



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:57 AM UTC

PDB ID : 4WOT / pdb_00004wot
Title : ROCK2 IN COMPLEX WITH 1426382-07-1
Authors : Augustin, M.; Krapp, S.; Boland, S.; Defert, O.; Bourin, A.; Alen, J.; Leysen, D.
Deposited on : 2014-10-16
Resolution : 2.93 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

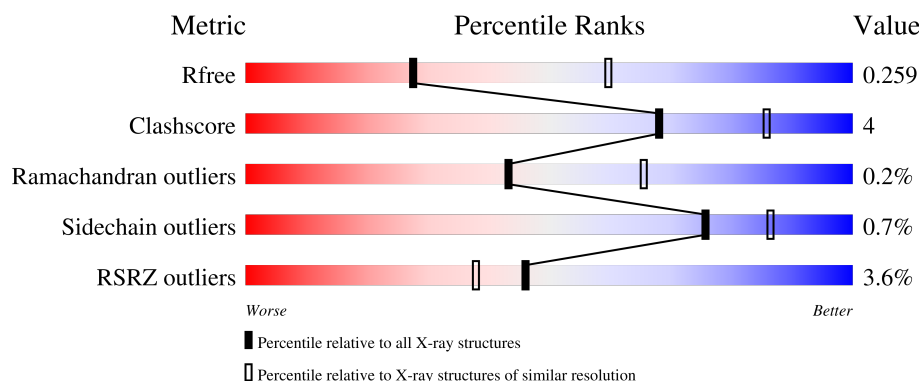
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	396	
1	B	396	
1	C	396	
1	D	396	

2 Entry composition [i](#)

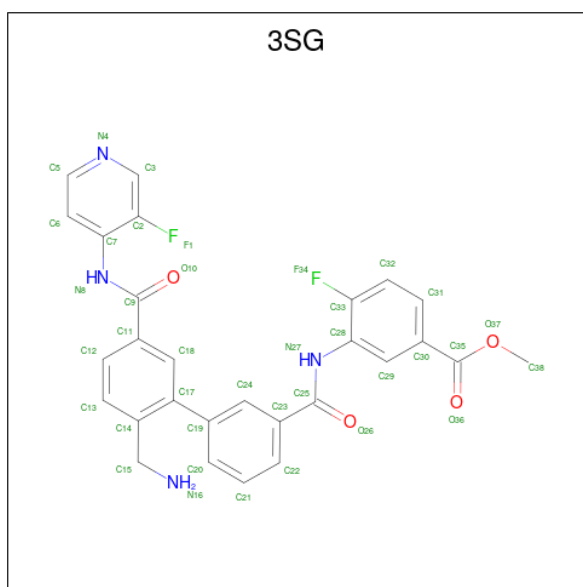
There are 3 unique types of molecules in this entry. The entry contains 12816 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Rho-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	217	0	0
			3149	2019	529	581	20			
1	B	394	Total	C	N	O	S	171	0	0
			3181	2036	534	591	20			
1	C	392	Total	C	N	O	S	260	0	0
			3169	2030	532	587	20			
1	D	389	Total	C	N	O	S	133	0	0
			3149	2019	529	581	20			

- Molecule 2 is methyl 3-[(2'-(aminomethyl)-5'-[(3-fluoropyridin-4-yl)carbamoyl]biphenyl-3-yl)carbonyl]amino]-4-fluorobenzoate (CCD ID: 3SG) (formula: C₂₈H₂₂F₂N₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	1	0
			38	28	2	4	4		
2	B	1	Total	C	F	N	O	1	0
			38	28	2	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	1	0
			38	28	2	4	4		
2	D	1	Total	C	F	N	O	1	0
			38	28	2	4	4		

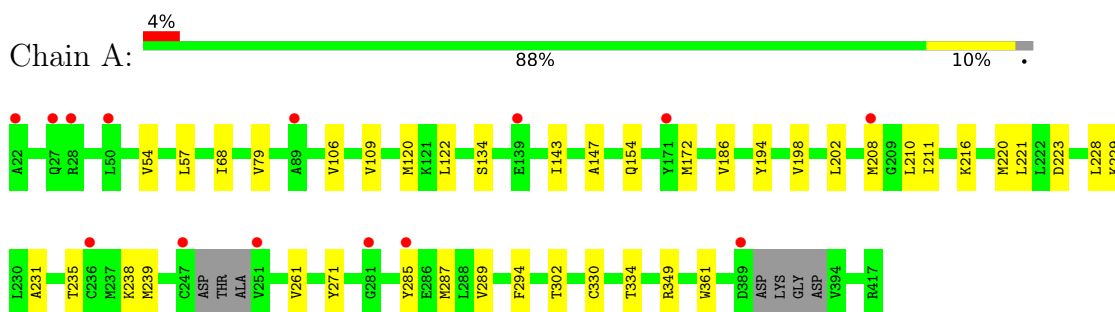
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		
3	C	4	Total	O	0	0
			4	4		
3	D	5	Total	O	0	0
			5	5		

