



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 01:30 pm BST

PDB ID : 9RVX / pdb_00009rvx
Title : Structure of CrtA with citrate
Authors : Hachmi, M.; Jacob-Dubuisson, F.; Arnoux, P.
Deposited on : 2025-07-09
Resolution : 2.29 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 : 1.8.4, CSD as541be (2020)
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

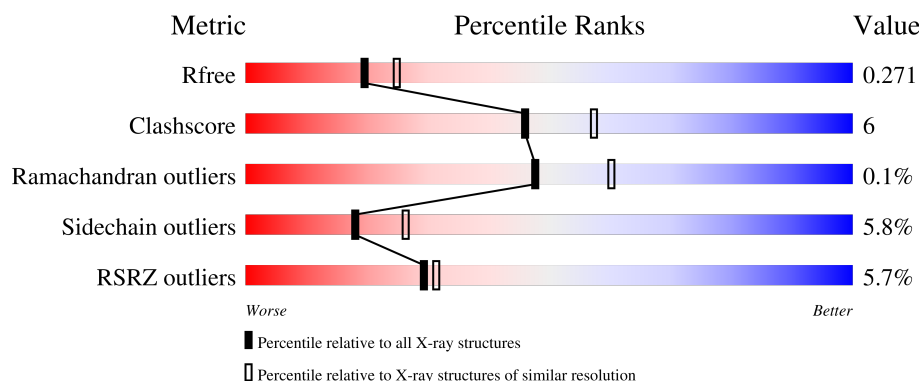
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	732	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	B	732	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 6%</div> </div> </div>

2 Entry composition [i](#)

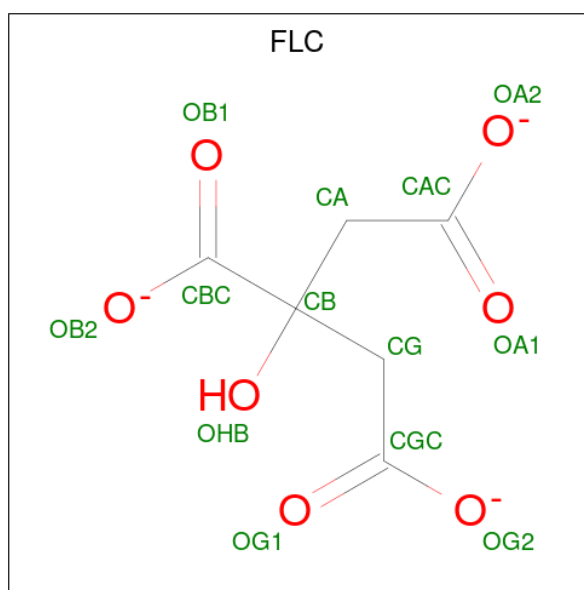
There are 3 unique types of molecules in this entry. The entry contains 10727 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TonB-dependent receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5287	3292	979	1012	4			
1	B	690	Total	C	N	O	S	0	0	0
			5310	3306	983	1017	4			

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

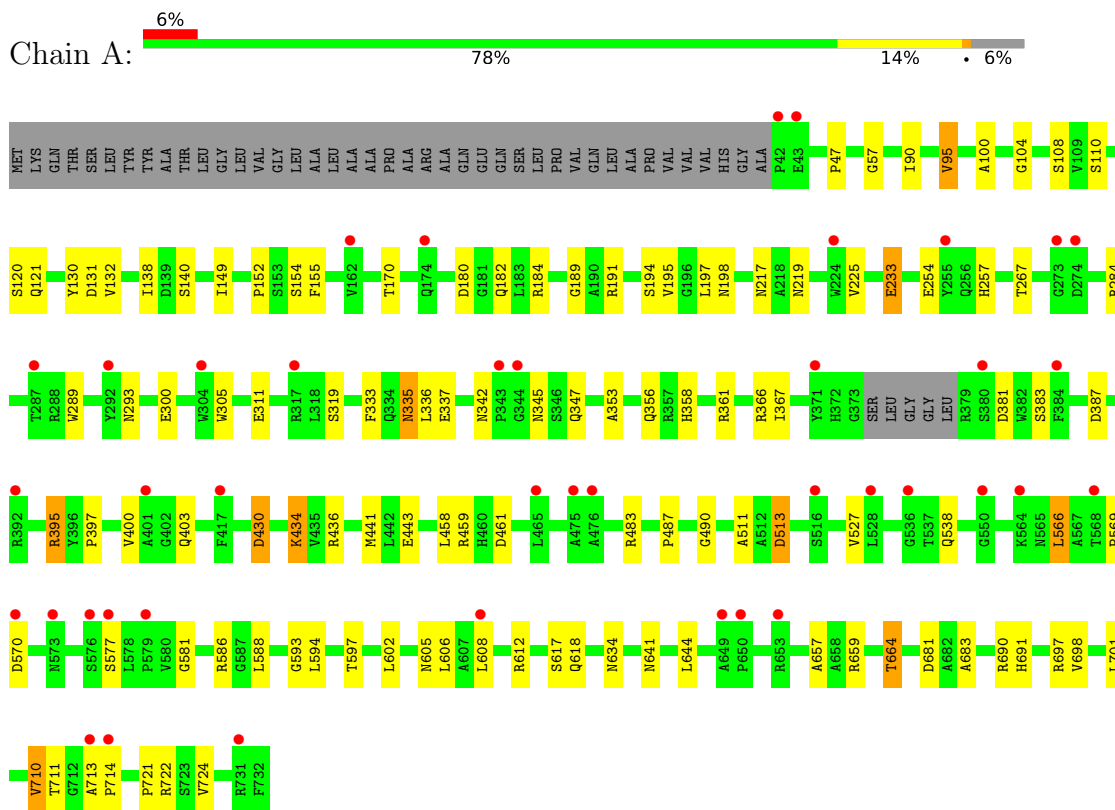
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total 46	O 46	0	0
3	B	58	Total 58	O 58	0	0

