



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:20 PM UTC

PDB ID : 7CFO / pdb_00007cfo
Title : Crystal structure of human RXRalpha ligand binding domain complexed with CBTF-EE.
Authors : Watanabe, M.; Fujihara, M.; Motoyama, T.; Kawasaki, M.; Yamada, S.; Takamura, Y.; Ito, S.; Makishima, M.; Nakano, S.; Kakuta, H.
Deposited on : 2020-06-27
Resolution : 2.15 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

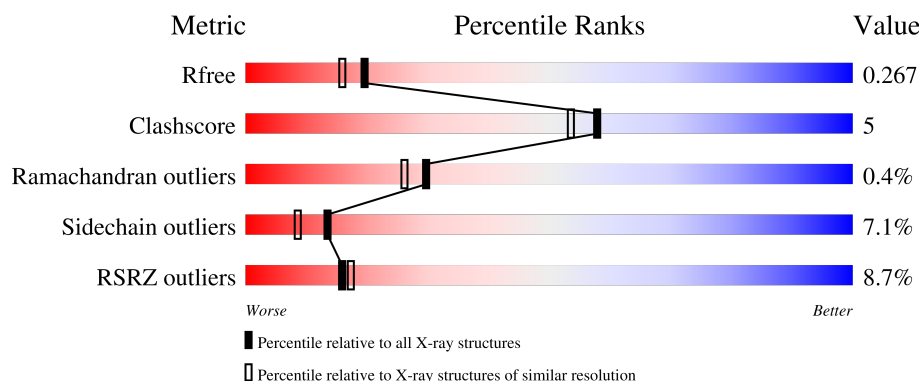
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	243	5% 72% 7% 21%
1	B	243	6% 72% 8% 5% 15%
1	C	243	12% 69% 11% •• 15%
1	D	243	5% 70% 6% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6481 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.

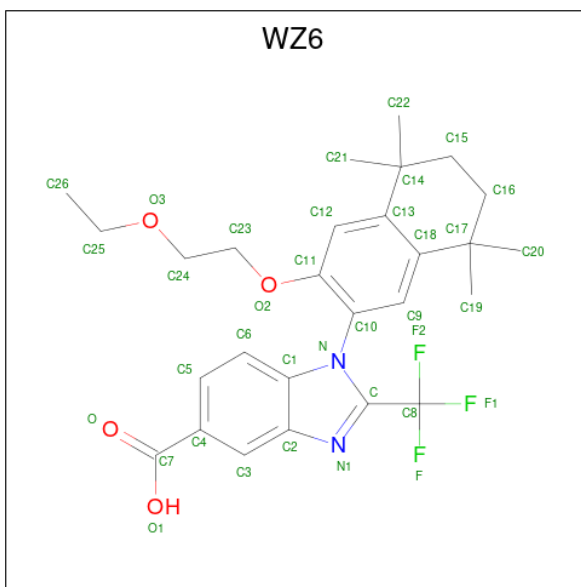
- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1528	986	264	269	9			
1	B	206	Total	C	N	O	S	0	0	0
			1625	1047	280	289	9			
1	C	206	Total	C	N	O	S	0	0	0
			1629	1049	280	291	9			
1	D	187	Total	C	N	O	S	0	0	0
			1486	959	257	261	9			

There are 16 discrepancies between the modelled and reference sequences:

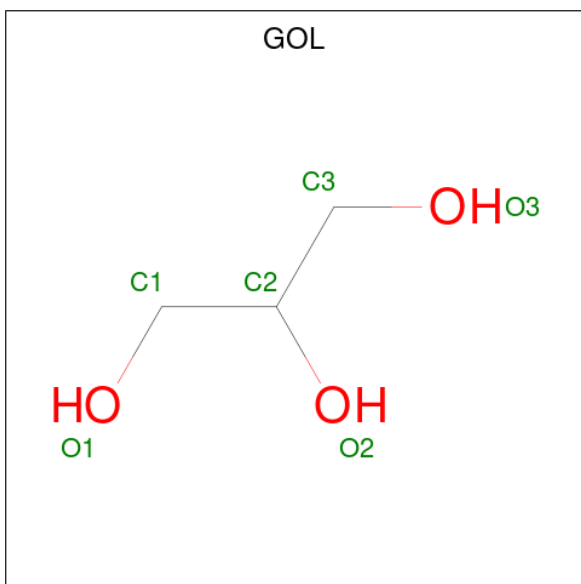
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	-	expression tag	UNP P19793
A	221	SER	-	expression tag	UNP P19793
A	222	SER	-	expression tag	UNP P19793
A	223	HIS	-	expression tag	UNP P19793
B	220	GLY	-	expression tag	UNP P19793
B	221	SER	-	expression tag	UNP P19793
B	222	SER	-	expression tag	UNP P19793
B	223	HIS	-	expression tag	UNP P19793
C	220	GLY	-	expression tag	UNP P19793
C	221	SER	-	expression tag	UNP P19793
C	222	SER	-	expression tag	UNP P19793
C	223	HIS	-	expression tag	UNP P19793
D	220	GLY	-	expression tag	UNP P19793
D	221	SER	-	expression tag	UNP P19793
D	222	SER	-	expression tag	UNP P19793
D	223	HIS	-	expression tag	UNP P19793

- Molecule 2 is 1-[3-(2-ethoxyethoxy)-5,5,8,8-tetramethyl-6,7-dihydronaphthalen-2-yl]-2-(trifluoromethyl)benzimidazole-5-carboxylic acid (CCD ID: WZ6) (formula: C₂₇H₃₁F₃N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			36	27	3	2	4		
2	B	1	Total	C	F	N	O	0	0
			36	27	3	2	4		
2	C	1	Total	C	F	N	O	0	0
			36	27	3	2	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

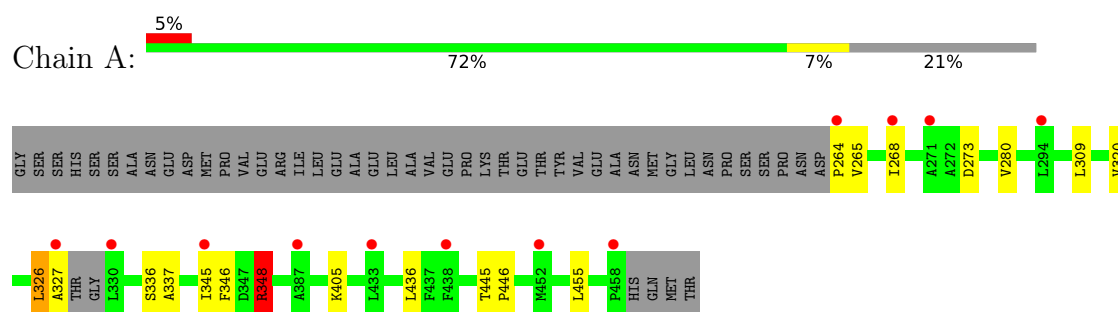
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	31	Total	O	0	0
			31	31		
4	C	24	Total	O	0	0
			24	24		
4	D	17	Total	O	0	0
			17	17		

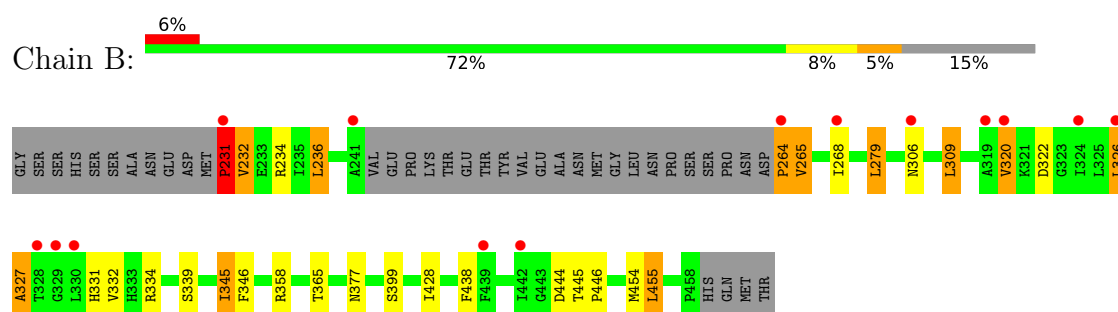
3 Residue-property plots

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.

