



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 5W4V / pdb_00005w4v
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

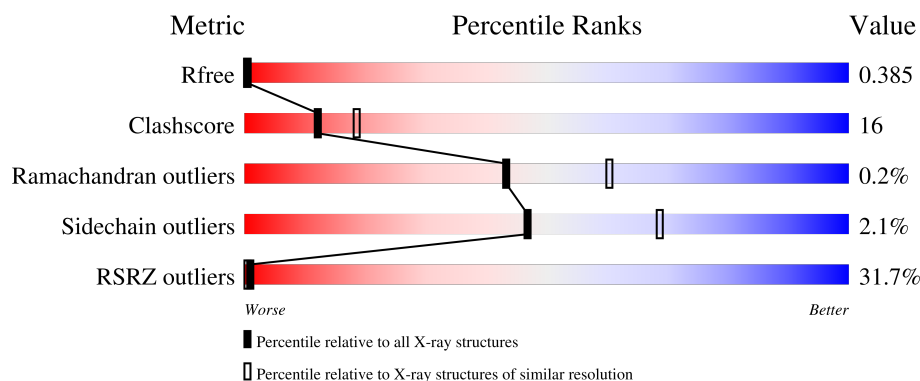
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	210	8% 77% 21% .
1	B	210	10% 68% 31%
1	C	210	40% 70% 27% ..
1	D	210	44% 63% 32% ..
1	E	210	40% 68% 27% ..

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Mol	Chain	Length	Quality of chain
1	F	210	45% 67% 28%

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.

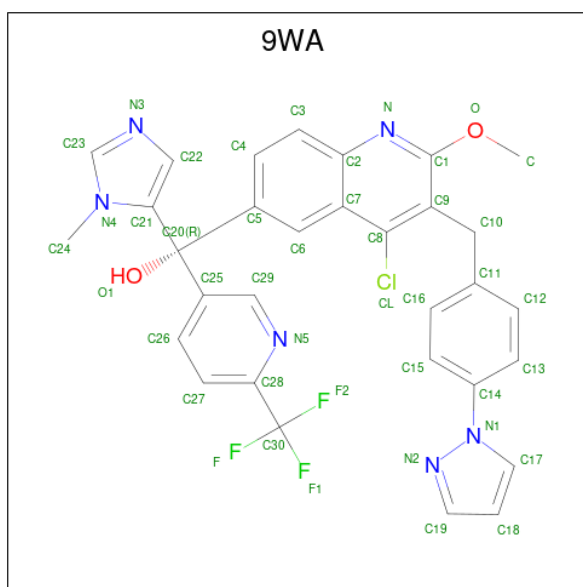
- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

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 (CCD ID: 9WA) (formula: C₃₁H₂₄ClF₃N₆O₂).



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		

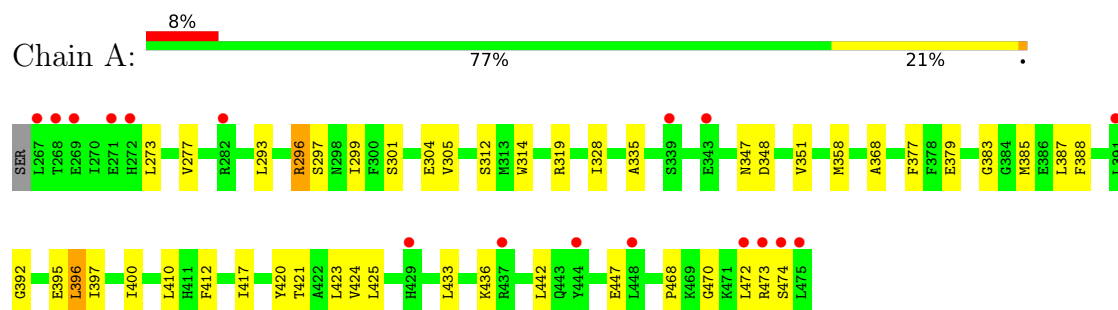
- Molecule 3 is water.

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

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.

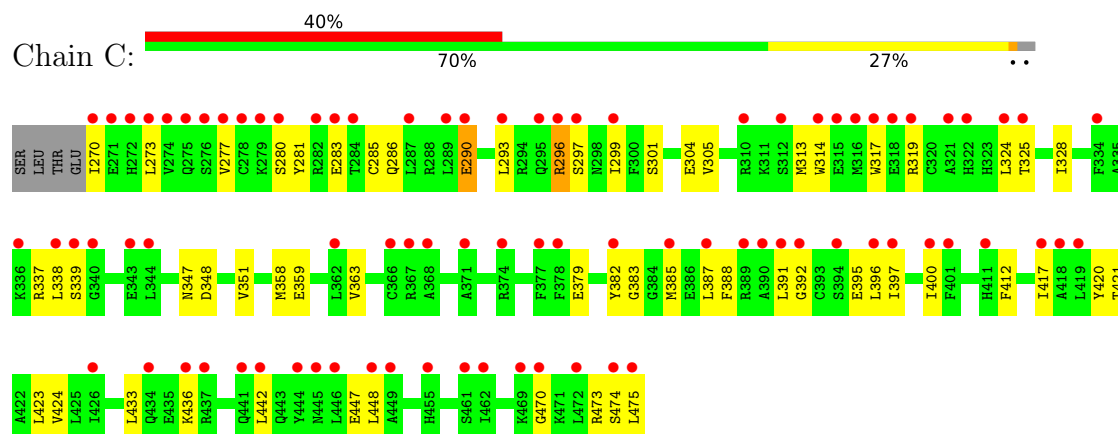
• Molecule 1: Nuclear receptor ROR-gamma



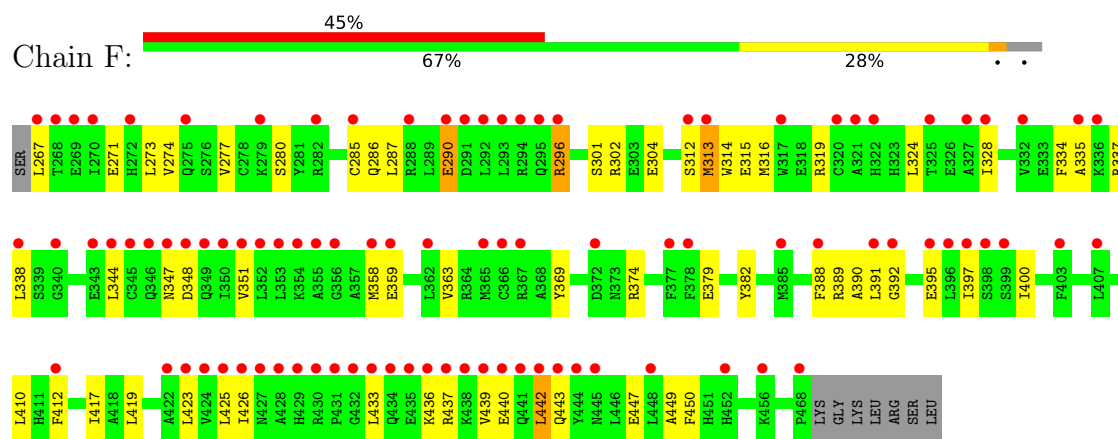
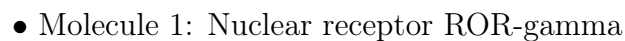
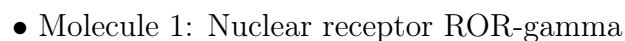
• Molecule 1: Nuclear receptor ROR-gamma



• 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, α , β , γ	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) 89.0 (29.35-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.343 , 0.384 0.350 , 0.385	Depositor DCC
R_{free} test set	2724 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.09	0/1746	0.26	0/2347
1	B	0.09	0/1746	0.27	0/2347
1	C	0.10	0/1722	0.28	0/2314
1	D	0.13	0/1697	0.43	3/2284 (0.1%)
1	E	0.10	0/1721	0.34	1/2314 (0.0%)
1	F	0.08	0/1691	0.26	0/2276
All	All	0.10	0/10323	0.31	4/13882 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	MET	N-CA-C	7.50	126.77	110.80
1	D	316	MET	CA-C-N	7.35	134.93	121.70
1	D	316	MET	C-N-CA	7.35	134.93	121.70
1	E	301	SER	N-CA-C	-5.65	103.46	110.41

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	51	0
1	B	1712	0	1715	61	0
1	C	1688	0	1691	59	0
1	D	1663	0	1651	59	0
1	E	1687	0	1686	61	1
1	F	1657	0	1646	52	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	320	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 16.

