
1	B	515	LYS
1	B	516	GLN
1	B	517	PHE
1	B	528	LEU
1	B	531	ASP
1	B	532	GLN
1	B	540	PHE
1	B	549	ASP
1	B	592	SER
1	B	604	SER
1	B	605	GLU
1	B	626	VAL
1	C	403	THR
1	C	407	GLU
1	C	430	LYS
1	C	431	MET

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Mol	Chain	Res	Type
1	C	450	MET
1	C	451	ASN
1	C	466	LYS
1	C	470	ILE
1	C	491	HIS
1	C	495	THR
1	C	510	GLU
1	C	516	GLN
1	C	528	LEU
1	C	531	ASP
1	C	532	GLN
1	C	540	PHE
1	C	569	LEU
1	C	649	SER
1	D	394	SER
1	D	403	THR
1	D	410	THR
1	D	430	LYS
1	D	444	GLU
1	D	455	GLU
1	D	465	THR
1	D	466	LYS
1	D	481	CYS
1	D	484	ASN
1	D	486	LEU
1	D	495	THR
1	D	540	PHE
1	D	547	LEU
1	D	553	SER
1	D	595	LYS
1	D	599	GLU
1	D	600	ARG
1	D	604	SER
1	D	612	GLN
1	D	624	GLU
1	D	628	THR
1	E	403	THR
1	E	405	LEU
1	E	407	GLU
1	E	425	TYR
1	E	430	LYS
1	E	431	MET

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Mol	Chain	Res	Type
1	E	436	SER
1	E	450	MET
1	E	451	ASN
1	E	465	THR
1	E	466	LYS
1	E	495	THR
1	E	496	GLN
1	E	528	LEU
1	E	529	VAL
1	E	567	GLU
1	E	600	ARG
1	E	604	SER
1	E	612	GLN
1	E	619	PRO
1	E	626	VAL
1	E	639	ASP
1	F	424	GLN
1	F	455	GLU
1	F	466	LYS
1	F	470	ILE
1	F	495	THR
1	F	496	GLN
1	F	517	PHE
1	F	520	ARG
1	F	531	ASP
1	F	532	GLN
1	F	540	PHE
1	F	552	THR
1	F	553	SER
1	F	554	SER
1	F	567	GLU
1	F	575	SER
1	F	586	LEU
1	F	599	GLU
1	F	600	ARG
1	F	649	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	GLN
1	A	484	ASN

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Mol	Chain	Res	Type
1	A	532	GLN
1	B	459	GLN
1	B	491	HIS
1	C	451	ASN
1	C	459	GLN
1	C	467	GLN
1	C	496	GLN
1	D	459	GLN
1	D	467	GLN
1	D	479	ASN
1	D	484	ASN
1	D	603	ASN
1	E	459	GLN
1	E	612	GLN
1	F	451	ASN
1	F	459	GLN
1	F	479	ASN

### 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 carbohydrates 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	9M3	F	701	-	46,46,46	1.68	3 (6%)	65,66,66	2.13	13 (20%)
2	9M3	B	701	-	46,46,46	1.76	4 (8%)	65,66,66	2.20	10 (15%)
2	9M3	C	701	-	46,46,46	1.74	3 (6%)	65,66,66	2.04	10 (15%)
2	9M3	E	701	-	46,46,46	1.70	3 (6%)	65,66,66	2.16	12 (18%)
2	9M3	A	701	-	46,46,46	1.71	4 (8%)	65,66,66	1.97	10 (15%)
2	9M3	D	701	-	46,46,46	1.70	3 (6%)	65,66,66	1.93	13 (20%)