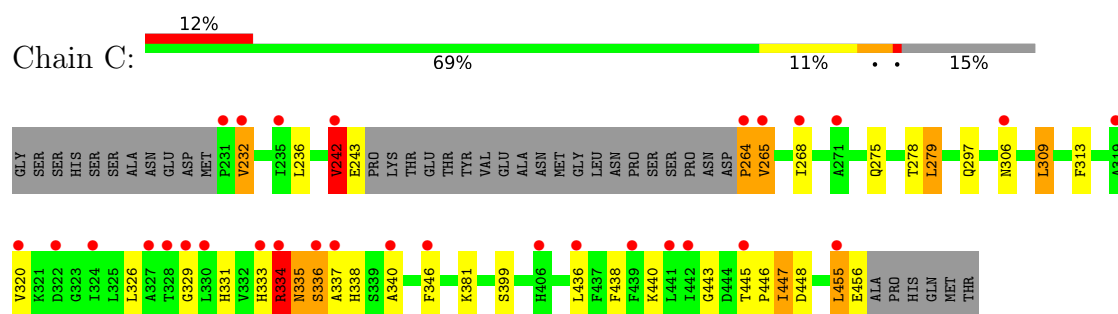
• Molecule 1: Retinoic acid receptor RXR-alpha



• Molecule 1: Retinoic acid receptor RXR-alpha

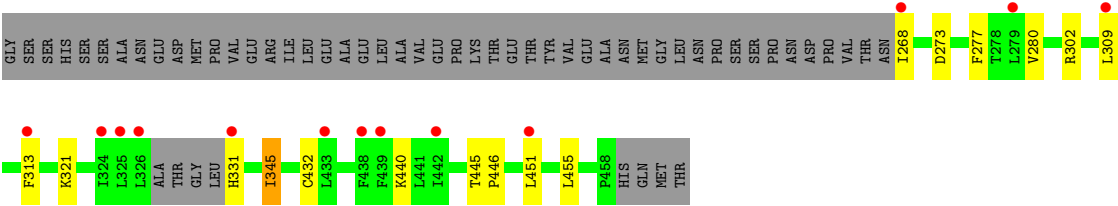


• Molecule 1: Retinoic acid receptor RXR-alpha



• Molecule 1: Retinoic acid receptor RXR-alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.76Å 99.43Å 93.60Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	47.14 – 2.15 47.14 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.6 (47.14-2.15) 95.7 (47.14-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.221 , 0.266 0.224 , 0.267	Depositor DCC
R_{free} test set	2423 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6481	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GOL, WZ6

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	1.10	0/1560	1.49	2/2107 (0.1%)
1	B	1.07	0/1658	1.54	1/2240 (0.0%)
1	C	1.07	0/1661	1.55	4/2243 (0.2%)
1	D	1.06	0/1517	1.45	1/2047 (0.0%)
All	All	1.07	0/6396	1.51	8/8637 (0.1%)

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	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	PRO	CA-N-CD	-9.35	98.91	112.00
1	A	348	ARG	CB-CG-CD	7.46	128.47	111.30
1	A	348	ARG	CG-CD-NE	5.79	124.75	112.00
1	C	242	VAL	CB-CA-C	5.71	116.00	110.63
1	C	313	PHE	CA-CB-CG	5.59	119.39	113.80
1	D	313	PHE	CA-CB-CG	5.13	118.93	113.80
1	C	329	GLY	CA-C-N	5.04	128.00	120.95
1	C	329	GLY	C-N-CA	5.04	128.00	120.95

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	231	PRO	Peptide
1	B	264	PRO	Peptide

5.2 Too-close contacts [i](#)

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	1528	0	1570	14	0
1	B	1625	0	1671	21	0
1	C	1629	0	1674	28	0
1	D	1486	0	1524	9	0
2	A	36	0	0	1	0
2	B	36	0	0	0	0
2	C	36	0	0	0	0
3	B	6	0	8	2	0
3	C	6	0	8	0	0
4	A	21	0	0	1	0
4	B	31	0	0	0	0
4	C	24	0	0	1	0
4	D	17	0	0	1	0
All	All	6481	0	6455	58	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 5.

All (58) 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:436:LEU:HD21	1:C:436:LEU:HD21	1.66	0.77
1:C:306:ASN:OD1	1:C:438:PHE:CE2	2.38	0.76
4:A:600:HOH:O	1:C:448:ASP:HB2	1.84	0.76
1:A:436:LEU:HD21	1:C:436:LEU:CD2	2.16	0.76
1:B:454:MET:HE1	1:D:277:PHE:CD1	2.25	0.71
1:C:334:ARG:HA	1:C:337:ALA:HB3	1.72	0.70
1:A:348:ARG:HG2	1:A:348:ARG:HH21	1.57	0.69
1:B:306:ASN:OD1	1:B:438:PHE:CE2	2.45	0.69
1:B:320:VAL:O	1:B:358:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ARG:O	1:C:338:HIS:HB2	1.97	0.64
1:A:264:PRO:O	1:A:268:ILE:HD13	1.98	0.63
1:B:377:ASN:HD21	3:B:501:GOL:H12	1.63	0.62
1:B:320:VAL:HG11	1:B:331:HIS:CE1	2.36	0.59
1:A:273:ASP:OD1	1:C:264:PRO:HA	2.02	0.59
1:C:445:THR:OG1	1:C:446:PRO:HD3	2.03	0.59
1:C:335:ASN:HD22	1:C:335:ASN:H	1.50	0.58
1:C:340:ALA:HB1	1:C:440:LYS:HB3	1.86	0.58
1:C:445:THR:OG1	1:C:446:PRO:CD	2.53	0.57
1:C:443:GLY:O	1:C:447:ILE:HD13	2.05	0.55
1:B:377:ASN:HD21	3:B:501:GOL:C1	2.19	0.55
1:B:265:VAL:HG13	1:D:273:ASP:CG	2.32	0.54
1:C:331:HIS:CE1	4:C:607:HOH:O	2.61	0.53
1:C:232:VAL:HG23	1:C:399:SER:OG	2.09	0.53
1:B:444:ASP:OD1	1:D:302:ARG:NH2	2.42	0.52
1:C:275:GLN:CG	1:C:309:LEU:HD21	2.41	0.50
1:A:436:LEU:HD21	1:C:436:LEU:HD22	1.94	0.50
1:B:232:VAL:HG23	1:B:399:SER:OG	2.12	0.49
1:C:335:ASN:HD22	1:C:335:ASN:N	2.10	0.49
1:B:454:MET:CE	1:D:277:PHE:CD1	2.96	0.48
1:C:242:VAL:HG22	1:C:278:THR:HG23	1.96	0.48
1:A:445:THR:HB	1:A:446:PRO:HD3	1.96	0.48
1:B:306:ASN:OD1	1:B:438:PHE:HE2	1.92	0.47
1:C:306:ASN:OD1	1:C:438:PHE:HE2	1.95	0.47
1:B:306:ASN:OD1	1:B:438:PHE:CZ	2.67	0.47
1:D:440:LYS:NZ	4:D:600:HOH:O	2.47	0.47
1:C:268:ILE:HD11	1:C:446:PRO:HB2	1.97	0.46
1:D:445:THR:HB	1:D:446:PRO:HD3	1.97	0.46
1:C:279:LEU:HD21	1:C:309:LEU:HD13	1.97	0.45
1:B:345:ILE:HD11	1:B:428:ILE:HG23	1.99	0.45
1:A:337:ALA:HB2	1:A:346:PHE:CD2	2.51	0.45
1:A:280:VAL:HG13	1:C:455:LEU:CD1	2.48	0.44
1:A:273:ASP:OD1	1:C:265:VAL:N	2.47	0.44
1:C:335:ASN:CG	1:C:336:SER:H	2.26	0.43
1:B:326:LEU:CD2	1:B:332:VAL:HG21	2.48	0.43
1:B:279:LEU:CD2	1:B:309:LEU:HD13	2.49	0.43
1:B:455:LEU:HD13	1:D:280:VAL:HG13	2.00	0.43
1:A:268:ILE:CG2	2:A:500:WZ6:C15	2.97	0.42
1:B:454:MET:HE2	1:D:280:VAL:HB	2.01	0.42
1:B:445:THR:HB	1:B:446:PRO:HD3	2.00	0.42
1:B:236:LEU:HG	1:B:365:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ILE:HD11	1:D:432:CYS:SG	2.60	0.42
1:A:273:ASP:OD1	1:C:264:PRO:CA	2.66	0.41
1:C:279:LEU:CD2	1:C:309:LEU:HD13	2.50	0.41
1:A:326:LEU:O	1:A:327:ALA:HB2	2.20	0.40
1:B:326:LEU:O	1:B:327:ALA:HB3	2.20	0.40
1:B:334:ARG:HA	1:B:346:PHE:CE1	2.55	0.40
1:C:306:ASN:OD1	1:C:438:PHE:CZ	2.73	0.40
1:A:455:LEU:HD22	1:C:297:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/243 (78%)	186 (98%)	3 (2%)	0	100	100
1	B	202/243 (83%)	195 (96%)	5 (2%)	2 (1%)	12	8
1	C	202/243 (83%)	194 (96%)	7 (4%)	1 (0%)	24	20
1	D	183/243 (75%)	180 (98%)	3 (2%)	0	100	100
All	All	776/972 (80%)	755 (97%)	18 (2%)	3 (0%)	30	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	334	ARG
1	B	322	ASP
1	B	327	ALA