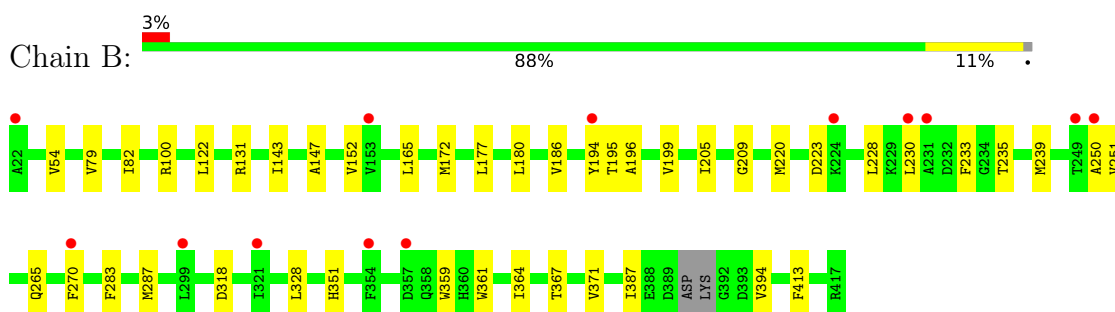
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

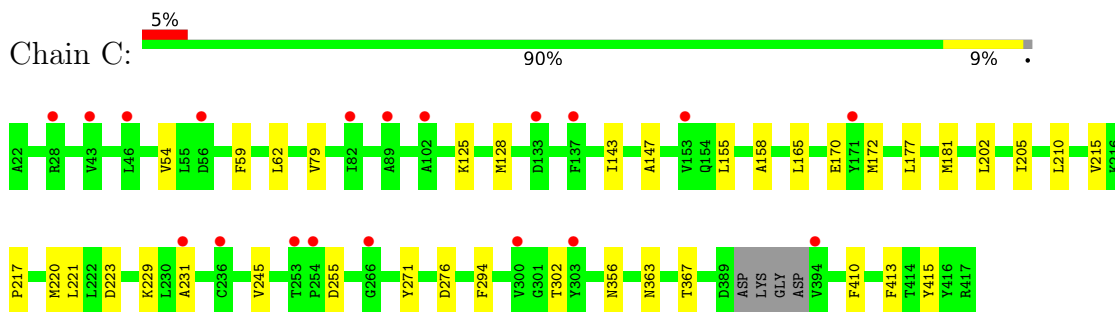
- Molecule 1: Rho-associated protein kinase 2



- Molecule 1: Rho-associated protein kinase 2

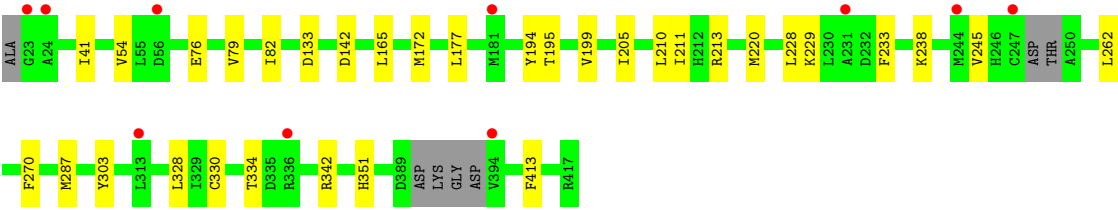


- Molecule 1: Rho-associated protein kinase 2



- Molecule 1: Rho-associated protein kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.19Å 148.23Å 117.38Å 90.00° 118.65° 90.00°	Depositor
Resolution (Å)	103.01 – 2.93 103.01 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (103.01-2.93) 99.9 (103.01-2.93)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.268 0.223 , 0.259	Depositor DCC
R_{free} test set	619 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	96.9	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12816	wwPDB-VP
Average B, all atoms (Å ²)	94.0	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 33.55 % 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 7.8582e-04. 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: 3SG

