



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:41 PM EDT

PDB ID : 6P7U / pdb_00006p7u
Title : CRYSTAL STRUCTURE OF THE CARBOXYLTRANSFERASE SUBUNIT
OF ACC (ACCD6) IN COMPLEX WITH INHIBITOR QUIZALOFOP-P
FROM MYCOBACTERIUM TUBERCULOSIS
Authors : Reddy, M.C.M.; Sacchettini, J.C.; Center for Structural Genomics of Infectious
Diseases (CSGID)
Deposited on : 2019-06-06
Resolution : 2.20 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](#) ①) 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

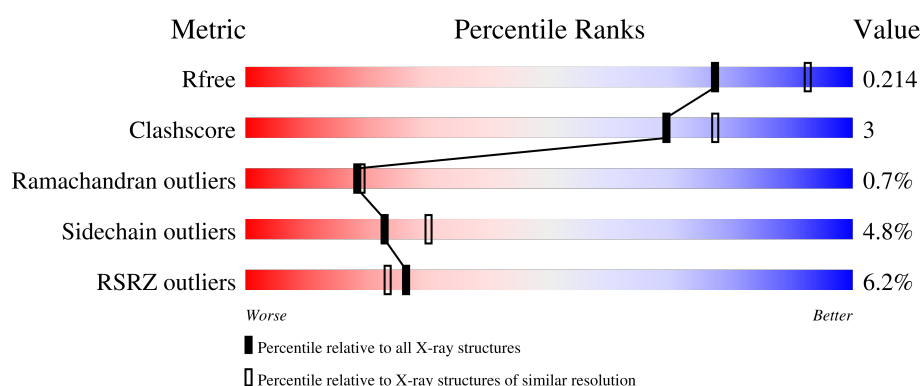
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	473	3% 79% 10% • 10%
1	B	473	3% 80% 9% • 10%
1	C	473	8% 77% 8% • 13%
1	D	473	8% 83% 7% • 10%

2 Entry composition [i](#)

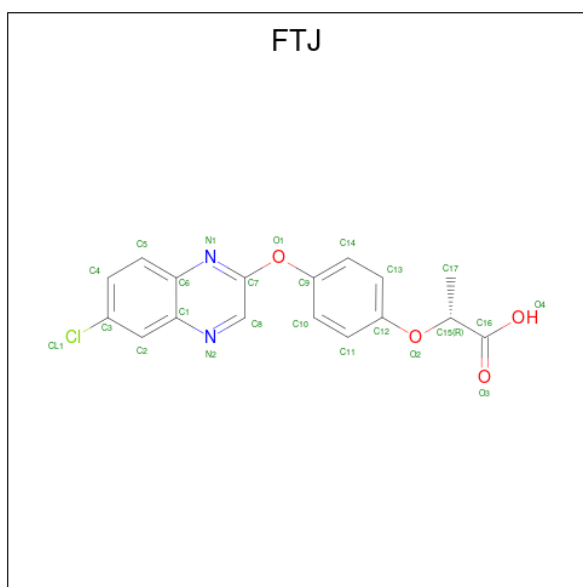
There are 3 unique types of molecules in this entry. The entry contains 13244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable propionyl-CoA carboxylase beta chain 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	1	0
			3147	1969	572	592	14			
1	B	424	Total	C	N	O	S	0	1	0
			3123	1958	569	582	14			
1	C	410	Total	C	N	O	S	0	2	0
			2992	1874	543	561	14			
1	D	428	Total	C	N	O	S	0	0	0
			3093	1940	558	581	14			

- Molecule 2 is (2R)-2-{4-[(6-chloroquinoxalin-2-yl)oxy]phenoxy}propanoic acid (CCD ID: FTJ) (formula: C₁₇H₁₃ClN₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N O	0	0
			24	17	1	2 4		
2	B	1	Total	C	Cl	N O	0	0
			24	17	1	2 4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	O	
			24	17	1	2	4	
2	D	1	Total	C	Cl	N	O	
			24	17	1	2	4	

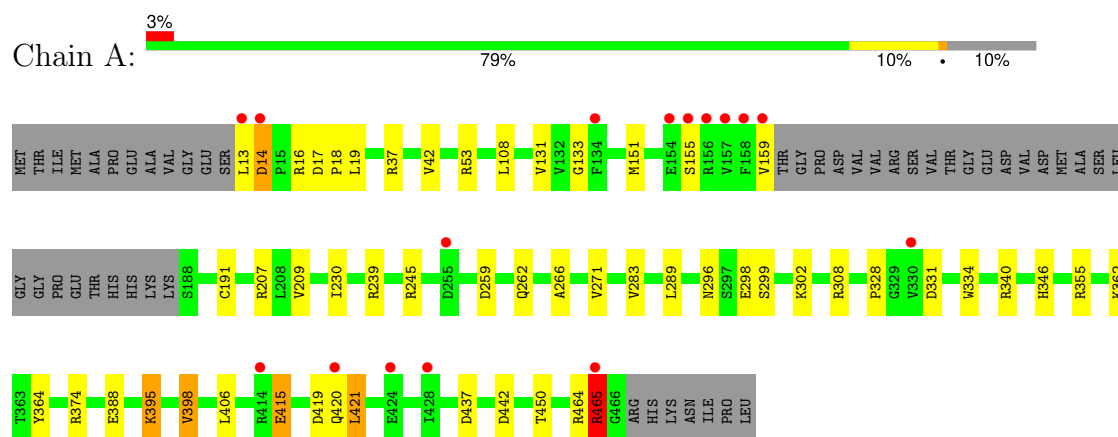
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total	O		
			234	234	0	0
3	B	175	Total	O		
			175	175	0	0
3	C	177	Total	O		
			177	177	0	0
3	D	207	Total	O		
			207	207	0	0