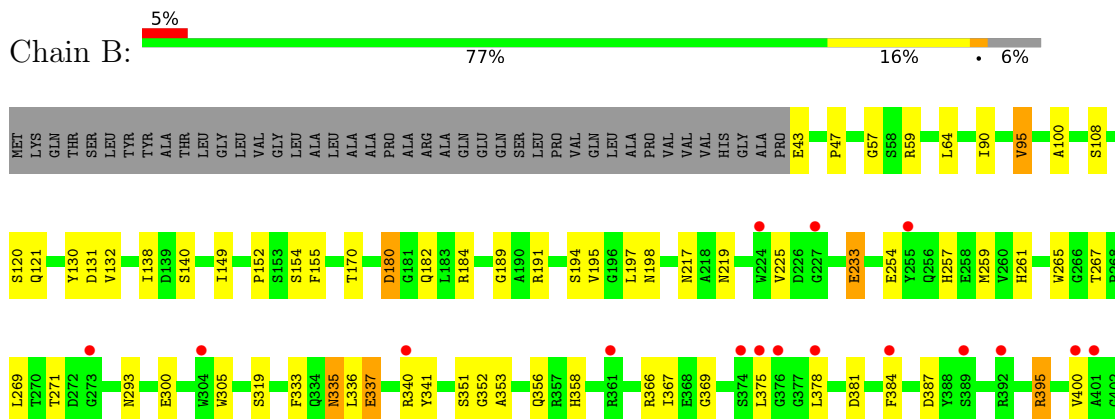
3 Residue-property plots [i](#)

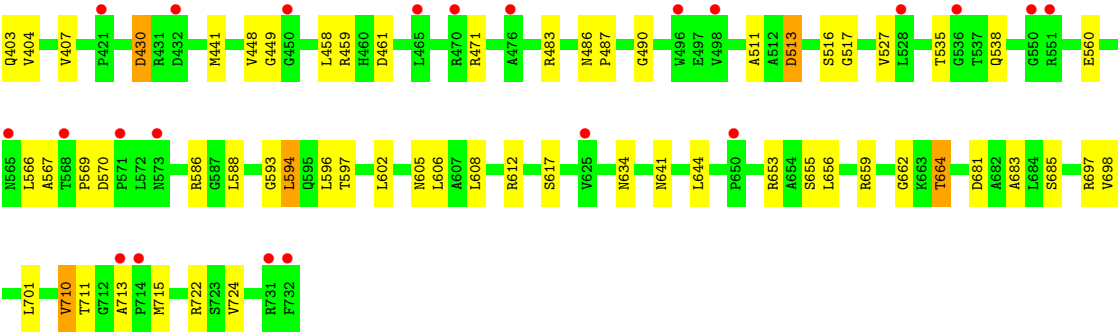
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: TonB-dependent receptor



• Molecule 1: TonB-dependent receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.14Å 67.90Å 102.52Å 89.27° 80.30° 68.56°	Depositor
Resolution (Å)	26.00 – 2.29 26.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	52.0 (26.00-2.29) 52.0 (26.00-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.234 , 0.272 0.225 , 0.271	Depositor DCC
R_{free} test set	1877 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.8	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	0.90	EDS
Total number of atoms	10727	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.69	0/5407	1.03	9/7362 (0.1%)
1	B	0.68	0/5430	1.03	17/7394 (0.2%)
All	All	0.68	0/10837	1.03	26/14756 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	TYR	CA-C-N	7.35	131.11	120.38
1	A	130	TYR	C-N-CA	7.35	131.11	120.38
1	B	130	TYR	CA-C-N	7.10	130.75	120.38
1	B	130	TYR	C-N-CA	7.10	130.75	120.38
1	A	337	GLU	N-CA-C	6.97	121.95	113.38
1	B	566	LEU	N-CA-CB	-6.11	101.01	110.29
1	A	513	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	513	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	430	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	337	GLU	N-CA-C	5.62	120.86	112.94
1	A	267	THR	CB-CA-C	5.59	116.06	109.47
1	B	267	THR	CB-CA-C	5.43	115.87	109.47
1	A	570	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	430	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	335	ASN	N-CA-C	5.28	116.83	108.96
1	B	570	ASP	CA-CB-CG	5.24	117.83	112.60
1	B	517	GLY	CA-C-N	5.23	130.28	123.06
1	B	517	GLY	C-N-CA	5.23	130.28	123.06
1	A	336	LEU	N-CA-C	-5.16	98.86	107.99
1	B	335	ASN	N-CA-C	5.11	116.57	108.96
1	B	64	LEU	CA-C-N	5.08	127.09	120.28
1	B	64	LEU	C-N-CA	5.08	127.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	LEU	N-CA-C	-5.03	99.09	107.99
1	B	662	GLY	CA-C-N	5.03	127.85	120.71
1	B	662	GLY	C-N-CA	5.03	127.85	120.71
1	B	180	ASP	CA-CB-CG	5.01	117.61	112.60

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	5287	0	5098	60	0
1	B	5310	0	5124	61	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
3	A	46	0	0	1	0
3	B	58	0	0	1	0
All	All	10727	0	10232	121	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 6.

