



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:39 PM EDT

PDB ID : 4TTV / pdb_00004ttv
Title : Crystal structure of human ThrRS complexing with a bioengineered macrolide BC194
Authors : Fang, P.; Guo, M.
Deposited on : 2014-06-23
Resolution : 2.80 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

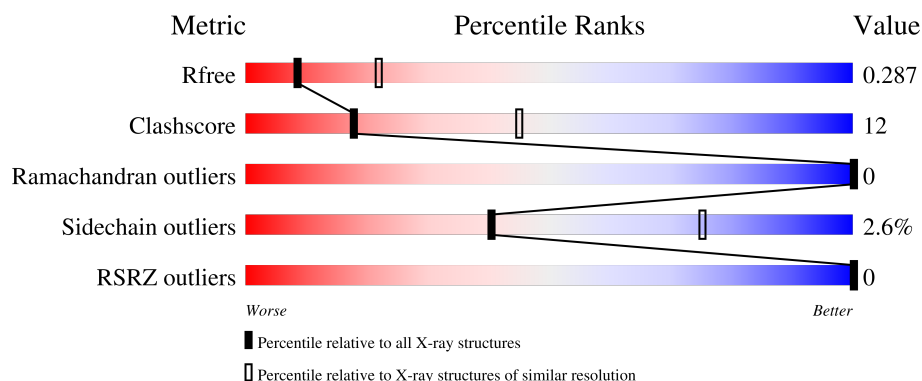
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	414	
1	B	414	
1	C	414	
1	D	414	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13247 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 Threonine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3263	2083	570	594	16			
1	B	403	Total	C	N	O	S	0	0	0
			3269	2086	573	594	16			
1	C	403	Total	C	N	O	S	0	0	0
			3257	2080	571	590	16			
1	D	403	Total	C	N	O	S	0	0	0
			3256	2079	573	588	16			

There are 48 discrepancies between the modelled and reference sequences:

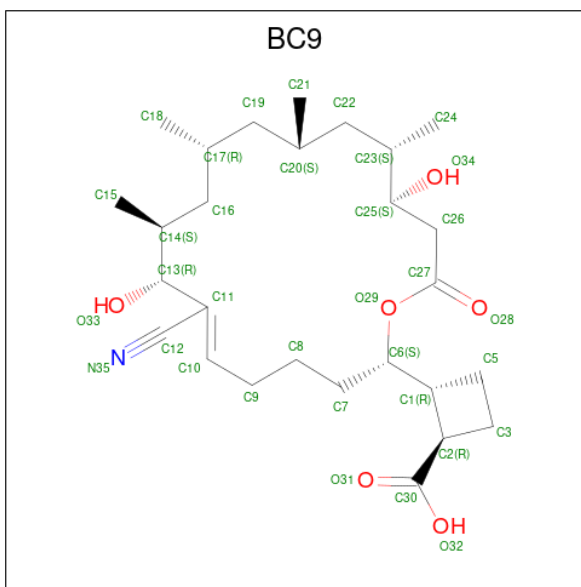
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	MET	-	initiating methionine	UNP P26639
A	311	GLY	-	expression tag	UNP P26639
A	312	SER	-	expression tag	UNP P26639
A	313	SER	-	expression tag	UNP P26639
A	314	HIS	-	expression tag	UNP P26639
A	315	HIS	-	expression tag	UNP P26639
A	316	HIS	-	expression tag	UNP P26639
A	317	HIS	-	expression tag	UNP P26639
A	318	HIS	-	expression tag	UNP P26639
A	319	HIS	-	expression tag	UNP P26639
A	320	SER	-	expression tag	UNP P26639
A	321	SER	-	expression tag	UNP P26639
B	310	MET	-	initiating methionine	UNP P26639
B	311	GLY	-	expression tag	UNP P26639
B	312	SER	-	expression tag	UNP P26639
B	313	SER	-	expression tag	UNP P26639
B	314	HIS	-	expression tag	UNP P26639
B	315	HIS	-	expression tag	UNP P26639
B	316	HIS	-	expression tag	UNP P26639
B	317	HIS	-	expression tag	UNP P26639
B	318	HIS	-	expression tag	UNP P26639

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Chain	Residue	Modelled	Actual	Comment	Reference
B	319	HIS	-	expression tag	UNP P26639
B	320	SER	-	expression tag	UNP P26639
B	321	SER	-	expression tag	UNP P26639
C	310	MET	-	initiating methionine	UNP P26639
C	311	GLY	-	expression tag	UNP P26639
C	312	SER	-	expression tag	UNP P26639
C	313	SER	-	expression tag	UNP P26639
C	314	HIS	-	expression tag	UNP P26639
C	315	HIS	-	expression tag	UNP P26639
C	316	HIS	-	expression tag	UNP P26639
C	317	HIS	-	expression tag	UNP P26639
C	318	HIS	-	expression tag	UNP P26639
C	319	HIS	-	expression tag	UNP P26639
C	320	SER	-	expression tag	UNP P26639
C	321	SER	-	expression tag	UNP P26639
D	310	MET	-	initiating methionine	UNP P26639
D	311	GLY	-	expression tag	UNP P26639
D	312	SER	-	expression tag	UNP P26639
D	313	SER	-	expression tag	UNP P26639
D	314	HIS	-	expression tag	UNP P26639
D	315	HIS	-	expression tag	UNP P26639
D	316	HIS	-	expression tag	UNP P26639
D	317	HIS	-	expression tag	UNP P26639
D	318	HIS	-	expression tag	UNP P26639
D	319	HIS	-	expression tag	UNP P26639
D	320	SER	-	expression tag	UNP P26639
D	321	SER	-	expression tag	UNP P26639

- Molecule 2 is (1R,2R)-2-[(2S,6E,8R,9S,11R,13S,15S,16S)-7-cyano-8,16-dihydroxy-9,11,13,15-tetramethyl-18-oxooxacyclooctadec-6-en-2-yl]cyclobutanecarboxylic acid (CCD ID: BC9) (formula: C₂₇H₄₃NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	27	1	6		
2	B	1	Total	C	N	O	0	0
			34	27	1	6		
2	C	1	Total	C	N	O	0	0
			34	27	1	6		
2	D	1	Total	C	N	O	0	0
			34	27	1	6		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		

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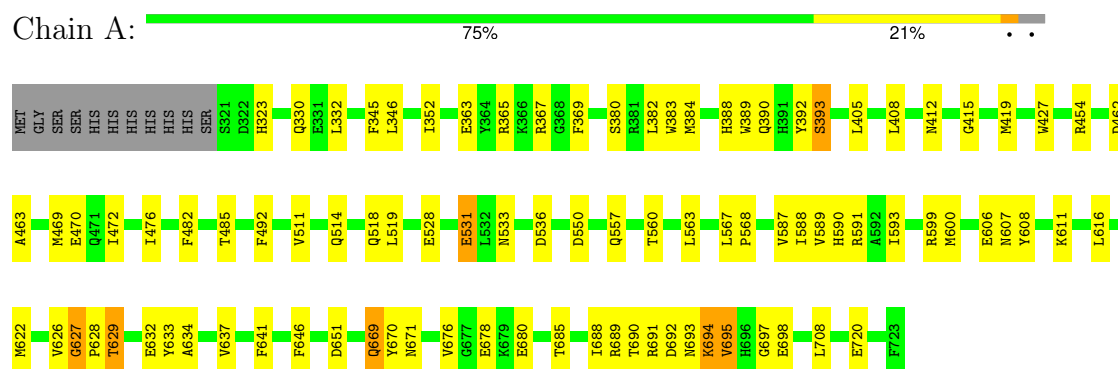
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	16	Total 16	O 16	0	0
4	C	11	Total 11	O 11	0	0
4	D	16	Total 16	O 16	0	0

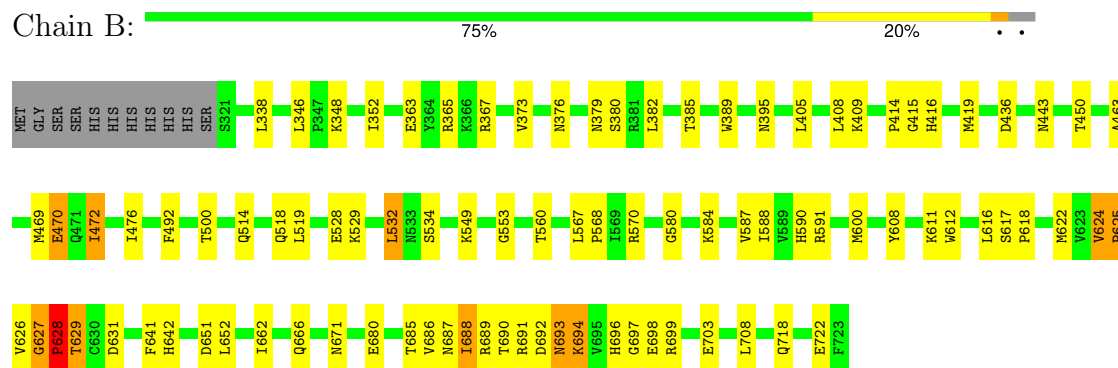
3 Residue-property plots

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.

