



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 28, 2020 – 10:09 AM JST

PDB ID : 7CFO
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

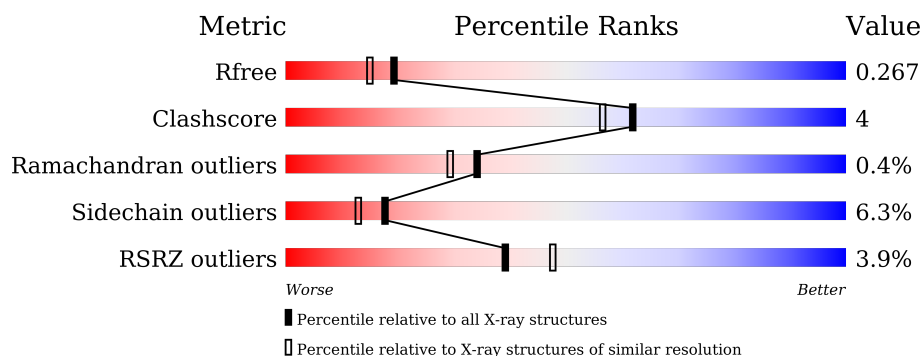
1 Overall quality at a glance

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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	<div> <div>0%</div> <div>71% 8% 21%</div> </div>
1	B	243	<div> <div>2%</div> <div>72% 9% 15%</div> </div>
1	C	243	<div> <div>7%</div> <div>71% 11% 15%</div> </div>
1	D	243	<div> <div>2%</div> <div>70% 7% 23%</div> </div>

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.

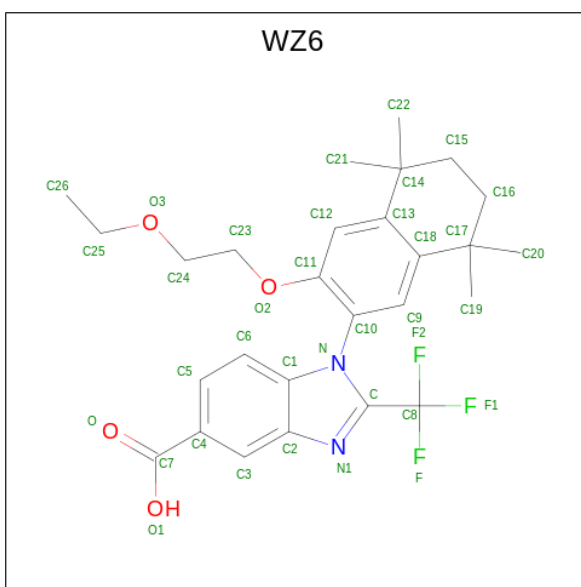
- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

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:

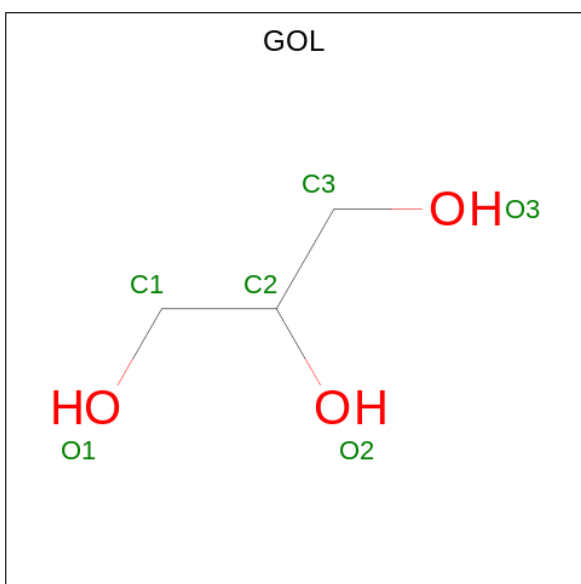
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	-	expression tag	UNP P19793
A	221	SER	-	expression tag	UNP P19793
A	222	SER	-	expression tag	UNP P19793
A	223	HIS	-	expression tag	UNP P19793
B	220	GLY	-	expression tag	UNP P19793
B	221	SER	-	expression tag	UNP P19793
B	222	SER	-	expression tag	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 (three-letter code: 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 (three-letter code: 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		

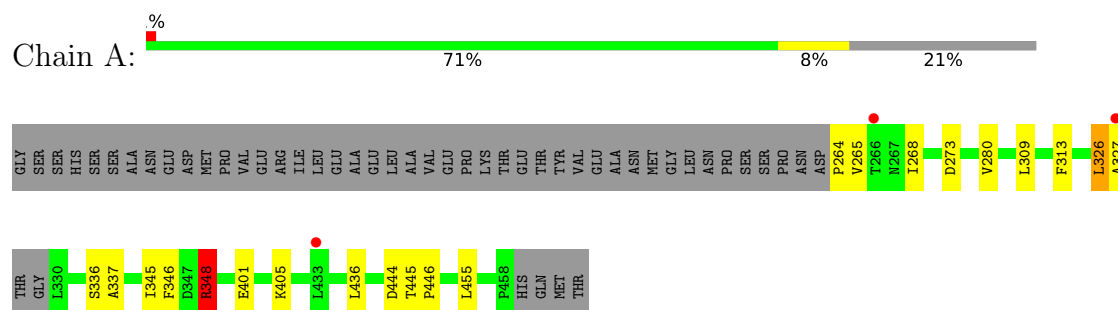
- Molecule 4 is water.