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	9M3	F	701	-	-	15/30/38/38	0/5/5/5
2	9M3	B	701	-	-	6/30/38/38	0/5/5/5
2	9M3	C	701	-	-	6/30/38/38	0/5/5/5
2	9M3	E	701	-	-	10/30/38/38	0/5/5/5
2	9M3	A	701	-	-	6/30/38/38	0/5/5/5
2	9M3	D	701	-	-	15/30/38/38	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	9M3	C3-C2	6.93	1.51	1.40
2	F	701	9M3	C3-C2	6.92	1.51	1.40
2	C	701	9M3	C3-C2	6.86	1.51	1.40
2	D	701	9M3	C3-C2	6.83	1.51	1.40
2	E	701	9M3	C7-C2	6.63	1.51	1.40
2	B	701	9M3	C3-C2	6.40	1.50	1.40
2	D	701	9M3	C7-C2	6.33	1.50	1.40
2	C	701	9M3	C7-C2	6.23	1.50	1.40
2	F	701	9M3	C7-C2	6.16	1.50	1.40
2	E	701	9M3	C3-C2	6.10	1.50	1.40
2	B	701	9M3	C7-C2	6.10	1.50	1.40
2	A	701	9M3	C7-C2	5.57	1.49	1.40
2	B	701	9M3	C31-N30	-3.36	1.26	1.35
2	E	701	9M3	C31-N30	-3.09	1.27	1.35
2	A	701	9M3	C31-N30	-3.06	1.27	1.35
2	D	701	9M3	C31-N30	-3.06	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	9M3	C31-N30	-2.97	1.27	1.35
2	F	701	9M3	C31-N30	-2.92	1.28	1.35
2	B	701	9M3	C19-C22	2.59	1.54	1.50
2	A	701	9M3	C33-C34	2.00	1.42	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	9M3	C11-N12-C13	12.04	122.28	114.60
2	B	701	9M3	C11-N12-C13	11.05	121.65	114.60
2	F	701	9M3	C11-N12-C13	10.50	121.30	114.60
2	C	701	9M3	C11-N12-C13	10.09	121.03	114.60
2	A	701	9M3	C11-N12-C13	9.92	120.92	114.60
2	D	701	9M3	C11-N12-C13	7.60	119.44	114.60
2	E	701	9M3	N10-C11-N12	-6.08	116.62	126.23
2	B	701	9M3	N10-C11-N12	-5.72	117.19	126.23
2	F	701	9M3	C24-N23-C28	5.67	123.55	112.62
2	C	701	9M3	N10-C11-N12	-5.64	117.32	126.23
2	A	701	9M3	N10-C11-N12	-5.43	117.64	126.23
2	D	701	9M3	N10-C11-N12	-5.25	117.94	126.23
2	F	701	9M3	N10-C11-N12	-5.19	118.02	126.23
2	D	701	9M3	C9-N10-C11	4.88	122.01	113.75
2	C	701	9M3	C9-N10-C11	4.68	121.67	113.75
2	D	701	9M3	C24-N23-C28	4.64	121.56	112.62
2	E	701	9M3	C9-N10-C11	4.45	121.28	113.75
2	B	701	9M3	C9-N10-C11	4.38	121.17	113.75
2	A	701	9M3	C9-N10-C11	4.38	121.16	113.75
2	F	701	9M3	C9-N10-C11	4.29	121.02	113.75
2	C	701	9M3	N14-C9-N10	4.13	123.67	117.25
2	B	701	9M3	N14-C9-N10	3.99	123.46	117.25
2	D	701	9M3	N10-C9-N8	-3.79	119.47	125.42
2	B	701	9M3	C25-C24-N23	3.61	117.54	109.84
2	B	701	9M3	C9-N8-C13	3.60	119.92	114.35
2	C	701	9M3	N10-C9-N8	-3.57	119.82	125.42
2	B	701	9M3	N12-C13-N8	-3.43	119.68	125.23
2	C	701	9M3	C9-N8-C13	3.42	119.63	114.35
2	A	701	9M3	C9-N8-C13	3.38	119.58	114.35
2	E	701	9M3	N14-C9-N10	3.38	122.50	117.25
2	B	701	9M3	C24-N23-C28	3.32	119.01	112.62
2	F	701	9M3	C9-N8-C13	3.32	119.47	114.35
2	F	701	9M3	N10-C9-N8	-3.31	120.23	125.42
2	A	701	9M3	N14-C9-N10	3.30	122.39	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	9M3	N12-C13-N8	-3.26	119.96	125.23
2	A	701	9M3	N10-C9-N8	-3.24	120.34	125.42
2	B	701	9M3	N10-C9-N8	-3.21	120.39	125.42
2	D	701	9M3	C9-N8-C13	3.16	119.23	114.35
2	E	701	9M3	N10-C9-N8	-3.09	120.57	125.42
2	A	701	9M3	N12-C13-N8	-3.01	120.36	125.23
2	D	701	9M3	N14-C9-N10	3.00	121.91	117.25
2	C	701	9M3	N12-C13-N8	-2.92	120.50	125.23
2	C	701	9M3	C24-N23-C28	2.92	118.24	112.62
2	E	701	9M3	N12-C13-N8	-2.90	120.55	125.23
2	F	701	9M3	N14-C9-N10	2.86	121.71	117.25
2	D	701	9M3	C19-C22-N23	2.84	122.32	118.72
2	E	701	9M3	C9-N8-C13	2.81	118.69	114.35
2	B	701	9M3	C42-C38-C35	-2.57	104.21	110.36
2	D	701	9M3	C41-C38-C35	-2.43	104.54	110.36
2	E	701	9M3	C41-C38-C35	-2.31	104.84	110.36
2	C	701	9M3	C25-O26-C27	2.27	117.48	109.89
2	F	701	9M3	C39-C38-C35	2.26	115.78	110.36
2	E	701	9M3	C24-N23-C28	2.24	116.93	112.62
2	F	701	9M3	C3-C13-N8	2.21	121.02	117.22
2	C	701	9M3	C3-C13-N8	2.21	121.01	117.22
2	D	701	9M3	C39-C38-C35	2.20	115.64	110.36
2	D	701	9M3	C4-C5-C6	2.19	123.35	120.25
2	F	701	9M3	C1-C2-C3	2.19	124.74	120.93
2	F	701	9M3	C2-C7-N30	-2.17	116.47	119.45
2	A	701	9M3	C36-C37-C32	2.15	123.28	120.78
2	E	701	9M3	C3-C13-N8	2.07	120.78	117.22
2	E	701	9M3	C39-C38-C42	-2.07	101.61	108.32
2	A	701	9M3	C33-C32-C37	-2.06	115.66	118.59
2	D	701	9M3	N12-C13-N8	-2.06	121.91	125.23
2	F	701	9M3	O29-C22-N23	-2.05	118.95	122.34
2	A	701	9M3	C3-C13-N8	2.04	120.73	117.22
2	D	701	9M3	N24-C11-N12	2.03	123.82	116.92
2	E	701	9M3	C42-C38-C35	2.03	115.22	110.36