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	0.62	0/3226	0.81	0/4356
1	B	0.62	0/3259	0.82	2/4403 (0.0%)
1	C	0.63	0/3247	0.82	0/4387
1	D	0.62	1/3226 (0.0%)	0.83	1/4356 (0.0%)
All	All	0.62	1/12958 (0.0%)	0.82	3/17502 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	133	ASP	CA-C	5.75	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	PHE	CA-CB-CG	6.46	120.26	113.80
1	D	270	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	186	VAL	N-CA-C	5.09	112.91	107.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	ARG	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	3149	0	3074	25	0
1	B	3181	0	3098	21	0
1	C	3169	0	3091	23	0
1	D	3149	0	3074	16	0
2	A	38	0	22	1	0
2	B	38	0	22	0	0
2	C	38	0	22	0	0
2	D	38	0	22	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	5	0	0	0	0
All	All	12816	0	12425	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (84) 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:A:186:VAL:HG11	1:A:287:MET:HE2	1.57	0.87
1:B:82:ILE:HD11	1:D:41:ILE:HD13	1.56	0.85
1:B:54:VAL:HG21	1:B:79:VAL:HG21	1.61	0.81
1:A:54:VAL:HG21	1:A:79:VAL:HG21	1.61	0.81
1:A:221:LEU:HD23	1:A:231:ALA:HB3	1.74	0.68
1:C:54:VAL:HG21	1:C:79:VAL:HG21	1.76	0.67
1:A:109:VAL:HG11	1:A:120:MET:HE2	1.76	0.66
1:C:221:LEU:HD23	1:C:231:ALA:HB3	1.83	0.60
1:A:57:LEU:HD22	1:A:68:ILE:HD13	1.86	0.57
1:D:330:CYS:O	1:D:334:THR:HG23	2.04	0.57
1:A:221:LEU:HD23	1:A:231:ALA:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:O	1:A:147:ALA:HB2	2.03	0.57
1:B:172:MET:HE1	1:B:223:ASP:HB3	1.86	0.57
1:C:172:MET:HE2	1:C:229:LYS:HB2	1.89	0.55
1:A:172:MET:HE1	1:A:223:ASP:HB3	1.88	0.54
1:D:205:ILE:HD11	1:D:233:PHE:HE1	1.72	0.54
1:C:177:LEU:HD13	1:C:220:MET:CB	2.38	0.54
1:B:165:LEU:HD22	1:B:413:PHE:CD2	2.44	0.53
1:A:172:MET:HE2	1:A:229:LYS:HB2	1.90	0.53
1:B:194:TYR:CD2	1:B:287:MET:HE1	2.45	0.52
1:C:172:MET:HE1	1:C:223:ASP:HB3	1.90	0.52
1:C:181:MET:HE1	1:C:217:PRO:HG3	1.91	0.52
1:A:261:VAL:HG22	1:A:271:TYR:CE2	2.45	0.52
1:C:125:LYS:HA	1:C:128:MET:HE3	1.92	0.52
1:C:158:ALA:HB3	1:C:415:TYR:HB3	1.93	0.51
1:B:152:VAL:HG13	1:B:233:PHE:CZ	2.46	0.50
1:A:349:ARG:HB2	1:A:361:TRP:CE2	2.46	0.50
1:D:262:LEU:HD13	1:D:303:TYR:CD1	2.47	0.50
1:A:210:LEU:HD23	1:A:238:LYS:HA	1.93	0.50
1:D:195:THR:O	1:D:199:VAL:HG23	2.12	0.50
1:B:209:GLY:HA2	1:B:239:MET:HE3	1.94	0.49
1:C:177:LEU:HD13	1:C:220:MET:HB2	1.94	0.49
1:C:245:VAL:HG12	1:C:271:TYR:O	2.13	0.48
1:B:250:ALA:HB2	1:B:265:GLN:HB2	1.96	0.48
1:D:172:MET:HE2	1:D:229:LYS:HB2	1.96	0.47
1:D:211:ILE:HD12	1:D:245:VAL:CG1	2.45	0.47
1:A:143:ILE:HG23	1:A:208:MET:HE1	1.97	0.47
1:D:165:LEU:HD22	1:D:413:PHE:CD2	2.49	0.47
1:B:328:LEU:HD13	1:B:351:HIS:CG	2.49	0.47
1:A:194:TYR:O	1:A:198:VAL:HG23	2.13	0.47
1:D:177:LEU:HD23	1:D:287:MET:HE3	1.95	0.47
1:B:122:LEU:HD12	1:B:122:LEU:N	2.29	0.47
1:D:194:TYR:CD2	1:D:287:MET:HE1	2.50	0.46
1:D:328:LEU:HD13	1:D:351:HIS:CG	2.50	0.46
1:A:216:LYS:C	1:A:220:MET:HE3	2.41	0.46
1:A:330:CYS:O	1:A:334:THR:HG23	2.16	0.46
1:B:177:LEU:HD23	1:B:283:PHE:CZ	2.52	0.45
1:C:205:ILE:HG22	1:C:210:LEU:O	2.16	0.44
1:A:106:VAL:HG23	2:A:501:3SG:H20	2.00	0.44
1:D:220:MET:HB3	1:D:228:LEU:HD11	1.99	0.44
1:A:285:TYR:CE1	1:A:289:VAL:HG21	2.52	0.44
1:C:143:ILE:O	1:C:147:ALA:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:HG12	1:A:202:LEU:HD12	2.01	0.43
1:B:195:THR:O	1:B:199:VAL:HG23	2.18	0.43
1:A:285:TYR:CZ	1:A:289:VAL:HG21	2.53	0.43
1:C:155:LEU:HD21	1:C:158:ALA:HB2	2.00	0.43
1:C:165:LEU:HD22	1:C:413:PHE:CD2	2.53	0.43
1:C:177:LEU:HD13	1:C:220:MET:HB3	2.00	0.43
1:D:211:ILE:HD12	1:D:245:VAL:HG12	1.99	0.43
1:B:196:ALA:HB1	1:B:361:TRP:CZ3	2.54	0.43
1:D:210:LEU:HD23	1:D:238:LYS:HA	2.01	0.43
1:B:235:THR:HG23	1:B:251:VAL:HB	2.01	0.43
1:C:363:ASN:O	1:C:367:THR:HG23	2.18	0.42
1:D:54:VAL:HG21	1:D:79:VAL:HG21	2.01	0.42
1:A:261:VAL:HG22	1:A:271:TYR:CD2	2.54	0.42
1:B:143:ILE:O	1:B:147:ALA:HB2	2.19	0.42
1:B:100:ARG:NH2	1:B:387:ILE:HG22	2.34	0.42
1:B:359:TRP:CD2	1:B:364:ILE:HD12	2.55	0.42
1:B:394:VAL:O	1:B:394:VAL:HG13	2.19	0.42
1:C:170:GLU:OE2	1:C:229:LYS:NZ	2.43	0.42
1:A:294:PHE:O	1:A:302:THR:HG23	2.20	0.42
1:C:165:LEU:HD11	1:C:410:PHE:CD1	2.55	0.41
1:A:228:LEU:HD23	1:A:229:LYS:N	2.34	0.41
1:C:294:PHE:O	1:C:302:THR:HG23	2.20	0.41
1:B:180:LEU:HD11	1:B:371:VAL:HG21	2.01	0.41
1:A:211:ILE:HG12	1:A:239:MET:HE2	2.02	0.41
1:B:177:LEU:HD13	1:B:220:MET:O	2.21	0.41
1:C:202:LEU:HD13	1:C:276:ASP:HB3	2.02	0.41
1:D:245:VAL:HG13	1:D:245:VAL:O	2.21	0.41
1:A:122:LEU:HD12	1:A:122:LEU:N	2.36	0.40
1:C:202:LEU:HD21	1:C:215:VAL:HG22	2.01	0.40
1:C:59:PHE:HB2	1:C:62:LEU:HD13	2.03	0.40
1:C:165:LEU:HD11	1:C:410:PHE:HD1	1.87	0.40
1:B:205:ILE:HD11	1:B:230:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/396 (97%)	364 (95%)	18 (5%)	1 (0%)	36	59
1	B	390/396 (98%)	374 (96%)	15 (4%)	1 (0%)	36	59
1	C	388/396 (98%)	369 (95%)	19 (5%)	0	100	100
1	D	383/396 (97%)	368 (96%)	14 (4%)	1 (0%)	36	59
All	All	1544/1584 (98%)	1475 (96%)	66 (4%)	3 (0%)	43	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	76	GLU
1	B	318	ASP
1	A	134	SER

