



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:17 pm BST

PDB ID : 4P3N  
Title : Structural Basis for Full-Spectrum Inhibition of Threonyl-tRNA Synthetase by Borrelidin 1  
Authors : Fang, P.; Yu, X.; Chen, K.; Chen, X.; Guo, M.  
Deposited on : 2014-03-09  
Resolution : 2.60 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

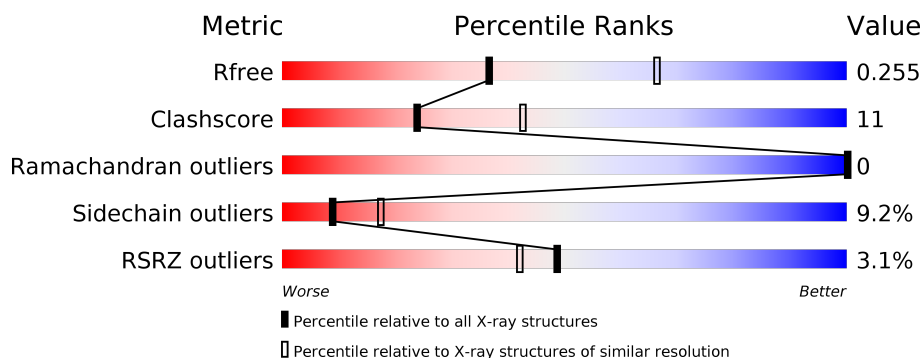
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	415	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	415	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
1	C	415	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>5% •</div> </div> </div>
1	D	415	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13506 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	402	Total	C	N	O	S	0	0	0
			3260	2081	571	592	16			
1	B	402	Total	C	N	O	S	0	0	0
			3253	2078	571	588	16			
1	C	402	Total	C	N	O	S	0	0	0
			3249	2077	566	590	16			
1	D	402	Total	C	N	O	S	0	0	0
			3211	2053	567	575	16			

There are 52 discrepancies between the modelled and reference sequences:

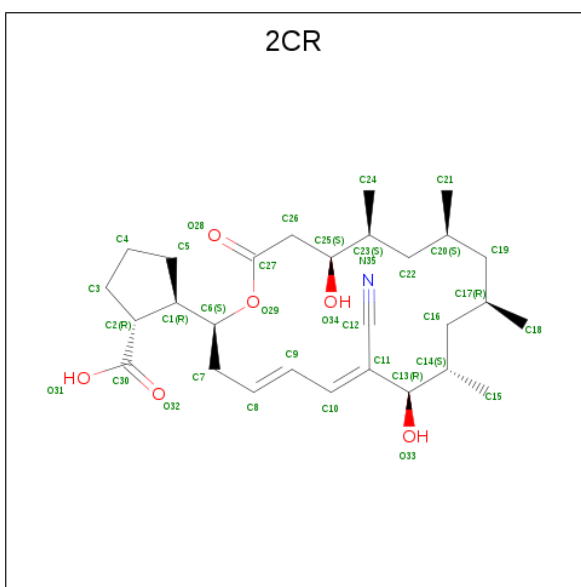
Chain	Residue	Modelled	Actual	Comment	Reference
A	309	MET	-	expression tag	UNP P26639
A	310	GLY	-	expression tag	UNP P26639
A	311	SER	-	expression tag	UNP P26639
A	312	SER	-	expression tag	UNP P26639
A	313	HIS	-	expression tag	UNP P26639
A	314	HIS	-	expression tag	UNP P26639
A	315	HIS	-	expression tag	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	SER	-	expression tag	UNP P26639
A	320	SER	-	expression tag	UNP P26639
A	321	GLY	-	expression tag	UNP P26639
B	309	MET	-	expression tag	UNP P26639
B	310	GLY	-	expression tag	UNP P26639
B	311	SER	-	expression tag	UNP P26639
B	312	SER	-	expression tag	UNP P26639
B	313	HIS	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	HIS	-	expression tag	UNP P26639
B	318	HIS	-	expression tag	UNP P26639
B	319	SER	-	expression tag	UNP P26639
B	320	SER	-	expression tag	UNP P26639
B	321	GLY	-	expression tag	UNP P26639
C	309	MET	-	expression tag	UNP P26639
C	310	GLY	-	expression tag	UNP P26639
C	311	SER	-	expression tag	UNP P26639
C	312	SER	-	expression tag	UNP P26639
C	313	HIS	-	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	SER	-	expression tag	UNP P26639
C	320	SER	-	expression tag	UNP P26639
C	321	GLY	-	expression tag	UNP P26639
D	309	MET	-	expression tag	UNP P26639
D	310	GLY	-	expression tag	UNP P26639
D	311	SER	-	expression tag	UNP P26639
D	312	SER	-	expression tag	UNP P26639
D	313	HIS	-	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	SER	-	expression tag	UNP P26639
D	320	SER	-	expression tag	UNP P26639
D	321	GLY	-	expression tag	UNP P26639

- Molecule 2 is (1R,2R)-2-[(2S,4E,6E,8R,9S,11R,13S,15S,16S)-7-cyano-8,16-dihydroxy-9,11,13,15-tetramethyl-18-oxooxacyclooctadeca-4,6-dien-2-yl]cyclopentanecarboxylic acid (three-letter code: 2CR) (formula: C<sub>28</sub>H<sub>43</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	1	6		
2	B	1	Total	C	N	O	0	0
			35	28	1	6		
2	C	1	Total	C	N	O	0	0
			35	28	1	6		
2	D	1	Total	C	N	O	0	0
			35	28	1	6		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		

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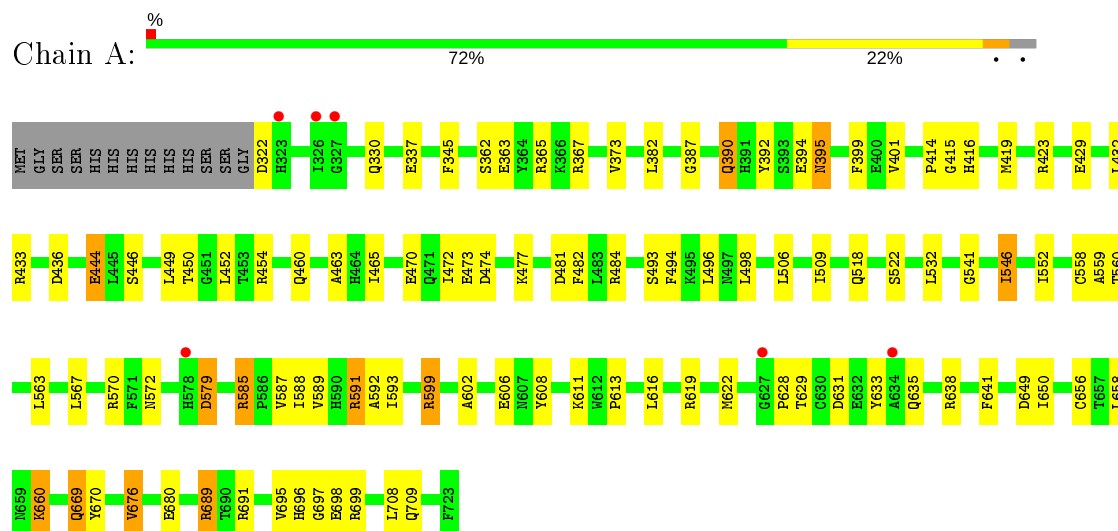
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	111	Total 111	O 111	0	0
4	C	90	Total 90	O 90	0	0
4	D	93	Total 93	O 93	0	0

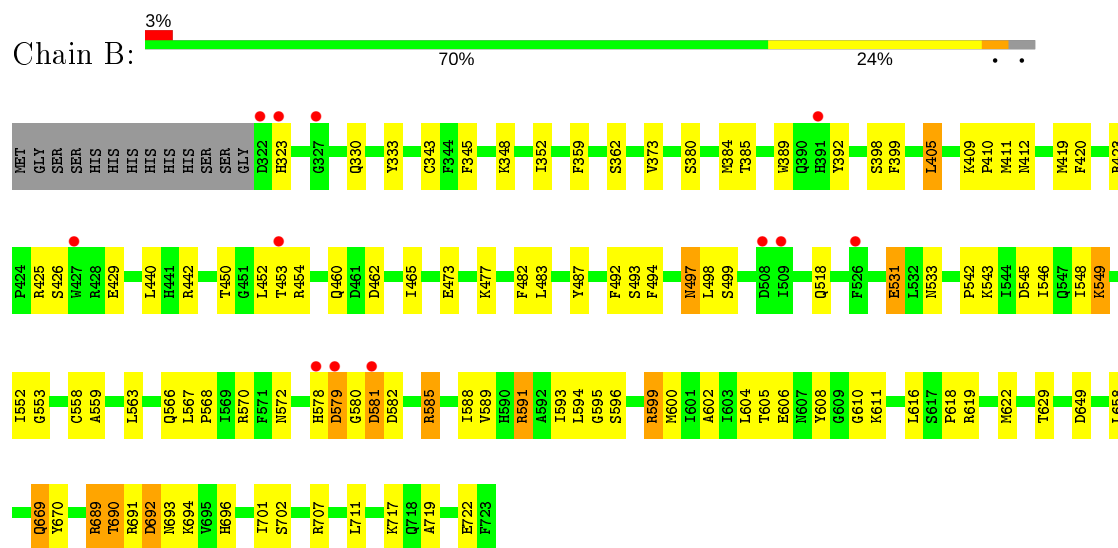
### 3 Residue-property plots [i](#)

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: Threonine-tRNA ligase, cytoplasmic