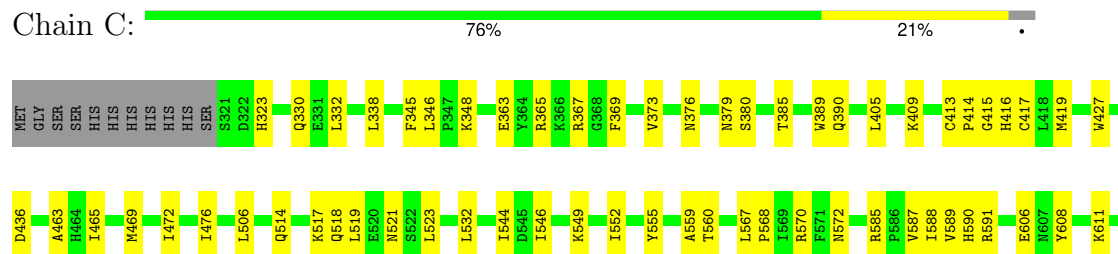
- Molecule 1: Threonine-tRNA ligase, cytoplasmic



- Molecule 1: Threonine-tRNA ligase, cytoplasmic



- Molecule 1: Threonine-tRNA ligase, cytoplasmic





● Molecule 1: Threonine-tRNA ligase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.02Å 134.61Å 128.67Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	46.51 – 2.80 46.51 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.51-2.80) 87.3 (46.51-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.255 , 0.288 0.260 , 0.287	Depositor DCC
R_{free} test set	3872 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13247	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0785e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BC9

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	0.55	1/3346 (0.0%)	0.82	5/4523 (0.1%)
1	B	0.51	2/3352 (0.1%)	0.85	7/4530 (0.2%)
1	C	0.50	3/3340 (0.1%)	0.83	4/4515 (0.1%)
1	D	0.51	1/3339 (0.0%)	0.83	5/4514 (0.1%)
All	All	0.52	7/13377 (0.1%)	0.83	21/18082 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	624	VAL	C-N	5.69	1.40	1.33
1	C	628	PRO	N-CD	5.55	1.55	1.47
1	B	628	PRO	N-CD	5.38	1.55	1.47
1	B	625	PRO	N-CD	5.06	1.54	1.47
1	D	628	PRO	N-CD	5.05	1.54	1.47
1	A	628	PRO	N-CD	5.03	1.54	1.47
1	C	625	PRO	N-CD	5.01	1.54	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	694	LYS	N-CA-C	-10.36	94.46	109.18
1	D	696	HIS	N-CA-C	-8.06	103.53	112.72
1	C	624	VAL	CA-C-N	-6.82	113.23	120.66
1	C	624	VAL	C-N-CA	-6.82	113.23	120.66
1	D	694	LYS	N-CA-C	-6.79	99.16	109.95
1	D	688	ILE	N-CA-C	6.10	117.80	108.71
1	A	688	ILE	N-CA-C	5.96	116.44	107.75
1	B	688	ILE	N-CA-C	5.70	116.50	108.36
1	C	688	ILE	N-CA-C	5.65	117.45	108.87
1	A	634	ALA	N-CA-C	-5.39	105.06	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	694	LYS	N-CA-C	-5.38	100.92	109.59
1	B	580	GLY	N-CA-C	-5.36	107.72	115.27
1	D	627	GLY	CA-C-N	-5.14	113.41	119.84
1	D	627	GLY	C-N-CA	-5.14	113.41	119.84
1	B	624	VAL	CA-C-N	-5.13	113.42	119.84
1	B	624	VAL	C-N-CA	-5.13	113.42	119.84
1	A	627	GLY	CA-C-N	-5.09	113.48	119.84
1	A	627	GLY	C-N-CA	-5.09	113.48	119.84
1	C	694	LYS	N-CA-C	-5.02	104.23	110.41
1	B	627	GLY	CA-C-N	-5.00	113.58	119.84
1	B	627	GLY	C-N-CA	-5.00	113.58	119.84