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	341/346 (99%)	339 (99%)	2 (1%)	78	89
1	B	344/346 (99%)	342 (99%)	2 (1%)	78	89
1	C	343/346 (99%)	341 (99%)	2 (1%)	78	89
1	D	341/346 (99%)	337 (99%)	4 (1%)	63	78
All	All	1369/1384 (99%)	1359 (99%)	10 (1%)	76	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	235	THR
1	B	228	LEU

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Mol	Chain	Res	Type
1	B	367	THR
1	C	255	ASP
1	C	356	ASN
1	D	82	ILE
1	D	142	ASP
1	D	213	ARG
1	D	342	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	70	ASN
1	A	154	GLN
1	A	265	GLN
1	A	360	HIS
1	B	70	ASN
1	B	86	GLN
1	C	70	ASN
1	C	111	HIS
1	D	27	GLN
1	D	115	GLN
1	D	327	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	3SG	B	501	-	41,41,41	0.85	1 (2%)	56,57,57	1.37	7 (12%)
2	3SG	D	501	-	41,41,41	0.75	1 (2%)	56,57,57	1.42	7 (12%)
2	3SG	C	501	-	41,41,41	0.80	1 (2%)	56,57,57	1.37	7 (12%)
2	3SG	A	501	-	41,41,41	0.67	0	56,57,57	1.31	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	3SG	B	501	-	-	9/28/28/28	0/4/4/4
2	3SG	D	501	-	-	9/28/28/28	0/4/4/4
2	3SG	C	501	-	-	7/28/28/28	0/4/4/4
2	3SG	A	501	-	-	8/28/28/28	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	3SG	O37-C38	-4.05	1.36	1.45
2	C	501	3SG	O37-C38	-3.35	1.37	1.45
2	D	501	3SG	O37-C38	2.41	1.50	1.45

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	3SG	O37-C35-C30	5.07	119.90	112.31
2	A	501	3SG	O37-C35-C30	4.85	119.58	112.31
2	B	501	3SG	C38-O37-C35	4.77	124.97	115.81
2	C	501	3SG	O37-C35-C30	4.75	119.42	112.31
2	B	501	3SG	O37-C35-C30	4.53	119.10	112.31
2	A	501	3SG	C23-C25-N27	3.37	124.08	115.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	3SG	C15-C14-C13	-3.09	114.00	120.12
2	C	501	3SG	C38-O37-C35	3.09	121.75	115.81
2	D	501	3SG	C5-N4-C3	3.06	122.21	116.85
2	D	501	3SG	C15-C14-C17	3.03	126.98	121.55
2	C	501	3SG	C5-N4-C3	2.86	121.85	116.85
2	B	501	3SG	C5-N4-C3	2.82	121.78	116.85
2	A	501	3SG	C5-N4-C3	2.81	121.77	116.85
2	A	501	3SG	C15-C14-C13	-2.79	114.59	120.12
2	D	501	3SG	C23-C25-N27	2.78	122.65	115.90
2	B	501	3SG	C15-C14-C13	-2.65	114.88	120.12
2	D	501	3SG	F34-C33-C28	-2.63	114.32	117.59
2	C	501	3SG	C23-C25-N27	2.46	121.87	115.90
2	A	501	3SG	C15-C14-C17	2.34	125.74	121.55
2	D	501	3SG	F34-C33-C32	2.27	123.91	118.65
2	B	501	3SG	C23-C25-N27	2.25	121.36	115.90
2	C	501	3SG	C29-C28-C33	2.25	119.80	117.65
2	B	501	3SG	C15-C14-C17	2.23	125.55	121.55
2	C	501	3SG	C15-C14-C13	-2.22	115.74	120.12
2	A	501	3SG	O26-C25-C23	-2.10	116.74	120.90
2	B	501	3SG	O37-C35-O36	-2.08	119.40	123.46
2	C	501	3SG	C15-C14-C17	2.05	125.23	121.55