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	701	9M3	C19-C22-N23-C28
2	F	701	9M3	C19-C22-N23-C24
2	F	701	9M3	O29-C22-N23-C28

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Mol	Chain	Res	Type	Atoms
2	F	701	9M3	O29-C22-N23-C24
2	B	701	9M3	C19-C22-N23-C28
2	B	701	9M3	O29-C22-N23-C24
2	C	701	9M3	C19-C22-N23-C28
2	C	701	9M3	C19-C22-N23-C24
2	C	701	9M3	O29-C22-N23-C28
2	C	701	9M3	O29-C22-N23-C24
2	E	701	9M3	C19-C22-N23-C28
2	E	701	9M3	C19-C22-N23-C24
2	E	701	9M3	O29-C22-N23-C28
2	E	701	9M3	O29-C22-N23-C24
2	A	701	9M3	C19-C22-N23-C28
2	A	701	9M3	C19-C22-N23-C24
2	A	701	9M3	O29-C22-N23-C28
2	A	701	9M3	O29-C22-N23-C24
2	D	701	9M3	C19-C22-N23-C28
2	D	701	9M3	C19-C22-N23-C24
2	D	701	9M3	O29-C22-N23-C28
2	D	701	9M3	O29-C22-N23-C24
2	B	701	9M3	O29-C22-N23-C28
2	B	701	9M3	C19-C22-N23-C24
2	F	701	9M3	C18-C19-C22-O29
2	F	701	9M3	C18-C19-C22-N23
2	F	701	9M3	C20-C19-C22-O29
2	C	701	9M3	C2-C7-N30-C31
2	C	701	9M3	C6-C7-N30-C31
2	B	701	9M3	C6-C7-N30-C31
2	B	701	9M3	C2-C7-N30-C31
2	A	701	9M3	C6-C7-N30-C31
2	F	701	9M3	C20-C19-C22-N23
2	A	701	9M3	C2-C7-N30-C31
2	D	701	9M3	C18-C19-C22-N23
2	F	701	9M3	C6-C7-N30-C31
2	D	701	9M3	C2-C7-N30-C31
2	D	701	9M3	C6-C7-N30-C31
2	E	701	9M3	C6-C7-N30-C31
2	F	701	9M3	C2-C7-N30-C31
2	D	701	9M3	C18-C19-C22-O29
2	E	701	9M3	C2-C7-N30-C31
2	D	701	9M3	C34-C35-C38-C41
2	E	701	9M3	C36-C35-C38-C41
2	E	701	9M3	C34-C35-C38-C41

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Mol	Chain	Res	Type	Atoms
2	D	701	9M3	C36-C35-C38-C41
2	F	701	9M3	C36-C35-C38-C41
2	F	701	9M3	C34-C35-C38-C41
2	F	701	9M3	C36-C35-C38-C42
2	E	701	9M3	C34-C35-C38-C42
2	D	701	9M3	C36-C35-C38-C39
2	F	701	9M3	C34-C35-C38-C42
2	E	701	9M3	C36-C35-C38-C42
2	D	701	9M3	C34-C35-C38-C39
2	D	701	9M3	C36-C35-C38-C42
2	D	701	9M3	C34-C35-C38-C42
2	F	701	9M3	C36-C35-C38-C39
2	D	701	9M3	C20-C19-C22-N23

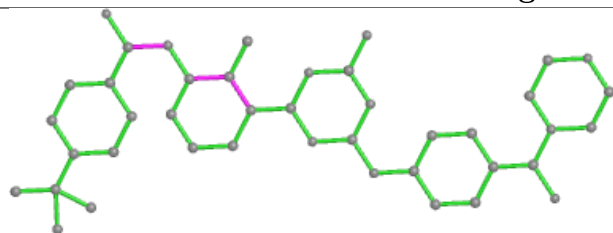
There are no ring outliers.

2 monomers are involved in 2 short contacts:

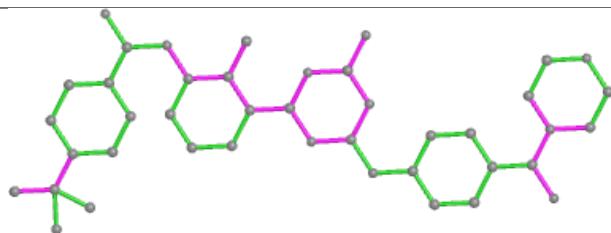
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	9M3	1	0
2	A	701	9M3	1	0

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.

