



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:53 AM UTC

PDB ID : 5ZZ4 / pdb_00005zz4
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

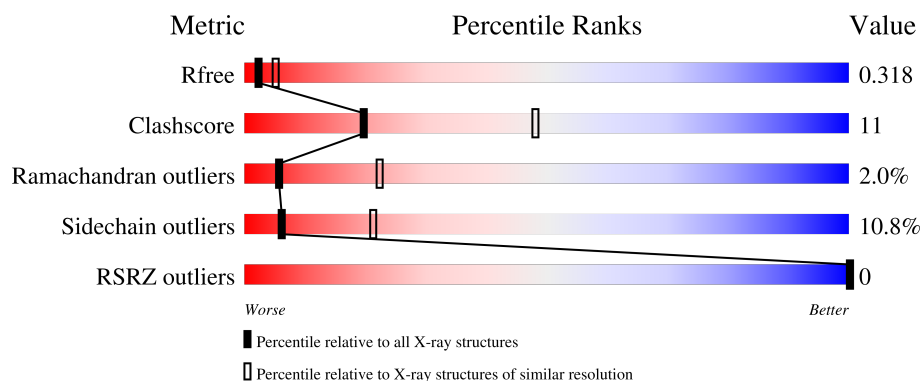
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	268	66% 26% 5% .
1	B	268	65% 27% 6% .
1	C	268	60% 35% . .
1	D	268	63% 28% 7% .
1	E	268	65% 28% 5% .

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Mol	Chain	Length	Quality of chain
1	F	268	70% 24% . .

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:

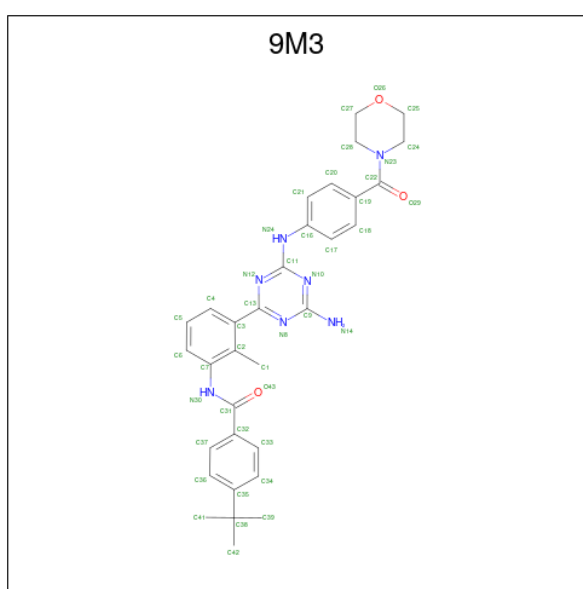
Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLY	-	expression tag	UNP Q06187
A	390	ALA	-	expression tag	UNP Q06187
A	391	MET	-	expression tag	UNP Q06187
A	392	GLY	-	expression tag	UNP Q06187
B	389	GLY	-	expression tag	UNP Q06187
B	390	ALA	-	expression tag	UNP Q06187
B	391	MET	-	expression tag	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 (CCD ID: 9M3) (formula: C₃₂H₃₅N₇O₃).

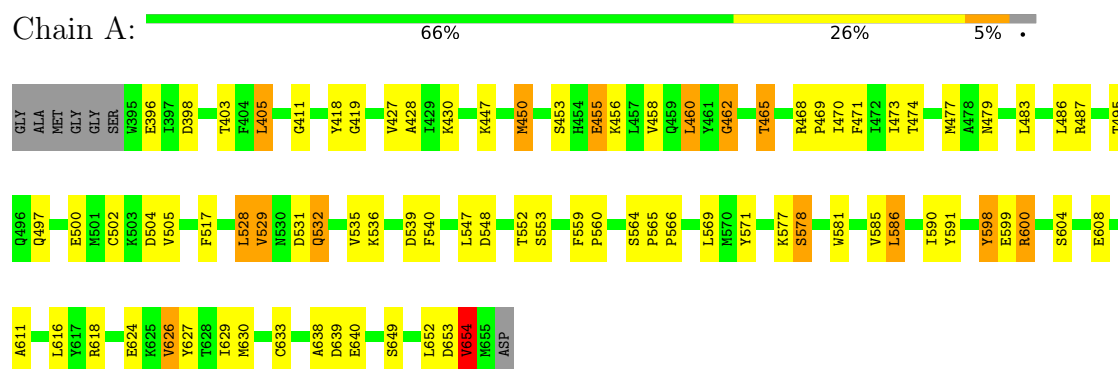


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	32	7	3		
2	B	1	Total	C	N	O	0	0
			42	32	7	3		
2	C	1	Total	C	N	O	0	0
			42	32	7	3		
2	D	1	Total	C	N	O	0	0
			42	32	7	3		
2	E	1	Total	C	N	O	0	0
			42	32	7	3		
2	F	1	Total	C	N	O	0	0
			42	32	7	3		

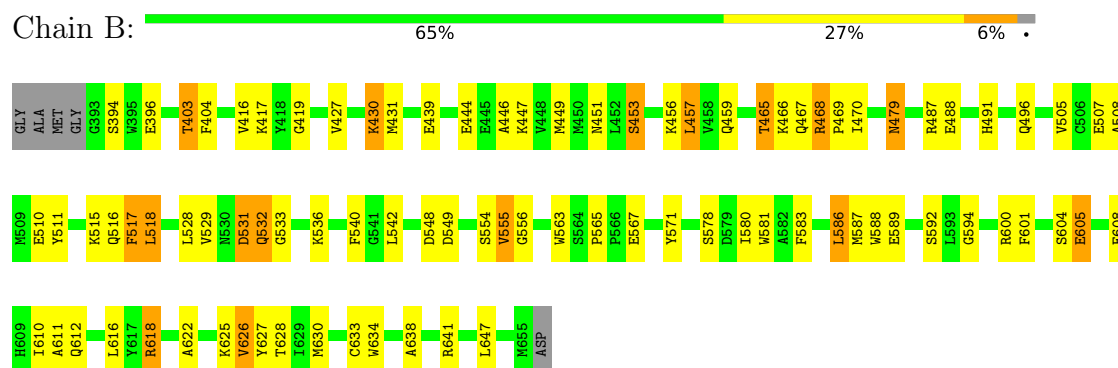
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

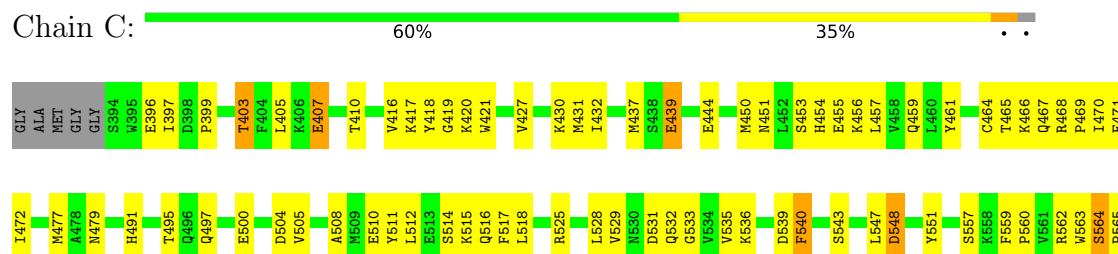
• Molecule 1: Tyrosine-protein kinase BTK

