



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:51 am BST

PDB ID : 5W4V  
Title : Structure of RORgt bound to a tertiary alcohol  
Authors : Spurlino, J.; Hars, U.  
Deposited on : 2017-06-13  
Resolution : 2.65 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](mailto: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.

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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 : 2.11  
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) : 2.11

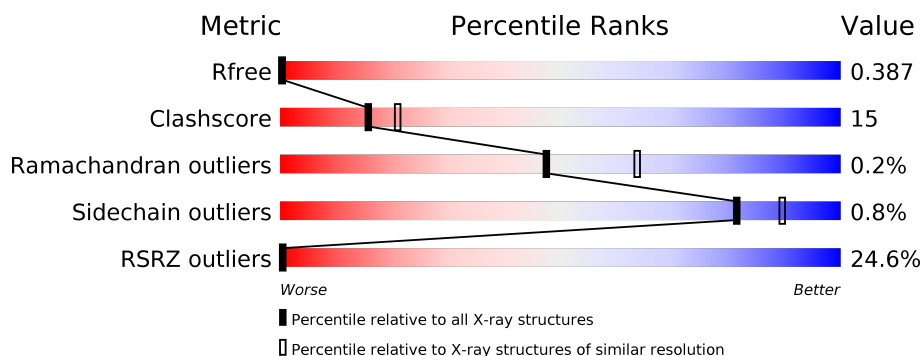
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	210	<div> <div>10%</div> <div>78%</div> <div>22%</div> </div>
1	B	210	<div> <div>11%</div> <div>70%</div> <div>30%</div> </div>
1	C	210	<div> <div>31%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>
1	D	210	<div> <div>30%</div> <div>63%</div> <div>32%</div> <div>..</div> </div>
1	E	210	<div> <div>32%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
1	F	210	<div> <div>30%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10553 atoms, of which 144 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.

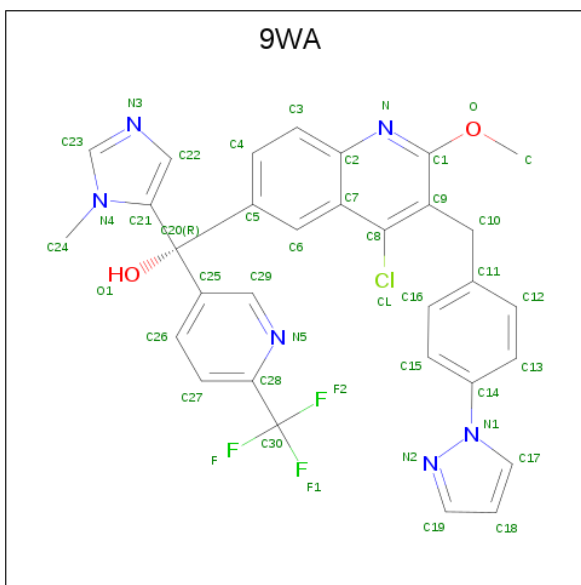
- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1712	1086	309	305	12			
1	B	209	Total	C	N	O	S	0	0	0
			1712	1086	309	305	12			
1	C	206	Total	C	N	O	S	0	0	0
			1688	1071	306	299	12			
1	D	203	Total	C	N	O	S	0	0	0
			1663	1054	298	299	12			
1	E	206	Total	C	N	O	S	0	0	0
			1687	1071	303	301	12			
1	F	202	Total	C	N	O	S	0	0	0
			1657	1051	297	297	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	HIS	CYS	conflict	UNP P51449
B	455	HIS	CYS	conflict	UNP P51449
C	455	HIS	CYS	conflict	UNP P51449
D	455	HIS	CYS	conflict	UNP P51449
E	455	HIS	CYS	conflict	UNP P51449
F	455	HIS	CYS	conflict	UNP P51449

- Molecule 2 is (R)-(4-chloro-2-methoxy-3-{[4-(1H-pyrazol-1-yl)phenyl]methyl}quinolin-6-yl)(1-methyl-1H-imidazol-5-yl)[6-(trifluoromethyl)pyridin-3-yl]methanol (three-letter code: 9WA) (formula: C<sub>31</sub>H<sub>24</sub>ClF<sub>3</sub>N<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	H	N	O	0	0
			67	31	1	3	24	6	2		
2	B	1	Total	C	Cl	F	H	N	O	0	0
			67	31	1	3	24	6	2		
2	C	1	Total	C	Cl	F	H	N	O	0	0
			67	31	1	3	24	6	2		
2	D	1	Total	C	Cl	F	H	N	O	0	0
			67	31	1	3	24	6	2		
2	E	1	Total	C	Cl	F	H	N	O	0	0
			67	31	1	3	24	6	2		
2	F	1	Total	C	Cl	F	H	N	O	0	0
			67	31	1	3	24	6	2		

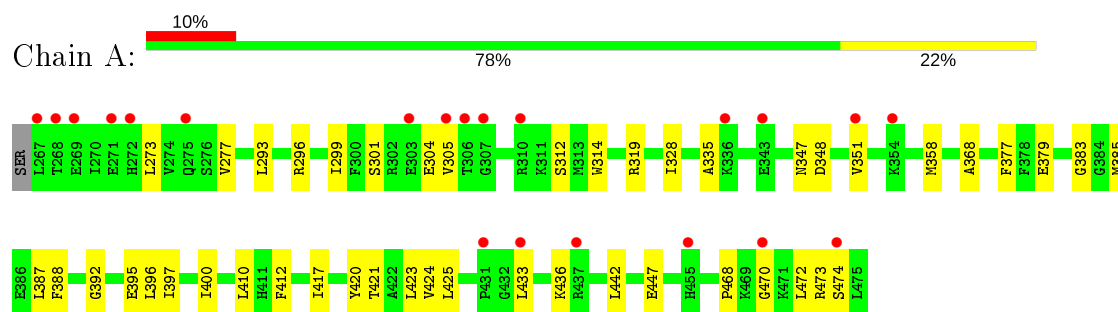
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	13	Total	O	0	0
			13	13		

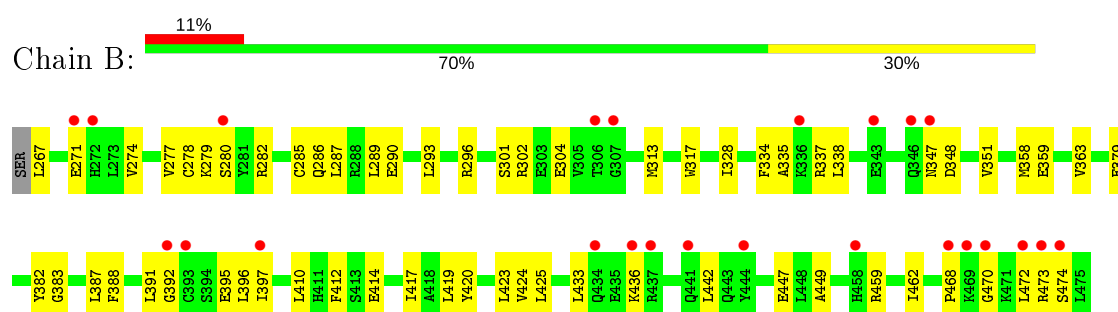
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

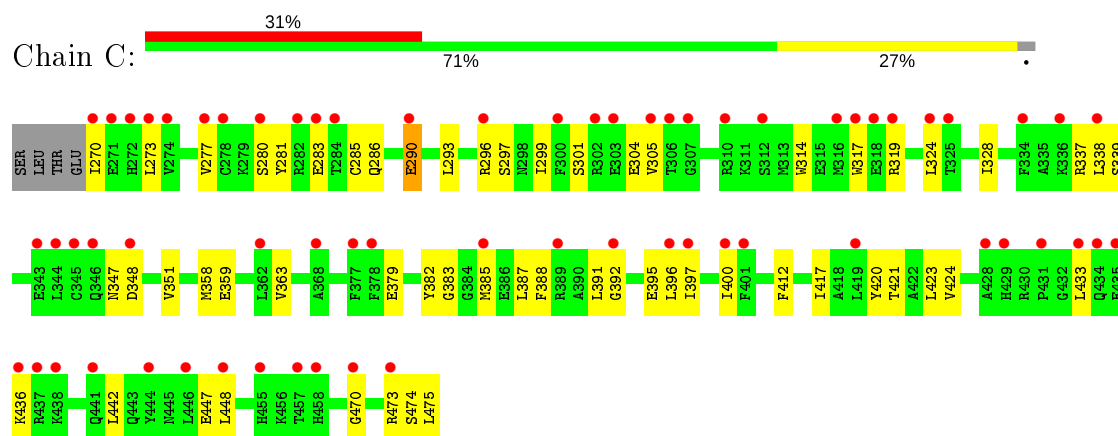
#### • Molecule 1: Nuclear receptor ROR-gamma



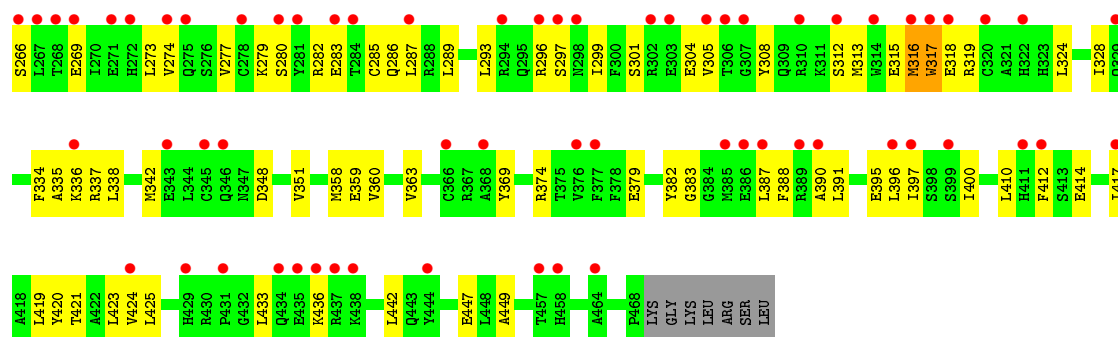
#### • Molecule 1: Nuclear receptor ROR-gamma



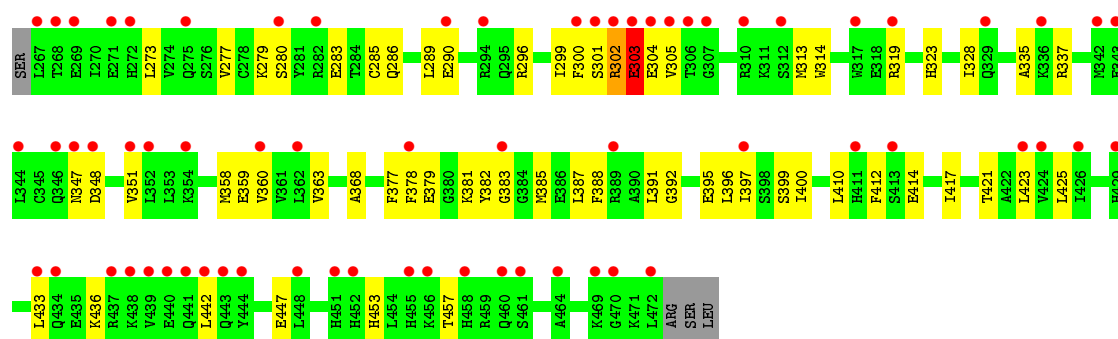
#### • Molecule 1: Nuclear receptor ROR-gamma



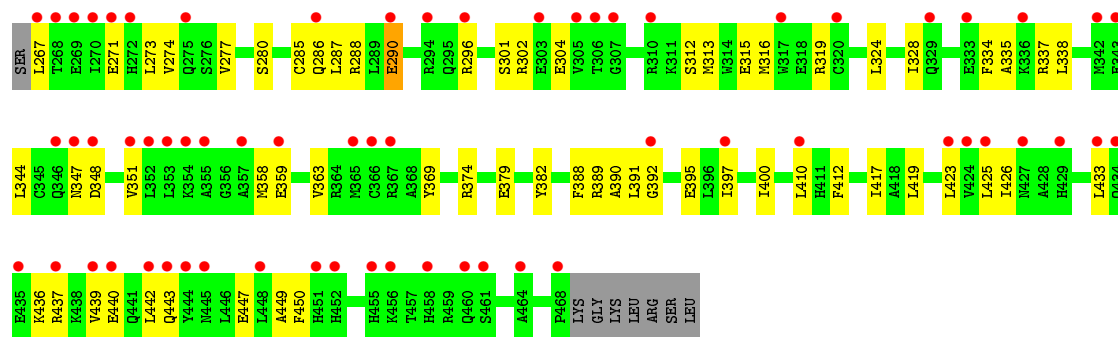
#### • Molecule 1: Nuclear receptor ROR-gamma