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	166/209 (79%)	158 (95%)	8 (5%)	23	20
1	B	176/209 (84%)	162 (92%)	14 (8%)	11	7
1	C	177/209 (85%)	158 (89%)	19 (11%)	6	3
1	D	161/209 (77%)	154 (96%)	7 (4%)	26	24
All	All	680/836 (81%)	632 (93%)	48 (7%)	13	8

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	VAL
1	A	309	LEU
1	A	320	VAL
1	A	326	LEU
1	A	336	SER
1	A	345	ILE
1	A	348	ARG
1	A	405	LYS
1	B	231	PRO
1	B	232	VAL
1	B	234	ARG
1	B	236	LEU
1	B	264	PRO
1	B	265	VAL
1	B	268	ILE
1	B	279	LEU
1	B	309	LEU
1	B	320	VAL
1	B	326	LEU
1	B	339	SER
1	B	345	ILE
1	B	455	LEU
1	C	232	VAL
1	C	236	LEU

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Mol	Chain	Res	Type
1	C	242	VAL
1	C	243	GLU
1	C	264	PRO
1	C	265	VAL
1	C	279	LEU
1	C	309	LEU
1	C	320	VAL
1	C	326	LEU
1	C	333	HIS
1	C	334	ARG
1	C	335	ASN
1	C	336	SER
1	C	346	PHE
1	C	381	LYS
1	C	447	ILE
1	C	455	LEU
1	C	456	GLU
1	D	268	ILE
1	D	309	LEU
1	D	321	LYS
1	D	331	HIS
1	D	345	ILE
1	D	451	LEU
1	D	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	275	GLN
1	A	335	ASN
1	C	335	ASN
1	D	335	ASN

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](#)

5 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	WZ6	C	500	-	39,39,39	2.48	8 (20%)	57,61,61	2.69	23 (40%)
3	GOL	C	501	-	5,5,5	0.13	0	5,5,5	0.14	0
2	WZ6	B	500	-	39,39,39	2.41	7 (17%)	57,61,61	4.26	33 (57%)
2	WZ6	A	500	-	39,39,39	2.63	10 (25%)	57,61,61	3.53	23 (40%)
3	GOL	B	501	-	5,5,5	0.52	0	5,5,5	0.83	0

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	WZ6	C	500	-	-	2/20/39/39	0/4/4/4
3	GOL	C	501	-	-	2/4/4/4	-
2	WZ6	B	500	-	-	5/20/39/39	0/4/4/4
2	WZ6	A	500	-	-	6/20/39/39	0/4/4/4
3	GOL	B	501	-	-	4/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	WZ6	C10-N	-10.24	1.33	1.44
2	A	500	WZ6	C10-C11	9.49	1.55	1.40
2	B	500	WZ6	C10-N	-7.68	1.36	1.44
2	B	500	WZ6	C1-C2	7.33	1.52	1.40
2	A	500	WZ6	C10-N	-7.11	1.37	1.44
2	B	500	WZ6	C10-C11	6.48	1.50	1.40
2	A	500	WZ6	C1-C2	6.05	1.50	1.40
2	C	500	WZ6	C1-C2	5.24	1.48	1.40
2	C	500	WZ6	C10-C11	4.56	1.47	1.40
2	A	500	WZ6	C18-C13	4.52	1.48	1.40
2	B	500	WZ6	C-N1	3.98	1.37	1.30
2	A	500	WZ6	C1-N	-3.92	1.34	1.40
2	B	500	WZ6	C18-C13	3.91	1.47	1.40
2	C	500	WZ6	C1-N	-3.87	1.34	1.40
2	C	500	WZ6	C-N	-3.80	1.34	1.37
2	B	500	WZ6	C1-N	-3.69	1.34	1.40
2	C	500	WZ6	C18-C13	3.66	1.46	1.40
2	A	500	WZ6	C-N1	3.04	1.35	1.30
2	C	500	WZ6	C-N1	3.02	1.35	1.30
2	A	500	WZ6	C12-C13	-2.97	1.35	1.39
2	A	500	WZ6	C17-C18	-2.95	1.49	1.53
2	A	500	WZ6	C14-C13	-2.62	1.50	1.53
2	C	500	WZ6	C14-C13	-2.44	1.50	1.53
2	B	500	WZ6	C14-C13	-2.12	1.50	1.53
2	A	500	WZ6	C8-C	2.11	1.54	1.50