All (320) 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:C:328:ILE:HD11	1:C:358:MET:HE2	1.58	0.83
1:E:302:ARG:H	1:E:305:VAL:HB	1.41	0.82
1:A:328:ILE:HD11	1:A:358:MET:HE2	1.61	0.80
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:E:328:ILE:HD11	1:E:358:MET:HE2	1.66	0.76
1:B:334:PHE:O	1:B:338:LEU:HD13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:336:LYS:HE3	1:D:342:MET:HE1	1.74	0.69
1:B:470:GLY:O	1:B:473:ARG:HG2	1.93	0.69
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:A:396:LEU:HD13	1:B:313:MET:HE2	1.77	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:VAL:HG11	1:F:433:LEU:HD23	1.84	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:E:301:SER:HB3	1:E:302:ARG:C	2.28	0.58
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
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:358:MET:HE3	1:B:314:TRP:CZ3	2.39	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: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:D:308:TYR:OH	1:D:379:GLU:OE1	2.18	0.56
1:A:348:ASP:HA	1:A:351:VAL:CG1	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:F:443:GLN:O	1:F:447:GLU:HG3	2.06	0.55
1:C:474:SER:C	1:C:475:LEU:HD12	2.31	0.55
1:D:314:TRP:CH2	1:E:358:MET:HE3	2.42	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:328:ILE:HD11	1:C:358:MET:CE	2.32	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:F:274:VAL:HG22	1:F:449:ALA:HB1	1.88	0.54
1:C:358:MET:HE3	1:F:314:TRP:CZ3	2.42	0.54
1:E:397:ILE:HA	1:E:400:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:VAL:HG11	1:D:433:LEU:HD23	1.90	0.54
1:E:436:LYS:NZ	1:E:436:LYS:HB3	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
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: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:B:290:GLU:H	1:B:290:GLU:CD	2.18	0.52
1:A:442:LEU:HD12	1:A:442:LEU:O	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:HD12	1:F:442:LEU:O	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:D:297:SER:C	1:D:299:ILE:HD12	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LYS:NZ	1:A:436:LYS:HB3	2.26	0.51
1:A:383:GLY:HA3	1:A:387:LEU:HD22	1.93	0.51
1:D:317:TRP:CD1	1:D:391:LEU:HD22	2.46	0.51
1:D:348:ASP:HA	1:D:351:VAL:HG12	1.92	0.51
1:B:348:ASP:HA	1:B:351:VAL:HG12	1.93	0.50
1:A:328:ILE:HD11	1:A:358:MET:CE	2.36	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:290:GLU:CD	1:C:290:GLU:H	2.20	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
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:F:290:GLU:CD	1:F:290:GLU:H	2.20	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:C:314:TRP:CD2	1:F:358:MET:HG2	2.47	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: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:HD12	1:B:442:LEU:O	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:324:LEU:HD11	2:D:501:9WA:C14	2.43	0.49
1:D:436:LYS:NZ	1:D:436:LYS:HB3	2.27	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:E:442:LEU:HD12	1:E:442:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:SER:C	1:C:299:ILE:HD12	2.38	0.48
1:C:319:ARG:NH1	1:C:379:GLU:OE2	2.47	0.47
1:E:328:ILE:HD11	1:E:358:MET:CE	2.38	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:336:LYS:HE3	1:D:342:MET:CE	2.43	0.47
1:C:392:GLY:O	1:F:395:GLU:HG2	2.15	0.47
1:C:396:LEU:HD13	1:F:313:MET:SD	2.53	0.47
1:D:289:LEU:HD13	1:D:414:GLU:OE2	2.13	0.47
1:A:273:LEU:O	1:A:277:VAL:HG23	2.14	0.47
1:A:385:MET:HG2	1:A:385:MET:O	2.14	0.47
1:A:319:ARG:NH1	1:A:379:GLU:OE2	2.48	0.47
2:C:501:9WA:O1	2:C:501:9WA:C24	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: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:HD2	1:B:302:ARG:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:E:302:ARG:HD3	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:A:358:MET:HE3	1:B:314:TRP:CE3	2.51	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:E:290:GLU:H	1:E:290:GLU:CD	2.23	0.45
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:297:SER:C	1:E:299:ILE:HD12	2.41	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:C:358:MET:HE3	1:F:314:TRP:CE3	2.52	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:A:297:SER:C	1:A:299:ILE:HD12	2.42	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:E:301:SER:CB	1:E:302:ARG:C	2.91	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:A:358:MET:HE3	1:B:314:TRP:CH2	2.54	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:A:395:GLU:HG2	1:B:392:GLY:O	2.18	0.43
1:B:301:SER:OG	1:B:304:GLU:HG3	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:C	1:B:267:LEU:HD23	2.43	0.43
1:B:289:LEU:HD22	1:B:414:GLU:OE2	2.18	0.43
1:D:313:MET:HE3	1:D:313:MET:HB2	1.95	0.43
2:D:501:9WA:O1	2:D:501:9WA:C24	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:A:436:LYS:HB3	1:A:436:LYS:HZ3	1.83	0.42
1:F:423:LEU:CD2	1:F:447:GLU:HG2	2.37	0.42
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.92	0.42
1:D:314:TRP:CZ2	1:E:358:MET:HE3	2.54	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
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:358:MET:HE3	1:F:314:TRP:CH2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:267:LEU:HD23	1:F:267:LEU:C	2.45	0.41
1:F:324:LEU:HD21	2:F:501:9WA:CL	2.58	0.41
1:C:396:LEU:C	1:C:400:ILE:HD12	2.44	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:D:328:ILE:HD11	1:D:358:MET:HE2	2.01	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:328:ILE:HD11	1:B:358:MET:HE2	2.03	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:297:SER:C	1:B:299:ILE:HD12	2.47	0.40
1:B:473:ARG:CG	1:B:474:SER:N	2.84	0.40
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%)	24	39
1	E	204/210 (97%)	195 (96%)	8 (4%)	1 (0%)	24	39
1	F	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
All	All	1223/1260 (97%)	1185 (97%)	36 (3%)	2 (0%)	43	60

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%)	184 (99%)	2 (1%)	65	80
1	B	186/187 (100%)	183 (98%)	3 (2%)	55	74
1	C	183/187 (98%)	178 (97%)	5 (3%)	39	61
1	D	181/187 (97%)	179 (99%)	2 (1%)	65	80
1	E	183/187 (98%)	177 (97%)	6 (3%)	33	55
1	F	180/187 (96%)	175 (97%)	5 (3%)	38	60
All	All	1099/1122 (98%)	1076 (98%)	23 (2%)	47	69

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	ARG

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Mol	Chain	Res	Type
1	A	396	LEU
1	B	290	GLU
1	B	317	TRP
1	B	325	THR
1	C	290	GLU
1	C	296	ARG
1	C	313	MET
1	C	325	THR
1	C	385	MET
1	D	318	GLU
1	D	319	ARG
1	E	290	GLU
1	E	296	ARG
1	E	302	ARG
1	E	303	GLU
1	E	313	MET
1	E	325	THR
1	F	290	GLU
1	F	296	ARG
1	F	302	ARG
1	F	313	MET
1	F	442	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	B	453	HIS
1	C	322	HIS
1	C	427	ASN
1	C	452	HIS
1	D	443	GLN
1	E	427	ASN
1	E	443	GLN
1	F	441	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	501	-	45,48,48	1.34	8 (17%)	59,72,72	1.66	6 (10%)
2	9WA	B	501	-	45,48,48	1.32	9 (20%)	59,72,72	1.63	5 (8%)
2	9WA	D	501	-	45,48,48	1.35	9 (20%)	59,72,72	1.67	6 (10%)
2	9WA	E	501	-	45,48,48	1.32	8 (17%)	59,72,72	1.72	5 (8%)
2	9WA	C	501	-	45,48,48	1.37	9 (20%)	59,72,72	1.65	6 (10%)
2	9WA	F	501	-	45,48,48	1.31	9 (20%)	59,72,72	1.72	6 (10%)

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	A	501	-	-	3/34/34/34	0/6/6/6
2	9WA	B	501	-	-	6/34/34/34	0/6/6/6
2	9WA	D	501	-	-	2/34/34/34	0/6/6/6
2	9WA	E	501	-	-	5/34/34/34	0/6/6/6
2	9WA	C	501	-	-	7/34/34/34	0/6/6/6
2	9WA	F	501	-	-	8/34/34/34	0/6/6/6

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	9WA	C8-C7	-3.13	1.37	1.42
2	D	501	9WA	C8-C7	-3.08	1.38	1.42
2	F	501	9WA	C8-C7	-3.04	1.38	1.42
2	E	501	9WA	C7-C2	-2.96	1.37	1.42
2	A	501	9WA	C8-C7	-2.89	1.38	1.42
2	C	501	9WA	C7-C2	-2.87	1.38	1.42
2	F	501	9WA	C7-C2	-2.86	1.38	1.42
2	A	501	9WA	C7-C2	-2.86	1.38	1.42
2	D	501	9WA	C7-C2	-2.86	1.38	1.42
2	B	501	9WA	C8-C7	-2.84	1.38	1.42
2	B	501	9WA	C7-C2	-2.84	1.38	1.42
2	E	501	9WA	C8-C7	-2.73	1.38	1.42
2	C	501	9WA	C20-C5	-2.67	1.49	1.53
2	D	501	9WA	C20-C5	-2.66	1.49	1.53
2	C	501	9WA	C20-C25	-2.57	1.49	1.53
2	E	501	9WA	C2-N	-2.55	1.33	1.37
2	C	501	9WA	C2-N	-2.54	1.33	1.37
2	A	501	9WA	C20-C5	-2.52	1.49	1.53
2	A	501	9WA	C3-C2	-2.50	1.37	1.41
2	E	501	9WA	C3-C2	-2.50	1.37	1.41
2	A	501	9WA	C2-N	-2.50	1.33	1.37
2	D	501	9WA	C3-C2	-2.50	1.37	1.41
2	D	501	9WA	C2-N	-2.49	1.33	1.37
2	D	501	9WA	C20-C25	-2.49	1.49	1.53
2	C	501	9WA	C3-C2	-2.48	1.37	1.41
2	F	501	9WA	C2-N	-2.44	1.33	1.37
2	E	501	9WA	C20-C5	-2.43	1.49	1.53
2	B	501	9WA	C20-C5	-2.41	1.49	1.53
2	B	501	9WA	C3-C2	-2.40	1.37	1.41
2	B	501	9WA	C2-N	-2.40	1.33	1.37
2	F	501	9WA	C20-C5	-2.39	1.49	1.53
2	F	501	9WA	C3-C2	-2.38	1.37	1.41
2	A	501	9WA	C20-C25	-2.35	1.49	1.53
2	B	501	9WA	C20-C25	-2.34	1.49	1.53
2	A	501	9WA	O-C1	2.26	1.38	1.35
2	B	501	9WA	O-C1	2.26	1.38	1.35
2	E	501	9WA	O-C1	2.25	1.38	1.35
2	E	501	9WA	C20-C25	-2.25	1.49	1.53
2	A	501	9WA	C9-C1	-2.24	1.37	1.39
2	B	501	9WA	C9-C1	-2.23	1.37	1.39
2	C	501	9WA	C9-C1	-2.20	1.37	1.39
2	F	501	9WA	O-C1	2.18	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	9WA	C9-C1	-2.14	1.37	1.39
2	D	501	9WA	C9-C1	-2.12	1.37	1.39
2	C	501	9WA	O-C1	2.12	1.38	1.35
2	C	501	9WA	C6-C7	-2.11	1.37	1.42
2	D	501	9WA	O-C1	2.10	1.38	1.35
2	E	501	9WA	C9-C1	-2.07	1.37	1.39
2	F	501	9WA	C20-C25	-2.07	1.50	1.53
2	F	501	9WA	C6-C7	-2.06	1.38	1.42
2	B	501	9WA	C6-C7	-2.05	1.38	1.42
2	D	501	9WA	C6-C7	-2.04	1.38	1.42