All (121) 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:A:586:ARG:HH21	1:A:612:ARG:NH2	1.51	1.08
1:B:586:ARG:HH21	1:B:612:ARG:NH2	1.51	1.06
1:A:154:SER:HB2	1:A:511:ALA:HA	1.51	0.93
1:B:293:ASN:HD21	1:B:335:ASN:HD22	1.11	0.92
1:B:154:SER:HB2	1:B:511:ALA:HA	1.52	0.90
1:A:293:ASN:HD21	1:A:335:ASN:HD22	1.12	0.90
1:A:586:ARG:HH21	1:A:612:ARG:HH21	1.23	0.86
1:B:586:ARG:HH21	1:B:612:ARG:HH21	1.23	0.85
1:A:690:ARG:HG3	1:A:691:HIS:HD2	1.41	0.84
1:A:217:ASN:HD21	1:A:219:ASN:HD22	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASN:HD21	1:B:219:ASN:HD22	1.32	0.76
1:B:254:GLU:HB3	1:B:305:TRP:HB2	1.67	0.76
1:A:254:GLU:HB2	1:A:305:TRP:HB2	1.68	0.75
1:A:586:ARG:NH2	1:A:612:ARG:NH2	2.32	0.75
1:A:690:ARG:HG3	1:A:691:HIS:CD2	2.21	0.75
1:B:586:ARG:NH2	1:B:612:ARG:NH2	2.33	0.70
1:A:233:GLU:OE2	1:A:257:HIS:HD2	1.81	0.64
1:A:293:ASN:ND2	1:A:335:ASN:HD22	1.92	0.64
1:B:233:GLU:OE2	1:B:257:HIS:HD2	1.81	0.64
1:A:397:PRO:HD3	1:A:430:ASP:HB2	1.80	0.63
1:A:634:ASN:HA	1:A:664:THR:HG23	1.82	0.61
1:A:217:ASN:ND2	1:A:219:ASN:HD22	1.99	0.61
1:B:217:ASN:ND2	1:B:219:ASN:HD22	2.00	0.60
1:B:634:ASN:HA	1:B:664:THR:HG23	1.83	0.60
1:A:441:MET:HG3	1:A:459:ARG:HD2	1.83	0.59
1:A:121:GLN:HB2	1:A:131:ASP:HB3	1.85	0.59
1:B:257:HIS:HE1	1:B:300:GLU:OE1	1.86	0.59
1:A:152:PRO:HD2	1:A:538:GLN:HB2	1.84	0.58
1:A:397:PRO:CD	1:A:430:ASP:HB2	2.33	0.58
1:B:333:PHE:HB2	1:B:356:GLN:HB3	1.85	0.58
1:A:155:PHE:HA	1:A:459:ARG:HB3	1.86	0.58
1:B:121:GLN:HB2	1:B:131:ASP:HB3	1.84	0.58
1:B:293:ASN:ND2	1:B:335:ASN:HD22	1.92	0.58
1:A:217:ASN:HD21	1:A:219:ASN:ND2	2.00	0.57
1:B:152:PRO:HD2	1:B:538:GLN:HB2	1.85	0.57
1:B:259:MET:HE2	1:B:261:HIS:CE1	2.40	0.57
1:A:95:VAL:HG13	1:A:605:ASN:HB2	1.86	0.57
1:A:333:PHE:HB2	1:A:356:GLN:HB3	1.85	0.57
1:A:257:HIS:HE1	1:A:300:GLU:OE1	1.87	0.57
1:B:95:VAL:HG13	1:B:605:ASN:HB2	1.85	0.57
1:B:337:GLU:HG2	1:B:352:GLY:O	2.04	0.56
1:B:57:GLY:HA2	1:B:149:ILE:HD12	1.87	0.56
1:B:217:ASN:HD21	1:B:219:ASN:ND2	2.01	0.56
1:A:104:GLY:O	2:A:801:FLC:HG2	2.05	0.56
1:B:293:ASN:HD21	1:B:335:ASN:ND2	1.93	0.56
1:A:57:GLY:HA2	1:A:149:ILE:HD12	1.86	0.55
1:B:340:ARG:NH1	1:B:351:SER:OG	2.40	0.55
1:A:441:MET:CG	1:A:459:ARG:HD2	2.37	0.54
1:B:155:PHE:HA	1:B:459:ARG:HB3	1.87	0.54
1:B:449:GLY:O	3:B:901:HOH:O	2.18	0.54
1:B:634:ASN:HD21	1:B:710:VAL:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ALA:HB3	1:A:681:ASP:HB2	1.89	0.54
1:B:483:ARG:HB2	1:B:527:VAL:HG13	1.90	0.54
1:A:566:LEU:HD23	1:A:581:GLY:HA3	1.90	0.54
1:A:483:ARG:HB2	1:A:527:VAL:HG13	1.90	0.53
1:A:634:ASN:HD21	1:A:710:VAL:H	1.54	0.53
1:B:698:VAL:HG22	1:B:724:VAL:HG22	1.90	0.53
1:B:560:GLU:HG3	1:B:586:ARG:HG2	1.89	0.53
1:B:711:THR:OG1	1:B:713:ALA:O	2.27	0.53
1:B:269:LEU:HG	1:B:715:MET:HA	1.90	0.52
1:A:641:ASN:HD21	1:A:659:ARG:NH1	2.07	0.52
1:B:641:ASN:HD21	1:B:659:ARG:NH1	2.08	0.51