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		

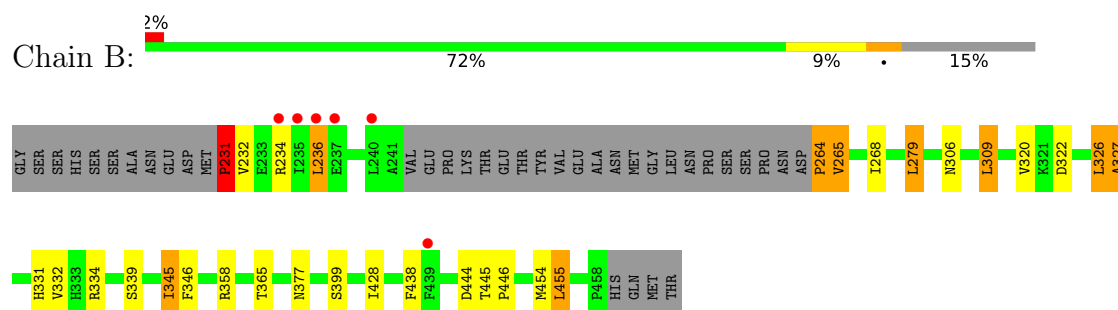
3 Residue-property plots [i](#)

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.

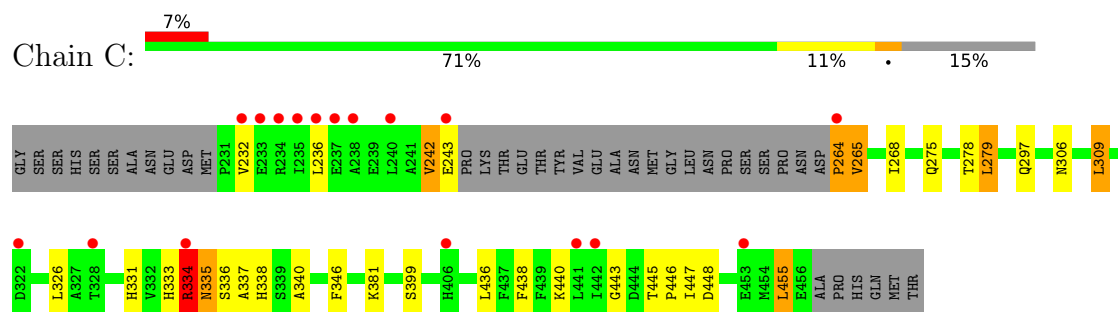
- Molecule 1: Retinoic acid receptor RXR-alpha



- Molecule 1: Retinoic acid receptor RXR-alpha

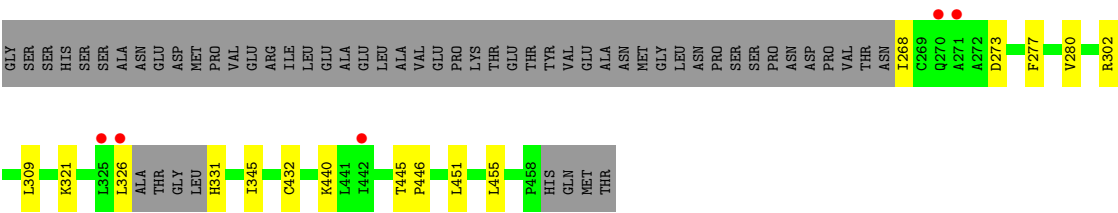


- Molecule 1: Retinoic acid receptor RXR-alpha



- 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 47.09 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.6 (47.14-2.15) 95.6 (47.09-2.15)	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 (5.05%)	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 , 32.3	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: WZ6, GOL

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	0.76	1/1560 (0.1%)	0.86	2/2107 (0.1%)
1	B	0.74	0/1658	0.90	1/2240 (0.0%)
1	C	0.72	0/1661	0.88	0/2243
1	D	0.74	0/1517	0.83	0/2047
All	All	0.74	1/6396 (0.0%)	0.87	3/8637 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	GLU	CD-OE2	-5.47	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	PRO	CA-N-CD	-8.99	98.91	111.50
1	A	348	ARG	CB-CG-CD	6.49	128.47	111.60
1	A	348	ARG	CG-CD-NE	6.17	124.75	111.80

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

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	20	0
1	C	1629	0	1674	27	0
1	D	1486	0	1524	8	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	56	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 (56) 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:C:334:ARG:HA	1:C:337:ALA:HB3	1.72	0.70
1:A:348:ARG:HH21	1:A:348:ARG:HG2	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
1:C:334:ARG:O	1:C:338:HIS:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:265:VAL:HG13	1:D:273:ASP:CG	2.32	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	0.49
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: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: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: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
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:B:454:MET:HE1	1:D:277:PHE:CD1	2.54	0.41
1:C:279:LEU:CD2	1:C:309:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:LYS:NZ	4:D:600:HOH:O	2.47	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%)	15	9
1	C	202/243 (83%)	194 (96%)	7 (4%)	1 (0%)	29	22
1	D	183/243 (75%)	180 (98%)	3 (2%)	0	100	100
All	All	776/972 (80%)	755 (97%)	18 (2%)	3 (0%)	34	29