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	9WA	C-O-C1	-10.79	107.11	117.20
2	D	501	9WA	C-O-C1	-10.22	107.64	117.20
2	F	501	9WA	C-O-C1	-10.17	107.68	117.20
2	B	501	9WA	C-O-C1	-10.09	107.77	117.20
2	A	501	9WA	C-O-C1	-10.07	107.78	117.20
2	C	501	9WA	C-O-C1	-9.99	107.85	117.20
2	F	501	9WA	C8-C7-C2	3.38	118.24	116.35
2	D	501	9WA	C8-C7-C2	3.17	118.12	116.35
2	C	501	9WA	C8-C7-C2	3.03	118.05	116.35
2	B	501	9WA	C8-C7-C2	2.80	117.92	116.35
2	A	501	9WA	C8-C7-C2	2.73	117.88	116.35
2	E	501	9WA	C10-C9-C8	2.59	122.75	118.67
2	D	501	9WA	C10-C9-C8	2.49	122.60	118.67
2	C	501	9WA	C10-C9-C8	2.49	122.60	118.67
2	D	501	9WA	N4-C23-N3	-2.39	111.52	112.94
2	C	501	9WA	N4-C23-N3	-2.37	111.53	112.94
2	C	501	9WA	C17-N1-N2	2.36	113.80	111.83
2	A	501	9WA	C17-N1-N2	2.36	113.80	111.83
2	F	501	9WA	C17-N1-N2	2.35	113.79	111.83
2	A	501	9WA	C10-C9-C8	2.34	122.35	118.67
2	B	501	9WA	C17-N1-N2	2.33	113.77	111.83
2	F	501	9WA	O1-C20-C21	-2.31	104.61	108.45
2	A	501	9WA	C25-C20-C5	2.31	116.28	111.70
2	D	501	9WA	C17-N1-N2	2.26	113.71	111.83
2	A	501	9WA	N4-C23-N3	-2.26	111.60	112.94
2	E	501	9WA	C17-N1-N2	2.25	113.71	111.83
2	F	501	9WA	C25-C20-C5	2.24	116.14	111.70
2	F	501	9WA	C10-C9-C8	2.23	122.19	118.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	9WA	C5-C6-C7	-2.16	120.16	122.34
2	B	501	9WA	C10-C9-C8	2.14	122.05	118.67
2	D	501	9WA	C5-C6-C7	-2.09	120.23	122.34
2	E	501	9WA	C8-C7-C2	2.08	117.51	116.35
2	E	501	9WA	C27-C28-C30	-2.07	118.06	120.98
2	B	501	9WA	N4-C23-N3	-2.05	111.72	112.94

There are no chirality outliers.

All (31) torsion outliers are listed below:

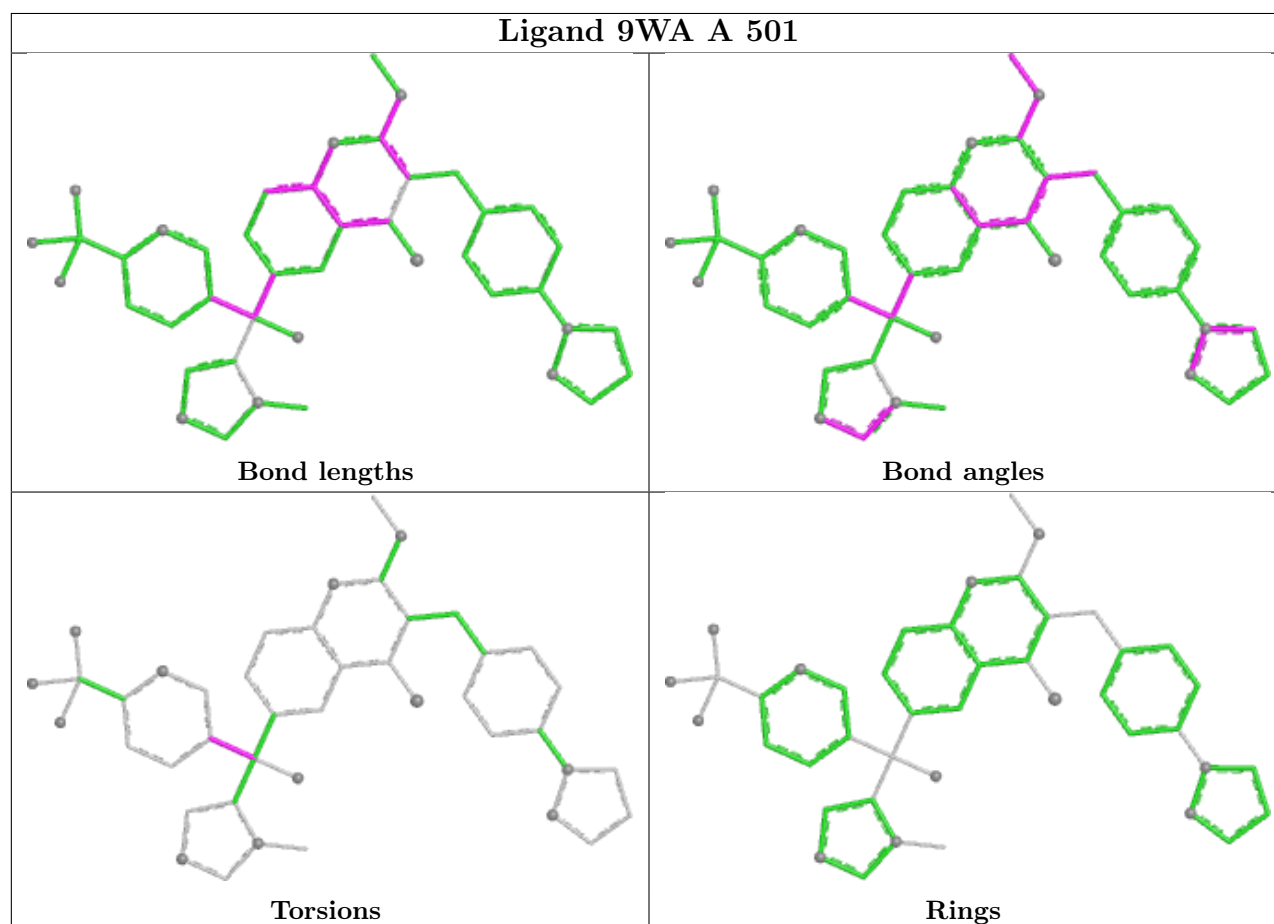
Mol	Chain	Res	Type	Atoms
2	F	501	9WA	C5-C20-C21-N4
2	F	501	9WA	O1-C20-C21-N4
2	A	501	9WA	C5-C20-C25-C29
2	E	501	9WA	C5-C20-C25-C29
2	F	501	9WA	C5-C20-C25-C29
2	E	501	9WA	N-C1-O-C
2	A	501	9WA	O1-C20-C25-C29
2	E	501	9WA	C9-C1-O-C
2	F	501	9WA	O1-C20-C25-C29
2	E	501	9WA	O1-C20-C25-C29
2	B	501	9WA	O1-C20-C25-C29
2	C	501	9WA	N5-C28-C30-F2
2	C	501	9WA	N5-C28-C30-F
2	C	501	9WA	N5-C28-C30-F1
2	C	501	9WA	C27-C28-C30-F2
2	B	501	9WA	C5-C20-C25-C29
2	C	501	9WA	C27-C28-C30-F1
2	C	501	9WA	O1-C20-C25-C29
2	C	501	9WA	C27-C28-C30-F
2	F	501	9WA	C25-C20-C21-C22
2	F	501	9WA	O1-C20-C21-C22
2	B	501	9WA	C11-C10-C9-C1
2	F	501	9WA	C5-C20-C25-C26
2	D	501	9WA	O1-C20-C25-C29
2	B	501	9WA	N5-C28-C30-F
2	B	501	9WA	N5-C28-C30-F1
2	F	501	9WA	C25-C20-C21-N4
2	B	501	9WA	N5-C28-C30-F2
2	A	501	9WA	C5-C20-C25-C26
2	D	501	9WA	O1-C20-C25-C26
2	E	501	9WA	C5-C20-C25-C26