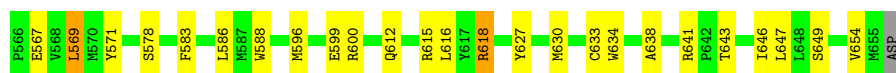


• Molecule 1: Tyrosine-protein kinase BTK



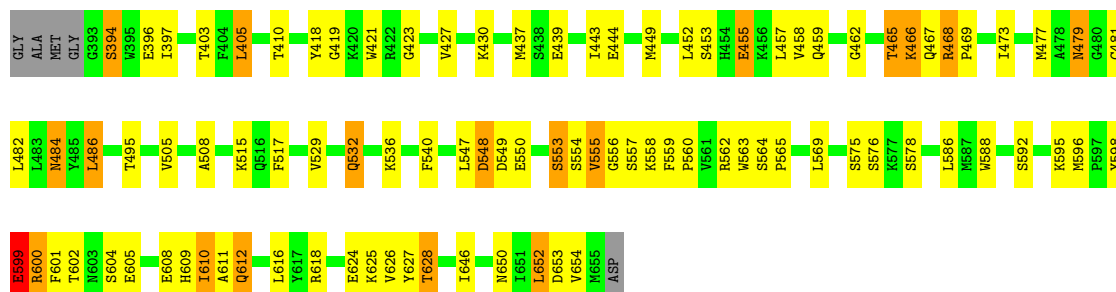
• Molecule 1: Tyrosine-protein kinase BTK





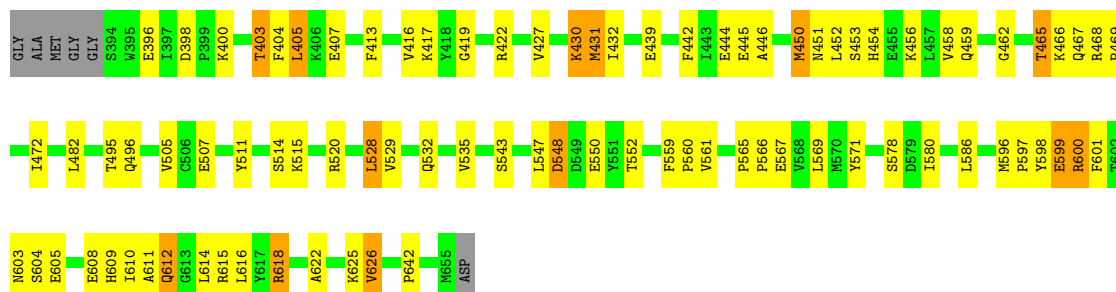
• Molecule 1: Tyrosine-protein kinase BTK

Chain D: 63% 28% 7%



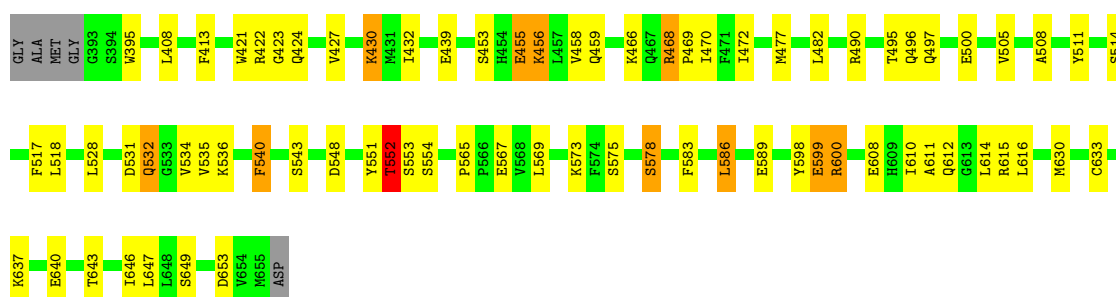
• Molecule 1: Tyrosine-protein kinase BTK

Chain E: 65% 28% 5%



• Molecule 1: Tyrosine-protein kinase BTK

Chain F: 70% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.27 Å 41.16 Å 587.94 Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	48.99 – 2.90 48.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.99-2.90) 99.8 (48.99-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.222 , 0.317 0.221 , 0.318	Depositor DCC
R_{free} test set	2042 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.934	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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	0.96	EDS
Total number of atoms	12800	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.92	0/2139	1.24	10/2889 (0.3%)
1	B	0.93	0/2139	1.25	6/2892 (0.2%)
1	C	0.94	0/2141	1.27	13/2894 (0.4%)
1	D	0.94	0/2155	1.26	7/2909 (0.2%)
1	E	0.93	0/2138	1.24	7/2888 (0.2%)
1	F	0.92	1/2128 (0.0%)	1.26	6/2876 (0.2%)
All	All	0.93	1/12840 (0.0%)	1.25	49/17348 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	456	LYS	CA-C	5.16	1.59	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	618	ARG	CA-C-N	-8.38	111.52	120.66
1	B	618	ARG	C-N-CA	-8.38	111.52	120.66
1	A	654	VAL	CB-CA-C	8.28	118.90	110.70
1	A	427	VAL	N-CA-C	8.23	120.73	108.46
1	F	427	VAL	N-CA-C	7.34	119.39	108.46
1	B	427	VAL	N-CA-C	7.11	118.97	108.45
1	E	571	TYR	N-CA-C	7.02	122.02	113.38
1	E	427	VAL	N-CA-C	6.90	118.75	108.46
1	A	571	TYR	N-CA-C	6.71	121.17	112.92
1	E	618	ARG	CA-C-N	-6.51	113.24	120.14
1	E	618	ARG	C-N-CA	-6.51	113.24	120.14
1	D	427	VAL	N-CA-C	6.43	118.05	108.46
1	F	552	THR	N-CA-C	6.36	119.52	111.69
1	A	578	SER	N-CA-C	-6.28	105.11	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	571	TYR	N-CA-C	6.08	120.32	113.02
1	D	599	GLU	CA-C-N	6.07	130.84	121.19
1	D	599	GLU	C-N-CA	6.07	130.84	121.19
1	C	461	TYR	N-CA-C	5.94	117.75	111.28
1	D	479	ASN	N-CA-C	5.89	119.23	112.57
1	C	548	ASP	N-CA-C	-5.85	98.33	110.80
1	E	454	HIS	N-CA-C	-5.81	99.69	108.46
1	F	578	SER	N-CA-C	-5.78	105.72	112.89
1	C	564	SER	CA-C-N	-5.77	114.43	120.38
1	C	564	SER	C-N-CA	-5.77	114.43	120.38
1	F	599	GLU	CA-C-N	5.72	128.75	120.79
1	F	599	GLU	C-N-CA	5.72	128.75	120.79
1	C	571	TYR	N-CA-C	5.72	120.26	112.88
1	C	518	LEU	N-CA-C	5.61	118.38	109.24
1	C	525	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	D	555	VAL	N-CA-C	-5.55	108.43	113.71
1	D	548	ASP	N-CA-C	-5.54	99.01	110.80
1	D	394	SER	N-CA-C	-5.53	105.15	112.94
1	A	591	TYR	N-CA-C	5.51	119.10	112.38
1	C	533	GLY	N-CA-C	5.45	122.78	115.59
1	B	518	LEU	N-CA-C	5.42	118.31	109.59
1	C	557	SER	N-CA-C	5.39	117.16	111.28
1	C	427	VAL	N-CA-C	5.37	117.61	108.86
1	C	618	ARG	CA-C-N	-5.32	114.47	119.85
1	C	618	ARG	C-N-CA	-5.32	114.47	119.85
1	F	518	LEU	N-CA-C	5.30	118.87	109.96
1	B	479	ASN	N-CA-C	5.27	118.73	112.72
1	A	599	GLU	CA-C-N	5.18	127.49	120.44
1	A	599	GLU	C-N-CA	5.18	127.49	120.44
1	C	539	ASP	N-CA-C	5.09	118.62	111.74
1	A	398	ASP	CA-C-N	5.05	125.33	119.47
1	A	398	ASP	C-N-CA	5.05	125.33	119.47
1	E	599	GLU	CA-C-N	5.04	127.80	120.79
1	E	599	GLU	C-N-CA	5.04	127.80	120.79
1	A	462	GLY	N-CA-C	5.03	117.40	110.56

