



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:25 PM UTC

PDB ID : 4P3N / pdb_00004p3n
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

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

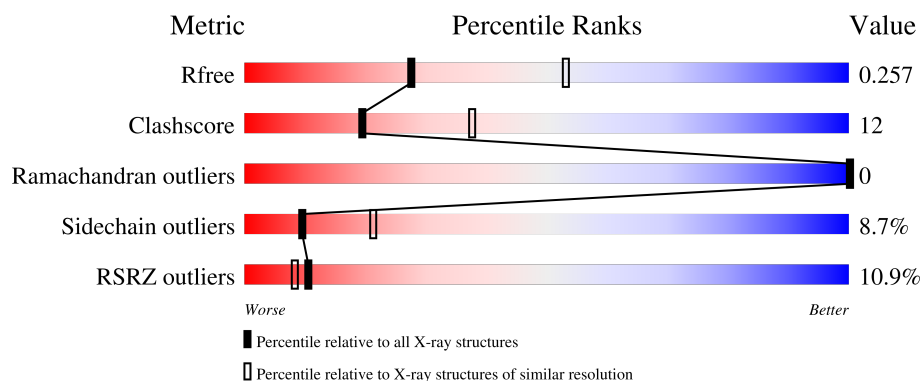
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	415	7% 71% 22% . .
1	B	415	7% 70% 22% . .
1	C	415	13% 69% 24% . .
1	D	415	15% 71% 24% . .

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:

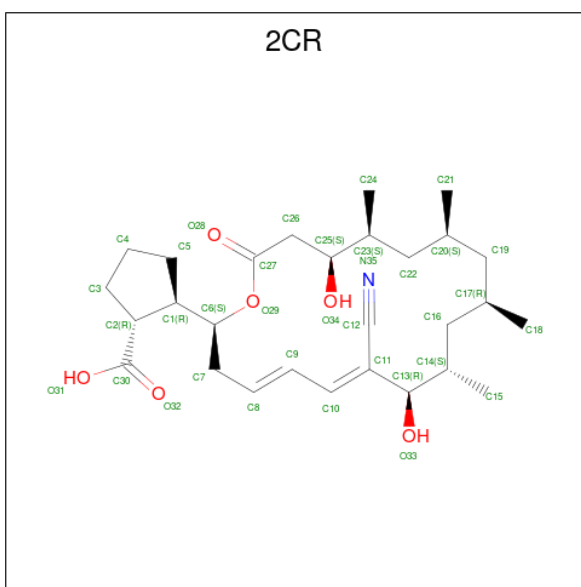
Chain	Residue	Modelled	Actual	Comment	Reference
A	309	MET	-	expression tag	UNP P26639
A	310	GLY	-	expression tag	UNP P26639
A	311	SER	-	expression tag	UNP P26639
A	312	SER	-	expression tag	UNP P26639
A	313	HIS	-	expression tag	UNP P26639
A	314	HIS	-	expression tag	UNP P26639
A	315	HIS	-	expression tag	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 (CCD ID: 2CR) (formula: C₂₈H₄₃NO₆).



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 (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	95	Total	O	0	0
			95	95		

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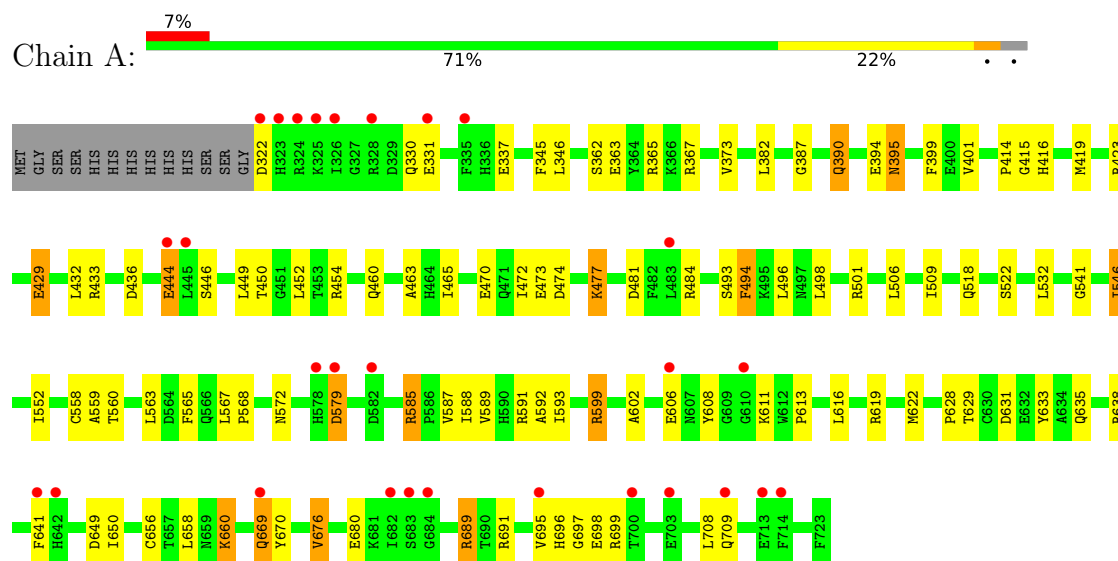
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	111	Total 111	O 111	0	0
4	C	90	Total 90	O 90	0	0
4	D	93	Total 93	O 93	0	0

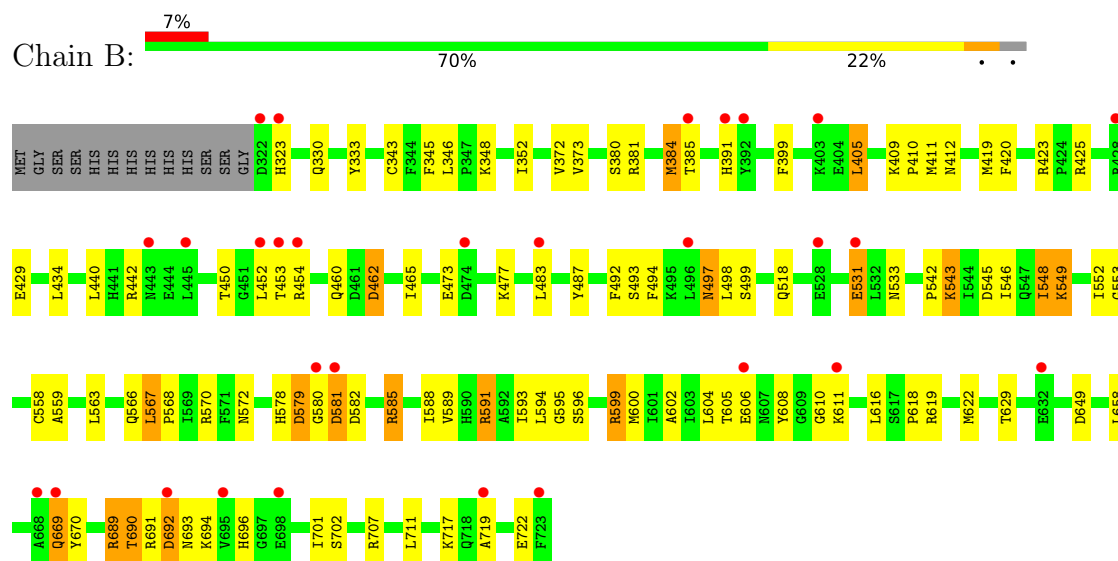
3 Residue-property plots

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.