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/209 (79%)	157 (95%)	9 (5%)	22	18
1	B	176/209 (84%)	164 (93%)	12 (7%)	16	10
1	C	177/209 (85%)	162 (92%)	15 (8%)	10	6
1	D	161/209 (77%)	154 (96%)	7 (4%)	29	27
All	All	680/836 (81%)	637 (94%)	43 (6%)	18	13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	VAL
1	A	309	LEU
1	A	313	PHE
1	A	326	LEU
1	A	336	SER
1	A	345	ILE
1	A	348	ARG
1	A	405	LYS
1	A	444	ASP
1	B	231	PRO
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	326	LEU
1	B	339	SER
1	B	345	ILE
1	B	455	LEU
1	C	236	LEU
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	326	LEU
1	C	333	HIS

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Mol	Chain	Res	Type
1	C	334	ARG
1	C	335	ASN
1	C	336	SER
1	C	346	PHE
1	C	381	LYS
1	C	455	LEU
1	D	268	ILE
1	D	309	LEU
1	D	321	LYS
1	D	326	LEU
1	D	331	HIS
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	335	ASN
1	B	331	HIS
1	C	335	ASN
1	D	335	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 monosaccharides 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	A	500	-	36,39,39	2.13	9 (25%)	48,61,61	3.95	22 (45%)
3	GOL	B	501	-	5,5,5	0.51	0	5,5,5	0.80	0
2	WZ6	C	500	-	36,39,39	2.39	10 (27%)	48,61,61	2.70	19 (39%)
2	WZ6	B	500	-	36,39,39	2.20	5 (13%)	48,61,61	4.80	30 (62%)
3	GOL	C	501	-	5,5,5	0.13	0	5,5,5	0.14	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	A	500	-	-	7/16/39/39	0/4/4/4
3	GOL	B	501	-	-	4/4/4/4	-
2	WZ6	C	500	-	-	2/16/39/39	0/4/4/4
2	WZ6	B	500	-	-	6/16/39/39	0/4/4/4
3	GOL	C	501	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	WZ6	C10-N	-10.28	1.33	1.45
2	B	500	WZ6	C10-N	-7.94	1.36	1.45
2	A	500	WZ6	C10-N	-7.43	1.37	1.45
2	B	500	WZ6	C1-C2	5.72	1.52	1.40
2	A	500	WZ6	C1-C2	4.71	1.50	1.40
2	B	500	WZ6	C4-C7	4.52	1.51	1.47
2	A	500	WZ6	C18-C13	4.47	1.48	1.40
2	C	500	WZ6	C1-C2	4.09	1.48	1.40
2	B	500	WZ6	C18-C13	3.87	1.47	1.40
2	C	500	WZ6	C4-C7	3.70	1.51	1.47
2	A	500	WZ6	C1-N	-3.64	1.34	1.39
2	C	500	WZ6	C18-C13	3.62	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	WZ6	C1-N	-3.59	1.34	1.39
2	B	500	WZ6	C1-N	-3.39	1.34	1.39
2	A	500	WZ6	C8-C	3.38	1.54	1.51
2	C	500	WZ6	C8-C	3.15	1.54	1.51
2	A	500	WZ6	C3-C2	-2.85	1.37	1.41
2	A	500	WZ6	C12-C13	-2.80	1.35	1.39
2	A	500	WZ6	C17-C18	-2.77	1.49	1.53
2	A	500	WZ6	C14-C13	-2.46	1.50	1.53
2	C	500	WZ6	C14-C13	-2.28	1.50	1.53
2	C	500	WZ6	C9-C10	2.19	1.42	1.38
2	C	500	WZ6	C6-C5	2.18	1.41	1.36
2	C	500	WZ6	C-N	-2.07	1.34	1.37