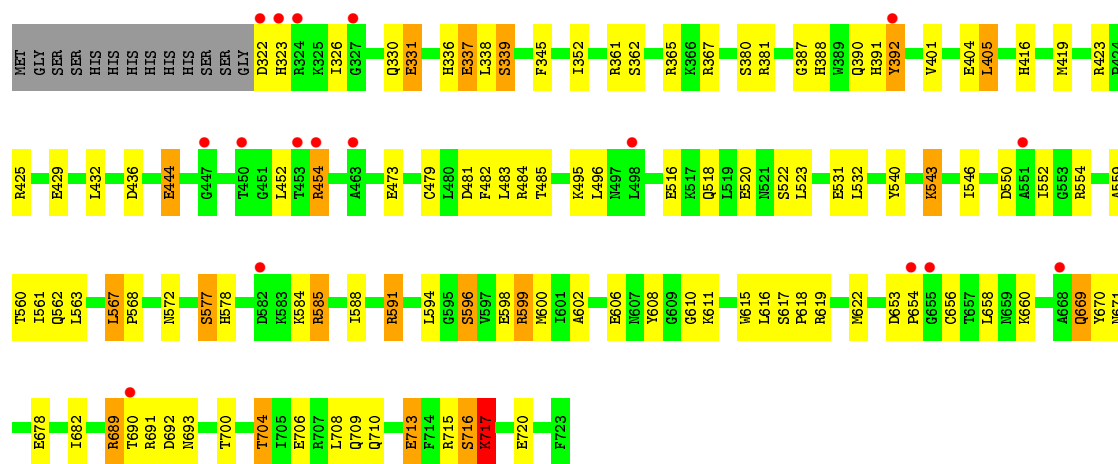


- Molecule 1: Threonine-tRNA ligase, cytoplasmic

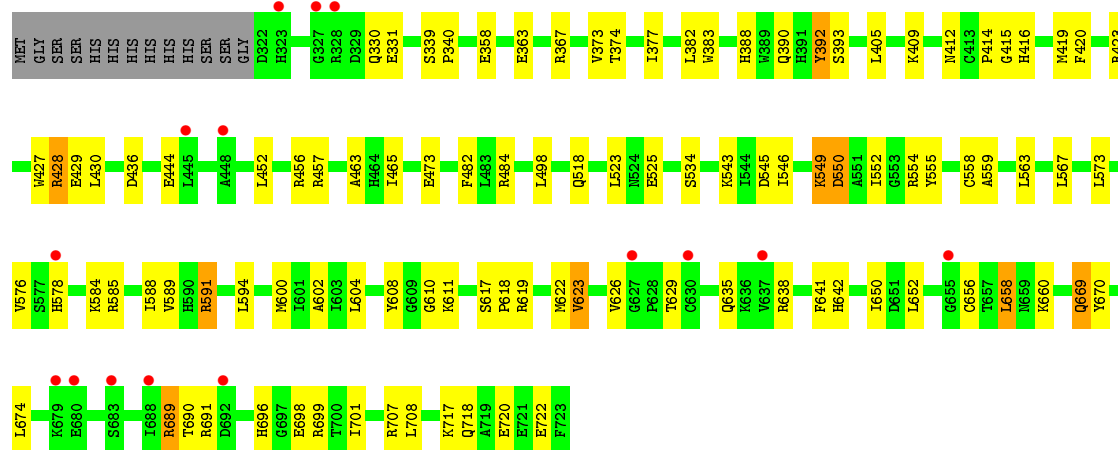


- Molecule 1: Threonine-tRNA ligase, cytoplasmic





• Molecule 1: Threonine-tRNA ligase, cytoplasmic





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.87Å 78.00Å 118.05Å 86.99° 83.32° 84.39°	Depositor
Resolution (Å)	47.71 – 2.60 63.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.71-2.60) 95.8 (63.47-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.228 , 0.255 0.228 , 0.255	Depositor DCC
$R_{free}$ test set	3365 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2CR

