Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:14 PM BST

PDB ID	:	6PK2
Title	:	CRYSTAL STRUCTURE OF THE CARBOXYLTRANSFERASE SUBUNIT OF ACC (ACCD6) IN COMPLEX WITH INHIBITOR QUIZALOFOP-P derivative FROM MYCOBACTERIUM TUBERCULOSIS
Authors	:	Reddy, M.C.M.; Nian, Z.; Michele, T.C.B.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2019-06-28
Resolution	:	2.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

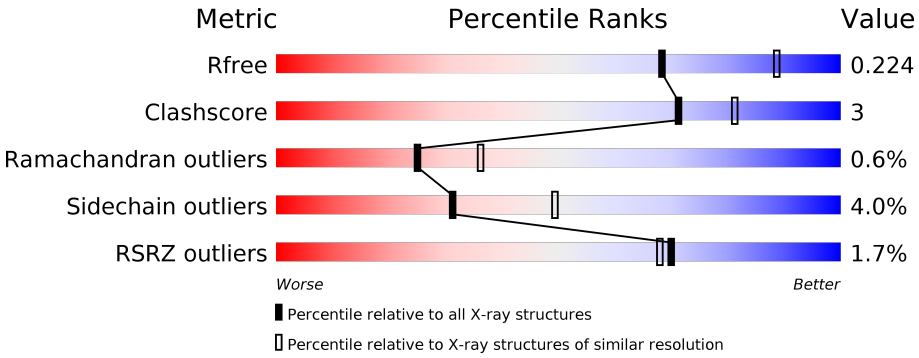
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	81% 8% • 10%
1	B	473	81% 8% 10%
1	C	473	2% 74% 11% • 13%
1	D	473	4% 82% 7% • 10%
1	E	473	% 82% 8% • 10%
1	F	473	81% 9% 10%

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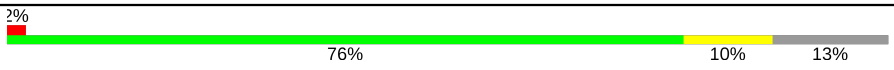
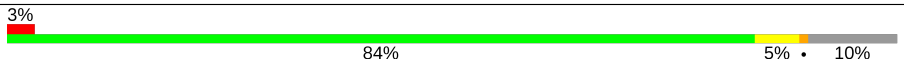
Mol	Chain	Length	Quality of chain
1	G	473	
1	H	473	

2 Entry composition

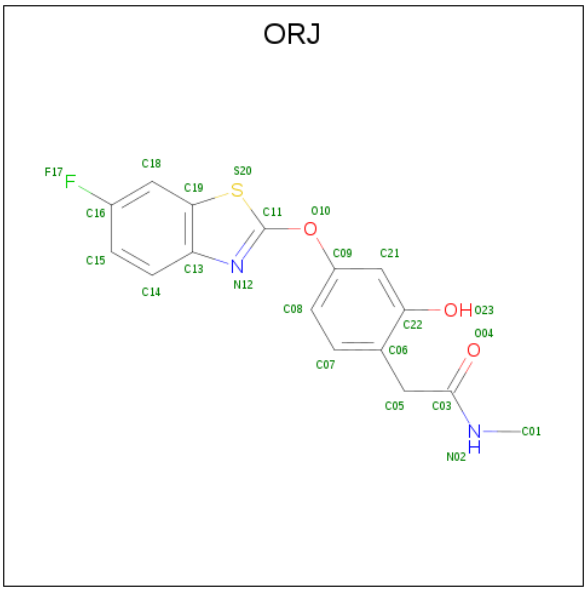
There are 3 unique types of molecules in this entry. The entry contains 25923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Propionyl-CoA carboxylase subunit beta.

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	0	0
			3115	1953	566	582	14			
1	C	410	Total	C	N	O	S	0	2	0
			2985	1871	539	561	14			
1	D	428	Total	C	N	O	S	0	0	0
			3101	1944	559	584	14			
1	E	426	Total	C	N	O	S	0	1	0
			3147	1969	572	592	14			
1	F	424	Total	C	N	O	S	0	1	0
			3123	1958	569	582	14			
1	G	410	Total	C	N	O	S	0	2	0
			2991	1874	542	561	14			
1	H	428	Total	C	N	O	S	0	0	0
			3097	1942	558	583	14			

- Molecule 2 is 2-{4-[(6-fluoro-1,3-benzothiazol-2-yl)oxy]-2-hydroxyphenyl}-N-methylacetamide (three-letter code: ORJ) (formula: $C_{16}H_{13}FN_2O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
2	C	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
2	D	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
2	E	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
2	F	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
2	G	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
2	G	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total	O	0	0
			143	143		
3	B	131	Total	O	0	0
			131	131		
3	C	130	Total	O	0	0
			130	130		
3	D	132	Total	O	0	0
			132	132		

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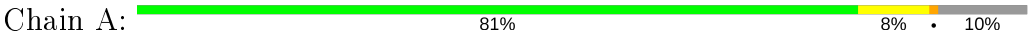
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	141	Total O 141 141	0	0
3	F	124	Total O 124 124	0	0
3	G	121	Total O 121 121	0	0
3	H	111	Total O 111 111	0	0

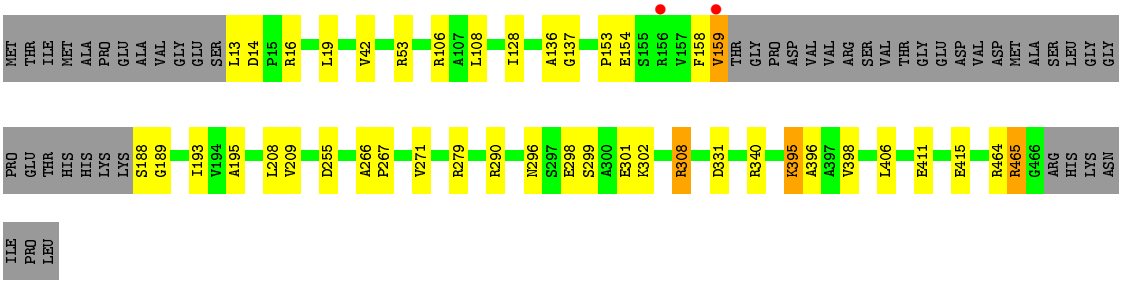
3 Residue-property plots (i)

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: Propionyl-CoA carboxylase subunit beta

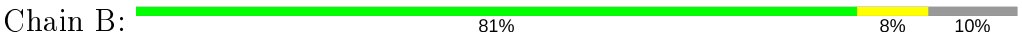
Chain A:

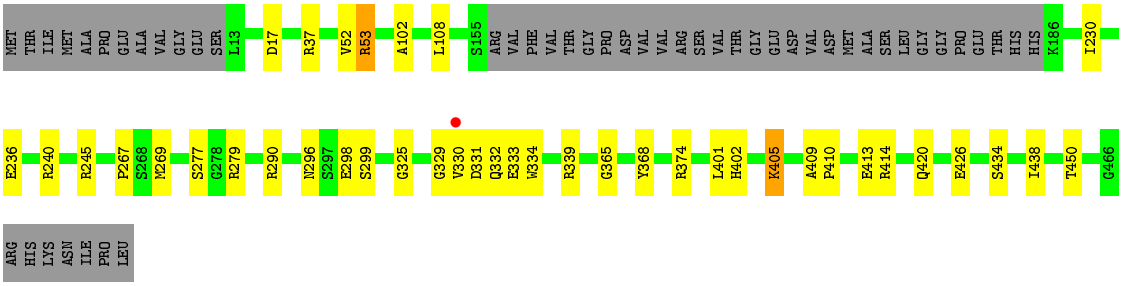




- Molecule 1: Propionyl-CoA carboxylase subunit beta

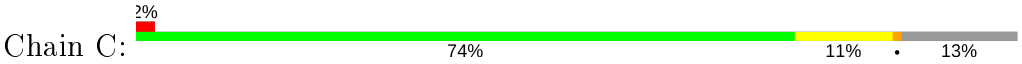
Chain B:

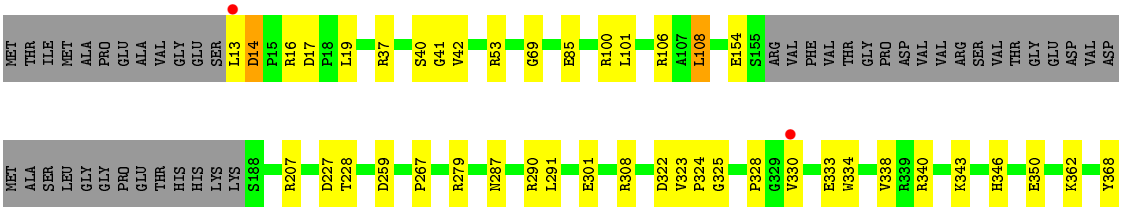


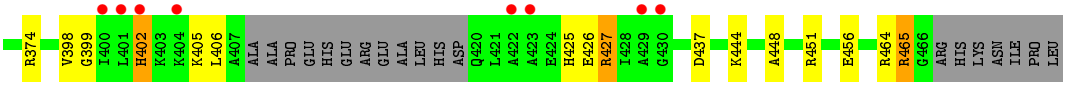


- Molecule 1: Propionyl-CoA carboxylase subunit beta

Chain C:

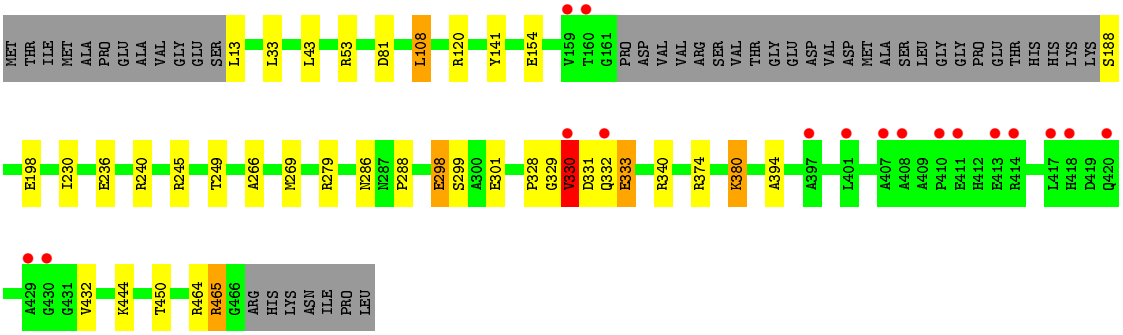






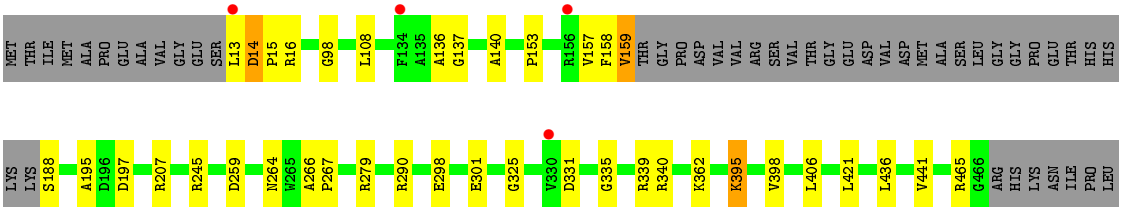
• Molecule 1: Propionyl-CoA carboxylase subunit beta

