Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 02:55 PM EDT

PDB ID	:	6P7U
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 (i) 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:

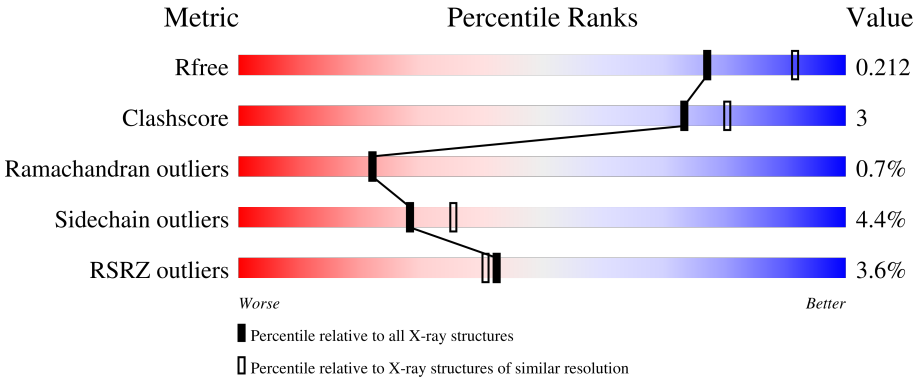
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	79% 10% • 10%
1	B	473	3% 81% 8% • 10%
1	C	473	4% 77% 8% • 13%
1	D	473	5% 84% 6% 10%

2 Entry composition

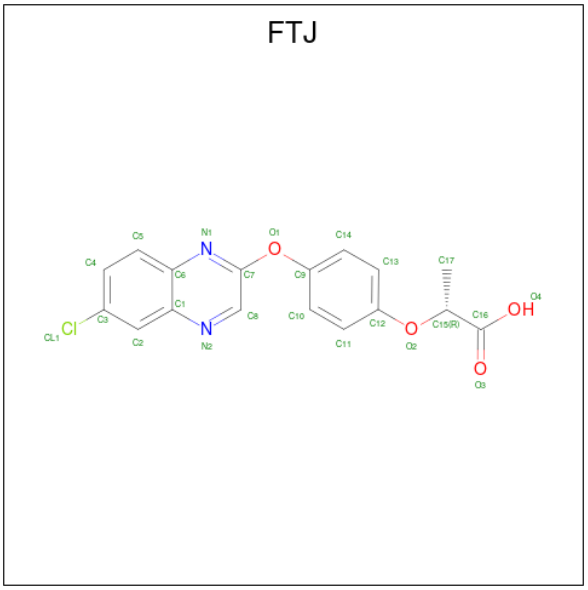
There are 3 unique types of molecules in this entry. The entry contains 13244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: FTJ) (formula: $C_{17}H_{13}ClN_2O_4$) (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	0	0
			24	17	1	2	4		
2	D	1	Total	C	Cl	N	O	0	0
			24	17	1	2	4		

- Molecule 3 is water.

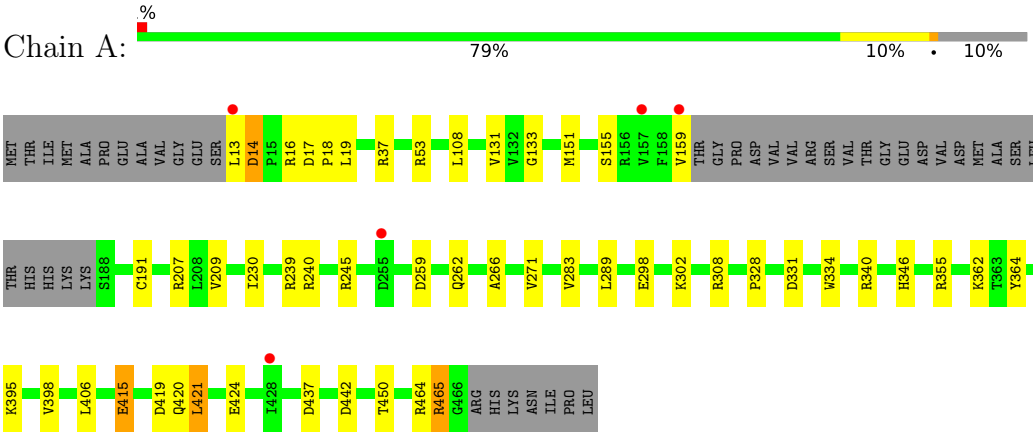
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total	O	0	0
			234	234		
3	B	175	Total	O	0	0
			175	175		
3	C	177	Total	O	0	0
			177	177		
3	D	207	Total	O	0	0
			207	207		

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.