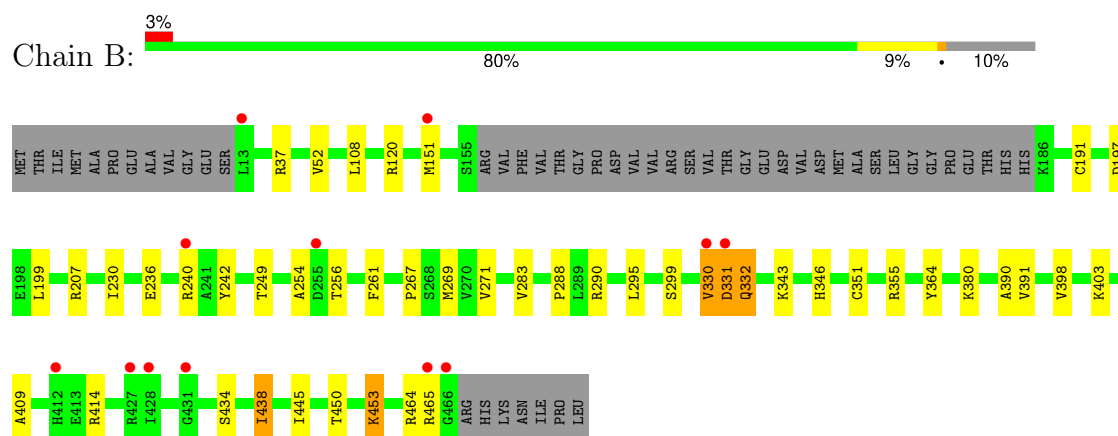
3 Residue-property plots [i](#)

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.

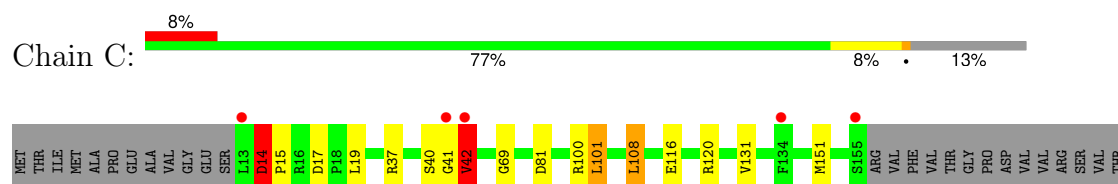
- Molecule 1: Probable propionyl-CoA carboxylase beta chain 6

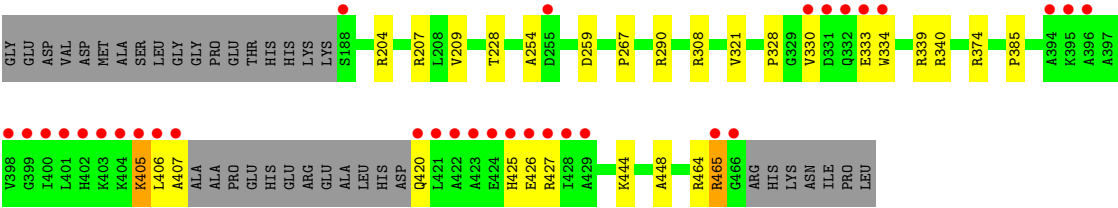


- Molecule 1: Probable propionyl-CoA carboxylase beta chain 6

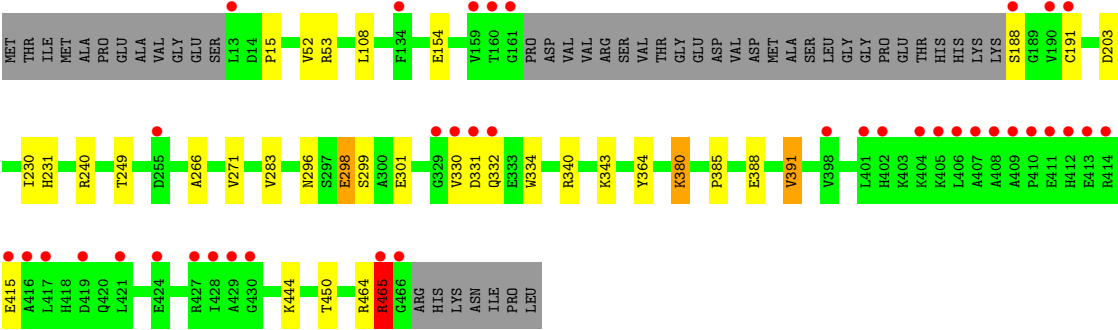
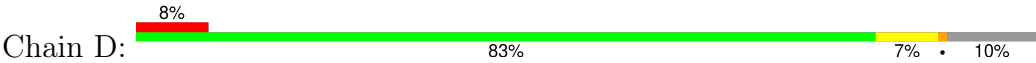