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	WZ6	C20-C17-C18	-13.68	86.56	110.10
2	A	500	WZ6	C22-C14-C13	-12.49	88.61	110.10
2	A	500	WZ6	O2-C11-C10	11.50	129.64	118.17
2	B	500	WZ6	C22-C14-C13	-10.61	91.84	110.10
2	B	500	WZ6	C22-C14-C21	-9.88	86.50	108.67
2	A	500	WZ6	C22-C14-C21	-9.87	86.53	108.67
2	B	500	WZ6	F-C8-C	9.71	121.75	111.32
2	B	500	WZ6	C16-C17-C18	7.77	122.69	110.16
2	A	500	WZ6	C21-C14-C13	7.75	123.43	110.10
2	B	500	WZ6	F2-C8-C	-7.15	103.64	111.32
2	B	500	WZ6	C21-C14-C13	7.06	122.25	110.10
2	C	500	WZ6	C22-C14-C21	-6.62	93.82	108.67
2	B	500	WZ6	C8-C-N1	-6.54	116.03	122.41
2	A	500	WZ6	C9-C10-C11	-6.45	113.98	121.21
2	B	500	WZ6	C19-C17-C20	-6.42	94.28	108.67
2	B	500	WZ6	C17-C18-C13	-6.37	115.83	122.70
2	A	500	WZ6	C8-C-N1	-6.33	116.23	122.41
2	B	500	WZ6	C9-C10-C11	-6.24	114.21	121.21
2	C	500	WZ6	C22-C14-C13	-6.18	99.47	110.10
2	C	500	WZ6	C14-C13-C18	-6.15	116.07	122.70
2	A	500	WZ6	O2-C11-C12	-6.06	109.66	123.58
2	B	500	WZ6	C19-C17-C18	5.88	120.22	110.10
2	B	500	WZ6	F1-C8-C	5.55	117.28	111.32
2	C	500	WZ6	C22-C14-C15	-5.21	88.31	109.20
2	B	500	WZ6	C20-C17-C16	-5.04	88.97	109.20
2	A	500	WZ6	C3-C4-C7	-4.85	113.98	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	WZ6	F-C8-C	-4.79	106.18	111.32
2	C	500	WZ6	C15-C14-C13	4.69	117.73	110.16
2	A	500	WZ6	C22-C14-C15	-4.49	91.20	109.20
2	B	500	WZ6	C15-C14-C13	4.48	117.38	110.16
2	B	500	WZ6	C10-N-C	4.36	131.17	124.60
2	B	500	WZ6	F1-C8-F2	-4.33	89.82	105.72
2	B	500	WZ6	O2-C11-C10	4.33	122.49	118.17
2	A	500	WZ6	C5-C4-C3	4.27	124.78	118.09
2	C	500	WZ6	C3-C2-C1	-4.23	116.76	121.10
2	C	500	WZ6	C21-C14-C15	3.94	124.99	109.20
2	A	500	WZ6	C10-N-C	3.93	130.53	124.60
2	A	500	WZ6	F1-C8-C	3.86	115.46	111.32
2	C	500	WZ6	C16-C17-C18	3.78	116.26	110.16
2	B	500	WZ6	O2-C11-C12	-3.57	115.37	123.58
2	B	500	WZ6	O2-C23-C24	3.54	120.69	108.72
2	C	500	WZ6	C9-C10-C11	-3.52	117.26	121.21
2	B	500	WZ6	C12-C11-C10	3.48	121.99	118.46
2	A	500	WZ6	C4-C3-C2	-3.47	118.40	121.44
2	C	500	WZ6	C21-C14-C13	3.45	116.04	110.10
2	B	500	WZ6	C3-C2-C1	-3.27	117.76	121.10
2	B	500	WZ6	F1-C8-F	3.17	117.33	105.72
2	A	500	WZ6	C3-C2-C1	-3.14	117.88	121.10
2	C	500	WZ6	C17-C18-C13	-3.13	119.33	122.70
2	A	500	WZ6	C21-C14-C15	3.08	121.56	109.20
2	C	500	WZ6	C16-C15-C14	-2.97	102.68	113.97
2	C	500	WZ6	C19-C17-C18	-2.95	105.03	110.10
2	A	500	WZ6	C15-C14-C13	2.91	114.85	110.16
2	B	500	WZ6	C22-C14-C15	-2.90	97.57	109.20
2	B	500	WZ6	C5-C4-C3	2.87	122.58	118.09
2	B	500	WZ6	F-C8-F2	-2.86	95.22	105.72
2	C	500	WZ6	F2-C8-C	2.81	114.34	111.32
2	A	500	WZ6	C25-O3-C24	2.71	122.61	112.90
2	B	500	WZ6	C21-C14-C15	2.71	120.06	109.20
2	A	500	WZ6	O2-C23-C24	2.44	116.98	108.72
2	B	500	WZ6	C4-C3-C2	-2.42	119.32	121.44
2	B	500	WZ6	C3-C4-C7	-2.37	117.24	120.36
2	A	500	WZ6	F2-C8-C	-2.32	108.83	111.32
2	A	500	WZ6	F-C8-C	2.29	113.78	111.32
2	C	500	WZ6	C5-C4-C3	2.27	121.65	118.09
2	A	500	WZ6	C23-O2-C11	2.22	123.12	117.69
2	A	500	WZ6	C12-C11-C10	2.21	120.71	118.46
2	B	500	WZ6	C9-C18-C17	2.19	125.06	119.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	WZ6	C10-N-C	2.18	127.89	124.60
2	C	500	WZ6	C19-C17-C20	2.13	113.44	108.67
2	C	500	WZ6	C12-C13-C14	2.01	124.60	119.39

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	WZ6	N-C-C8-F2
2	A	500	WZ6	N-C-C8-F
2	A	500	WZ6	N-C-C8-F1
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
2	B	500	WZ6	N-C-C8-F2
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	O2-C23-C24-O3
2	B	500	WZ6	C10-C11-O2-C23
2	C	500	WZ6	O2-C23-C24-O3
2	B	500	WZ6	N-C-C8-F
2	B	500	WZ6	C24-C23-O2-C11
2	B	500	WZ6	C12-C11-O2-C23
2	A	500	WZ6	C26-C25-O3-C24
2	C	500	WZ6	C26-C25-O3-C24
2	A	500	WZ6	O2-C23-C24-O3
2	A	500	WZ6	C24-C23-O2-C11