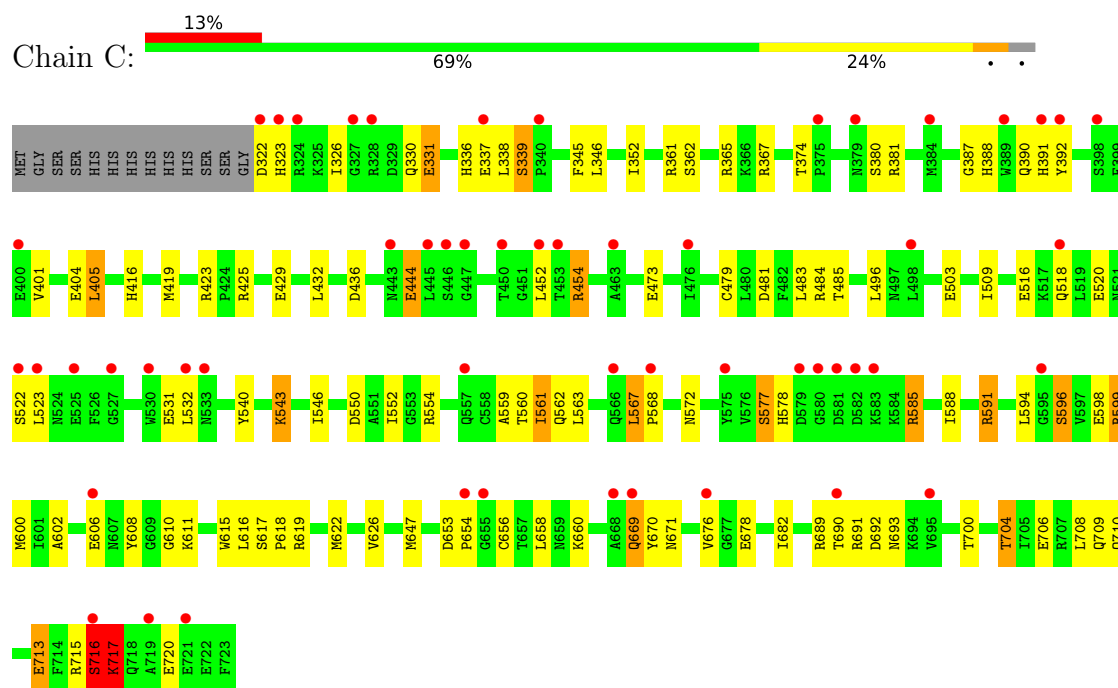
- Molecule 1: Threonine-tRNA ligase, cytoplasmic



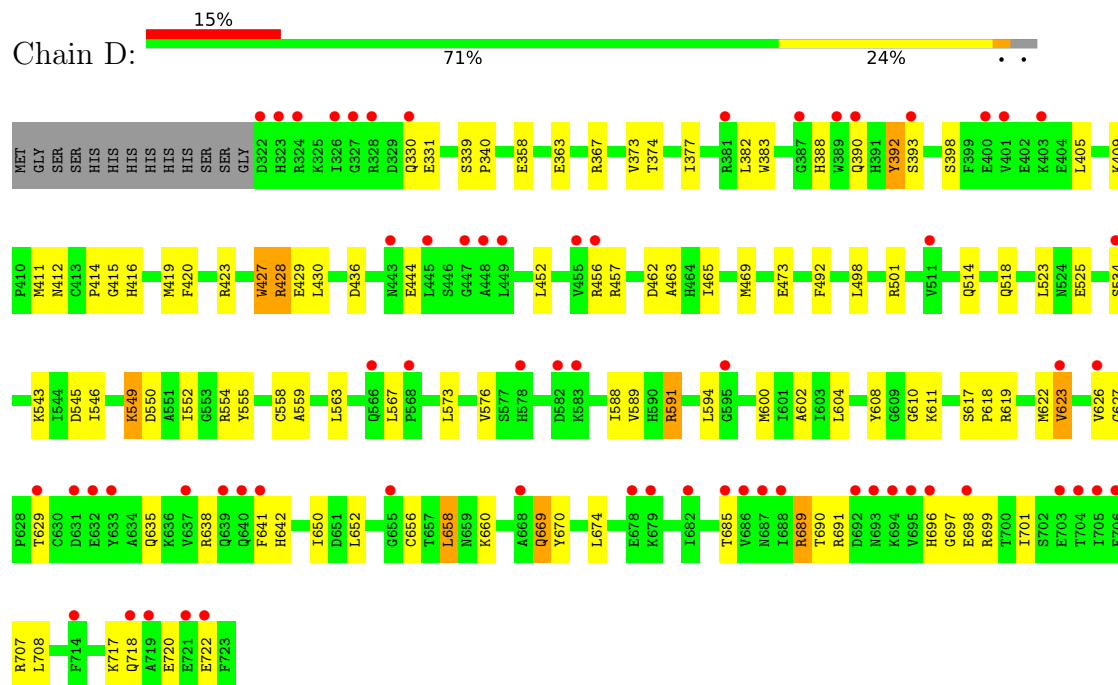
- Molecule 1: Threonine-tRNA ligase, cytoplasmic



- Molecule 1: Threonine-tRNA ligase, cytoplasmic



- Molecule 1: Threonine-tRNA ligase, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.87Å 78.00Å 118.05Å 86.99° 83.32° 84.39°	Depositor
Resolution (Å)	47.71 – 2.60 47.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.71-2.60) 95.8 (47.71-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.228 , 0.255 0.229 , 0.257	Depositor DCC
R_{free} test set	3365 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.802	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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: 2CR, ZN

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	0.45	0/3343	0.79	3/4520 (0.1%)
1	B	0.61	1/3336 (0.0%)	0.82	3/4510 (0.1%)
1	C	0.60	1/3332 (0.0%)	0.84	2/4507 (0.0%)
1	D	0.56	2/3294 (0.1%)	0.87	6/4459 (0.1%)
All	All	0.56	4/13305 (0.0%)	0.83	14/17996 (0.1%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	561	ILE	C-O	-5.43	1.18	1.24
1	D	427	TRP	CA-C	-5.40	1.45	1.53
1	B	462	ASP	C-O	-5.13	1.18	1.24
1	D	462	ASP	C-O	-5.01	1.17	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	427	TRP	N-CA-C	-9.70	97.73	110.53
1	B	692	ASP	N-CA-C	9.22	124.79	113.17
1	C	716	SER	N-CA-C	8.41	120.06	111.07
1	B	391	HIS	N-CA-C	6.46	120.78	113.02
1	C	626	VAL	N-CA-C	5.94	116.12	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	PHE	N-CA-C	5.68	117.92	108.99
1	D	627	GLY	CA-C-N	5.52	125.61	119.32
1	D	627	GLY	C-N-CA	5.52	125.61	119.32
1	A	501	ARG	CA-C-N	5.36	125.34	120.03
1	A	501	ARG	C-N-CA	5.36	125.34	120.03
1	D	501	ARG	CA-C-N	5.30	125.77	120.52
1	D	501	ARG	C-N-CA	5.30	125.77	120.52
1	B	543	LYS	N-CA-C	5.18	117.12	108.99
1	D	697	GLY	N-CA-C	5.14	121.83	112.58