1:A:293:ASN:HD21	1:A:335:ASN:ND2	1.94	0.51
1:A:698:VAL:HG22	1:A:724:VAL:HG22	1.93	0.51
1:B:353:ALA:HB3	1:B:400:VAL:HB	1.93	0.50
1:B:47:PRO:HA	1:B:593:GLY:HA3	1.95	0.49
1:B:182:GLN:HB3	1:B:194:SER:HB2	1.95	0.49
1:A:711:THR:OG1	1:A:713:ALA:O	2.30	0.49
1:A:47:PRO:HA	1:A:593:GLY:HA3	1.94	0.48
1:A:353:ALA:HB3	1:A:400:VAL:HB	1.93	0.48
1:B:358:HIS:CD2	1:B:395:ARG:HG2	2.49	0.47
1:B:59:ARG:NH1	1:B:441:MET:SD	2.87	0.47
1:B:259:MET:CE	1:B:261:HIS:CE1	2.97	0.47
1:A:182:GLN:HB3	1:A:194:SER:HB2	1.97	0.47
1:A:333:PHE:HB3	3:A:915:HOH:O	2.14	0.47
1:B:655:SER:HB2	1:B:683:ALA:HB3	1.96	0.47
1:B:90:ILE:HD11	1:B:140:SER:HB2	1.97	0.47
1:B:271:THR:HG23	1:B:341:TYR:HB2	1.97	0.46
1:B:602:LEU:HD13	1:B:644:LEU:HD13	1.96	0.46
1:A:602:LEU:HD13	1:A:644:LEU:HD13	1.97	0.46
1:B:366:ARG:HD3	1:B:387:ASP:OD2	2.16	0.46
1:B:155:PHE:HB3	1:B:490:GLY:HA2	1.98	0.46
1:A:358:HIS:CD2	1:A:395:ARG:HG2	2.51	0.45
1:B:100:ALA:O	1:B:108:SER:HB2	2.16	0.45
1:A:155:PHE:HB3	1:A:490:GLY:HA2	1.99	0.45
1:A:100:ALA:O	1:A:108:SER:HB2	2.17	0.45
1:A:90:ILE:HD11	1:A:140:SER:HB2	1.98	0.44
1:A:366:ARG:HD3	1:A:387:ASP:OD2	2.16	0.44
1:B:701:LEU:O	1:B:722:ARG:HD3	2.17	0.44
1:A:701:LEU:O	1:A:722:ARG:HD3	2.17	0.44
1:B:265:TRP:CE3	1:B:337:GLU:HB2	2.52	0.44
1:A:683:ALA:HB2	1:A:697:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ASP:HB2	1:A:487:PRO:HG2	2.00	0.43
1:B:683:ALA:HB2	1:B:697:ARG:HG3	2.00	0.43
1:B:461:ASP:HB2	1:B:487:PRO:HG2	1.99	0.43
1:B:369:GLY:HA3	1:B:384:PHE:CE2	2.53	0.43
1:A:586:ARG:NH2	1:A:612:ARG:HH21	2.02	0.43
1:B:653:ARG:HB3	1:B:685:SER:HB2	2.01	0.42
1:B:656:LEU:HD23	1:B:656:LEU:HA	1.94	0.42
1:B:90:ILE:HD11	1:B:140:SER:CB	2.50	0.42
1:A:342:ASN:ND2	1:A:347:GLN:HB2	2.35	0.42
1:B:516:SER:HB3	1:B:567:ALA:HB3	2.01	0.42
1:A:289:TRP:HZ3	1:A:721:PRO:HG3	1.85	0.42
1:B:569:PRO:HD2	1:B:617:SER:HB2	2.01	0.41
1:B:594:LEU:HD23	1:B:596:LEU:HD21	2.01	0.41
1:A:641:ASN:ND2	1:A:659:ARG:NH1	2.68	0.41
1:A:90:ILE:HD11	1:A:140:SER:CB	2.50	0.41
1:A:586:ARG:NH2	1:A:612:ARG:HH22	2.14	0.41
1:B:375:LEU:HD12	1:B:375:LEU:HA	1.99	0.41
1:A:569:PRO:HD2	1:A:617:SER:HB2	2.01	0.41
1:B:430:ASP:HA	1:B:471:ARG:HE	1.85	0.41
1:B:588:LEU:HD23	1:B:608:LEU:HD12	2.02	0.41
1:A:588:LEU:HD23	1:A:608:LEU:HD12	2.02	0.41
1:B:189:GLY:O	1:B:191:ARG:NH1	2.54	0.41
1:B:641:ASN:ND2	1:B:659:ARG:NH1	2.69	0.41
1:A:434:LYS:HD3	1:A:436:ARG:HG3	2.02	0.41
1:A:284:ARG:NH1	1:A:345:ASN:O	2.54	0.40
1:B:586:ARG:NH2	1:B:612:ARG:HH21	2.04	0.40
1:A:383:SER:OG	1:A:443:GLU:HB2	2.22	0.40
1:A:189:GLY:O	1:A:191:ARG:NH1	2.55	0.40
1:A:664:THR:HG22	1:A:710:VAL:HG23	2.02	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	682/732 (93%)	660 (97%)	21 (3%)	1 (0%)	48	60
1	B	688/732 (94%)	666 (97%)	22 (3%)	0	100	100
All	All	1370/1464 (94%)	1326 (97%)	43 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	PRO