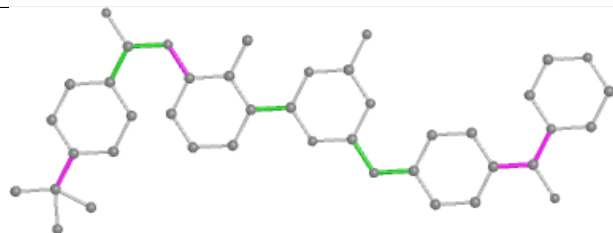
## Ligand 9M3 F 701



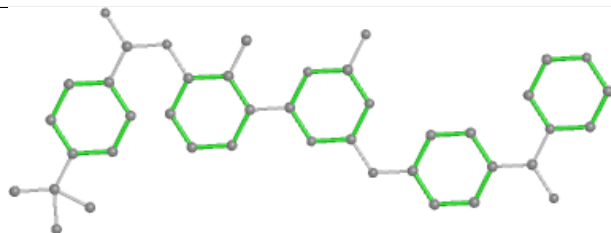
Bond lengths



Bond angles

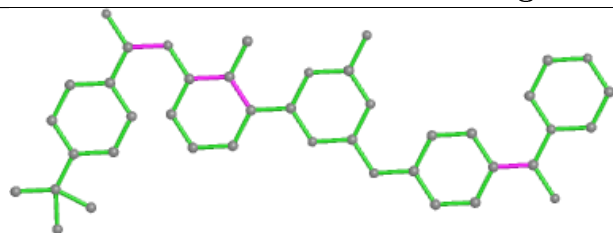


Torsions

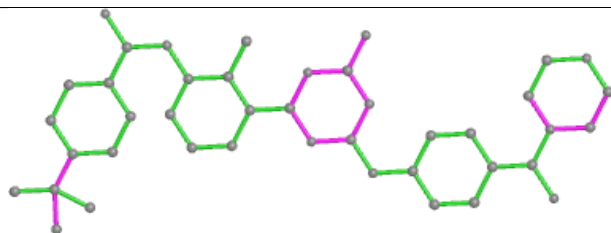


Rings

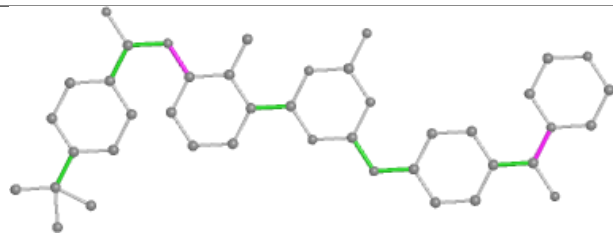
## Ligand 9M3 B 701



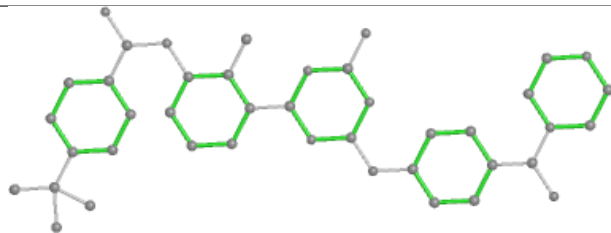
Bond lengths



Bond angles

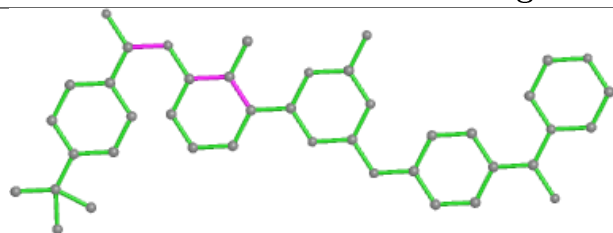


Torsions

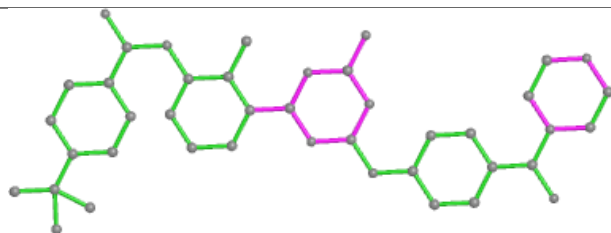


Rings

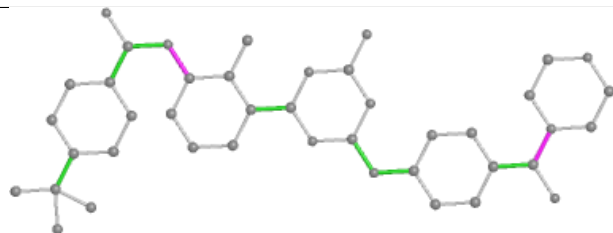
## Ligand 9M3 C 701



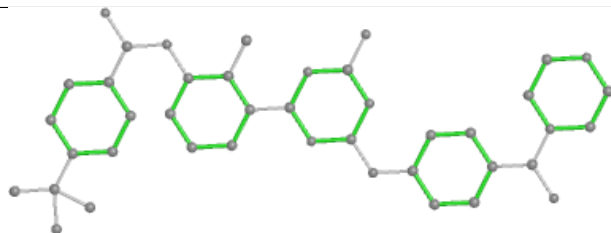
Bond lengths



Bond angles

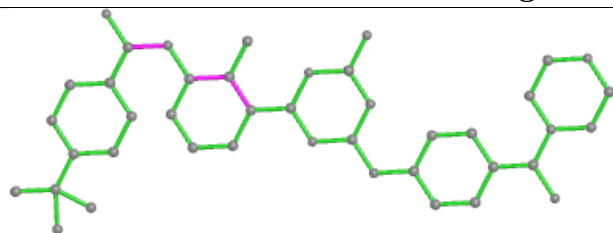


Torsions

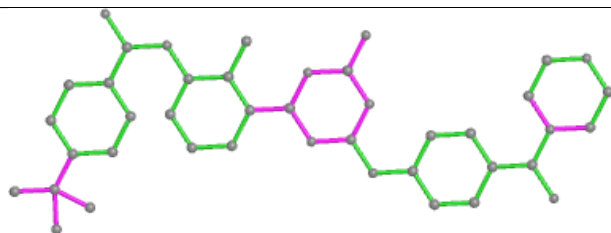


Rings

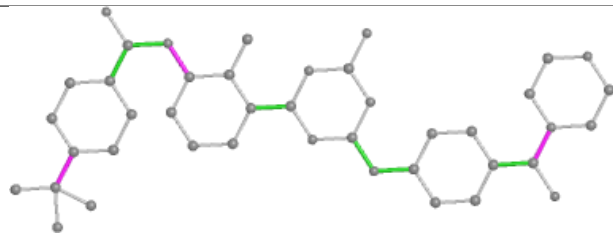