Chain D:



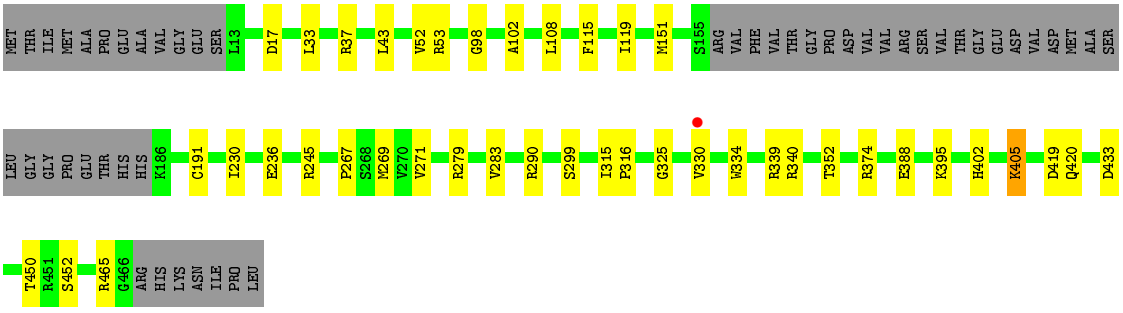
• Molecule 1: Propionyl-CoA carboxylase subunit beta

Chain E:



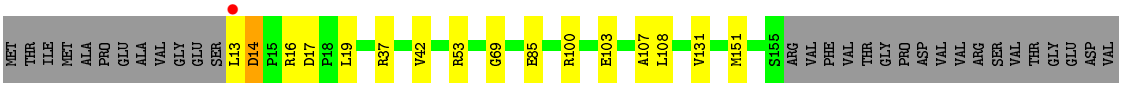
• Molecule 1: Propionyl-CoA carboxylase subunit beta

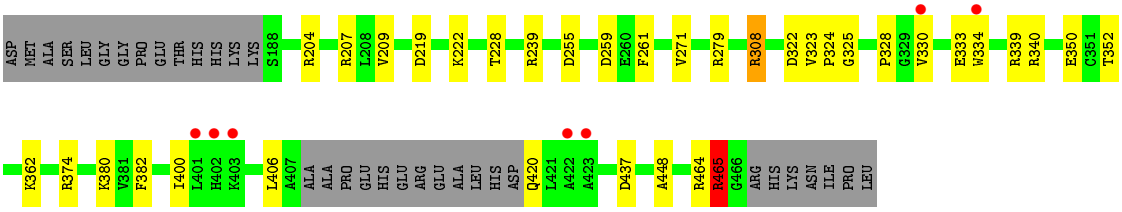
Chain F:



• Molecule 1: Propionyl-CoA carboxylase subunit beta

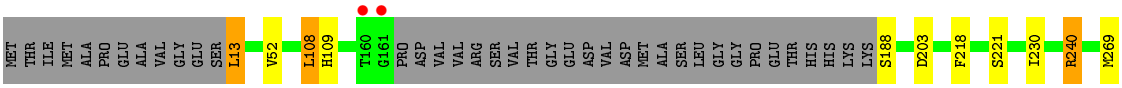
Chain G:

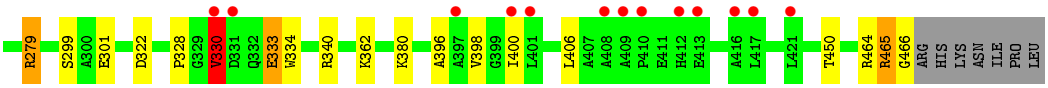




- Molecule 1: Propionyl-CoA carboxylase subunit beta

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.12Å 149.80Å 152.96Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	48.44 – 2.40 48.44 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.44-2.40) 98.6 (48.44-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.173 , 0.222 0.175 , 0.224	Depositor DCC
R_{free} test set	2017 reflections (1.14%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 26.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k 0.008 for -h,-l,-k 0.477 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25923	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.35% 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: ORJ

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	0.41	0/3209	0.54	0/4365
1	B	0.40	0/3174	0.55	0/4316
1	C	0.44	0/3045	0.57	0/4144
1	D	0.45	1/3159 (0.0%)	0.55	0/4304
1	E	0.42	0/3209	0.54	0/4365
1	F	0.40	0/3185	0.54	0/4330
1	G	0.41	0/3051	0.56	0/4151
1	H	0.41	0/3155	0.54	0/4299
All	All	0.42	1/25187 (0.0%)	0.55	0/34274

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	329	GLY	N-CA	-5.78	1.37	1.46