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	WZ6	C20-C17-C18	-13.69	86.56	110.12
2	A	500	WZ6	C22-C14-C13	-12.50	88.61	110.12
2	B	500	WZ6	C22-C14-C13	-10.62	91.84	110.12
2	B	500	WZ6	C22-C14-C21	-10.01	86.50	108.63
2	A	500	WZ6	C22-C14-C21	-9.99	86.53	108.63
2	A	500	WZ6	O2-C11-C10	9.17	129.64	116.07
2	B	500	WZ6	C8-C-N1	-8.04	116.03	122.44
2	B	500	WZ6	C16-C17-C18	7.87	122.69	110.11
2	A	500	WZ6	C8-C-N1	-7.78	116.23	122.44
2	A	500	WZ6	C21-C14-C13	7.74	123.43	110.12
2	B	500	WZ6	F-C8-C	7.12	121.75	111.95
2	B	500	WZ6	C21-C14-C13	7.05	122.25	110.12
2	C	500	WZ6	C22-C14-C21	-6.70	93.82	108.63
2	B	500	WZ6	C19-C17-C20	-6.49	94.28	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	WZ6	O2-C11-C12	-6.40	109.66	123.49
2	B	500	WZ6	C17-C18-C13	-6.19	115.83	122.76
2	C	500	WZ6	C22-C14-C13	-6.18	99.47	110.12
2	B	500	WZ6	F2-C8-C	-6.04	103.64	111.95
2	C	500	WZ6	C14-C13-C18	-5.98	116.07	122.76
2	B	500	WZ6	C19-C17-C18	5.87	120.22	110.12
2	A	500	WZ6	C9-C10-N	-5.35	110.61	119.18
2	C	500	WZ6	C22-C14-C15	-5.10	88.31	109.15
2	B	500	WZ6	C20-C17-C16	-4.94	88.97	109.15
2	A	500	WZ6	C5-C4-C3	4.78	124.78	119.25
2	C	500	WZ6	C15-C14-C13	4.77	117.73	110.11
2	B	500	WZ6	C15-C14-C13	4.55	117.38	110.11
2	A	500	WZ6	C22-C14-C15	-4.39	91.20	109.15
2	B	500	WZ6	O2-C11-C10	4.34	122.49	116.07
2	C	500	WZ6	C1-N-C	4.30	113.25	106.07
2	C	500	WZ6	F-C8-C	-4.19	106.18	111.95
2	A	500	WZ6	C9-C10-C11	-3.94	113.98	119.78
2	C	500	WZ6	C21-C14-C15	3.88	124.99	109.15
2	B	500	WZ6	F1-C8-C	3.87	117.28	111.95
2	C	500	WZ6	C16-C17-C18	3.85	116.26	110.11
2	B	500	WZ6	F1-C8-F2	-3.80	89.82	106.20
2	C	500	WZ6	C9-C10-N	3.79	125.26	119.18
2	B	500	WZ6	C9-C10-C11	-3.78	114.21	119.78
2	B	500	WZ6	O2-C11-C12	-3.76	115.37	123.49
2	C	500	WZ6	C3-C2-C1	-3.70	116.76	120.16
2	C	500	WZ6	C6-C1-N	3.64	137.16	130.54
2	C	500	WZ6	C2-C1-N	-3.62	102.56	105.25
2	B	500	WZ6	O2-C23-C24	3.58	120.69	108.71
2	C	500	WZ6	C21-C14-C13	3.44	116.04	110.12
2	A	500	WZ6	C3-C4-C7	-3.34	113.98	119.96
2	A	500	WZ6	C2-C1-N	-3.31	102.79	105.25
2	C	500	WZ6	O1-C7-C4	3.25	123.19	114.84
2	C	500	WZ6	C17-C18-C13	-3.07	119.33	122.76
2	C	500	WZ6	C16-C15-C14	-3.04	102.68	113.84
2	A	500	WZ6	C21-C14-C15	3.04	121.56	109.15
2	B	500	WZ6	O1-C7-C4	3.01	122.57	114.84
2	A	500	WZ6	C15-C14-C13	2.97	114.85	110.11
2	C	500	WZ6	C19-C17-C18	-2.96	105.03	110.12
2	C	500	WZ6	C3-C2-N1	2.90	135.55	129.31
2	B	500	WZ6	C5-C4-C3	2.88	122.58	119.25
2	B	500	WZ6	C22-C14-C15	-2.84	97.57	109.15
2	A	500	WZ6	C6-C1-N	2.82	135.67	130.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	WZ6	C9-C10-N	2.73	123.56	119.18
2	A	500	WZ6	C25-O3-C24	2.72	122.61	113.06
2	B	500	WZ6	C6-C1-N	2.70	135.45	130.54
2	B	500	WZ6	C21-C14-C15	2.67	120.06	109.15
2	A	500	WZ6	C1-N-C	2.66	110.50	106.07
2	B	500	WZ6	C3-C2-C1	-2.62	117.76	120.16
2	B	500	WZ6	F1-C8-F	2.58	117.33	106.20
2	A	500	WZ6	F1-C8-C	2.55	115.46	111.95
2	B	500	WZ6	F-C8-F2	-2.55	95.22	106.20
2	B	500	WZ6	O1-C7-O	-2.48	118.01	123.35
2	A	500	WZ6	C3-C2-C1	-2.48	117.88	120.16
2	A	500	WZ6	C10-N-C1	-2.48	118.50	123.89
2	A	500	WZ6	O2-C23-C24	2.47	116.98	108.71
2	B	500	WZ6	C9-C18-C17	2.34	125.06	119.22
2	C	500	WZ6	C10-N-C1	-2.31	118.86	123.89
2	A	500	WZ6	F2-C8-C	-2.26	108.83	111.95
2	B	500	WZ6	C2-C1-N	-2.25	103.58	105.25
2	A	500	WZ6	C23-O2-C11	2.25	123.12	117.69
2	B	500	WZ6	C10-N-C1	-2.19	119.12	123.89
2	B	500	WZ6	C1-N-C	2.18	109.71	106.07
2	C	500	WZ6	C19-C17-C20	2.18	113.44	108.63
2	C	500	WZ6	C12-C13-C14	2.16	124.60	119.22
2	C	500	WZ6	C5-C4-C3	2.07	121.65	119.25

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	GOL	O1-C1-C2-O2
3	B	501	GOL	O1-C1-C2-C3
3	B	501	GOL	C1-C2-C3-O3
3	B	501	GOL	O2-C2-C3-O3
3	C	501	GOL	C1-C2-C3-O3
3	C	501	GOL	O2-C2-C3-O3
2	A	500	WZ6	C23-C24-O3-C25
2	B	500	WZ6	C10-C11-O2-C23
2	B	500	WZ6	O2-C23-C24-O3
2	C	500	WZ6	O2-C23-C24-O3
2	B	500	WZ6	C12-C11-O2-C23
2	B	500	WZ6	C24-C23-O2-C11
2	A	500	WZ6	C26-C25-O3-C24
2	B	500	WZ6	N-C-C8-F

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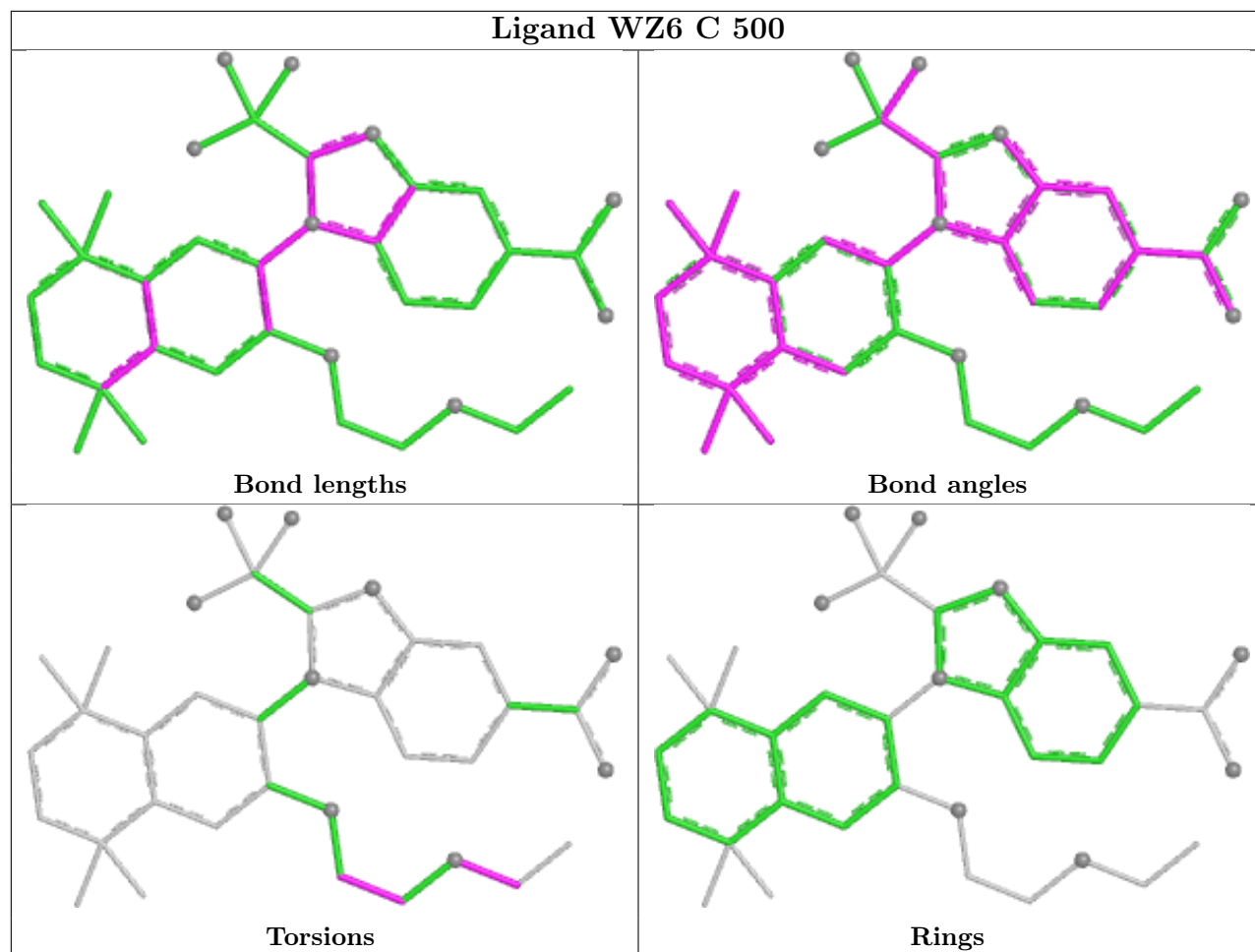
Mol	Chain	Res	Type	Atoms
2	C	500	WZ6	C26-C25-O3-C24
2	A	500	WZ6	N-C-C8-F1
2	A	500	WZ6	O2-C23-C24-O3
2	A	500	WZ6	N-C-C8-F2
2	A	500	WZ6	C24-C23-O2-C11