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	73	0
1	B	3253	0	3105	81	0
1	C	3249	0	3091	78	0
1	D	3211	0	3036	74	0
2	A	35	0	42	5	0
2	B	35	0	42	1	0
2	C	35	0	42	5	0
2	D	35	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	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	298	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 (298) 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:HH21	1:A:689:ARG:HG3	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:HG3	1:A:689:ARG:NH2	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
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:D:429:GLU:C	1:D:430:LEU:HD23	2.07	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:B:581:ASP:OD2	1:B:581:ASP:C	2.30	0.75
1:B:409:LYS:NZ	1:B:412:ASN:OD1	2.16	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:PHE:HE2	1:B:600:MET:HE1	1.57	0.69
1:D:611:LYS:HA	1:D:669:GLN:HG2	1.76	0.68
1:B:497:ASN:C	1:B:497:ASN:ND2	2.51	0.68
1:A:330:GLN:HG2	1:A:619:ARG:NH1	2.08	0.68
1:A:394:GLU:C	1:A:395:ASN:HD22	2.02	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:B:497:ASN:C	1:B:497:ASN:HD22	2.03	0.66
1:A:641:PHE:HE1	1:A:708:LEU:HD12	1.60	0.65
1:B:497:ASN:ND2	1:B:497:ASN:O	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
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:579:ASP:OD2	1:B:579:ASP:N	2.30	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: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:600:MET:HE3	1:B:604:LEU:HG	1.81	0.61
1:D:641:PHE:HE1	1:D:708:LEU:HD12	1.65	0.61
1:D:550:ASP:C	1:D:550:ASP:OD1	2.42	0.60
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: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:330:GLN:O	1:B:619:ARG:NH2	2.36	0.58
1:B:452:LEU:HB2	1:B:602:ALA:HB2	1.84	0.58
1:A:591:ARG:HG3	1:A:591:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:608:TYR:HB3	1:C:611:LYS:O	2.04	0.58
1:A:599:ARG:NH1	1:A:599:ARG:HG2	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:373:VAL:HB	1:B:345:PHE:HB2	1.87	0.57
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.05	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:381:ARG:HA	1:B:384:MET:HE2	1.86	0.56
1:B:563:LEU:HD22	1:B:589:VAL:HG22	1.88	0.56
1:B:572:ASN:OD1	1:B:585:ARG:NH2	2.34	0.56
1:D:388:HIS:NE2	1:D:411:MET:HE2	2.20	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:626:VAL:HG12	1:D:658:LEU:HD11	1.87	0.55
1:D:492:PHE:HE2	1:D:600:MET:HE1	1.71	0.55
1:C:656:CYS:HB3	1:C:660:LYS:HD3	1.89	0.55
1:B:600:MET:HE3	1:B:604:LEU:CG	2.35	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:A:346:LEU:HD23	1:B:419:MET:HE3	1.90	0.54
1:B:352:ILE:HG23	1:B:616:LEU:HD22	1.89	0.54
1:C:540:TYR:OH	2:C:800:2CR:O34	2.20	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:B:372:VAL:HG11	1:B:419:MET:HE1	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:395:ASN:N	1:A:395:ASN:ND2	2.31	0.53
1:C:700:THR:O	1:C:704:THR:HG23	2.06	0.52
1:C:484:ARG:HG2	1:C:484:ARG:HH11	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:A:419:MET:HE2	1:B:346:LEU:HD23	1.91	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:B:693:ASN:CG	1:B:693:ASN:O	2.54	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
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:591:ARG:C	1:C:591:ARG:HH11	2.21	0.48
1:C:387:GLY:HA2	1:C:390:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:HD12	1:B:460:GLN:HE21	1.78	0.48
1:B:549:LYS:HB3	1:B:549:LYS:HE3	1.41	0.48
1:D:416:HIS:HE2	1:D:436:ASP:HB2	1.78	0.48
1:A:470:GLU:CD	1:A:470:GLU:H	2.20	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:345:PHE:HB2	1:B:373:VAL:HB	1.97	0.47
1:A:613:PRO:HG2	1:A:616:LEU:HB2	1.95	0.47
1:B:707:ARG:NH2	1:B:722:GLU:O	2.46	0.47
1:D:416:HIS:CE1	1:D:436:ASP:HB2	2.49	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
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:HH11	1:A:599:ARG:CG	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
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:B:419:MET:HE2	1:B:419:MET:HB3	1.75	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:HG2	1:A:599:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:388:HIS:O	1:D:392:TYR:N	2.42	0.44
1:D:549:LYS:HZ3	1:D:549:LYS:HG2	1.63	0.43
1:D:670:TYR:O	1:D:691:ARG:HB2	2.17	0.43
2:D:800:2CR:H35	2:D:800:2CR:H42	1.61	0.43
1:A:599:ARG:NH1	1:A:599:ARG:CG	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
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:OD2	1:A:579:ASP:N	2.40	0.42
1:C:338:LEU:HD13	1:D:382:LEU:HB2	2.00	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:374:THR:OG1	1:C:436:ASP:OD2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:THR:OG1	1:D:698:GLU:OE2	2.21	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:HD23	1:D:652:LEU:HA	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: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:D:411:MET:HE1	2:D:800:2CR:C9	2.50	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:HE	1:D:689:ARG:HB2	1.45	0.42
1:C:367:ARG:NH2	1:C:481:ASP:OD2	2.47	0.41
1:D:591:ARG:NH1	1:D:591:ARG:C	2.77	0.41
1:C:346:LEU:HD23	1:D:419:MET:HE2	2.01	0.41
1:C:361:ARG:O	1:C:365:ARG:HG3	2.20	0.41
1:C:567:LEU:HD12	1:C:567:LEU:HA	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
1:C:552:ILE:HD12	1:C:552:ILE:HA	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:565:PHE:C	1:A:568:PRO:HD2	2.45	0.41
1:D:469:MET:HE2	1:D:514:GLN:HB3	2.03	0.41
1:A:465:ILE:HB	1:A:589:VAL:HB	2.03	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:591:ARG:NH2	1:A:593:ILE:HG13	2.35	0.41
1:B:409:LYS:HA	1:B:410:PRO:HD2	1.94	0.41
1:B:548:ILE:HD13	1:B:548:ILE:HA	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:693:ASN:OD1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	312 (91%)	30 (9%)	9	21
1	B	339/368 (92%)	312 (92%)	27 (8%)	11	25
1	C	338/368 (92%)	305 (90%)	33 (10%)	7	17
1	D	328/368 (89%)	301 (92%)	27 (8%)	10	24
All	All	1347/1472 (92%)	1230 (91%)	117 (9%)	9	21

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	GLU
1	A	337	GLU
1	A	390	GLN
1	A	395	ASN
1	A	401	VAL
1	A	429	GLU
1	A	432	LEU
1	A	444	GLU
1	A	450	THR
1	A	477	LYS
1	A	493	SER
1	A	498	LEU
1	A	506	LEU
1	A	509	ILE
1	A	522	SER
1	A	532	LEU
1	A	546	ILE
1	A	552	ILE
1	A	579	ASP
1	A	585	ARG
1	A	599	ARG
1	A	622	MET
1	A	629	THR
1	A	635	GLN

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Mol	Chain	Res	Type
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	405	LEU
1	B	434	LEU
1	B	453	THR
1	B	477	LYS
1	B	497	ASN
1	B	498	LEU
1	B	531	GLU
1	B	548	ILE
1	B	549	LYS
1	B	552	ILE
1	B	558	CYS
1	B	567	LEU
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
1	B	701	ILE
1	B	702	SER
1	B	717	LYS
1	C	331	GLU
1	C	339	SER
1	C	380	SER
1	C	401	VAL
1	C	405	LEU
1	C	432	LEU
1	C	444	GLU
1	C	454	ARG
1	C	485	THR

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Mol	Chain	Res	Type
1	C	496	LEU
1	C	503	GLU
1	C	509	ILE
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	585	ARG
1	C	591	ARG
1	C	596	SER
1	C	599	ARG
1	C	622	MET
1	C	647	MET
1	C	658	LEU
1	C	669	GLN
1	C	676	VAL
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
1	D	398	SER
1	D	405	LEU
1	D	428	ARG
1	D	444	GLU
1	D	457	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	591	ARG
1	D	622	MET

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	HIS
1	A	395	ASN
1	A	460	GLN
1	A	497	ASN
1	A	533	ASN
1	A	669	GLN
1	B	422	HIS
1	B	460	GLN
1	B	497	ASN
1	B	518	GLN
1	B	666	GLN
1	B	709	GLN
1	B	710	GLN
1	C	497	ASN
1	C	547	GLN
1	C	710	GLN
1	D	441	HIS
1	D	547	GLN
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 [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	2CR	D	800	-	35,36,36	2.99	6 (17%)	39,49,49	1.83	8 (20%)
2	2CR	A	800	-	35,36,36	3.09	9 (25%)	39,49,49	2.22	13 (33%)
2	2CR	C	800	-	35,36,36	2.92	5 (14%)	39,49,49	1.72	7 (17%)
2	2CR	B	800	-	35,36,36	2.89	10 (28%)	39,49,49	1.97	11 (28%)