- Molecule 1: Probable propionyl-CoA carboxylase beta chain 6





● Molecule 1: Probable propionyl-CoA carboxylase beta chain 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.60Å 153.34Å 102.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.20 48.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.76-2.20) 97.5 (48.76-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.171 , 0.206 0.179 , 0.214	Depositor DCC
R_{free} test set	5916 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13244	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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: FTJ

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	0.47	0/3209	0.79	0/4365
1	B	0.49	1/3185 (0.0%)	0.78	1/4330 (0.0%)
1	C	0.51	1/3052 (0.0%)	0.84	6/4151 (0.1%)
1	D	0.48	0/3151	0.79	0/4294
All	All	0.49	2/12597 (0.0%)	0.80	7/17140 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	SER	C-O	-7.92	1.14	1.24
1	B	120	ARG	C-O	-5.42	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	SER	N-CA-C	6.53	119.72	111.69
1	C	42	VAL	N-CA-C	6.19	115.98	108.06
1	C	254	ALA	N-CA-C	5.92	117.73	111.28
1	B	254	ALA	N-CA-C	5.44	116.89	111.07
1	C	321	VAL	N-CA-C	5.17	115.40	108.17
1	C	14	ASP	CA-C-N	-5.16	114.30	119.56
1	C	14	ASP	C-N-CA	-5.16	114.30	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3147	0	3090	24	0
1	B	3123	0	3075	19	0
1	C	2992	0	2921	23	0
1	D	3093	0	3000	23	0
2	A	24	0	0	1	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	0	0
3	A	234	0	0	2	0
3	B	175	0	0	1	0
3	C	177	0	0	1	0
3	D	207	0	0	7	0
All	All	13244	0	12086	85	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 3.