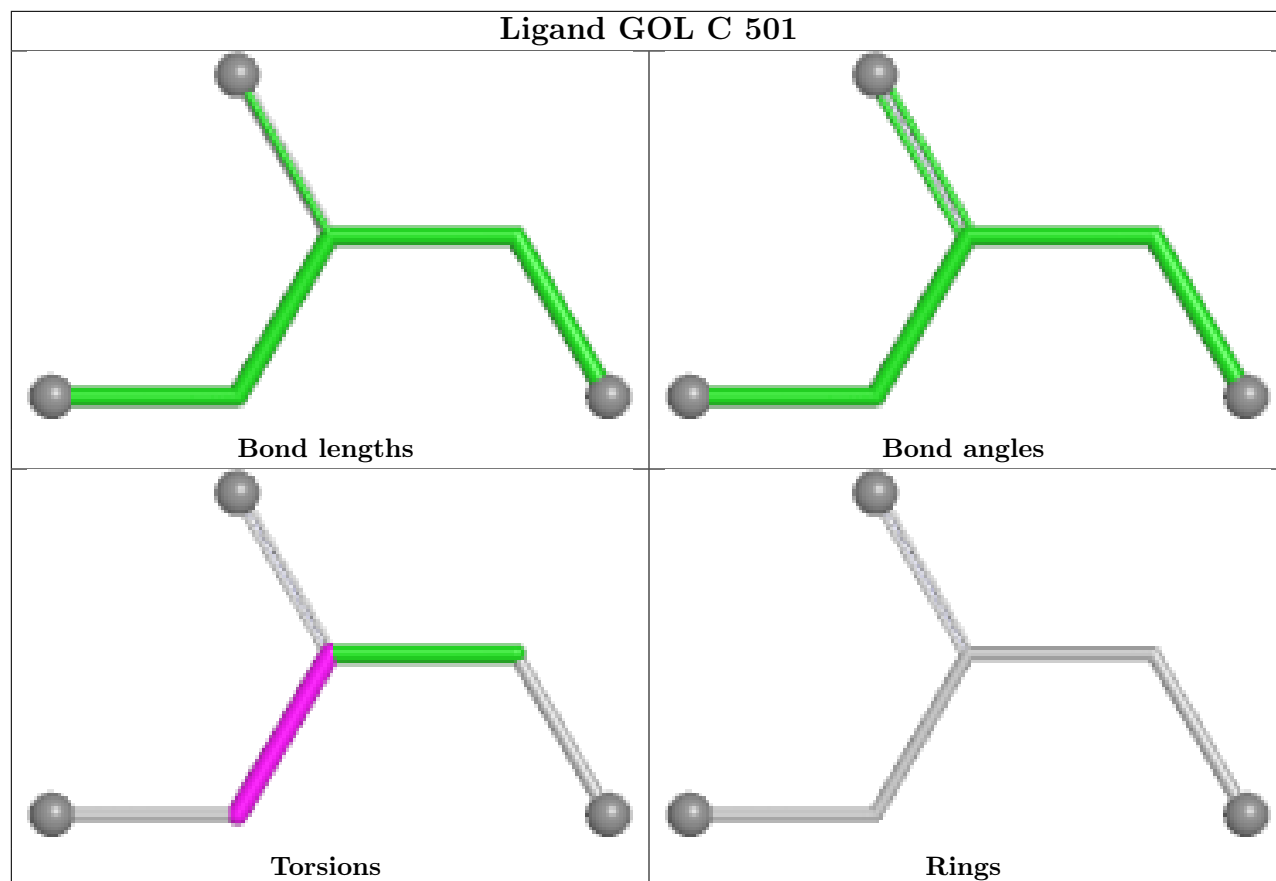
There are no ring outliers.

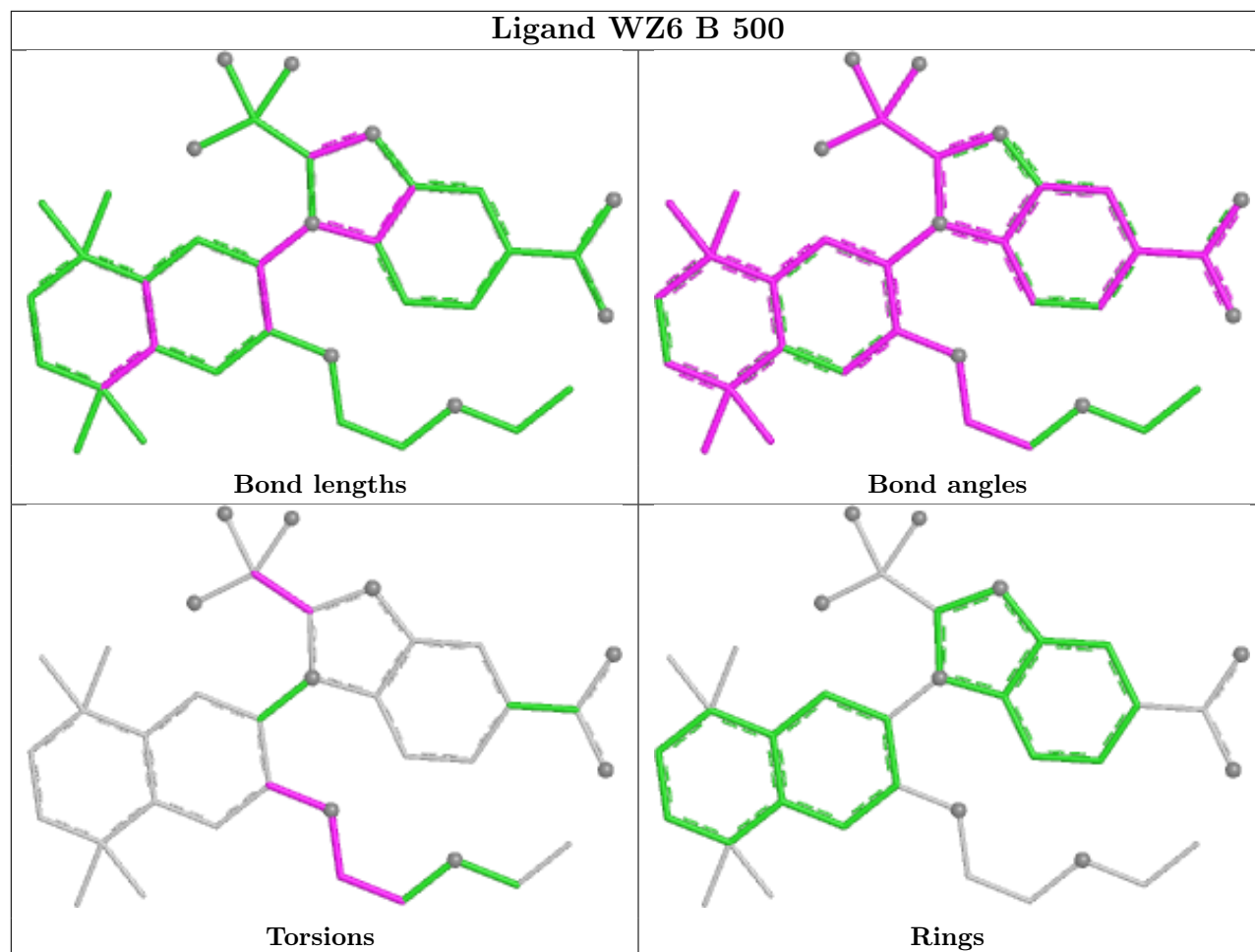
2 monomers are involved in 3 short contacts:

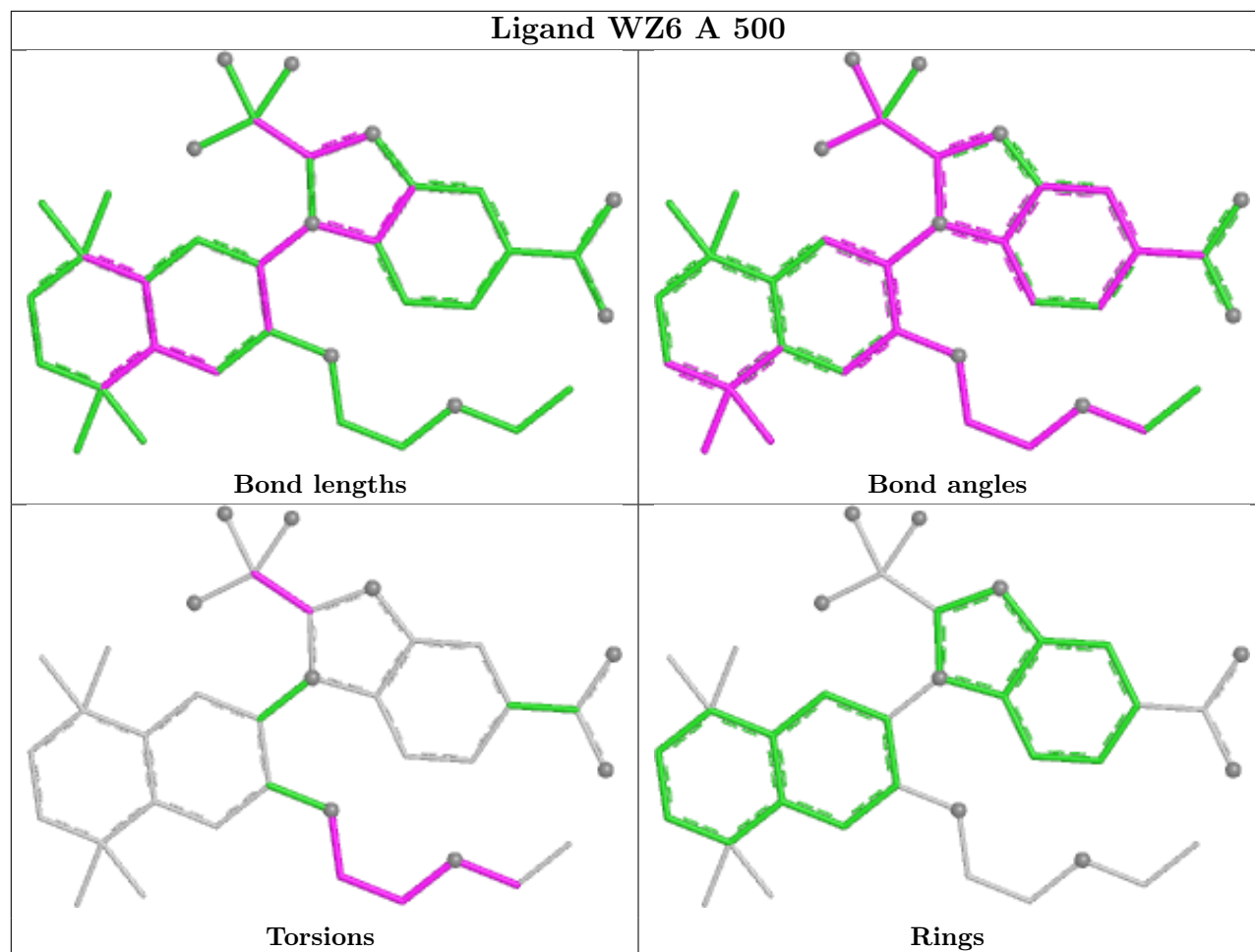
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	WZ6	1	0
3	B	501	GOL	2	0

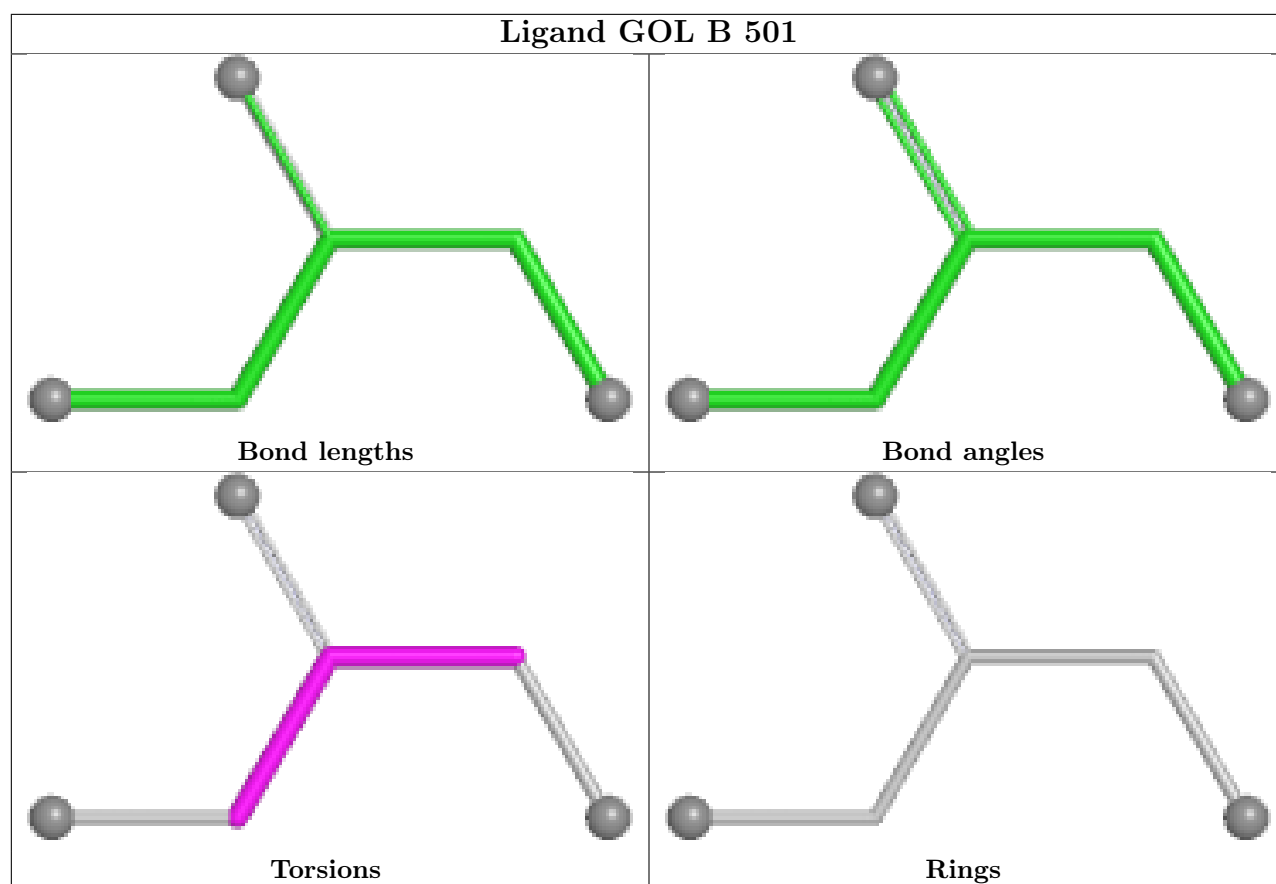
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	193/243 (79%)	0.33	12 (6%) 26 30	27, 47, 80, 103	0
1	B	206/243 (84%)	0.44	14 (6%) 23 26	30, 48, 75, 89	0
1	C	206/243 (84%)	0.76	30 (14%) 6 6	33, 54, 89, 116	0
1	D	187/243 (76%)	0.66	13 (6%) 22 25	31, 56, 81, 99	0
All	All	792/972 (81%)	0.55	69 (8%) 16 17	27, 51, 84, 116	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	PRO	7.0
1	D	268	ILE	6.8
1	B	264	PRO	6.6
1	A	327	ALA	5.5
1	C	442	ILE	5.4
1	B	231	PRO	5.1
1	D	438	PHE	4.4
1	C	330	LEU	4.3
1	B	439	PHE	4.2
1	C	328	THR	4.1
1	C	231	PRO	4.1
1	D	433	LEU	4.0
1	C	265	VAL	4.0
1	A	268	ILE	3.6
1	D	313	PHE	3.3
1	D	325	LEU	3.2
1	C	406	HIS	3.2
1	A	264	PRO	3.1
1	C	322	ASP	3.1
1	B	320	VAL	3.1
1	B	326	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	346	PHE	3.0
1	B	328	THR	3.0
1	A	458	PRO	2.9
1	B	319	ALA	2.9
1	C	340	ALA	2.9
1	C	337	ALA	2.8
1	D	326	LEU	2.8
1	A	330	LEU	2.8
1	D	439	PHE	2.7
1	C	334	ARG	2.7
1	C	324	ILE	2.7
1	B	442	ILE	2.6
1	C	445	THR	2.6
1	C	306	ASN	2.6
1	C	268	ILE	2.6
1	D	442	ILE	2.6
1	C	439	PHE	2.5
1	B	329	GLY	2.5
1	C	319	ALA	2.5
1	C	242	VAL	2.5
1	B	330	LEU	2.5
1	C	327	ALA	2.5
1	B	306	ASN	2.4
1	A	271	ALA	2.4
1	A	433	LEU	2.4
1	C	235	ILE	2.4
1	C	436	LEU	2.3
1	D	279	LEU	2.3
1	C	320	VAL	2.3
1	C	336	SER	2.2
1	A	438	PHE	2.2
1	B	268	ILE	2.2
1	A	387	ALA	2.2
1	C	232	VAL	2.2
1	D	309	LEU	2.2
1	C	329	GLY	2.2
1	B	241	ALA	2.2
1	A	294	LEU	2.2
1	C	441	LEU	2.1
1	A	452	MET	2.1
1	C	333	HIS	2.1
1	D	324	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	324	ILE	2.1
1	C	455	LEU	2.0
1	A	345	ILE	2.0
1	C	271	ALA	2.0
1	D	451	LEU	2.0
1	D	331	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