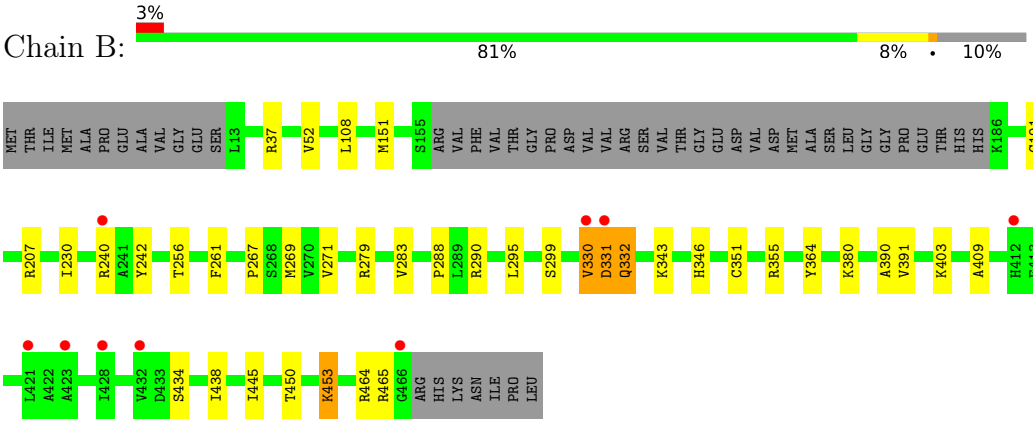
• Molecule 1: Probable propionyl-CoA carboxylase beta chain 6

Chain A:



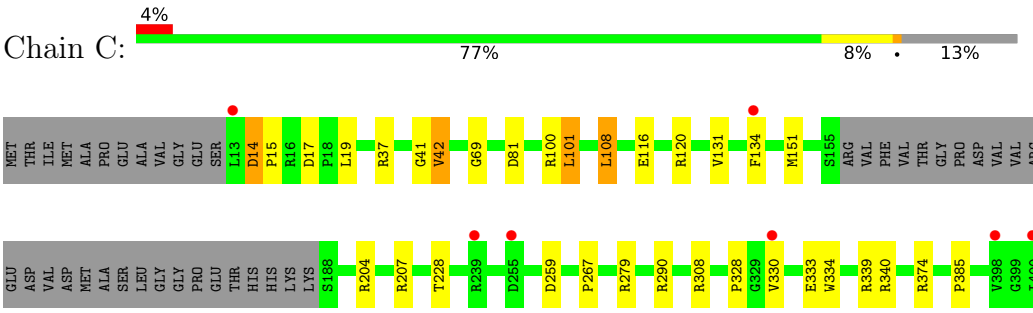
• Molecule 1: Probable propionyl-CoA carboxylase beta chain 6

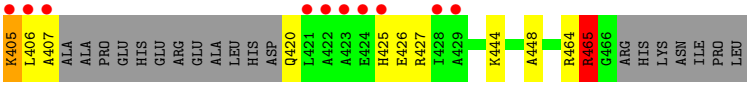
Chain B:



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

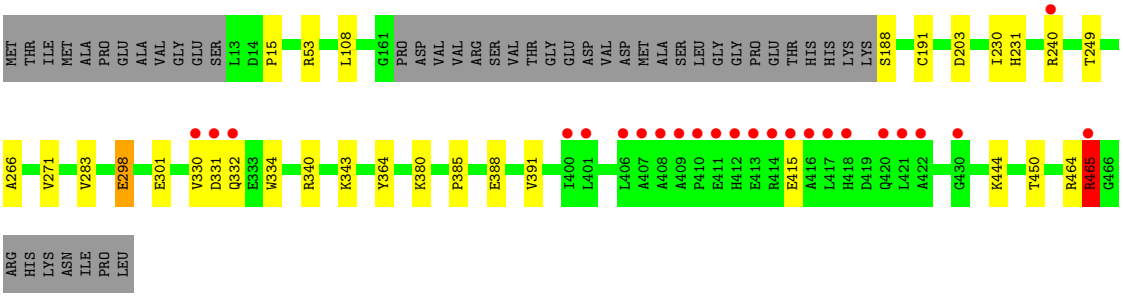
Chain C:





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

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.45 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.171 , 0.206 0.176 , 0.212	Depositor DCC
R_{free} test set	5914 reflections (5.02%)	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 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.38	0/3209	0.54	0/4365
1	B	0.40	0/3185	0.52	0/4330
1	C	0.40	0/3052	0.55	0/4151
1	D	0.38	0/3151	0.52	0/4294
All	All	0.39	0/12597	0.53	0/17140

There are no bond length outliers.

There are no bond angle outliers.