All (85) 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:B:330:VAL:O	1:B:331:ASP:CB	2.24	0.83
1:C:41:GLY:O	1:C:42:VAL:HG12	1.79	0.83
1:B:331:ASP:O	1:B:332:GLN:CB	2.31	0.76
1:D:301:GLU:HB2	1:D:340:ARG:HD2	1.67	0.75
1:C:204[B]:ARG:NH2	1:C:259:ASP:OD1	2.25	0.68
1:C:41:GLY:C	1:C:42:VAL:CG1	2.66	0.67
1:D:465:ARG:CG	3:D:799:HOH:O	2.44	0.65
1:B:445:ILE:HG21	1:B:453:LYS:HG2	1.80	0.61
1:A:17:ASP:OD1	1:A:37:ARG:NH2	2.33	0.60
1:C:41:GLY:O	1:C:42:VAL:CG1	2.49	0.60
1:A:464:ARG:O	1:A:465:ARG:HB2	2.02	0.59
1:A:53:ARG:NH1	3:A:601:HOH:O	2.30	0.57
1:A:398:VAL:HG11	1:A:421:LEU:HB3	1.86	0.57
1:A:340:ARG:NE	3:A:604:HOH:O	2.38	0.57
1:C:385:PRO:HA	1:C:444:LYS:HD2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:LYS:NZ	3:D:601:HOH:O	2.39	0.56
1:B:151:MET:SD	1:B:191:CYS:HB2	2.45	0.56
1:C:464:ARG:O	1:C:465:ARG:HB2	2.06	0.55
1:B:409:ALA:O	1:B:414:ARG:NH2	2.37	0.53
1:D:465:ARG:CD	3:D:799:HOH:O	2.56	0.53
1:D:331:ASP:O	1:D:332:GLN:CB	2.58	0.52
1:D:230:ILE:HD12	1:D:450:THR:HB	1.92	0.51
1:D:53:ARG:HD2	3:D:610:HOH:O	2.09	0.51
1:C:81:ASP:OD1	1:C:120:ARG:NH2	2.31	0.50
1:D:332:GLN:O	1:D:334:TRP:CD1	2.65	0.50
1:D:465:ARG:HG3	3:D:799:HOH:O	2.10	0.49
1:D:465:ARG:CB	3:D:799:HOH:O	2.60	0.49
1:C:405:LYS:O	1:C:407:ALA:N	2.45	0.49
1:D:364:TYR:OH	1:D:388:GLU:OE1	2.21	0.49
1:C:101:LEU:HD13	1:D:391:VAL:HG21	1.95	0.49
1:D:330:VAL:O	1:D:331:ASP:CB	2.61	0.48
1:B:267:PRO:HB2	1:B:290:ARG:HG3	1.96	0.48
1:A:266:ALA:HB3	1:A:302:LYS:HD2	1.96	0.48
1:C:425:HIS:C	1:C:427:ARG:H	2.21	0.47
1:C:41:GLY:C	1:C:42:VAL:HG13	2.36	0.47
1:A:296:ASN:H	1:A:299:SER:HG	1.63	0.47
1:C:69:GLY:HA3	1:C:100:ARG:HD2	1.97	0.47
1:A:230:ILE:HD12	1:A:450:THR:HB	1.97	0.47
1:B:464:ARG:O	1:B:465:ARG:HB2	2.14	0.47
1:A:13:LEU:CB	1:A:16:ARG:HH21	2.28	0.46
1:C:108:LEU:HD21	1:D:391:VAL:HA	1.97	0.46
1:D:385:PRO:HA	1:D:444:LYS:HD3	1.98	0.46
1:C:339:ARG:NH1	1:D:188:SER:O	2.49	0.45
1:A:207:ARG:HD2	1:A:259:ASP:OD2	2.17	0.45
1:C:116:GLU:OE1	1:C:120:ARG:HD3	2.17	0.45
1:A:151:MET:SD	1:A:191:CYS:HB2	2.57	0.45
1:D:464:ARG:O	1:D:465:ARG:CG	2.65	0.44
1:B:364:TYR:HA	1:B:390:ALA:O	2.17	0.44
1:B:230:ILE:HD12	1:B:450:THR:HB	1.99	0.44
1:C:267:PRO:HB2	1:C:290:ARG:HG3	1.99	0.44
1:D:231:HIS:HD2	3:D:604:HOH:O	2.01	0.44
1:A:262:GLN:HB2	1:A:302:LYS:HE3	2.00	0.44
1:D:271:VAL:HA	1:D:283:VAL:O	2.18	0.44
1:C:207:ARG:HD2	1:C:259:ASP:OD2	2.17	0.43
2:A:501:FTJ:CL1	1:B:295:LEU:HD13	2.55	0.43
1:B:434:SER:O	1:B:438:ILE:HD12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:HB	1:A:151:MET:HG2	2.00	0.43
1:B:242:TYR:CE1	1:B:288:PRO:HG2	2.54	0.43
1:A:133:GLY:C	1:A:155:SER:HB2	2.44	0.43
1:B:269:MET:HB2	1:B:299:SER:HB2	2.01	0.43
1:B:351:CYS:HB3	1:B:355:ARG:NE	2.35	0.42
1:C:14:ASP:N	1:C:15:PRO:HD2	2.34	0.42
1:A:328:PRO:HB3	1:A:334:TRP:CD2	2.55	0.42
1:C:328:PRO:HB3	1:C:334:TRP:CE2	2.54	0.42
1:B:261:PHE:HB2	1:B:271:VAL:HG23	2.02	0.42
1:A:271:VAL:HA	1:A:283:VAL:O	2.19	0.42
1:B:453:LYS:HE3	3:B:734:HOH:O	2.19	0.42
1:D:296:ASN:H	1:D:299:SER:HG	1.67	0.42
1:B:271:VAL:HA	1:B:283:VAL:O	2.20	0.41
1:A:364:TYR:HE1	1:A:388:GLU:HG2	1.85	0.41
1:C:131:VAL:HB	1:C:151:MET:HG2	2.01	0.41
1:C:228:THR:O	1:C:448:ALA:HA	2.21	0.41
1:A:17:ASP:HA	1:A:18:PRO:HD3	1.93	0.41
1:A:331:ASP:OD1	1:A:331:ASP:N	2.53	0.41
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.82	0.41
1:A:133:GLY:O	1:A:155:SER:HB2	2.20	0.40
1:A:289:LEU:HD21	1:D:15:PRO:HD2	2.03	0.40
1:A:374:ARG:NH2	1:A:442:ASP:OD2	2.51	0.40
1:D:266:ALA:HB2	1:D:298:GLU:HB2	2.03	0.40
1:D:343:LYS:HA	1:D:343:LYS:HD3	1.86	0.40
1:A:239:ARG:HE	1:A:239:ARG:HB3	1.66	0.40
1:A:395:LYS:C	1:A:395:LYS:HE2	2.46	0.40
1:B:207:ARG:HH11	1:B:207:ARG:HD3	1.76	0.40
1:C:17:ASP:OD2	1:C:37:ARG:NH2	2.49	0.40
1:C:340:ARG:NE	3:C:612:HOH:O	2.55	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	423/473 (89%)	412 (97%)	8 (2%)	3 (1%)	18	19
1	B	421/473 (89%)	406 (96%)	13 (3%)	2 (0%)	24	27
1	C	406/473 (86%)	387 (95%)	14 (3%)	5 (1%)	10	8
1	D	424/473 (90%)	407 (96%)	15 (4%)	2 (0%)	24	27
All	All	1674/1892 (88%)	1612 (96%)	50 (3%)	12 (1%)	18	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	ARG
1	B	332	GLN
1	C	330	VAL
1	C	465	ARG
1	D	465	ARG
1	A	415	GLU
1	B	331	ASP
1	C	406	LEU
1	C	426	GLU
1	C	405	LYS
1	D	415	GLU
1	A	14	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/362 (87%)	294 (93%)	22 (7%)	14	16
1	B	311/362 (86%)	294 (94%)	17 (6%)	19	24
1	C	295/362 (82%)	284 (96%)	11 (4%)	30	41
1	D	302/362 (83%)	291 (96%)	11 (4%)	31	42
All	All	1224/1448 (84%)	1163 (95%)	61 (5%)	23	28