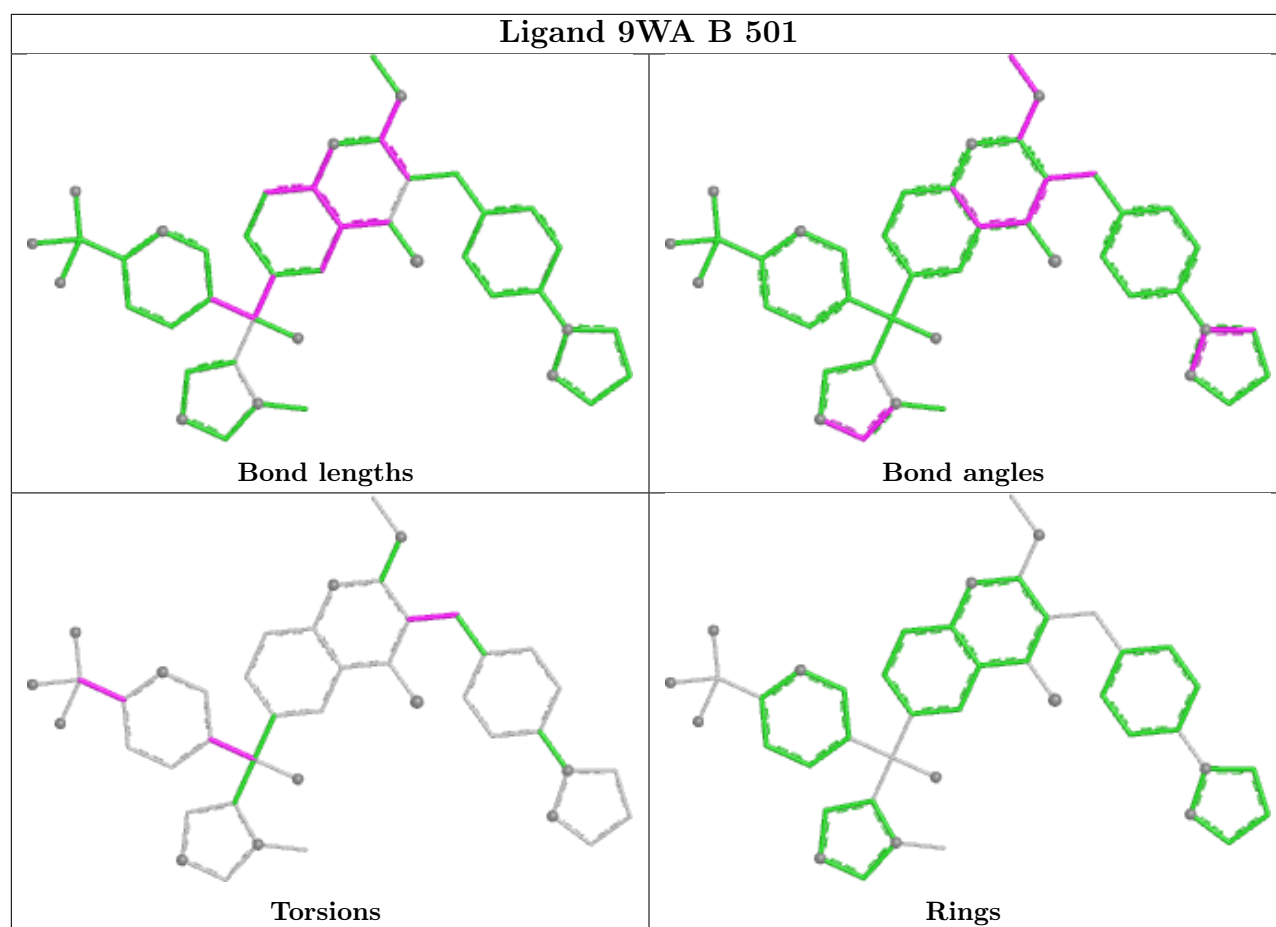
There are no ring outliers.

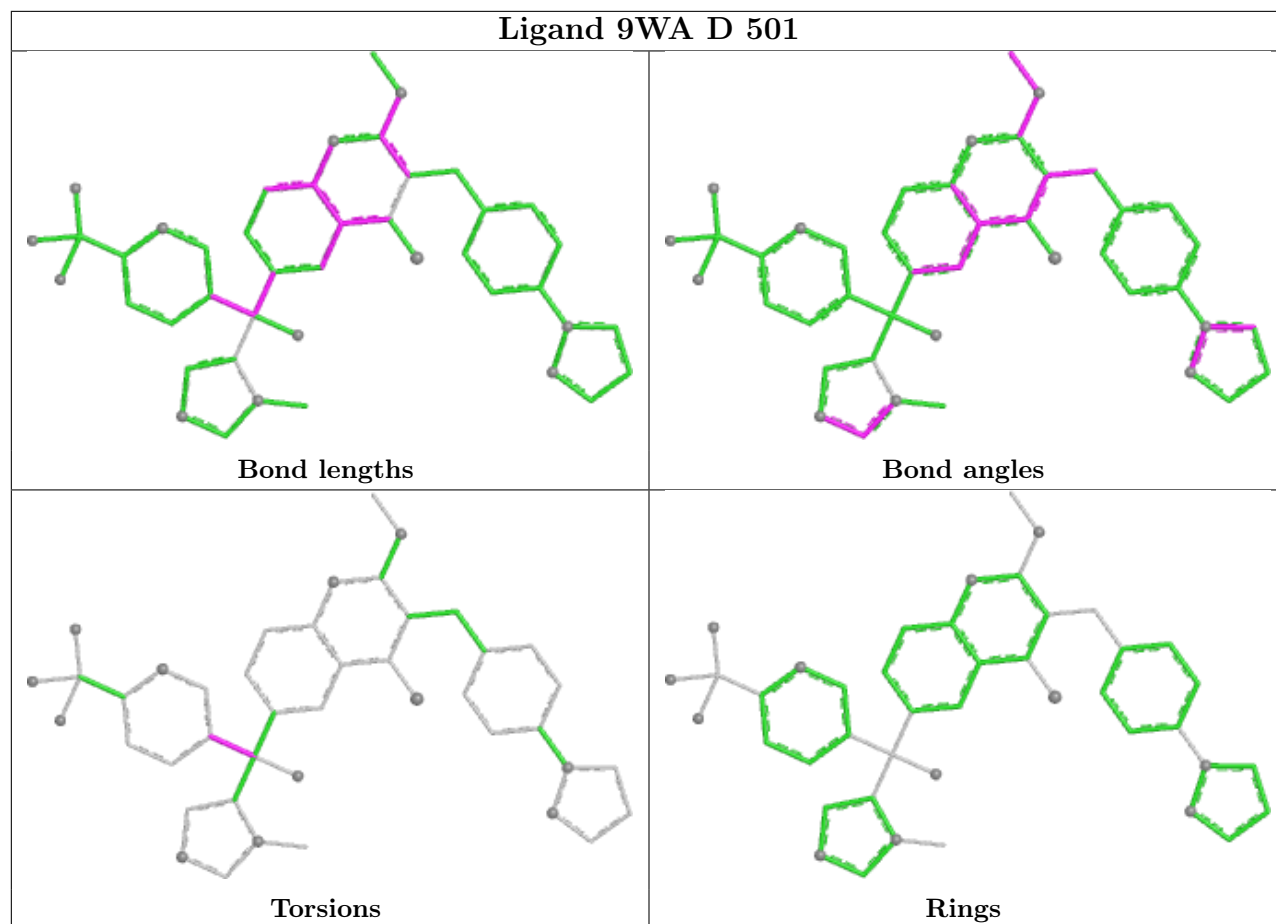
4 monomers are involved in 10 short contacts:

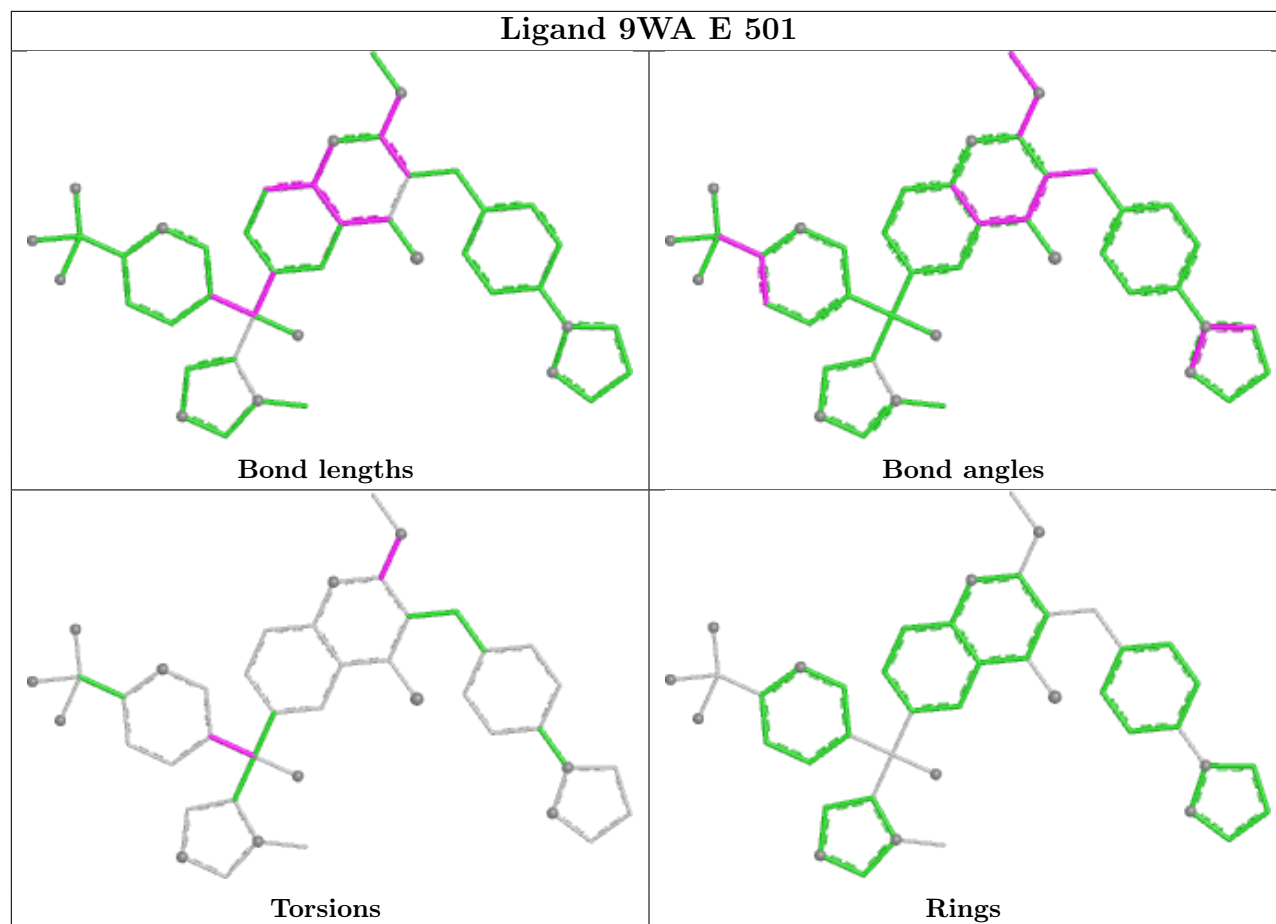
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	9WA	3	0
2	D	501	9WA	3	0
2	C	501	9WA	2	0
2	F	501	9WA	2	0

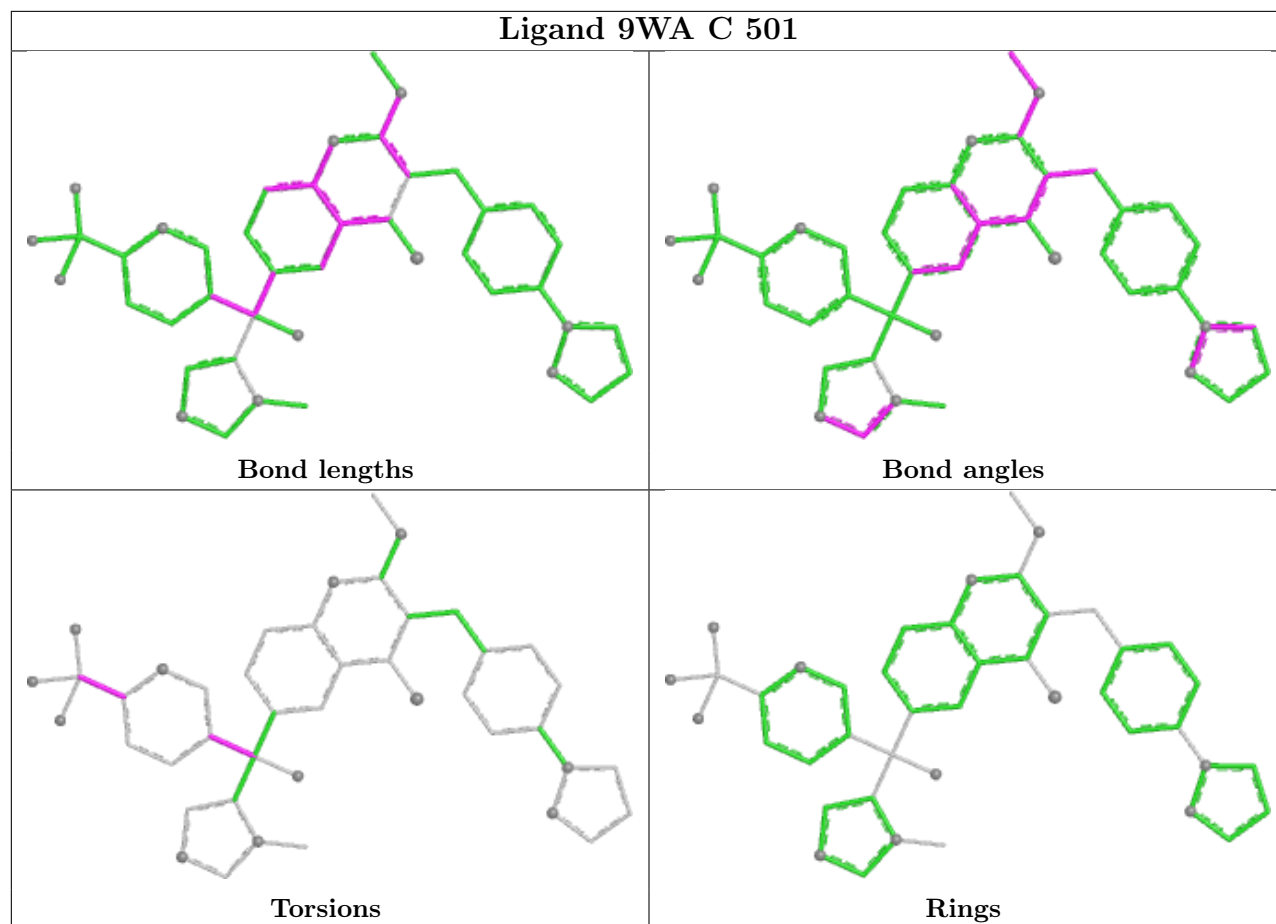
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

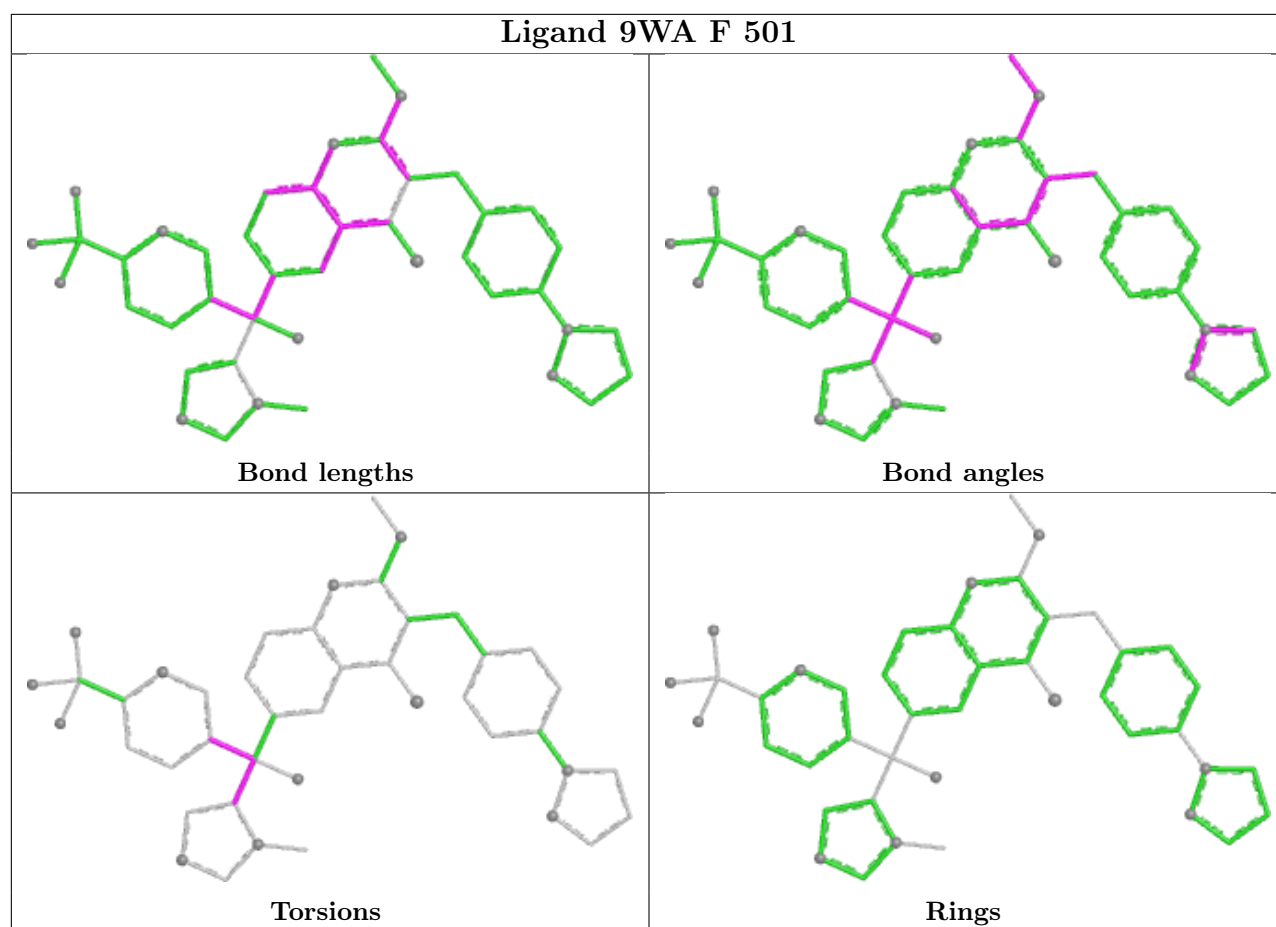












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	209/210 (99%)	0.72	17 (8%)	18 13	12, 28, 60, 73	0
1	B	209/210 (99%)	0.80	21 (10%)	12 10	12, 29, 70, 103	0
1	C	206/210 (98%)	1.91	84 (40%)	0 0	18, 36, 67, 82	0
1	D	203/210 (96%)	1.86	92 (45%)	0 0	15, 37, 64, 75	0
1	E	206/210 (98%)	1.83	84 (40%)	0 0	18, 37, 65, 74	0
1	F	202/210 (96%)	1.97	94 (46%)	0 0	17, 39, 68, 88	0
All	All	1235/1260 (98%)	1.51	392 (31%)	1 0	12, 36, 67, 103	0