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	3SG	C30-C35-O37-C38
2	B	501	3SG	C30-C35-O37-C38
2	D	501	3SG	C17-C14-C15-N16
2	D	501	3SG	C30-C35-O37-C38
2	D	501	3SG	O36-C35-O37-C38
2	C	501	3SG	C31-C30-C35-O36
2	B	501	3SG	O36-C35-O37-C38
2	C	501	3SG	C30-C35-O37-C38
2	A	501	3SG	C31-C30-C35-O36
2	A	501	3SG	C31-C30-C35-O37
2	A	501	3SG	C29-C30-C35-O37
2	C	501	3SG	C31-C30-C35-O37
2	C	501	3SG	C29-C30-C35-O37
2	A	501	3SG	C29-C30-C35-O36
2	C	501	3SG	C29-C30-C35-O36
2	A	501	3SG	O36-C35-O37-C38

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Mol	Chain	Res	Type	Atoms
2	C	501	3SG	O36-C35-O37-C38
2	D	501	3SG	C31-C30-C35-O37
2	D	501	3SG	C29-C30-C35-O37
2	D	501	3SG	C31-C30-C35-O36
2	B	501	3SG	C31-C30-C35-O37
2	D	501	3SG	C29-C30-C35-O36
2	B	501	3SG	C29-C30-C35-O37
2	D	501	3SG	C33-C28-N27-C25
2	B	501	3SG	C31-C30-C35-O36
2	B	501	3SG	C29-C30-C35-O36
2	A	501	3SG	C17-C14-C15-N16
2	C	501	3SG	C33-C28-N27-C25
2	A	501	3SG	C33-C28-N27-C25
2	B	501	3SG	C33-C28-N27-C25
2	D	501	3SG	C29-C28-N27-C25
2	B	501	3SG	C18-C11-C9-N8
2	B	501	3SG	C18-C11-C9-O10

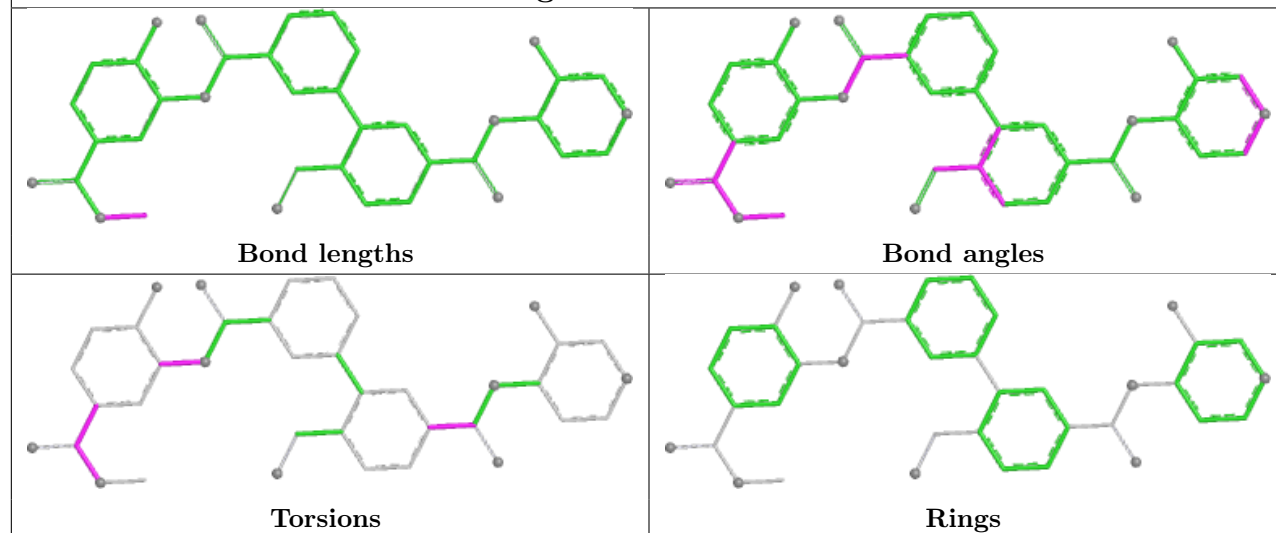
There are no ring outliers.

1 monomer is involved in 1 short contact:

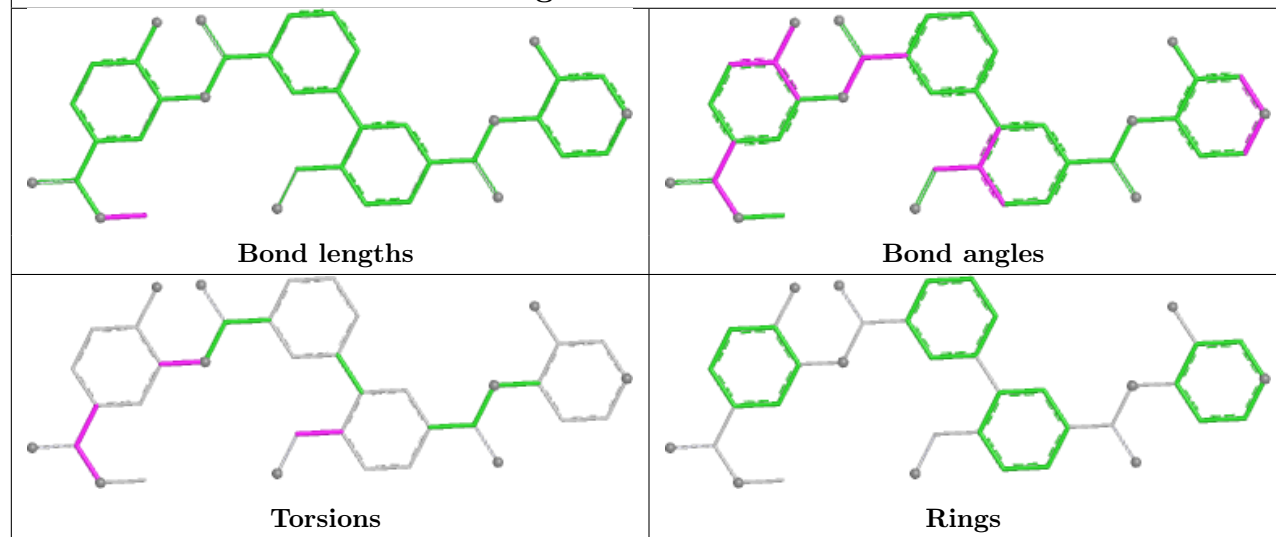
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	3SG	1	0