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	19	LEU
1	A	42	VAL
1	A	108	LEU
1	A	159	VAL
1	A	209	VAL
1	A	245	ARG
1	A	298	GLU
1	A	308[A]	ARG
1	A	308[B]	ARG
1	A	346	HIS
1	A	355	ARG
1	A	362	LYS
1	A	395	LYS
1	A	398	VAL
1	A	406	LEU
1	A	415	GLU
1	A	419	ASP
1	A	420	GLN
1	A	421	LEU
1	A	437	ASP
1	A	465	ARG
1	B	37	ARG
1	B	52	VAL
1	B	108	LEU
1	B	197	ASP
1	B	236	GLU
1	B	240	ARG
1	B	249	THR
1	B	256	THR
1	B	330	VAL
1	B	343	LYS
1	B	346	HIS
1	B	380	LYS
1	B	391	VAL
1	B	398	VAL
1	B	403	LYS
1	B	438	ILE
1	B	453	LYS
1	C	14	ASP
1	C	19	LEU
1	C	42	VAL
1	C	101	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	108	LEU
1	C	209	VAL
1	C	308[A]	ARG
1	C	308[B]	ARG
1	C	333	GLU
1	C	374	ARG
1	C	420	GLN
1	D	52	VAL
1	D	108	LEU
1	D	154	GLU
1	D	191	CYS
1	D	203	ASP
1	D	240	ARG
1	D	249	THR
1	D	298	GLU
1	D	380	LYS
1	D	391	VAL
1	D	465	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	420	GLN
1	B	420	GLN
1	D	127	GLN
1	D	231	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	FTJ	C	501	-	26,26,26	1.14	2 (7%)	36,36,36	2.07	6 (16%)
2	FTJ	B	501	-	26,26,26	1.27	2 (7%)	36,36,36	2.28	7 (19%)
2	FTJ	D	501	-	26,26,26	1.17	1 (3%)	36,36,36	2.27	4 (11%)
2	FTJ	A	501	-	26,26,26	1.18	1 (3%)	36,36,36	2.17	6 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FTJ	C	501	-	-	0/12/12/12	0/3/3/3
2	FTJ	B	501	-	-	0/12/12/12	0/3/3/3
2	FTJ	D	501	-	-	0/12/12/12	0/3/3/3
2	FTJ	A	501	-	-	3/12/12/12	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FTJ	O2-C15	-3.70	1.37	1.43
2	C	501	FTJ	O2-C15	-3.43	1.37	1.43
2	A	501	FTJ	O2-C15	-3.19	1.37	1.43
2	D	501	FTJ	O2-C15	-2.91	1.38	1.43
2	C	501	FTJ	C6-C1	-2.20	1.38	1.42
2	B	501	FTJ	C6-C1	-2.08	1.38	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FTJ	C8-C7-N1	-10.07	119.04	124.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FTJ	C8-C7-N1	-9.15	119.50	124.03
2	A	501	FTJ	C8-C7-N1	-8.98	119.58	124.03
2	C	501	FTJ	C8-C7-N1	-8.11	120.01	124.03
2	B	501	FTJ	C7-N1-C6	6.78	120.93	115.85
2	D	501	FTJ	C7-N1-C6	6.26	120.54	115.85
2	C	501	FTJ	C7-N1-C6	6.00	120.34	115.85
2	A	501	FTJ	C7-N1-C6	5.50	119.97	115.85
2	C	501	FTJ	C7-C8-N2	-2.92	120.24	121.89
2	B	501	FTJ	O2-C15-C16	-2.88	107.70	111.34
2	C	501	FTJ	C12-O2-C15	2.69	122.80	118.40
2	B	501	FTJ	C7-C8-N2	-2.69	120.37	121.89
2	A	501	FTJ	O1-C7-N1	2.52	126.59	119.39
2	A	501	FTJ	C5-C6-N1	2.45	122.26	118.69
2	D	501	FTJ	C8-N2-C1	2.32	119.64	116.96
2	B	501	FTJ	C8-N2-C1	2.29	119.61	116.96
2	B	501	FTJ	C1-C6-N1	-2.27	118.41	121.18
2	C	501	FTJ	C8-N2-C1	2.20	119.50	116.96
2	A	501	FTJ	C1-C6-N1	-2.18	118.51	121.18
2	D	501	FTJ	C5-C6-N1	2.16	121.85	118.69
2	A	501	FTJ	O2-C15-C16	-2.10	108.68	111.34
2	B	501	FTJ	C12-O2-C15	2.09	121.82	118.40
2	C	501	FTJ	C1-C6-N1	-2.07	118.65	121.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FTJ	C17-C15-C16-O4
2	A	501	FTJ	C17-C15-C16-O3
2	A	501	FTJ	O2-C15-C16-O4