• Molecule 1: Nuclear receptor ROR-gamma



• Molecule 1: Nuclear receptor ROR-gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.12Å 133.12Å 181.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.35 – 2.65 29.35 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.35-2.65) 89.1 (29.35-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.343 , 0.384 0.354 , 0.387	Depositor DCC
$R_{free}$ test set	2724 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6886e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9WA

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	0.23	0/1746	0.37	0/2347
1	B	0.23	0/1746	0.37	0/2347
1	C	0.23	0/1722	0.37	0/2314
1	D	0.24	0/1697	0.45	2/2284 (0.1%)
1	E	0.24	0/1721	0.39	0/2314
1	F	0.23	0/1691	0.37	0/2276
All	All	0.24	0/10323	0.39	2/13882 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	316	MET	N-CA-C	5.84	126.77	111.00
1	D	316	MET	C-N-CA	5.29	134.93	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	316	MET	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1712	0	1715	46	0
1	B	1712	0	1715	55	0
1	C	1688	0	1691	55	0
1	D	1663	0	1651	55	0
1	E	1687	0	1686	57	1
1	F	1657	0	1646	48	1
2	A	43	24	0	0	0
2	B	43	24	0	3	0
2	C	43	24	0	2	0
2	D	43	24	0	3	0
2	E	43	24	0	0	0
2	F	43	24	0	2	0
3	A	19	0	0	0	0
3	B	13	0	0	0	0
All	All	10409	144	10104	301	1

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 15.