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

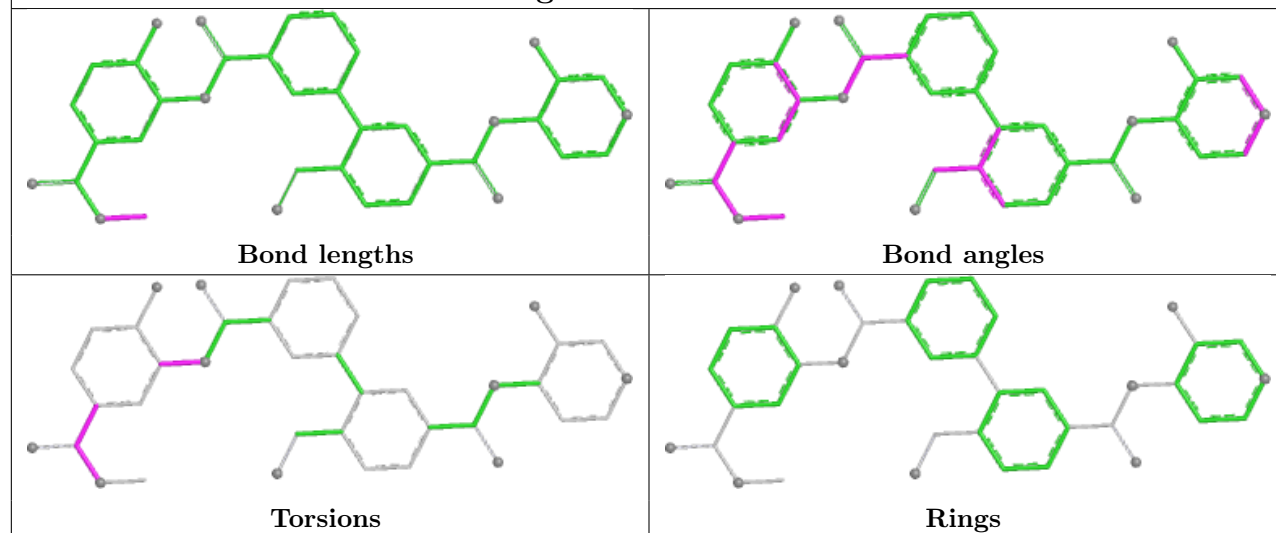
Ligand 3SG B 501

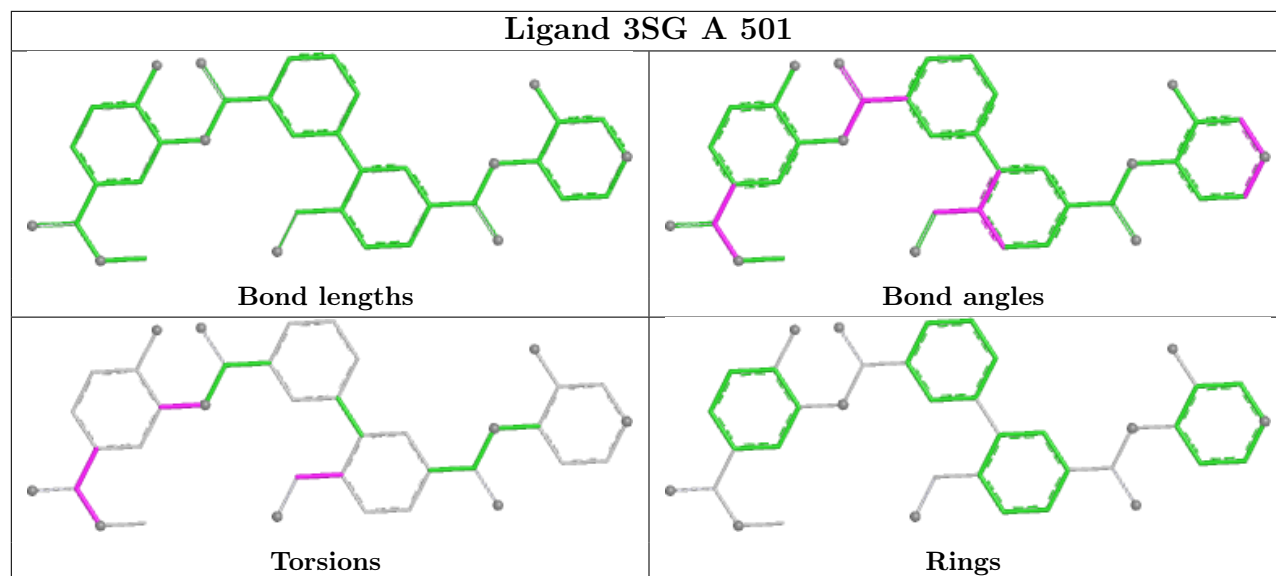


Ligand 3SG D 501



Ligand 3SG C 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	389/396 (98%)	0.26	14 (3%)	46 38	46, 84, 123, 149	76 (19%)
1	B	394/396 (99%)	0.22	13 (3%)	49 41	41, 84, 127, 158	57 (14%)
1	C	392/396 (98%)	0.42	19 (4%)	35 29	51, 93, 134, 165	98 (25%)
1	D	389/396 (98%)	0.20	10 (2%)	57 48	46, 79, 115, 161	49 (12%)
All	All	1564/1584 (98%)	0.27	56 (3%)	46 38	41, 85, 128, 165	280 (17%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	ILE	3.7
1	D	244	MET	3.5
1	D	394	VAL	3.1
1	C	394	VAL	3.1
1	A	281	GLY	3.0
1	C	56	ASP	3.0
1	C	303	TYR	3.0
1	C	236	CYS	2.9
1	C	46	LEU	2.9
1	B	22	ALA	2.9
1	C	43	VAL	2.9
1	A	50	LEU	2.9
1	D	231	ALA	2.8
1	D	247	CYS	2.8
1	B	194	TYR	2.8