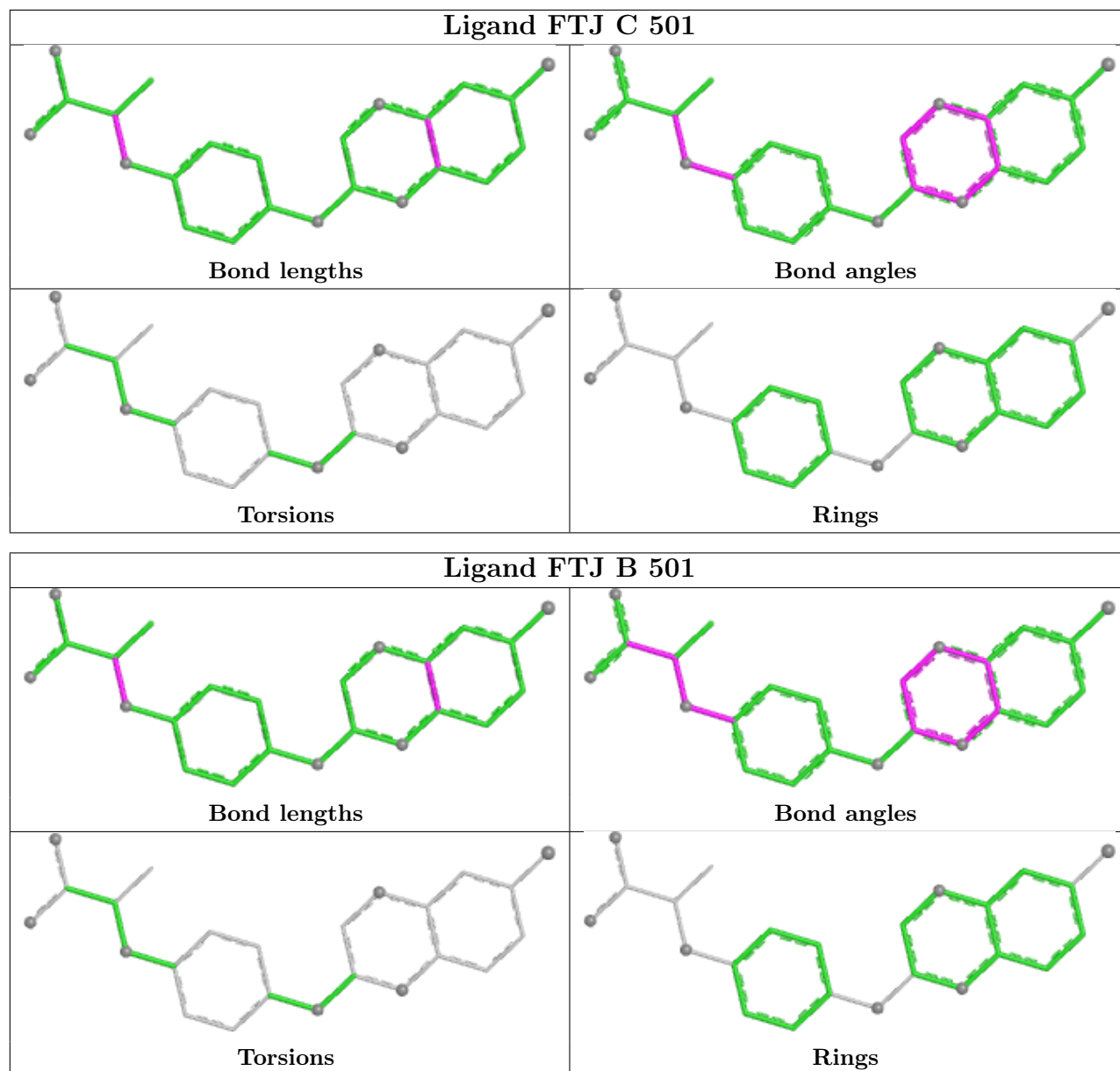
There are no ring outliers.