All (301) 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:279:LYS:HA	1:B:282:ARG:HD3	1.36	1.05
1:F:423:LEU:HD21	1:F:447:GLU:HG2	1.58	0.84
1:E:302:ARG:H	1:E:305:VAL:HB	1.41	0.82
1:E:301:SER:O	1:E:305:VAL:HG23	1.82	0.80
1:C:423:LEU:HD11	1:C:447:GLU:HG2	1.66	0.78
1:B:334:PHE:O	1:B:338:LEU:HD13	1.85	0.76
1:E:335:ALA:HB2	1:E:425:LEU:HD21	1.68	0.76
1:C:396:LEU:O	1:C:400:ILE:HD12	1.88	0.74
1:F:388:PHE:HB2	1:F:397:ILE:HD13	1.70	0.74
1:B:388:PHE:HB2	1:B:397:ILE:HD13	1.70	0.73
1:D:319:ARG:NH1	1:D:379:GLU:OE2	2.20	0.73
1:E:396:LEU:O	1:E:400:ILE:HD12	1.88	0.73
1:E:301:SER:HB3	1:E:302:ARG:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:PHE:HB2	1:E:397:ILE:HD13	1.70	0.72
1:D:388:PHE:HB2	1:D:397:ILE:HD13	1.73	0.71
1:F:334:PHE:O	1:F:338:LEU:HD13	1.90	0.71
1:A:388:PHE:HB2	1:A:397:ILE:HD13	1.73	0.71
1:C:388:PHE:HB2	1:C:397:ILE:HD13	1.73	0.70
1:E:302:ARG:O	1:E:303:GLU:HB2	1.91	0.70
1:F:335:ALA:HB2	1:F:425:LEU:HD21	1.73	0.69
1:B:470:GLY:O	1:B:473:ARG:HG2	1.93	0.69
1:A:396:LEU:HD13	1:B:313:MET:HE2	1.75	0.68
1:D:277:VAL:HG11	1:D:419:LEU:HD23	1.75	0.67
1:B:279:LYS:HA	1:B:282:ARG:CD	2.20	0.67
1:B:277:VAL:HG11	1:B:419:LEU:HD23	1.76	0.67
1:E:279:LYS:NZ	1:E:283:GLU:OE2	2.24	0.67
1:A:335:ALA:HB2	1:A:425:LEU:HD21	1.77	0.67
1:D:423:LEU:HD11	1:D:447:GLU:HG2	1.76	0.67
1:B:379:GLU:HA	2:B:501:9WA:F1	1.84	0.67
1:C:473:ARG:HG3	1:C:474:SER:H	1.62	0.65
1:A:397:ILE:HA	1:A:400:ILE:HD12	1.78	0.65
1:F:423:LEU:HD21	1:F:447:GLU:CG	2.28	0.64
1:D:312:SER:OG	1:D:315:GLU:HG3	1.98	0.64
1:D:317:TRP:N	1:D:391:LEU:HD21	2.13	0.63
1:A:470:GLY:O	1:A:473:ARG:HG2	1.98	0.63
1:A:396:LEU:HD11	1:A:400:ILE:HD11	1.80	0.63
1:B:391:LEU:HD12	1:B:397:ILE:HD11	1.80	0.63
1:C:470:GLY:O	1:C:473:ARG:HG2	1.99	0.62
1:A:385:MET:HG3	1:A:397:ILE:HG22	1.80	0.62
1:A:312:SER:HB2	1:B:473:ARG:HB2	1.82	0.62
1:B:335:ALA:HB2	1:B:425:LEU:HD21	1.80	0.62
1:A:301:SER:O	1:A:305:VAL:HG23	2.00	0.61
1:C:283:GLU:OE1	1:C:337:ARG:NH1	2.33	0.61
1:B:423:LEU:HD11	1:B:447:GLU:HG2	1.82	0.61
1:F:277:VAL:HG11	1:F:419:LEU:HD23	1.83	0.61
1:C:301:SER:O	1:C:305:VAL:HG23	2.01	0.61
1:F:351:VAL:HG11	1:F:433:LEU:HD23	1.84	0.60
1:C:328:ILE:HD11	1:C:358:MET:CE	2.32	0.60
1:D:383:GLY:HA3	1:D:387:LEU:HD22	1.83	0.60
1:F:319:ARG:HD3	1:F:379:GLU:OE2	2.01	0.59
1:D:324:LEU:HD11	2:D:501:9WA:C15	2.33	0.59
1:C:273:LEU:O	1:C:277:VAL:HG23	2.02	0.58
1:C:270:ILE:HD11	1:C:448:LEU:HD23	1.84	0.58
1:D:301:SER:OG	1:D:304:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ALA:HB2	1:D:425:LEU:HD21	1.84	0.58
1:D:279:LYS:HA	1:D:282:ARG:HG2	1.86	0.58
1:F:359:GLU:O	1:F:363:VAL:HG23	2.04	0.57
1:B:379:GLU:CA	2:B:501:9WA:F1	2.43	0.57
1:A:388:PHE:CB	1:A:397:ILE:HD13	2.34	0.57
1:D:317:TRP:H	1:D:391:LEU:HD21	1.69	0.57
1:C:328:ILE:HD11	1:C:358:MET:HE1	1.85	0.57
1:C:293:LEU:HA	1:C:296:ARG:HD3	1.87	0.57
1:F:344:LEU:HD13	1:F:439:VAL:HG22	1.87	0.57
1:A:312:SER:CB	1:B:473:ARG:HB2	2.34	0.56
1:A:351:VAL:HG11	1:A:433:LEU:HD23	1.88	0.56
1:A:473:ARG:HG3	1:A:474:SER:N	2.20	0.56
1:E:385:MET:HG3	1:E:397:ILE:HG22	1.88	0.56
1:C:324:LEU:HD11	2:C:501:9WA:C15	2.36	0.56
1:A:396:LEU:CD1	1:A:400:ILE:HD11	2.36	0.56
1:B:351:VAL:HG11	1:B:433:LEU:HD23	1.87	0.56
1:A:348:ASP:HA	1:A:351:VAL:CG1	2.36	0.55
1:A:328:ILE:HD11	1:A:358:MET:CE	2.36	0.55
1:A:473:ARG:HG3	1:A:474:SER:H	1.69	0.55
1:B:286:GLN:HG2	1:B:287:LEU:HD13	1.88	0.55
1:D:266:SER:HB3	1:D:269:GLU:HB2	1.88	0.55
1:E:328:ILE:HD11	1:E:358:MET:HE2	1.88	0.55
1:F:443:GLN:O	1:F:447:GLU:HG3	2.06	0.55
1:D:336:LYS:HE3	1:D:342:MET:HE1	1.89	0.55
1:C:473:ARG:HG3	1:C:474:SER:N	2.21	0.55
1:A:396:LEU:HD13	1:B:313:MET:CE	2.36	0.55
1:C:388:PHE:CB	1:C:397:ILE:HD13	2.37	0.54
1:D:266:SER:HB3	1:D:269:GLU:CB	2.37	0.54
1:E:385:MET:HG3	1:E:397:ILE:CG2	2.37	0.54
1:E:328:ILE:HD11	1:E:358:MET:CE	2.38	0.54
1:F:274:VAL:HG22	1:F:449:ALA:HB1	1.88	0.54
1:E:301:SER:HB3	1:E:302:ARG:C	2.28	0.54
1:E:397:ILE:HA	1:E:400:ILE:HD13	1.89	0.54
1:D:351:VAL:HG11	1:D:433:LEU:HD23	1.90	0.54
1:E:436:LYS:HB3	1:E:436:LYS:NZ	2.23	0.54
1:C:383:GLY:HA3	1:C:387:LEU:HD22	1.90	0.53
1:F:388:PHE:CB	1:F:397:ILE:HD13	2.36	0.53
1:C:296:ARG:HA	1:C:382:TYR:CE1	2.43	0.53
1:E:289:LEU:HD22	1:E:414:GLU:OE2	2.08	0.53
1:E:348:ASP:HA	1:E:351:VAL:HG12	1.91	0.53
1:F:391:LEU:HD12	1:F:397:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ASP:HA	1:C:351:VAL:CG1	2.39	0.53
1:C:348:ASP:HA	1:C:351:VAL:HG12	1.91	0.53
1:E:348:ASP:HA	1:E:351:VAL:CG1	2.39	0.53
1:B:468:PRO:O	1:B:472:LEU:HD22	2.07	0.53
1:B:473:ARG:HG3	1:B:474:SER:H	1.73	0.53
1:E:300:PHE:HB3	1:E:301:SER:O	2.08	0.53
1:B:420:TYR:O	1:B:424:VAL:HG23	2.08	0.53
1:D:391:LEU:HD12	1:D:397:ILE:HD11	1.91	0.53
1:E:412:PHE:HB3	1:E:417:ILE:HG13	1.90	0.53
1:B:348:ASP:HA	1:B:351:VAL:CG1	2.38	0.52
1:E:351:VAL:HG11	1:E:433:LEU:HD23	1.91	0.52
1:A:348:ASP:HA	1:A:351:VAL:HG12	1.92	0.52
1:F:436:LYS:NZ	1:F:436:LYS:HB3	2.25	0.52
1:A:328:ILE:HD11	1:A:358:MET:HE1	1.91	0.52
1:D:388:PHE:CB	1:D:397:ILE:HD13	2.38	0.52
1:B:388:PHE:CB	1:B:397:ILE:HD13	2.36	0.52
1:A:410:LEU:HD23	1:A:412:PHE:CZ	2.45	0.52
1:E:359:GLU:O	1:E:363:VAL:HG23	2.09	0.52
1:B:278:CYS:O	1:B:282:ARG:HG3	2.10	0.52
1:A:442:LEU:O	1:A:442:LEU:HD12	2.10	0.51
1:B:436:LYS:NZ	1:B:436:LYS:HB3	2.25	0.51
1:C:281:TYR:CE1	1:C:417:ILE:HG22	2.45	0.51
1:D:397:ILE:HA	1:D:400:ILE:HD12	1.91	0.51
1:F:442:LEU:O	1:F:442:LEU:HD12	2.11	0.51
1:D:358:MET:HG2	1:E:314:TRP:CG	2.46	0.51
1:E:410:LEU:HD23	1:E:412:PHE:CZ	2.45	0.51
1:C:285:CYS:O	1:C:286:GLN:HB3	2.11	0.51
1:D:277:VAL:CG1	1:D:419:LEU:HD23	2.41	0.51
1:C:423:LEU:CD1	1:C:447:GLU:HG2	2.40	0.51
1:E:395:GLU:HG2	1:E:396:LEU:H	1.75	0.51
1:F:348:ASP:HA	1:F:351:VAL:HG12	1.92	0.51
1:F:412:PHE:HB3	1:F:417:ILE:HG13	1.92	0.51
1:A:436:LYS:HB3	1:A:436:LYS:NZ	2.26	0.51
1:A:383:GLY:HA3	1:A:387:LEU:HD22	1.93	0.51
1:D:348:ASP:HA	1:D:351:VAL:HG12	1.92	0.51
1:D:317:TRP:CD1	1:D:391:LEU:HD22	2.46	0.51
1:B:348:ASP:HA	1:B:351:VAL:HG12	1.93	0.50
1:E:396:LEU:CD1	1:E:400:ILE:HD11	2.41	0.50
1:A:314:TRP:CG	1:B:358:MET:HG2	2.47	0.50
1:C:396:LEU:CD1	1:C:400:ILE:HD11	2.42	0.50
1:E:301:SER:HB2	1:E:304:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:SER:C	1:C:475:LEU:HD12	2.31	0.50
1:E:391:LEU:HD12	1:E:397:ILE:HD11	1.92	0.49
1:A:385:MET:HG3	1:A:397:ILE:CG2	2.42	0.49
1:C:474:SER:O	1:C:475:LEU:HD12	2.12	0.49
1:E:395:GLU:HG2	1:E:396:LEU:N	2.27	0.49
1:A:314:TRP:CD2	1:B:358:MET:HG2	2.47	0.49
1:A:293:LEU:HA	1:A:296:ARG:HD3	1.94	0.49
1:C:436:LYS:HB3	1:C:436:LYS:NZ	2.28	0.49
1:E:453:HIS:O	1:E:457:THR:HG23	2.11	0.49
1:A:420:TYR:O	1:A:424:VAL:HG23	2.13	0.49
1:E:388:PHE:CB	1:E:397:ILE:HD13	2.41	0.49
1:E:423:LEU:HD21	1:E:447:GLU:CG	2.43	0.49
1:E:423:LEU:HD21	1:E:447:GLU:HG2	1.94	0.49
1:C:314:TRP:CD2	1:F:358:MET:HG2	2.47	0.49
1:D:301:SER:O	1:D:305:VAL:HG23	2.13	0.49
1:F:312:SER:OG	1:F:315:GLU:HG3	2.13	0.49
1:B:442:LEU:O	1:B:442:LEU:HD12	2.12	0.49
1:B:473:ARG:HG3	1:B:474:SER:N	2.27	0.49
1:D:293:LEU:HA	1:D:296:ARG:HG3	1.94	0.49
1:D:436:LYS:NZ	1:D:436:LYS:HB3	2.27	0.49
1:D:324:LEU:HD11	2:D:501:9WA:C14	2.43	0.49
1:E:301:SER:HB2	1:E:304:GLU:HG3	1.95	0.49
1:F:437:ARG:HA	1:F:440:GLU:HB2	1.95	0.49
1:F:348:ASP:HA	1:F:351:VAL:CG1	2.43	0.48
1:D:359:GLU:O	1:D:363:VAL:HG23	2.13	0.48
1:E:368:ALA:HB1	1:E:377:PHE:HB3	1.95	0.48
1:A:423:LEU:HD21	1:A:447:GLU:CG	2.43	0.48
1:A:392:GLY:O	1:B:395:GLU:HG2	2.14	0.48
1:D:358:MET:HG2	1:E:314:TRP:CD2	2.48	0.48
1:D:336:LYS:HE3	1:D:342:MET:CE	2.43	0.48
1:E:442:LEU:HD12	1:E:442:LEU:O	2.13	0.48
1:A:412:PHE:HB3	1:A:417:ILE:HG13	1.96	0.48
1:D:442:LEU:O	1:D:442:LEU:HD12	2.13	0.48
1:B:280:SER:OG	1:B:337:ARG:HB2	2.14	0.48
1:C:319:ARG:NH1	1:C:379:GLU:OE2	2.47	0.47
1:F:410:LEU:HD23	1:F:412:PHE:CZ	2.49	0.47
1:C:338:LEU:O	1:C:339:SER:OG	2.20	0.47
1:C:420:TYR:O	1:C:424:VAL:HG23	2.15	0.47
1:D:274:VAL:CG2	1:D:449:ALA:HB1	2.44	0.47
1:A:347:ASN:O	1:A:351:VAL:HG12	2.14	0.47
1:D:289:LEU:HD13	1:D:414:GLU:OE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:LEU:HD13	1:F:313:MET:SD	2.53	0.47
1:C:392:GLY:O	1:F:395:GLU:HG2	2.15	0.47
1:A:273:LEU:O	1:A:277:VAL:HG23	2.14	0.47
1:A:385:MET:O	1:A:385:MET:HG2	2.14	0.47
1:A:319:ARG:NH1	1:A:379:GLU:OE2	2.48	0.47
2:C:501:9WA:C24	2:C:501:9WA:O1	2.62	0.47
1:E:335:ALA:HB2	1:E:425:LEU:CD2	2.41	0.47
1:F:426:ILE:O	1:F:443:GLN:HG3	2.15	0.47
1:F:397:ILE:HA	1:F:400:ILE:HD12	1.97	0.47
1:B:347:ASN:O	1:B:351:VAL:HG12	2.15	0.47
1:E:383:GLY:HA3	1:E:387:LEU:HD22	1.96	0.47
1:B:274:VAL:HG22	1:B:449:ALA:HB1	1.97	0.47
1:B:328:ILE:HD11	1:B:358:MET:CE	2.45	0.47
1:D:328:ILE:HD11	1:D:358:MET:CE	2.45	0.47
1:D:395:GLU:HG2	1:E:392:GLY:O	2.15	0.47
1:B:412:PHE:HB3	1:B:417:ILE:HG13	1.97	0.46
1:F:280:SER:OG	1:F:337:ARG:HB2	2.15	0.46
1:B:296:ARG:HA	1:B:382:TYR:CE1	2.51	0.46
1:C:301:SER:OG	1:C:304:GLU:HG3	2.16	0.46
1:F:296:ARG:HA	1:F:382:TYR:CE1	2.51	0.46
1:D:297:SER:C	1:D:299:ILE:HD12	2.36	0.46
1:B:290:GLU:CD	1:B:290:GLU:H	2.18	0.46
1:C:442:LEU:HD12	1:C:442:LEU:O	2.14	0.46
1:D:286:GLN:HG2	1:D:287:LEU:HD13	1.98	0.46
1:D:412:PHE:HB3	1:D:417:ILE:HG13	1.97	0.46
1:B:383:GLY:HA3	1:B:387:LEU:HD22	1.98	0.46
1:E:300:PHE:CE1	1:E:381:LYS:HB2	2.50	0.46
1:B:302:ARG:HA	1:B:302:ARG:HD2	1.82	0.46
1:C:317:TRP:HA	1:C:391:LEU:HD21	1.98	0.45
1:C:395:GLU:HG2	1:F:392:GLY:O	2.16	0.45
1:E:360:VAL:HG13	1:E:421:THR:HB	1.98	0.45
1:E:273:LEU:O	1:E:277:VAL:HG23	2.15	0.45
1:E:319:ARG:NH1	1:E:379:GLU:OE2	2.49	0.45
1:D:273:LEU:O	1:D:277:VAL:HG23	2.17	0.45
1:E:302:ARG:HD3	1:E:302:ARG:HA	1.51	0.45
1:A:423:LEU:HD21	1:A:447:GLU:HG2	1.98	0.45
1:A:335:ALA:HB2	1:A:425:LEU:CD2	2.45	0.45
1:C:290:GLU:CD	1:C:290:GLU:H	2.20	0.45
1:C:351:VAL:HG11	1:C:433:LEU:HD23	1.98	0.45
1:A:301:SER:OG	1:A:304:GLU:HG3	2.17	0.45
1:F:290:GLU:CD	1:F:290:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:SER:OG	1:C:337:ARG:HB2	2.18	0.44
1:C:423:LEU:HD23	1:C:423:LEU:HA	1.83	0.44
1:E:300:PHE:CZ	1:E:381:LYS:HB2	2.52	0.44
1:F:351:VAL:CG1	1:F:433:LEU:HD23	2.47	0.44
1:C:347:ASN:O	1:C:351:VAL:HG12	2.17	0.44
1:C:359:GLU:O	1:C:363:VAL:HG23	2.17	0.44
1:E:347:ASN:O	1:E:351:VAL:HG12	2.17	0.44
1:D:285:CYS:O	1:D:286:GLN:HB3	2.18	0.44
1:E:302:ARG:N	1:E:305:VAL:HB	2.21	0.44
1:B:410:LEU:HD23	1:B:412:PHE:CZ	2.53	0.44
1:C:395:GLU:HG2	1:C:396:LEU:N	2.33	0.44
1:C:412:PHE:HB3	1:C:417:ILE:HG13	2.00	0.44
1:C:395:GLU:HG2	1:C:396:LEU:H	1.82	0.44
1:C:314:TRP:CG	1:F:358:MET:HG2	2.53	0.44
1:D:280:SER:OG	1:D:337:ARG:HB2	2.17	0.44
1:A:395:GLU:HG2	1:A:396:LEU:N	2.33	0.43
1:D:308:TYR:OH	1:D:379:GLU:OE1	2.18	0.43
1:B:423:LEU:HD21	1:B:447:GLU:CG	2.48	0.43
1:F:286:GLN:HG2	1:F:287:LEU:HD13	2.00	0.43
1:C:296:ARG:HG3	1:C:382:TYR:CZ	2.53	0.43
1:E:280:SER:OG	1:E:337:ARG:HB2	2.18	0.43
1:D:296:ARG:HA	1:D:382:TYR:CE1	2.54	0.43
1:B:301:SER:OG	1:B:304:GLU:HG3	2.19	0.43
1:A:395:GLU:HG2	1:B:392:GLY:O	2.18	0.43
1:C:297:SER:C	1:C:299:ILE:HD12	2.38	0.43
1:C:299:ILE:HD12	1:C:299:ILE:N	2.33	0.43
1:D:274:VAL:HG22	1:D:449:ALA:HB1	2.00	0.43
1:B:289:LEU:HD22	1:B:414:GLU:OE2	2.18	0.43
2:D:501:9WA:C24	2:D:501:9WA:O1	2.67	0.43
1:E:397:ILE:HA	1:E:400:ILE:CD1	2.49	0.43
1:F:267:LEU:HD21	1:F:271:GLU:OE1	2.19	0.43
1:A:468:PRO:O	1:A:472:LEU:HD22	2.19	0.43
1:C:473:ARG:CG	1:C:474:SER:H	2.30	0.43
1:F:287:LEU:HD22	2:F:501:9WA:C24	2.48	0.43
1:F:423:LEU:CD2	1:F:447:GLU:HG2	2.37	0.42
1:C:391:LEU:HA	1:C:391:LEU:HD23	1.92	0.42
1:D:420:TYR:O	1:D:424:VAL:HG23	2.20	0.42
1:B:285:CYS:O	1:B:286:GLN:HB3	2.19	0.42
1:C:417:ILE:O	1:C:421:THR:HG23	2.19	0.42
1:F:273:LEU:O	1:F:277:VAL:HG23	2.18	0.42
1:F:335:ALA:HB2	1:F:425:LEU:CD2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ASP:HA	1:D:351:VAL:CG1	2.49	0.42
1:B:359:GLU:O	1:B:363:VAL:HG23	2.20	0.42
1:C:397:ILE:HA	1:C:400:ILE:CD1	2.49	0.42
1:D:279:LYS:NZ	1:D:283:GLU:OE2	2.40	0.42
1:F:436:LYS:O	1:F:440:GLU:N	2.48	0.42
1:A:299:ILE:HD12	1:A:299:ILE:N	2.35	0.42
1:F:285:CYS:O	1:F:286:GLN:HB3	2.20	0.42
1:C:397:ILE:HA	1:C:400:ILE:HD12	2.01	0.42
1:D:410:LEU:HD23	1:D:412:PHE:CZ	2.54	0.42
1:E:296:ARG:HA	1:E:382:TYR:CE1	2.54	0.42
1:B:379:GLU:N	2:B:501:9WA:F1	2.43	0.42
1:F:369:TYR:OH	1:F:374:ARG:HG2	2.20	0.42
1:B:267:LEU:HD21	1:B:271:GLU:OE1	2.19	0.41
1:D:423:LEU:CD1	1:D:447:GLU:HG2	2.46	0.41
1:B:293:LEU:HA	1:B:296:ARG:HG3	2.01	0.41
1:A:368:ALA:HB1	1:A:377:PHE:HB3	2.02	0.41
1:E:423:LEU:HD11	1:E:447:GLU:HG2	2.01	0.41
1:F:316:MET:HG3	1:F:390:ALA:HB3	2.02	0.41
1:D:396:LEU:HA	1:E:313:MET:CE	2.50	0.41
1:F:447:GLU:O	1:F:450:PHE:HB3	2.21	0.41
1:A:417:ILE:O	1:A:421:THR:HG23	2.20	0.41
1:B:267:LEU:HD23	1:B:267:LEU:O	2.21	0.41
1:F:301:SER:OG	1:F:304:GLU:HG3	2.21	0.41
1:F:347:ASN:O	1:F:351:VAL:HG12	2.21	0.41
1:C:473:ARG:CG	1:C:474:SER:N	2.83	0.41
1:D:334:PHE:O	1:D:338:LEU:HG	2.20	0.41
1:E:323:HIS:HD2	1:E:378:PHE:HE1	1.68	0.41
1:F:324:LEU:HD21	2:F:501:9WA:CL	2.58	0.41
1:D:369:TYR:OH	1:D:374:ARG:HG2	2.21	0.41
1:D:395:GLU:HG2	1:D:396:LEU:N	2.36	0.41
1:E:299:ILE:HD12	1:E:299:ILE:N	2.36	0.41
1:E:285:CYS:O	1:E:286:GLN:HB3	2.21	0.40
1:D:313:MET:HG3	1:D:390:ALA:O	2.21	0.40
1:D:360:VAL:HG13	1:D:421:THR:HB	2.03	0.40
1:B:274:VAL:CG2	1:B:449:ALA:HB1	2.50	0.40
1:B:459:ARG:O	1:B:462:ILE:HG12	2.21	0.40
1:B:473:ARG:CG	1:B:474:SER:H	2.32	0.40
1:B:395:GLU:HG2	1:B:396:LEU:N	2.36	0.40
1:A:473:ARG:CG	1:A:474:SER:N	2.83	0.40
1:B:473:ARG:CG	1:B:474:SER:N	2.84	0.40
1:E:290:GLU:CD	1:E:290:GLU:H	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:ILE:HD11	1:F:358:MET:CE	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:SER:OG	1:F:389:ARG:NH1[5_664]	2.06	0.14