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	D	800	-	-	6/47/59/59	0/1/2/2
2	2CR	A	800	-	-	9/47/59/59	0/1/2/2
2	2CR	C	800	-	-	7/47/59/59	0/1/2/2
2	2CR	B	800	-	-	5/47/59/59	0/1/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	2CR	C12-C11	-15.73	1.25	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	2CR	C12-C11	-15.55	1.25	1.43
2	C	800	2CR	C12-C11	-15.02	1.25	1.43
2	B	800	2CR	C12-C11	-14.17	1.26	1.43
2	A	800	2CR	O29-C6	-4.23	1.38	1.46
2	C	800	2CR	O29-C6	-4.05	1.39	1.46
2	B	800	2CR	O29-C6	-3.80	1.39	1.46
2	D	800	2CR	O29-C6	-3.52	1.40	1.46
2	B	800	2CR	C2-C30	-2.90	1.46	1.51
2	B	800	2CR	C22-C23	-2.76	1.49	1.54
2	D	800	2CR	O29-C27	2.69	1.41	1.34
2	B	800	2CR	O29-C27	2.67	1.41	1.34
2	A	800	2CR	C26-C25	-2.65	1.49	1.53
2	B	800	2CR	O31-C30	-2.65	1.22	1.30
2	C	800	2CR	O29-C27	2.64	1.41	1.34
2	B	800	2CR	C3-C2	-2.58	1.49	1.54
2	A	800	2CR	O29-C27	2.56	1.41	1.34
2	A	800	2CR	C2-C1	-2.51	1.48	1.54
2	D	800	2CR	C16-C14	-2.45	1.50	1.54
2	A	800	2CR	C3-C2	-2.44	1.49	1.54
2	A	800	2CR	C22-C23	-2.42	1.50	1.54
2	D	800	2CR	O31-C30	-2.41	1.23	1.30
2	C	800	2CR	C23-C25	-2.36	1.50	1.53
2	A	800	2CR	O31-C30	-2.34	1.23	1.30
2	A	800	2CR	C2-C30	-2.34	1.47	1.51
2	C	800	2CR	O31-C30	-2.30	1.23	1.30
2	B	800	2CR	C26-C25	-2.28	1.49	1.53
2	B	800	2CR	C2-C1	-2.24	1.49	1.54
2	D	800	2CR	C22-C23	-2.14	1.50	1.54
2	B	800	2CR	C23-C25	-2.04	1.50	1.53

All (39) 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	A	800	2CR	C9-C10-C11	5.60	136.49	127.04
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	B	800	2CR	C9-C10-C11	4.82	135.19	127.04
2	C	800	2CR	O29-C27-C26	4.48	119.47	111.43
2	D	800	2CR	O29-C27-C26	4.13	118.83	111.43
2	D	800	2CR	C5-C1-C2	4.09	108.72	103.97
2	C	800	2CR	C10-C9-C8	-4.08	114.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	2CR	C9-C10-C11	3.77	133.41	127.04
2	B	800	2CR	C10-C11-C12	3.77	129.66	122.08
2	D	800	2CR	C9-C10-C11	3.74	133.35	127.04
2	A	800	2CR	C5-C1-C2	3.71	108.28	103.97
2	B	800	2CR	O29-C27-C26	3.70	118.07	111.43
2	A	800	2CR	C24-C23-C22	-3.35	105.61	110.68
2	B	800	2CR	C5-C1-C2	3.23	107.72	103.97
2	B	800	2CR	C14-C16-C17	-3.20	108.64	116.59
2	A	800	2CR	C24-C23-C25	-3.14	107.52	111.61
2	A	800	2CR	C10-C11-C12	3.14	128.40	122.08
2	C	800	2CR	C24-C23-C25	-3.13	107.54	111.61
2	A	800	2CR	O29-C27-C26	3.09	116.96	111.43
2	D	800	2CR	C14-C16-C17	-3.08	108.92	116.59
2	A	800	2CR	C14-C16-C17	-3.02	109.08	116.59
2	D	800	2CR	O29-C6-C7	3.00	112.51	107.45
2	A	800	2CR	O32-C30-C2	-2.93	116.08	123.01
2	B	800	2CR	C24-C23-C22	-2.90	106.29	110.68
2	A	800	2CR	C25-C26-C27	-2.59	108.34	114.02
2	C	800	2CR	C5-C1-C2	2.45	106.82	103.97
2	B	800	2CR	C3-C2-C30	-2.42	106.87	112.52
2	C	800	2CR	C10-C11-C12	2.38	126.87	122.08
2	A	800	2CR	C11-C12-N35	-2.37	174.81	177.87
2	A	800	2CR	O29-C6-C7	2.37	111.45	107.45
2	D	800	2CR	C10-C11-C12	2.34	126.78	122.08
2	A	800	2CR	O31-C30-C2	2.26	119.79	113.93
2	D	800	2CR	C24-C23-C22	-2.25	107.27	110.68
2	C	800	2CR	C14-C16-C17	-2.23	111.03	116.59
2	B	800	2CR	C24-C23-C25	-2.22	108.72	111.61
2	B	800	2CR	C3-C2-C1	2.05	106.99	103.63
2	B	800	2CR	O32-C30-C2	-2.02	118.23	123.01

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C	800	2CR	C22-C23-C25-C26
2	C	800	2CR	C22-C23-C25-O34
2	C	800	2CR	C24-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
2	C	800	2CR	C24-C23-C25-O34
2	D	800	2CR	C11-C13-C14-C16
2	A	800	2CR	C1-C6-C7-C8
2	B	800	2CR	C1-C6-C7-C8
2	C	800	2CR	C1-C6-C7-C8
2	D	800	2CR	C1-C6-C7-C8
2	A	800	2CR	O29-C6-C7-C8
2	B	800	2CR	O29-C6-C7-C8
2	B	800	2CR	C22-C23-C25-C26
2	C	800	2CR	O29-C6-C7-C8
2	D	800	2CR	O29-C6-C7-C8
2	B	800	2CR	C20-C22-C23-C25
2	D	800	2CR	C15-C14-C16-C17
2	D	800	2CR	C1-C2-C30-O31
2	D	800	2CR	C1-C2-C30-O32
2	A	800	2CR	C15-C14-C16-C17
2	A	800	2CR	C20-C22-C23-C24
2	B	800	2CR	C17-C19-C20-C21
2	C	800	2CR	C3-C2-C30-O31
2	A	800	2CR	C20-C22-C23-C25