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	21	0
1	B	3123	0	3075	19	0
1	C	2992	0	2921	23	0
1	D	3093	0	3000	21	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	175	0	0	1	0
3	C	177	0	0	1	0
3	D	207	0	0	6	0
All	All	13244	0	12086	80	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 (80) 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:D:465:ARG:CG	3:D:799:HOH:O	2.44	0.65
1:C:41:GLY:C	1:C:42:VAL:CG1	2.66	0.63
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:41:GLY:C	1:C:42:VAL:HG13	2.36	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
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:B:269:MET:HB2	1:B:299:SER:HB2	2.01	0.43
1:C:425:HIS:C	1:C:427:ARG:H	2.21	0.42
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/473 (89%)	412 (97%)	8 (2%)	3 (1%)	22	22
1	B	421/473 (89%)	406 (96%)	13 (3%)	2 (0%)	29	31
1	C	406/473 (86%)	387 (95%)	14 (3%)	5 (1%)	13	10
1	D	424/473 (90%)	407 (96%)	15 (4%)	2 (0%)	29	31
All	All	1674/1892 (88%)	1612 (96%)	50 (3%)	12 (1%)	22	22

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/362 (87%)	295 (93%)	21 (7%)	16	19
1	B	311/362 (86%)	297 (96%)	14 (4%)	27	34
1	C	295/362 (82%)	282 (96%)	13 (4%)	28	35
1	D	302/362 (83%)	294 (97%)	8 (3%)	46	58
All	All	1224/1448 (84%)	1168 (95%)	56 (5%)	28	34

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	19	LEU
1	A	108	LEU
1	A	159	VAL
1	A	209	VAL
1	A	240	ARG
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	406	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	415	GLU
1	A	419	ASP
1	A	420	GLN
1	A	421	LEU
1	A	424	GLU
1	A	437	ASP
1	B	37	ARG
1	B	52	VAL
1	B	108	LEU
1	B	197	ASP
1	B	240	ARG
1	B	256	THR
1	B	279	ARG
1	B	330	VAL
1	B	343	LYS
1	B	346	HIS
1	B	380	LYS
1	B	391	VAL
1	B	403	LYS
1	B	453	LYS
1	C	14	ASP
1	C	19	LEU
1	C	42	VAL
1	C	101	LEU
1	C	108	LEU
1	C	134	PHE
1	C	279	ARG
1	C	308[A]	ARG
1	C	308[B]	ARG
1	C	333	GLU
1	C	374	ARG
1	C	420	GLN
1	C	465	ARG
1	D	108	LEU
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	465	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	501	-	26,26,26	1.37	3 (11%)	36,36,36	2.35	6 (16%)
2	FTJ	A	501	-	26,26,26	1.44	2 (7%)	36,36,36	2.30	6 (16%)
2	FTJ	B	501	-	26,26,26	1.44	4 (15%)	36,36,36	2.31	8 (22%)
2	FTJ	C	501	-	26,26,26	1.31	3 (11%)	36,36,36	2.11	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	D	501	-	-	1/12/12/12	0/3/3/3
2	FTJ	A	501	-	-	4/12/12/12	0/3/3/3
2	FTJ	B	501	-	-	0/12/12/12	0/3/3/3
2	FTJ	C	501	-	-	0/12/12/12	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FTJ	C7-N1	4.46	1.36	1.30
2	D	501	FTJ	C7-N1	3.90	1.35	1.30
2	B	501	FTJ	O2-C15	-3.77	1.37	1.43
2	B	501	FTJ	C7-N1	3.67	1.35	1.30
2	C	501	FTJ	C7-N1	3.63	1.35	1.30
2	C	501	FTJ	O2-C15	-3.49	1.37	1.43
2	A	501	FTJ	O2-C15	-3.25	1.37	1.43
2	D	501	FTJ	O2-C15	-2.95	1.38	1.43
2	B	501	FTJ	C15-C16	-2.13	1.48	1.52
2	C	501	FTJ	C6-C1	-2.11	1.38	1.42
2	D	501	FTJ	C15-C16	-2.07	1.48	1.52
2	B	501	FTJ	C6-C1	-2.00	1.38	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FTJ	C8-C7-N1	-9.99	119.04	124.09
2	B	501	FTJ	C8-C7-N1	-9.08	119.50	124.09
2	A	501	FTJ	C8-C7-N1	-8.92	119.58	124.09
2	C	501	FTJ	C8-C7-N1	-8.06	120.01	124.09
2	B	501	FTJ	C7-N1-C6	7.02	120.93	115.79
2	D	501	FTJ	C7-N1-C6	6.49	120.54	115.79
2	C	501	FTJ	C7-N1-C6	6.22	120.34	115.79
2	A	501	FTJ	C7-N1-C6	5.71	119.97	115.79
2	A	501	FTJ	O1-C7-N1	5.08	126.59	120.14
2	D	501	FTJ	O1-C7-N1	3.89	125.08	120.14
2	C	501	FTJ	O1-C7-N1	3.07	124.04	120.14
2	B	501	FTJ	O1-C7-N1	3.02	123.97	120.14
2	B	501	FTJ	O2-C15-C16	-2.84	107.70	111.34
2	C	501	FTJ	C7-C8-N2	-2.68	120.24	121.86
2	C	501	FTJ	C12-O2-C15	2.61	122.80	118.29
2	B	501	FTJ	C7-C8-N2	-2.47	120.37	121.86
2	A	501	FTJ	C5-C6-N1	2.34	122.26	118.69
2	D	501	FTJ	C8-N2-C1	2.27	119.64	116.91
2	B	501	FTJ	C8-N2-C1	2.24	119.61	116.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FTJ	O2-C15-C17	2.18	110.87	106.82
2	C	501	FTJ	C8-N2-C1	2.15	119.50	116.91
2	B	501	FTJ	C1-C6-N1	-2.13	118.41	121.18
2	A	501	FTJ	O2-C15-C16	-2.07	108.68	111.34
2	D	501	FTJ	C5-C6-N1	2.07	121.85	118.69
2	A	501	FTJ	C1-C6-N1	-2.05	118.51	121.18
2	B	501	FTJ	C12-O2-C15	2.04	121.82	118.29