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	26	0
1	B	3115	0	3062	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2985	0	2908	28	0
1	D	3101	0	3010	26	0
1	E	3147	0	3090	20	0
1	F	3123	0	3075	22	0
1	G	2991	0	2919	24	0
1	H	3097	0	3004	18	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
2	E	23	0	0	1	0
2	F	23	0	0	1	0
2	G	46	0	0	0	0
3	A	143	0	0	4	0
3	B	131	0	0	2	0
3	C	130	0	0	5	0
3	D	132	0	0	6	0
3	E	141	0	0	2	0
3	F	124	0	0	2	0
3	G	121	0	0	2	0
3	H	111	0	0	2	0
All	All	25923	0	24158	170	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 (170) 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:D:330:VAL:CG1	1:D:331:ASP:H	1.21	1.33
1:D:330:VAL:HG13	1:D:331:ASP:H	0.98	1.11
1:D:330:VAL:HG12	1:D:331:ASP:H	1.12	1.10
1:D:330:VAL:CG1	1:D:331:ASP:N	1.98	1.08
1:D:330:VAL:HG13	1:D:331:ASP:N	1.68	1.03
1:G:464:ARG:O	1:G:465:ARG:HB2	1.55	0.99
1:D:330:VAL:HG12	1:D:331:ASP:N	1.76	0.86
1:F:405:LYS:H	1:F:405:LYS:HE3	1.44	0.79
1:A:395:LYS:HD3	1:A:395:LYS:H	1.47	0.78
1:E:395:LYS:HD3	1:E:395:LYS:H	1.49	0.77
1:D:330:VAL:HB	1:D:333:GLU:HB2	1.67	0.76
1:D:245:ARG:NH1	3:D:601:HOH:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HA	1:C:16:ARG:HH21	1.51	0.74
1:F:17:ASP:OD1	1:F:37:ARG:NH2	2.21	0.73
1:A:188:SER:O	1:B:339:ARG:NH1	2.21	0.73
1:C:308[A]:ARG:NH2	1:C:350:GLU:OE2	2.22	0.73
1:A:415:GLU:HG2	3:A:642:HOH:O	1.90	0.71
1:F:53:ARG:NH2	3:F:601:HOH:O	2.24	0.70
1:D:266:ALA:HB2	1:D:298:GLU:HB3	1.75	0.69
1:A:53:ARG:NE	3:A:601:HOH:O	2.27	0.68
1:C:402:HIS:HB3	1:C:406:LEU:HG	1.74	0.68
1:F:325:GLY:HA2	3:F:644:HOH:O	1.98	0.63
1:B:17:ASP:OD1	1:B:37:ARG:NH2	2.26	0.62
1:D:380:LYS:NZ	3:D:602:HOH:O	2.25	0.62
1:F:98:GLY:HA3	2:F:501:ORJ:C01	2.31	0.60
1:A:464:ARG:O	1:A:465:ARG:HB2	2.01	0.60
1:F:402:HIS:HA	1:F:405:LYS:HD2	1.82	0.60
1:E:188:SER:O	1:F:339:ARG:NH1	2.36	0.59
1:B:267:PRO:HB2	1:B:290:ARG:HG3	1.85	0.59
1:C:301:GLU:HB2	1:C:340:ARG:HD2	1.85	0.59
1:B:325:GLY:HA2	3:B:634:HOH:O	2.02	0.58
1:G:308[A]:ARG:NH2	1:G:350:GLU:OE1	2.37	0.58
1:H:328:PRO:HD3	1:H:334:TRP:CH2	2.38	0.58
1:C:13:LEU:HA	1:C:16:ARG:NH2	2.20	0.57
1:B:331:ASP:O	1:B:333:GLU:N	2.34	0.57
1:B:410:PRO:HB2	1:B:413:GLU:HG2	1.87	0.56
1:A:106:ARG:NE	1:B:438:ILE:HD12	2.21	0.55
1:G:339:ARG:NH2	1:H:188:SER:O	2.34	0.55
1:H:340:ARG:NE	3:H:511:HOH:O	2.39	0.55
1:E:159:VAL:HG23	1:F:334:TRP:CD2	2.41	0.55
1:B:230:ILE:HD12	1:B:450:THR:HB	1.89	0.55
1:C:17:ASP:OD1	1:C:37:ARG:NH2	2.40	0.55
1:B:102:ALA:CB	1:G:14:ASP:HB3	2.37	0.54
1:A:154:GLU:N	3:A:602:HOH:O	2.28	0.54
1:A:13:LEU:CB	1:A:16:ARG:HH21	2.21	0.54
1:A:266:ALA:HB2	1:A:298:GLU:HB2	1.91	0.53
1:A:267:PRO:HB2	1:A:290:ARG:HG3	1.91	0.53
1:H:230:ILE:HD12	1:H:450:THR:HB	1.91	0.53
1:F:269:MET:HB2	1:F:299:SER:HB2	1.91	0.52
1:F:352:THR:HB	1:F:465:ARG:H	1.74	0.52
1:G:17:ASP:OD2	1:G:37:ARG:NH2	2.43	0.52
1:F:267:PRO:HB2	1:F:290:ARG:HG3	1.92	0.52
1:A:136:ALA:HA	1:A:158:PHE:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLU:HB2	1:A:340:ARG:HD2	1.92	0.51
1:D:53:ARG:HG3	3:D:612:HOH:O	2.10	0.51
1:C:425:HIS:O	1:C:427:ARG:N	2.42	0.51
1:D:81:ASP:OD1	1:D:120:ARG:NH2	2.28	0.51
1:G:131:VAL:HB	1:G:151:MET:HG2	1.93	0.51
1:C:287:ASN:ND2	3:C:604:HOH:O	2.34	0.51
1:C:14:ASP:HB3	1:F:102:ALA:CB	2.40	0.51
1:F:230:ILE:HD12	1:F:450:THR:HB	1.93	0.51
1:E:266:ALA:HB2	1:E:298:GLU:HB2	1.93	0.50
1:E:136:ALA:HA	1:E:158:PHE:O	2.12	0.50
1:C:308[B]:ARG:HH22	1:C:343:LYS:HE3	1.75	0.50
1:E:98:GLY:HA3	2:E:501:ORJ:C01	2.42	0.50
1:B:402:HIS:HA	1:B:405:LYS:HE2	1.94	0.49
1:E:335:GLY:O	1:E:339:ARG:HG3	2.12	0.49
1:H:330:VAL:HG23	1:H:333:GLU:HB2	1.94	0.49
1:E:207:ARG:NH1	1:E:259:ASP:OD1	2.45	0.49
1:D:240:ARG:NH1	3:D:615:HOH:O	2.45	0.49
1:A:159:VAL:HG23	1:B:334:TRP:CD2	2.48	0.49
1:D:301:GLU:HB2	1:D:340:ARG:HD2	1.94	0.49
1:B:330:VAL:N	1:B:331:ASP:O	2.46	0.49
1:G:465:ARG:HA	1:G:465:ARG:HD2	1.47	0.48
1:C:323:VAL:HA	1:C:324:PRO:HD3	1.69	0.48
1:G:374:ARG:HG3	1:H:109:HIS:HE1	1.79	0.48
1:G:69:GLY:HA3	1:G:100:ARG:HD2	1.95	0.48
1:F:115:PHE:O	1:F:119:ILE:HG12	2.13	0.48
1:C:464:ARG:O	1:C:465:ARG:HB2	2.12	0.48
1:G:204[B]:ARG:NH2	1:G:259:ASP:OD1	2.47	0.48
1:G:207:ARG:HD2	1:G:259:ASP:OD2	2.14	0.48
1:G:323:VAL:HA	1:G:324:PRO:HD3	1.71	0.48
1:A:271:VAL:HG22	1:A:302:LYS:HE2	1.95	0.47
1:D:230:ILE:HG13	1:D:450:THR:HB	1.95	0.47
1:D:53:ARG:NH1	3:D:612:HOH:O	2.40	0.47
1:D:432:VAL:HB	1:D:444:LYS:HE2	1.95	0.47
1:A:331:ASP:N	1:A:331:ASP:OD1	2.41	0.47
1:C:41:GLY:HA2	3:C:628:HOH:O	2.14	0.47
1:H:465:ARG:HG3	1:H:466:GLY:H	1.79	0.47
1:A:308[A]:ARG:NH1	3:A:606:HOH:O	2.37	0.47
1:G:13:LEU:HA	1:G:16:ARG:HH21	1.79	0.47
1:C:228:THR:O	1:C:448:ALA:HA	2.15	0.46
1:D:464:ARG:O	1:D:465:ARG:HB2	2.15	0.46
1:E:301:GLU:HB2	1:E:340:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:396:ALA:O	1:H:400:ILE:HG12	2.16	0.46
1:G:322:ASP:OD1	1:G:362:LYS:HG2	2.16	0.46
1:E:153:PRO:HD3	1:E:195:ALA:O	2.16	0.45
1:H:464:ARG:O	1:H:465:ARG:HB2	2.15	0.45
1:E:159:VAL:HG23	1:F:334:TRP:CE3	2.51	0.45
1:C:328:PRO:HD3	1:C:334:TRP:CH2	2.51	0.45
1:A:153:PRO:HD3	1:A:195:ALA:O	2.16	0.45
1:C:14:ASP:OD2	3:C:601:HOH:O	2.21	0.45
1:G:325:GLY:HA2	3:G:661:HOH:O	2.17	0.45
1:A:128:ILE:HD12	1:A:209:VAL:HG12	1.99	0.45
1:A:395:LYS:HZ2	1:A:396:ALA:H	1.64	0.45
1:D:13:LEU:N	3:D:618:HOH:O	2.50	0.45
1:F:33:LEU:HD22	1:F:43:LEU:HD11	1.99	0.44
1:G:328:PRO:HD3	1:G:334:TRP:CH2	2.52	0.44
1:G:219:ASP:OD2	1:G:222:LYS:HE2	2.17	0.44
1:C:207:ARG:HD2	1:C:259:ASP:OD2	2.18	0.44
1:G:261:PHE:HB2	1:G:271:VAL:HG23	1.99	0.43
1:G:380:LYS:HE2	1:G:382:PHE:CE1	2.53	0.43
1:B:434:SER:O	1:B:438:ILE:HG12	2.18	0.43
1:A:106:ARG:NE	1:B:438:ILE:CD1	2.82	0.43
1:C:267:PRO:HB2	1:C:290:ARG:HG3	2.00	0.43
1:E:436:LEU:HD23	1:E:441:VAL:O	2.19	0.43
1:H:218:PHE:CZ	1:H:279:ARG:HD2	2.53	0.43
1:B:269:MET:HB2	1:B:299:SER:HB2	2.01	0.43
1:C:108:LEU:HD12	1:C:108:LEU:HA	1.83	0.43
1:D:236:GLU:H	1:D:236:GLU:CD	2.21	0.43
1:D:286:ASN:O	1:D:288:PRO:HD3	2.19	0.43
1:G:308[A]:ARG:HD2	3:G:604:HOH:O	2.18	0.43
1:G:103:GLU:HB2	1:G:107:ALA:HB2	2.01	0.43
1:A:189:GLY:HA3	1:B:339:ARG:NH1	2.33	0.43
1:B:365:GLY:O	1:B:368:TYR:HB3	2.19	0.43
1:H:269:MET:HB2	1:H:299:SER:HB2	2.00	0.43
1:A:296:ASN:H	1:A:299:SER:HG	1.64	0.43
1:F:151:MET:HB2	1:F:191:CYS:SG	2.59	0.43
1:B:409:ALA:O	1:B:414:ARG:NH2	2.51	0.42
1:G:228:THR:O	1:G:448:ALA:HA	2.18	0.42
1:D:108:LEU:HA	1:D:108:LEU:HD12	1.84	0.42
1:E:137:GLY:HA2	1:E:159:VAL:HG12	2.02	0.42
1:E:14:ASP:N	1:E:15:PRO:HD2	2.34	0.42
1:F:315:ILE:HA	1:F:316:PRO:HD3	1.81	0.42
1:H:398:VAL:HG12	1:H:406:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:VAL:HG23	1:C:399:GLY:H	1.85	0.42
1:A:159:VAL:HG23	1:B:334:TRP:CE3	2.54	0.42
1:C:322:ASP:OD1	1:C:362:LYS:HG2	2.20	0.42
1:C:227:ASP:OD1	1:C:451:ARG:HB3	2.20	0.42
1:E:140:ALA:HB1	1:E:157:VAL:HG13	2.01	0.42
1:F:405:LYS:CE	1:F:405:LYS:H	2.23	0.42
1:C:338:VAL:HA	1:D:141:TYR:CE2	2.54	0.42
1:H:322:ASP:OD1	1:H:362:LYS:HG2	2.20	0.42
1:D:269:MET:HB2	1:D:299:SER:HB2	2.01	0.42
1:C:40:SER:HB2	1:C:42:VAL:H	1.85	0.41
1:C:69:GLY:HA3	1:C:100:ARG:HD2	2.01	0.41
1:G:340:ARG:HH22	1:H:301:GLU:CD	2.23	0.41
1:A:193:ILE:HD12	1:A:208:LEU:HD11	2.01	0.41
1:B:331:ASP:C	1:B:333:GLU:H	2.19	0.41
1:F:395:LYS:NZ	1:F:419:ASP:OD1	2.53	0.41
1:G:352:THR:HB	1:G:465:ARG:H	1.85	0.41
1:H:13:LEU:HD22	1:H:13:LEU:HA	1.93	0.41
1:D:33:LEU:HD22	1:D:43:LEU:HD11	2.02	0.41
1:E:13:LEU:CB	1:E:16:ARG:HE	2.34	0.41
1:E:325:GLY:HA2	3:E:655:HOH:O	2.20	0.41
1:H:108:LEU:HA	1:H:108:LEU:HD12	1.95	0.41
1:H:221:SER:OG	3:H:501:HOH:O	2.22	0.41
1:C:325:GLY:HA2	3:C:624:HOH:O	2.21	0.41
1:E:267:PRO:HB2	1:E:290:ARG:HG3	2.03	0.41
1:C:106:ARG:NE	3:C:602:HOH:O	2.22	0.41
1:E:264:ASN:OD1	3:E:601:HOH:O	2.21	0.41
1:D:154:GLU:OE1	1:D:198:GLU:HB2	2.22	0.40
1:F:340:ARG:HD3	1:F:340:ARG:HA	1.89	0.40
1:B:53:ARG:NH2	3:B:614:HOH:O	2.52	0.40
1:A:137:GLY:HA2	1:A:159:VAL:HG12	2.02	0.40
1:B:296:ASN:H	1:B:299:SER:HG	1.69	0.40
1:E:331:ASP:OD1	1:E:331:ASP:N	2.52	0.40
1:H:240:ARG:HH11	1:H:240:ARG:HB2	1.86	0.40
1:F:271:VAL:HA	1:F:283:VAL:O	2.22	0.40
1:A:411:GLU:HB2	1:C:291:LEU:HD22	2.04	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%)	409 (97%)	12 (3%)	2 (0%)	29	41
1	B	420/473 (89%)	409 (97%)	9 (2%)	2 (0%)	29	41
1	C	406/473 (86%)	384 (95%)	16 (4%)	6 (2%)	10	14
1	D	424/473 (90%)	403 (95%)	17 (4%)	4 (1%)	17	25
1	E	423/473 (89%)	411 (97%)	12 (3%)	0	100	100
1	F	421/473 (89%)	411 (98%)	9 (2%)	1 (0%)	47	62
1	G	406/473 (86%)	385 (95%)	18 (4%)	3 (1%)	22	32
1	H	424/473 (90%)	410 (97%)	12 (3%)	2 (0%)	29	41
All	All	3347/3784 (88%)	3222 (96%)	105 (3%)	20 (1%)	25	36

All (20) 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	330	VAL
1	D	394	ALA
1	G	330	VAL
1	H	330	VAL
1	C	405	LYS
1	C	427	ARG
1	D	465	ARG
1	G	465	ARG
1	C	426	GLU
1	H	465	ARG
1	D	328	PRO
1	A	14	ASP
1	G	400	ILE

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Mol	Chain	Res	Type
1	B	329	GLY
1	C	14	ASP
1	F	330	VAL

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%)	305 (96%)	11 (4%)	36	55
1	B	310/362 (86%)	296 (96%)	14 (4%)	27	44
1	C	294/362 (81%)	279 (95%)	15 (5%)	24	39
1	D	304/362 (84%)	294 (97%)	10 (3%)	38	57
1	E	316/362 (87%)	304 (96%)	12 (4%)	33	51
1	F	311/362 (86%)	300 (96%)	11 (4%)	36	55
1	G	295/362 (82%)	278 (94%)	17 (6%)	20	32
1	H	303/362 (84%)	294 (97%)	9 (3%)	41	61
All	All	2449/2896 (85%)	2350 (96%)	99 (4%)	31	49