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	540/573 (94%)	509 (94%)	31 (6%)	18	27
1	B	542/573 (95%)	510 (94%)	32 (6%)	18	26
All	All	1082/1146 (94%)	1019 (94%)	63 (6%)	18	26

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	110	SER
1	A	120	SER
1	A	132	VAL
1	A	138	ILE
1	A	170	THR
1	A	180	ASP
1	A	184	ARG
1	A	195	VAL
1	A	197	LEU
1	A	198	ASN
1	A	225	VAL
1	A	233	GLU
1	A	311	GLU
1	A	319	SER

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Mol	Chain	Res	Type
1	A	361	ARG
1	A	367	ILE
1	A	381	ASP
1	A	395	ARG
1	A	403	GLN
1	A	434	LYS
1	A	458	LEU
1	A	513	ASP
1	A	566	LEU
1	A	577	SER
1	A	594	LEU
1	A	597	THR
1	A	606	LEU
1	A	618	GLN
1	A	664	THR
1	A	710	VAL
1	B	43	GLU
1	B	95	VAL
1	B	120	SER
1	B	132	VAL
1	B	138	ILE
1	B	170	THR
1	B	180	ASP
1	B	184	ARG
1	B	195	VAL
1	B	197	LEU
1	B	198	ASN
1	B	225	VAL
1	B	233	GLU
1	B	319	SER
1	B	367	ILE
1	B	378	LEU
1	B	381	ASP
1	B	395	ARG
1	B	403	GLN
1	B	404	VAL
1	B	407	VAL
1	B	448	VAL
1	B	458	LEU
1	B	486	ASN
1	B	513	ASP
1	B	535	THR

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Mol	Chain	Res	Type
1	B	594	LEU
1	B	597	THR
1	B	606	LEU
1	B	664	THR
1	B	681	ASP
1	B	710	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	121	GLN
1	A	182	GLN
1	A	192	GLN
1	A	217	ASN
1	A	231	HIS
1	A	257	HIS
1	A	322	ASN
1	A	335	ASN
1	A	365	ASN
1	A	393	GLN
1	A	495	ASN
1	A	529	ASN
1	A	530	ASN
1	A	634	ASN
1	A	641	ASN
1	A	729	GLN
1	B	88	GLN
1	B	121	GLN
1	B	182	GLN
1	B	192	GLN
1	B	217	ASN
1	B	231	HIS
1	B	257	HIS
1	B	261	HIS
1	B	322	ASN
1	B	335	ASN
1	B	365	ASN
1	B	393	GLN
1	B	507	GLN
1	B	583	GLN
1	B	634	ASN

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Mol	Chain	Res	Type
1	B	641	ASN
1	B	729	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FLC	A	801	-	12,12,12	1.11	0	17,17,17	1.63	5 (29%)
2	FLC	B	801	-	12,12,12	1.12	1 (8%)	17,17,17	1.48	4 (23%)

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	FLC	A	801	-	-	5/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	B	801	-	-	8/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FLC	OG2-CGC	-2.01	1.24	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FLC	CB-CG-CGC	3.30	121.81	113.81
2	A	801	FLC	OB1-CBC-CB	-3.13	117.83	122.25
2	B	801	FLC	OHB-CB-CA	-2.72	103.05	109.40
2	A	801	FLC	OB2-CBC-CB	2.60	117.57	113.05
2	B	801	FLC	OB1-CBC-CB	-2.33	118.96	122.25
2	A	801	FLC	CB-CA-CAC	2.31	119.40	113.81
2	B	801	FLC	CB-CA-CAC	2.30	119.37	113.81
2	B	801	FLC	CB-CG-CGC	2.16	119.05	113.81
2	A	801	FLC	OHB-CB-CG	-2.12	104.44	109.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