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	40	0
1	B	2090	0	1988	50	0
1	C	2092	0	2006	58	0
1	D	2106	0	2046	53	0
1	E	2089	0	2003	51	0
1	F	2080	0	1985	40	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	285	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 11.

All (285) 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:B:404:PHE:HE2	1:B:431:MET:HE2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:PHE:CD2	1:C:647:LEU:HD13	2.28	0.69
1:F:453:SER:HA	1:F:459:GLN:HE22	1.57	0.68
1:A:477:MET:HE1	1:A:536:LYS:HD2	1.74	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:B:517:PHE:CD1	1:B:517:PHE:C	2.74	0.65
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:449:MET:HE1	1:B:542:LEU:HD13	1.82	0.61
1:B:465:THR:C	1:B:467:GLN:H	2.08	0.61
1:F:477:MET:HE2	1:F:536:LYS:HB2	1.83	0.60
1:C:396:GLU:OE2	1:C:465:THR:HG23	2.01	0.60
1:C:540:PHE:H	1:C:540:PHE:HD1	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: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:D:627:TYR:O	1:D:628:THR:C	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:PHE:CD1	1:C:517:PHE:C	2.83	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:D:477:MET:HE1	1:D:536:LYS:HD2	1.86	0.57
1:D:517:PHE:CD1	1:D:517:PHE:C	2.82	0.56
1:A:468:ARG:HA	1:A:469:PRO:C	2.29	0.56
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
1:D:652:LEU:C	1:D:654:VAL:H	2.13	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:F:468:ARG:HA	1:F:469:PRO:C	2.30	0.56
1:D:553:SER:C	1:D:555:VAL:H	2.14	0.56
1:D:600:ARG:HD2	1:D:601:PHE:CE2	2.41	0.56
1:E:596:MET:HE3	1:E:599:GLU:HA	1.86	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:F:517:PHE:CD1	1:F:517:PHE:C	2.83	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:E:547:LEU:O	1:E:548:ASP:HB2	2.09	0.53
1:E:450:MET:HE3	1:E:462:GLY:HA2	1.89	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:E:465:THR:C	1:E:467:GLN:H	2.17	0.53
1:E:559:PHE:CG	1:E:560:PRO:HD2	2.44	0.53
1:B:517:PHE:C	1:B:517:PHE:HD1	2.15	0.52
1:E:404:PHE:CZ	1:E:431:MET:HE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:497:GLN:O	1:F:500:GLU:HB3	2.09	0.52
1:B:531:ASP:C	1:B:533:GLY:H	2.18	0.52
1:C:600:ARG:HG3	1:D:600:ARG:HB3	1.90	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:497:GLN:O	1:A:500:GLU:HB3	2.09	0.52
1:C:468:ARG:HA	1:C:469:PRO:C	2.34	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
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: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:A:577:LYS:HD2	1:A:638:ALA:O	2.11	0.51
1:C:465:THR:C	1:C:467:GLN:H	2.19	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:A:652:LEU:C	1:A:654:VAL:H	2.20	0.50
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:468:ARG:HA	1:E:469:PRO:C	2.36	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:456:LYS:HA	1:C:536:LYS:HG2	1.95	0.48
1:D:532:GLN:N	1:D:532:GLN:CD	2.71	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:B:417:LYS:HE3	1:B:431:MET:CE	2.44	0.48
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: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:E:596:MET:HE2	1:E:596:MET:HB3	1.81	0.47
1:B:456:LYS:NZ	1:B:507:GLU:OE2	2.47	0.47
1:B:488:GLU:HB3	1:B:491:HIS:HD2	1.79	0.47
1:E:600:ARG:HD3	1:F:600:ARG:HD3	1.96	0.47
1:B:587:MET:O	1:B:588:TRP:C	2.58	0.47
1:C:403:THR:O	1:C:419:GLY:HA3	2.14	0.47
1:C:477:MET:HE1	1:C:536:LYS:HD2	1.97	0.47
1:F:508:ALA:O	1:F:511:TYR:HB3	2.15	0.47
1:A:477:MET:CE	1:A:536:LYS:HD2	2.42	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:D:465:THR:C	1:D:467:GLN:H	2.23	0.47
1:B:505:VAL:HG11	1:B:586:LEU:HD21	1.97	0.46
1:F:600:ARG:H	1:F:600:ARG:HG3	1.45	0.46
1:C:405:LEU:HG	1:C:419:GLY:HA2	1.97	0.46
1:A:405:LEU:HD12	1:A:418:TYR:HE2	1.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:PRO:HA	1:A:569:LEU:HD12	1.98	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
1:D:455:GLU:O	1:D:536:LYS:HE2	2.15	0.45
1:F:421:TRP:C	1:F:423:GLY:H	2.25	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:A:517:PHE:CD1	1:A:517:PHE:C	2.95	0.45
1:B:549:ASP:OD1	1:B:549:ASP:N	2.50	0.45
1:C:437:MET:C	1:C:439:GLU:H	2.25	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:477:MET:HE1	1:F:536:LYS:HD2	1.99	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: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:D:575:SER:O	1:D:576:SER:C	2.61	0.44
1:E:442:PHE:CZ	1:E:472:ILE:HD11	2.52	0.44
1:B:417:LYS:HE3	1:B:431:MET:HE3	1.99	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:D:556:GLY:C	1:D:558:LYS:H	2.26	0.43
1:B:468:ARG:HA	1:B:469:PRO:C	2.42	0.43
1:F:408:LEU:HD22	2:F:701:9M3:C17	2.49	0.43
1:A:616:LEU:O	1:A:627:TYR:OH	2.32	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:468:ARG:HA	1:D:469:PRO:C	2.42	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:C:596:MET:HE3	1:C:599:GLU:HA	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:SER:O	1:B:555:VAL:C	2.61	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:H	1:E:600:ARG:HG3	1.32	0.43
1:B:465:THR:C	1:B:467:GLN:N	2.77	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:A:560:PRO:O	1:A:564:SER:OG	2.25	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:B:404:PHE:CE2	1:B:431:MET:HE2	2.44	0.42
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
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:D:477:MET:HE2	1:D:536:LYS:HB2	2.01	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:A:430:LYS:NZ	1:A:539:ASP:OD1	2.53	0.42
1:B:554:SER:C	1:B:556:GLY:N	2.78	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:F:517:PHE:C	1:F:517:PHE:HD1	2.26	0.42
1:E:482:LEU:HD22	1:E:535:VAL:HG11	2.01	0.41
1:C:477:MET:HE2	1:C:536:LYS:HB2	2.02	0.41
1:C:565:PRO:HG3	1:C:578:SER:HA	2.02	0.41
1:E:450:MET:C	1:E:452:LEU:H	2.28	0.41
1:A:430:LYS:O	1:A:471:PHE:HA	2.20	0.41
1:F:477:MET:CE	1:F:536:LYS:HB2	2.48	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:C:454:HIS:C	1:C:456:LYS:N	2.79	0.41
1:D:588:TRP:O	1:D:592:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:GLU:O	1:E:446:ALA:C	2.64	0.41
1:A:450:MET:HG2	1:A:460:LEU:HD23	2.03	0.41
1:A:502:CYS:SG	1:A:590:ILE:HD13	2.61	0.41
1:B:457:LEU:HD11	1:B:511:TYR:CE2	2.55	0.41
1:E:404:PHE:C	1:E:405:LEU:HD23	2.45	0.41
1:F:569:LEU:HD12	1:F:610:ILE:HD11	2.03	0.41
1:B:449:MET:HE2	1:B:449:MET:HB3	1.99	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:A:483:LEU:HD21	1:A:487:ARG:NH2	2.36	0.40
1:B:446:ALA:O	1:B:447:LYS:C	2.64	0.40
1:D:437:MET:C	1:D:439:GLU:H	2.29	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:599:GLU:H	1:D:599:GLU:CD	2.28	0.40
1:D:646:ILE:HG22	1:D:650:ASN:ND2	2.37	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 [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	259/268 (97%)	225 (87%)	30 (12%)	4 (2%)	8 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	261/268 (97%)	227 (87%)	28 (11%)	6 (2%)	5	19
1	C	260/268 (97%)	233 (90%)	23 (9%)	4 (2%)	8	28
1	D	261/268 (97%)	215 (82%)	38 (15%)	8 (3%)	3	14
1	E	260/268 (97%)	230 (88%)	26 (10%)	4 (2%)	8	28
1	F	261/268 (97%)	231 (88%)	25 (10%)	5 (2%)	6	23
All	All	1562/1608 (97%)	1361 (87%)	170 (11%)	31 (2%)	6	22