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	42	VAL
1	A	108	LEU
1	A	159	VAL
1	A	255	ASP
1	A	279	ARG
1	A	308[A]	ARG
1	A	308[B]	ARG
1	A	395	LYS
1	A	398	VAL
1	A	406	LEU
1	B	52	VAL

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Mol	Chain	Res	Type
1	B	53	ARG
1	B	108	LEU
1	B	236	GLU
1	B	240	ARG
1	B	245	ARG
1	B	277	SER
1	B	279	ARG
1	B	298	GLU
1	B	374	ARG
1	B	401	LEU
1	B	405	LYS
1	B	420	GLN
1	B	426	GLU
1	C	19	LEU
1	C	53	ARG
1	C	85	GLU
1	C	101	LEU
1	C	108	LEU
1	C	154	GLU
1	C	279	ARG
1	C	333	GLU
1	C	346	HIS
1	C	368	TYR
1	C	374	ARG
1	C	402	HIS
1	C	437	ASP
1	C	444	LYS
1	C	456	GLU
1	D	108	LEU
1	D	188	SER
1	D	249	THR
1	D	279	ARG
1	D	298	GLU
1	D	330	VAL
1	D	332	GLN
1	D	333	GLU
1	D	374	ARG
1	D	380	LYS
1	E	14	ASP
1	E	108	LEU
1	E	159	VAL
1	E	197	ASP

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Mol	Chain	Res	Type
1	E	245	ARG
1	E	279	ARG
1	E	362	LYS
1	E	395	LYS
1	E	398	VAL
1	E	406	LEU
1	E	421	LEU
1	E	465	ARG
1	F	52	VAL
1	F	108	LEU
1	F	236	GLU
1	F	245	ARG
1	F	279	ARG
1	F	374	ARG
1	F	388	GLU
1	F	405	LYS
1	F	420	GLN
1	F	433	ASP
1	F	452	SER
1	G	14	ASP
1	G	19	LEU
1	G	42	VAL
1	G	53	ARG
1	G	85	GLU
1	G	108	LEU
1	G	209	VAL
1	G	239	ARG
1	G	255	ASP
1	G	279	ARG
1	G	308[A]	ARG
1	G	308[B]	ARG
1	G	333	GLU
1	G	406	LEU
1	G	420	GLN
1	G	437	ASP
1	G	465	ARG
1	H	13	LEU
1	H	52	VAL
1	H	108	LEU
1	H	203	ASP
1	H	240	ARG
1	H	279	ARG

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Mol	Chain	Res	Type
1	H	330	VAL
1	H	333	GLU
1	H	380	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

8 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	ORJ	G	502	-	22,25,25	2.03	6 (27%)	29,35,35	1.78	6 (20%)
2	ORJ	A	501	-	22,25,25	2.06	6 (27%)	29,35,35	1.75	6 (20%)
2	ORJ	G	501	-	22,25,25	1.99	6 (27%)	29,35,35	1.75	6 (20%)
2	ORJ	C	501	-	22,25,25	1.95	6 (27%)	29,35,35	1.68	6 (20%)
2	ORJ	E	501	-	22,25,25	2.03	6 (27%)	29,35,35	2.16	9 (31%)
2	ORJ	F	501	-	22,25,25	2.02	5 (22%)	29,35,35	2.11	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ORJ	D	501	-	22,25,25	1.98	5 (22%)	29,35,35	1.81	6 (20%)
2	ORJ	B	501	-	22,25,25	2.05	5 (22%)	29,35,35	1.82	6 (20%)

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	ORJ	G	502	-	-	0/8/10/10	0/3/3/3
2	ORJ	A	501	-	-	0/8/10/10	0/3/3/3
2	ORJ	G	501	-	-	0/8/10/10	0/3/3/3
2	ORJ	C	501	-	-	0/8/10/10	0/3/3/3
2	ORJ	E	501	-	-	3/8/10/10	0/3/3/3
2	ORJ	F	501	-	-	3/8/10/10	0/3/3/3
2	ORJ	D	501	-	-	0/8/10/10	0/3/3/3
2	ORJ	B	501	-	-	0/8/10/10	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	502	ORJ	O10-C11	4.93	1.42	1.36
2	A	501	ORJ	O10-C11	4.90	1.42	1.36
2	E	501	ORJ	O10-C11	4.85	1.42	1.36
2	B	501	ORJ	O10-C11	4.69	1.42	1.36
2	C	501	ORJ	O10-C11	4.66	1.42	1.36
2	F	501	ORJ	O10-C11	4.54	1.41	1.36
2	G	501	ORJ	O10-C11	4.50	1.41	1.36
2	D	501	ORJ	C18-C16	4.38	1.43	1.36
2	D	501	ORJ	O10-C11	4.20	1.41	1.36
2	B	501	ORJ	C18-C16	4.06	1.42	1.36
2	A	501	ORJ	C18-C16	3.96	1.42	1.36
2	G	501	ORJ	O23-C22	3.92	1.44	1.36
2	D	501	ORJ	O23-C22	3.92	1.44	1.36
2	G	502	ORJ	O23-C22	3.87	1.44	1.36
2	G	501	ORJ	C18-C16	3.87	1.42	1.36
2	F	501	ORJ	O23-C22	3.85	1.44	1.36
2	B	501	ORJ	O23-C22	3.84	1.44	1.36
2	C	501	ORJ	O23-C22	3.82	1.44	1.36
2	F	501	ORJ	C18-C16	3.73	1.42	1.36
2	E	501	ORJ	C18-C16	3.73	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ORJ	O23-C22	3.57	1.43	1.36
2	G	502	ORJ	C18-C16	3.42	1.41	1.36
2	E	501	ORJ	O23-C22	3.42	1.43	1.36
2	C	501	ORJ	C18-C16	3.10	1.41	1.36
2	G	502	ORJ	C13-N12	2.53	1.47	1.38
2	B	501	ORJ	C13-N12	2.43	1.46	1.38
2	C	501	ORJ	C13-N12	2.43	1.46	1.38
2	A	501	ORJ	C14-C13	2.42	1.46	1.41
2	G	501	ORJ	C13-N12	2.40	1.46	1.38
2	C	501	ORJ	C14-C13	2.35	1.45	1.41
2	F	501	ORJ	C13-N12	2.34	1.46	1.38
2	D	501	ORJ	C13-N12	2.32	1.46	1.38
2	C	501	ORJ	C03-N02	2.28	1.44	1.34
2	A	501	ORJ	C03-N02	2.26	1.44	1.34
2	E	501	ORJ	C13-N12	2.26	1.46	1.38
2	G	502	ORJ	C14-C13	2.25	1.45	1.41
2	F	501	ORJ	C21-C09	2.22	1.42	1.38
2	E	501	ORJ	O04-C03	-2.21	1.18	1.23
2	A	501	ORJ	C13-N12	2.20	1.46	1.38
2	G	502	ORJ	C03-N02	2.17	1.44	1.34
2	B	501	ORJ	C03-N02	2.17	1.44	1.34
2	E	501	ORJ	C14-C13	2.17	1.45	1.41
2	D	501	ORJ	C03-N02	2.17	1.44	1.34
2	G	501	ORJ	C03-N02	2.13	1.44	1.34
2	G	501	ORJ	C14-C13	2.04	1.45	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	ORJ	C05-C03-N02	5.36	123.11	115.45
2	D	501	ORJ	C18-C19-S20	4.84	134.78	125.10
2	F	501	ORJ	C13-C19-S20	-4.67	105.66	111.85
2	B	501	ORJ	C18-C19-S20	4.62	134.35	125.10
2	G	501	ORJ	C18-C19-S20	4.61	134.32	125.10
2	A	501	ORJ	C18-C19-S20	4.61	134.32	125.10
2	B	501	ORJ	C13-C19-S20	-4.60	105.75	111.85
2	F	501	ORJ	C18-C19-S20	4.38	133.86	125.10
2	G	502	ORJ	C13-C19-S20	-4.37	106.05	111.85
2	E	501	ORJ	C18-C19-S20	4.34	133.78	125.10
2	G	502	ORJ	C18-C19-S20	4.33	133.77	125.10
2	G	501	ORJ	C13-C19-S20	-4.25	106.22	111.85
2	D	501	ORJ	C13-C19-S20	-4.23	106.24	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	ORJ	C18-C19-S20	4.20	133.50	125.10
2	F	501	ORJ	C05-C03-N02	4.10	121.31	115.45
2	C	501	ORJ	C13-C19-S20	-4.05	106.48	111.85
2	A	501	ORJ	C13-C19-S20	-3.97	106.58	111.85
2	F	501	ORJ	C19-C13-N12	3.81	116.91	108.04
2	E	501	ORJ	C13-C19-S20	-3.81	106.80	111.85
2	B	501	ORJ	C19-C13-N12	3.75	116.77	108.04
2	G	502	ORJ	C19-C13-N12	3.72	116.69	108.04
2	D	501	ORJ	C19-C13-N12	3.66	116.56	108.04
2	A	501	ORJ	C19-C13-N12	3.58	116.37	108.04
2	G	501	ORJ	C19-C13-N12	3.53	116.26	108.04
2	C	501	ORJ	C19-C13-N12	3.43	116.02	108.04
2	E	501	ORJ	C19-C13-N12	3.41	115.97	108.04
2	C	501	ORJ	C15-C16-C18	-3.37	119.51	123.23
2	G	502	ORJ	C15-C16-C18	-3.23	119.67	123.23
2	B	501	ORJ	C15-C16-C18	-3.18	119.72	123.23
2	E	501	ORJ	C05-C06-C22	3.17	124.41	120.88
2	F	501	ORJ	C15-C16-C18	-3.08	119.83	123.23
2	E	501	ORJ	C15-C16-C18	-3.00	119.92	123.23
2	D	501	ORJ	C14-C13-N12	-2.88	122.44	130.78
2	G	502	ORJ	C05-C03-N02	2.86	119.54	115.45
2	A	501	ORJ	C14-C13-N12	-2.85	122.52	130.78
2	D	501	ORJ	C15-C16-C18	-2.81	120.13	123.23
2	F	501	ORJ	C14-C13-N12	-2.77	122.74	130.78
2	D	501	ORJ	C05-C03-N02	2.75	119.37	115.45
2	G	501	ORJ	C14-C13-N12	-2.74	122.83	130.78
2	G	501	ORJ	C05-C03-N02	2.72	119.33	115.45
2	A	501	ORJ	C05-C03-N02	2.68	119.28	115.45
2	B	501	ORJ	C14-C13-N12	-2.67	123.03	130.78
2	E	501	ORJ	C14-C13-N12	-2.64	123.13	130.78
2	A	501	ORJ	C15-C16-C18	-2.60	120.36	123.23
2	E	501	ORJ	C05-C06-C07	-2.58	115.62	120.06
2	G	502	ORJ	C14-C13-N12	-2.48	123.60	130.78
2	F	501	ORJ	C05-C06-C22	2.32	123.47	120.88
2	G	501	ORJ	C15-C16-C18	-2.32	120.67	123.23
2	F	501	ORJ	C05-C06-C07	-2.31	116.09	120.06
2	C	501	ORJ	C14-C13-N12	-2.24	124.29	130.78
2	C	501	ORJ	C05-C03-N02	2.21	118.61	115.45
2	F	501	ORJ	C01-N02-C03	-2.17	105.36	121.93
2	F	501	ORJ	C07-C06-C22	2.15	120.45	118.16
2	E	501	ORJ	C06-C05-C03	2.14	117.55	113.43
2	B	501	ORJ	C07-C06-C22	2.04	120.34	118.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	ORJ	O04-C03-C05-C06
2	E	501	ORJ	O04-C03-C05-C06
2	E	501	ORJ	N02-C03-C05-C06
2	F	501	ORJ	N02-C03-C05-C06
2	F	501	ORJ	C03-C05-C06-C07
2	E	501	ORJ	C03-C05-C06-C07