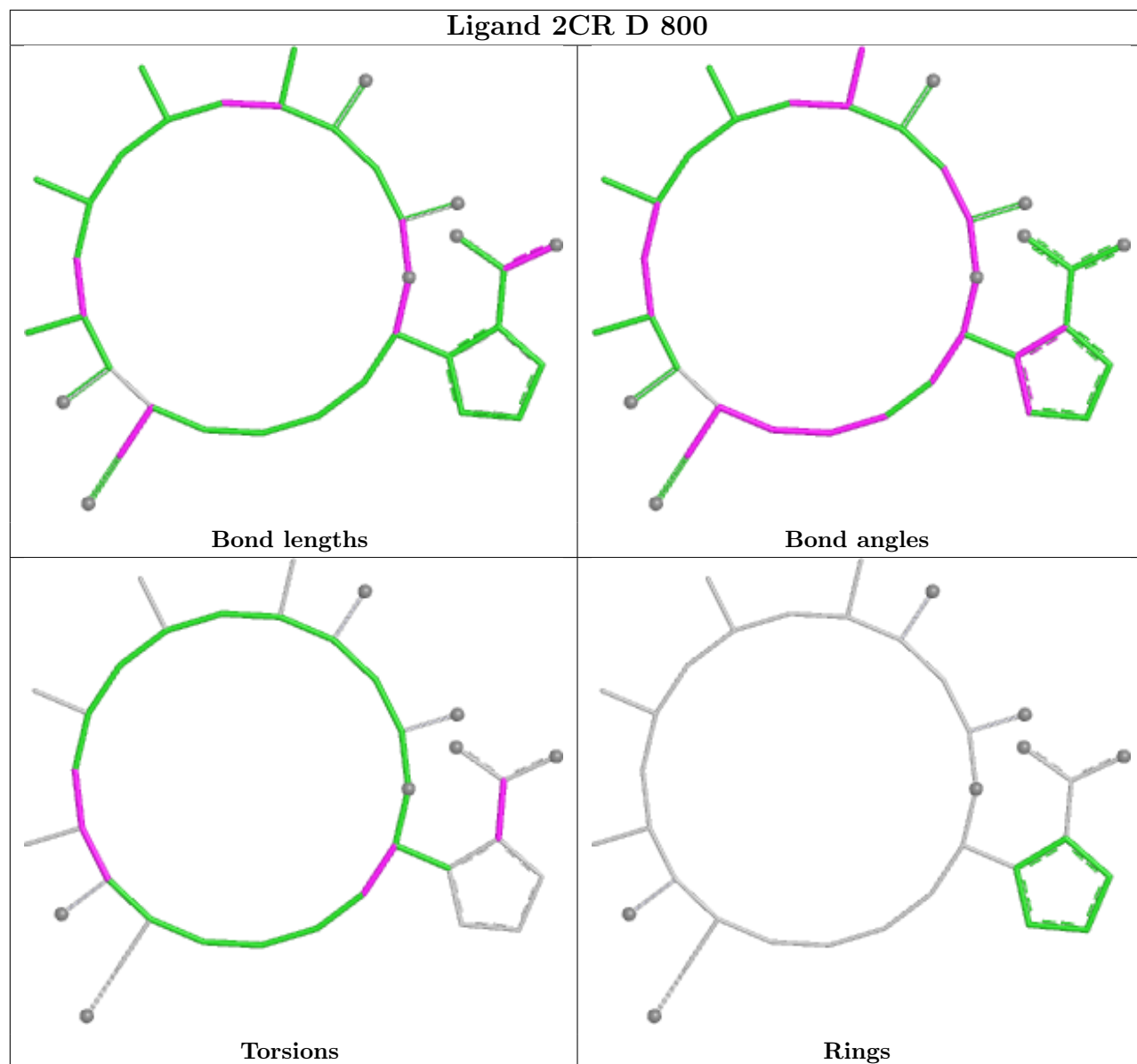
There are no ring outliers.

4 monomers are involved in 13 short contacts:

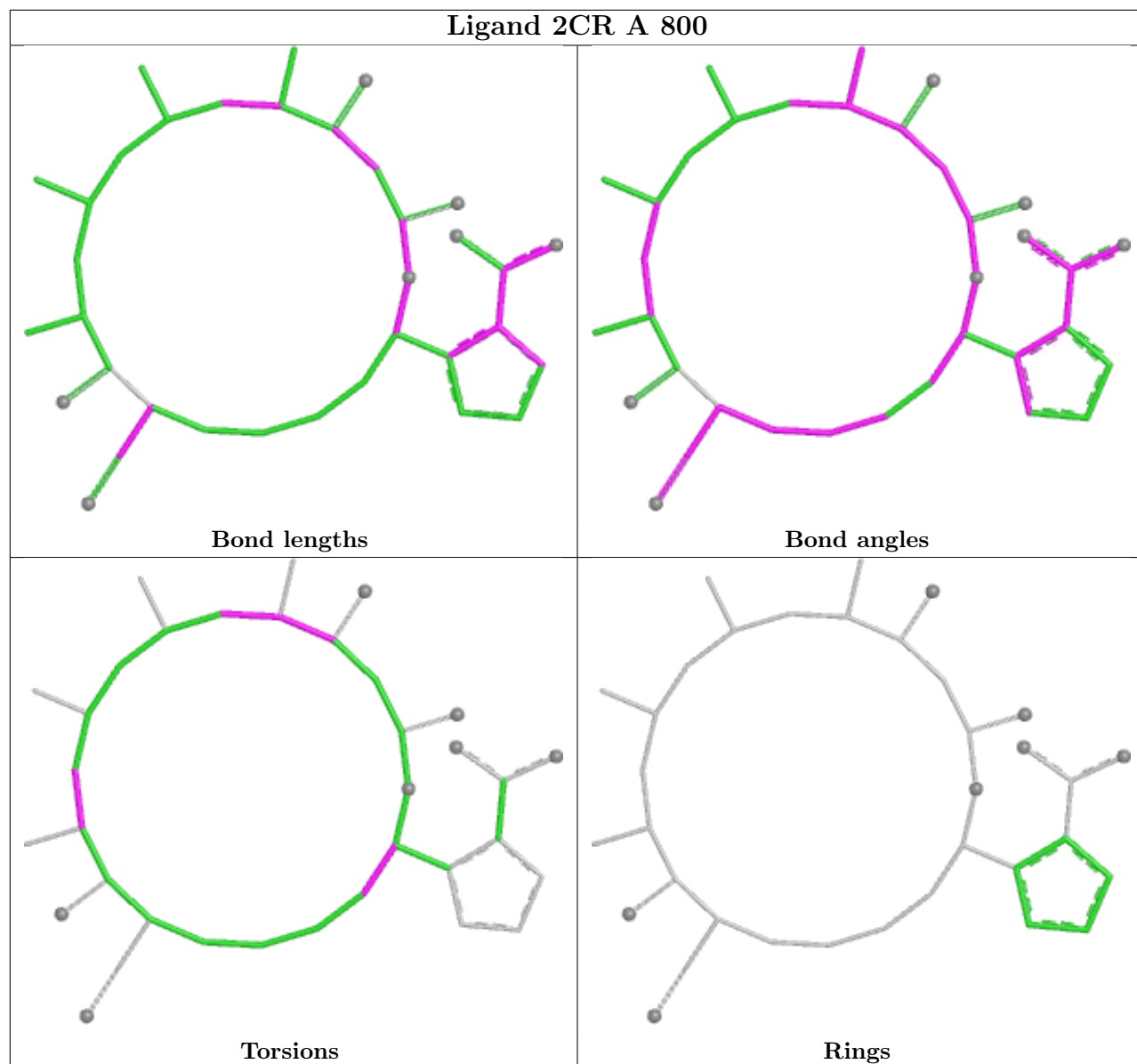
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	800	2CR	2	0
2	A	800	2CR	5	0
2	C	800	2CR	5	0
2	B	800	2CR	1	0

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.