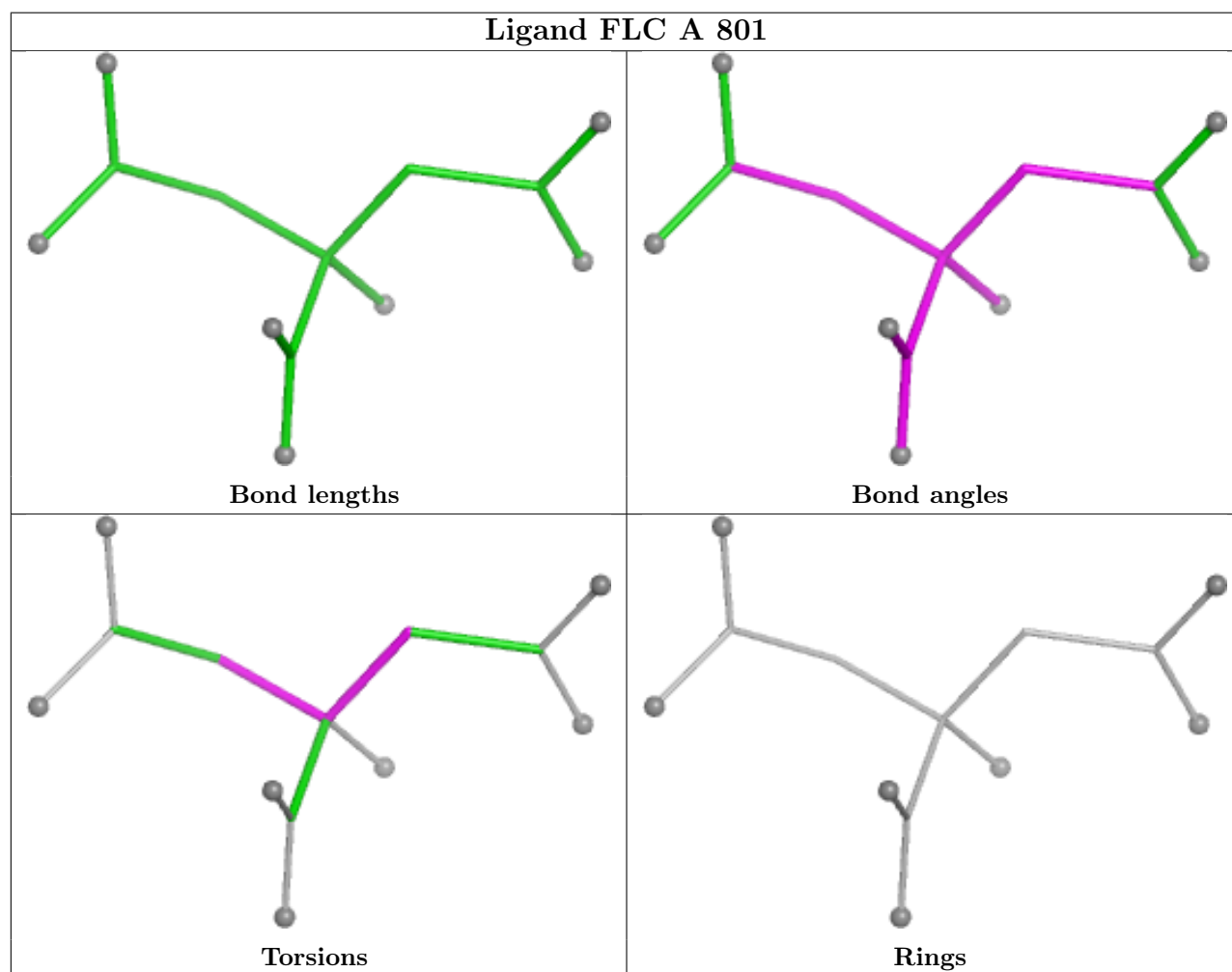
Mol	Chain	Res	Type	Atoms
2	B	801	FLC	CG-CB-CBC-OB1
2	B	801	FLC	CG-CB-CBC-OB2
2	B	801	FLC	OHB-CB-CBC-OB1
2	B	801	FLC	OHB-CB-CBC-OB2
2	A	801	FLC	CAC-CA-CB-CBC
2	A	801	FLC	OHB-CB-CG-CGC
2	A	801	FLC	CAC-CA-CB-CG
2	A	801	FLC	CAC-CA-CB-OHB
2	B	801	FLC	CA-CB-CG-CGC
2	B	801	FLC	CBC-CB-CG-CGC
2	A	801	FLC	CA-CB-CG-CGC
2	B	801	FLC	CAC-CA-CB-OHB
2	B	801	FLC	OHB-CB-CG-CGC