## 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	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
1	B	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
1	C	204/210 (97%)	198 (97%)	6 (3%)	0	100	100
1	D	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	43
1	E	204/210 (97%)	195 (96%)	8 (4%)	1 (0%)	29	43
1	F	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
All	All	1223/1260 (97%)	1185 (97%)	36 (3%)	2 (0%)	47	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	303	GLU
1	D	317	TRP

### 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	186/187 (100%)	186 (100%)	0	100	100
1	B	186/187 (100%)	185 (100%)	1 (0%)	88	94
1	C	183/187 (98%)	181 (99%)	2 (1%)	73	85
1	D	181/187 (97%)	180 (99%)	1 (1%)	86	92
1	E	183/187 (98%)	181 (99%)	2 (1%)	73	85
1	F	180/187 (96%)	177 (98%)	3 (2%)	60	77
All	All	1099/1122 (98%)	1090 (99%)	9 (1%)	81	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	317	TRP
1	C	290	GLU
1	C	385	MET
1	D	318	GLU
1	E	302	ARG
1	E	303	GLU
1	F	288	ARG
1	F	290	GLU
1	F	302	ARG

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 carbohydrates in this entry.

## 5.6 Ligand geometry

6 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	9WA	B	501	-	43,48,48	1.38	9 (20%)	61,72,72	1.60	4 (6%)
2	9WA	F	501	-	43,48,48	1.37	8 (18%)	61,72,72	1.84	9 (14%)
2	9WA	E	501	-	43,48,48	1.38	7 (16%)	61,72,72	1.70	6 (9%)
2	9WA	C	501	-	43,48,48	1.44	9 (20%)	61,72,72	1.61	5 (8%)
2	9WA	A	501	-	43,48,48	1.40	8 (18%)	61,72,72	1.62	5 (8%)
2	9WA	D	501	-	43,48,48	1.42	8 (18%)	61,72,72	1.65	6 (9%)

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	9WA	B	501	-	-	10/28/34/34	0/6/6/6
2	9WA	F	501	-	-	5/28/34/34	0/6/6/6
2	9WA	E	501	-	-	6/28/34/34	0/6/6/6
2	9WA	C	501	-	-	11/28/34/34	0/6/6/6
2	9WA	A	501	-	-	4/28/34/34	0/6/6/6
2	9WA	D	501	-	-	4/28/34/34	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	9WA	C8-C7	-3.07	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	9WA	C20-C5	-3.07	1.49	1.53
2	D	501	9WA	C20-C5	-3.05	1.49	1.53
2	D	501	9WA	C8-C7	-3.02	1.38	1.42
2	F	501	9WA	C8-C7	-2.98	1.38	1.42
2	C	501	9WA	C20-C25	-2.96	1.49	1.53
2	A	501	9WA	C20-C5	-2.91	1.49	1.53
2	D	501	9WA	C20-C25	-2.87	1.49	1.53
2	A	501	9WA	C8-C7	-2.83	1.38	1.42
2	E	501	9WA	C7-C2	-2.83	1.37	1.42
2	E	501	9WA	C20-C5	-2.81	1.49	1.53
2	B	501	9WA	C20-C5	-2.79	1.49	1.53
2	B	501	9WA	C8-C7	-2.78	1.38	1.42
2	F	501	9WA	C20-C5	-2.76	1.49	1.53
2	C	501	9WA	C7-C2	-2.75	1.38	1.42
2	F	501	9WA	C7-C2	-2.74	1.38	1.42
2	A	501	9WA	C20-C25	-2.73	1.49	1.53
2	A	501	9WA	C7-C2	-2.73	1.38	1.42
2	D	501	9WA	C7-C2	-2.73	1.38	1.42
2	B	501	9WA	C20-C25	-2.72	1.49	1.53
2	B	501	9WA	C7-C2	-2.72	1.38	1.42
2	E	501	9WA	C8-C7	-2.67	1.38	1.42
2	E	501	9WA	C20-C25	-2.62	1.49	1.53
2	E	501	9WA	C2-N	-2.44	1.33	1.37
2	C	501	9WA	C2-N	-2.44	1.33	1.37
2	F	501	9WA	C20-C25	-2.42	1.50	1.53
2	E	501	9WA	C3-C2	-2.40	1.37	1.41
2	A	501	9WA	C3-C2	-2.40	1.37	1.41
2	A	501	9WA	C2-N	-2.40	1.33	1.37
2	D	501	9WA	C3-C2	-2.40	1.37	1.41
2	D	501	9WA	C2-N	-2.39	1.33	1.37
2	C	501	9WA	C3-C2	-2.38	1.37	1.41
2	F	501	9WA	C2-N	-2.34	1.33	1.37
2	B	501	9WA	C3-C2	-2.30	1.37	1.41
2	B	501	9WA	C2-N	-2.30	1.33	1.37
2	F	501	9WA	C3-C2	-2.28	1.37	1.41
2	A	501	9WA	O-C1	2.18	1.38	1.35
2	B	501	9WA	O-C1	2.17	1.38	1.35
2	E	501	9WA	O-C1	2.17	1.38	1.35
2	C	501	9WA	C6-C7	-2.13	1.37	1.42
2	F	501	9WA	O-C1	2.10	1.38	1.35
2	F	501	9WA	C6-C7	-2.08	1.38	1.42
2	A	501	9WA	C9-C1	-2.08	1.37	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	9WA	C9-C1	-2.07	1.37	1.39
2	B	501	9WA	C6-C7	-2.07	1.38	1.42
2	D	501	9WA	C6-C7	-2.06	1.38	1.42
2	C	501	9WA	C9-C1	-2.05	1.37	1.39
2	C	501	9WA	O-C1	2.04	1.38	1.35
2	D	501	9WA	O-C1	2.03	1.38	1.35

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	9WA	C-O-C1	-10.20	107.11	117.21
2	D	501	9WA	C-O-C1	-9.66	107.64	117.21
2	F	501	9WA	C-O-C1	-9.62	107.68	117.21
2	B	501	9WA	C-O-C1	-9.53	107.77	117.21
2	A	501	9WA	C-O-C1	-9.52	107.78	117.21
2	C	501	9WA	C-O-C1	-9.45	107.85	117.21
2	F	501	9WA	C24-N4-C21	4.39	129.76	124.35
2	F	501	9WA	C21-C20-C25	3.60	116.80	110.77
2	E	501	9WA	C30-C28-N5	3.26	118.53	114.61
2	F	501	9WA	C8-C7-C2	3.08	118.24	116.41
2	F	501	9WA	O1-C20-C21	-3.03	104.61	108.29
2	A	501	9WA	C30-C28-N5	2.91	118.11	114.61
2	D	501	9WA	C8-C7-C2	2.89	118.12	116.41
2	B	501	9WA	C30-C28-N5	2.88	118.07	114.61
2	F	501	9WA	C30-C28-N5	2.76	117.93	114.61
2	C	501	9WA	C8-C7-C2	2.76	118.05	116.41
2	C	501	9WA	C17-N1-N2	2.75	113.80	111.94
2	A	501	9WA	C17-N1-N2	2.75	113.80	111.94
2	D	501	9WA	C30-C28-N5	2.75	117.92	114.61
2	F	501	9WA	C17-N1-N2	2.74	113.79	111.94
2	B	501	9WA	C17-N1-N2	2.71	113.77	111.94
2	D	501	9WA	C17-N1-N2	2.63	113.71	111.94
2	E	501	9WA	C17-N1-N2	2.62	113.71	111.94
2	B	501	9WA	C8-C7-C2	2.54	117.92	116.41
2	C	501	9WA	C30-C28-N5	2.53	117.65	114.61
2	A	501	9WA	C8-C7-C2	2.47	117.88	116.41
2	E	501	9WA	C24-N4-C21	2.20	127.07	124.35
2	D	501	9WA	C21-C20-C5	-2.18	107.13	110.77
2	A	501	9WA	C25-C20-C5	2.17	116.28	110.96
2	C	501	9WA	C5-C6-C7	-2.14	120.16	122.31
2	E	501	9WA	C13-C14-N1	2.12	121.01	119.15
2	F	501	9WA	C25-C20-C5	2.12	116.14	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	9WA	C5-C6-C7	-2.07	120.23	122.31
2	E	501	9WA	C27-C28-C30	-2.06	118.06	121.01
2	F	501	9WA	C21-C20-C5	-2.05	107.34	110.77

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	9WA	C5-C20-C25-C29
2	E	501	9WA	C5-C20-C25-C29
2	A	501	9WA	C5-C20-C25-C29
2	A	501	9WA	O1-C20-C25-C29
2	E	501	9WA	N-C1-O-C
2	E	501	9WA	C9-C1-O-C
2	E	501	9WA	C15-C14-N1-C17
2	F	501	9WA	O1-C20-C25-C29
2	E	501	9WA	C13-C14-N1-C17
2	B	501	9WA	O1-C20-C25-C29
2	E	501	9WA	O1-C20-C25-C29
2	B	501	9WA	C11-C10-C9-C1
2	C	501	9WA	N5-C28-C30-F2
2	B	501	9WA	C5-C20-C25-C29
2	A	501	9WA	C15-C14-N1-C17
2	A	501	9WA	C13-C14-N1-C17
2	D	501	9WA	C13-C14-N1-C17
2	C	501	9WA	N5-C28-C30-F
2	C	501	9WA	O1-C20-C25-C29
2	F	501	9WA	C11-C10-C9-C1
2	C	501	9WA	N5-C28-C30-F1
2	C	501	9WA	C27-C28-C30-F2
2	C	501	9WA	C27-C28-C30-F1
2	F	501	9WA	C15-C14-N1-C17
2	F	501	9WA	C13-C14-N1-C17
2	D	501	9WA	C15-C14-N1-C17
2	C	501	9WA	C27-C28-C30-F
2	D	501	9WA	O1-C20-C25-C29
2	D	501	9WA	O1-C20-C25-C26
2	B	501	9WA	N5-C28-C30-F
2	B	501	9WA	N5-C28-C30-F1
2	B	501	9WA	C15-C14-N1-C17
2	B	501	9WA	C13-C14-N1-C17
2	C	501	9WA	C15-C14-N1-C17