## Ligand 9M3 E 701



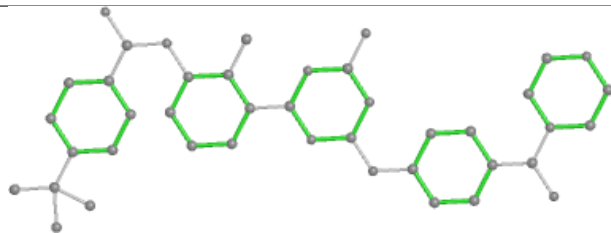
Bond lengths



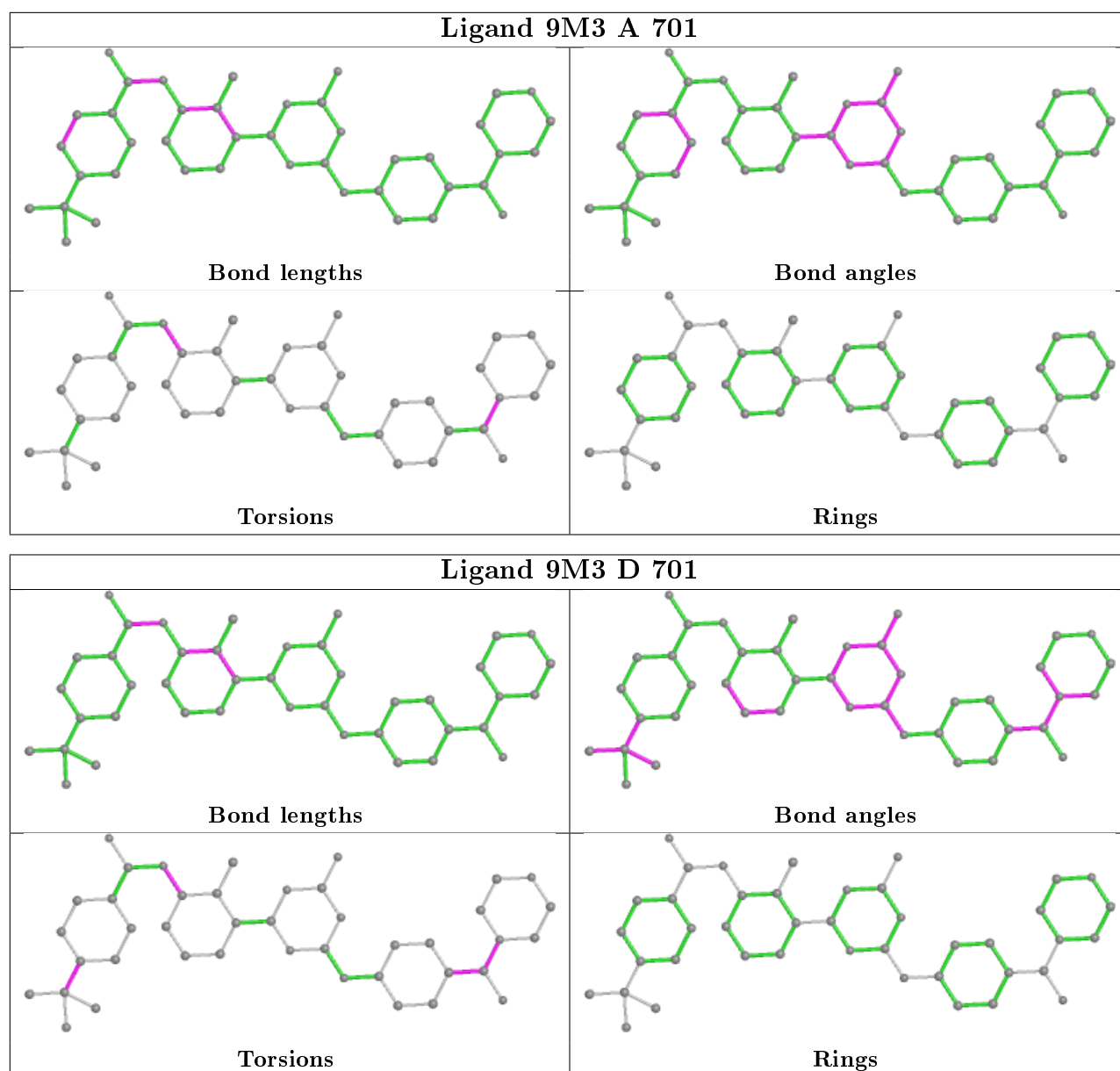
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	261/268 (97%)	-0.11	2 (0%) 86 86	25, 49, 71, 99	0
1	B	263/268 (98%)	-0.13	1 (0%) 92 93	21, 48, 74, 95	0
1	C	262/268 (97%)	-0.13	4 (1%) 73 73	23, 48, 75, 97	0
1	D	263/268 (98%)	-0.15	2 (0%) 86 86	24, 47, 73, 106	0
1	E	262/268 (97%)	-0.10	1 (0%) 92 93	23, 48, 74, 95	0
1	F	263/268 (98%)	-0.17	0 100 100	29, 49, 72, 94	0
All	All	1574/1608 (97%)	-0.13	10 (0%) 89 89	21, 48, 74, 106	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	TRP	3.1
1	D	569	LEU	2.5
1	A	489	MET	2.5
1	E	495	THR	2.3
1	C	471	PHE	2.2
1	A	473	ILE	2.2
1	C	462	GLY	2.2
1	C	453	SER	2.2
1	D	583	PHE	2.1
1	C	474	THR	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