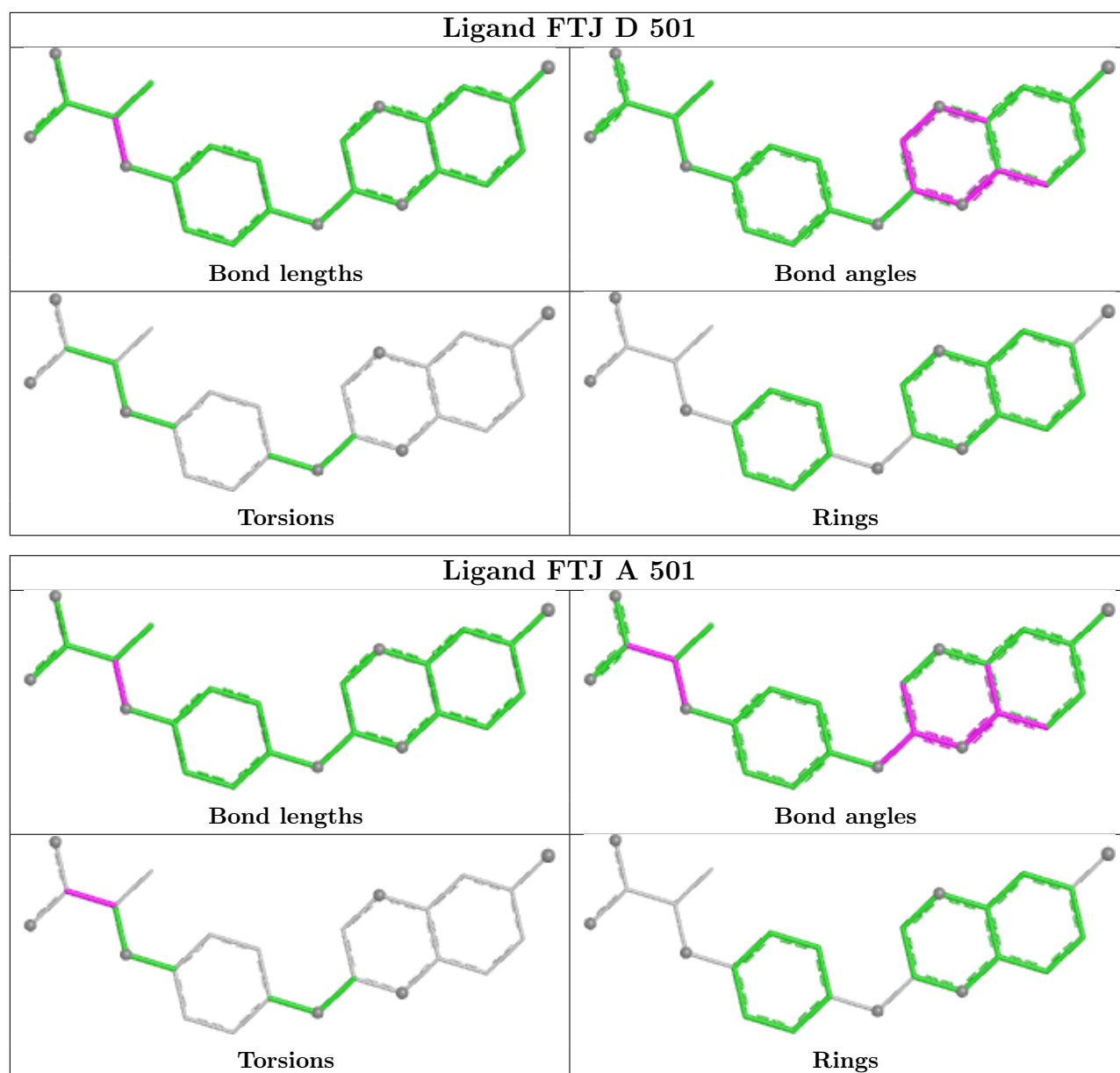
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FTJ	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	426/473 (90%)	-0.27	16 (3%)	44	41	12, 29, 56, 89	1 (0%)
1	B	424/473 (89%)	-0.28	12 (2%)	55	52	10, 28, 59, 86	1 (0%)
1	C	410/473 (86%)	-0.03	37 (9%)	15	12	13, 30, 77, 118	2 (0%)
1	D	428/473 (90%)	-0.09	39 (9%)	15	12	16, 28, 70, 97	0
All	All	1688/1892 (89%)	-0.17	104 (6%)	26	23	10, 29, 67, 118	4 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	332	GLN	8.8
1	B	330	VAL	7.6
1	D	465	ARG	6.8
1	C	421	LEU	6.2
1	A	159	VAL	5.4
1	D	330	VAL	5.3
1	C	407	ALA	5.2
1	C	13	LEU	5.1
1	C	404	LYS	5.1
1	C	406	LEU	5.1
1	B	466	GLY	5.0
1	A	158	PHE	5.0
1	D	413	GLU	4.8
1	C	466	GLY	4.7
1	D	331	ASP	4.7
1	A	157	VAL	4.7
1	C	330	VAL	4.6
1	C	423	ALA	4.6
1	A	13	LEU	4.6
1	C	401	LEU	4.6
1	B	331	ASP	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	134	PHE	4.5
1	D	161	GLY	4.5
1	D	401	LEU	4.5
1	D	416	ALA	4.4
1	D	160	THR	4.3
1	D	410	PRO	4.3
1	C	425	HIS	4.3
1	B	13	LEU	4.2
1	D	408	ALA	4.0
1	D	428	ILE	4.0
1	D	412	HIS	4.0
1	D	411	GLU	3.9
1	B	465	ARG	3.8
1	C	429	ALA	3.8
1	C	41	GLY	3.8
1	C	403	LYS	3.7
1	C	465	ARG	3.7
1	C	405	LYS	3.7
1	C	332	GLN	3.6
1	C	331	ASP	3.5
1	C	398	VAL	3.5
1	D	415	GLU	3.5
1	C	422	ALA	3.4
1	D	414	ARG	3.4
1	D	134	PHE	3.3
1	C	394	ALA	3.2
1	D	417	LEU	3.2
1	A	156	ARG	3.2
1	A	330	VAL	3.1
1	C	428	ILE	3.1
1	C	426	GLU	3.1
1	A	134	PHE	3.1
1	C	399	GLY	3.1
1	C	334	TRP	3.1
1	A	255	ASP	3.1
1	D	466	GLY	3.0
1	D	255	ASP	3.0
1	C	395	LYS	3.0
1	C	42	VAL	3.0
1	D	159	VAL	2.9
1	D	13	LEU	2.9
1	D	409	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	402	HIS	2.9
1	A	465	ARG	2.9
1	A	154	GLU	2.8
1	C	420	GLN	2.8
1	B	431	GLY	2.8
1	D	404	LYS	2.8
1	B	428	ILE	2.8
1	D	421	LEU	2.7
1	D	406	LEU	2.7
1	C	255	ASP	2.6
1	C	155	SER	2.6
1	D	405	LYS	2.6
1	B	240	ARG	2.6
1	D	419	ASP	2.6
1	C	188	SER	2.6
1	C	424	GLU	2.6
1	A	424	GLU	2.5
1	D	430	GLY	2.5
1	C	427	ARG	2.5
1	A	155	SER	2.5
1	C	333	GLU	2.5
1	C	400	ILE	2.5
1	D	190	VAL	2.4
1	D	398	VAL	2.4
1	C	396	ALA	2.4
1	A	14	ASP	2.4
1	D	407	ALA	2.3
1	D	424	GLU	2.3
1	D	329	GLY	2.3
1	D	188	SER	2.2
1	A	414	ARG	2.2
1	B	151	MET	2.2
1	D	427	ARG	2.1
1	B	255	ASP	2.1
1	D	402	HIS	2.1
1	D	429	ALA	2.1
1	A	420	GLN	2.1
1	A	428	ILE	2.1
1	D	191	CYS	2.0
1	B	427	ARG	2.0
1	B	412	HIS	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](#)