There are no chirality outliers.

All (5) 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	D	501	FTJ	C17-C15-C16-O4
2	A	501	FTJ	O2-C15-C16-O4
2	A	501	FTJ	O2-C15-C16-O3

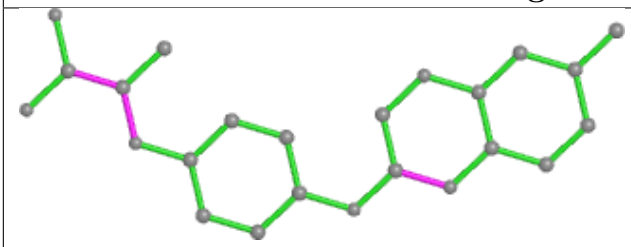
There are no ring outliers.

1 monomer is involved in 1 short contact:

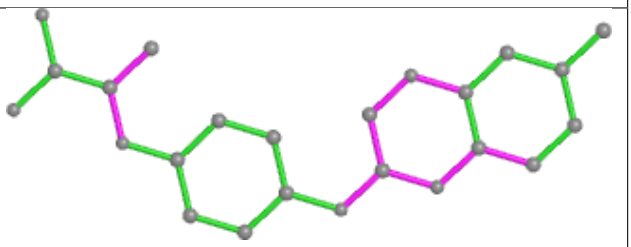
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FTJ	1	0

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 then 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.