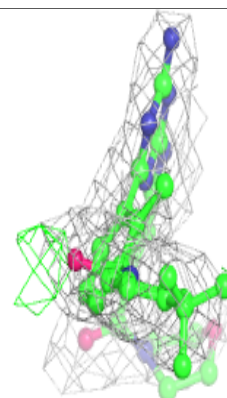
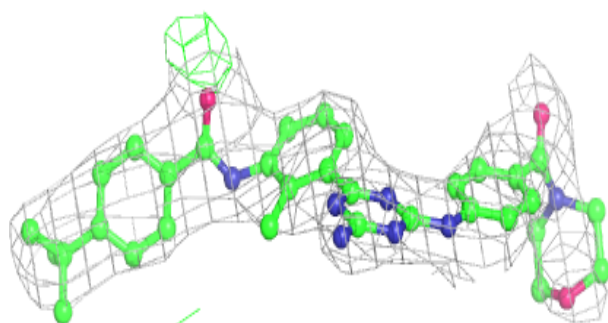
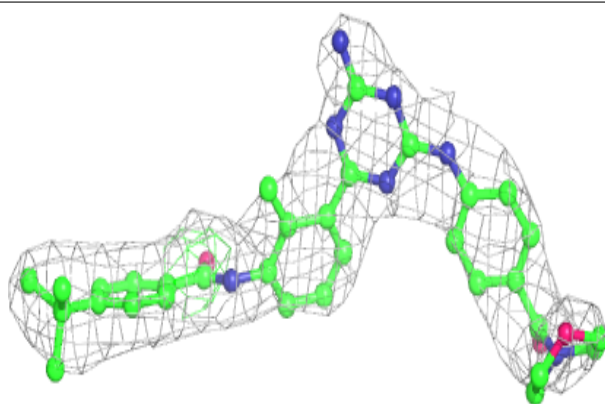
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	9M3	E	701	42/42	0.90	0.28	36,45,87,94	0
2	9M3	A	701	42/42	0.90	0.24	37,48,81,85	0
2	9M3	F	701	42/42	0.91	0.21	38,48,75,79	0
2	9M3	B	701	42/42	0.92	0.28	40,48,78,84	0
2	9M3	D	701	42/42	0.92	0.24	38,46,80,83	0
2	9M3	C	701	42/42	0.94	0.28	36,43,81,86	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.