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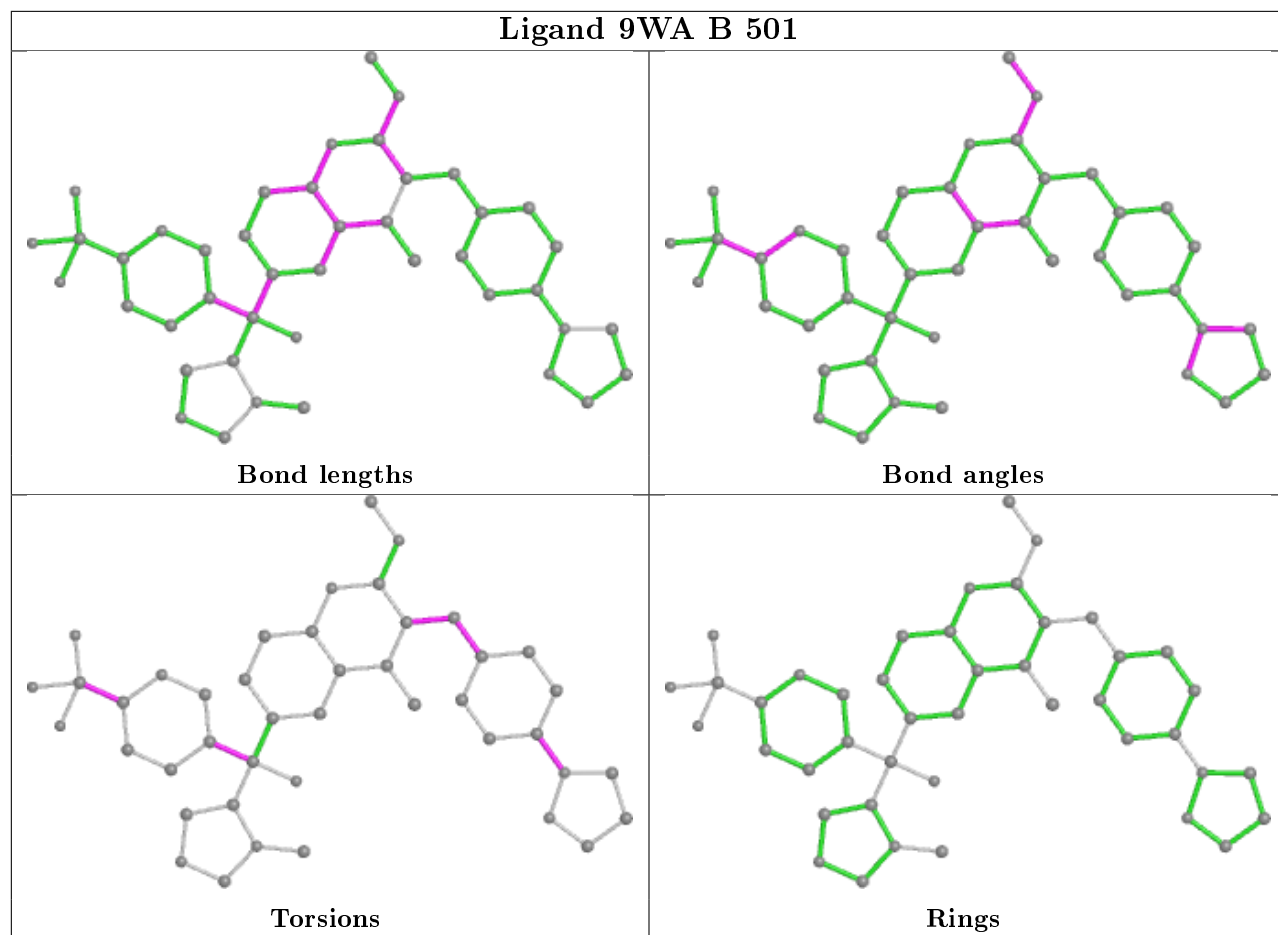
Mol	Chain	Res	Type	Atoms
2	C	501	9WA	C13-C14-N1-C17
2	C	501	9WA	O1-C20-C25-C26
2	C	501	9WA	C5-C20-C25-C29
2	B	501	9WA	N5-C28-C30-F2
2	B	501	9WA	C9-C10-C11-C12
2	B	501	9WA	C27-C28-C30-F1

There are no ring outliers.

4 monomers are involved in 10 short contacts:

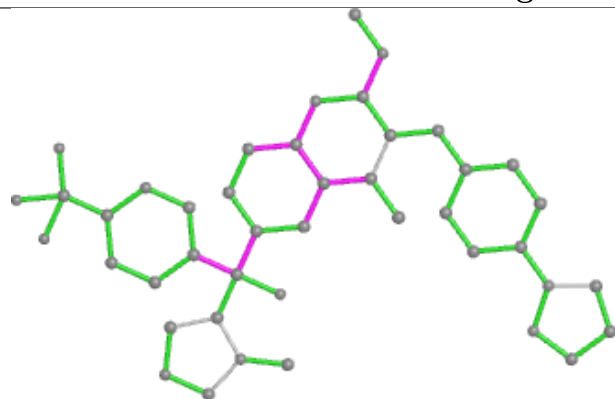
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	9WA	3	0
2	F	501	9WA	2	0
2	C	501	9WA	2	0
2	D	501	9WA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