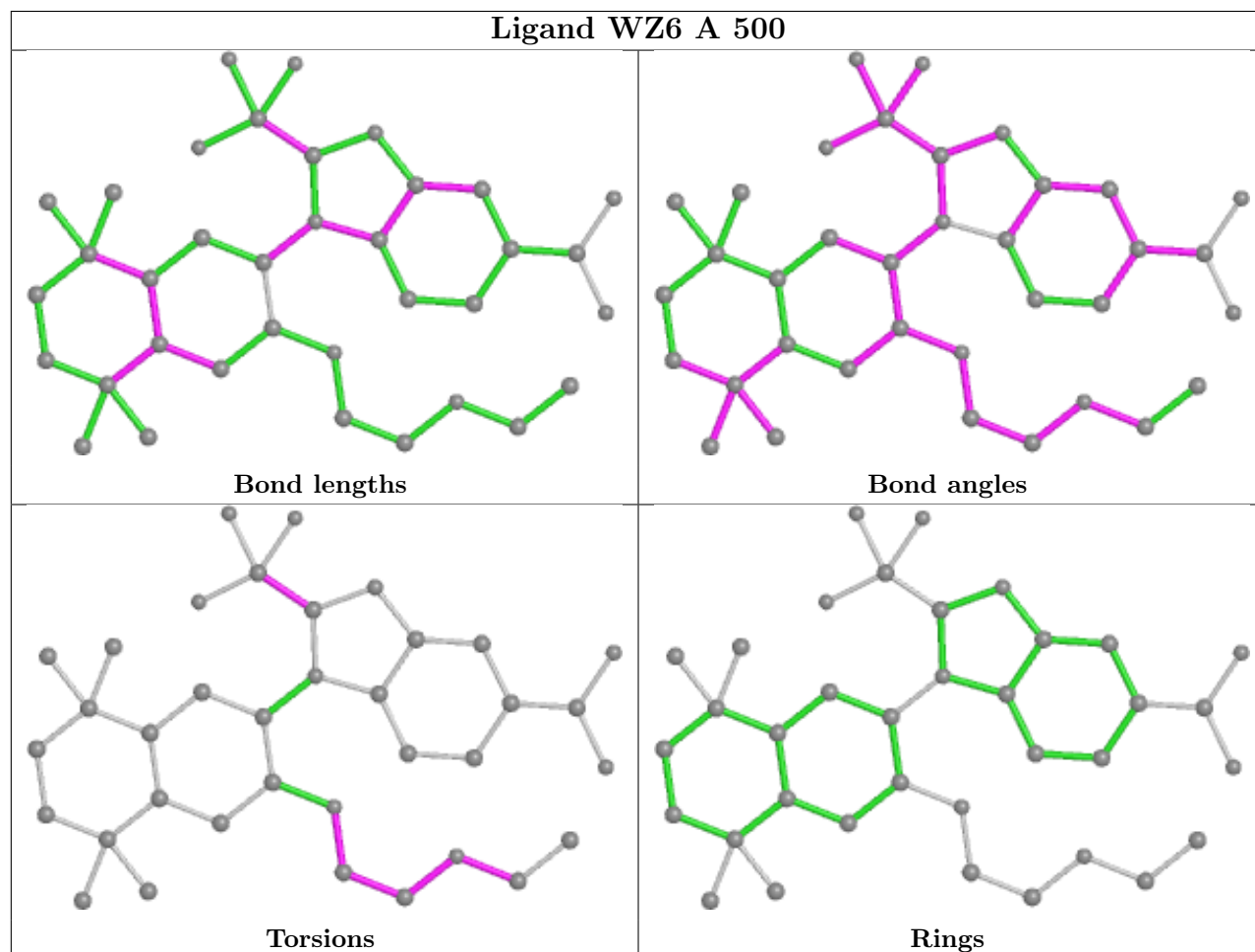
There are no ring outliers.