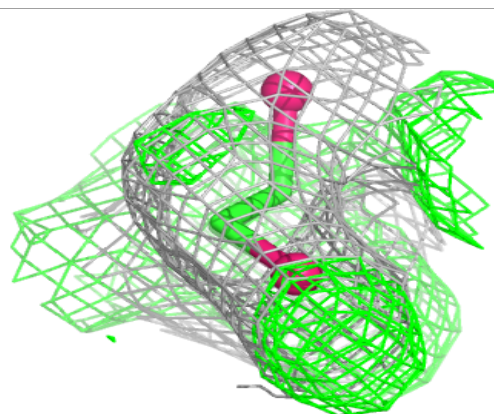
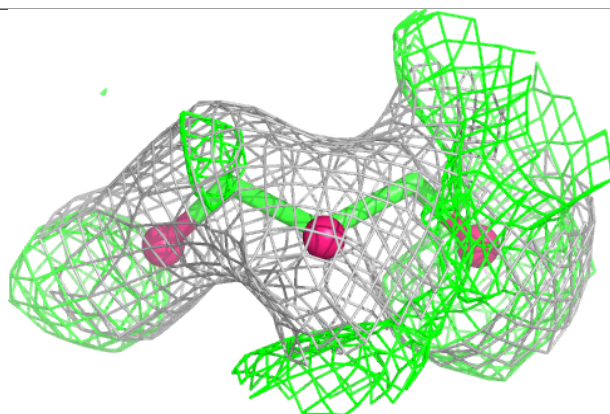
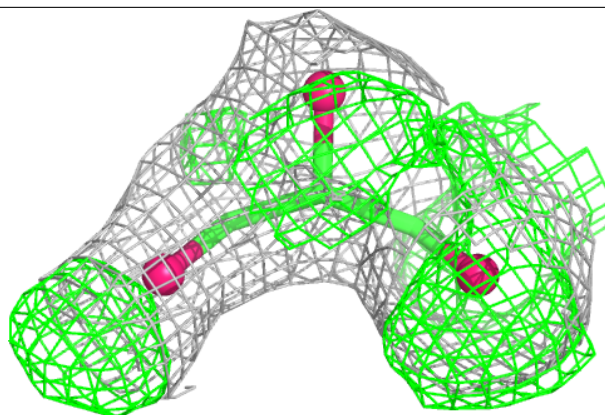
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	GOL	B	501	6/6	0.63	0.23	42,57,62,65	0
2	WZ6	A	500	36/36	0.77	0.26	87,115,167,172	0
3	GOL	C	501	6/6	0.83	0.13	48,55,57,62	0
2	WZ6	B	500	36/36	0.85	0.15	58,74,80,81	0
2	WZ6	C	500	36/36	0.89	0.12	45,55,65,74	0

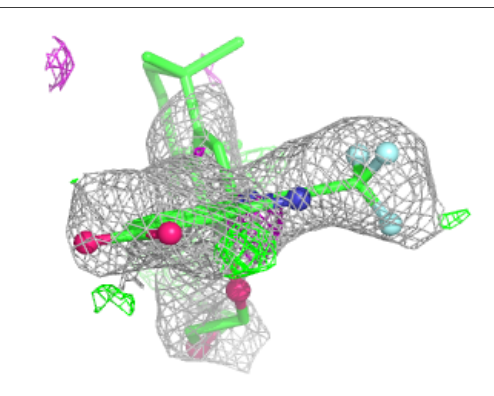
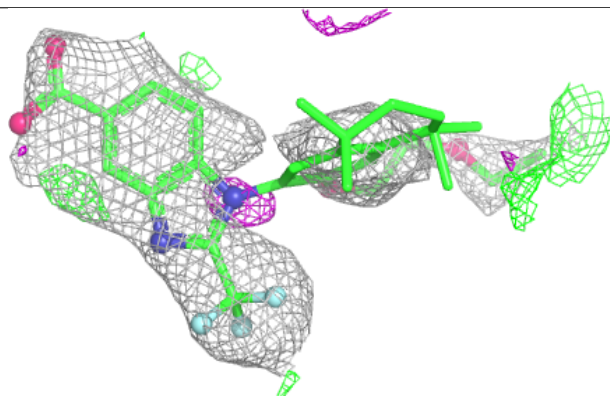
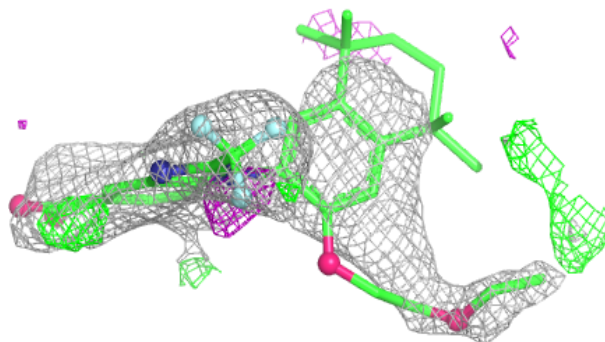
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GOL 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)