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	0.35	0/3343	0.46	0/4520
1	B	0.44	0/3336	0.49	1/4510 (0.0%)
1	C	0.44	0/3332	0.51	0/4507
1	D	0.44	0/3294	0.51	1/4459 (0.0%)
All	All	0.42	0/13305	0.49	2/17996 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	550	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	B	692	ASP	N-CA-C	5.11	124.79	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	717	LYS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3260	0	3114	70	0
1	B	3253	0	3105	76	0
1	C	3249	0	3091	76	0
1	D	3211	0	3036	67	0
2	A	35	0	42	6	0
2	B	35	0	42	1	0
2	C	35	0	42	5	0
2	D	35	0	42	1	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	95	0	0	1	0
4	B	111	0	0	3	0
4	C	90	0	0	0	0
4	D	93	0	0	1	0
All	All	13506	0	12514	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:C:331:GLU:OE1	1:D:423:ARG:NH1	1.81	1.13
1:A:689:ARG:HG3	1:A:689:ARG:HH21	0.96	1.09
1:C:444:GLU:OE1	1:C:454:ARG:NH1	1.99	0.96
1:A:395:ASN:N	1:A:395:ASN:HD22	1.58	0.95
1:A:689:ARG:NH2	1:A:689:ARG:HG3	1.77	0.94
1:B:385:THR:O	1:B:570:ARG:NH1	2.00	0.94
1:C:709:GLN:O	1:C:713:GLU:HG3	1.68	0.94
1:C:543:LYS:HB3	1:C:562:GLN:OE1	1.70	0.91
1:A:689:ARG:HH21	1:A:689:ARG:CG	1.82	0.91
1:C:690:THR:HG22	1:C:692:ASP:H	1.37	0.89
1:B:594:LEU:HD22	1:B:600:MET:HG2	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:CYS:SG	1:D:660:LYS:NZ	2.48	0.85
1:B:323:HIS:HB3	1:B:606:GLU:HG3	1.58	0.84
1:A:591:ARG:HG3	1:A:591:ARG:HH11	1.46	0.81
1:D:427:TRP:O	1:D:428:ARG:CG	2.30	0.80
1:A:560:THR:CG2	2:A:800:2CR:H5	2.10	0.80
1:A:463:ALA:HB3	1:A:591:ARG:HH11	1.47	0.79
1:C:700:THR:O	1:C:704:THR:CG2	2.31	0.78
1:B:567:LEU:HB3	1:B:588:ILE:HD12	1.67	0.76
1:D:429:GLU:C	1:D:430:LEU:HD23	2.07	0.75
1:A:423:ARG:NH1	1:A:429:GLU:OE2	2.20	0.75
1:C:689:ARG:NH2	1:C:693:ASN:OD1	2.19	0.75
1:D:698:GLU:O	1:D:699:ARG:HG2	1.88	0.74
1:B:531:GLU:OE2	1:B:533:ASN:ND2	2.20	0.74
1:D:591:ARG:O	1:D:591:ARG:NH1	2.19	0.74
1:A:669:GLN:HG3	1:A:691:ARG:HD2	1.69	0.73
1:A:567:LEU:HB3	1:A:588:ILE:HD12	1.70	0.73
1:A:395:ASN:N	1:A:395:ASN:ND2	2.31	0.72
1:A:560:THR:HG21	2:A:800:2CR:H5	1.70	0.72
1:D:429:GLU:O	1:D:430:LEU:HD23	1.90	0.72
1:A:649:ASP:OD2	1:A:670:TYR:OH	2.04	0.72
1:C:546:ILE:HB	1:C:559:ALA:HB3	1.69	0.72
1:B:499:SER:HB2	1:B:543:LYS:HG2	1.72	0.70
1:B:581:ASP:OD2	1:B:581:ASP:C	2.30	0.70
1:C:543:LYS:CB	1:C:562:GLN:OE1	2.38	0.70
1:A:463:ALA:HB3	1:A:591:ARG:NH1	2.06	0.69
1:D:567:LEU:HB3	1:D:588:ILE:HD12	1.73	0.69
1:D:611:LYS:HA	1:D:669:GLN:HG2	1.76	0.68
1:A:330:GLN:HG2	1:A:619:ARG:NH1	2.08	0.68
1:B:546:ILE:HB	1:B:559:ALA:HB3	1.74	0.67
1:C:700:THR:O	1:C:704:THR:HG22	1.93	0.67
1:C:669:GLN:HG3	1:C:691:ARG:HD2	1.77	0.67
1:D:427:TRP:O	1:D:428:ARG:HG2	1.94	0.67
1:C:560:THR:CG2	2:C:800:2CR:H5	2.25	0.66
1:B:649:ASP:OD2	1:B:670:TYR:OH	2.08	0.66
1:D:623:VAL:HG21	1:D:638:ARG:HB2	1.78	0.66
1:A:363:GLU:HG3	1:A:367:ARG:HE	1.61	0.66
1:A:641:PHE:HE1	1:A:708:LEU:HD12	1.60	0.65
1:B:497:ASN:O	1:B:497:ASN:ND2	2.30	0.65
1:C:423:ARG:NH2	1:C:429:GLU:OE1	2.29	0.65
1:B:581:ASP:OD2	1:B:582:ASP:N	2.30	0.65
1:A:638:ARG:HG3	1:A:650:ILE:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:ARG:NH2	4:B:972:HOH:O	2.29	0.64
1:B:585:ARG:NH1	4:B:961:HOH:O	2.29	0.64
1:C:452:LEU:HB2	1:C:602:ALA:HB2	1.79	0.64
1:C:716:SER:O	1:C:717:LYS:CB	2.46	0.64
1:C:567:LEU:HB3	1:C:588:ILE:HD12	1.78	0.64
1:B:497:ASN:C	1:B:497:ASN:ND2	2.51	0.63
1:B:579:ASP:N	1:B:579:ASP:OD2	2.30	0.63
1:A:394:GLU:C	1:A:395:ASN:HD22	2.02	0.63
1:A:689:ARG:NH2	1:A:689:ARG:CG	2.49	0.63
1:B:380:SER:HB3	1:B:405:LEU:HB3	1.79	0.63
1:B:409:LYS:NZ	1:B:412:ASN:OD1	2.16	0.62
1:D:340:PRO:HG2	1:D:456:ARG:NH1	2.15	0.62
1:A:572:ASN:OD1	1:A:585:ARG:NH2	2.33	0.62
1:A:628:PRO:HA	1:A:631:ASP:OD2	2.01	0.61
1:B:497:ASN:HD22	1:B:497:ASN:C	2.03	0.61
1:D:641:PHE:HE1	1:D:708:LEU:HD12	1.65	0.61
1:A:611:LYS:HA	1:A:669:GLN:HG2	1.83	0.60
1:A:656:CYS:SG	1:A:660:LYS:NZ	2.69	0.60
1:C:540:TYR:OH	2:C:800:2CR:O34	2.20	0.59
1:B:579:ASP:N	1:B:580:GLY:HA2	2.16	0.59
1:B:692:ASP:N	1:B:693:ASN:HA	2.18	0.58
1:A:330:GLN:HG2	1:A:619:ARG:HH12	1.67	0.58
1:B:452:LEU:HB2	1:B:602:ALA:HB2	1.84	0.58
1:B:330:GLN:O	1:B:619:ARG:NH2	2.36	0.58
1:A:591:ARG:NH1	1:A:591:ARG:HG3	2.18	0.58
1:C:608:TYR:HB3	1:C:611:LYS:O	2.04	0.58
1:A:599:ARG:HG2	1:A:599:ARG:NH1	2.19	0.58
1:B:460:GLN:HA	1:B:596:SER:HA	1.86	0.58
1:C:381:ARG:NH2	1:C:404:GLU:OE1	2.35	0.58
1:D:546:ILE:HB	1:D:559:ALA:HB3	1.86	0.58
1:B:460:GLN:HB2	1:B:595:GLY:O	2.04	0.57
1:C:716:SER:O	1:C:717:LYS:HB3	2.03	0.57
1:A:444:GLU:OE1	1:A:444:GLU:HA	2.05	0.57
1:A:373:VAL:HB	1:B:345:PHE:HB2	1.87	0.57
1:D:543:LYS:HE3	1:D:545:ASP:OD2	2.05	0.57
1:D:427:TRP:O	1:D:428:ARG:CB	2.52	0.57
1:B:492:PHE:HB3	1:B:548:ILE:HD12	1.87	0.57
1:C:690:THR:HG22	1:C:692:ASP:N	2.15	0.57
1:D:330:GLN:O	1:D:619:ARG:NH2	2.37	0.56
1:B:494:PHE:HB3	1:B:548:ILE:HD13	1.87	0.56
1:B:572:ASN:OD1	1:B:585:ARG:NH2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:LEU:HD22	1:B:589:VAL:HG22	1.88	0.56
1:C:550:ASP:OD1	1:C:554:ARG:N	2.38	0.56
1:C:323:HIS:HB3	1:C:606:GLU:HG3	1.87	0.56
1:B:323:HIS:HB2	1:B:605:THR:HB	1.88	0.56
1:B:423:ARG:NH1	1:B:429:GLU:OE2	2.37	0.56
1:A:680:GLU:OE2	1:A:698:GLU:OE2	2.24	0.55
1:D:550:ASP:OD1	1:D:550:ASP:C	2.42	0.55
1:D:626:VAL:HG12	1:D:658:LEU:HD11	1.87	0.55
1:C:656:CYS:HB3	1:C:660:LYS:HD3	1.89	0.55
1:D:608:TYR:HB3	1:D:611:LYS:O	2.07	0.55
1:D:619:ARG:HB3	1:D:670:TYR:CE1	2.42	0.55
1:B:619:ARG:HB3	1:B:670:TYR:CE1	2.42	0.55
1:D:374:THR:OG1	1:D:436:ASP:OD2	2.16	0.54
1:B:352:ILE:HG23	1:B:616:LEU:HD22	1.89	0.54
1:C:387:GLY:O	1:C:391:HIS:HB2	2.07	0.54
1:B:348:LYS:HE2	1:B:619:ARG:NH1	2.22	0.53
1:B:608:TYR:HB3	1:B:611:LYS:O	2.09	0.53
1:C:572:ASN:OD1	1:C:585:ARG:NH2	2.41	0.53
1:D:363:GLU:HG3	1:D:367:ARG:HE	1.73	0.53
1:D:430:LEU:HD23	1:D:430:LEU:N	2.20	0.53
1:D:452:LEU:HB2	1:D:602:ALA:HB2	1.91	0.53
1:C:700:THR:O	1:C:704:THR:HG23	2.06	0.52
1:C:484:ARG:HH11	1:C:484:ARG:HG2	1.73	0.52
1:D:463:ALA:HB3	1:D:591:ARG:NH1	2.24	0.52
1:B:543:LYS:CE	1:B:545:ASP:OD2	2.58	0.52
1:C:560:THR:HG22	2:C:800:2CR:H5	1.91	0.52
1:C:339:SER:OG	1:D:377:ILE:O	2.28	0.52
1:D:427:TRP:CD2	1:D:428:ARG:HB3	2.46	0.52
1:C:419:MET:O	1:C:425:ARG:NH2	2.41	0.51
1:A:608:TYR:HB3	1:A:611:LYS:O	2.09	0.51
1:C:473:GLU:HB2	1:C:518:GLN:HB3	1.92	0.51
1:C:615:TRP:CD2	1:C:715:ARG:HD3	2.45	0.51
1:A:496:LEU:HD23	1:A:546:ILE:HB	1.93	0.51
1:C:670:TYR:O	1:C:691:ARG:HB2	2.10	0.51
1:D:549:LYS:HB2	1:D:555:TYR:CE1	2.46	0.51
1:A:362:SER:HA	1:A:365:ARG:NH1	2.26	0.50
1:C:598:GLU:OE2	1:C:598:GLU:N	2.38	0.50
1:A:481:ASP:OD1	1:A:484:ARG:NH1	2.42	0.50
1:C:594:LEU:HD22	1:C:600:MET:HG2	1.92	0.50
1:D:420:PHE:HD2	1:D:573:LEU:HD22	1.76	0.50
1:C:416:HIS:CE1	1:C:436:ASP:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:VAL:HG12	1:D:674:LEU:HB2	1.94	0.50
1:B:411:MET:HG2	1:B:442:ARG:HH21	1.76	0.49
1:C:560:THR:HG21	2:C:800:2CR:H5	1.93	0.49
1:D:330:GLN:NE2	1:D:610:GLY:O	2.43	0.49
1:D:669:GLN:HG3	1:D:691:ARG:HH11	1.78	0.49