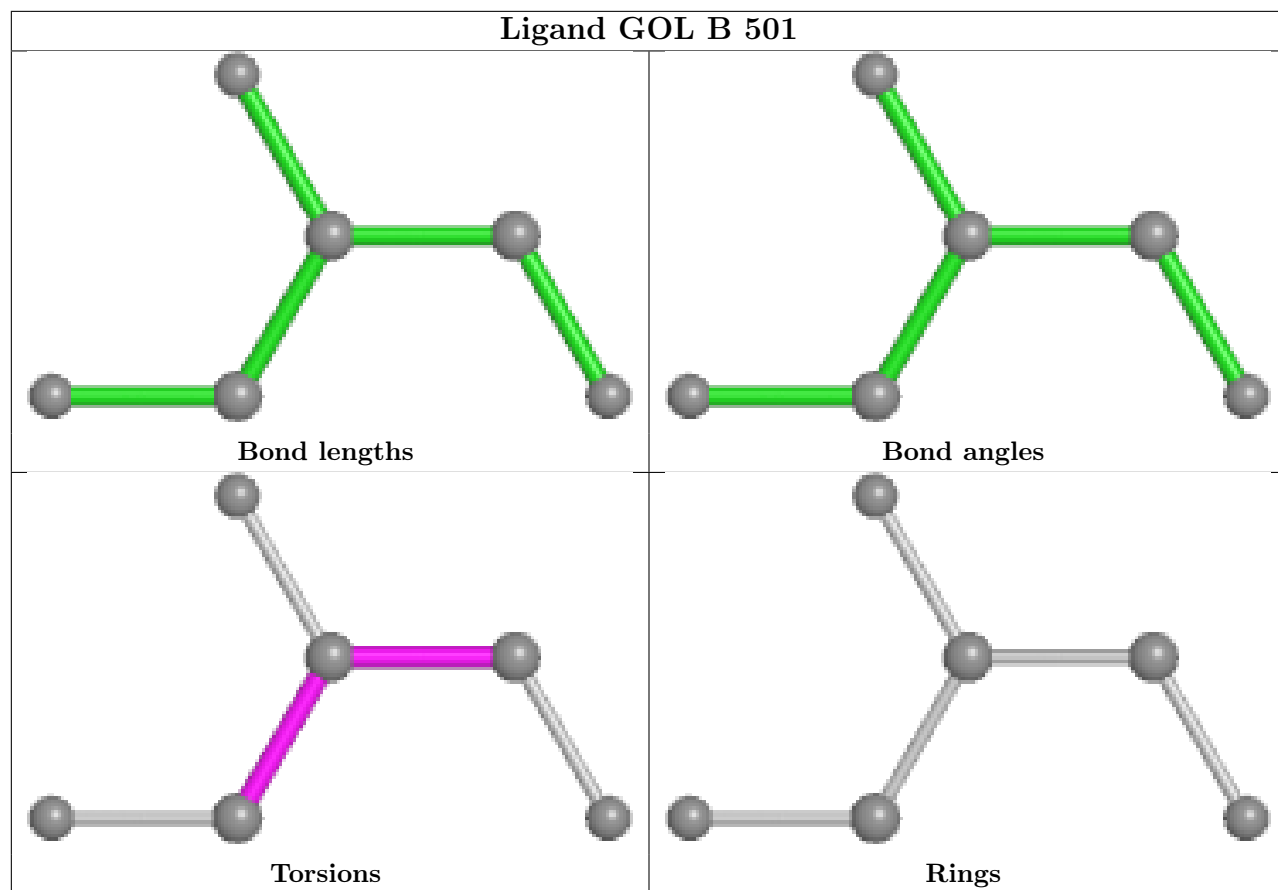
2 monomers are involved in 3 short contacts:

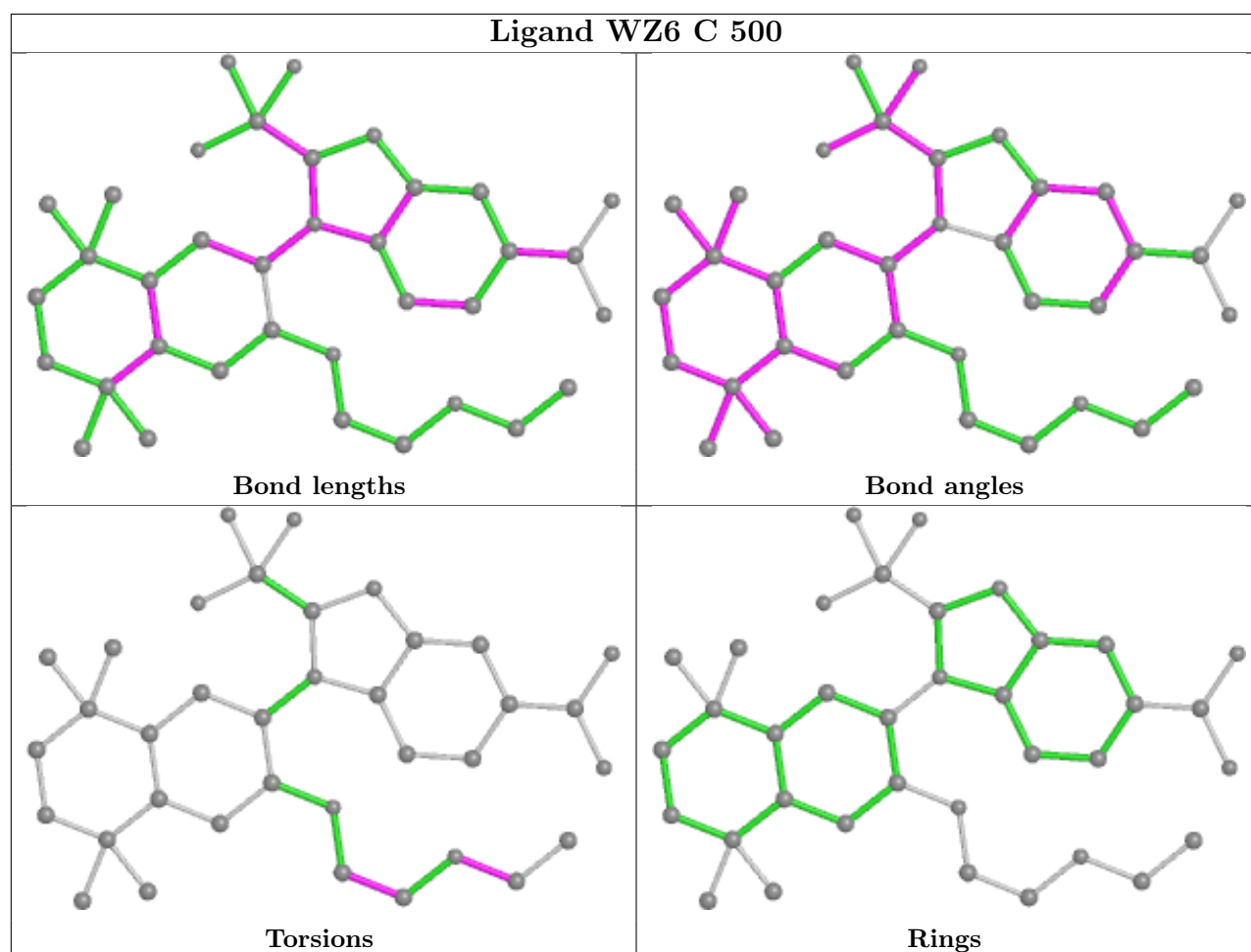
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	WZ6	1	0
3	B	501	GOL	2	0