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	3263	0	3114	74	0
1	B	3269	0	3122	85	0
1	C	3257	0	3106	67	0
1	D	3256	0	3110	99	0
2	A	34	0	42	6	0
2	B	34	0	42	4	0
2	C	34	0	42	4	0
2	D	34	0	42	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	19	0	0	2	0
4	B	16	0	0	2	0
4	C	11	0	0	0	0
4	D	16	0	0	0	0
All	All	13247	0	12620	316	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 12.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:LYS:CG	1:D:691:ARG:NH1	1.82	1.43
1:D:611:LYS:HG3	1:D:691:ARG:NH1	1.34	1.28
1:B:611:LYS:CG	1:B:691:ARG:NH1	1.98	1.27
1:B:611:LYS:HG2	1:B:691:ARG:NH1	1.57	1.19
1:D:611:LYS:HG2	1:D:691:ARG:HH12	1.10	1.13
1:D:690:THR:HG21	1:D:720:GLU:HB3	1.31	1.10
1:D:611:LYS:HG2	1:D:691:ARG:NH1	1.65	1.09
1:D:611:LYS:CG	1:D:691:ARG:HH11	1.56	1.06
1:B:611:LYS:CG	1:B:691:ARG:HH11	1.64	1.05
1:B:611:LYS:HG3	1:B:691:ARG:NH1	1.78	0.99
1:A:690:THR:HG21	1:A:720:GLU:HB3	1.46	0.95
1:A:463:ALA:HB3	1:A:591:ARG:HH11	1.31	0.94
1:B:690:THR:O	1:B:693:ASN:N	1.98	0.94
1:C:463:ALA:HB3	1:C:591:ARG:HH11	1.37	0.90
1:B:463:ALA:HB3	1:B:591:ARG:HH11	1.35	0.89
1:D:463:ALA:HB3	1:D:591:ARG:HH11	1.36	0.89
1:D:611:LYS:HE3	1:D:691:ARG:HD2	1.54	0.88
1:C:611:LYS:HG3	1:C:691:ARG:NH1	1.91	0.86
1:B:611:LYS:HG2	1:B:691:ARG:HH12	1.37	0.86
1:B:689:ARG:HH21	1:B:689:ARG:HG3	1.40	0.85
1:D:611:LYS:CG	1:D:691:ARG:HH12	1.69	0.84
1:B:611:LYS:CD	1:B:691:ARG:HH11	1.92	0.82
1:D:611:LYS:HG3	1:D:691:ARG:HH11	1.06	0.82
1:D:690:THR:HG21	1:D:720:GLU:CB	2.11	0.78
1:A:690:THR:CG2	1:A:720:GLU:HB3	2.16	0.75
1:D:611:LYS:CE	1:D:691:ARG:HH11	2.00	0.74
1:B:611:LYS:HE3	1:B:691:ARG:NH1	2.04	0.73
1:D:463:ALA:HB3	1:D:591:ARG:NH1	2.03	0.72
1:A:633:TYR:HD2	1:A:676:VAL:HG11	1.54	0.72
1:B:685:THR:OG1	1:B:699:ARG:O	2.06	0.72
1:D:633:TYR:HD2	1:D:676:VAL:HG11	1.53	0.71
1:B:560:THR:HG21	2:B:801:BC9:H3	1.72	0.71
1:D:514:GLN:O	1:D:518:GLN:HG3	1.91	0.71
1:C:690:THR:HG21	1:C:720:GLU:HB3	1.72	0.71
1:A:680:GLU:HA	1:A:685:THR:HG23	1.73	0.69
1:A:560:THR:HG21	2:A:801:BC9:H3	1.75	0.69
1:B:698:GLU:O	1:B:699:ARG:HG2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:BC9:H28	2:B:801:BC9:O34	1.93	0.68
1:D:611:LYS:CD	1:D:691:ARG:HH11	2.06	0.68
1:D:626:VAL:HG23	1:D:676:VAL:O	1.94	0.68
1:C:590:HIS:CE1	2:C:801:BC9:H12	2.29	0.68
1:B:472:ILE:HD11	1:B:587:VAL:HG11	1.75	0.67
1:C:622:MET:HE3	1:C:651:ASP:HB2	1.78	0.66
1:B:690:THR:HB	1:B:694:LYS:H	1.59	0.65
1:C:690:THR:HG22	1:C:691:ARG:N	2.10	0.65
1:B:671:ASN:ND2	1:B:691:ARG:NH2	2.44	0.65
1:D:696:HIS:O	1:D:699:ARG:NH1	2.30	0.65
1:A:671:ASN:ND2	1:A:691:ARG:NH2	2.44	0.65
1:B:611:LYS:CE	1:B:691:ARG:HH11	2.10	0.65
1:B:689:ARG:HG3	1:B:689:ARG:NH2	2.12	0.65
1:C:696:HIS:O	1:C:699:ARG:NH1	2.29	0.64
1:B:611:LYS:HE3	1:B:691:ARG:HH11	1.61	0.64
1:A:557:GLN:O	1:A:599:ARG:NH1	2.31	0.63
1:D:323:HIS:HB3	1:D:606:GLU:HG3	1.79	0.63
1:A:472:ILE:HD11	1:A:587:VAL:HG11	1.80	0.63
1:B:532:LEU:HD11	1:B:534:SER:HB3	1.81	0.62
1:C:472:ILE:HD11	1:C:587:VAL:HG11	1.80	0.62
1:C:626:VAL:HG23	1:C:676:VAL:O	1.99	0.62
1:B:626:VAL:HG23	1:B:627:GLY:N	2.13	0.62
1:C:572:ASN:OD1	1:C:585:ARG:NH2	2.32	0.62
1:A:419:MET:HE2	1:B:346:LEU:HD23	1.81	0.62
1:B:380:SER:HB3	1:B:405:LEU:HB3	1.81	0.62
1:C:463:ALA:HB3	1:C:591:ARG:NH1	2.13	0.62
1:D:689:ARG:HH21	1:D:693:ASN:ND2	1.97	0.62
1:A:690:THR:HG22	1:A:691:ARG:N	2.15	0.62
1:C:611:LYS:CG	1:C:691:ARG:NH1	2.62	0.61
1:D:560:THR:HG21	2:D:801:BC9:H3	1.81	0.61
1:B:718:GLN:O	1:B:722:GLU:HG3	2.00	0.61
1:B:567:LEU:HB3	1:B:588:ILE:HD12	1.83	0.61
1:D:611:LYS:HE3	1:D:691:ARG:HH11	1.65	0.61
1:C:591:ARG:HH11	1:C:591:ARG:HG3	1.66	0.61
1:A:611:LYS:HG3	1:A:691:ARG:NH1	2.16	0.60
1:D:685:THR:OG1	1:D:686:VAL:N	2.33	0.60
1:D:670:TYR:O	1:D:691:ARG:HB2	2.03	0.59
1:D:591:ARG:HH11	1:D:591:ARG:HG3	1.66	0.59
1:C:611:LYS:HG3	1:C:691:ARG:CZ	2.32	0.59
1:B:696:HIS:O	1:B:699:ARG:NH1	2.36	0.59
1:B:492:PHE:HE2	1:B:600:MET:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ASN:HB3	1:A:536:ASP:OD2	2.03	0.59
1:C:346:LEU:HD23	1:D:419:MET:HE2	1.84	0.58
1:A:363:GLU:HG3	1:A:367:ARG:HE	1.69	0.57
1:D:683:SER:HB2	1:D:685:THR:HG22	1.87	0.57
1:A:469:MET:O	1:A:518:GLN:NE2	2.33	0.57
1:B:463:ALA:HB3	1:B:591:ARG:NH1	2.11	0.57
1:B:628:PRO:HA	1:B:631:ASP:OD1	2.04	0.57
1:C:469:MET:O	1:C:518:GLN:NE2	2.33	0.57
1:A:670:TYR:O	1:A:691:ARG:HB2	2.05	0.57
1:C:685:THR:OG1	1:C:699:ARG:O	2.19	0.56
1:A:323:HIS:HB3	1:A:606:GLU:HG3	1.88	0.56
1:B:532:LEU:HD13	1:B:534:SER:N	2.20	0.56
1:C:560:THR:HG21	2:C:801:BC9:H3	1.86	0.56
1:D:690:THR:HG22	1:D:691:ARG:N	2.20	0.56
1:A:463:ALA:HB3	1:A:591:ARG:NH1	2.10	0.56
1:C:549:LYS:HD3	1:C:555:TYR:CZ	2.41	0.56
1:C:348:LYS:HD2	1:C:618:PRO:HB2	1.86	0.56
1:A:685:THR:HG21	1:A:698:GLU:OE2	2.06	0.55
1:D:363:GLU:HG3	1:D:367:ARG:HE	1.70	0.55
1:A:633:TYR:O	1:A:637:VAL:HG23	2.05	0.55
1:B:699:ARG:HD2	1:B:703:GLU:OE2	2.06	0.55
1:B:611:LYS:HG3	1:B:691:ARG:CZ	2.35	0.55
1:B:591:ARG:HH11	1:B:591:ARG:HG3	1.72	0.55
1:A:568:PRO:HG3	1:A:588:ILE:HG13	1.87	0.54
1:B:532:LEU:CD1	1:B:534:SER:HB3	2.37	0.54
1:C:323:HIS:HB3	1:C:606:GLU:HG3	1.89	0.54
1:D:572:ASN:OD1	1:D:585:ARG:NH2	2.40	0.54
1:D:469:MET:O	1:D:518:GLN:NE2	2.36	0.54
1:D:680:GLU:HA	1:D:685:THR:HG23	1.89	0.54
1:D:690:THR:CG2	1:D:720:GLU:CG	2.86	0.54
1:B:469:MET:O	1:B:518:GLN:NE2	2.35	0.54
1:B:568:PRO:HG3	1:B:588:ILE:HG13	1.90	0.54
1:C:363:GLU:HG3	1:C:367:ARG:HE	1.72	0.53
1:B:363:GLU:HG3	1:B:367:ARG:HE	1.73	0.53
1:B:698:GLU:C	1:B:699:ARG:HG2	2.33	0.53
1:C:646:PHE:O	1:D:365:ARG:NH2	2.42	0.53
1:A:346:LEU:HD23	1:B:419:MET:HE2	1.90	0.53
1:A:695:VAL:HG13	1:A:695:VAL:O	2.09	0.53
1:D:568:PRO:HG3	1:D:588:ILE:HG13	1.90	0.52
1:B:380:SER:HB2	1:B:389:TRP:HE1	1.74	0.52
1:D:495:LYS:HE2	1:D:555:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:LYS:CE	1:D:691:ARG:NH1	2.68	0.52
1:A:641:PHE:HE2	1:A:708:LEU:HD12	1.75	0.52
1:B:662:ILE:O	1:B:666:GLN:HG3	2.10	0.52
1:D:608:TYR:HB3	1:D:611:LYS:O	2.09	0.52
1:D:633:TYR:O	1:D:637:VAL:HG23	2.09	0.52
1:B:626:VAL:CG2	1:B:627:GLY:N	2.73	0.52
1:D:508:ASP:OD1	1:D:509:ILE:N	2.43	0.52
1:D:413:CYS:HA	1:D:464:HIS:CE1	2.43	0.52
1:B:671:ASN:ND2	1:B:691:ARG:HH21	2.08	0.51
1:D:379:ASN:OD1	1:D:380:SER:N	2.42	0.51
1:D:472:ILE:HD11	1:D:587:VAL:HG11	1.92	0.51
1:A:608:TYR:HB3	1:A:611:LYS:O	2.11	0.51
1:D:458:PHE:HB2	1:D:596:SER:HB2	1.93	0.51
1:B:590:HIS:CE1	2:B:801:BC9:H12	2.45	0.51
1:B:611:LYS:CE	1:B:691:ARG:NH1	2.69	0.51
1:D:497:ASN:OD1	1:D:545:ASP:HB2	2.10	0.51
1:A:669:GLN:HE21	1:A:691:ARG:HD3	1.75	0.51
1:A:383:TRP:HB2	1:A:389:TRP:CD1	2.47	0.50
1:C:419:MET:HE2	1:D:346:LEU:HD23	1.94	0.50
1:C:611:LYS:HZ2	1:C:691:ARG:NE	2.09	0.50
1:D:390:GLN:OE1	1:D:390:GLN:N	2.38	0.50
1:B:690:THR:HG22	1:B:692:ASP:H	1.76	0.50
1:A:482:PHE:HD2	4:A:907:HOH:O	1.95	0.50
1:A:690:THR:CG2	1:A:691:ARG:N	2.75	0.50
1:B:395:ASN:O	1:B:443:ASN:N	2.40	0.50
1:C:690:THR:CG2	1:C:691:ARG:N	2.74	0.50
1:A:567:LEU:HB3	1:A:588:ILE:HD12	1.94	0.50
1:B:622:MET:HE2	1:B:651:ASP:HB2	1.94	0.50
1:C:476:ILE:HG13	1:C:519:LEU:HD23	1.93	0.49
1:D:690:THR:HG22	1:D:691:ARG:H	1.76	0.49
1:D:700:THR:HG22	1:D:703:GLU:HG3	1.94	0.49
1:A:380:SER:HB3	1:A:405:LEU:HB3	1.93	0.49
1:B:476:ILE:HG13	1:B:519:LEU:HD23	1.95	0.49
1:C:611:LYS:NZ	1:C:691:ARG:NE	2.60	0.49
1:A:671:ASN:ND2	1:A:691:ARG:HH22	2.10	0.49
1:C:517:LYS:O	1:C:521:ASN:ND2	2.43	0.49
1:A:345:PHE:HB2	1:B:373:VAL:HB	1.95	0.49
1:A:690:THR:HG21	1:A:720:GLU:CB	2.30	0.49
1:B:385:THR:O	1:B:570:ARG:HD3	2.13	0.49
1:B:608:TYR:HB3	1:B:611:LYS:O	2.12	0.49