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
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

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Mol	Chain	Res	Type
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%)	198 (88%)	26 (12%)	5	18
1	B	222/239 (93%)	197 (89%)	25 (11%)	5	19
1	C	223/239 (93%)	202 (91%)	21 (9%)	8	26
1	D	227/239 (95%)	198 (87%)	29 (13%)	4	14
1	E	223/239 (93%)	201 (90%)	22 (10%)	7	24
1	F	220/239 (92%)	199 (90%)	21 (10%)	8	26
All	All	1339/1434 (93%)	1195 (89%)	144 (11%)	6	21

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	THR
1	A	405	LEU
1	A	447	LYS
1	A	450	MET
1	A	453	SER
1	A	455	GLU
1	A	460	LEU
1	A	465	THR
1	A	470	ILE
1	A	486	LEU
1	A	495	THR
1	A	528	LEU
1	A	529	VAL
1	A	540	PHE
1	A	547	LEU
1	A	552	THR
1	A	553	SER

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Mol	Chain	Res	Type
1	A	586	LEU
1	A	598	TYR
1	A	600	ARG
1	A	604	SER
1	A	626	VAL
1	A	639	ASP
1	A	640	GLU
1	A	649	SER
1	A	654	VAL
1	B	394	SER
1	B	403	THR
1	B	430	LYS
1	B	451	ASN
1	B	453	SER
1	B	457	LEU
1	B	465	THR
1	B	468	ARG
1	B	470	ILE
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	567	GLU
1	B	586	LEU
1	B	592	SER
1	B	604	SER
1	B	605	GLU
1	B	610	ILE
1	B	626	VAL
1	C	403	THR
1	C	407	GLU
1	C	410	THR
1	C	431	MET
1	C	450	MET
1	C	466	LYS
1	C	470	ILE
1	C	491	HIS

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Mol	Chain	Res	Type
1	C	495	THR
1	C	510	GLU
1	C	515	LYS
1	C	516	GLN
1	C	528	LEU
1	C	531	ASP
1	C	532	GLN
1	C	540	PHE
1	C	547	LEU
1	C	567	GLU
1	C	569	LEU
1	C	649	SER
1	C	654	VAL
1	D	394	SER
1	D	403	THR
1	D	405	LEU
1	D	410	THR
1	D	430	LYS
1	D	444	GLU
1	D	449	MET
1	D	455	GLU
1	D	465	THR
1	D	466	LYS
1	D	468	ARG
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	610	ILE
1	D	612	GLN
1	D	624	GLU
1	D	625	LYS
1	D	626	VAL
1	D	628	THR
1	D	652	LEU

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Mol	Chain	Res	Type
1	E	403	THR
1	E	405	LEU
1	E	407	GLU
1	E	417	LYS
1	E	430	LYS
1	E	431	MET
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	515	LYS
1	E	528	LEU
1	E	529	VAL
1	E	552	THR
1	E	567	GLU
1	E	600	ARG
1	E	604	SER
1	E	612	GLN
1	E	625	LYS
1	E	626	VAL
1	F	424	GLN
1	F	430	LYS
1	F	455	GLU
1	F	466	LYS
1	F	468	ARG
1	F	470	ILE
1	F	495	THR
1	F	496	GLN
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	573	LYS
1	F	575	SER
1	F	586	LEU
1	F	599	GLU
1	F	600	ARG

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Mol	Chain	Res	Type
1	F	649	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	GLN
1	A	479	ASN
1	A	484	ASN
1	A	497	GLN
1	A	532	GLN
1	B	412	GLN
1	B	451	ASN
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	C	650	ASN
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	497	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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	1.70	3 (6%)	65,66,66	2.14	13 (20%)
2	9M3	B	701	-	46,46,46	1.78	4 (8%)	65,66,66	2.22	10 (15%)
2	9M3	E	701	-	46,46,46	1.72	4 (8%)	65,66,66	2.18	12 (18%)
2	9M3	D	701	-	46,46,46	1.72	3 (6%)	65,66,66	1.94	14 (21%)
2	9M3	A	701	-	46,46,46	1.74	4 (8%)	65,66,66	1.99	10 (15%)
2	9M3	C	701	-	46,46,46	1.77	3 (6%)	65,66,66	2.07	11 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9M3	F	701	-	-	16/30/38/38	0/5/5/5
2	9M3	B	701	-	-	6/30/38/38	0/5/5/5
2	9M3	E	701	-	-	12/30/38/38	0/5/5/5
2	9M3	D	701	-	-	14/30/38/38	0/5/5/5
2	9M3	A	701	-	-	6/30/38/38	0/5/5/5
2	9M3	C	701	-	-	6/30/38/38	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	9M3	C3-C2	6.94	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	9M3	C3-C2	6.93	1.51	1.40
2	C	701	9M3	C3-C2	6.87	1.51	1.40
2	E	701	9M3	C7-C2	6.84	1.51	1.40
2	D	701	9M3	C3-C2	6.83	1.51	1.40
2	D	701	9M3	C7-C2	6.54	1.50	1.40
2	C	701	9M3	C7-C2	6.43	1.50	1.40
2	B	701	9M3	C3-C2	6.40	1.50	1.40
2	F	701	9M3	C7-C2	6.37	1.50	1.40
2	B	701	9M3	C7-C2	6.30	1.50	1.40
2	E	701	9M3	C3-C2	6.10	1.50	1.40
2	A	701	9M3	C7-C2	5.75	1.49	1.40
2	B	701	9M3	C31-N30	-3.07	1.26	1.35
2	E	701	9M3	C31-N30	-2.82	1.27	1.35
2	A	701	9M3	C31-N30	-2.80	1.27	1.35
2	D	701	9M3	C31-N30	-2.79	1.27	1.35
2	C	701	9M3	C31-N30	-2.71	1.27	1.35
2	F	701	9M3	C31-N30	-2.67	1.28	1.35
2	B	701	9M3	C19-C22	2.54	1.54	1.50
2	A	701	9M3	C33-C34	2.22	1.42	1.38
2	E	701	9M3	C9-N10	2.03	1.38	1.35