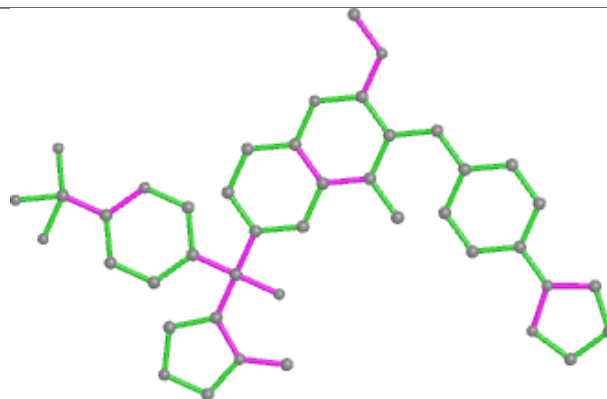




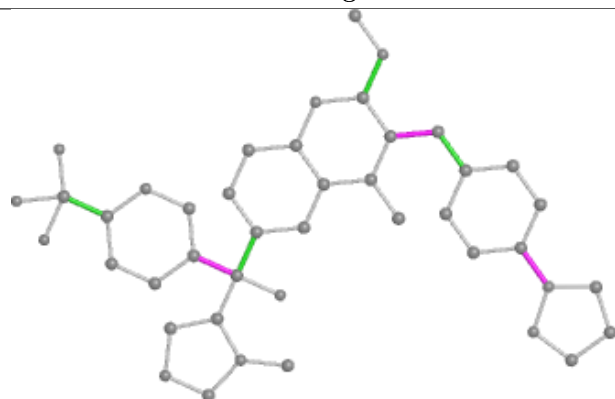
## Ligand 9WA F 501



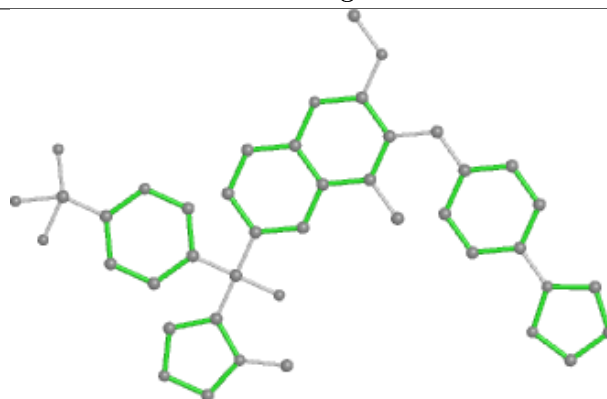
Bond lengths



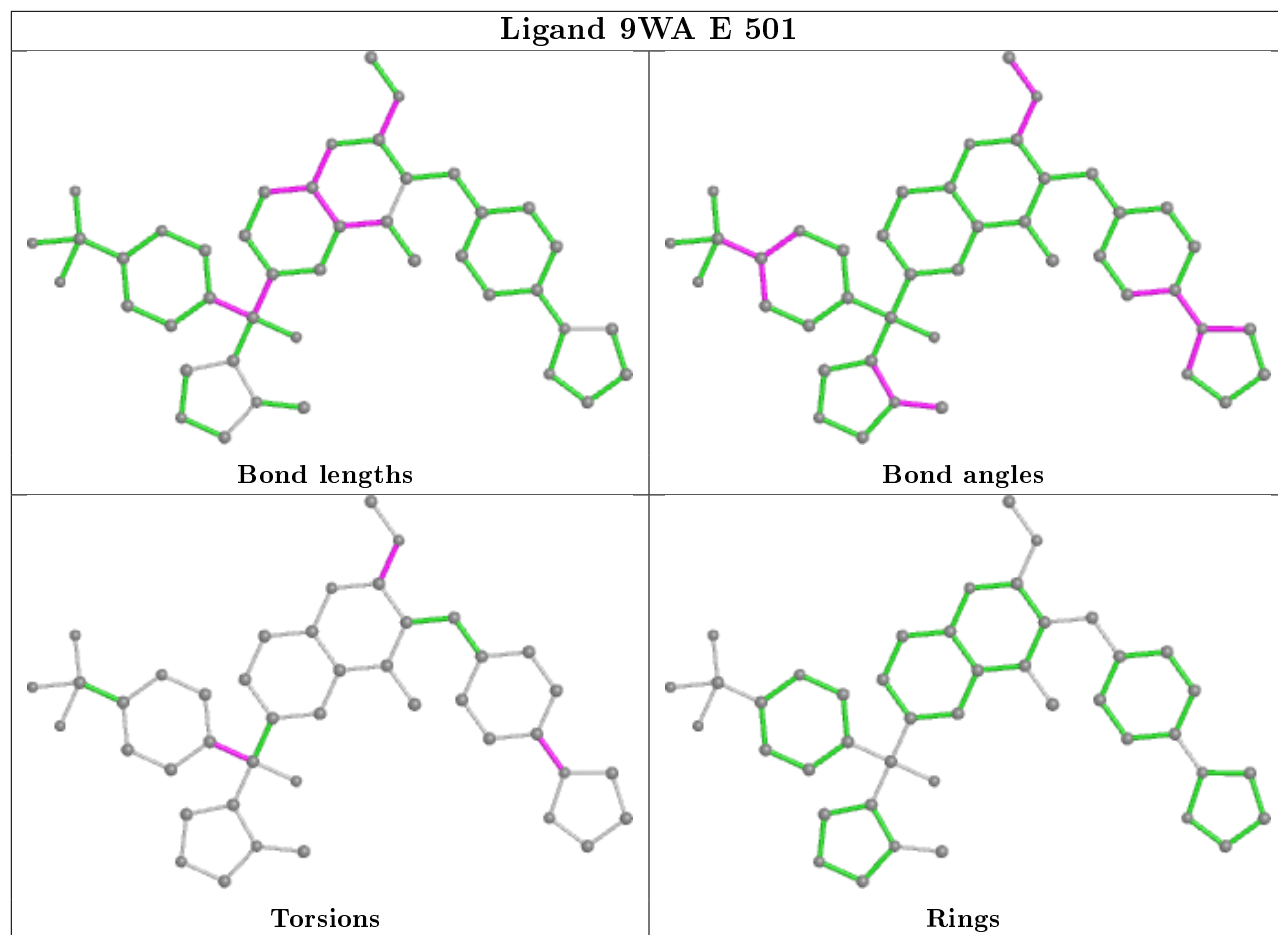
Bond angles

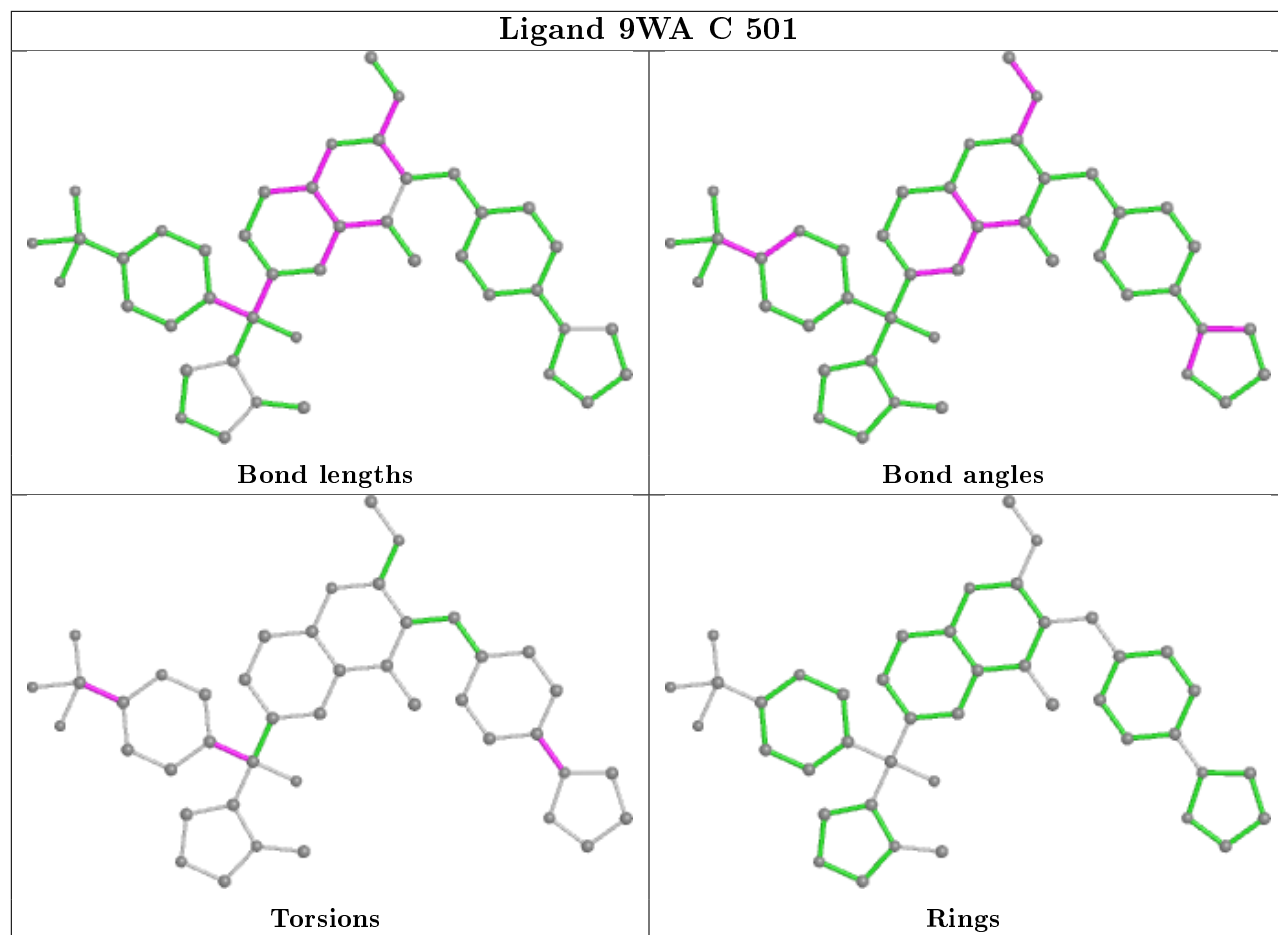


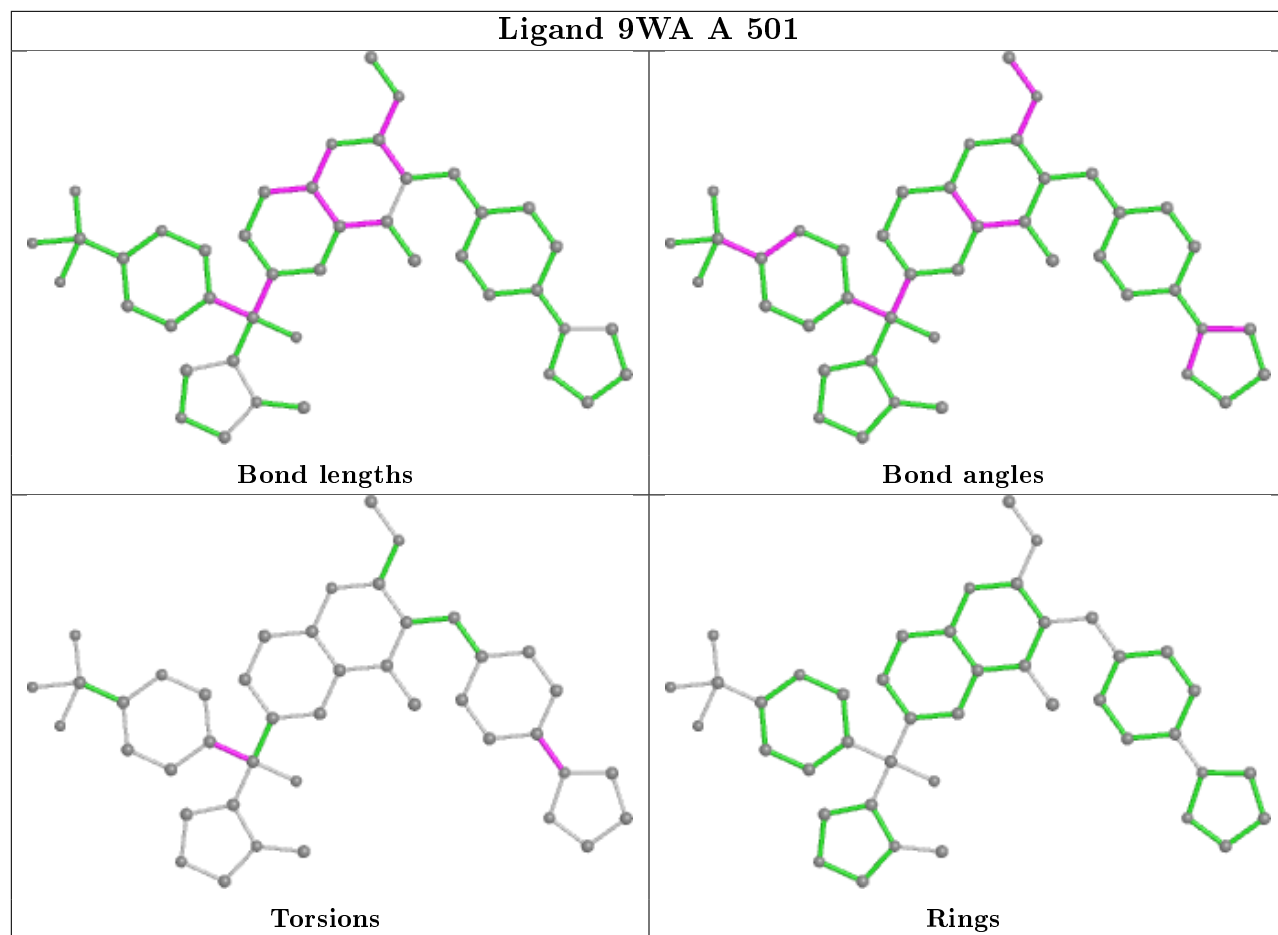
Torsions

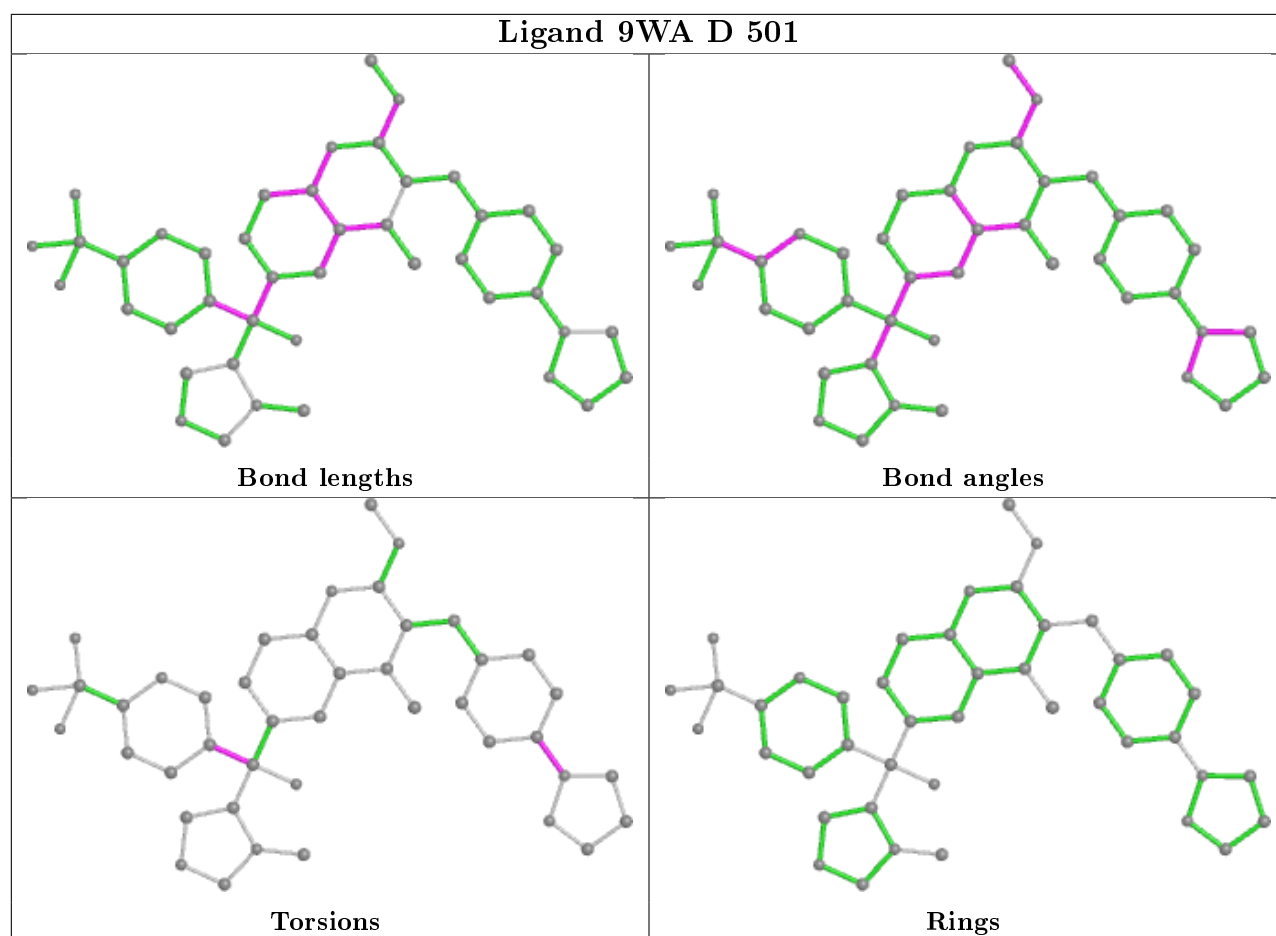


Rings









## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	209/210 (99%)	0.66	21 (10%) 7 5	12, 28, 60, 73	0
1	B	209/210 (99%)	0.67	24 (11%) 4 3	12, 29, 70, 103	0
1	C	206/210 (98%)	1.66	65 (31%) 0 0	18, 36, 67, 82	0
1	D	203/210 (96%)	1.64	63 (31%) 0 0	15, 37, 64, 75	0
1	E	206/210 (98%)	1.72	67 (32%) 0 0	18, 37, 65, 74	0
1	F	202/210 (96%)	1.70	64 (31%) 0 0	17, 39, 68, 88	0
All	All	1235/1260 (98%)	1.34	304 (24%) 0 0	12, 36, 67, 103	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	351	VAL	8.1
1	E	351	VAL	7.2
1	D	303	GLU	7.2
1	D	268	THR	7.2
1	F	272	HIS	7.0
1	E	267	LEU	6.7
1	B	444	TYR	6.5
1	C	437	ARG	6.5
1	C	310	ARG	6.2
1	B	472	LEU	6.2
1	E	301	SER	6.2
1	A	267	LEU	6.1
1	E	354	LYS	5.8
1	F	439	VAL	5.8
1	B	470	GLY	5.8
1	F	444	TYR	5.8
1	C	336	LYS	5.7
1	D	343	GLU	5.6
1	C	273	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	470	GLY	5.6
1	C	271	GLU	5.4
1	C	306	THR	5.4
1	F	268	THR	5.4
1	F	452	HIS	5.3
1	B	473	ARG	5.3
1	D	312	SER	5.3
1	D	444	TYR	5.3
1	F	270	ILE	5.3
1	F	267	LEU	5.2
1	E	444	TYR	5.1
1	C	303	GLU	5.1
1	F	348	ASP	5.1
1	D	458	HIS	5.1
1	E	271	GLU	5.0
1	E	346	GLN	5.0
1	F	456	LYS	4.9
1	C	296	ARG	4.9
1	C	470	GLY	4.8
1	E	269	GLU	4.8
1	E	452	HIS	4.8
1	C	284	THR	4.7
1	C	280	SER	4.7
1	E	389	ARG	4.7
1	E	437	ARG	4.6
1	B	474	SER	4.6
1	E	469	LYS	4.5
1	D	306	THR	4.5
1	D	267	LEU	4.5
1	E	302	ARG	4.5
1	C	277	VAL	4.5
1	E	268	THR	4.4
1	D	284	THR	4.4
1	A	271	GLU	4.3
1	B	272	HIS	4.3
1	C	458	HIS	4.2
1	E	455	HIS	4.2
1	F	434	GLN	4.2
1	A	269	GLU	4.2
1	A	437	ARG	4.2
1	C	343	GLU	4.2
1	C	455	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	348	ASP	4.0
1	B	343	GLU	4.0
1	F	305	VAL	4.0
1	D	269	GLU	4.0
1	D	316	MET	3.9
1	F	303	GLU	3.9
1	F	290	GLU	3.9
1	F	269	GLU	3.9
1	A	268	THR	3.8
1	E	290	GLU	3.8
1	E	433	LEU	3.8
1	E	306	THR	3.8
1	D	271	GLU	3.7
1	C	431	PRO	3.7
1	C	444	TYR	3.7
1	E	460	GLN	3.7
1	D	437	ARG	3.7
1	F	427	ASN	3.7
1	F	354	LYS	3.7
1	D	296	ARG	3.6
1	B	437	ARG	3.6
1	C	433	LEU	3.6
1	F	346	GLN	3.6
1	D	280	SER	3.6
1	C	307	GLY	3.6
1	F	442	LEU	3.5
1	C	305	VAL	3.5
1	D	272	HIS	3.5
1	D	336	LYS	3.5
1	E	378	PHE	3.5
1	F	424	VAL	3.5
1	E	451	HIS	3.5
1	A	272	HIS	3.4
1	E	424	VAL	3.4
1	C	278	CYS	3.4
1	F	271	GLU	3.4
1	F	310	ARG	3.3
1	D	436	LYS	3.3
1	D	310	ARG	3.3
1	D	345	CYS	3.3
1	F	342	MET	3.2
1	F	448	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	429	HIS	3.2
1	E	438	LYS	3.2
1	D	376	VAL	3.2
1	E	305	VAL	3.2
1	E	456	LYS	3.2
1	C	434	GLN	3.2
1	B	434	GLN	3.1
1	B	468	PRO	3.1
1	D	346	GLN	3.1
1	E	272	HIS	3.1
1	F	333	GLU	3.1
1	B	469	LYS	3.1
1	D	424	VAL	3.1
1	C	302	ARG	3.1
1	E	317	TRP	3.0
1	E	303	GLU	3.0
1	C	282	ARG	3.0
1	F	437	ARG	3.0
1	E	434	GLN	3.0
1	C	272	HIS	3.0
1	E	282	ARG	3.0
1	F	306	THR	3.0
1	E	343	GLU	3.0
1	C	274	VAL	2.9
1	C	283	GLU	2.9
1	C	377	PHE	2.9
1	F	359	GLU	2.9
1	C	448	LEU	2.9
1	E	310	ARG	2.9
1	E	342	MET	2.9