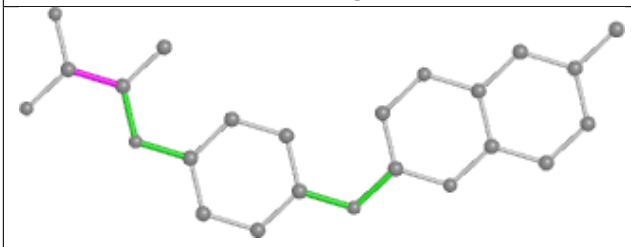
Ligand FTJ D 501



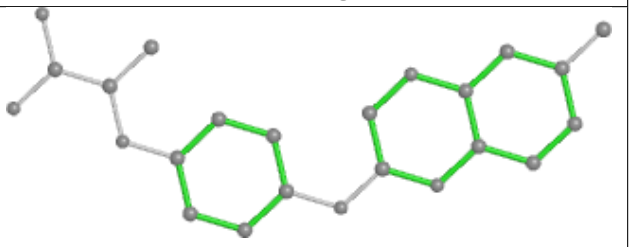
Bond lengths



Bond angles

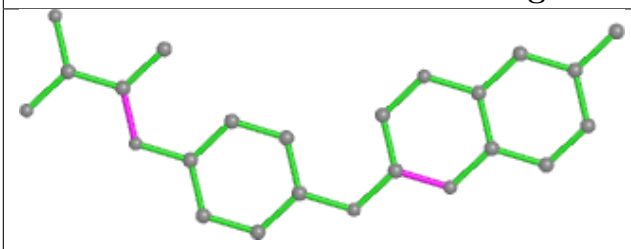


Torsions

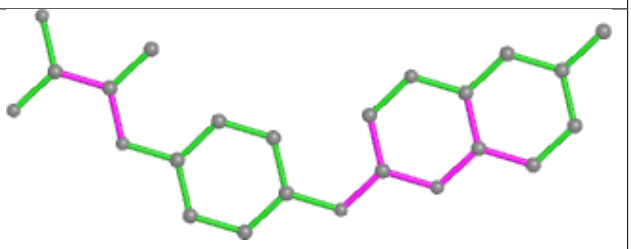


Rings

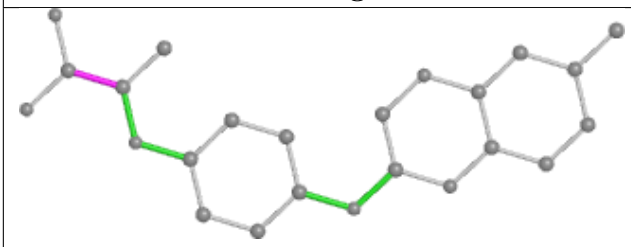
Ligand FTJ A 501



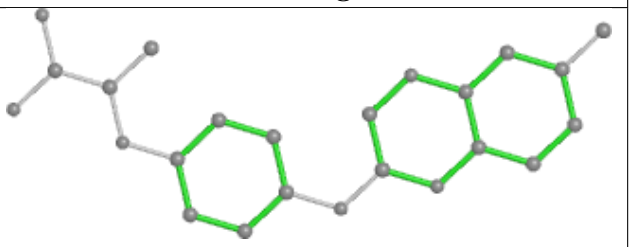
Bond lengths



Bond angles

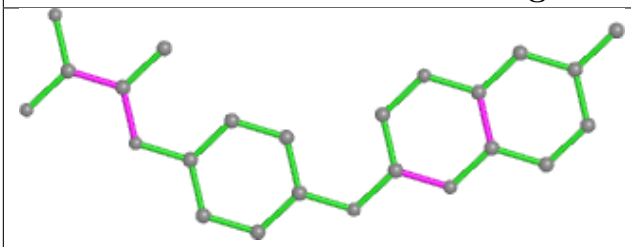


Torsions

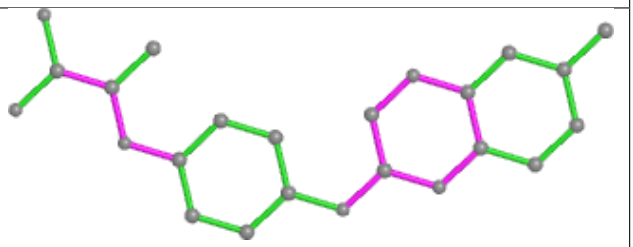


Rings

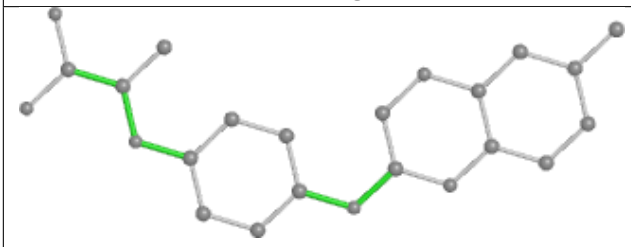
Ligand FTJ B 501



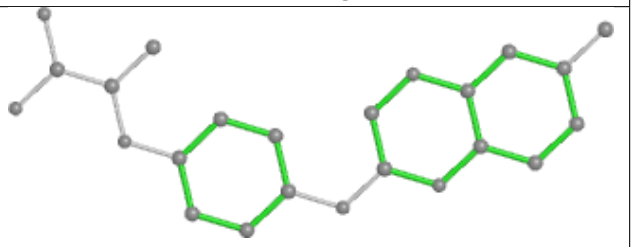
Bond lengths



Bond angles

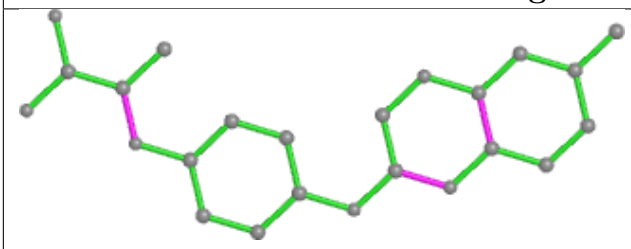


Torsions

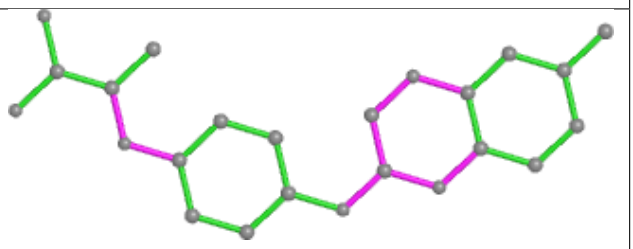


Rings

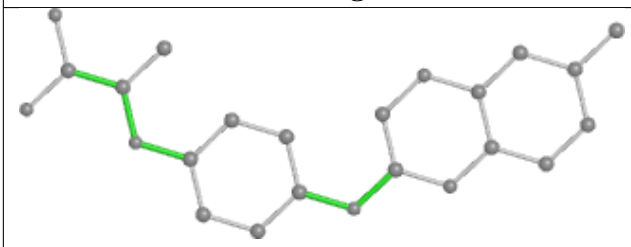
Ligand FTJ C 501



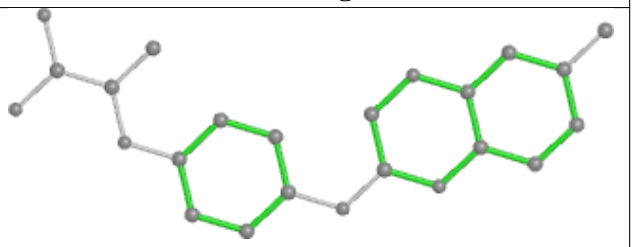
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.26	5 (1%)	79	77	14, 29, 56, 89	0
1	B	424/473 (89%)	-0.12	12 (2%)	53	51	13, 28, 59, 86	0
1	C	410/473 (86%)	-0.04	20 (4%)	29	28	17, 30, 77, 118	0
1	D	428/473 (90%)	-0.15	24 (5%)	24	23	16, 28, 70, 97	0
All	All	1688/1892 (89%)	-0.14	61 (3%)	42	41	13, 29, 67, 118	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	330	VAL	7.1