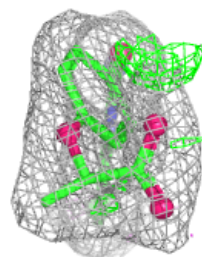
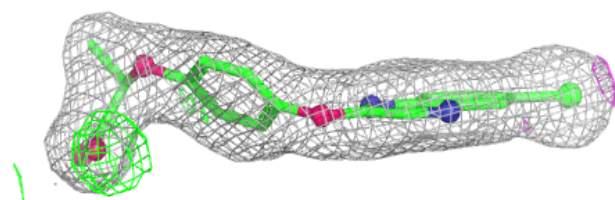
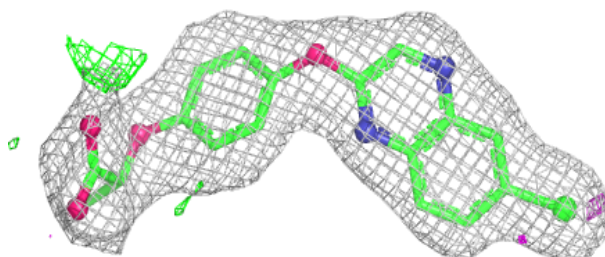
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FTJ	A	501	24/24	0.96	0.07	20,27,51,55	0
2	FTJ	B	501	24/24	0.97	0.06	15,21,37,44	0
2	FTJ	D	501	24/24	0.97	0.06	20,28,37,41	0
2	FTJ	C	501	24/24	0.98	0.05	24,30,42,43	0

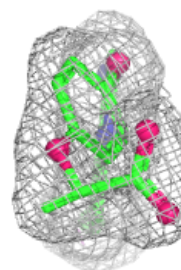
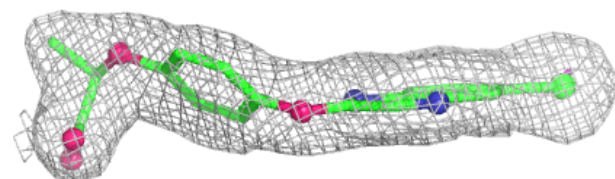
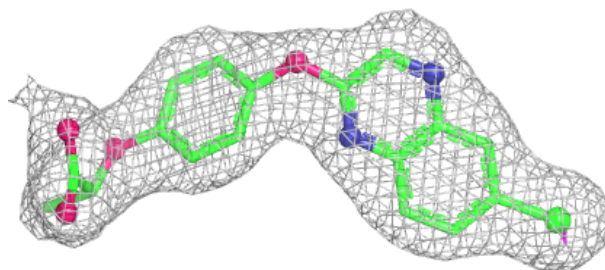
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FTJ A 501:

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

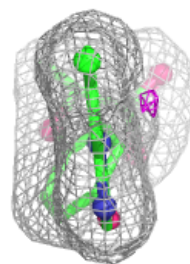
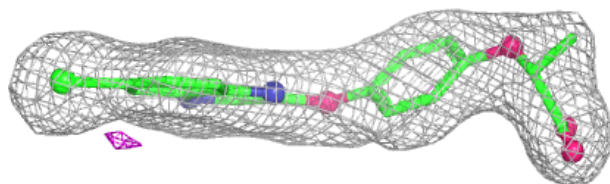
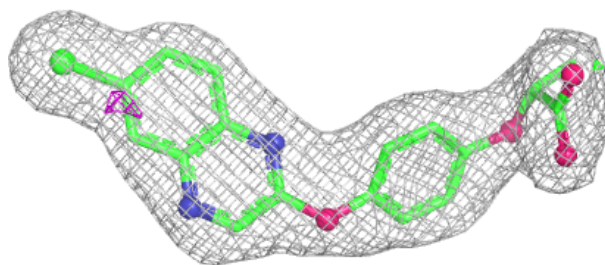
**Electron density around FTJ B 501:**

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

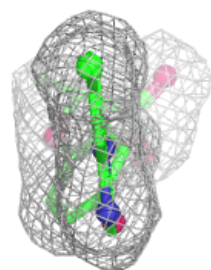
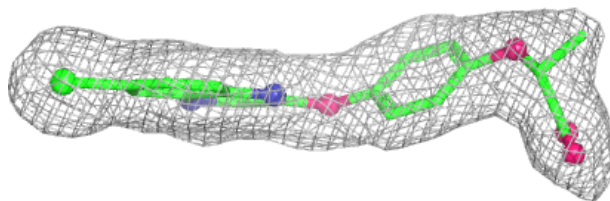
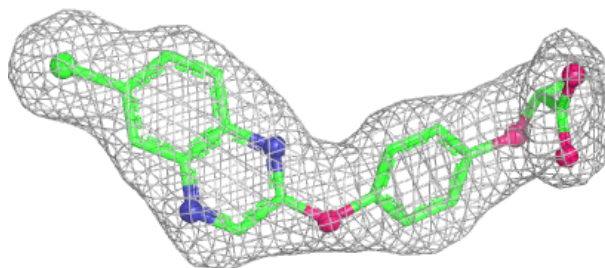


Electron density around FTJ D 501:

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

**Electron density around FTJ C 501:**

$2mF_o-DF_c$ (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.