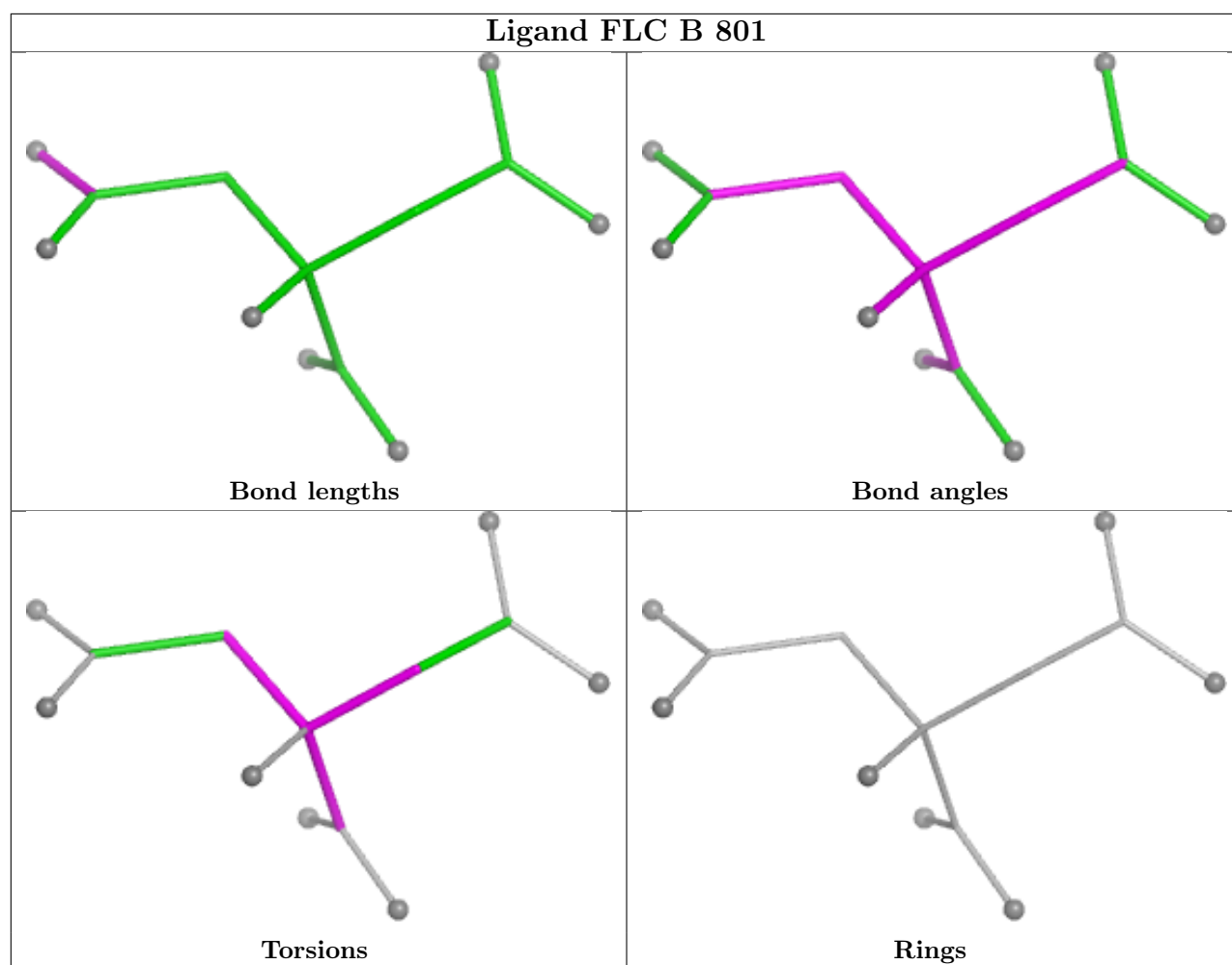
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FLC	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.





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	686/732 (93%)	0.46	41 (5%) 27 29	19, 35, 53, 63	0
1	B	690/732 (94%)	0.59	38 (5%) 30 32	22, 38, 55, 72	0
All	All	1376/1464 (93%)	0.53	79 (5%) 29 31	19, 37, 54, 72	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	GLY	7.1
1	B	374	SER	7.0
1	B	375	LEU	5.5
1	A	401	ALA	4.4
1	B	255	TYR	4.3
1	B	536	GLY	4.0
1	A	371	TYR	4.0
1	A	650	PRO	3.9
1	B	496	TRP	3.9
1	A	42	PRO	3.8
1	B	470	ARG	3.7
1	B	273	GLY	3.7
1	B	732	PHE	3.5
1	A	568	THR	3.4
1	B	465	LEU	3.3
1	B	384	PHE	3.2
1	B	498	VAL	3.2
1	B	227	GLY	3.2
1	A	576	SER	3.1
1	A	476	ALA	3.1
1	A	43	GLU	3.1
1	A	731	ARG	3.1
1	B	340	ARG	3.0
1	B	401	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	392	ARG	2.9
1	A	287	THR	2.9
1	A	255	TYR	2.9
1	A	274	ASP	2.8
1	B	650	PRO	2.8
1	A	608	LEU	2.8
1	A	384	PHE	2.8
1	A	273	GLY	2.8
1	B	731	ARG	2.8
1	A	579	PRO	2.7
1	A	465	LEU	2.7
1	A	344	GLY	2.7
1	B	713	ALA	2.7
1	B	550	GLY	2.7
1	B	450	GLY	2.6
1	B	361	ARG	2.6
1	B	400	VAL	2.6
1	A	317	ARG	2.5
1	A	343	PRO	2.5
1	A	174	GLN	2.5
1	A	714	PRO	2.5
1	B	528	LEU	2.4
1	A	224	TRP	2.4
1	B	392	ARG	2.4
1	A	475	ALA	2.3
1	A	516	SER	2.3
1	B	551	ARG	2.3
1	B	421	PRO	2.3
1	A	577	SER	2.3
1	B	568	THR	2.3
1	B	432	ASP	2.2
1	B	714	PRO	2.2
1	A	162	VAL	2.2
1	A	564	LYS	2.2
1	B	224	TRP	2.2
1	B	625	VAL	2.2
1	A	550	GLY	2.2
1	A	649	ALA	2.1
1	A	292	TYR	2.1
1	A	528	LEU	2.1
1	A	570	ASP	2.1
1	A	304	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	417	PHE	2.1
1	A	653	ARG	2.1
1	A	380	SER	2.1
1	B	565	ASN	2.1
1	A	536	GLY	2.1
1	B	571	PRO	2.1
1	A	713	ALA	2.0
1	A	573	ASN	2.0
1	B	573	ASN	2.0
1	B	304	TRP	2.0
1	B	389	SER	2.0
1	B	476	ALA	2.0
1	B	378	LEU	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](#)