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	9M3	C11-N12-C13	12.20	122.28	114.50
2	B	701	9M3	C11-N12-C13	11.21	121.65	114.50
2	F	701	9M3	C11-N12-C13	10.66	121.30	114.50
2	C	701	9M3	C11-N12-C13	10.25	121.03	114.50
2	A	701	9M3	C11-N12-C13	10.07	120.92	114.50
2	D	701	9M3	C11-N12-C13	7.75	119.44	114.50
2	E	701	9M3	N10-C11-N12	-5.88	116.62	126.26
2	B	701	9M3	N10-C11-N12	-5.54	117.19	126.26
2	C	701	9M3	N10-C11-N12	-5.46	117.32	126.26
2	F	701	9M3	C24-N23-C28	5.33	123.55	112.68
2	A	701	9M3	N10-C11-N12	-5.26	117.64	126.26
2	D	701	9M3	N10-C11-N12	-5.08	117.94	126.26
2	F	701	9M3	N10-C11-N12	-5.03	118.02	126.26
2	D	701	9M3	C9-N10-C11	4.96	122.01	113.77
2	C	701	9M3	C9-N10-C11	4.76	121.67	113.77
2	E	701	9M3	C9-N10-C11	4.53	121.28	113.77
2	B	701	9M3	C9-N10-C11	4.46	121.17	113.77
2	A	701	9M3	C9-N10-C11	4.45	121.16	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	9M3	C9-N10-C11	4.37	121.02	113.77
2	D	701	9M3	C24-N23-C28	4.35	121.56	112.68
2	C	701	9M3	N14-C9-N10	4.30	123.67	117.22
2	B	701	9M3	N14-C9-N10	4.16	123.46	117.22
2	D	701	9M3	N10-C9-N8	-3.92	119.47	125.48
2	C	701	9M3	N10-C9-N8	-3.69	119.82	125.48
2	B	701	9M3	C9-N8-C13	3.69	119.92	114.36
2	B	701	9M3	C25-C24-N23	3.67	117.54	109.82
2	E	701	9M3	N14-C9-N10	3.52	122.50	117.22
2	C	701	9M3	C9-N8-C13	3.50	119.63	114.36
2	A	701	9M3	C9-N8-C13	3.46	119.58	114.36
2	A	701	9M3	N14-C9-N10	3.44	122.39	117.22
2	F	701	9M3	N10-C9-N8	-3.43	120.23	125.48
2	F	701	9M3	C9-N8-C13	3.39	119.47	114.36
2	A	701	9M3	N10-C9-N8	-3.36	120.34	125.48
2	B	701	9M3	N10-C9-N8	-3.32	120.39	125.48
2	B	701	9M3	N12-C13-N8	-3.31	119.68	125.13
2	D	701	9M3	C9-N8-C13	3.23	119.23	114.36
2	E	701	9M3	N10-C9-N8	-3.21	120.57	125.48
2	F	701	9M3	N12-C13-N8	-3.14	119.96	125.13
2	D	701	9M3	N14-C9-N10	3.13	121.91	117.22
2	B	701	9M3	C24-N23-C28	3.10	119.01	112.68
2	F	701	9M3	N14-C9-N10	2.99	121.71	117.22
2	D	701	9M3	C19-C22-N23	2.93	122.32	118.66
2	A	701	9M3	N12-C13-N8	-2.90	120.36	125.13
2	E	701	9M3	C9-N8-C13	2.88	118.69	114.36
2	C	701	9M3	N12-C13-N8	-2.81	120.50	125.13
2	E	701	9M3	N12-C13-N8	-2.79	120.55	125.13
2	C	701	9M3	C24-N23-C28	2.73	118.24	112.68
2	B	701	9M3	C42-C38-C35	-2.60	104.21	110.35
2	D	701	9M3	C41-C38-C35	-2.47	104.54	110.35
2	F	701	9M3	C3-C13-N8	2.46	121.02	117.22
2	C	701	9M3	C3-C13-N8	2.45	121.01	117.22
2	D	701	9M3	C4-C5-C6	2.42	123.35	120.24
2	C	701	9M3	C25-O26-C27	2.35	117.48	109.88
2	E	701	9M3	C41-C38-C35	-2.34	104.84	110.35
2	A	701	9M3	C36-C37-C32	2.33	123.28	120.80
2	F	701	9M3	C39-C38-C35	2.30	115.78	110.35
2	E	701	9M3	C3-C13-N8	2.30	120.78	117.22
2	A	701	9M3	C33-C32-C37	-2.29	115.66	118.57
2	E	701	9M3	C39-C38-C42	-2.27	101.61	108.36
2	A	701	9M3	C3-C13-N8	2.27	120.73	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	9M3	C39-C38-C35	2.24	115.64	110.35
2	F	701	9M3	C1-C2-C3	2.19	124.74	120.78
2	F	701	9M3	O29-C22-N23	-2.16	118.95	122.35
2	D	701	9M3	O29-C22-N23	-2.09	119.05	122.35
2	E	701	9M3	C24-N23-C28	2.08	116.93	112.68
2	D	701	9M3	C3-C13-N8	2.08	120.44	117.22
2	E	701	9M3	C42-C38-C35	2.07	115.22	110.35
2	C	701	9M3	O26-C27-C28	2.05	116.18	111.77
2	D	701	9M3	N24-C11-N12	2.01	123.82	116.90
2	F	701	9M3	C2-C7-N30	-2.01	116.47	119.34

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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	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	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	F	701	9M3	C19-C22-N23-C28
2	F	701	9M3	C19-C22-N23-C24
2	F	701	9M3	O29-C22-N23-C28
2	F	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	C	701	9M3	C2-C7-N30-C31
2	F	701	9M3	C18-C19-C22-N23

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Mol	Chain	Res	Type	Atoms
2	F	701	9M3	C20-C19-C22-O29
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	A	701	9M3	C2-C7-N30-C31
2	F	701	9M3	C20-C19-C22-N23
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	E	701	9M3	C36-C35-C38-C41
2	D	701	9M3	C34-C35-C38-C41
2	D	701	9M3	C36-C35-C38-C41
2	E	701	9M3	C34-C35-C38-C41
2	D	701	9M3	C18-C19-C22-O29
2	F	701	9M3	C36-C35-C38-C41
2	F	701	9M3	C34-C35-C38-C41
2	E	701	9M3	C2-C7-N30-C31
2	E	701	9M3	C34-C35-C38-C42
2	F	701	9M3	C34-C35-C38-C42
2	D	701	9M3	C36-C35-C38-C39
2	D	701	9M3	C34-C35-C38-C39
2	E	701	9M3	C36-C35-C38-C42
2	D	701	9M3	C34-C35-C38-C42
2	D	701	9M3	C36-C35-C38-C42
2	F	701	9M3	C36-C35-C38-C42
2	F	701	9M3	C36-C35-C38-C39
2	E	701	9M3	C36-C35-C38-C39
2	E	701	9M3	C34-C35-C38-C39
2	F	701	9M3	C34-C35-C38-C39