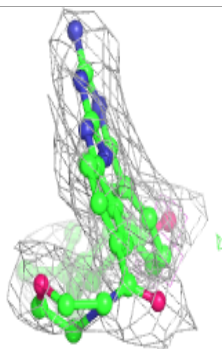
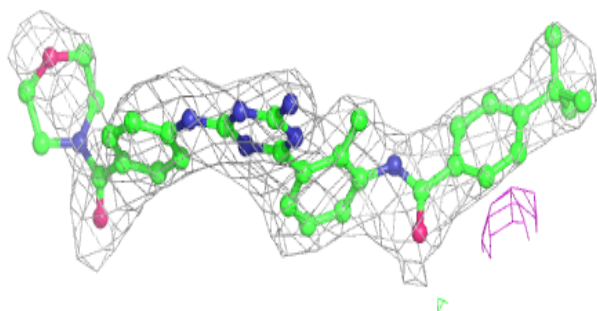
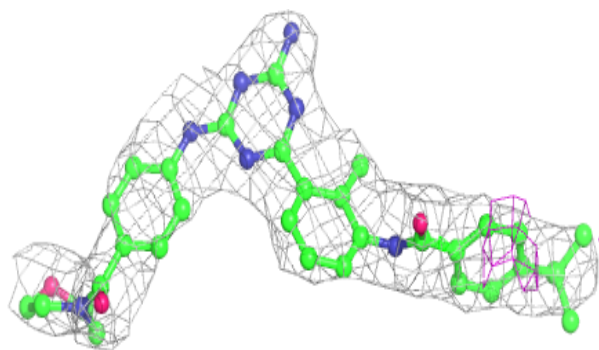
### Electron density around 9M3 E 701:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

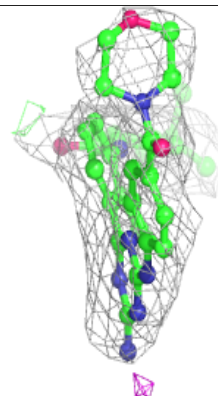
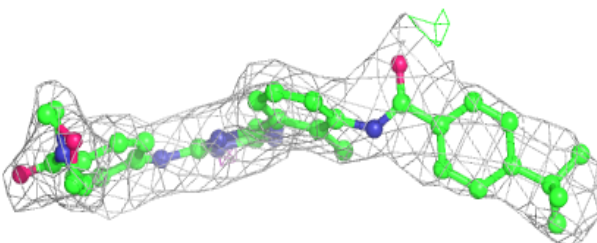
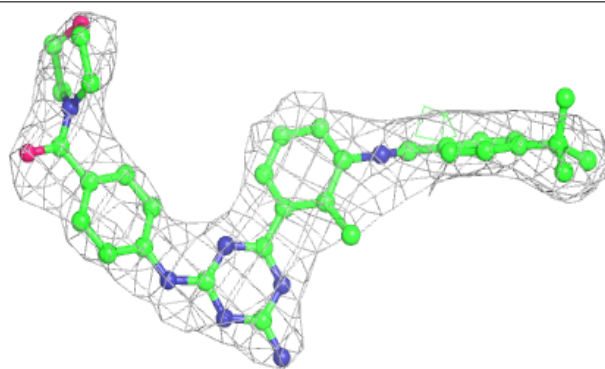


**Electron density around 9M3 A 701:**

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

**Electron density around 9M3 F 701:**

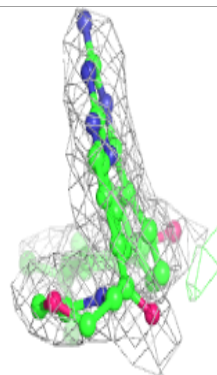
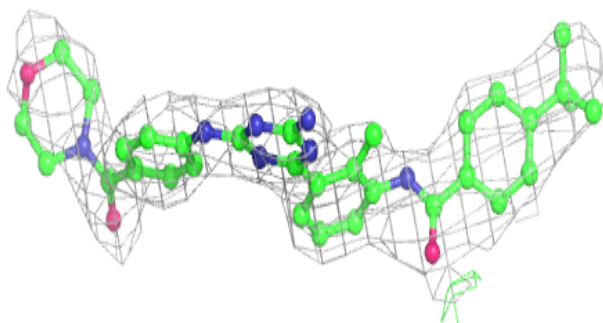
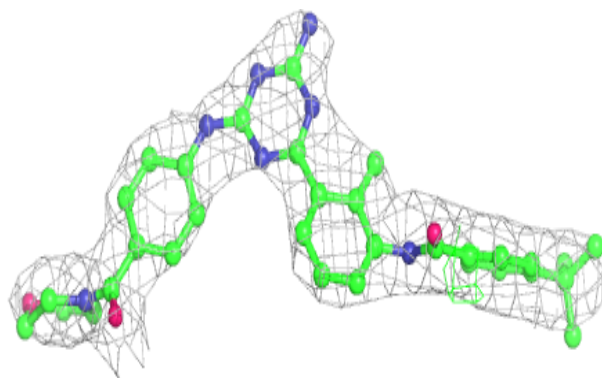
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