1	A	389	ASP	2.7
1	C	89	ALA	2.7
1	A	236	CYS	2.6
1	B	357	ASP	2.6
1	C	254	PRO	2.6
1	C	253	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	251	VAL	2.6
1	C	300	VAL	2.6
1	D	313	LEU	2.5
1	A	27	GLN	2.5
1	C	231	ALA	2.5
1	C	266	GLY	2.4
1	A	171	TYR	2.4
1	D	24	ALA	2.4
1	B	249	THR	2.4
1	A	22	ALA	2.3
1	A	285	TYR	2.3
1	D	23	GLY	2.3
1	D	181	MET	2.3
1	B	270	PHE	2.3
1	B	224	LYS	2.2
1	A	247	CYS	2.2
1	B	250	ALA	2.2
1	C	153	VAL	2.2
1	D	56	ASP	2.2
1	B	354	PHE	2.1
1	D	336	ARG	2.1
1	B	153	VAL	2.1
1	B	230	LEU	2.1
1	B	231	ALA	2.1
1	B	321	ILE	2.1
1	B	299	LEU	2.0
1	C	28	ARG	2.0
1	C	137	PHE	2.0
1	A	89	ALA	2.0
1	C	102	ALA	2.0
1	A	139	GLU	2.0
1	C	171	TYR	2.0
1	A	28	ARG	2.0
1	C	133	ASP	2.0
1	A	208	MET	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](#)

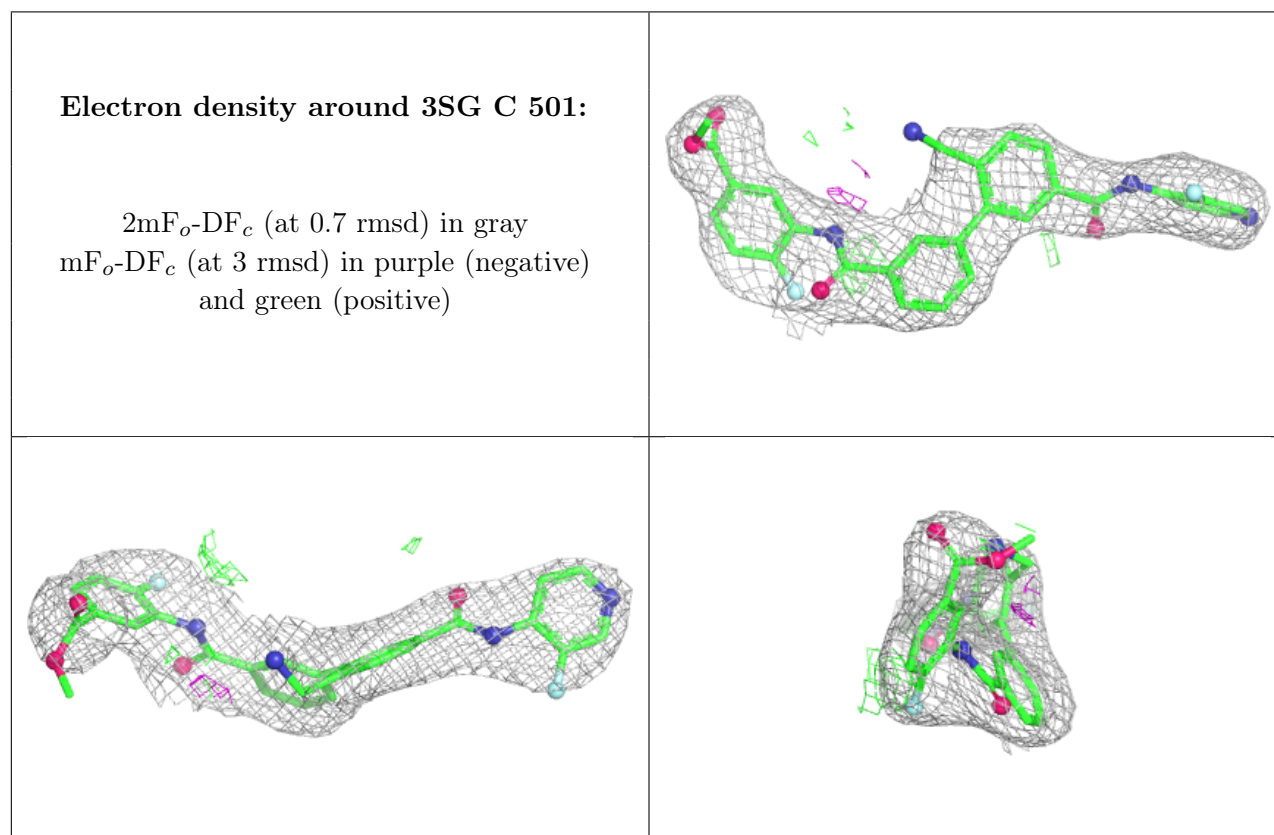
There are no oligosaccharides in this entry.