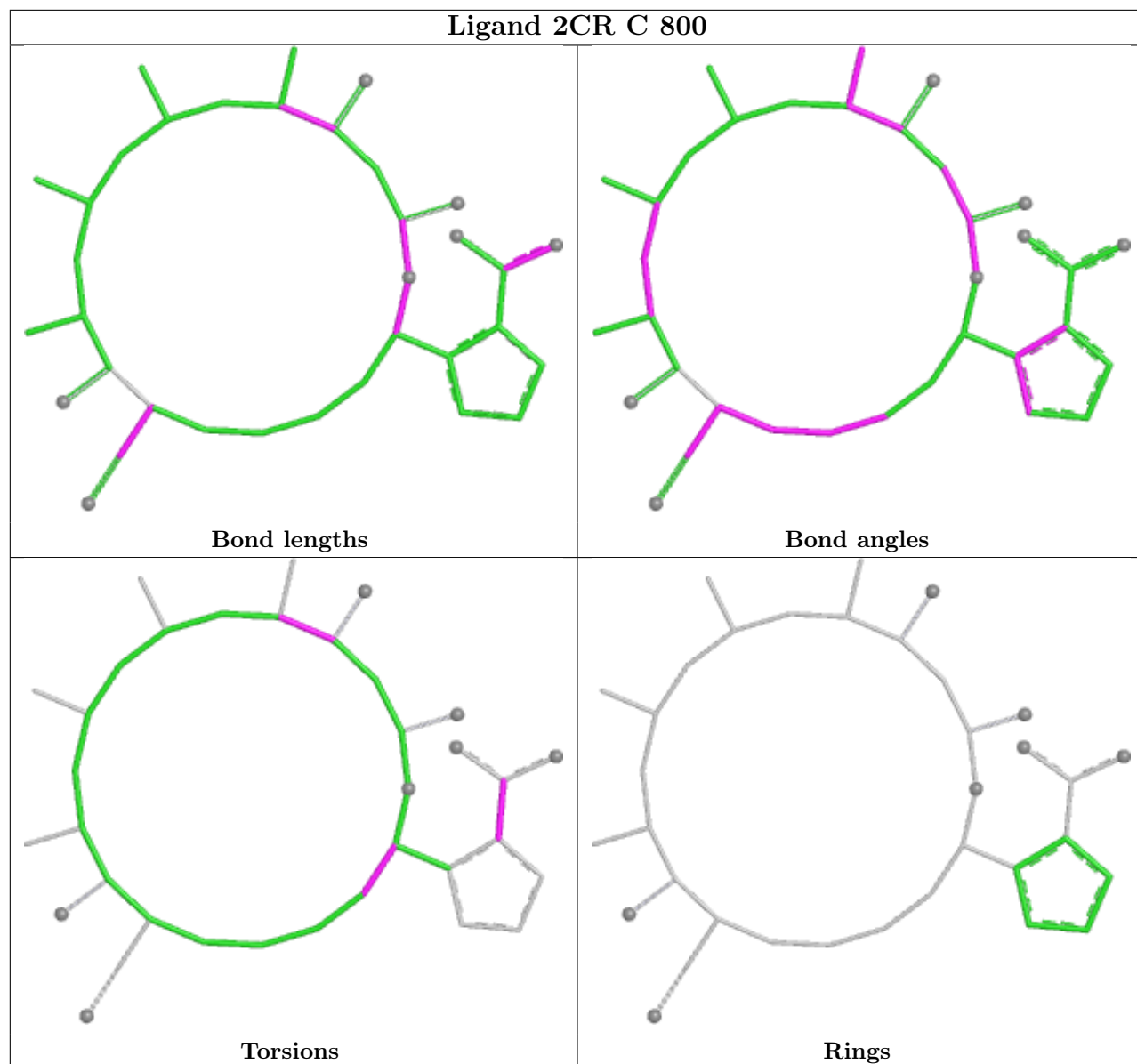
Ligand 2CR D 800

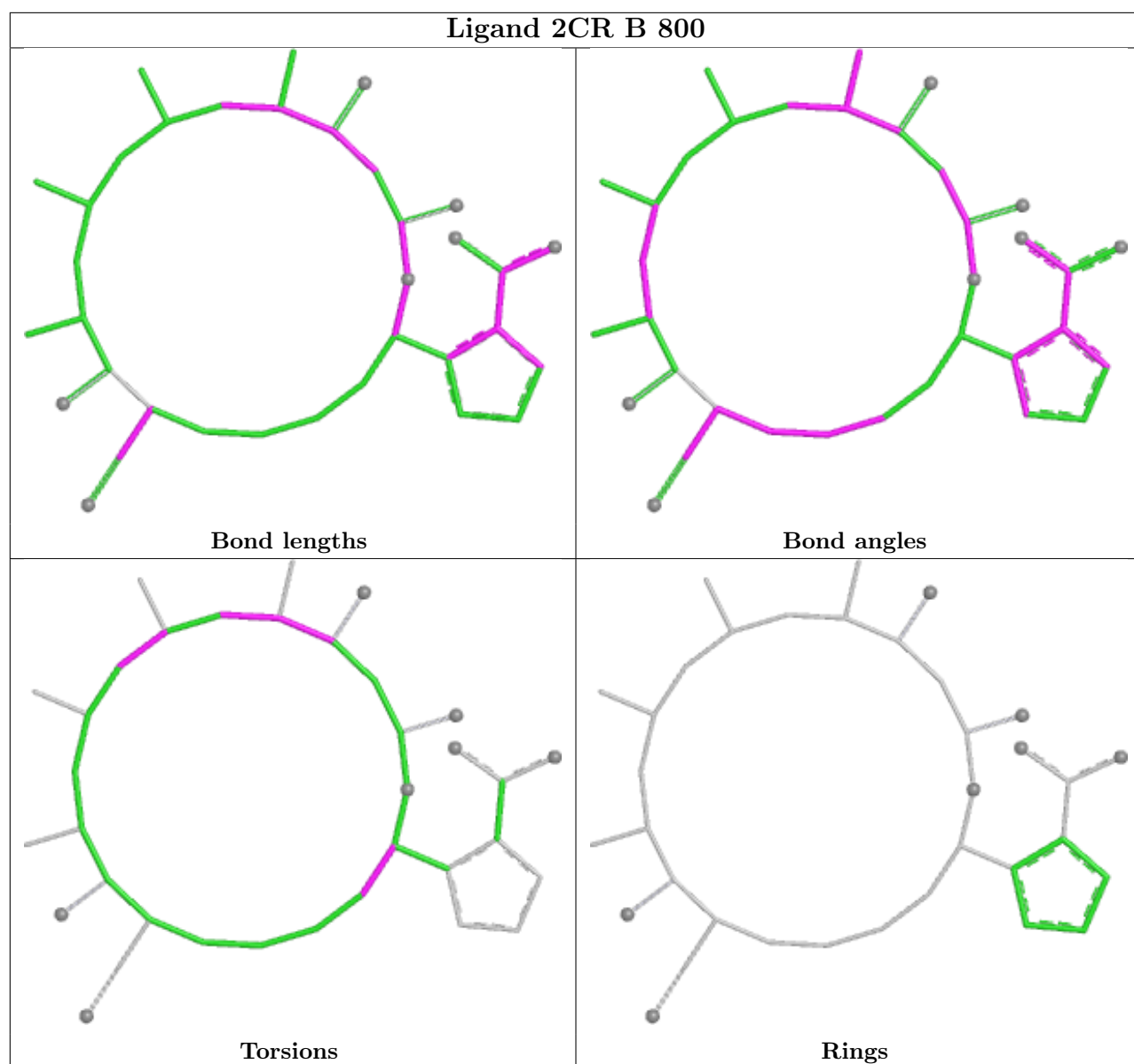


Ligand 2CR A 800



Ligand 2CR C 800





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, 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	402/415 (96%)	0.85	28 (6%) 22 18	33, 51, 74, 95	0
1	B	402/415 (96%)	0.86	29 (7%) 21 17	35, 53, 72, 97	0
1	C	402/415 (96%)	1.07	54 (13%) 7 5	35, 58, 84, 100	0
1	D	402/415 (96%)	1.21	64 (15%) 5 4	36, 56, 89, 104	0
All	All	1608/1660 (96%)	1.00	175 (10%) 10 8	33, 54, 84, 104	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	322	ASP	4.8
1	D	679	LYS	4.5
1	D	322	ASP	4.4
1	A	328	ARG	4.3
1	A	323	HIS	4.3
1	C	323	HIS	3.9
1	C	450	THR	3.7
1	D	389	TRP	3.7
1	D	688	ILE	3.6
1	C	445	LEU	3.6
1	D	403	LYS	3.5
1	D	328	ARG	3.5
1	A	322	ASP	3.4
1	C	327	GLY	3.4
1	D	323	HIS	3.4
1	D	695	VAL	3.4
1	C	463	ALA	3.4
1	D	692	ASP	3.4
1	D	578	HIS	3.3
1	A	684	GLY	3.3
1	A	713	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	669	GLN	3.3
1	C	453	THR	3.2
1	D	703	GLU	3.2
1	B	385	THR	3.2
1	D	678	GLU	3.2
1	C	668	ALA	3.1
1	C	532	LEU	3.1
1	A	326	ILE	3.1
1	A	335	PHE	3.1
1	C	324	ARG	3.1
1	A	579	ASP	3.0
1	C	582	ASP	3.0
1	D	448	ALA	3.0
1	C	389	TRP	2.9
1	D	704	THR	2.9
1	C	583	LYS	2.9
1	A	324	ARG	2.9
1	D	631	ASP	2.9
1	C	654	PRO	2.8
1	C	655	GLY	2.8
1	A	714	PHE	2.8
1	C	398	SER	2.8
1	D	534	SER	2.8
1	A	578	HIS	2.8
1	B	453	THR	2.8
1	C	328	ARG	2.8
1	D	443	ASN	2.7
1	D	706	GLU	2.7
1	D	568	PRO	2.7
1	A	606	GLU	2.7
1	D	632	GLU	2.7
1	D	626	VAL	2.7
1	D	682	ILE	2.7
1	B	581	ASP	2.7
1	D	633	TYR	2.7
1	D	698	GLU	2.7
1	D	714	PHE	2.7
1	D	390	GLN	2.6
1	D	456	ARG	2.6
1	D	400	GLU	2.6
1	D	655	GLY	2.6
1	D	583	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	687	ASN	2.6
1	B	695	VAL	2.6
1	D	685	THR	2.6
1	B	323	HIS	2.6
1	C	669	GLN	2.6
1	C	579	ASP	2.6
1	B	528	GLU	2.6
1	C	566	GLN	2.6
1	C	498	LEU	2.6
1	D	447	GLY	2.5
1	D	693	ASN	2.5
1	D	694	LYS	2.5
1	C	379	ASN	2.5
1	A	444	GLU	2.5
1	C	568	PRO	2.5
1	D	511	VAL	2.5
1	A	641	PHE	2.5
1	D	719	ALA	2.5
1	B	391	HIS	2.5
1	B	698	GLU	2.5
1	B	496	LEU	2.4
1	D	445	LEU	2.4
1	A	331	GLU	2.4
1	D	324	ARG	2.4
1	A	483	LEU	2.4