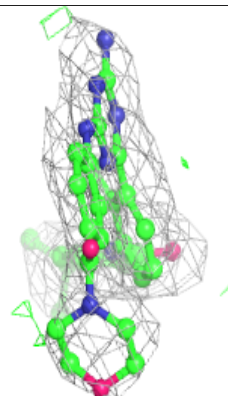
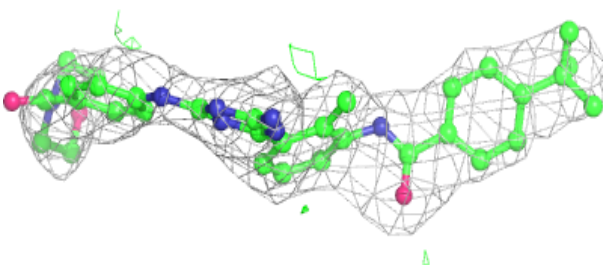
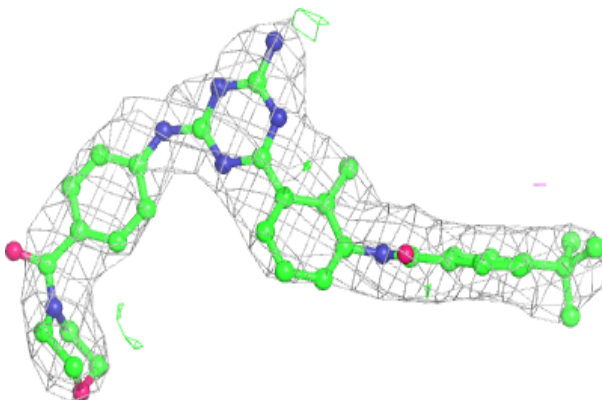


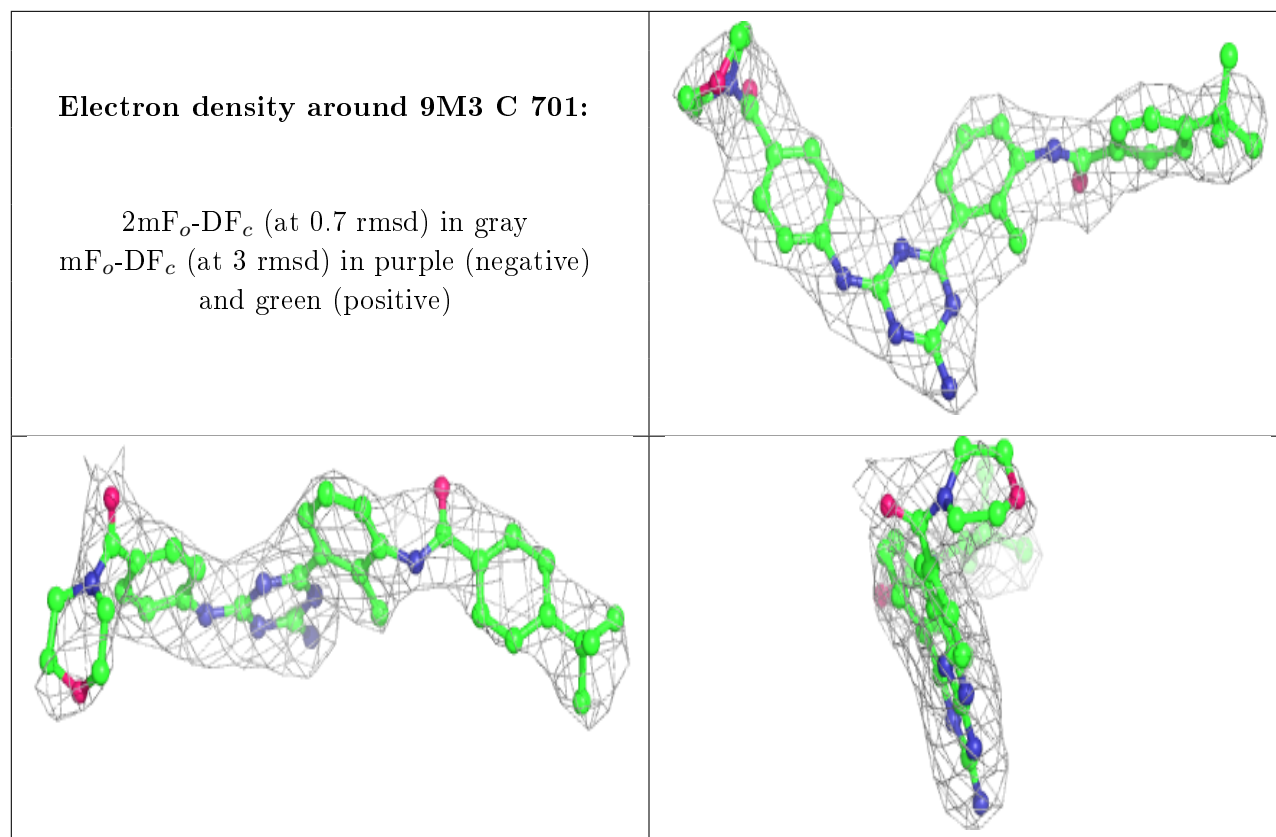
**Electron density around 9M3 B 701:**

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

**Electron density around 9M3 D 701:**

$2mF_o-DF_c$  (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.