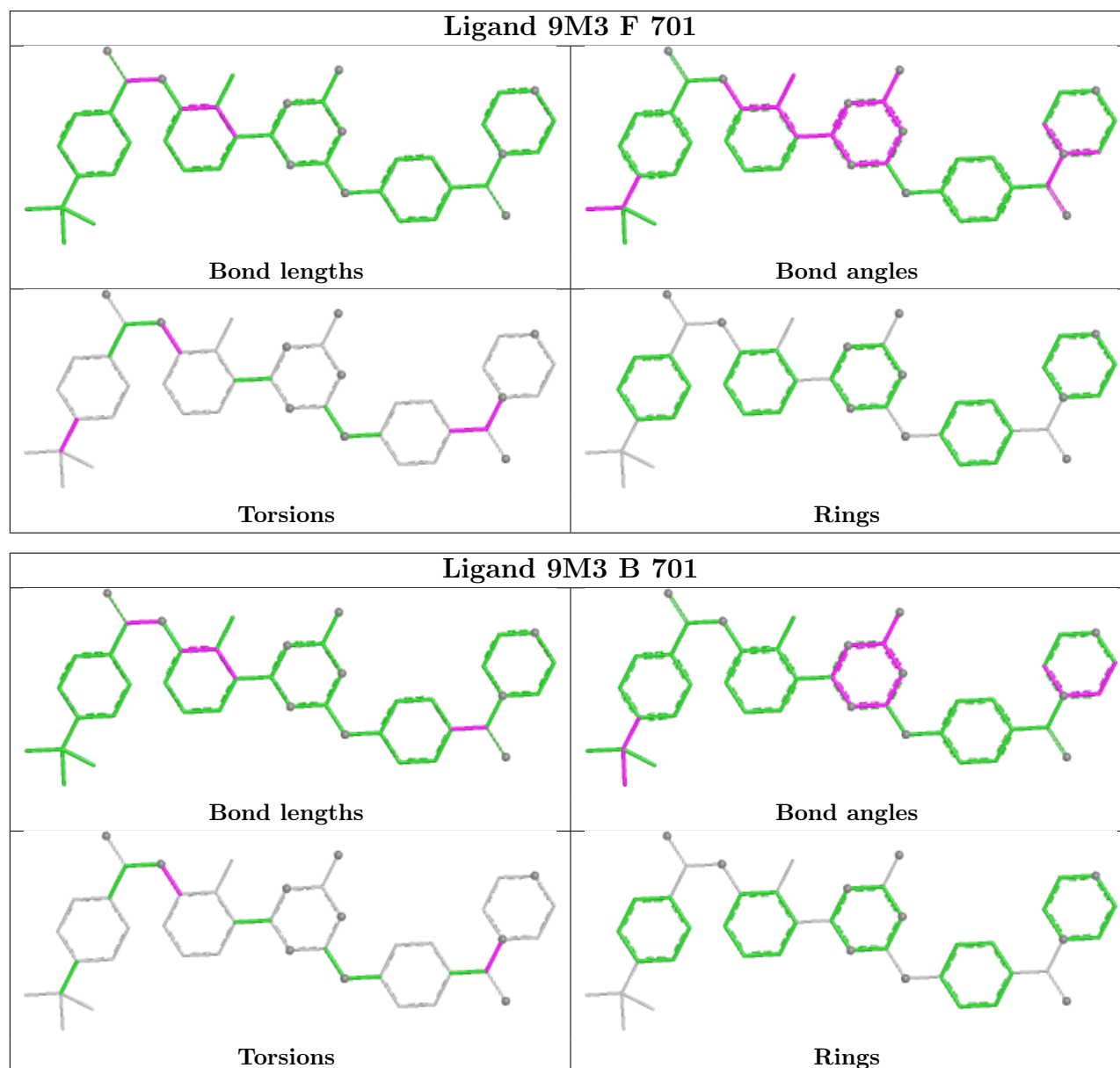
There are no ring outliers.

2 monomers are involved in 2 short contacts:

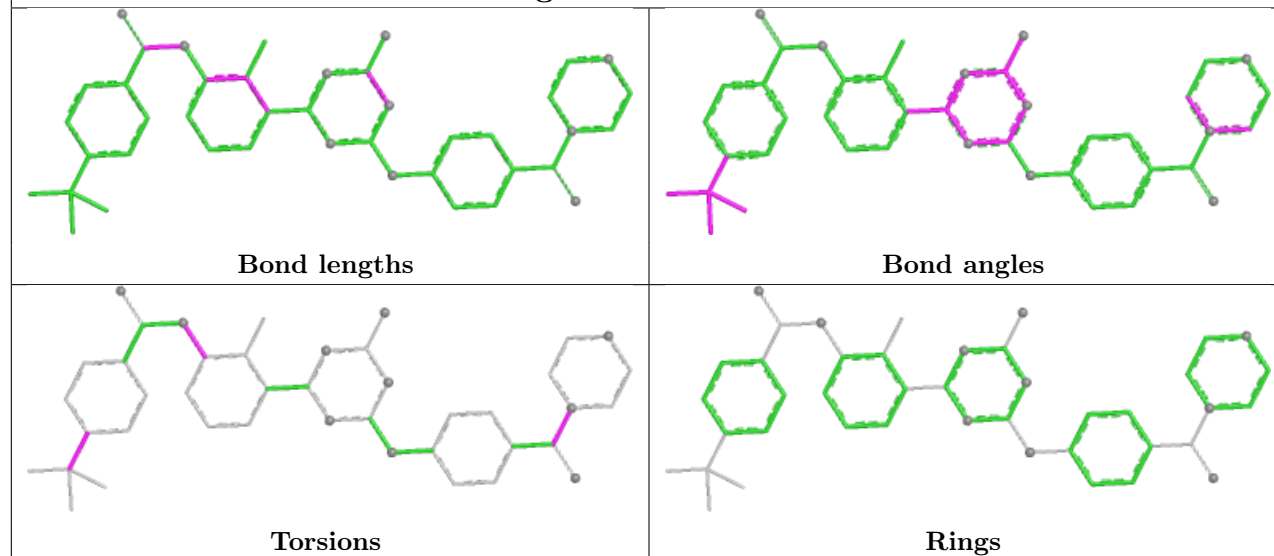
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	9M3	1	0
2	A	701	9M3	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