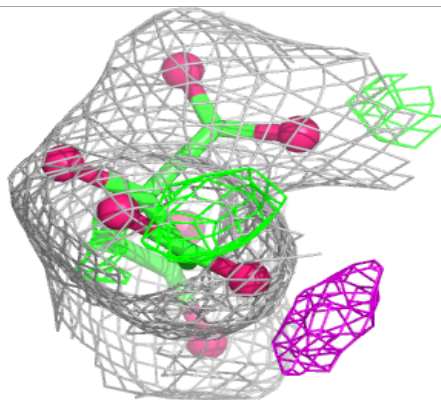
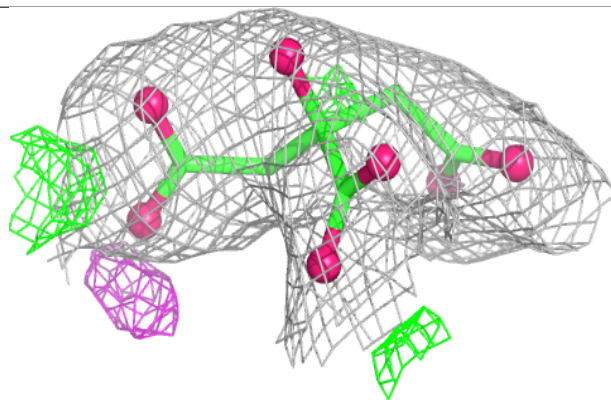
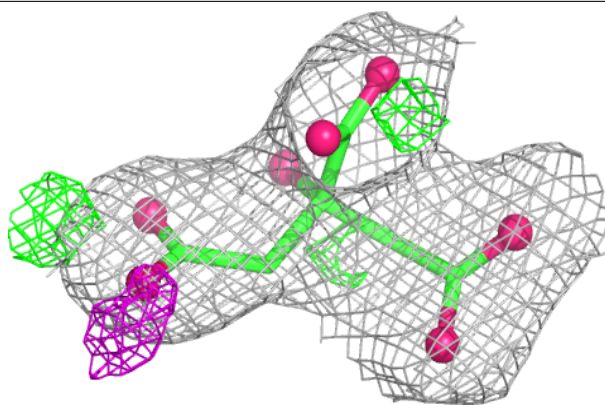
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FLC	B	801	13/13	0.86	0.11	28,29,31,31	0
2	FLC	A	801	13/13	0.91	0.08	25,26,28,28	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.

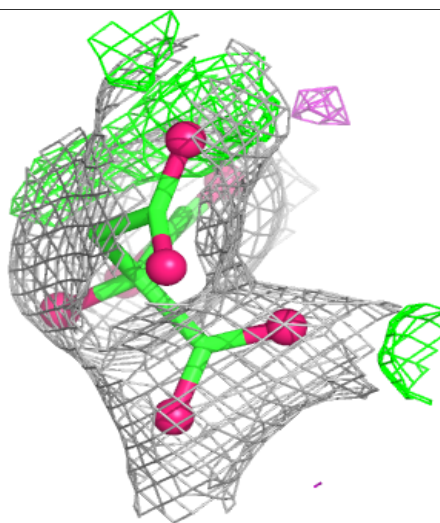
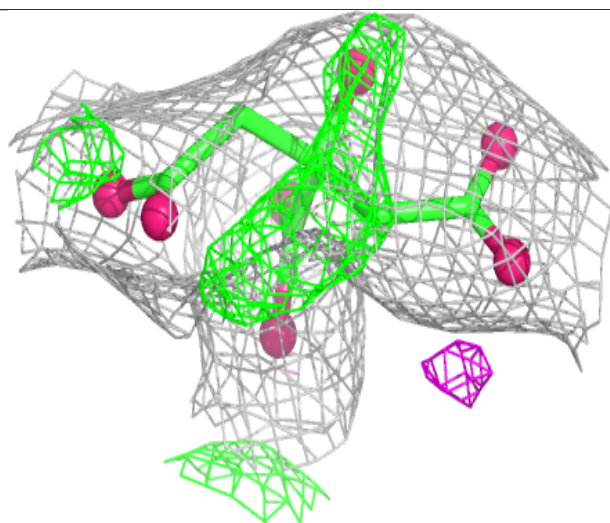
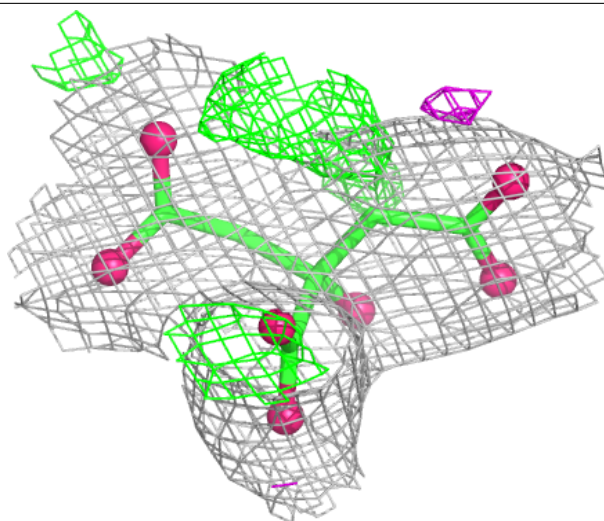
Electron density around FLC B 801:

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



Electron density around FLC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.