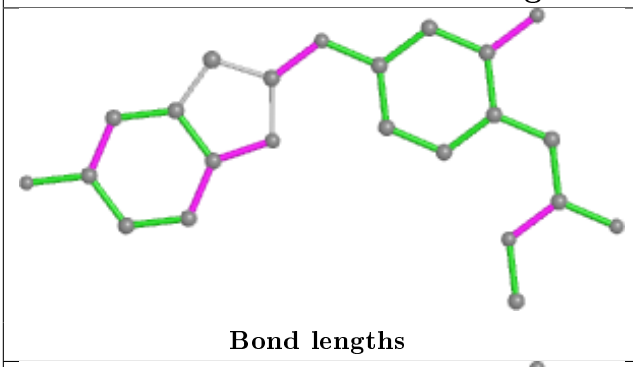
There are no ring outliers.

2 monomers are involved in 2 short contacts:

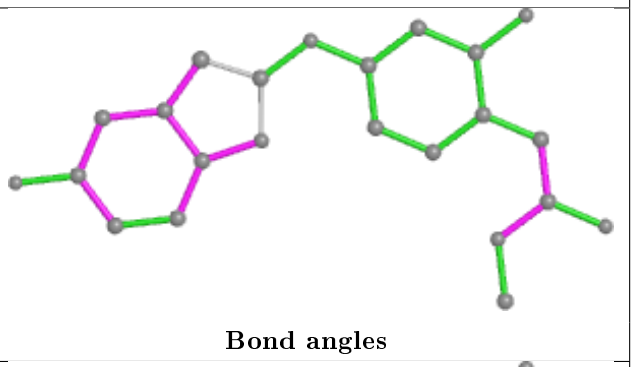
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	ORJ	1	0
2	F	501	ORJ	1	0

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.

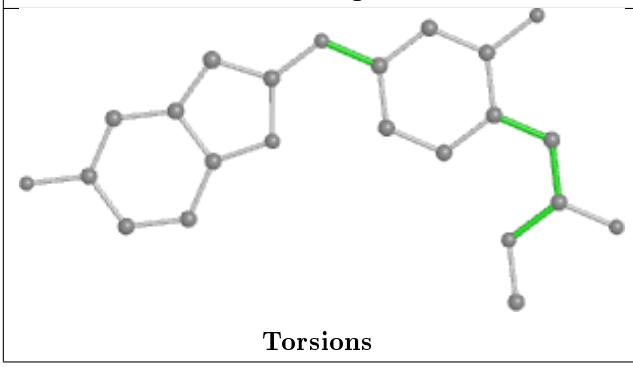
Ligand ORJ G 502



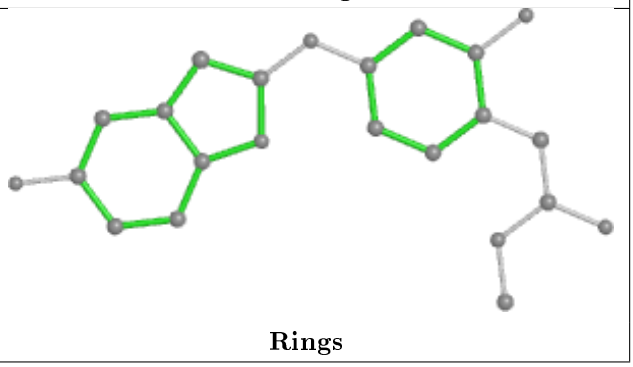
Bond lengths



Bond angles

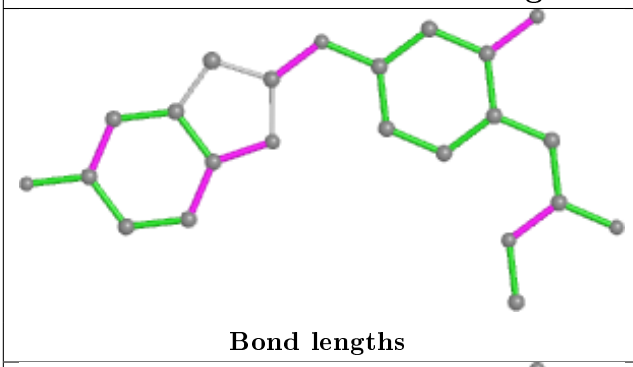


Torsions

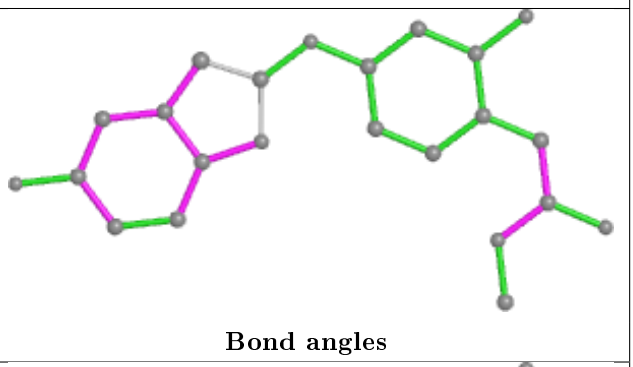


Rings

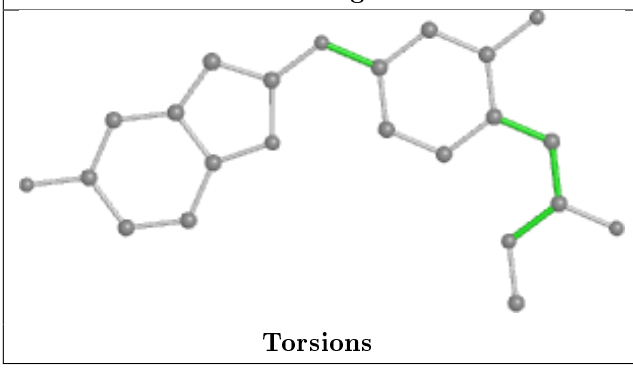
Ligand ORJ A 501



Bond lengths



Bond angles



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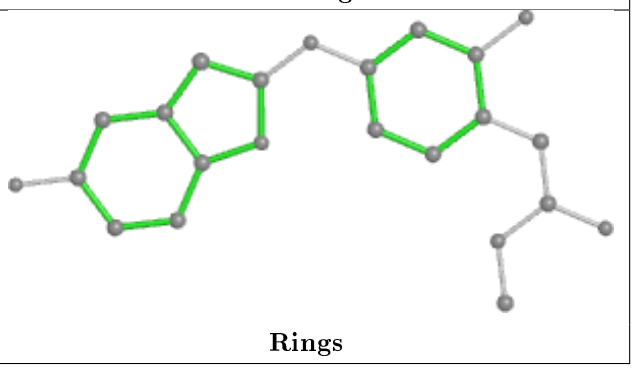
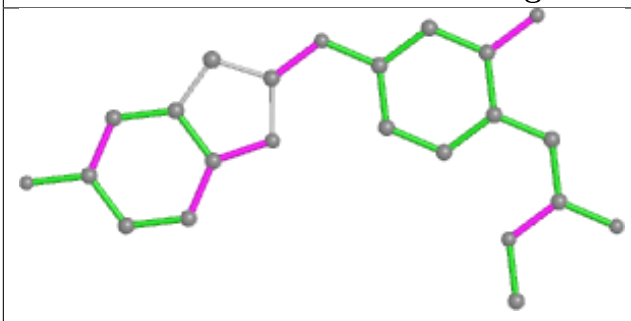
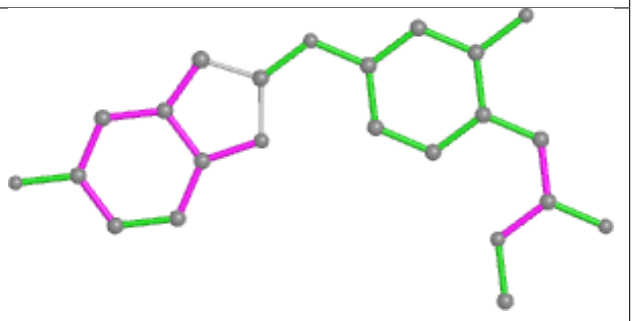