1	C	401	LEU	7.0
1	D	408	ALA	6.2
1	A	13	LEU	5.8
1	D	416	ALA	5.5
1	D	332	GLN	5.5
1	C	402	HIS	5.1
1	D	330	VAL	4.8
1	C	406	LEU	4.7
1	D	421	LEU	4.7
1	D	465	ARG	4.6
1	C	13	LEU	4.5
1	C	404	LYS	4.5
1	D	409	ALA	4.3
1	D	417	LEU	4.2
1	A	428	ILE	4.2
1	D	430	GLY	4.1
1	C	407	ALA	4.1
1	C	422	ALA	4.1
1	D	401	LEU	3.9
1	D	414	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	405	LYS	3.8
1	C	398	VAL	3.8
1	D	407	ALA	3.7
1	A	157	VAL	3.7
1	D	410	PRO	3.6
1	D	400	ILE	3.6
1	C	425	HIS	3.5
1	B	412	HIS	3.4
1	B	330	VAL	3.4
1	D	413	GLU	3.3
1	D	418	HIS	3.3
1	D	331	ASP	3.2
1	B	331	ASP	3.2
1	D	420	GLN	3.2
1	C	421	LEU	3.1
1	C	423	ALA	3.1
1	B	428	ILE	3.1
1	B	466	GLY	2.9
1	C	429	ALA	2.8
1	B	423	ALA	2.8
1	C	424	GLU	2.8
1	A	255	ASP	2.8
1	D	412	HIS	2.8
1	C	428	ILE	2.7
1	B	416	ALA	2.4
1	D	411	GLU	2.4
1	D	240	ARG	2.4
1	C	239	ARG	2.4
1	B	414	ARG	2.3
1	D	422	ALA	2.3
1	B	421	LEU	2.3
1	A	159	VAL	2.3
1	B	417	LEU	2.3
1	B	240	ARG	2.3
1	B	432	VAL	2.1
1	C	134	PHE	2.1
1	C	400	ILE	2.0
1	D	406	LEU	2.0
1	D	415	GLU	2.0
1	C	255	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

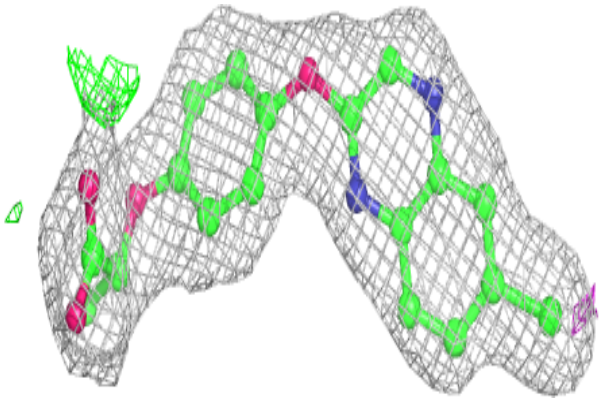
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