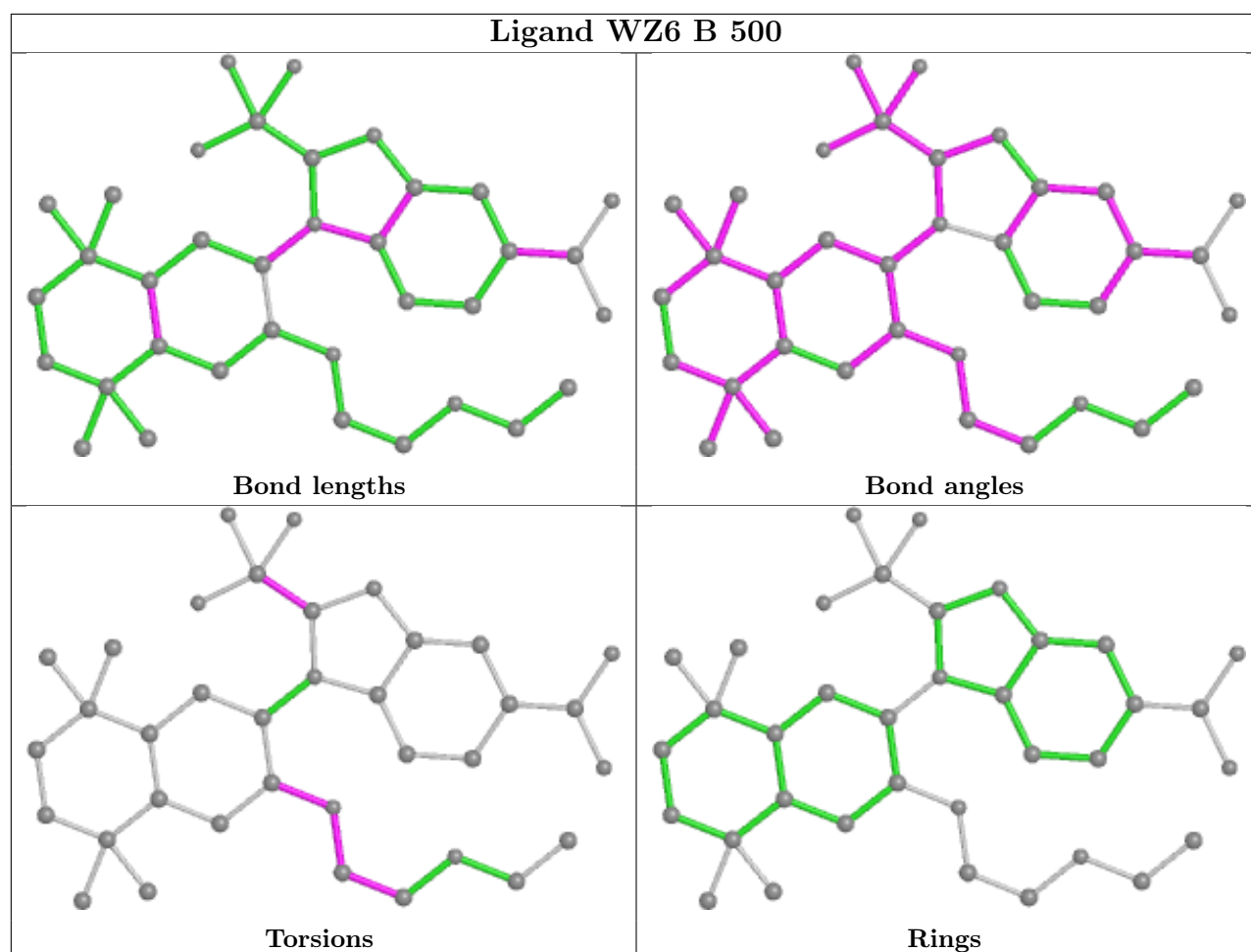
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