All (392) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	LEU	8.6
1	A	267	LEU	7.7
1	C	271	GLU	7.7
1	F	444	TYR	7.0
1	F	439	VAL	6.9
1	B	474	SER	6.8
1	E	267	LEU	6.8
1	F	442	LEU	6.7
1	E	354	LYS	6.7
1	C	282	ARG	6.3
1	B	444	TYR	6.1
1	A	271	GLU	6.0
1	D	287	LEU	6.0
1	D	312	SER	5.9
1	F	290	GLU	5.8
1	C	296	ARG	5.8
1	F	359	GLU	5.8
1	C	273	LEU	5.8
1	E	301	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	354	LYS	5.4
1	E	290	GLU	5.3
1	D	316	MET	5.3
1	C	287	LEU	5.3
1	F	351	VAL	5.3
1	C	270	ILE	5.3
1	E	378	PHE	5.2
1	E	470	GLY	5.2
1	E	442	LEU	5.2
1	E	268	THR	5.1
1	E	444	TYR	5.1
1	C	448	LEU	5.0
1	B	469	LYS	4.9
1	A	268	THR	4.9
1	E	351	VAL	4.9
1	F	468	PRO	4.9
1	D	296	ARG	4.8
1	E	469	LYS	4.8
1	D	271	GLU	4.7
1	F	424	VAL	4.7
1	E	362	LEU	4.6
1	E	347	ASN	4.6
1	C	368	ALA	4.5
1	C	277	VAL	4.5
1	E	282	ARG	4.5
1	B	470	GLY	4.5
1	B	473	ARG	4.5
1	C	339	SER	4.5
1	C	338	LEU	4.5
1	C	475	LEU	4.4
1	F	355	ALA	4.3
1	E	424	VAL	4.3
1	E	271	GLU	4.3
1	B	475	LEU	4.3
1	D	368	ALA	4.2
1	D	444	TYR	4.2
1	F	348	ASP	4.2
1	D	442	LEU	4.2
1	F	288	ARG	4.2
1	C	312	SER	4.1
1	F	431	PRO	4.1
1	F	448	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	436	LYS	4.0
1	D	322	HIS	4.0
1	C	474	SER	4.0
1	E	472	LEU	4.0
1	F	291	ASP	4.0
1	E	429	HIS	3.9
1	C	274	VAL	3.9
1	D	314	TRP	3.9
1	C	290	GLU	3.9
1	C	391	LEU	3.9
1	F	425	LEU	3.9
1	D	317	TRP	3.9
1	B	468	PRO	3.8
1	D	280	SER	3.8
1	D	272	HIS	3.8
1	F	272	HIS	3.8
1	F	427	ASN	3.8
1	B	272	HIS	3.8
1	F	362	LEU	3.8
1	A	474	SER	3.8
1	F	443	GLN	3.7
1	C	280	SER	3.7
1	F	428	ALA	3.7
1	D	340	GLY	3.7
1	F	327	ALA	3.7
1	E	441	GLN	3.7
1	D	426	ILE	3.7
1	E	317	TRP	3.7
1	F	282	ARG	3.6
1	C	315	GLU	3.6
1	D	400	ILE	3.6
1	F	317	TRP	3.6
1	B	280	SER	3.6
1	E	350	ILE	3.6
1	E	426	ILE	3.6
1	D	298	ASN	3.6
1	C	340	GLY	3.6
1	E	389	ARG	3.5
1	D	321	ALA	3.5
1	C	272	HIS	3.5
1	C	324	LEU	3.5
1	F	350	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	432	GLY	3.4
1	A	272	HIS	3.4
1	F	397	ILE	3.4
1	E	288	ARG	3.4
1	F	268	THR	3.4
1	B	343	GLU	3.4
1	D	389	ARG	3.4
1	B	471	LYS	3.4
1	D	267	LEU	3.4
1	F	267	LEU	3.4
1	D	318	GLU	3.3
1	E	437	ARG	3.3
1	E	468	PRO	3.3
1	D	295	GLN	3.3
1	D	366	CYS	3.3
1	C	377	PHE	3.3
1	E	295	GLN	3.3
1	C	284	THR	3.3
1	D	297	SER	3.3
1	A	475	LEU	3.3
1	C	400	ILE	3.3
1	C	442	LEU	3.3
1	C	446	LEU	3.3
1	D	266	SER	3.3
1	E	428	ALA	3.3
1	F	429	HIS	3.2
1	D	339	SER	3.2
1	F	441	GLN	3.2
1	D	320	CYS	3.2
1	F	345	CYS	3.2
1	F	430	ARG	3.2
1	D	385	MET	3.2
1	D	447	GLU	3.2
1	E	436	LYS	3.2
1	C	322	HIS	3.2
1	E	346	GLN	3.2
1	D	399	SER	3.2
1	D	413	SER	3.2
1	E	355	ALA	3.2
1	F	293	LEU	3.2
1	D	371	ALA	3.2
1	A	472	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	338	LEU	3.2
1	E	448	LEU	3.2
1	D	289	LEU	3.1
1	F	352	LEU	3.1
1	F	433	LEU	3.1
1	D	397	ILE	3.1
1	D	412	PHE	3.1
1	C	385	MET	3.1
1	D	391	LEU	3.1
1	E	433	LEU	3.1
1	D	458	HIS	3.1
1	E	313	MET	3.1
1	F	365	MET	3.1
1	E	440	GLU	3.1
1	D	268	THR	3.1
1	C	426	ILE	3.1
1	D	299	ILE	3.1
1	A	437	ARG	3.1
1	D	303	GLU	3.0
1	E	275	GLN	3.0
1	D	365	MET	3.0
1	C	276	SER	3.0
1	C	297	SER	3.0
1	E	443	GLN	3.0
1	D	270	ILE	3.0
1	D	417	ILE	3.0
1	C	334	PHE	3.0
1	C	401	PHE	3.0
1	E	353	LEU	3.0
1	E	387	LEU	3.0
1	F	372	ASP	3.0
1	C	299	ILE	3.0
1	E	397	ILE	3.0
1	F	325	THR	3.0
1	C	455	HIS	2.9
1	F	366	CYS	2.9
1	C	397	ILE	2.9
1	E	352	LEU	2.9
1	E	413	SER	2.9
1	C	310	ARG	2.9
1	F	294	ARG	2.9
1	D	324	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	371	ALA	2.9
1	A	282	ARG	2.9
1	D	288	ARG	2.9
1	C	362	LEU	2.9
1	C	419	LEU	2.9
1	B	271	GLU	2.8
1	F	313	MET	2.8
1	D	294	ARG	2.8
1	D	367	ARG	2.8
1	C	317	TRP	2.8
1	D	380	GLY	2.8
1	A	448	LEU	2.8
1	F	440	GLU	2.8
1	F	385	MET	2.8
1	F	392	GLY	2.8
1	F	321	ALA	2.8
1	C	462	ILE	2.8
1	F	312	SER	2.8
1	F	456	LYS	2.8
1	E	348	ASP	2.8
1	C	444	TYR	2.8
1	D	411	HIS	2.8
1	E	388	PHE	2.8
1	F	320	CYS	2.8
1	D	275	GLN	2.8
1	E	398	SER	2.8
1	E	412	PHE	2.8
1	C	366	CYS	2.7
1	C	275	GLN	2.7
1	E	396	LEU	2.7
1	C	319	ARG	2.7
1	F	396	LEU	2.7
1	E	451	HIS	2.7
1	D	343	GLU	2.7
1	D	274	VAL	2.7
1	D	282	ARG	2.7
1	C	411	HIS	2.7
1	D	290	GLU	2.7
1	F	347	ASN	2.7
1	F	398	SER	2.7
1	F	335	ALA	2.7
1	F	346	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	426	ILE	2.7
1	D	319	ARG	2.7
1	F	437	ARG	2.7
1	C	336	LYS	2.7
1	F	332	VAL	2.7
1	F	434	GLN	2.6
1	E	438	LYS	2.6
1	F	399	SER	2.6
1	F	275	GLN	2.6
1	E	391	LEU	2.6
1	D	313	MET	2.6
1	E	423	LEU	2.6
1	F	353	LEU	2.6
1	D	269	GLU	2.6
1	E	392	GLY	2.6
1	B	441	GLN	2.6
1	E	280	SER	2.6
1	E	372	ASP	2.6
1	C	396	LEU	2.6
1	C	279	LYS	2.6
1	D	336	LYS	2.6
1	D	414	GLU	2.6
1	D	278	CYS	2.6
1	E	431	PRO	2.6
1	E	439	VAL	2.6
1	D	291	ASP	2.5
1	D	310	ARG	2.5
1	C	318	GLU	2.5
1	C	470	GLY	2.5
1	C	278	CYS	2.5
1	D	334	PHE	2.5
1	F	403	PHE	2.5
1	A	473	ARG	2.5
1	C	472	LEU	2.5
1	C	378	PHE	2.5
1	C	394	SER	2.5
1	D	273	LEU	2.5
1	E	283	GLU	2.5
1	B	442	LEU	2.5
1	E	289	LEU	2.5
1	F	423	LEU	2.5
1	F	395	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	382	TYR	2.5
1	F	340	GLY	2.5
1	C	295	GLN	2.5
1	D	377	PHE	2.5
1	C	445	ASN	2.4
1	E	294	ARG	2.4
1	D	362	LEU	2.4
1	A	429	HIS	2.4
1	C	316	MET	2.4
1	D	422	ALA	2.4
1	F	378	PHE	2.4
1	C	437	ARG	2.4
1	D	284	THR	2.4
1	D	292	LEU	2.4
1	D	293	LEU	2.4
1	F	438	LYS	2.4
1	B	282	ARG	2.4
1	B	437	ARG	2.4
1	E	327	ALA	2.4
1	F	412	PHE	2.4
1	F	407	LEU	2.4
1	D	445	ASN	2.4
1	E	272	HIS	2.4
1	C	343	GLU	2.4
1	F	356	GLY	2.4
1	C	418	ALA	2.4
1	D	281	TYR	2.4
1	E	390	ALA	2.4
1	E	430	ARG	2.4
1	A	391	LEU	2.4
1	F	270	ILE	2.4
1	E	427	ASN	2.4
1	E	269	GLU	2.4
1	C	469	LYS	2.4
1	E	291	ASP	2.3
1	C	392	GLY	2.3
1	C	367	ARG	2.3
1	E	425	LEU	2.3
1	F	338	LEU	2.3
1	A	269	GLU	2.3
1	C	436	LYS	2.3
1	F	269	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	314	TRP	2.3
1	E	360	VAL	2.3
1	C	449	ALA	2.3
1	D	423	LEU	2.3
1	E	365	MET	2.3
1	D	379	GLU	2.3
1	F	343	GLU	2.3
1	D	401	PHE	2.3
1	F	328	ILE	2.3
1	D	374	ARG	2.3
1	C	441	GLN	2.3
1	F	295	GLN	2.3
1	B	267	LEU	2.3
1	D	376	VAL	2.3
1	C	321	ALA	2.2
1	F	279	LYS	2.2
1	E	359	GLU	2.2
1	F	435	GLU	2.2
1	C	461	SER	2.2
1	D	392	GLY	2.2
1	E	321	ALA	2.2
1	F	452	HIS	2.2
1	F	285	CYS	2.2
1	A	343	GLU	2.2
1	D	382	TYR	2.2
1	E	349	GLN	2.2
1	D	276	SER	2.2
1	B	397	ILE	2.2
1	C	390	ALA	2.2
1	A	444	TYR	2.2
1	C	293	LEU	2.2
1	F	336	LYS	2.2
1	F	422	ALA	2.2
1	E	435	GLU	2.2
1	C	374	ARG	2.2
1	B	275	GLN	2.2
1	F	349	GLN	2.2
1	C	289	LEU	2.2
1	C	344	LEU	2.2
1	E	293	LEU	2.2
1	F	292	LEU	2.2
1	E	312	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	394	SER	2.2
1	F	322	HIS	2.2
1	E	335	ALA	2.1
1	E	345	CYS	2.1
1	F	344	LEU	2.1
1	F	358	MET	2.1
1	D	415	ASP	2.1
1	D	388	PHE	2.1
1	C	283	GLU	2.1
1	F	296	ARG	2.1
1	D	354	LYS	2.1
1	F	388	PHE	2.1
1	C	325	THR	2.1
1	D	325	THR	2.1
1	D	396	LEU	2.1
1	F	445	ASN	2.1
1	D	378	PHE	2.1
1	F	377	PHE	2.1
1	D	315	GLU	2.1
1	E	357	ALA	2.1
1	E	399	SER	2.1
1	C	434	GLN	2.1
1	E	332	VAL	2.1
1	D	386	GLU	2.0
1	A	339	SER	2.0
1	E	292	LEU	2.0
1	E	434	GLN	2.0
1	D	285	CYS	2.0
1	B	389	ARG	2.0
1	F	367	ARG	2.0
1	C	387	LEU	2.0
1	D	346	GLN	2.0
1	F	391	LEU	2.0
1	C	417	ILE	2.0
1	C	389	ARG	2.0
1	D	424	VAL	2.0
1	E	363	VAL	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 [i](#)