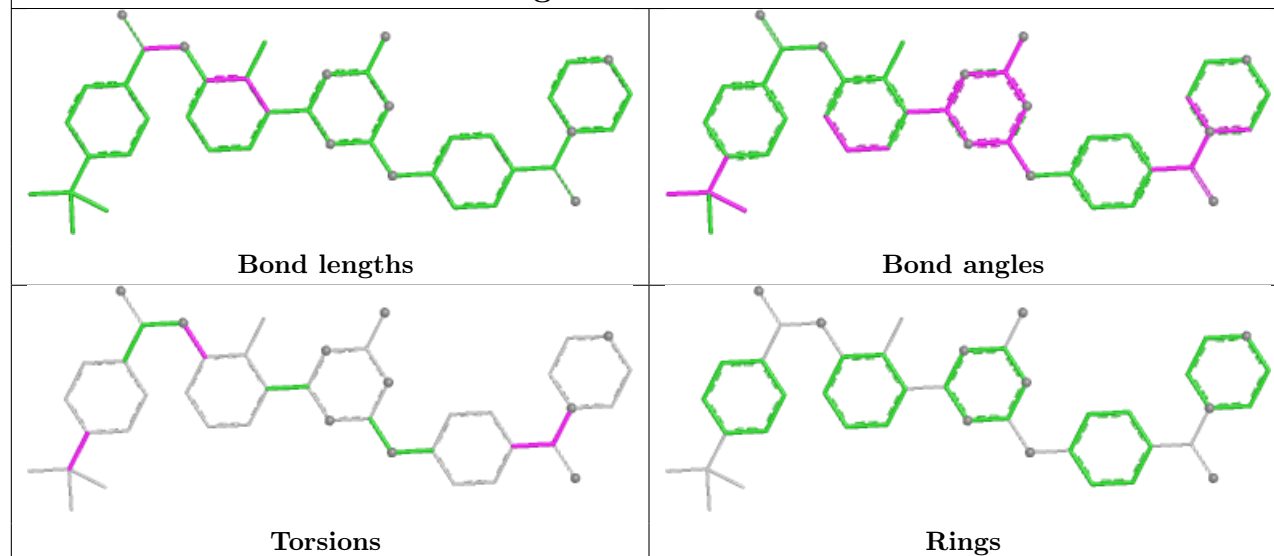
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

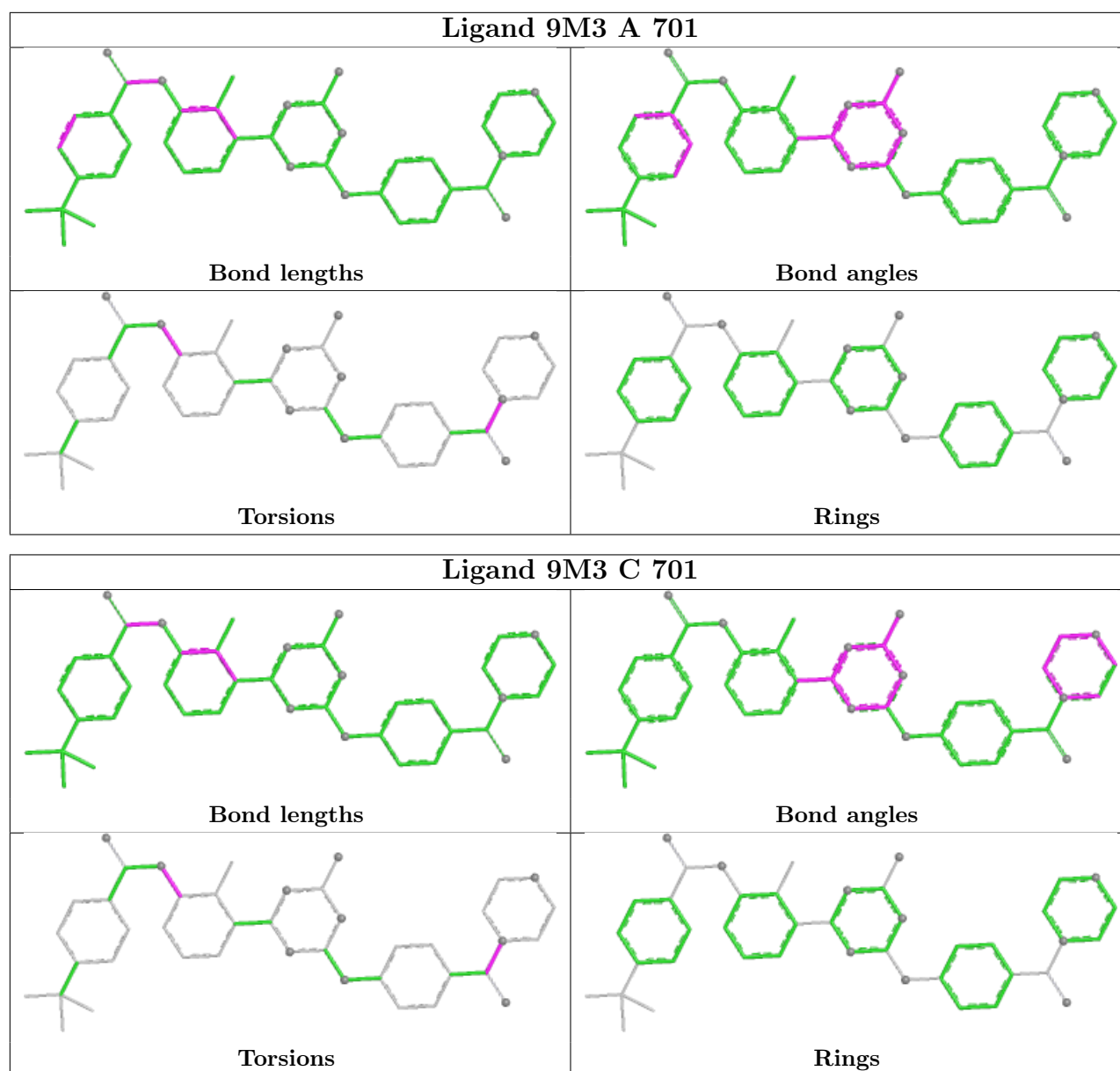


Ligand 9M3 E 701



Ligand 9M3 D 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/268 (97%)	-1.35	0 100 100	25, 49, 71, 99	0
1	B	263/268 (98%)	-1.35	0 100 100	21, 48, 74, 95	0
1	C	262/268 (97%)	-1.32	0 100 100	23, 48, 75, 97	0
1	D	263/268 (98%)	-1.37	0 100 100	24, 47, 73, 106	0
1	E	262/268 (97%)	-1.33	0 100 100	23, 48, 74, 95	0
1	F	263/268 (98%)	-1.36	0 100 100	29, 49, 72, 94	0
All	All	1574/1608 (97%)	-1.35	0 100 100	21, 48, 74, 106	0

There are no RSRZ outliers to report.

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	9M3	A	701	42/42	0.99	0.04	37,48,81,85	0

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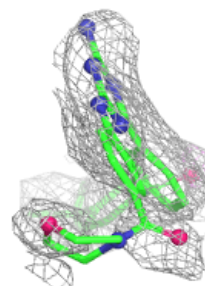
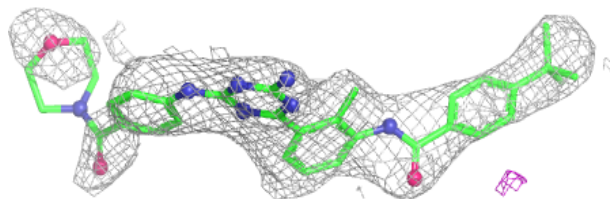
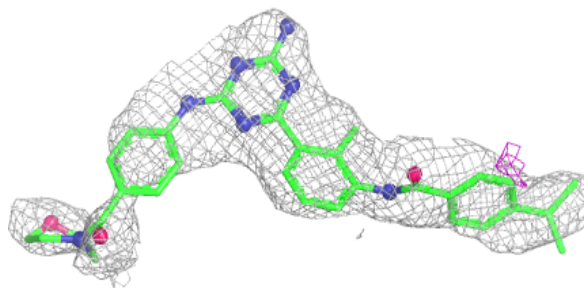
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	9M3	B	701	42/42	0.99	0.05	40,48,78,84	0
2	9M3	C	701	42/42	0.99	0.04	36,43,81,86	0
2	9M3	D	701	42/42	0.99	0.05	38,46,80,83	0
2	9M3	E	701	42/42	0.99	0.05	36,45,87,94	0
2	9M3	F	701	42/42	0.99	0.04	38,48,75,79	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.