1:B:543:LYS:HE2	1:B:545:ASP:OD2	2.12	0.49
1:C:336:HIS:ND1	1:C:337:GLU:N	2.60	0.49
1:A:416:HIS:CE1	1:A:436:ASP:HB2	2.48	0.49
1:C:577:SER:OG	1:C:578:HIS:N	2.46	0.49
1:A:563:LEU:HD22	1:A:589:VAL:HG22	1.95	0.49
1:D:669:GLN:HG3	1:D:691:ARG:HD2	1.95	0.49
1:B:568:PRO:HG3	1:B:588:ILE:HG13	1.95	0.48
1:D:718:GLN:O	1:D:722:GLU:HB2	2.13	0.48
1:A:559:ALA:HA	1:A:592:ALA:O	2.13	0.48
1:C:387:GLY:HA2	1:C:390:GLN:OE1	2.13	0.48
1:B:440:LEU:HD12	1:B:460:GLN:HE21	1.78	0.48
1:B:549:LYS:HE3	1:B:549:LYS:HB3	1.41	0.48
1:D:416:HIS:HE2	1:D:436:ASP:HB2	1.78	0.48
1:C:619:ARG:HB3	1:C:670:TYR:CE1	2.48	0.48
1:C:669:GLN:HG3	1:C:691:ARG:HH11	1.79	0.48
1:B:549:LYS:HD2	1:B:553:GLY:HA2	1.95	0.47
1:D:427:TRP:CE3	1:D:428:ARG:HB3	2.49	0.47
1:D:638:ARG:HD2	1:D:650:ILE:HB	1.96	0.47
1:A:613:PRO:HG2	1:A:616:LEU:HB2	1.95	0.47
1:A:345:PHE:HB2	1:B:373:VAL:HB	1.97	0.47
1:D:416:HIS:CE1	1:D:436:ASP:HB2	2.49	0.47
1:B:707:ARG:NH2	1:B:722:GLU:O	2.46	0.47
1:A:415:GLY:O	1:A:419:MET:HG3	2.15	0.47
1:B:493:SER:OG	1:B:549:LYS:HE2	2.14	0.47
2:A:800:2CR:O28	2:A:800:2CR:O34	2.30	0.47
1:A:619:ARG:HB3	1:A:670:TYR:CD1	2.50	0.47
1:D:549:LYS:HD3	1:D:555:TYR:CZ	2.49	0.47
1:A:599:ARG:CG	1:A:599:ARG:HH11	2.28	0.46
1:A:696:HIS:O	1:A:699:ARG:NH1	2.44	0.46
1:A:446:SER:HA	1:A:449:LEU:HD12	1.97	0.46
1:D:416:HIS:NE2	1:D:436:ASP:HB2	2.30	0.46
1:A:382:LEU:HD21	1:A:414:PRO:HB2	1.97	0.46
1:B:450:THR:H	1:B:454:ARG:HB3	1.80	0.46
1:C:405:LEU:HD23	1:C:405:LEU:HA	1.70	0.46
1:B:591:ARG:O	1:B:591:ARG:NH1	2.45	0.46
1:D:383:TRP:CZ3	1:D:414:PRO:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:ASN:CG	1:B:693:ASN:O	2.54	0.45
1:C:388:HIS:O	1:C:392:TYR:N	2.40	0.45
1:A:322:ASP:OD1	1:A:606:GLU:HG3	2.16	0.45
1:D:594:LEU:HD22	1:D:600:MET:HG2	1.98	0.45
1:C:531:GLU:HG2	1:C:532:LEU:H	1.81	0.45
1:A:599:ARG:HH11	1:A:599:ARG:HG2	1.81	0.45
1:B:578:HIS:HD2	4:B:931:HOH:O	1.98	0.45
2:B:800:2CR:H7	2:B:800:2CR:H11	1.74	0.45
1:C:671:ASN:ND2	1:C:720:GLU:OE2	2.29	0.45
1:A:433:ARG:HG2	1:A:465:ILE:HG23	1.98	0.45
1:B:483:LEU:HD23	1:B:593:ILE:HG23	1.99	0.45
1:A:695:VAL:HG12	1:A:697:GLY:H	1.82	0.45
1:B:566:GLN:O	1:B:570:ARG:HG3	2.16	0.45
1:B:465:ILE:HB	1:B:589:VAL:HB	1.99	0.45
1:C:479:CYS:O	1:C:483:LEU:HD13	2.17	0.45
1:C:352:ILE:HG23	1:C:616:LEU:HD22	1.98	0.45
1:D:465:ILE:HB	1:D:589:VAL:HB	1.98	0.44
1:B:333:TYR:HB2	1:B:343:CYS:SG	2.57	0.44
1:B:689:ARG:HE	1:B:693:ASN:HD22	1.66	0.44
2:C:800:2CR:H31	2:C:800:2CR:H36	1.79	0.44
1:A:470:GLU:H	1:A:470:GLU:CD	2.20	0.44
1:B:473:GLU:HB2	1:B:518:GLN:HB3	1.98	0.44
1:B:669:GLN:HG3	1:B:691:ARG:HD2	1.99	0.44
1:C:326:ILE:O	1:C:330:GLN:HB2	2.18	0.44
1:D:707:ARG:NH2	1:D:722:GLU:O	2.51	0.44
1:D:656:CYS:HB3	1:D:660:LYS:HD3	2.00	0.44
1:A:494:PHE:HB2	1:A:546:ILE:CD1	2.47	0.44
1:B:487:TYR:CD2	1:B:548:ILE:HD11	2.53	0.44
1:B:690:THR:CG2	1:B:696:HIS:CD2	3.01	0.44
1:C:591:ARG:C	1:C:591:ARG:HH11	2.21	0.44
1:D:388:HIS:O	1:D:392:TYR:N	2.42	0.44
1:D:549:LYS:HG2	1:D:549:LYS:HZ3	1.63	0.43
1:D:670:TYR:O	1:D:691:ARG:HB2	2.17	0.43
2:D:800:2CR:H42	2:D:800:2CR:H35	1.61	0.43
1:A:599:ARG:CG	1:A:599:ARG:NH1	2.81	0.43
1:C:611:LYS:HA	1:C:669:GLN:HG2	1.99	0.43
1:C:716:SER:O	1:C:717:LYS:HG2	2.18	0.43
1:A:399:PHE:HB3	1:B:399:PHE:HB3	1.99	0.43
1:A:619:ARG:HD3	1:A:670:TYR:CE2	2.53	0.43
2:A:800:2CR:H7	2:A:800:2CR:H11	1.78	0.43
1:B:604:LEU:HD22	1:B:608:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:TYR:HD2	1:A:676:VAL:HG13	1.83	0.43
1:B:543:LYS:HE3	1:B:545:ASP:OD2	2.19	0.43
1:B:610:GLY:O	1:B:669:GLN:HG2	2.19	0.43
1:C:653:ASP:HA	1:C:654:PRO:HD3	1.88	0.43
1:A:641:PHE:CE1	1:A:708:LEU:HD12	2.45	0.43
2:A:800:2CR:H35	2:A:800:2CR:H42	1.54	0.43
1:C:330:GLN:HG2	1:C:619:ARG:NH1	2.34	0.43
1:A:444:GLU:OE2	1:A:454:ARG:NH2	2.42	0.43
1:B:596:SER:OG	1:B:599:ARG:HB2	2.19	0.43
1:A:619:ARG:HB3	1:A:670:TYR:CE1	2.54	0.42
1:D:415:GLY:O	1:D:419:MET:HG3	2.19	0.42
1:A:558:CYS:O	4:A:932:HOH:O	2.21	0.42
1:A:579:ASP:N	1:A:579:ASP:OD2	2.40	0.42
1:C:362:SER:HA	1:C:365:ARG:NH1	2.34	0.42
1:C:610:GLY:O	1:C:669:GLN:HG2	2.18	0.42
1:C:338:LEU:HD13	1:D:382:LEU:HB2	2.00	0.42
1:A:387:GLY:HA2	1:A:390:GLN:OE1	2.20	0.42
1:C:423:ARG:NH1	1:D:331:GLU:OE1	2.52	0.42
1:D:427:TRP:HD1	1:D:576:VAL:O	2.02	0.42
1:D:652:LEU:HA	1:D:652:LEU:HD23	1.82	0.42
1:C:365:ARG:O	1:D:642:HIS:HE1	2.01	0.42
1:D:358:GLU:OE2	4:D:992:HOH:O	2.21	0.42
1:C:345:PHE:HB2	1:D:373:VAL:HB	2.01	0.42
1:B:389:TRP:HH2	1:B:398:SER:HG	1.67	0.42
1:B:420:PHE:CE1	1:B:425:ARG:HD2	2.55	0.42
1:B:711:LEU:HD13	1:B:719:ALA:HB1	2.02	0.42
1:C:619:ARG:HB3	1:C:670:TYR:CD1	2.54	0.42
1:A:460:GLN:NE2	2:A:800:2CR:H4	2.35	0.42
1:D:409:LYS:NZ	1:D:412:ASN:OD1	2.26	0.42
1:D:689:ARG:HB2	1:D:689:ARG:HE	1.45	0.42
1:B:359:PHE:O	1:B:362:SER:OG	2.30	0.41
1:B:419:MET:HB3	1:B:419:MET:HE3	1.87	0.41
1:C:367:ARG:NH2	1:C:481:ASP:OD2	2.47	0.41
1:C:361:ARG:O	1:C:365:ARG:HG3	2.20	0.41
1:C:567:LEU:HA	1:C:567:LEU:HD12	1.87	0.41
1:C:617:SER:HA	1:C:618:PRO:HD3	1.81	0.41
1:C:678:GLU:O	1:C:682:ILE:HD13	2.20	0.41
1:A:452:LEU:HB2	1:A:602:ALA:HB2	2.02	0.41
1:C:619:ARG:HD3	1:C:670:TYR:CE2	2.55	0.41
1:B:542:PRO:HD2	1:B:563:LEU:HB2	2.02	0.41
1:B:412:ASN:HB2	1:B:462:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:ILE:HA	1:C:552:ILE:HD12	1.91	0.41
1:C:596:SER:HB2	1:C:599:ARG:H	1.85	0.41
1:D:604:LEU:HD22	1:D:608:TYR:CE2	2.56	0.41
1:A:474:ASP:O	1:A:477:LYS:HB3	2.19	0.41
1:D:617:SER:HA	1:D:618:PRO:HD3	1.92	0.41
1:A:473:GLU:HB2	1:A:518:GLN:HB3	2.01	0.41
1:A:541:GLY:HA3	1:A:563:LEU:O	2.20	0.41
1:A:465:ILE:HB	1:A:589:VAL:HB	2.03	0.41
1:A:591:ARG:NH2	1:A:593:ILE:HG13	2.35	0.41
1:B:548:ILE:HD13	1:B:548:ILE:HA	1.87	0.41
1:B:409:LYS:HA	1:B:410:PRO:HD2	1.94	0.41
1:C:336:HIS:CE1	1:C:338:LEU:HG	2.56	0.41
1:A:699:ARG:NH1	1:D:525:GLU:HG2	2.36	0.41
1:D:473:GLU:HB2	1:D:518:GLN:HB3	2.02	0.41
1:D:563:LEU:HD22	1:D:589:VAL:HG22	2.02	0.41
1:D:619:ARG:HB3	1:D:670:TYR:CZ	2.56	0.41
1:D:696:HIS:CE1	1:D:720:GLU:O	2.74	0.41
1:C:568:PRO:HG3	1:C:588:ILE:HG13	2.03	0.40
1:C:516:GLU:O	1:C:520:GLU:HG3	2.21	0.40
1:A:472:ILE:HD11	1:A:587:VAL:HG11	2.02	0.40
1:B:690:THR:HG23	1:B:694:LYS:O	2.21	0.40
1:D:549:LYS:HD3	1:D:555:TYR:OH	2.21	0.40
1:B:348:LYS:HB3	1:B:618:PRO:HB3	2.02	0.40
1:B:579:ASP:N	1:B:580:GLY:CA	2.84	0.40
1:C:322:ASP:HB3	1:C:606:GLU:HG2	2.03	0.40
1:C:322:ASP:O	1:C:326:ILE:HG13	2.22	0.40
1:C:706:GLU:O	1:C:710:GLN:HG3	2.22	0.40
1:B:693:ASN:OD1	1:B:693:ASN:O	2.40	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	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
1	B	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
1	C	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
1	D	400/415 (96%)	393 (98%)	7 (2%)	0	100	100
All	All	1600/1660 (96%)	1572 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	342/368 (93%)	311 (91%)	31 (9%)	9	18
1	B	339/368 (92%)	312 (92%)	27 (8%)	12	24
1	C	338/368 (92%)	303 (90%)	35 (10%)	7	13
1	D	328/368 (89%)	297 (90%)	31 (10%)	8	16
All	All	1347/1472 (92%)	1223 (91%)	124 (9%)	9	17