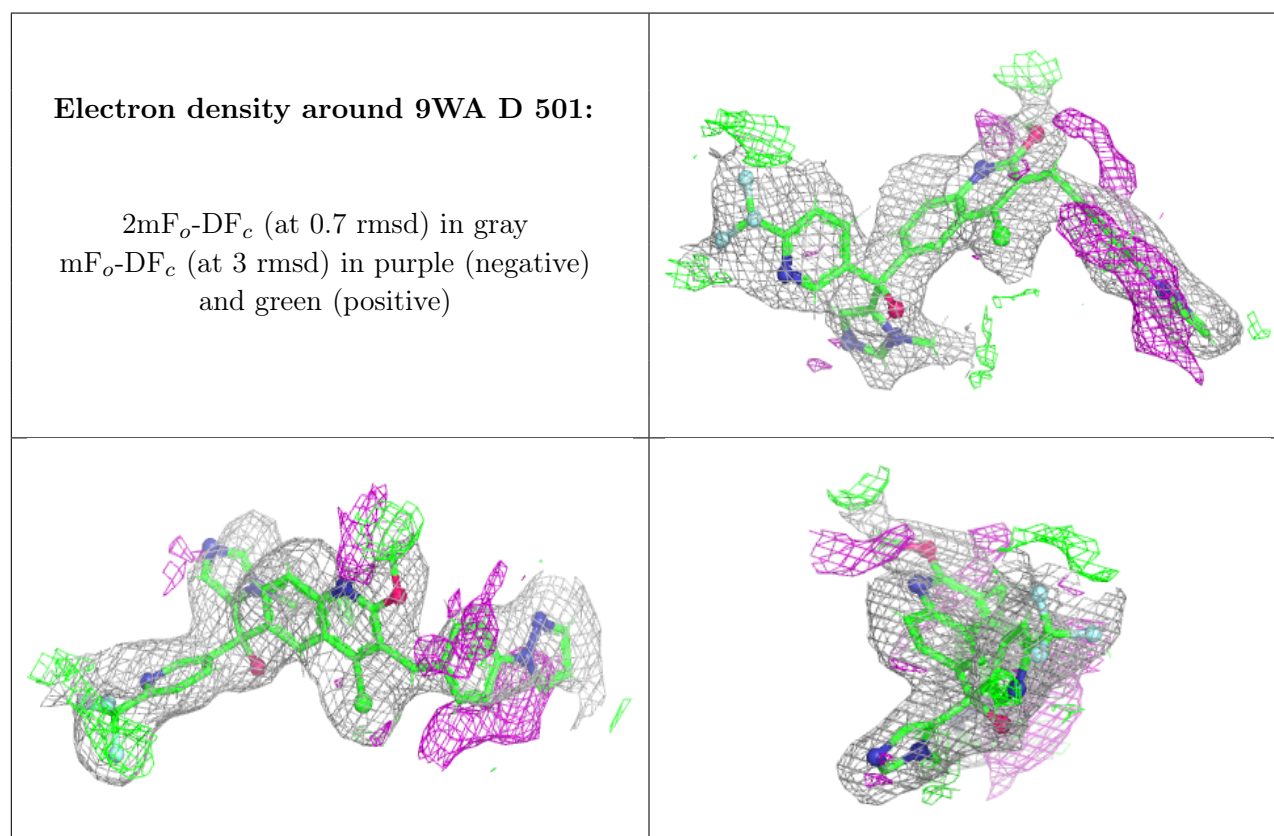
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

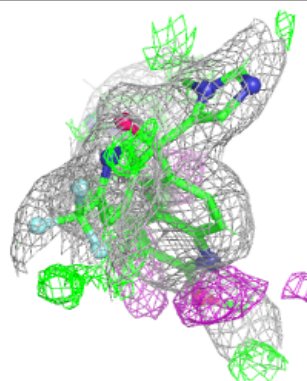
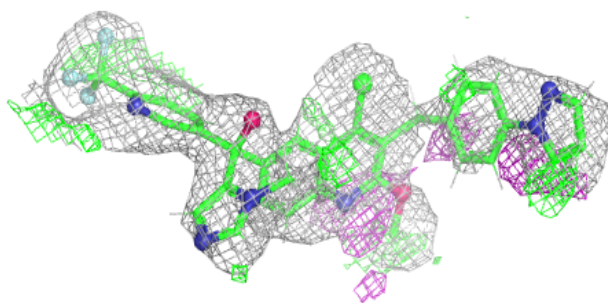
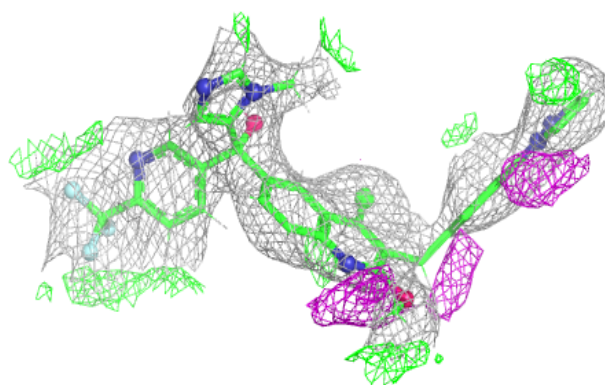
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	9WA	D	501	43/43	0.76	0.17	18,34,46,68	0
2	9WA	C	501	43/43	0.77	0.17	13,32,51,73	0
2	9WA	E	501	43/43	0.80	0.25	28,49,67,80	0
2	9WA	F	501	43/43	0.83	0.16	11,29,46,57	0
2	9WA	A	501	43/43	0.90	0.10	9,22,37,60	0
2	9WA	B	501	43/43	0.90	0.11	7,19,31,56	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.