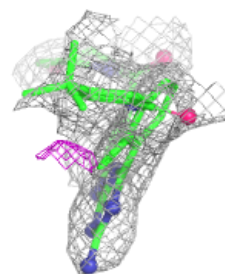
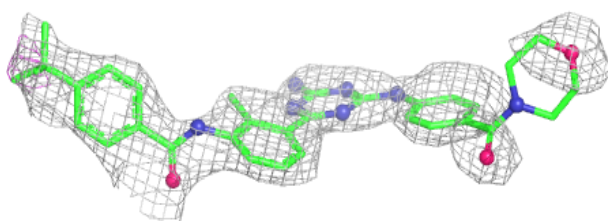
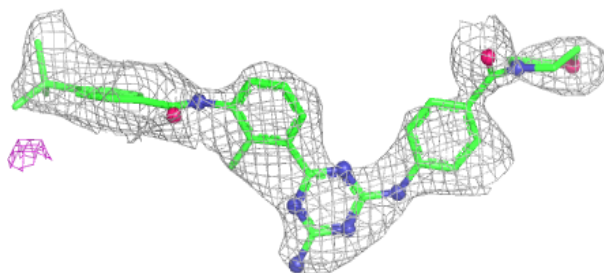
Electron density around 9M3 A 701:

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

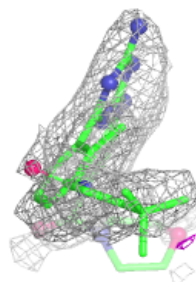
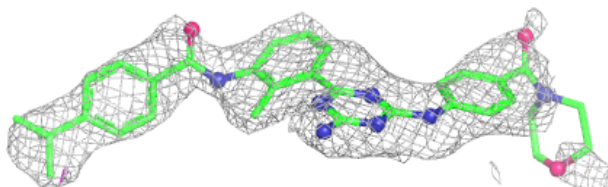
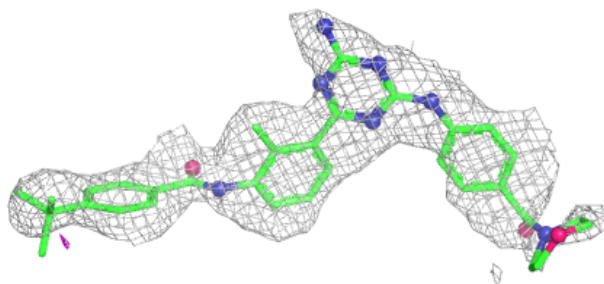


Electron density around 9M3 B 701:

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

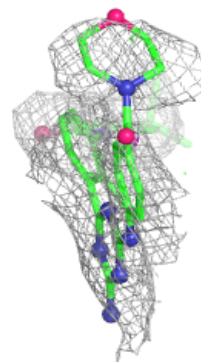
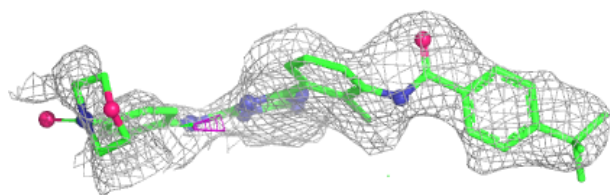
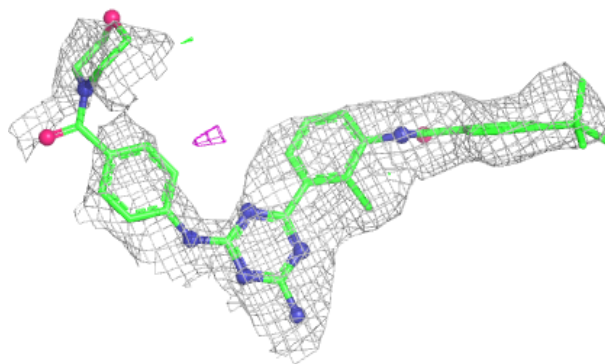
**Electron density around 9M3 C 701:**

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

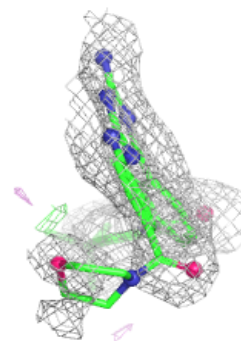
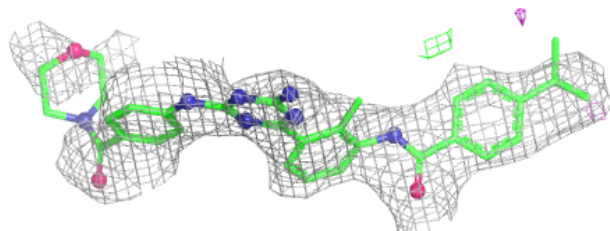
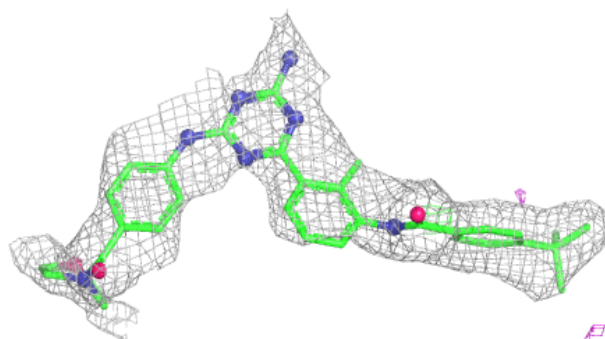


Electron density around 9M3 D 701:

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

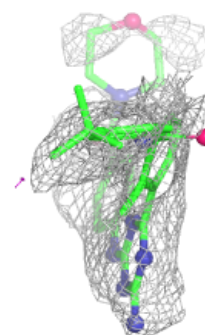
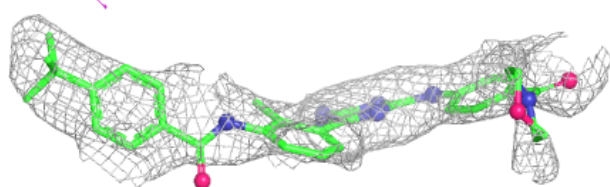
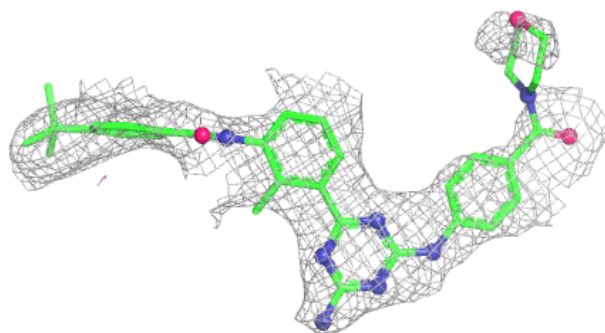
**Electron density around 9M3 E 701:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.