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	GLU
1	A	390	GLN
1	A	392	TYR
1	A	395	ASN
1	A	401	VAL
1	A	432	LEU
1	A	444	GLU
1	A	450	THR
1	A	482	PHE
1	A	493	SER
1	A	498	LEU
1	A	506	LEU
1	A	509	ILE

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Mol	Chain	Res	Type
1	A	522	SER
1	A	532	LEU
1	A	546	ILE
1	A	552	ILE
1	A	570	ARG
1	A	579	ASP
1	A	585	ARG
1	A	591	ARG
1	A	599	ARG
1	A	622	MET
1	A	629	THR
1	A	635	GLN
1	A	658	LEU
1	A	660	LYS
1	A	669	GLN
1	A	676	VAL
1	A	689	ARG
1	A	709	GLN
1	B	384	MET
1	B	392	TYR
1	B	405	LEU
1	B	426	SER
1	B	453	THR
1	B	477	LYS
1	B	482	PHE
1	B	497	ASN
1	B	498	LEU
1	B	531	GLU
1	B	549	LYS
1	B	552	ILE
1	B	558	CYS
1	B	579	ASP
1	B	581	ASP
1	B	585	ARG
1	B	591	ARG
1	B	599	ARG
1	B	622	MET
1	B	629	THR
1	B	658	LEU
1	B	669	GLN
1	B	689	ARG
1	B	690	THR

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Mol	Chain	Res	Type
1	B	701	ILE
1	B	702	SER
1	B	717	LYS
1	C	331	GLU
1	C	337	GLU
1	C	339	SER
1	C	380	SER
1	C	392	TYR
1	C	401	VAL
1	C	405	LEU
1	C	432	LEU
1	C	444	GLU
1	C	454	ARG
1	C	482	PHE
1	C	485	THR
1	C	495	LYS
1	C	496	LEU
1	C	522	SER
1	C	523	LEU
1	C	543	LYS
1	C	561	ILE
1	C	563	LEU
1	C	567	LEU
1	C	577	SER
1	C	584	LYS
1	C	585	ARG
1	C	591	ARG
1	C	596	SER
1	C	599	ARG
1	C	622	MET
1	C	658	LEU
1	C	669	GLN
1	C	689	ARG
1	C	704	THR
1	C	708	LEU
1	C	713	GLU
1	C	716	SER
1	C	717	LYS
1	D	339	SER
1	D	390	GLN
1	D	392	TYR
1	D	393	SER

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Mol	Chain	Res	Type
1	D	405	LEU
1	D	428	ARG
1	D	444	GLU
1	D	457	ARG
1	D	482	PHE
1	D	484	ARG
1	D	498	LEU
1	D	523	LEU
1	D	534	SER
1	D	549	LYS
1	D	552	ILE
1	D	554	ARG
1	D	558	CYS
1	D	578	HIS
1	D	584	LYS
1	D	585	ARG
1	D	591	ARG
1	D	622	MET
1	D	623	VAL
1	D	629	THR
1	D	635	GLN
1	D	658	LEU
1	D	669	GLN
1	D	689	ARG
1	D	690	THR
1	D	701	ILE
1	D	717	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	ASN
1	A	497	ASN
1	A	533	ASN
1	B	460	GLN
1	B	497	ASN
1	B	666	GLN
1	C	497	ASN
1	D	422	HIS
1	D	642	HIS
1	D	696	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	2CR	C	800	-	32,36,36	2.84	5 (15%)	33,49,49	1.68	6 (18%)
2	2CR	D	800	-	32,36,36	2.91	6 (18%)	33,49,49	1.85	8 (24%)
2	2CR	A	800	-	32,36,36	3.02	7 (21%)	33,49,49	2.12	11 (33%)
2	2CR	B	800	-	32,36,36	2.80	8 (25%)	33,49,49	1.88	9 (27%)

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	2CR	C	800	-	-	8/42/59/59	0/1/2/2
2	2CR	D	800	-	-	5/42/59/59	0/1/2/2
2	2CR	A	800	-	-	9/42/59/59	0/1/2/2
2	2CR	B	800	-	-	4/42/59/59	0/1/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	2CR	C12-C11	-14.40	1.25	1.43
2	D	800	2CR	C12-C11	-14.24	1.25	1.43
2	C	800	2CR	C12-C11	-13.76	1.25	1.43
2	B	800	2CR	C12-C11	-12.98	1.26	1.43
2	A	800	2CR	O29-C6	-4.27	1.38	1.46
2	A	800	2CR	C2-C1	-4.12	1.48	1.55
2	C	800	2CR	O29-C6	-4.10	1.39	1.46
2	B	800	2CR	O29-C6	-3.83	1.39	1.46
2	B	800	2CR	C2-C1	-3.71	1.49	1.55
2	D	800	2CR	O29-C6	-3.56	1.40	1.46
2	C	800	2CR	C2-C1	-2.97	1.50	1.55
2	D	800	2CR	C2-C1	-2.81	1.50	1.55
2	D	800	2CR	O29-C27	2.68	1.41	1.34
2	B	800	2CR	O29-C27	2.67	1.41	1.34
2	B	800	2CR	C22-C23	-2.64	1.49	1.54
2	C	800	2CR	O29-C27	2.63	1.41	1.34
2	A	800	2CR	C26-C25	-2.57	1.49	1.53
2	A	800	2CR	O29-C27	2.55	1.41	1.34
2	B	800	2CR	C3-C2	-2.45	1.49	1.54
2	C	800	2CR	C23-C25	-2.34	1.50	1.53
2	D	800	2CR	C16-C14	-2.34	1.50	1.54
2	A	800	2CR	C3-C2	-2.32	1.49	1.54
2	A	800	2CR	C22-C23	-2.31	1.50	1.54
2	B	800	2CR	C26-C25	-2.21	1.49	1.53
2	D	800	2CR	C22-C23	-2.04	1.50	1.54
2	B	800	2CR	C23-C25	-2.01	1.50	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	2CR	C10-C9-C8	-6.58	108.22	123.63
2	D	800	2CR	C10-C9-C8	-5.16	111.54	123.63
2	B	800	2CR	C10-C9-C8	-5.15	111.57	123.63
2	C	800	2CR	O29-C27-C26	4.36	119.47	111.46
2	B	800	2CR	C10-C11-C12	4.22	129.66	122.42
2	C	800	2CR	C10-C9-C8	-4.08	114.06	123.63
2	D	800	2CR	O29-C27-C26	4.01	118.83	111.46
2	D	800	2CR	C5-C1-C2	3.93	108.72	104.05
2	B	800	2CR	O29-C27-C26	3.60	118.07	111.46
2	A	800	2CR	C5-C1-C2	3.56	108.28	104.05
2	A	800	2CR	C10-C11-C12	3.48	128.40	122.42
2	A	800	2CR	C24-C23-C22	-3.39	105.61	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	2CR	C24-C23-C25	-3.36	107.52	111.64
2	C	800	2CR	C24-C23-C25	-3.34	107.54	111.64
2	D	800	2CR	O29-C6-C7	3.19	112.51	107.27
2	B	800	2CR	C5-C1-C2	3.09	107.72	104.05
2	A	800	2CR	O29-C27-C26	3.00	116.96	111.46
2	B	800	2CR	C14-C16-C17	-2.97	108.64	116.43
2	B	800	2CR	C24-C23-C22	-2.93	106.29	110.69
2	D	800	2CR	C14-C16-C17	-2.87	108.92	116.43
2	A	800	2CR	C14-C16-C17	-2.81	109.08	116.43
2	A	800	2CR	C25-C26-C27	-2.62	108.34	114.07
2	C	800	2CR	C10-C11-C12	2.60	126.87	122.42
2	A	800	2CR	C4-C3-C2	2.58	108.34	104.28
2	A	800	2CR	O29-C6-C7	2.55	111.45	107.27
2	D	800	2CR	C10-C11-C12	2.54	126.78	122.42
2	B	800	2CR	C24-C23-C25	-2.38	108.72	111.64
2	C	800	2CR	C5-C1-C2	2.33	106.82	104.05
2	D	800	2CR	C24-C23-C22	-2.28	107.27	110.69
2	A	800	2CR	C11-C12-N35	-2.20	174.81	177.82
2	B	800	2CR	C3-C2-C1	2.12	106.99	103.60
2	C	800	2CR	C14-C16-C17	-2.06	111.03	116.43
2	D	800	2CR	C4-C3-C2	2.06	107.52	104.28
2	B	800	2CR	C4-C3-C2	2.02	107.45	104.28