1:B:641:PHE:HE2	1:B:708:LEU:HD12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:HD13	1:B:534:SER:H	1.77	0.48
1:D:690:THR:CG2	1:D:720:GLU:HB3	2.22	0.48
1:D:622:MET:HG2	1:D:670:TYR:CE2	2.47	0.48
1:A:622:MET:HE3	1:A:651:ASP:HB2	1.95	0.48
1:C:385:THR:O	1:C:570:ARG:NH1	2.43	0.48
1:D:660:LYS:HE3	1:D:664:ASN:HD21	1.78	0.48
1:D:476:ILE:HG13	1:D:519:LEU:HD23	1.96	0.48
1:A:384:MET:HE1	1:D:389:TRP:CD2	2.49	0.47
1:D:633:TYR:HD2	1:D:676:VAL:CG1	2.22	0.47
1:B:528:GLU:HG3	1:B:529:LYS:H	1.79	0.47
1:D:533:ASN:N	1:D:533:ASN:ND2	2.61	0.47
1:B:689:ARG:NH2	1:B:689:ARG:CG	2.73	0.47
1:C:608:TYR:HB3	1:C:611:LYS:O	2.14	0.47
1:A:412:ASN:HB2	1:A:462:ASP:OD2	2.14	0.47
1:A:492:PHE:HE2	1:A:600:MET:HE1	1.79	0.47
1:C:642:HIS:CE1	1:D:365:ARG:NH1	2.82	0.47
1:D:383:TRP:HB2	1:D:389:TRP:NE1	2.30	0.47
1:D:330:GLN:HB2	1:D:332:LEU:HG	1.97	0.47
1:D:415:GLY:O	1:D:419:MET:HG3	2.15	0.47
1:A:689:ARG:HA	1:A:694:LYS:O	2.15	0.47
1:C:567:LEU:HB3	1:C:588:ILE:HD12	1.97	0.47
1:D:685:THR:HG1	1:D:699:ARG:C	2.17	0.47
1:C:376:ASN:HA	1:C:409:LYS:HE2	1.97	0.46
1:C:568:PRO:HG3	1:C:588:ILE:HG13	1.97	0.46
1:B:352:ILE:HG23	1:B:616:LEU:HD22	1.97	0.46
1:D:465:ILE:HB	1:D:589:VAL:HB	1.97	0.46
1:D:720:GLU:H	1:D:720:GLU:CD	2.23	0.46
1:B:500:THR:OG1	1:B:534:SER:HA	2.15	0.46
1:D:532:LEU:C	1:D:533:ASN:HD22	2.24	0.46
1:A:389:TRP:CE3	1:D:390:GLN:HG3	2.50	0.46
1:C:380:SER:HB3	1:C:405:LEU:HB3	1.97	0.46
1:A:514:GLN:O	1:A:518:GLN:HG3	2.16	0.46
1:A:591:ARG:HH11	1:A:591:ARG:HG3	1.81	0.46
1:A:695:VAL:HG22	1:A:697:GLY:H	1.81	0.46
1:B:685:THR:OG1	1:B:686:VAL:N	2.48	0.46
1:D:689:ARG:HA	1:D:694:LYS:O	2.15	0.46
1:A:476:ILE:HG13	1:A:519:LEU:HD23	1.98	0.46
1:C:373:VAL:HB	1:D:345:PHE:HB2	1.97	0.46
1:A:591:ARG:NH2	1:A:593:ILE:HG13	2.31	0.46
1:B:628:PRO:HA	1:B:631:ASP:CG	2.40	0.46
1:D:632:GLU:HA	1:D:635:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:TRP:CE3	1:A:393:SER:HB3	2.51	0.45
1:B:514:GLN:O	1:B:518:GLN:HG3	2.17	0.45
1:B:627:GLY:C	1:B:629:THR:N	2.73	0.45
1:A:330:GLN:HB2	1:A:332:LEU:HG	1.99	0.45
1:A:692:ASP:HA	4:A:918:HOH:O	2.16	0.45
2:D:801:BC9:H11	2:D:801:BC9:H1	1.71	0.45
1:D:385:THR:O	1:D:570:ARG:HD2	2.16	0.45
1:D:591:ARG:NH1	1:D:591:ARG:HG3	2.32	0.45
1:B:685:THR:HG21	1:B:698:GLU:OE2	2.17	0.45
1:D:622:MET:HE1	1:D:651:ASP:HB2	1.97	0.45
1:D:492:PHE:HE2	1:D:600:MET:HE1	1.81	0.45
1:D:690:THR:HG21	1:D:720:GLU:CG	2.46	0.45
1:B:584:LYS:HA	4:B:911:HOH:O	2.16	0.44
1:C:622:MET:HB2	1:C:670:TYR:CD2	2.52	0.44
1:C:689:ARG:HE	1:C:689:ARG:HB2	1.64	0.44
1:A:629:THR:HG21	1:A:678:GLU:OE2	2.17	0.44
1:B:382:LEU:HD21	1:B:414:PRO:HB2	2.00	0.44
1:A:469:MET:HE1	1:A:511:VAL:HG13	1.99	0.44
1:A:388:HIS:O	1:A:392:TYR:N	2.43	0.44
1:A:611:LYS:HA	1:A:669:GLN:HG2	1.98	0.44
1:A:531:GLU:CG	1:A:533:ASN:HD21	2.30	0.44
1:D:380:SER:HB2	1:D:405:LEU:HB3	1.99	0.44
1:A:463:ALA:CB	1:A:591:ARG:HH11	2.17	0.44
1:C:330:GLN:HB2	1:C:332:LEU:HG	1.98	0.44
1:D:493:SER:OG	1:D:549:LYS:HE3	2.17	0.44
1:C:413:CYS:HB2	1:C:414:PRO:HD3	2.00	0.44
1:A:627:GLY:C	1:A:629:THR:N	2.73	0.44
1:A:720:GLU:CD	1:A:720:GLU:H	2.25	0.44
1:B:612:TRP:O	1:B:691:ARG:NH2	2.36	0.44
1:C:617:SER:HA	1:C:618:PRO:HD2	1.91	0.44
2:A:801:BC9:H24	2:A:801:BC9:H16	1.80	0.43
1:B:685:THR:HG1	1:B:686:VAL:H	1.64	0.43
1:C:628:PRO:C	1:C:630:CYS:N	2.73	0.43
1:A:415:GLY:O	1:A:419:MET:HG3	2.18	0.43
2:A:801:BC9:H33	2:A:801:BC9:H40	1.61	0.43
1:C:338:LEU:HD13	1:D:382:LEU:HD13	2.01	0.43
1:C:591:ARG:NH1	1:C:591:ARG:HG3	2.31	0.43
1:D:550:ASP:HB2	1:D:607:ASN:OD1	2.17	0.43
2:A:801:BC9:H29	2:A:801:BC9:H34	1.79	0.43
1:B:690:THR:HB	1:B:694:LYS:N	2.31	0.43
1:C:546:ILE:HB	1:C:559:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASP:HB2	1:A:607:ASN:OD1	2.19	0.43
1:B:611:LYS:HG3	1:B:691:ARG:HH11	1.51	0.43
1:C:345:PHE:HB2	1:D:373:VAL:HB	2.00	0.43
1:D:550:ASP:OD2	1:D:554:ARG:HB2	2.19	0.43
1:B:680:GLU:OE1	1:B:680:GLU:N	2.47	0.42
1:C:680:GLU:OE1	1:C:680:GLU:N	2.52	0.42
1:D:484:ARG:HH11	1:D:526:PHE:HE1	1.67	0.42
1:D:567:LEU:HB3	1:D:588:ILE:HD12	2.00	0.42
1:A:611:LYS:HE3	1:A:691:ARG:HH11	1.84	0.42
1:A:690:THR:O	1:A:693:ASN:N	2.46	0.42
1:B:687:ASN:OD1	1:B:697:GLY:HA2	2.18	0.42
1:C:379:ASN:OD1	1:C:380:SER:N	2.53	0.42
1:C:514:GLN:O	1:C:518:GLN:HG3	2.18	0.42
1:C:619:ARG:HB3	1:C:670:TYR:CD2	2.54	0.42
1:C:380:SER:HB2	1:C:389:TRP:HE1	1.85	0.42
1:D:689:ARG:HH21	1:D:693:ASN:HD21	1.67	0.42
1:D:629:THR:OG1	1:D:678:GLU:OE2	2.38	0.42
1:D:690:THR:CG2	1:D:720:GLU:CB	2.91	0.42
1:A:367:ARG:NH2	1:A:485:THR:OG1	2.52	0.42
1:B:652:LEU:O	4:B:915:HOH:O	2.22	0.42
1:D:413:CYS:HB2	1:D:414:PRO:HD3	2.01	0.42
1:C:552:ILE:HD11	1:C:606:GLU:O	2.19	0.42
1:A:611:LYS:CG	1:A:691:ARG:NH1	2.83	0.42
2:B:801:BC9:H22	2:B:801:BC9:H30	1.82	0.42
1:C:690:THR:HG22	1:C:691:ARG:H	1.82	0.42
1:D:493:SER:OG	1:D:549:LYS:HB3	2.20	0.42
1:C:416:HIS:CE1	1:C:436:ASP:HB2	2.54	0.42
1:C:663:ARG:HD2	1:C:663:ARG:HA	1.85	0.42
1:A:427:TRP:H	1:A:427:TRP:CD1	2.37	0.41
1:D:690:THR:O	1:D:693:ASN:N	2.47	0.41
1:B:416:HIS:CE1	1:B:436:ASP:HB2	2.55	0.41
1:A:622:MET:HB2	1:A:670:TYR:CD2	2.55	0.41
1:A:633:TYR:CD2	1:A:676:VAL:HG11	2.42	0.41
1:A:590:HIS:CE1	2:A:801:BC9:H12	2.55	0.41
1:A:646:PHE:O	1:B:365:ARG:NH2	2.54	0.41
1:B:376:ASN:HA	1:B:409:LYS:HE2	2.03	0.41
1:C:365:ARG:NH2	1:D:646:PHE:O	2.53	0.41
1:C:369:PHE:CE2	1:C:591:ARG:HD3	2.55	0.41
1:C:632:GLU:O	1:C:635:GLN:HB2	2.20	0.41
1:C:690:THR:CG2	1:C:720:GLU:HB3	2.47	0.41
1:C:465:ILE:HB	1:C:589:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:NH2	1:B:642:HIS:O	2.49	0.41
1:C:417:CYS:SG	1:C:567:LEU:HG	2.61	0.41
1:A:408:LEU:HD21	1:B:408:LEU:HD11	2.02	0.41
2:A:801:BC9:H21	2:A:801:BC9:H28	1.88	0.41
1:D:641:PHE:HE2	1:D:708:LEU:HD12	1.85	0.41
1:B:492:PHE:CE2	1:B:600:MET:HE1	2.53	0.41
1:B:617:SER:HA	1:B:618:PRO:HD2	1.94	0.41
1:C:463:ALA:HB3	1:C:591:ARG:HG3	2.03	0.41
1:B:348:LYS:HD2	1:B:618:PRO:HB2	2.02	0.41
1:B:379:ASN:OD1	1:B:380:SER:N	2.54	0.41
1:D:680:GLU:OE1	1:D:680:GLU:N	2.49	0.41
1:B:549:LYS:HE2	1:B:553:GLY:HA2	2.03	0.41
1:C:427:TRP:CD1	1:C:427:TRP:H	2.39	0.41
1:D:505:PHE:C	1:D:506:LEU:HD12	2.46	0.41
1:A:384:MET:HE1	1:D:389:TRP:CE2	2.56	0.40
1:B:415:GLY:O	1:B:419:MET:HG3	2.20	0.40
1:C:523:LEU:HD21	1:C:544:ILE:HD13	2.04	0.40
1:A:352:ILE:HG23	1:A:616:LEU:HD22	2.03	0.40
1:A:369:PHE:CE2	1:A:591:ARG:HD3	2.56	0.40
1:B:470:GLU:H	1:B:470:GLU:HG3	1.51	0.40
2:C:801:BC9:H33	2:C:801:BC9:H40	1.61	0.40
1:D:348:LYS:HD2	1:D:618:PRO:HB2	2.04	0.40
1:D:416:HIS:CE1	1:D:436:ASP:HB2	2.56	0.40
1:D:638:ARG:NH2	1:D:638:ARG:HG2	2.35	0.40
1:D:695:VAL:C	1:D:697:GLY:H	2.28	0.40
1:C:670:TYR:O	1:C:691:ARG:HB2	2.21	0.40
1:A:382:LEU:HD13	1:B:338:LEU:HD13	2.03	0.40
1:A:563:LEU:HD22	1:A:589:VAL:HG22	2.03	0.40
1:C:415:GLY:O	1:C:419:MET:HG3	2.21	0.40
2:C:801:BC9:H21	2:C:801:BC9:H28	1.78	0.40
1:D:549:LYS:HB2	1:D:555:TYR:CE1	2.56	0.40
1:D:627:GLY:C	1:D:629:THR:N	2.77	0.40
1:D:631:ASP:O	1:D:635:GLN:HG2	2.22	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	401/414 (97%)	388 (97%)	13 (3%)	0	100	100
1	B	401/414 (97%)	382 (95%)	19 (5%)	0	100	100
1	C	401/414 (97%)	392 (98%)	9 (2%)	0	100	100
1	D	401/414 (97%)	386 (96%)	15 (4%)	0	100	100
All	All	1604/1656 (97%)	1548 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/368 (93%)	331 (97%)	11 (3%)	34	70
1	B	343/368 (93%)	333 (97%)	10 (3%)	37	73
1	C	340/368 (92%)	333 (98%)	7 (2%)	47	79
1	D	340/368 (92%)	332 (98%)	8 (2%)	43	77
All	All	1365/1472 (93%)	1329 (97%)	36 (3%)	40	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	A	393	SER