1	C	368	ALA	2.9
1	D	317	TRP	2.9
1	E	458	HIS	2.9
1	F	461	SER	2.9
1	A	275	GLN	2.9
1	E	448	LEU	2.9
1	F	429	HIS	2.9
1	C	397	ILE	2.9
1	F	392	GLY	2.9
1	D	386	GLU	2.9
1	F	343	GLU	2.9
1	D	266	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	329	GLN	2.8
1	C	438	LYS	2.8
1	B	306	THR	2.8
1	D	294	ARG	2.8
1	F	336	LYS	2.8
1	F	455	HIS	2.8
1	F	294	ARG	2.8
1	A	455	HIS	2.8
1	E	275	GLN	2.8
1	D	438	LYS	2.8
1	D	434	GLN	2.7
1	F	443	GLN	2.7
1	C	312	SER	2.7
1	F	410	LEU	2.7
1	F	347	ASN	2.7
1	B	441	GLN	2.7
1	F	307	GLY	2.7
1	E	442	LEU	2.7
1	F	451	HIS	2.7
1	F	317	TRP	2.7
1	E	464	ALA	2.7
1	D	305	VAL	2.7
1	C	435	GLU	2.7
1	C	473	ARG	2.7
1	E	347	ASN	2.7
1	F	275	GLN	2.7
1	E	304	GLU	2.7
1	D	322	HIS	2.7
1	C	385	MET	2.7
1	D	314	TRP	2.7
1	E	397	ILE	2.7
1	B	458	HIS	2.7
1	E	411	HIS	2.7
1	D	368	ALA	2.6
1	F	320	CYS	2.6
1	A	306	THR	2.6
1	F	365	MET	2.6
1	E	352	LEU	2.6
1	F	353	LEU	2.6
1	E	329	GLN	2.6
1	C	436	LYS	2.6
1	E	362	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	468	PRO	2.6
1	D	275	GLN	2.6
1	E	423	LEU	2.6
1	A	354	LYS	2.6
1	D	457	THR	2.6
1	B	346	GLN	2.6
1	C	396	LEU	2.6
1	E	307	GLY	2.6
1	B	271	GLU	2.6
1	C	419	LEU	2.5
1	D	287	LEU	2.5
1	F	352	LEU	2.5
1	C	389	ARG	2.5
1	D	329	GLN	2.5
1	F	460	GLN	2.5
1	A	474	SER	2.5
1	C	290	GLU	2.5
1	E	319	ARG	2.5
1	F	397	ILE	2.5
1	C	317	TRP	2.5
1	C	334	PHE	2.5
1	E	280	SER	2.5
1	D	307	GLY	2.5
1	C	344	LEU	2.5
1	F	425	LEU	2.5
1	D	366	CYS	2.5
1	C	446	LEU	2.4
1	C	346	GLN	2.4
1	A	310	ARG	2.4
1	C	392	GLY	2.4
1	C	400	ILE	2.4
1	D	283	GLU	2.4
1	E	383	GLY	2.4
1	A	303	GLU	2.4
1	C	441	GLN	2.4
1	D	298	ASN	2.4
1	E	440	GLU	2.4
1	D	399	SER	2.4
1	E	344	LEU	2.4
1	D	464	ALA	2.3
1	E	461	SER	2.3
1	B	336	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	423	LEU	2.3
1	C	270	ILE	2.3
1	D	318	GLU	2.3
1	C	316	MET	2.3
1	F	458	HIS	2.3
1	C	457	THR	2.3
1	E	300	PHE	2.3
1	A	305	VAL	2.3
1	D	396	LEU	2.2
1	B	436	LYS	2.2
1	F	296	ARG	2.2
1	C	401	PHE	2.2
1	C	345	CYS	2.2
1	D	397	ILE	2.2
1	C	428	ALA	2.2
1	A	336	LYS	2.2
1	D	320	CYS	2.2
1	D	302	ARG	2.2
1	E	336	LYS	2.2
1	A	431	PRO	2.2
1	D	429	HIS	2.2
1	B	393	CYS	2.2
1	F	286	GLN	2.2
1	A	307	GLY	2.2
1	C	319	ARG	2.2
1	E	441	GLN	2.2
1	D	278	CYS	2.2
1	A	351	VAL	2.1
1	D	274	VAL	2.1
1	E	426	ILE	2.1
1	D	389	ARG	2.1
1	C	300	PHE	2.1
1	A	433	LEU	2.1
1	C	324	LEU	2.1
1	C	429	HIS	2.1
1	F	367	ARG	2.1
1	F	355	ALA	2.1
1	F	464	ALA	2.1
1	D	431	PRO	2.1
1	D	377	PHE	2.1
1	F	366	CYS	2.1
1	B	392	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	397	ILE	2.1
1	E	360	VAL	2.1
1	B	307	GLY	2.1
1	C	362	LEU	2.1
1	F	433	LEU	2.1
1	F	440	GLU	2.1
1	C	325	THR	2.1
1	D	385	MET	2.1
1	E	413	SER	2.1
1	D	435	GLU	2.1
1	D	387	LEU	2.1
1	F	357	ALA	2.1
1	C	318	GLU	2.1
1	A	470	GLY	2.1
1	C	348	ASP	2.1
1	E	312	SER	2.1
1	C	338	LEU	2.0
1	E	439	VAL	2.0
1	D	417	ILE	2.0
1	D	281	TYR	2.0
1	B	280	SER	2.0
1	D	297	SER	2.0
1	D	412	PHE	2.0
1	F	435	GLU	2.0
1	B	347	ASN	2.0
1	F	445	ASN	2.0
1	E	443	GLN	2.0
1	D	411	HIS	2.0
1	A	343	GLU	2.0
1	D	390	ALA	2.0
1	C	378	PHE	2.0
1	E	294	ARG	2.0
1	E	472	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

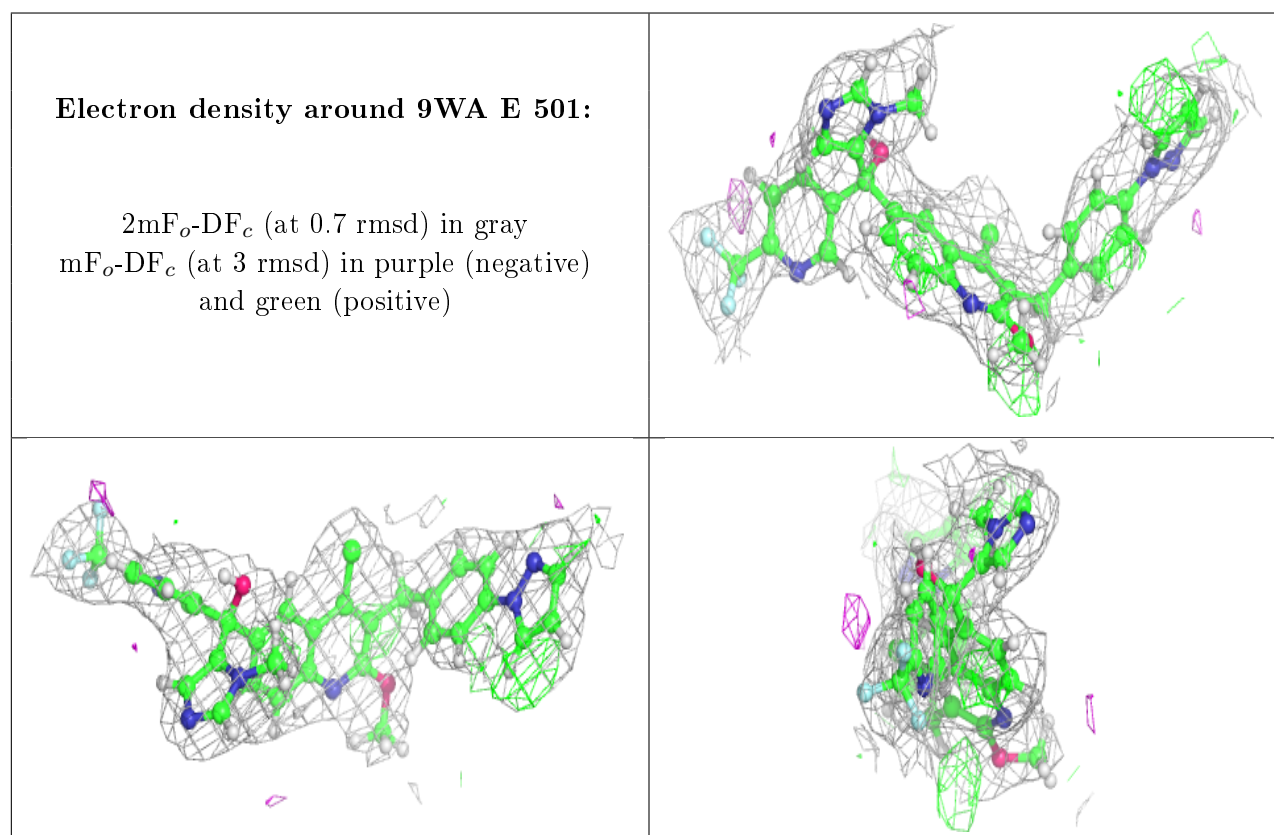
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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.