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	800	2CR	C22-C23-C25-C26
2	C	800	2CR	C22-C23-C25-O34
2	C	800	2CR	C24-C23-C25-C26
2	C	800	2CR	C24-C23-C25-O34
2	A	800	2CR	C22-C23-C25-C26
2	A	800	2CR	C22-C23-C25-O34
2	A	800	2CR	C24-C23-C25-C26
2	A	800	2CR	C24-C23-C25-O34
2	D	800	2CR	C11-C13-C14-C15
2	D	800	2CR	C15-C14-C16-C17
2	A	800	2CR	C15-C14-C16-C17
2	C	800	2CR	C1-C6-C7-C8
2	C	800	2CR	O29-C6-C7-C8
2	D	800	2CR	C1-C6-C7-C8
2	D	800	2CR	O29-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	800	2CR	C1-C6-C7-C8
2	A	800	2CR	O29-C6-C7-C8
2	B	800	2CR	C1-C6-C7-C8
2	B	800	2CR	O29-C6-C7-C8
2	D	800	2CR	C11-C13-C14-C16
2	B	800	2CR	C22-C23-C25-C26
2	A	800	2CR	C20-C22-C23-C25
2	B	800	2CR	C20-C22-C23-C25
2	A	800	2CR	C20-C22-C23-C24
2	C	800	2CR	C20-C22-C23-C24
2	C	800	2CR	C20-C22-C23-C25

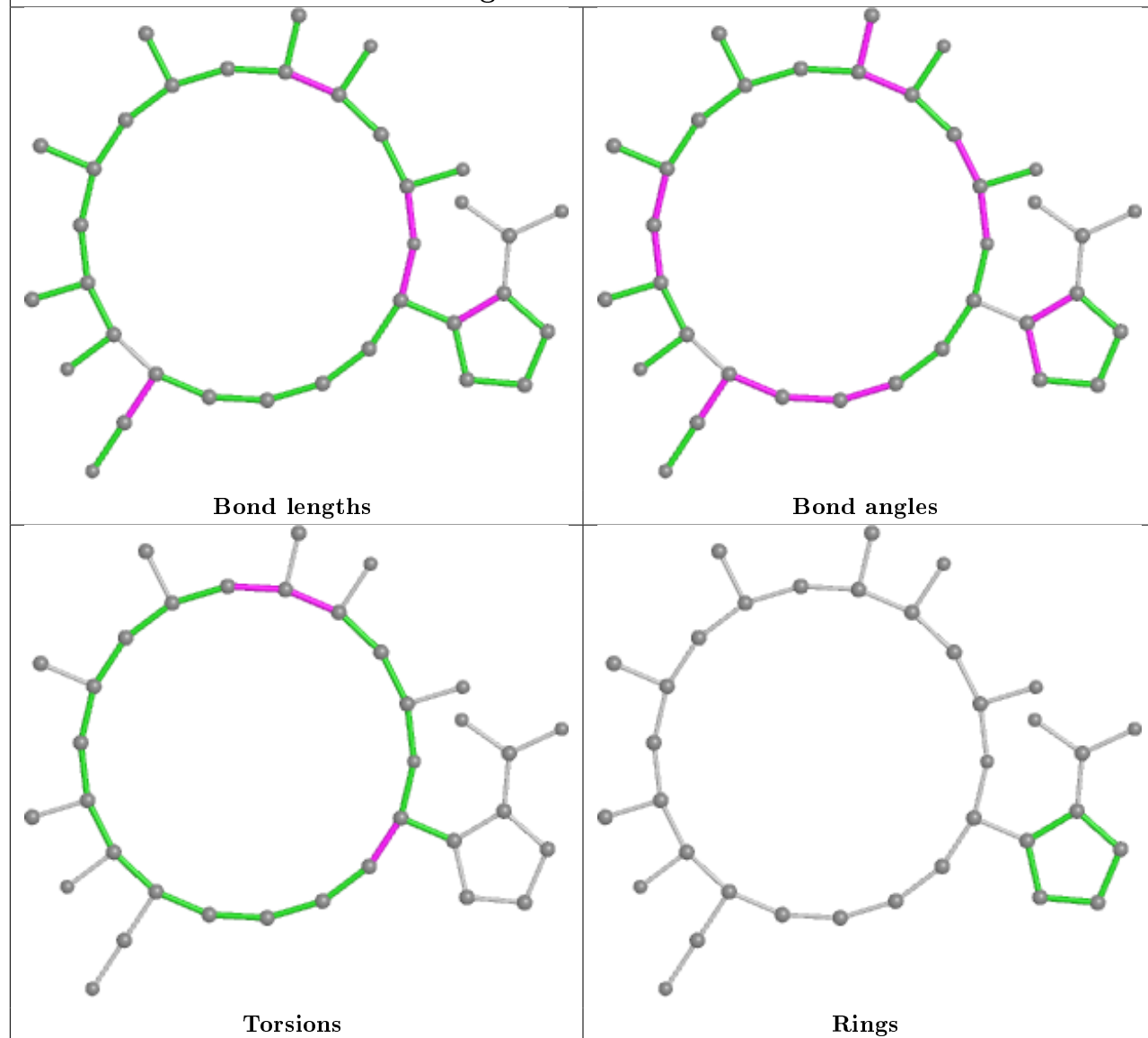
There are no ring outliers.

4 monomers are involved in 13 short contacts:

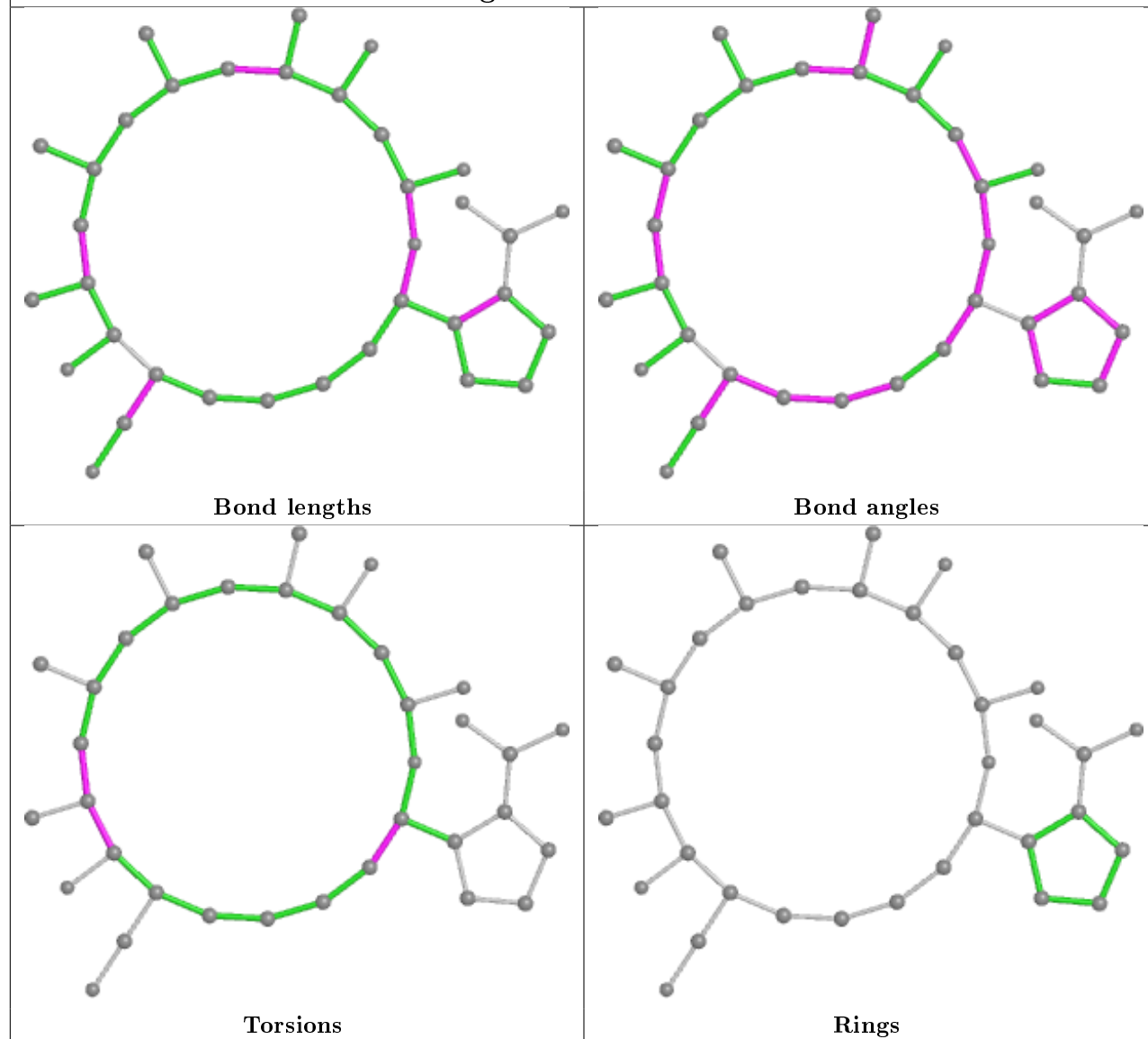
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	800	2CR	5	0
2	D	800	2CR	1	0
2	A	800	2CR	6	0
2	B	800	2CR	1	0

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.