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Mol	Chain	Res	Type
1	A	454	ARG
1	A	470	GLU
1	A	528	GLU
1	A	531	GLU
1	A	626	VAL
1	A	629	THR
1	A	632	GLU
1	A	669	GLN
1	A	695	VAL
1	B	450	THR
1	B	470	GLU
1	B	472	ILE
1	B	532	LEU
1	B	624	VAL
1	B	625	PRO
1	B	628	PRO
1	B	629	THR
1	B	688	ILE
1	B	693	ASN
1	C	390	GLN
1	C	506	LEU
1	C	532	LEU
1	C	624	VAL
1	C	625	PRO
1	C	628	PRO
1	C	693	ASN
1	D	405	LEU
1	D	470	GLU
1	D	514	GLN
1	D	533	ASN
1	D	629	THR
1	D	685	THR
1	D	693	ASN
1	D	695	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	GLN
1	A	497	ASN
1	A	521	ASN
1	A	533	ASN

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Mol	Chain	Res	Type
1	A	669	GLN
1	B	422	HIS
1	B	666	GLN
1	C	390	GLN
1	C	422	HIS
1	C	460	GLN
1	C	566	GLN
1	D	460	GLN
1	D	521	ASN
1	D	533	ASN
1	D	635	GLN
1	D	664	ASN
1	D	693	ASN
1	D	696	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BC9	A	801	-	34,35,35	3.40	11 (32%)	35,48,48	1.67	7 (20%)
2	BC9	D	801	-	34,35,35	3.30	10 (29%)	35,48,48	2.07	9 (25%)
2	BC9	C	801	-	34,35,35	3.27	10 (29%)	35,48,48	2.07	9 (25%)
2	BC9	B	801	-	34,35,35	3.33	10 (29%)	35,48,48	1.87	6 (17%)

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	BC9	A	801	-	-	8/46/58/58	0/1/2/2
2	BC9	D	801	-	-	11/46/58/58	0/1/2/2
2	BC9	C	801	-	-	9/46/58/58	0/1/2/2
2	BC9	B	801	-	-	4/46/58/58	0/1/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	BC9	C12-C11	-16.63	1.23	1.43
2	D	801	BC9	C12-C11	-16.49	1.24	1.43
2	B	801	BC9	C12-C11	-16.20	1.24	1.43
2	C	801	BC9	C12-C11	-15.97	1.24	1.43
2	A	801	BC9	C8-C9	-4.91	1.31	1.52
2	C	801	BC9	C8-C9	-4.86	1.31	1.52
2	B	801	BC9	C8-C9	-4.79	1.32	1.52
2	A	801	BC9	C2-C1	-4.72	1.49	1.55
2	D	801	BC9	C8-C9	-4.68	1.32	1.52
2	B	801	BC9	C2-C1	-4.64	1.49	1.55
2	C	801	BC9	C2-C1	-4.19	1.49	1.55
2	D	801	BC9	C2-C1	-3.66	1.50	1.55
2	D	801	BC9	O29-C27	3.24	1.43	1.34
2	C	801	BC9	O29-C27	3.17	1.43	1.34
2	A	801	BC9	O29-C27	3.15	1.43	1.34
2	B	801	BC9	O29-C27	3.05	1.42	1.34
2	C	801	BC9	O29-C6	-2.94	1.41	1.46
2	B	801	BC9	O29-C6	-2.77	1.41	1.46
2	A	801	BC9	O29-C6	-2.68	1.41	1.46
2	B	801	BC9	O32-C30	-2.50	1.22	1.30
2	D	801	BC9	O32-C30	-2.48	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	BC9	O29-C6	-2.47	1.41	1.46
2	C	801	BC9	C9-C10	-2.46	1.43	1.50
2	B	801	BC9	C9-C10	-2.43	1.43	1.50
2	A	801	BC9	O32-C30	-2.42	1.22	1.30
2	B	801	BC9	C2-C30	-2.40	1.47	1.51
2	C	801	BC9	C16-C14	-2.37	1.50	1.54
2	B	801	BC9	C22-C23	-2.35	1.50	1.54
2	A	801	BC9	C22-C23	-2.32	1.50	1.54
2	A	801	BC9	C3-C2	-2.29	1.50	1.54
2	A	801	BC9	C9-C10	-2.25	1.43	1.50
2	C	801	BC9	C3-C2	-2.24	1.50	1.54
2	C	801	BC9	O32-C30	-2.21	1.23	1.30
2	A	801	BC9	C2-C30	-2.20	1.47	1.51
2	D	801	BC9	C23-C25	-2.20	1.50	1.53
2	D	801	BC9	C22-C23	-2.17	1.50	1.54
2	D	801	BC9	C3-C2	-2.13	1.50	1.54
2	D	801	BC9	C9-C10	-2.10	1.44	1.50
2	B	801	BC9	C3-C2	-2.08	1.50	1.54
2	C	801	BC9	C14-C13	-2.03	1.49	1.53
2	A	801	BC9	C16-C14	-2.02	1.50	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	BC9	C8-C9-C10	6.49	125.69	112.79
2	D	801	BC9	C7-C8-C9	6.01	127.51	114.47
2	C	801	BC9	O29-C27-C26	5.75	121.73	111.43
2	B	801	BC9	C7-C8-C9	5.57	126.54	114.47
2	C	801	BC9	C7-C8-C9	5.09	125.51	114.47
2	D	801	BC9	O29-C27-C26	4.90	120.22	111.43
2	A	801	BC9	O29-C27-C26	4.64	119.75	111.43
2	C	801	BC9	C8-C9-C10	-4.53	103.79	112.79
2	B	801	BC9	O29-C27-C26	4.48	119.46	111.43
2	B	801	BC9	C8-C9-C10	-4.35	104.14	112.79
2	A	801	BC9	C7-C8-C9	4.10	123.36	114.47
2	C	801	BC9	C14-C16-C17	-3.35	108.25	116.59
2	A	801	BC9	C24-C23-C22	-3.16	105.89	110.68
2	C	801	BC9	C9-C10-C11	3.03	135.23	127.47
2	B	801	BC9	C24-C23-C22	-2.98	106.16	110.68
2	C	801	BC9	O28-C27-C26	-2.67	118.44	124.65
2	D	801	BC9	O32-C30-C2	2.41	120.18	113.93
2	D	801	BC9	O28-C27-C26	-2.40	119.06	124.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BC9	C9-C10-C11	2.40	133.62	127.47
2	D	801	BC9	C3-C2-C1	2.32	90.85	88.54
2	A	801	BC9	C8-C9-C10	-2.31	108.19	112.79
2	B	801	BC9	C15-C14-C13	-2.27	105.17	111.42
2	C	801	BC9	O32-C30-C2	2.26	119.80	113.93
2	D	801	BC9	O31-C30-C2	-2.18	117.85	123.01
2	D	801	BC9	C24-C23-C25	-2.11	108.86	111.61
2	A	801	BC9	C26-C25-C23	-2.09	108.78	112.90
2	C	801	BC9	O29-C6-C1	2.08	110.69	107.29
2	D	801	BC9	C26-C25-C23	-2.04	108.88	112.90
2	A	801	BC9	O29-C27-O28	-2.02	118.98	123.70
2	A	801	BC9	O31-C30-C2	-2.02	118.25	123.01
2	C	801	BC9	C5-C3-C2	2.01	90.95	88.94