Rings

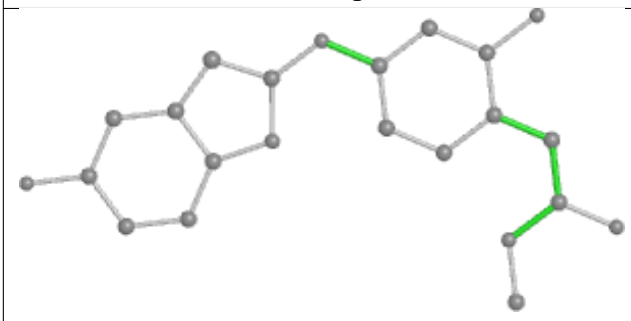
Ligand ORJ G 501



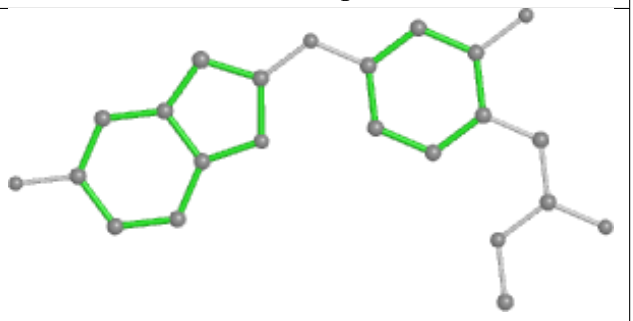
Bond lengths



Bond angles

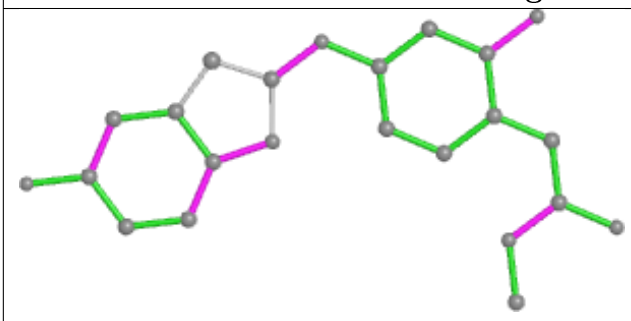


Torsions

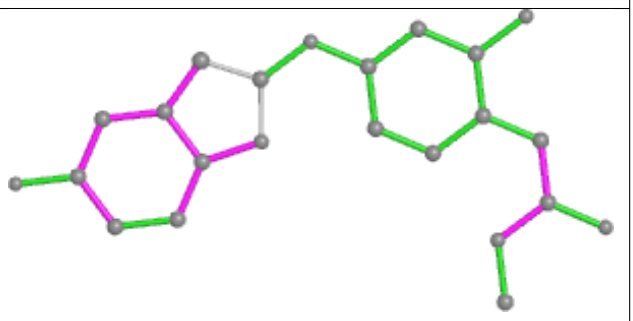


Rings

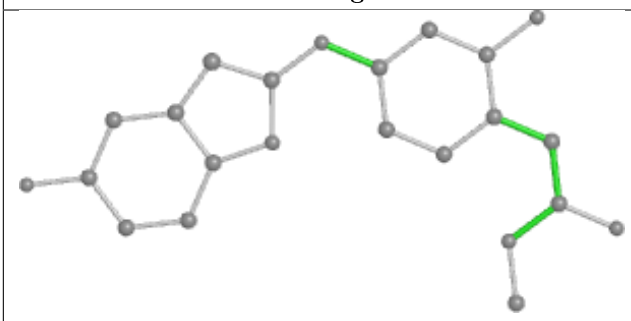
Ligand ORJ C 501



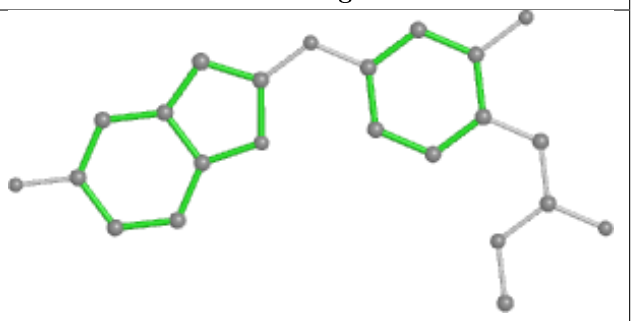
Bond lengths



Bond angles

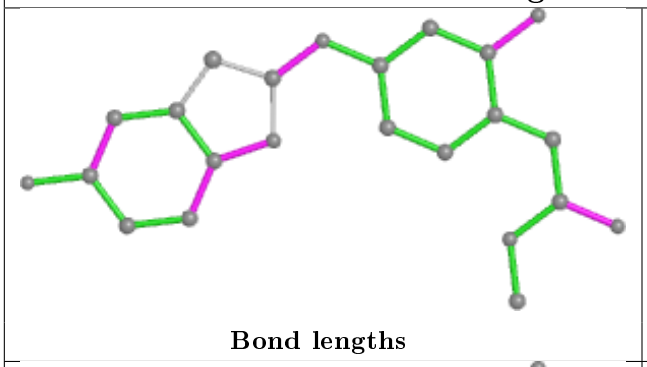


Torsions

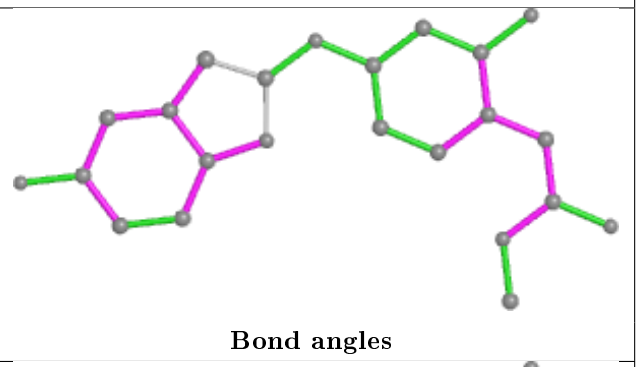


Rings

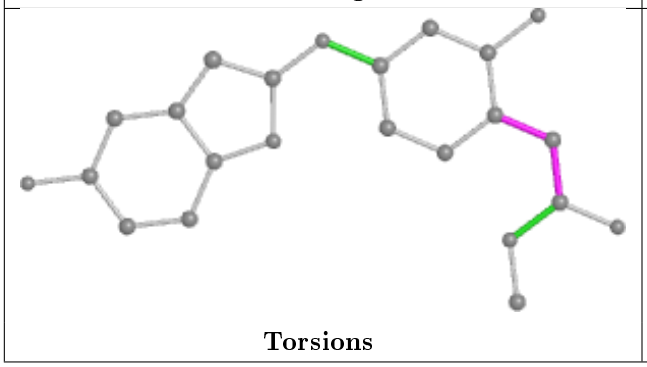
Ligand ORJ E 501



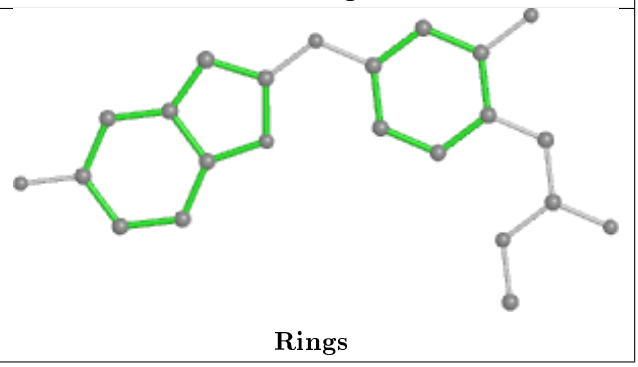
Bond lengths



Bond angles

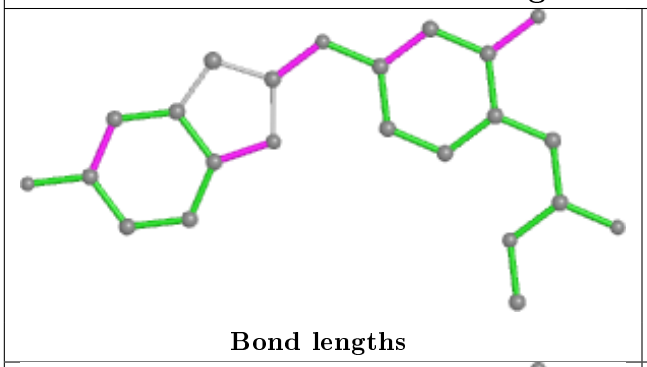


Torsions

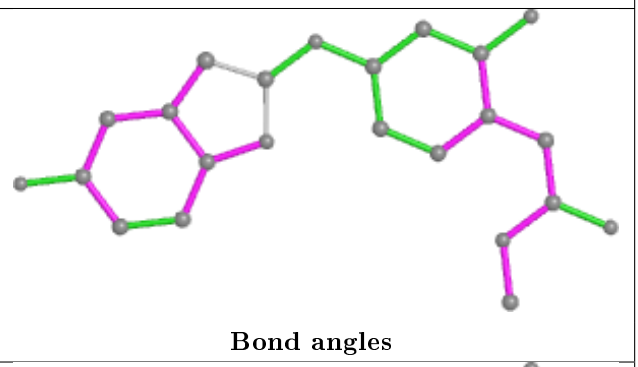


Rings

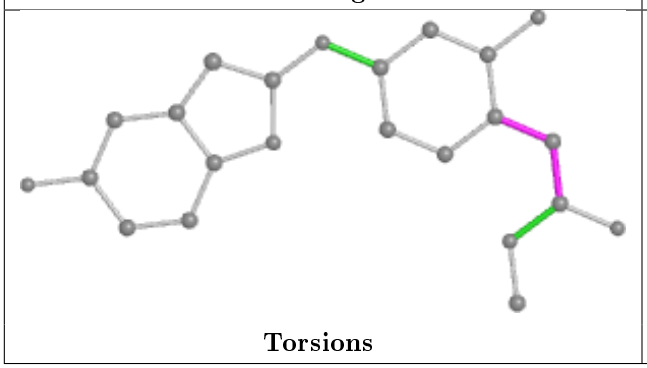
Ligand ORJ F 501



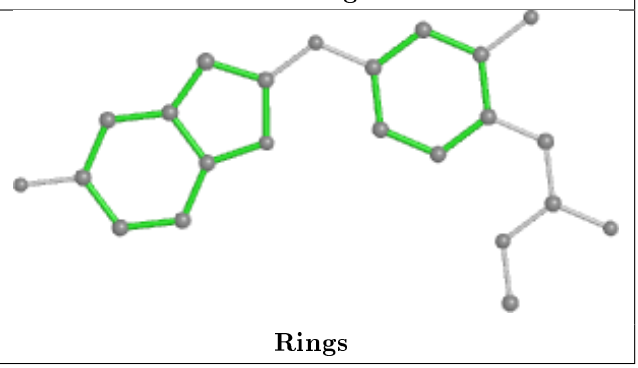
Bond lengths



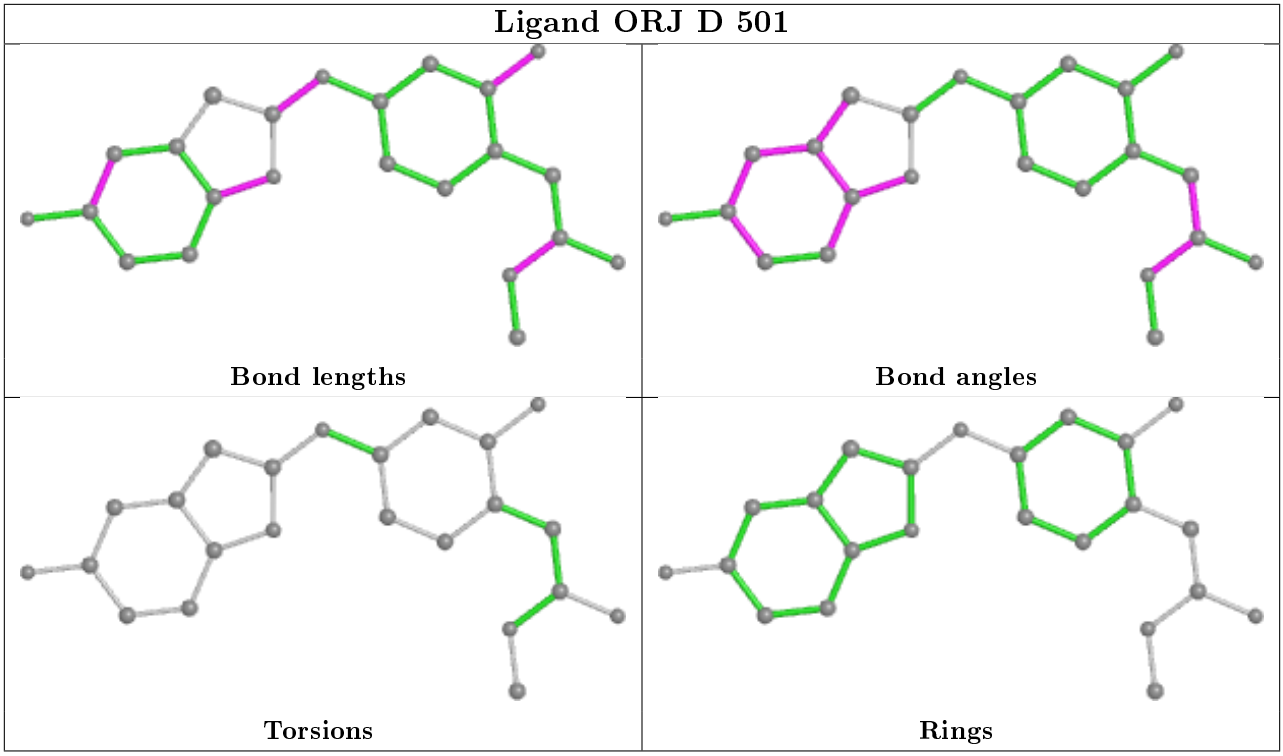
Bond angles

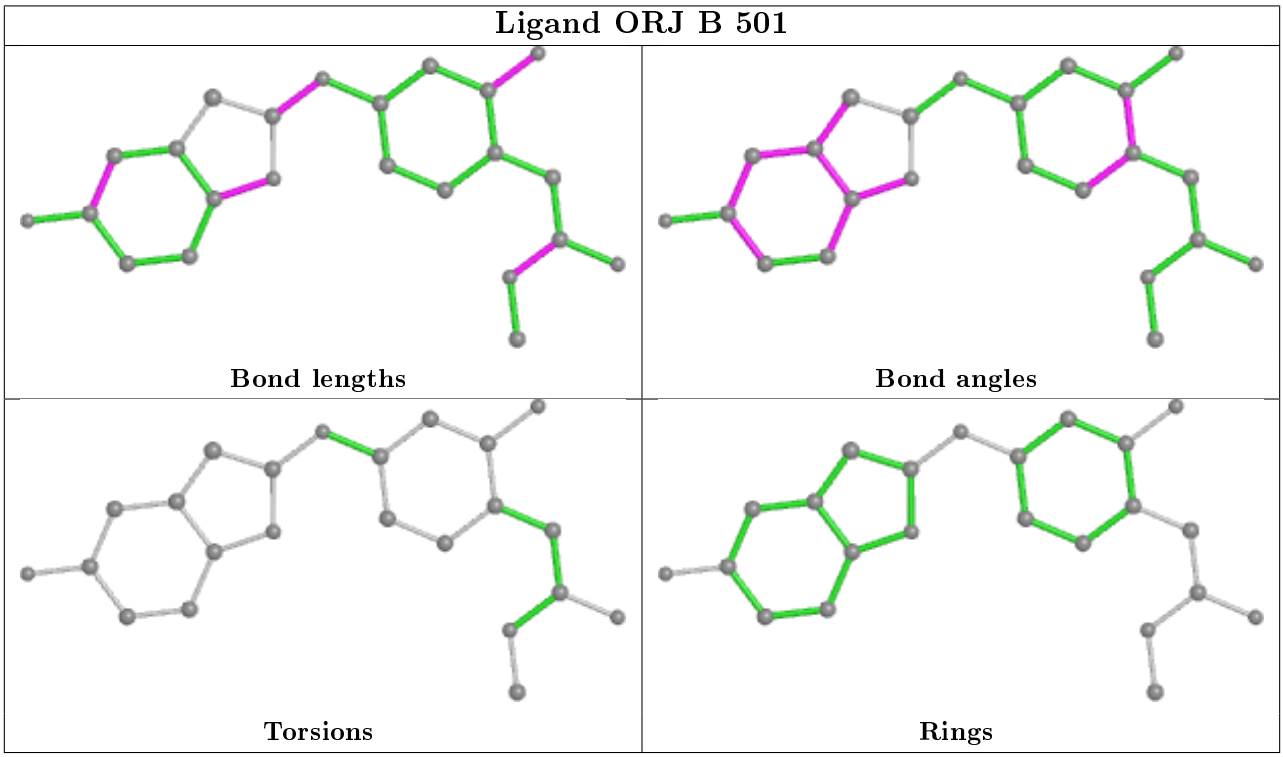


Torsions



Rings





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.29	2 (0%)	91	89	26, 40, 62, 78	0
1	B	424/473 (89%)	-0.30	1 (0%)	95	94	26, 40, 66, 92	0
1	C	410/473 (86%)	-0.22	10 (2%)	59	57	27, 39, 86, 116	0
1	D	428/473 (90%)	-0.13	17 (3%)	38	37	28, 41, 85, 99	0
1	E	426/473 (90%)	-0.27	4 (0%)	84	82	26, 40, 62, 80	0
1	F	424/473 (89%)	-0.29	1 (0%)	95	94	26, 41, 66, 92	0
1	G	410/473 (86%)	-0.22	8 (1%)	65	63	27, 39, 83, 114	0
1	H	428/473 (90%)	-0.18	15 (3%)	44	43	28, 40, 84, 101	0
All	All	3376/3784 (89%)	-0.24	58 (1%)	70	68	26, 40, 72, 116	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	VAL	5.4