1	D	641	PHE	2.4
1	C	391	HIS	2.4
1	C	446	SER	2.4
1	D	393	SER	2.4
1	C	322	ASP	2.4
1	B	403	LYS	2.4
1	B	580	GLY	2.4
1	C	595	GLY	2.4
1	D	629	THR	2.4
1	C	400	GLU	2.4
1	C	525	GLU	2.4
1	D	387	GLY	2.4
1	A	445	LEU	2.3
1	A	682	ILE	2.3
1	C	447	GLY	2.3
1	D	623	VAL	2.3
1	B	452	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	705	ILE	2.3
1	A	700	THR	2.3
1	D	640	GLN	2.3
1	B	445	LEU	2.3
1	C	523	LEU	2.3
1	B	392	TYR	2.3
1	D	595	GLY	2.3
1	C	676	VAL	2.3
1	B	668	ALA	2.2
1	C	375	PRO	2.2
1	C	581	ASP	2.2
1	D	582	ASP	2.2
1	A	709	GLN	2.2
1	B	669	GLN	2.2
1	C	557	GLN	2.2
1	C	527	GLY	2.2
1	C	716	SER	2.2
1	C	452	LEU	2.2
1	C	392	TYR	2.2
1	B	692	ASP	2.2
1	D	637	VAL	2.2
1	D	686	VAL	2.2
1	D	326	ILE	2.2
1	D	696	HIS	2.2
1	D	381	ARG	2.2
1	C	340	PRO	2.2
1	C	533	ASN	2.2
1	C	518	GLN	2.2
1	A	325	LYS	2.2
1	C	522	SER	2.2
1	B	428	ARG	2.1
1	A	695	VAL	2.1
1	B	723	PHE	2.1
1	A	703	GLU	2.1
1	B	531	GLU	2.1
1	B	483	LEU	2.1
1	B	719	ALA	2.1
1	C	719	ALA	2.1
1	B	632	GLU	2.1
1	C	606	GLU	2.1
1	D	639	GLN	2.1
1	C	443	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	610	GLY	2.1
1	A	582	ASP	2.1
1	D	668	ALA	2.1
1	D	722	GLU	2.1
1	C	530	TRP	2.1
1	C	384	MET	2.1
1	C	575	TYR	2.1
1	D	401	VAL	2.1
1	B	474	ASP	2.0
1	B	606	GLU	2.0
1	D	721	GLU	2.0
1	B	611	LYS	2.0
1	D	330	GLN	2.0
1	D	449	LEU	2.0
1	D	566	GLN	2.0
1	D	718	GLN	2.0
1	C	476	ILE	2.0
1	C	580	GLY	2.0
1	D	327	GLY	2.0
1	C	695	VAL	2.0
1	D	455	VAL	2.0
1	C	337	GLU	2.0
1	C	721	GLU	2.0
1	A	683	SER	2.0
1	C	690	THR	2.0
1	A	642	HIS	2.0
1	B	443	ASN	2.0
1	B	454	ARG	2.0

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,

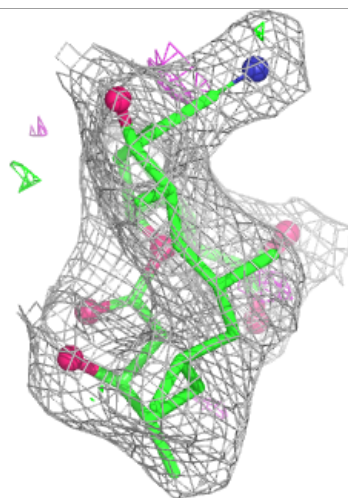
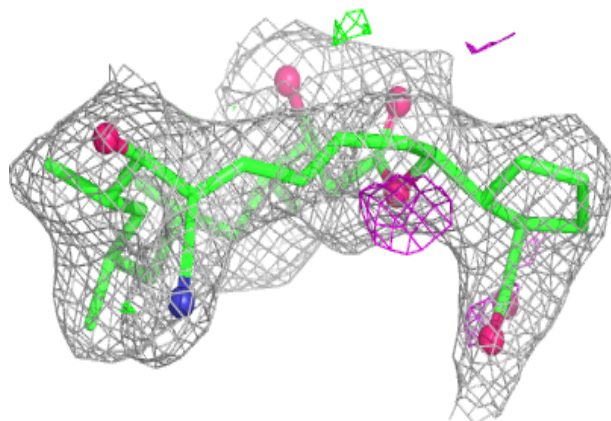
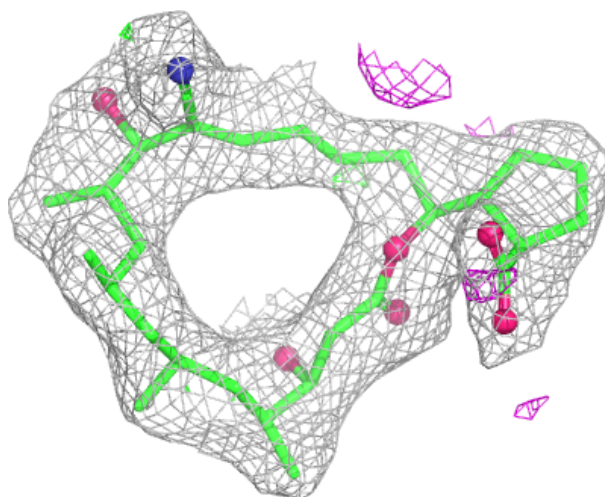
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	801	1/1	0.89	0.09	44,44,44,44	0
2	2CR	C	800	35/35	0.91	0.13	52,53,55,55	0
3	ZN	C	801	1/1	0.91	0.11	58,58,58,58	0
2	2CR	D	800	35/35	0.92	0.13	50,52,54,55	0
2	2CR	A	800	35/35	0.93	0.11	38,41,43,45	0
2	2CR	B	800	35/35	0.93	0.12	45,46,50,51	0
3	ZN	D	801	1/1	0.93	0.10	52,52,52,52	0
3	ZN	B	801	1/1	0.94	0.07	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.