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BC9	C1-C6-C7-C8
2	B	801	BC9	C1-C6-C7-C8
2	B	801	BC9	O29-C6-C7-C8
2	C	801	BC9	C1-C6-C7-C8
2	C	801	BC9	O29-C6-C7-C8
2	C	801	BC9	O34-C25-C26-C27
2	D	801	BC9	C7-C8-C9-C10
2	D	801	BC9	C21-C20-C22-C23
2	D	801	BC9	O34-C25-C26-C27
2	A	801	BC9	O29-C6-C7-C8
2	C	801	BC9	C23-C25-C26-C27
2	D	801	BC9	C23-C25-C26-C27
2	B	801	BC9	C6-C7-C8-C9
2	D	801	BC9	C1-C6-C7-C8
2	C	801	BC9	C6-C7-C8-C9
2	A	801	BC9	C21-C20-C22-C23
2	A	801	BC9	O34-C25-C26-C27
2	A	801	BC9	C24-C23-C25-O34
2	B	801	BC9	C24-C23-C25-O34
2	C	801	BC9	C1-C2-C30-O32
2	A	801	BC9	C6-C7-C8-C9
2	C	801	BC9	C1-C2-C30-O31
2	D	801	BC9	C6-C7-C8-C9
2	D	801	BC9	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	A	801	BC9	C16-C17-C19-C20
2	D	801	BC9	C1-C2-C30-O32
2	A	801	BC9	C20-C22-C23-C24
2	C	801	BC9	C24-C23-C25-O34
2	D	801	BC9	C24-C23-C25-O34
2	D	801	BC9	C14-C16-C17-C18
2	C	801	BC9	C20-C22-C23-C25
2	D	801	BC9	C20-C22-C23-C25

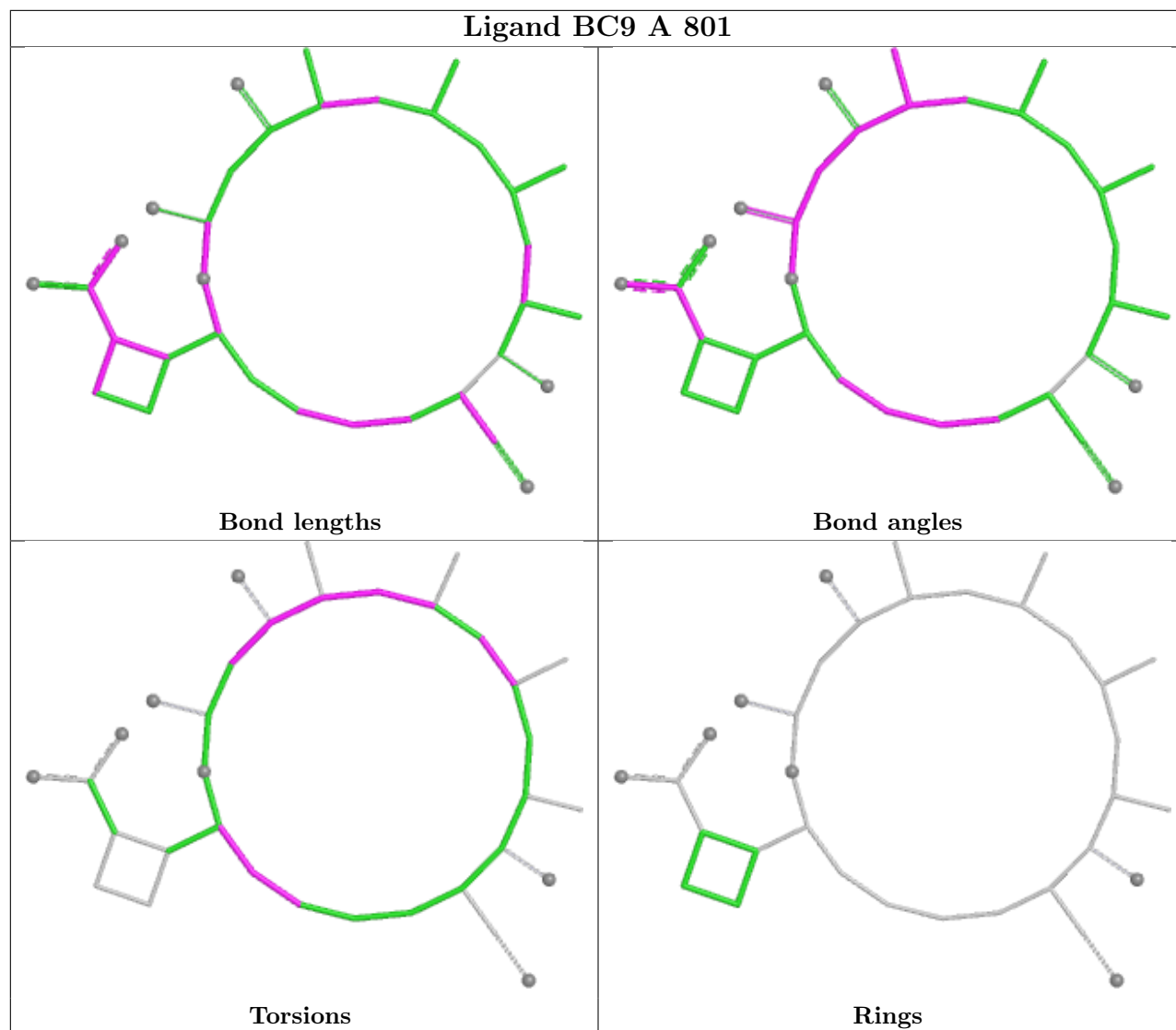
There are no ring outliers.

4 monomers are involved in 16 short contacts:

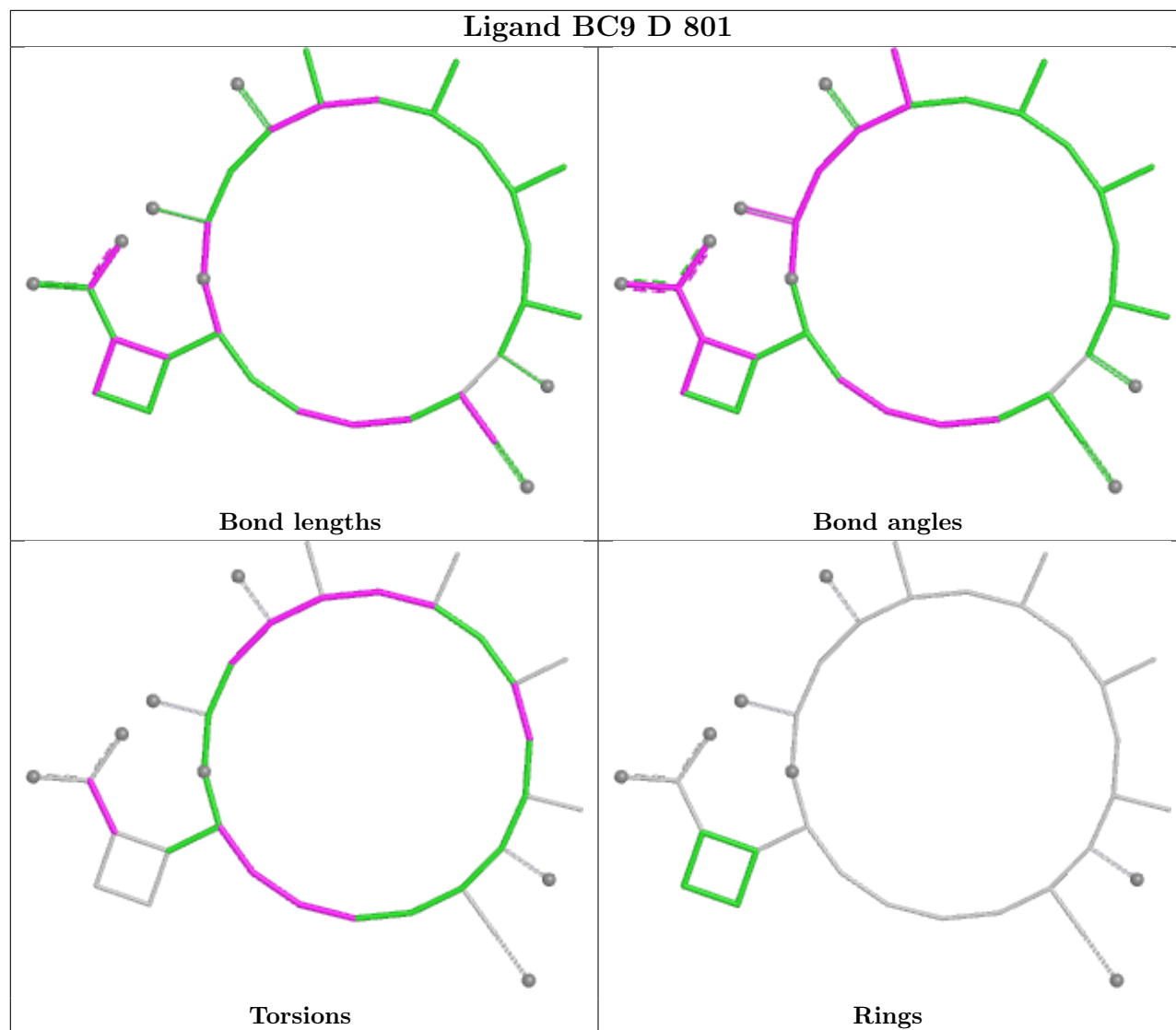
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BC9	6	0
2	D	801	BC9	2	0
2	C	801	BC9	4	0
2	B	801	BC9	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