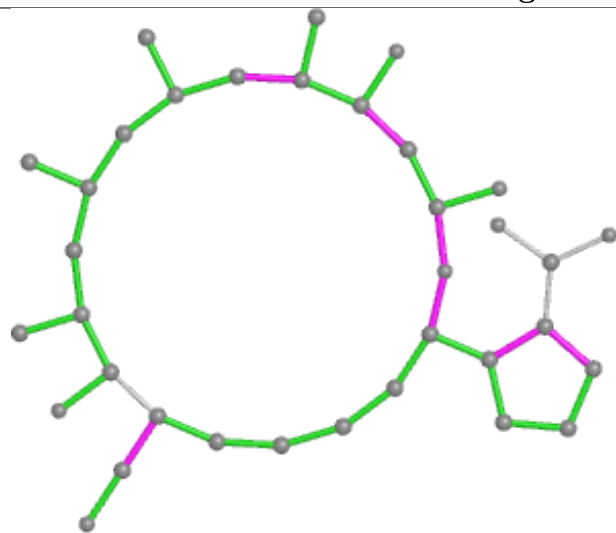
## Ligand 2CR C 800



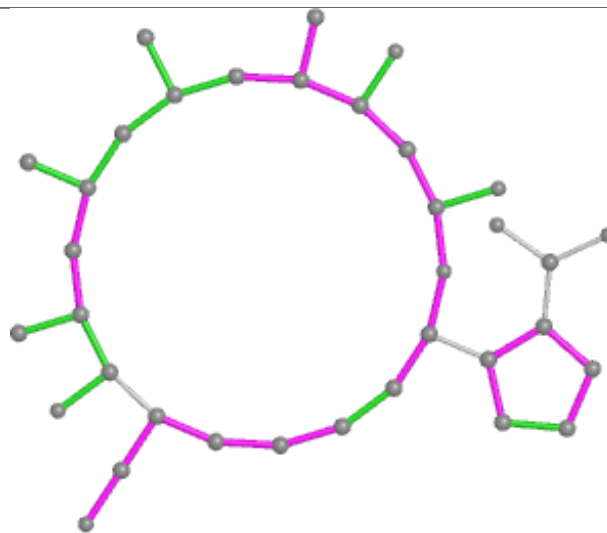
## Ligand 2CR D 800



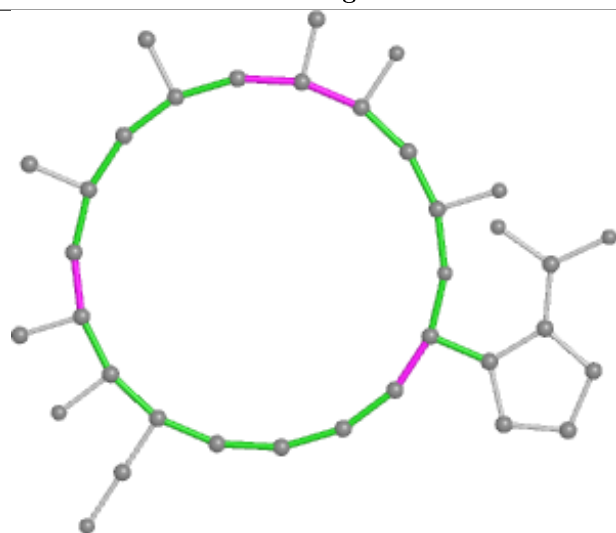
## Ligand 2CR A 800



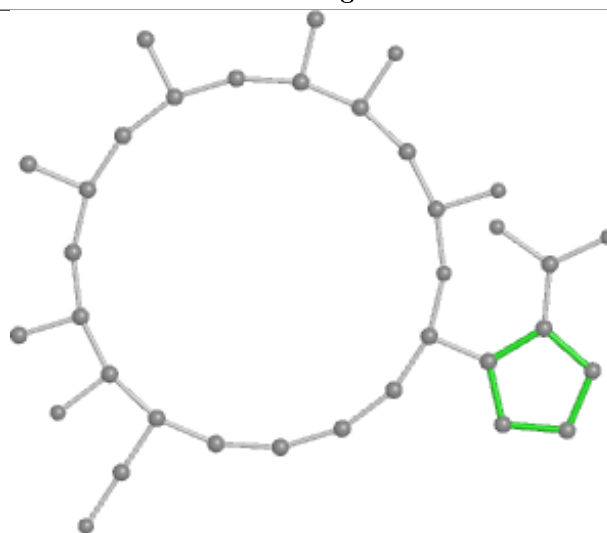
Bond lengths



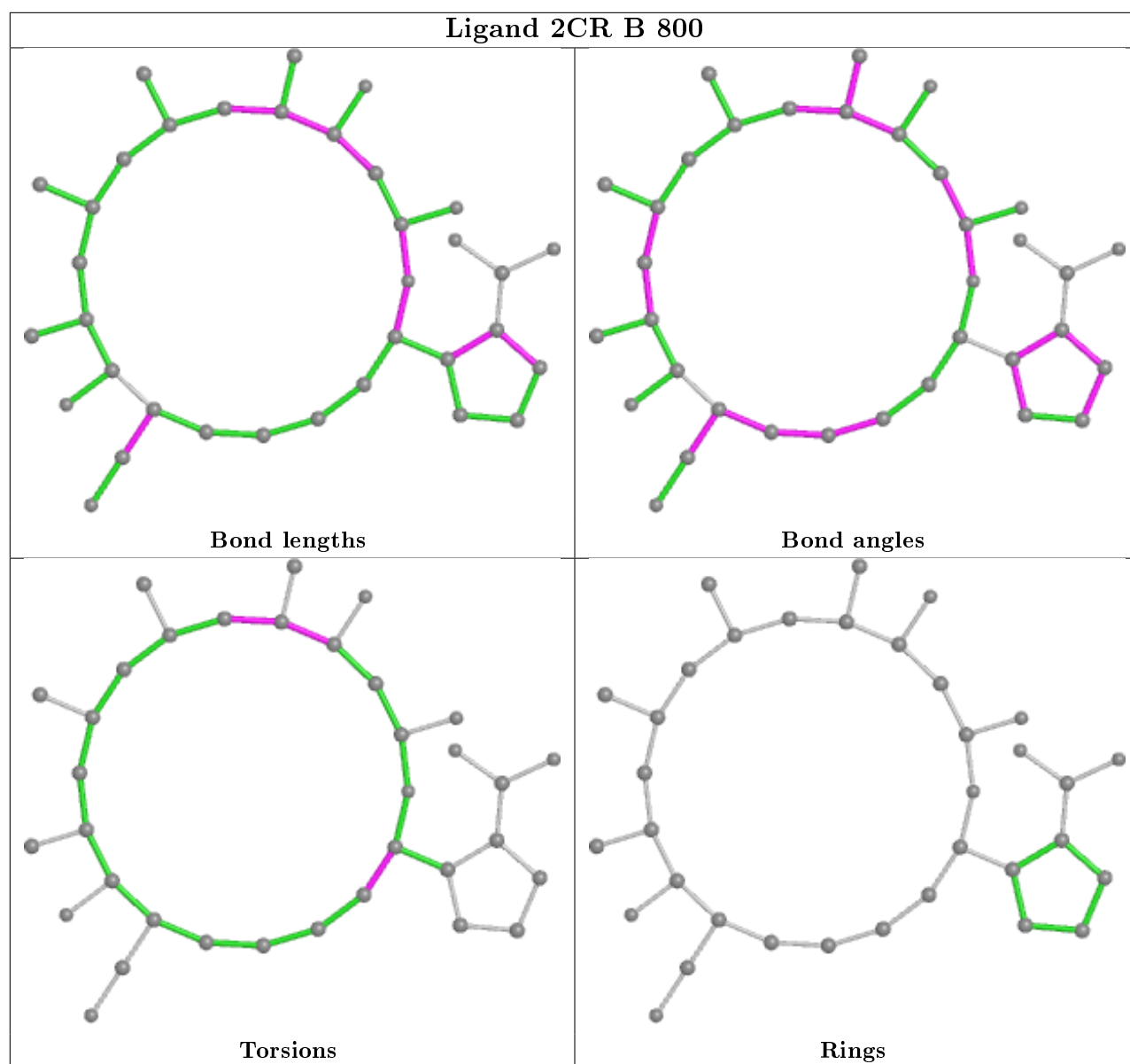
Bond angles



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	402/415 (96%)	0.29	6 (1%) 73 70	33, 51, 74, 95	0
1	B	402/415 (96%)	0.39	12 (2%) 50 43	35, 53, 72, 97	0
1	C	402/415 (96%)	0.38	17 (4%) 36 29	35, 58, 84, 100	0
1	D	402/415 (96%)	0.46	15 (3%) 41 34	36, 56, 89, 104	0
All	All	1608/1660 (96%)	0.38	50 (3%) 49 42	33, 54, 84, 104	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	HIS	4.9
1	B	322	ASP	4.2
1	C	322	ASP	4.0
1	C	327	GLY	3.9
1	D	679	LYS	3.8
1	C	323	HIS	3.7
1	D	323	HIS	3.7
1	D	627	GLY	3.5
1	D	448	ALA	3.5
1	B	578	HIS	3.5
1	C	453	THR	3.0
1	B	579	ASP	2.9
1	C	450	THR	2.9
1	C	447	GLY	2.8
1	C	582	ASP	2.8
1	C	668	ALA	2.8
1	D	688	ILE	2.7
1	B	327	GLY	2.6
1	B	581	ASP	2.6
1	B	509	ILE	2.6
1	D	327	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLY	2.6
1	A	326	ILE	2.5
1	D	445	LEU	2.5
1	B	323	HIS	2.5
1	B	526	PHE	2.5
1	B	508	ASP	2.4
1	C	454	ARG	2.4
1	D	683	SER	2.4
1	A	634	ALA	2.3
1	C	324	ARG	2.3
1	D	578	HIS	2.3
1	D	655	GLY	2.2
1	D	328	ARG	2.2
1	B	427	TRP	2.2
1	B	391	HIS	2.2
1	C	463	ALA	2.2
1	C	392	TYR	2.2
1	A	578	HIS	2.2
1	D	630	CYS	2.2
1	D	680	GLU	2.2
1	D	692	ASP	2.2
1	D	637	VAL	2.1
1	B	453	THR	2.1
1	A	627	GLY	2.1
1	C	690	THR	2.1
1	C	654	PRO	2.1
1	C	498	LEU	2.0
1	C	551	ALA	2.0
1	C	655	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands

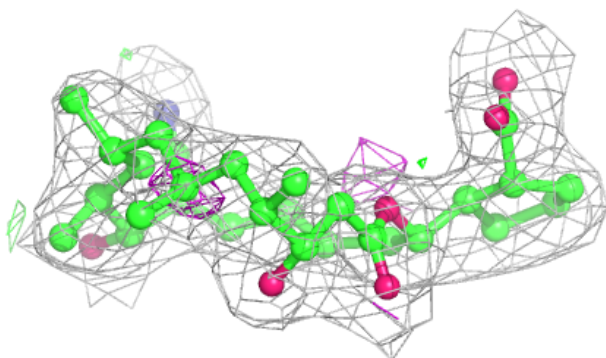
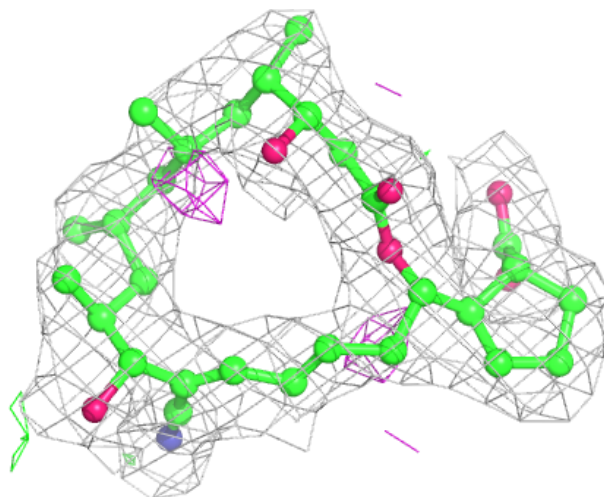
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	801	1/1	0.82	0.16	44,44,44,44	0
3	ZN	C	801	1/1	0.91	0.16	58,58,58,58	0
2	2CR	D	800	35/35	0.91	0.21	50,52,54,55	0
2	2CR	C	800	35/35	0.92	0.19	52,53,55,55	0
2	2CR	B	800	35/35	0.93	0.20	45,46,50,51	0
3	ZN	D	801	1/1	0.93	0.19	52,52,52,52	0
2	2CR	A	800	35/35	0.94	0.16	38,41,43,45	0
3	ZN	B	801	1/1	0.96	0.15	50,50,50,50	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.

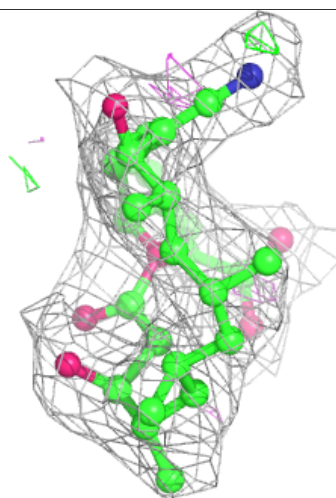
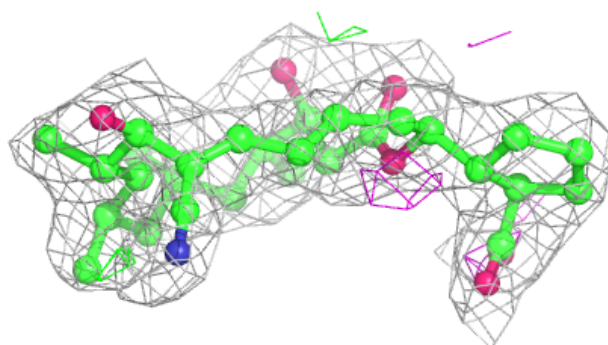
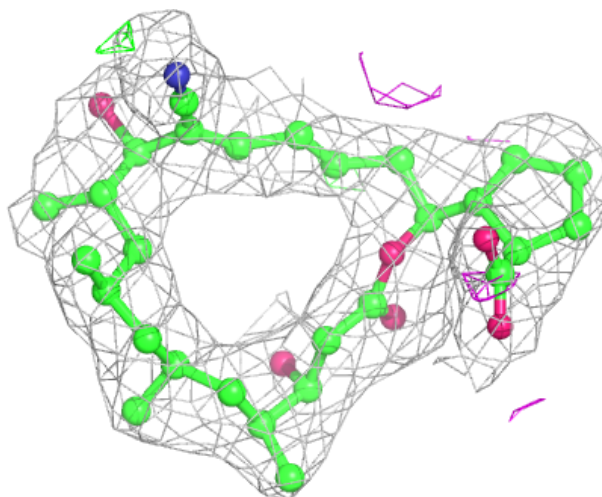
**Electron density around 2CR D 800:**

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



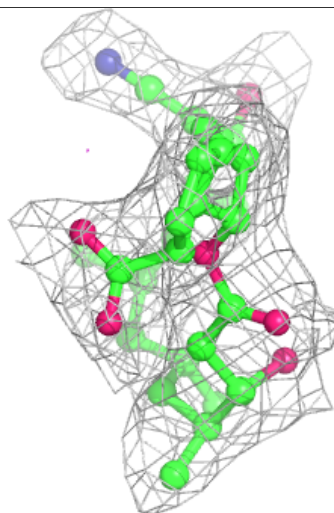
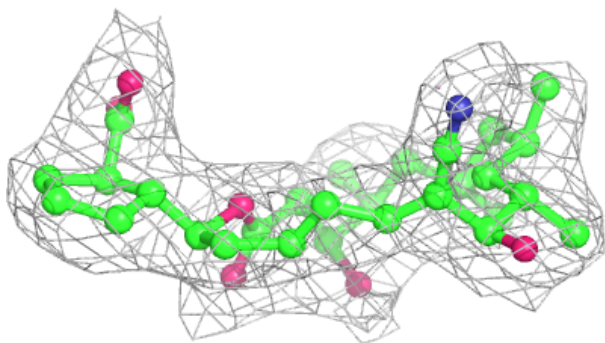
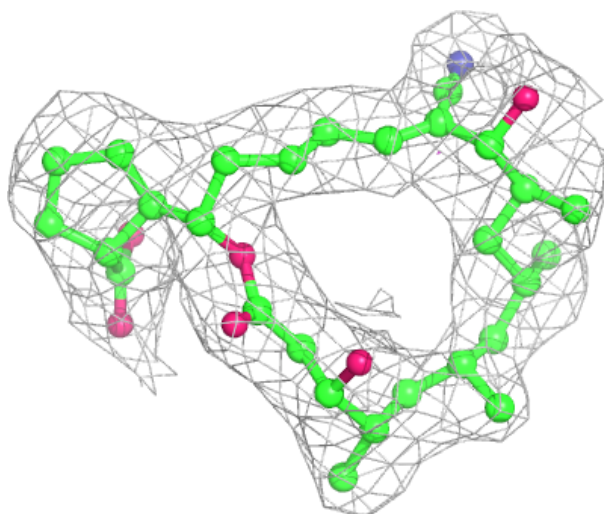
**Electron density around 2CR C 800:**

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



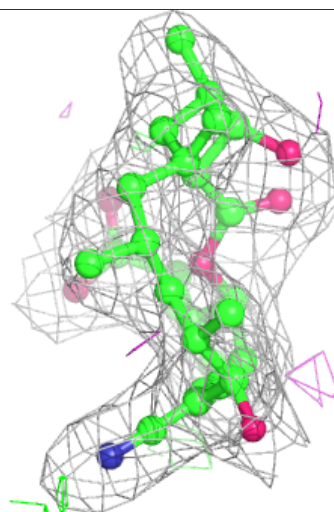
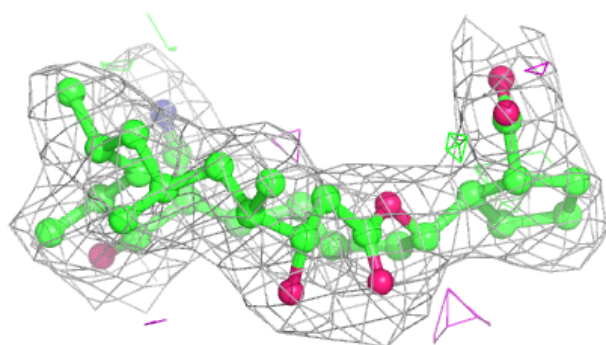
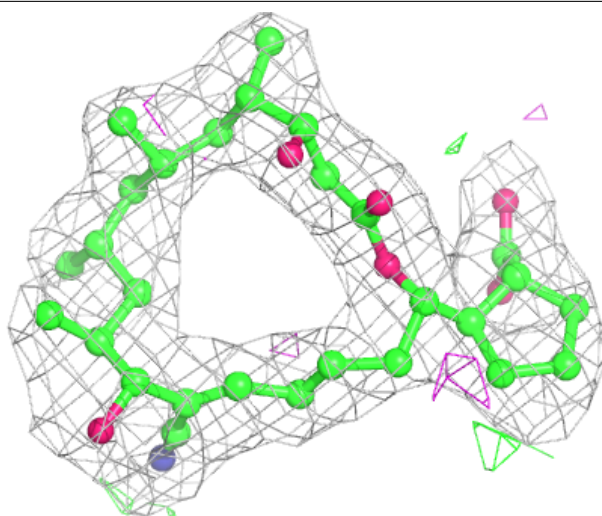
**Electron density around 2CR B 800:**

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



**Electron density around 2CR A 800:**

$2mF_o-DF_c$  (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.