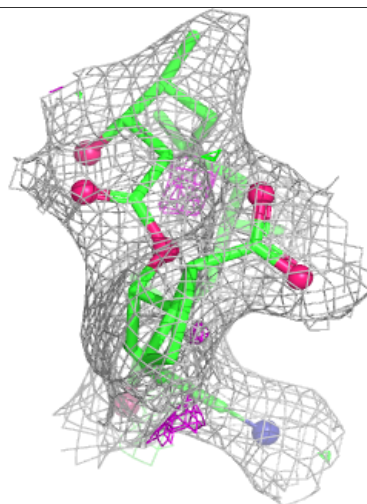
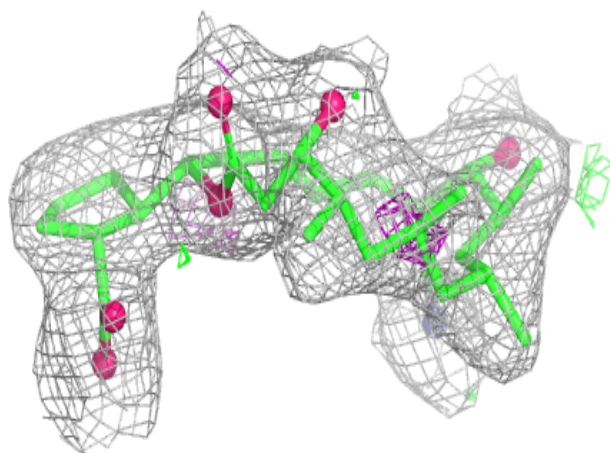
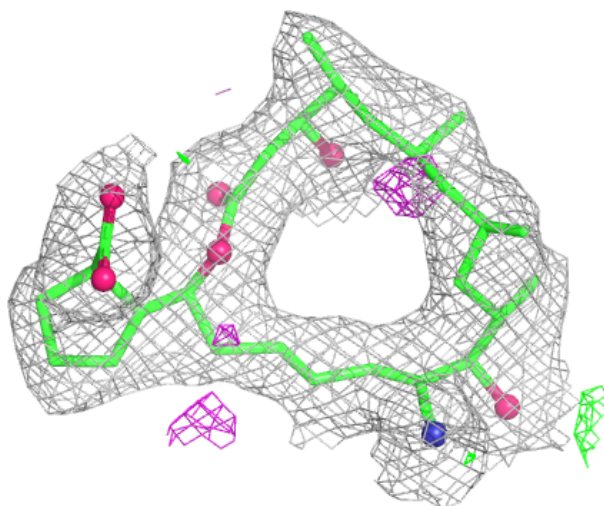
Electron density around 2CR C 800:

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



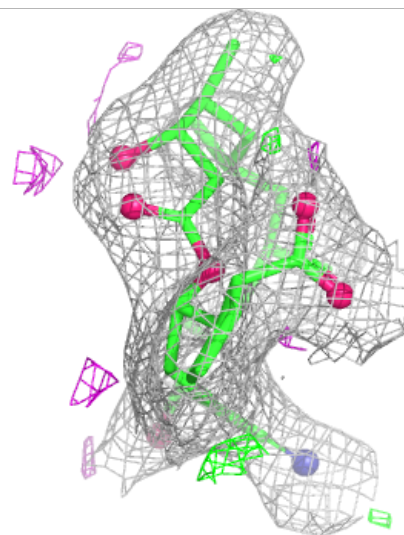
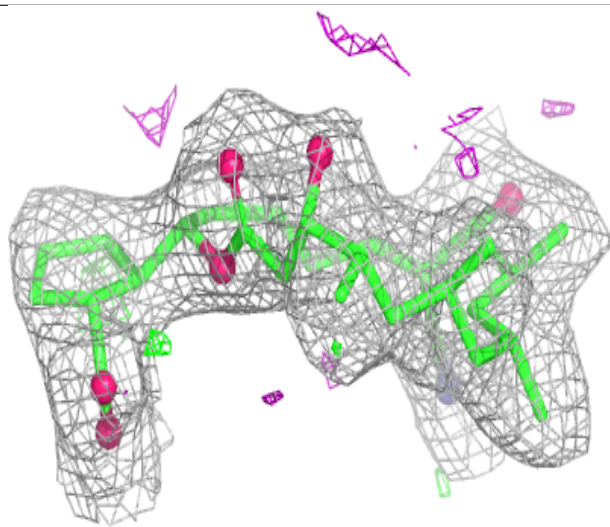
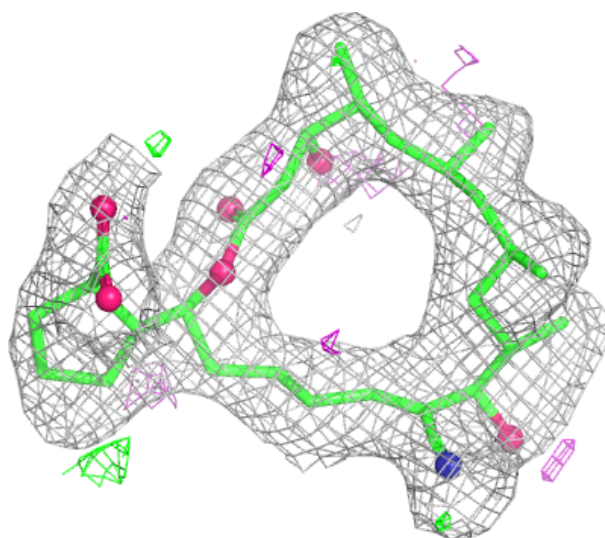
Electron density around 2CR D 800:

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



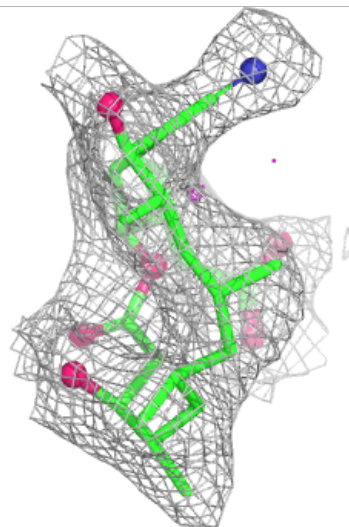
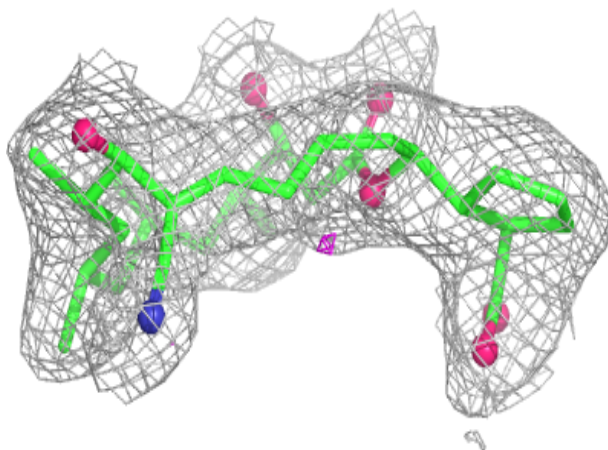
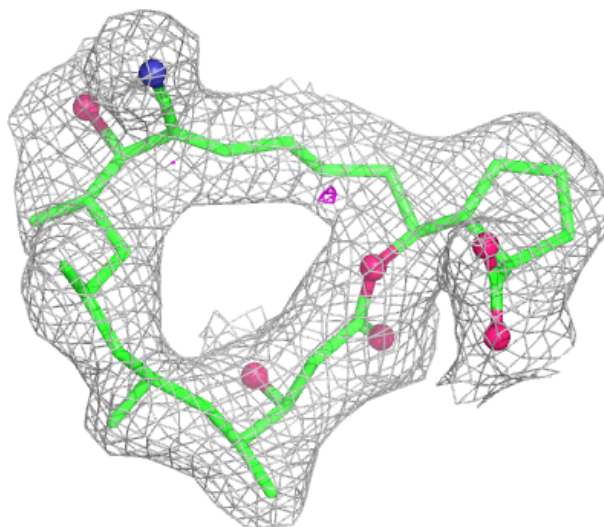
Electron density around 2CR A 800:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.