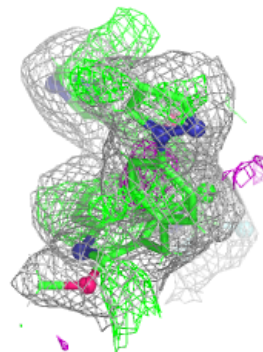
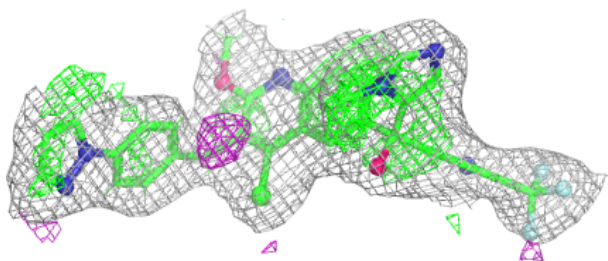
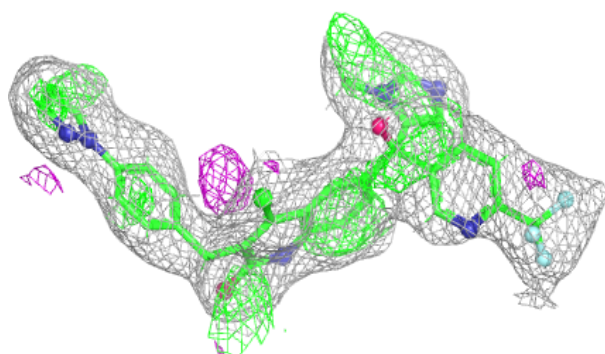


Electron density around 9WA C 501:

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

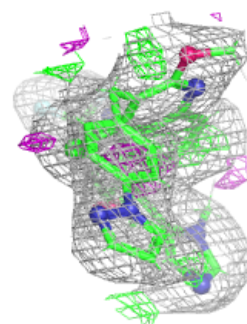
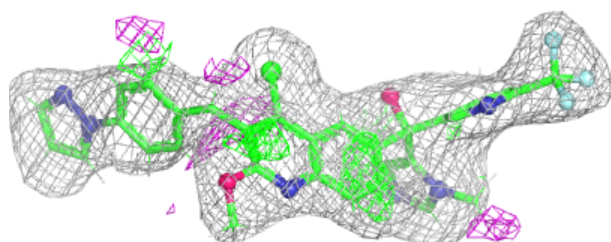
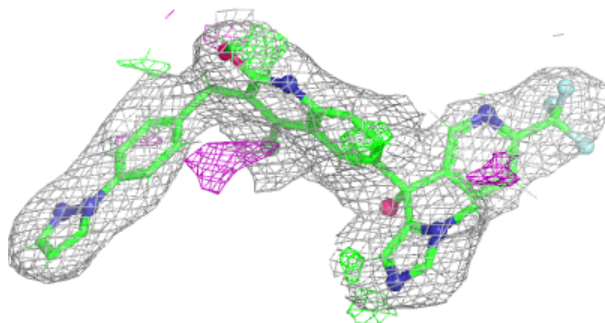
**Electron density around 9WA E 501:**

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

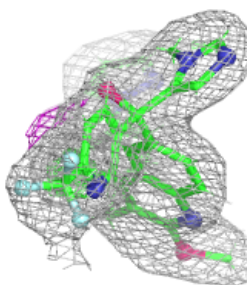
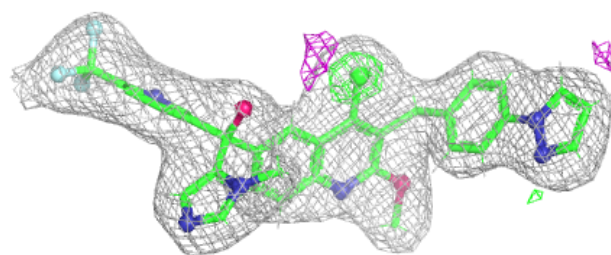
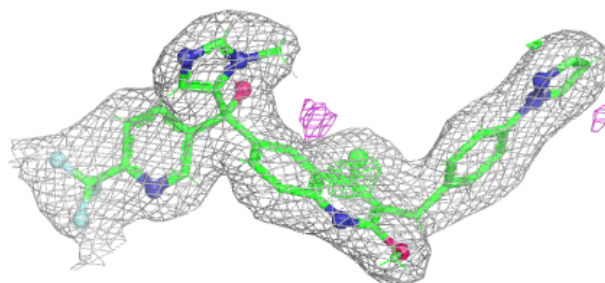


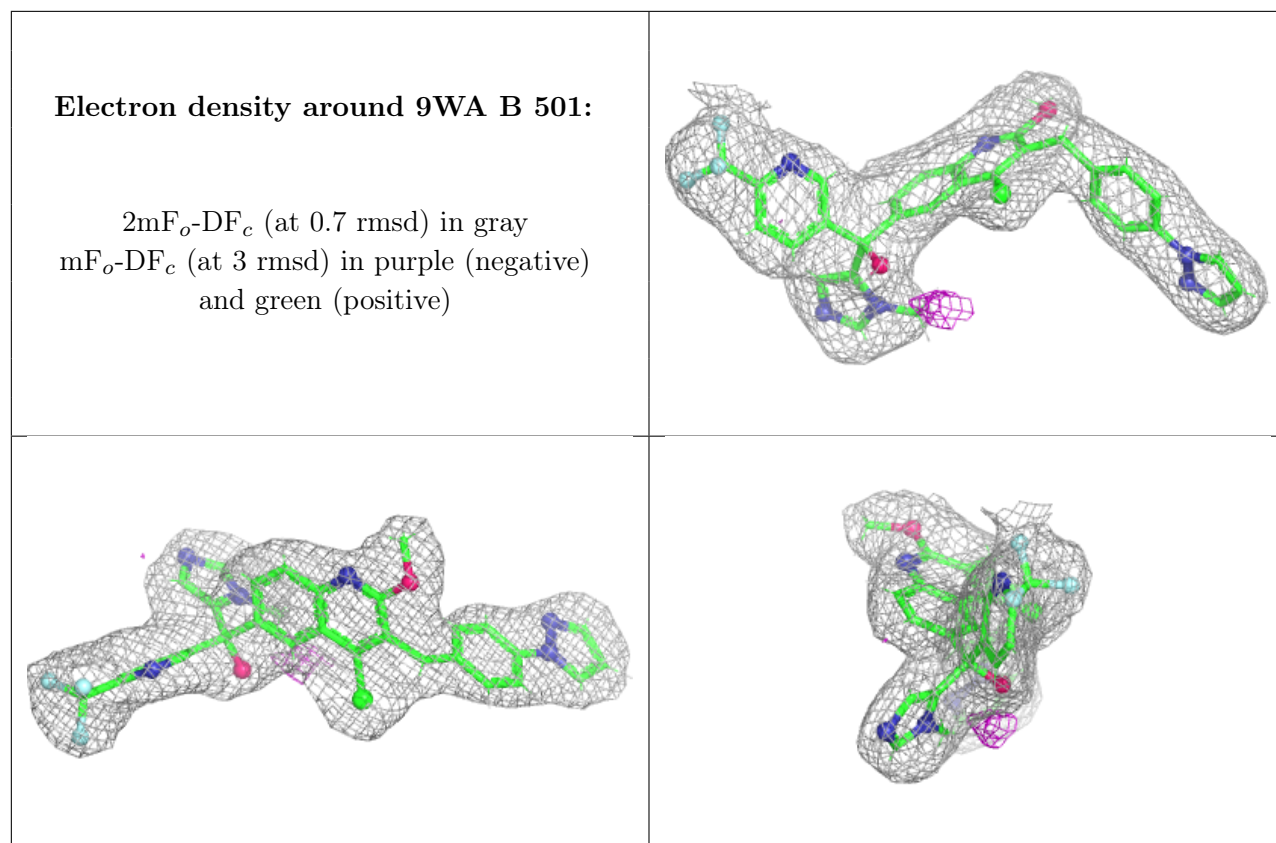
Electron density around 9WA F 501:

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

**Electron density around 9WA 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.