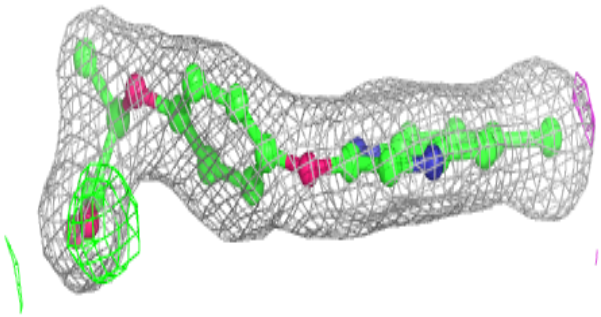
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FTJ	A	501	24/24	0.97	0.10	20,27,51,55	0
2	FTJ	B	501	24/24	0.97	0.11	15,21,37,44	0
2	FTJ	D	501	24/24	0.97	0.10	20,28,37,41	0
2	FTJ	C	501	24/24	0.98	0.09	24,30,42,43	0

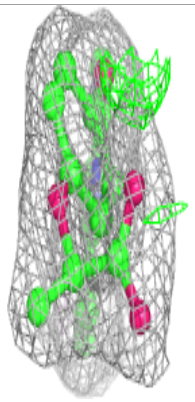
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

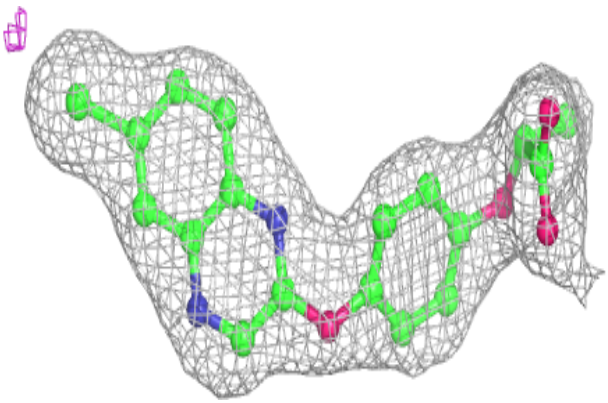


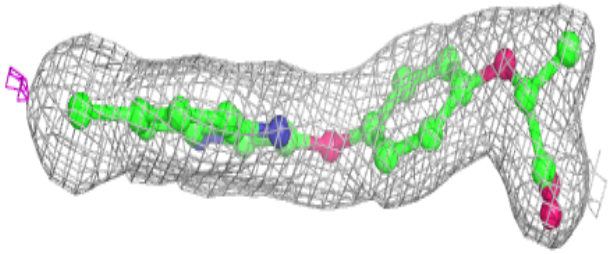


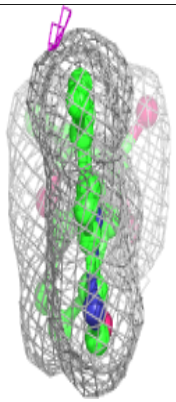


Electron density around FTJ B 501:

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

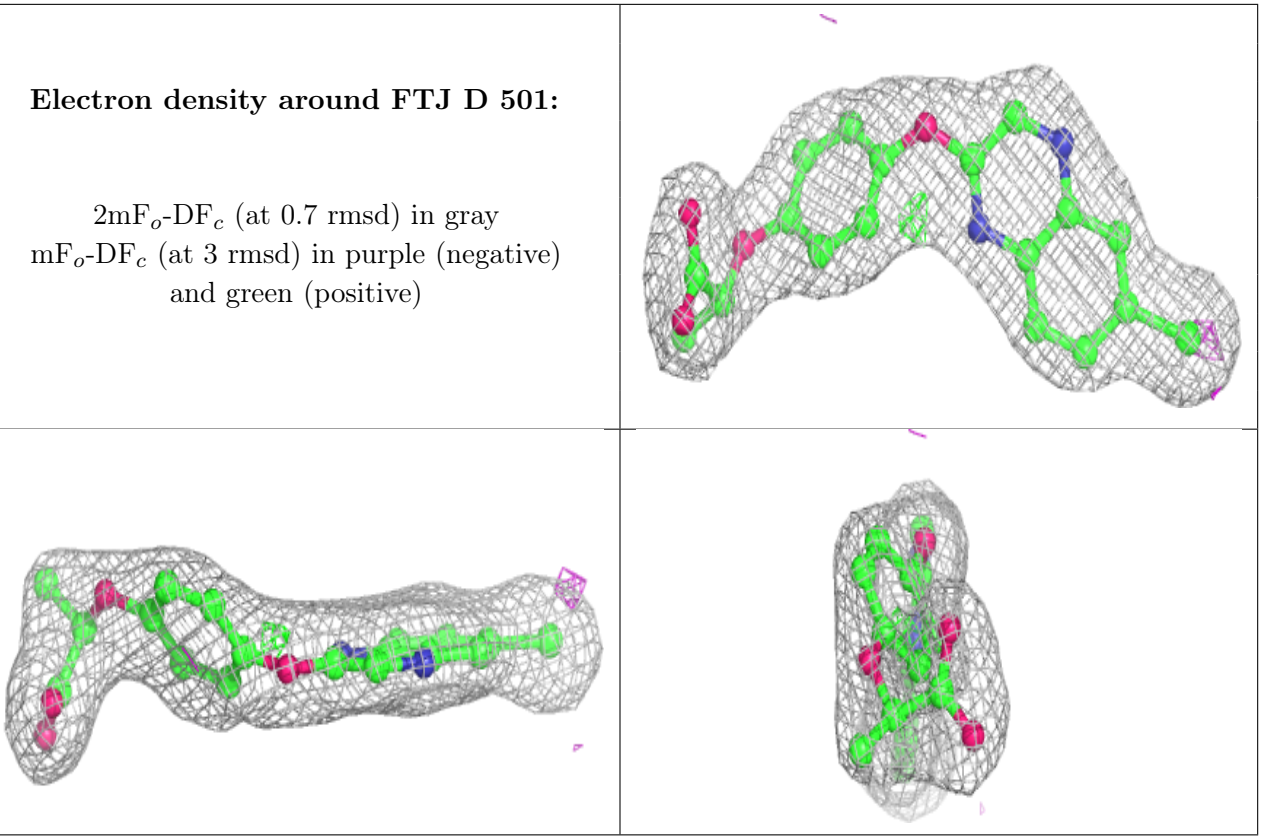






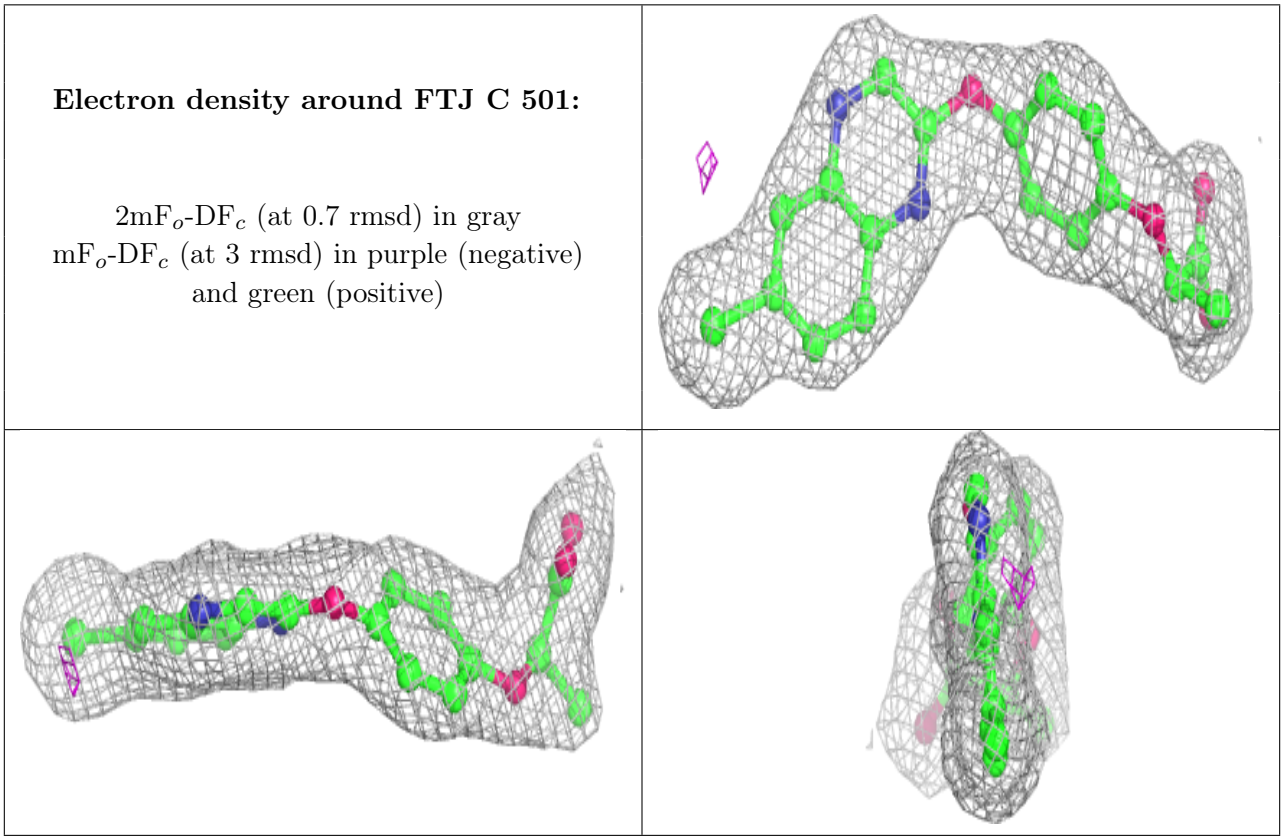
Electron density around FTJ D 501:

$2mF_o$-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.