1	E	13	LEU	5.4
1	D	408	ALA	5.2
1	D	407	ALA	5.0
1	H	409	ALA	4.9
1	D	420	GLN	4.7
1	D	417	LEU	4.7
1	G	422	ALA	4.6
1	H	408	ALA	4.5
1	D	410	PRO	4.4
1	C	400	ILE	4.3
1	H	421	LEU	4.2
1	D	401	LEU	4.1
1	H	417	LEU	4.1
1	H	401	LEU	4.0
1	G	403	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	332	GLN	3.7
1	E	156	ARG	3.7
1	D	430	GLY	3.7
1	D	414	ARG	3.6
1	D	160	THR	3.6
1	H	410	PRO	3.5
1	D	429	ALA	3.5
1	G	423	ALA	3.4
1	E	330	VAL	3.3
1	C	402	HIS	3.3
1	D	330	VAL	3.3
1	H	160	THR	3.3
1	D	411	GLU	3.2
1	C	429	ALA	3.1
1	H	416	ALA	3.0
1	H	397	ALA	3.0
1	G	402	HIS	3.0
1	G	401	LEU	2.9
1	C	404	LYS	2.9
1	H	330	VAL	2.8
1	C	13	LEU	2.8
1	H	400	ILE	2.8
1	D	418	HIS	2.6
1	H	412	HIS	2.6
1	D	413	GLU	2.5
1	H	161	GLY	2.4
1	G	13	LEU	2.4
1	A	156	ARG	2.4
1	A	159	VAL	2.3
1	F	330	VAL	2.3
1	D	159	VAL	2.3
1	C	423	ALA	2.3
1	E	134	PHE	2.3
1	C	422	ALA	2.3
1	H	331	ASP	2.3
1	C	401	LEU	2.3
1	G	334	TRP	2.2
1	H	413	GLU	2.2
1	D	397	ALA	2.1
1	C	330	VAL	2.1
1	G	330	VAL	2.1
1	C	430	GLY	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)

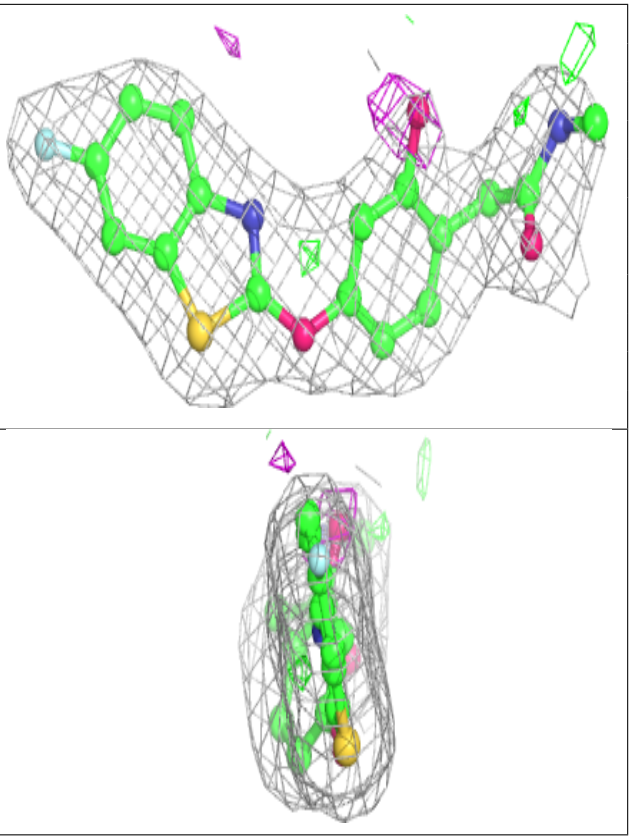
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ORJ	G	501	23/23	0.95	0.14	31,39,45,49	0
2	ORJ	G	502	23/23	0.96	0.14	31,37,44,46	0
2	ORJ	A	501	23/23	0.97	0.13	32,40,47,49	0
2	ORJ	D	501	23/23	0.97	0.13	31,36,46,49	0
2	ORJ	B	501	23/23	0.97	0.13	28,32,38,46	0
2	ORJ	F	501	23/23	0.98	0.13	28,31,44,49	0
2	ORJ	C	501	23/23	0.98	0.12	31,35,44,46	0
2	ORJ	E	501	23/23	0.98	0.12	35,38,46,57	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.