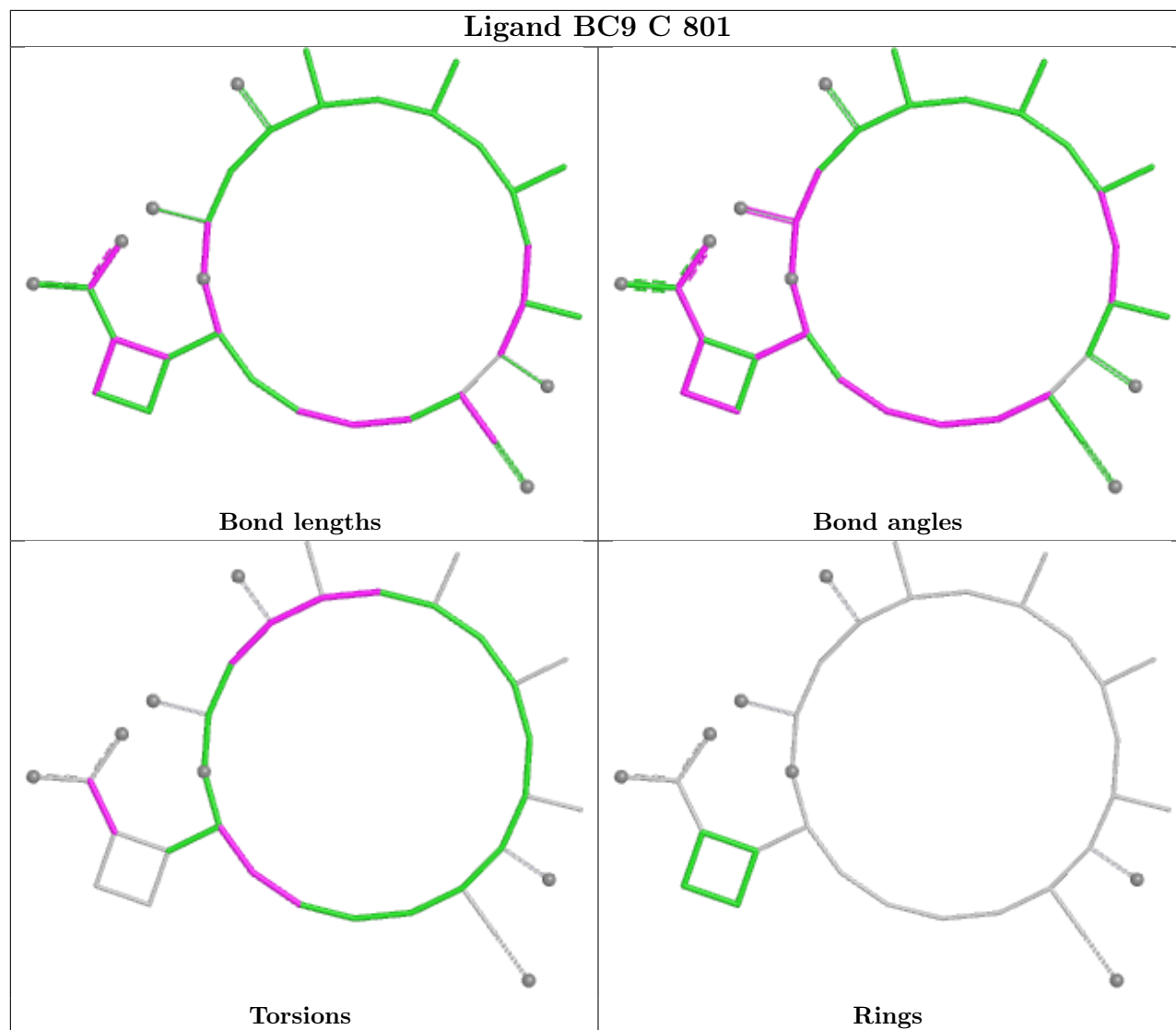
Ligand BC9 A 801

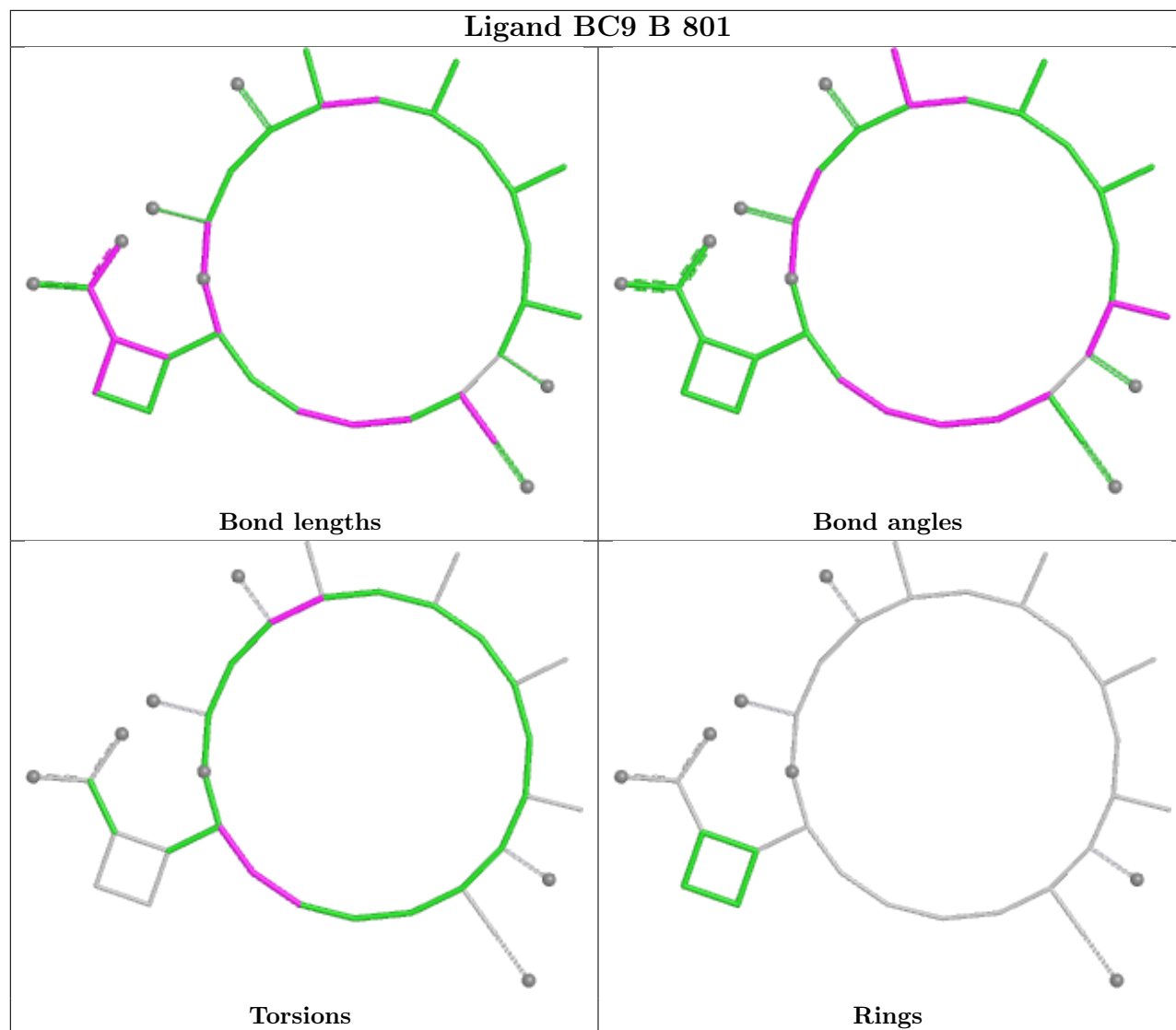


Ligand BC9 D 801



Ligand BC9 C 801





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	403/414 (97%)	-1.36	0 100 100	32, 53, 78, 91	0
1	B	403/414 (97%)	-1.25	0 100 100	33, 59, 88, 101	0
1	C	403/414 (97%)	-1.20	0 100 100	33, 58, 89, 106	0
1	D	403/414 (97%)	-1.36	0 100 100	30, 53, 80, 93	0
All	All	1612/1656 (97%)	-1.29	0 100 100	30, 56, 85, 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	BC9	A	801	34/34	0.99	0.04	41,46,49,49	0
2	BC9	B	801	34/34	0.99	0.05	50,52,53,54	0
2	BC9	C	801	34/34	0.99	0.05	49,50,52,53	0
2	BC9	D	801	34/34	0.99	0.04	45,48,50,50	0