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.

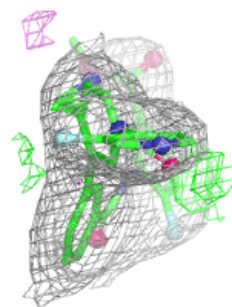
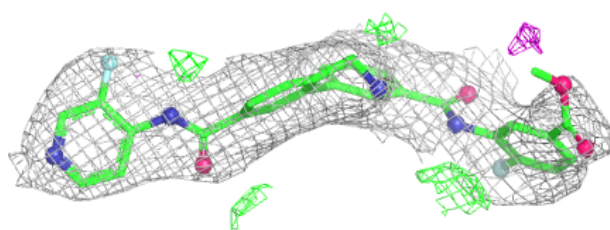
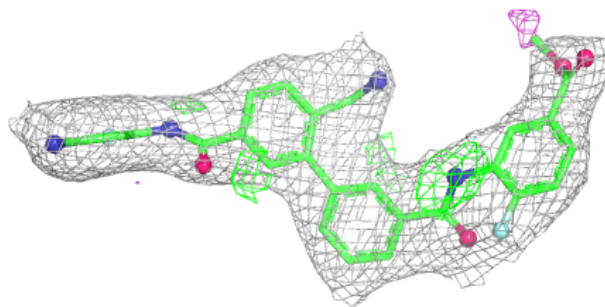
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3SG	C	501	38/38	0.90	0.11	76,83,93,96	1
2	3SG	B	501	38/38	0.92	0.10	53,69,87,89	1
2	3SG	A	501	38/38	0.92	0.10	68,78,105,110	1
2	3SG	D	501	38/38	0.93	0.11	60,77,103,107	1

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.

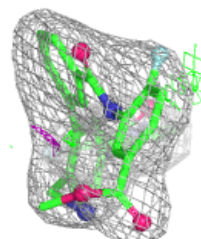
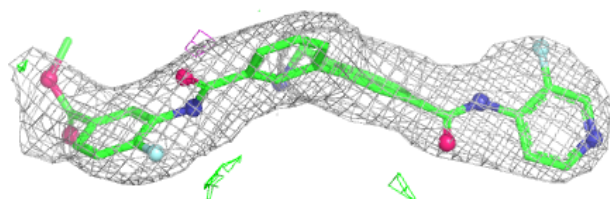
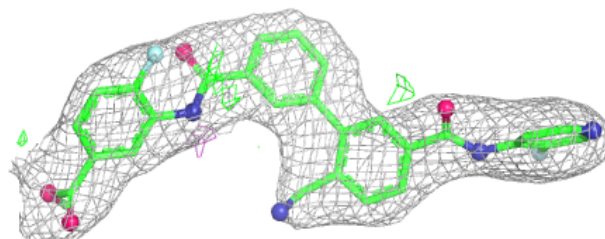


Electron density around 3SG B 501:

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

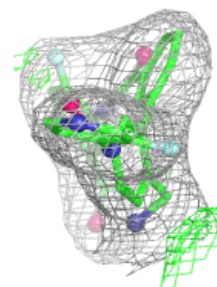
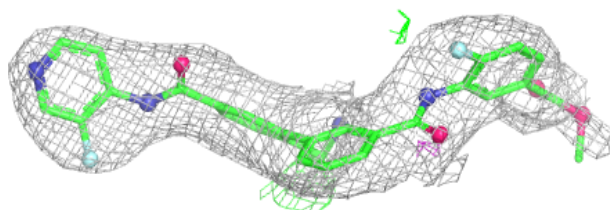
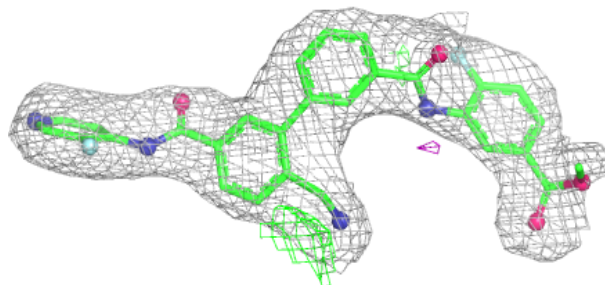
**Electron density around 3SG A 501:**

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



Electron density around 3SG 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.