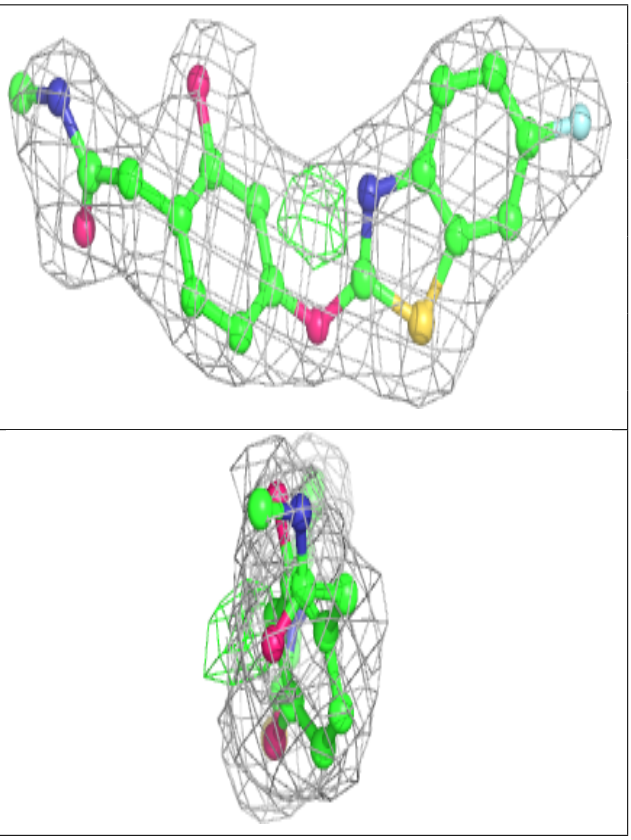
Electron density around ORJ G 501:

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



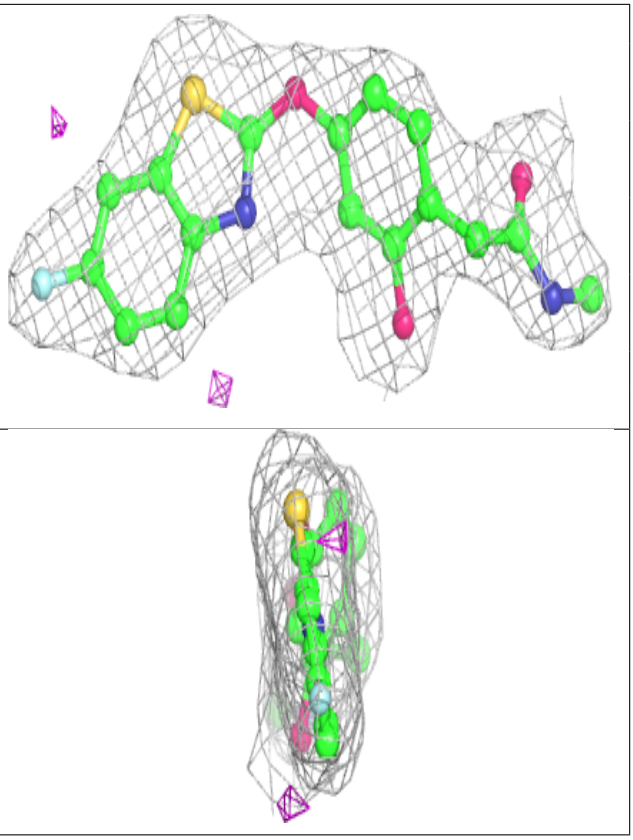
Electron density around ORJ G 502:

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



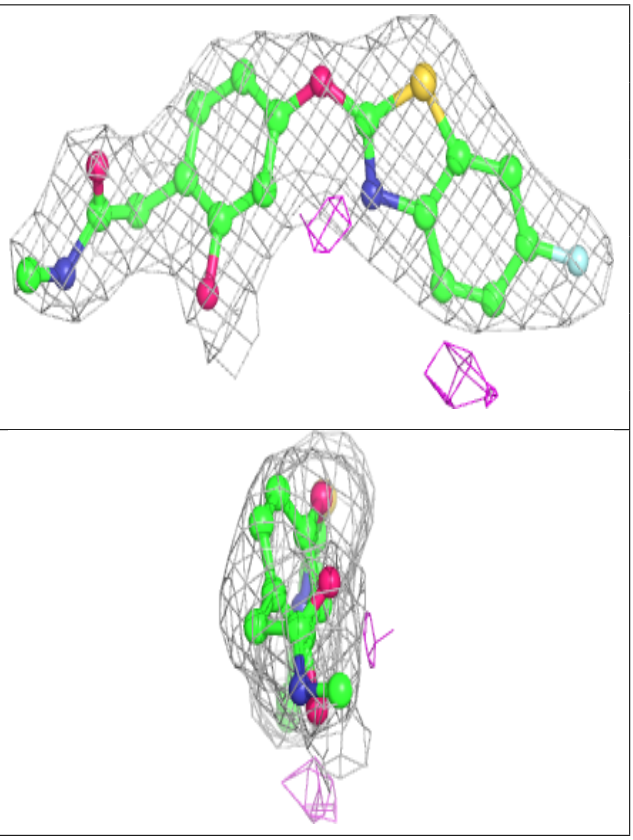
Electron density around ORJ A 501:

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



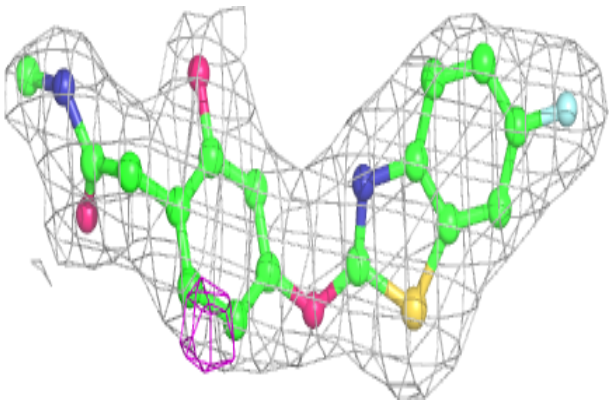
Electron density around ORJ D 501:

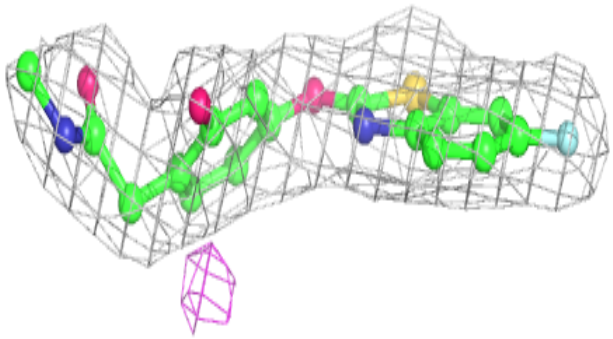
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

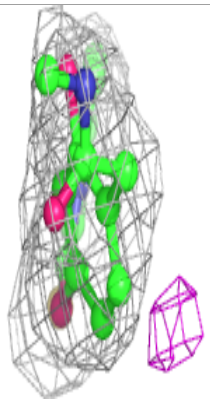


Electron density around ORJ B 501:

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

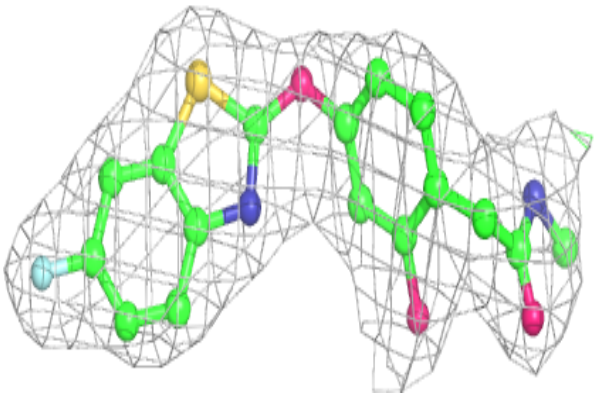


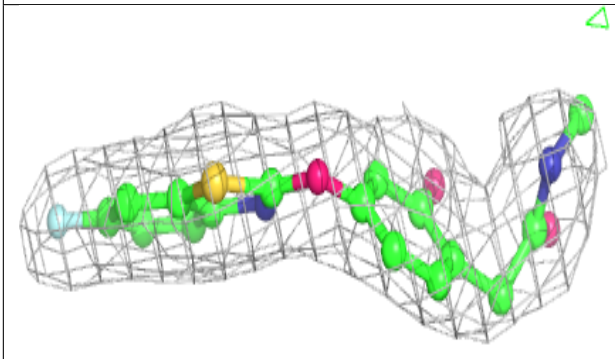


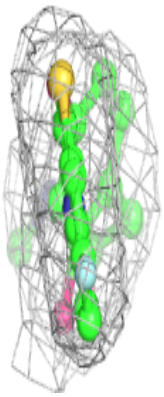


Electron density around ORJ F 501:

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

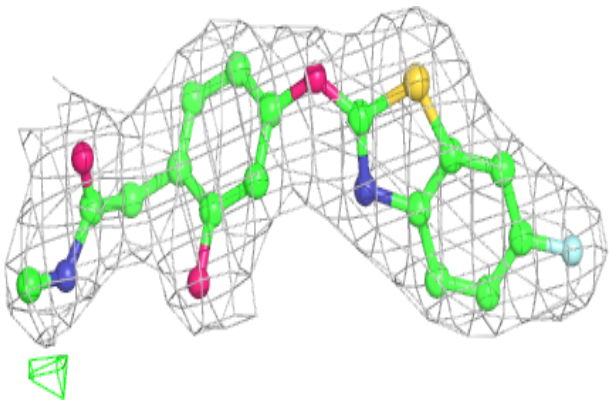


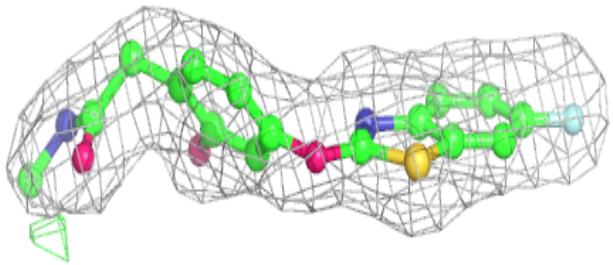


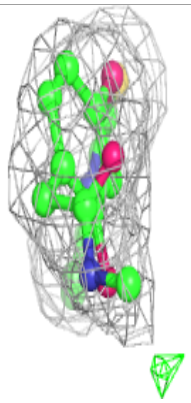


Electron density around ORJ C 501:

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

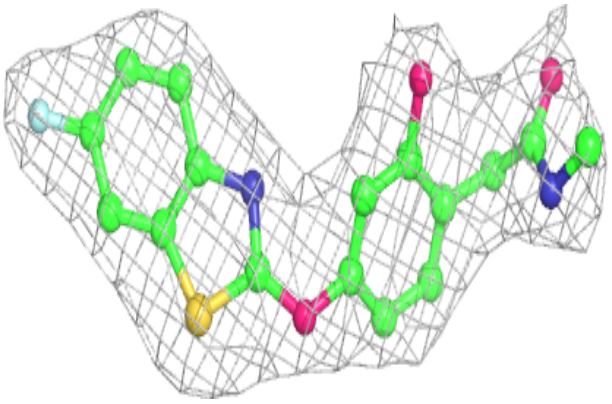


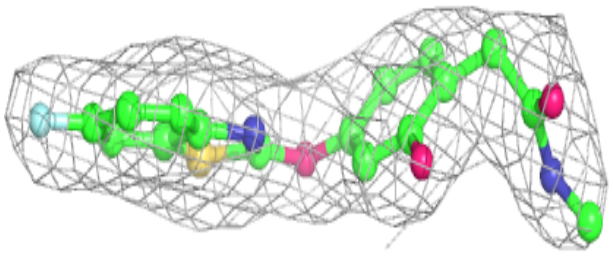


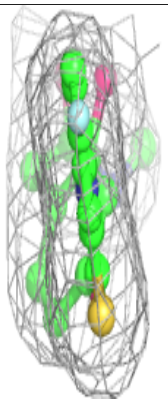


Electron density around ORJ E 501:

$2mF_o$-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.