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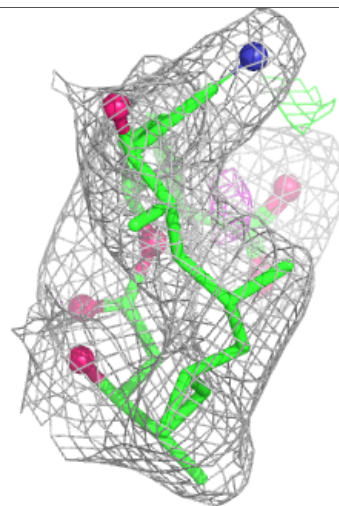
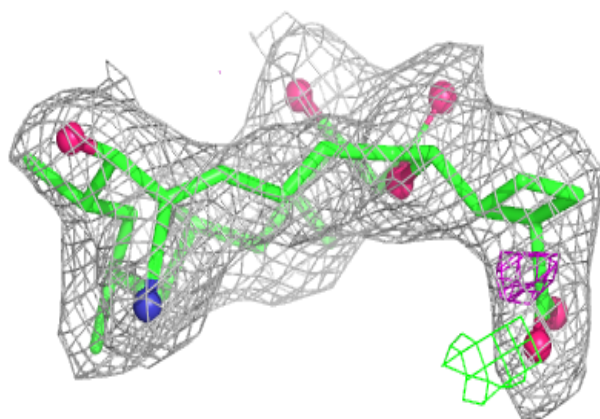
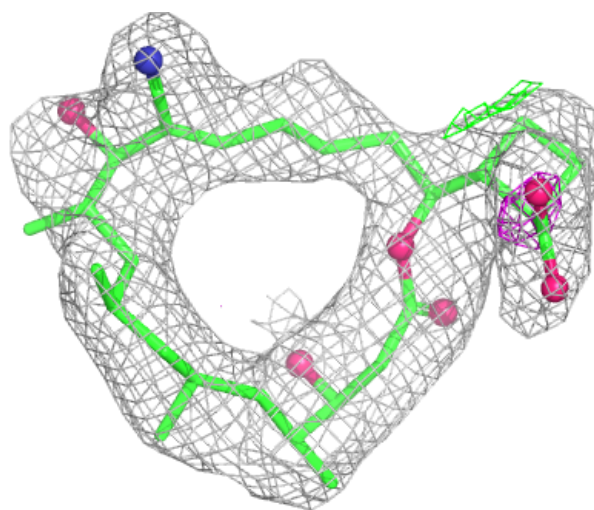
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	802	1/1	1.00	0.02	71,71,71,71	0
3	ZN	B	802	1/1	1.00	0.02	57,57,57,57	0
3	ZN	C	802	1/1	1.00	0.02	65,65,65,65	0
3	ZN	D	802	1/1	1.00	0.03	61,61,61,61	0

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.

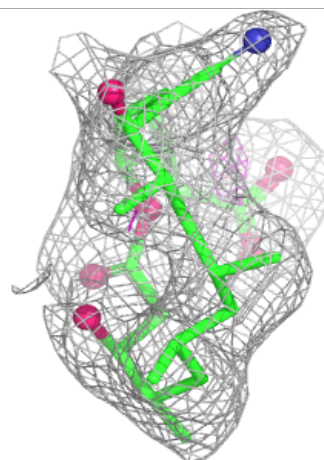
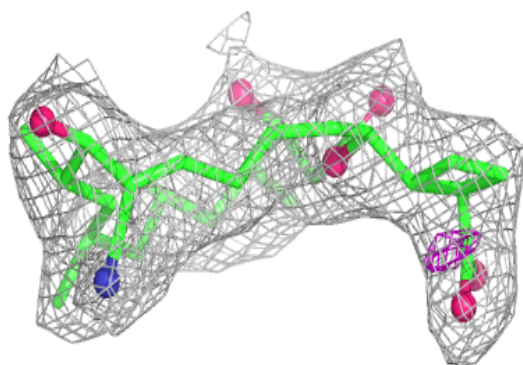
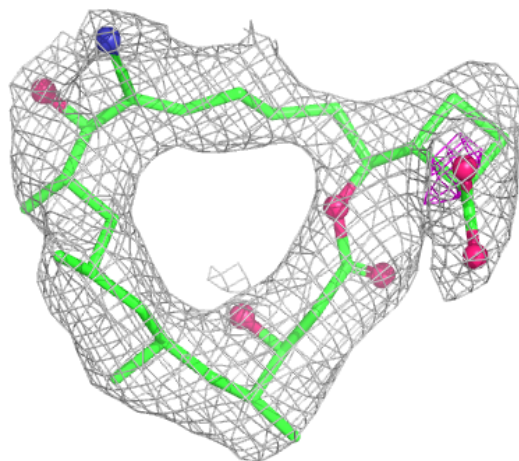
Electron density around BC9 A 801:

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



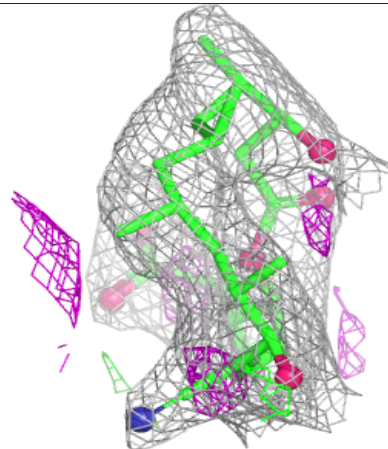
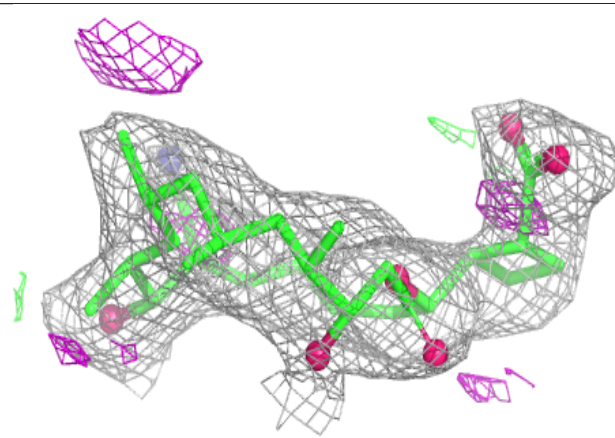
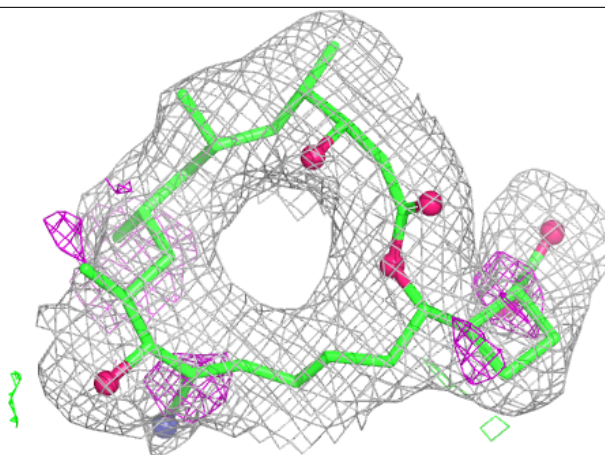
Electron density around BC9 B 801:

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



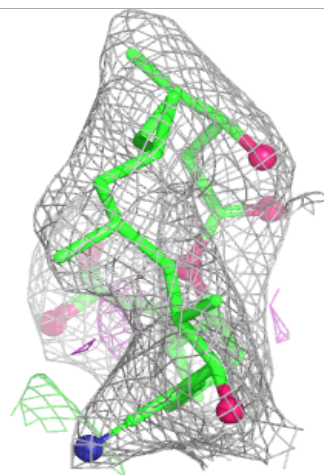
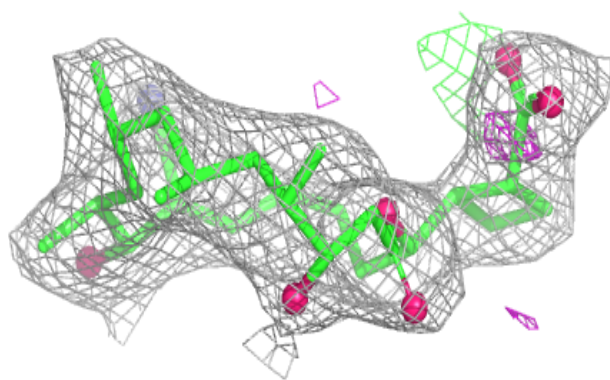
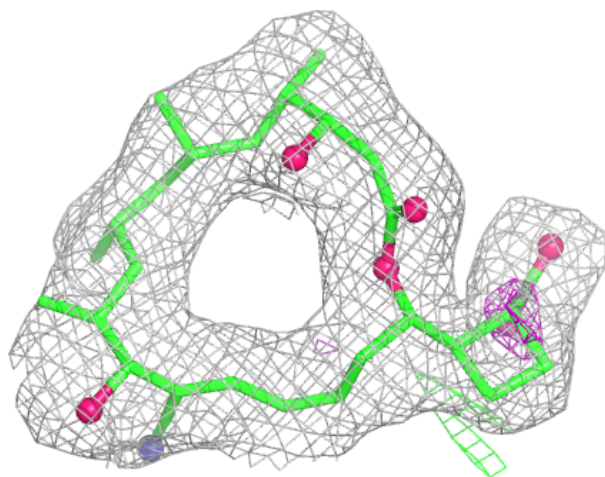
Electron density around BC9 C 801:

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



Electron density around BC9 D 801:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.