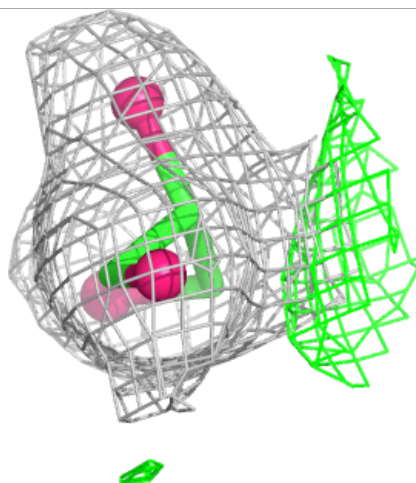
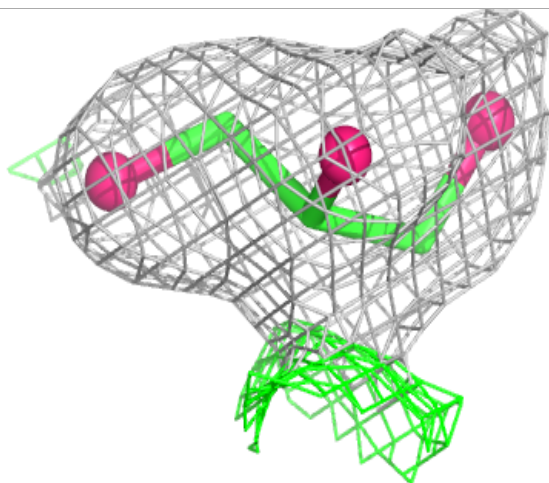
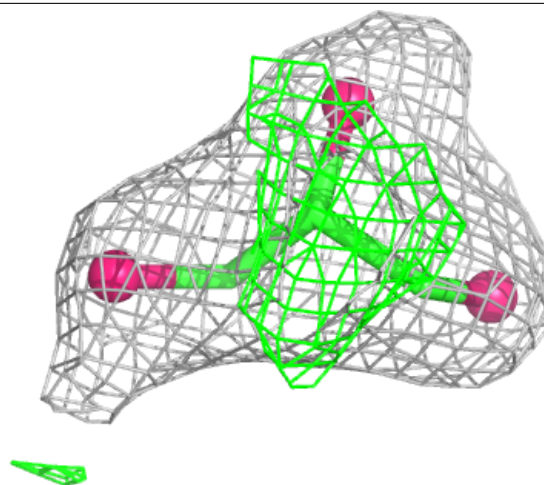
**Electron density around WZ6 A 500:**

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



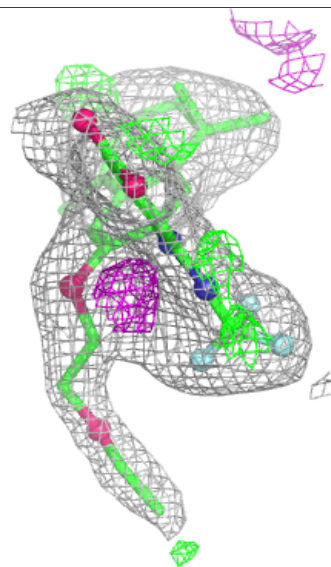
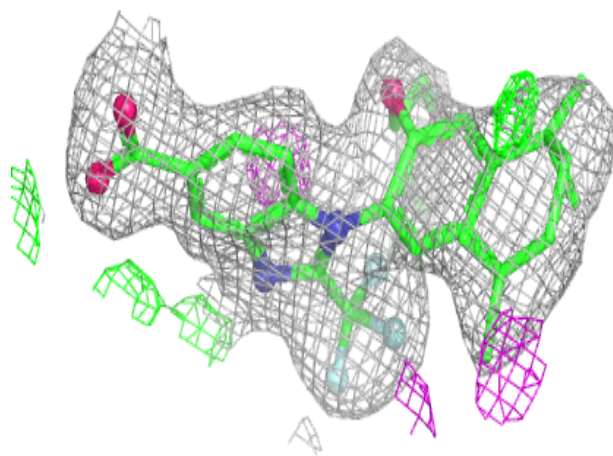
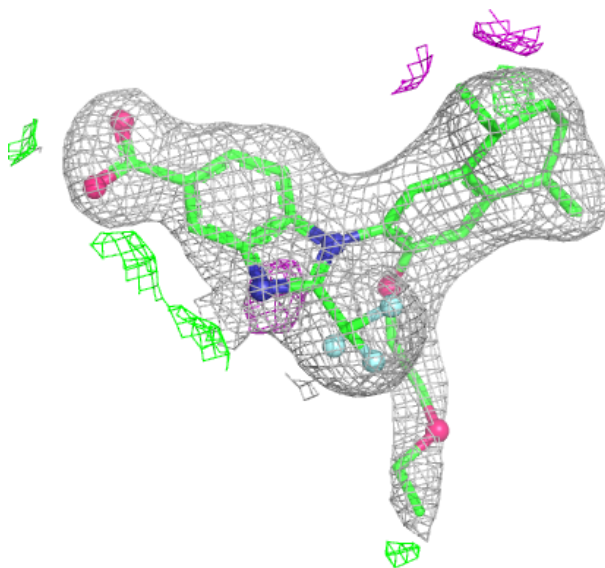
Electron density around GOL C 501:

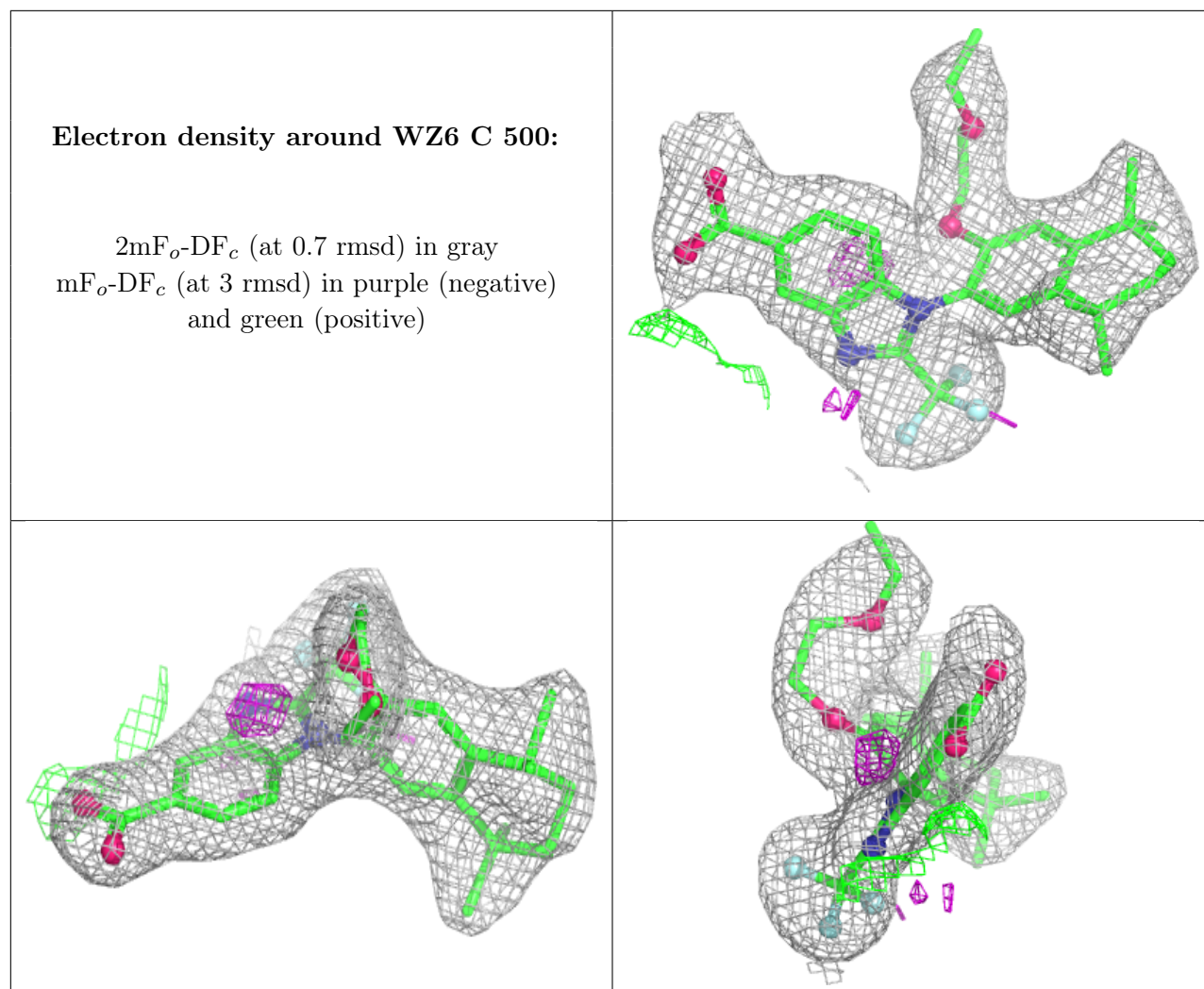
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around WZ6 B 500:

$2mF_o-DF_c$ (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.