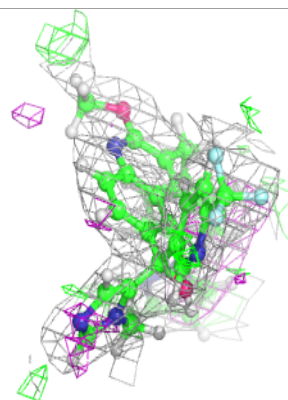
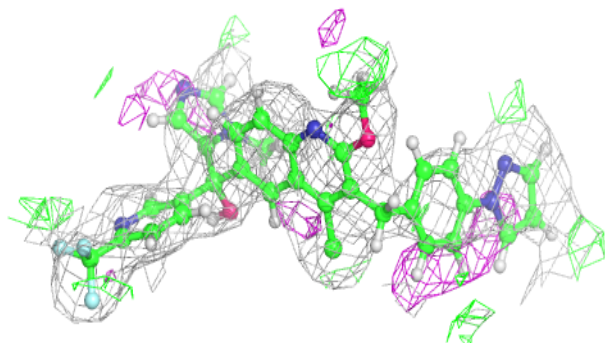
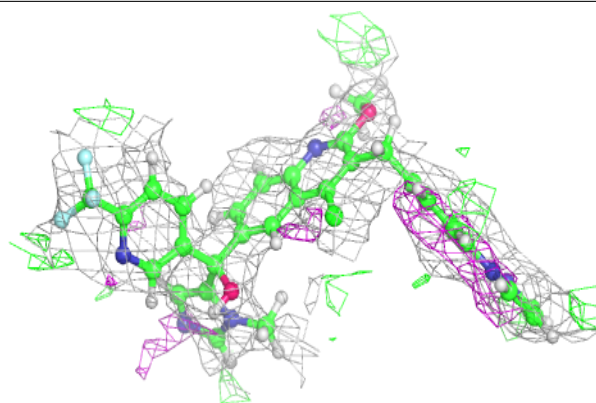
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	9WA	E	501	43/43	0.75	0.35	28,49,67,80	0
2	9WA	D	501	43/43	0.78	0.29	18,34,46,68	0
2	9WA	F	501	43/43	0.80	0.27	11,29,46,57	0
2	9WA	C	501	43/43	0.81	0.28	13,32,51,73	0
2	9WA	B	501	43/43	0.89	0.19	7,19,31,56	0
2	9WA	A	501	43/43	0.90	0.19	9,22,37,60	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.

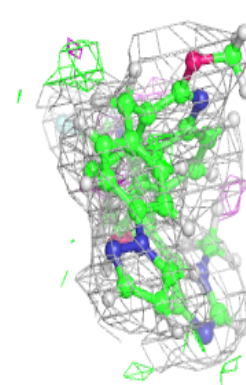
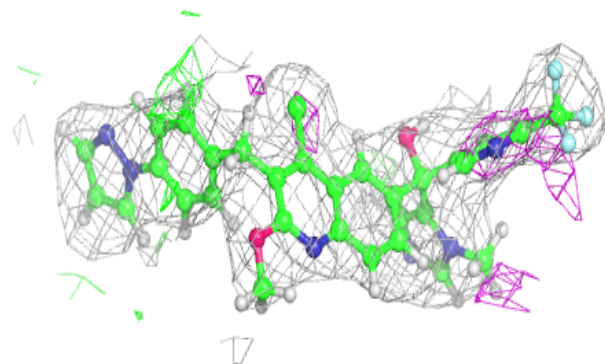
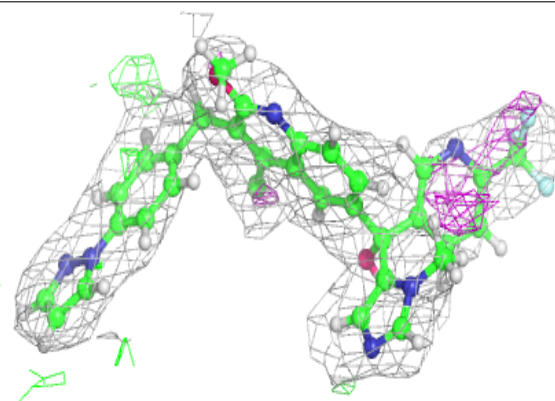


**Electron density around 9WA D 501:**

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

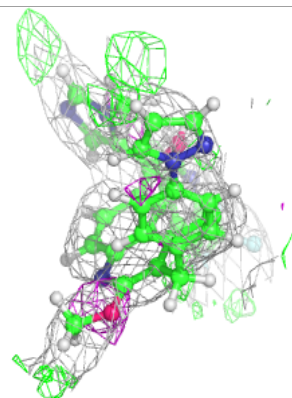
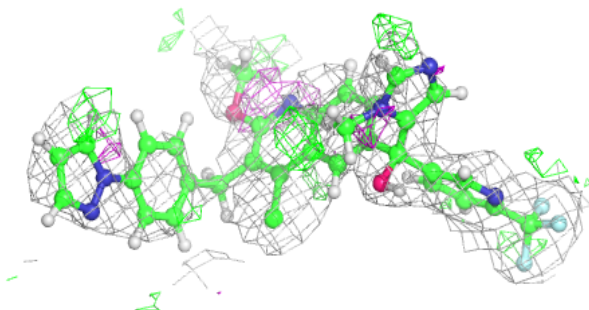
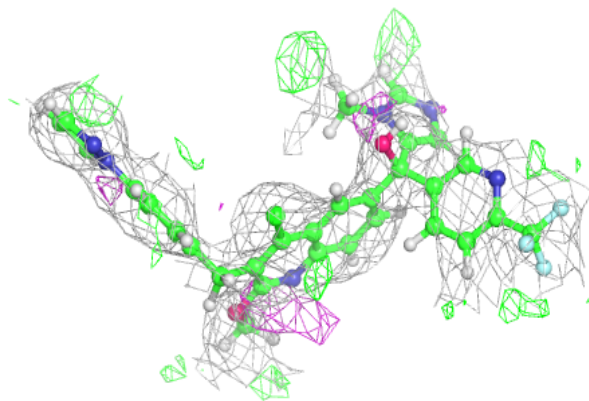
**Electron density around 9WA F 501:**

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

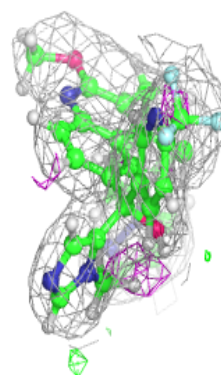
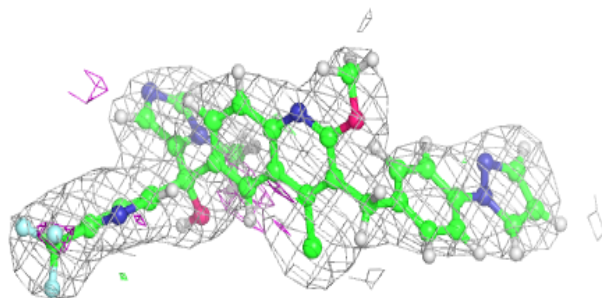
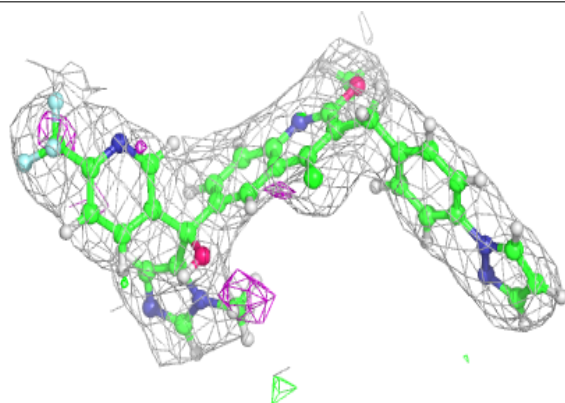


**Electron density around 9WA C 501:**

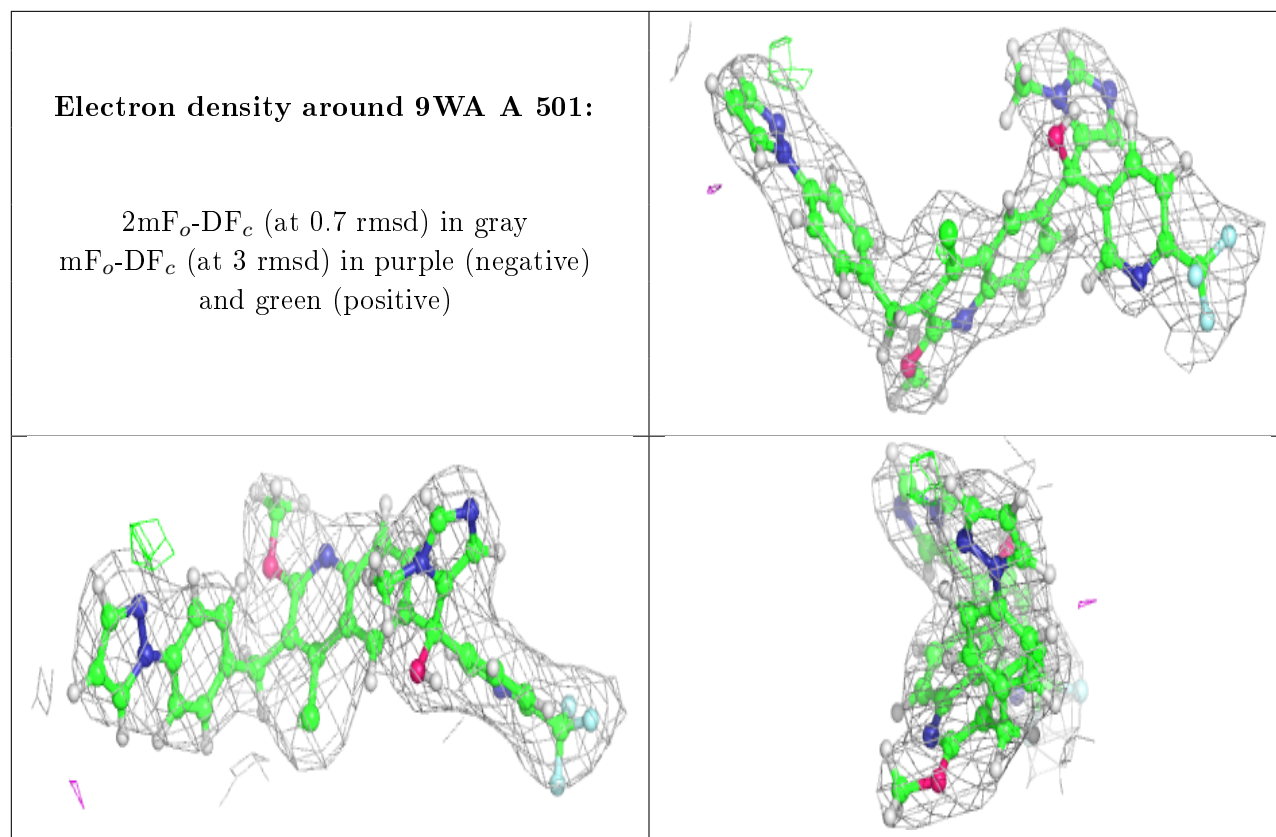
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 9WA 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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.