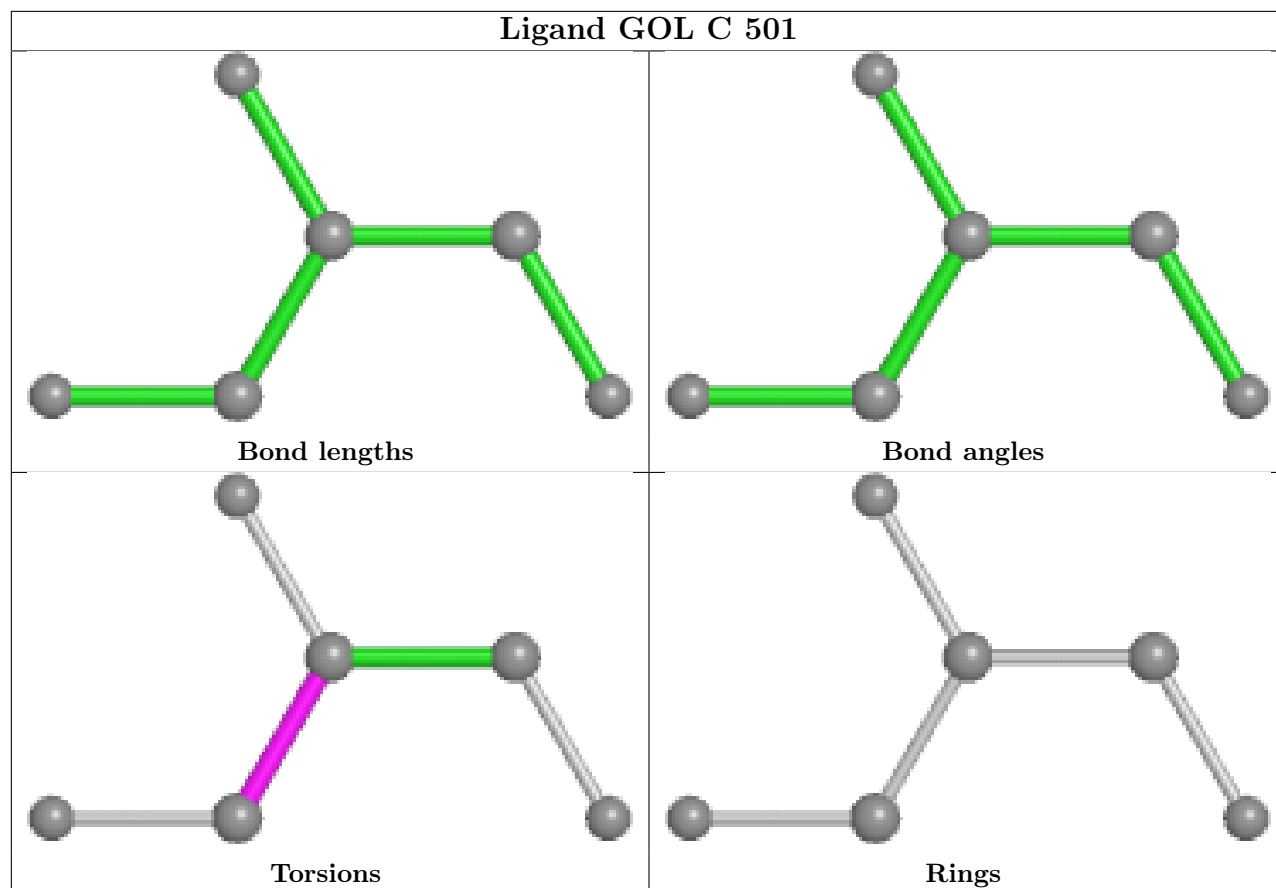
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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%)	0.09	3 (1%) 72 77	27, 47, 80, 103	0
1	B	206/243 (84%)	0.25	6 (2%) 51 61	30, 48, 75, 89	0
1	C	206/243 (84%)	0.46	17 (8%) 11 15	33, 54, 89, 116	0
1	D	187/243 (76%)	0.15	5 (2%) 54 63	31, 56, 81, 99	0
All	All	792/972 (81%)	0.24	31 (3%) 39 48	27, 51, 84, 116	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	442	ILE	6.4
1	A	327	ALA	4.6
1	C	237	GLU	4.3
1	B	234	ARG	4.3
1	C	233	GLU	4.1
1	D	270	GLN	3.7
1	C	328	THR	3.7
1	C	235	ILE	3.7
1	C	232	VAL	3.7
1	C	238	ALA	3.7
1	B	439	PHE	3.6
1	C	236	LEU	3.5
1	C	240	LEU	3.5
1	D	325	LEU	3.4
1	C	453	GLU	3.2
1	C	322	ASP	3.2
1	A	433	LEU	2.7
1	C	234	ARG	2.6
1	C	406	HIS	2.5
1	B	235	ILE	2.4
1	B	236	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	271	ALA	2.2
1	C	441	LEU	2.2
1	B	240	LEU	2.2
1	C	264	PRO	2.2
1	D	326	LEU	2.2
1	C	243	GLU	2.2
1	B	237	GLU	2.1
1	A	266	THR	2.0
1	C	334	ARG	2.0
1	D	442	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

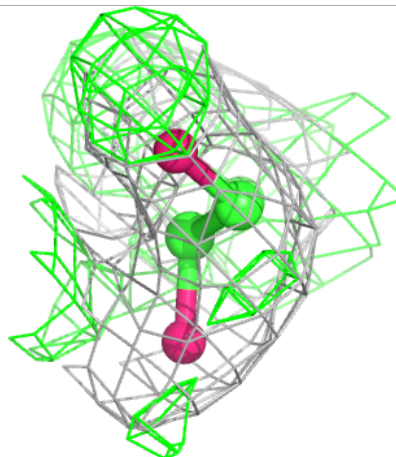
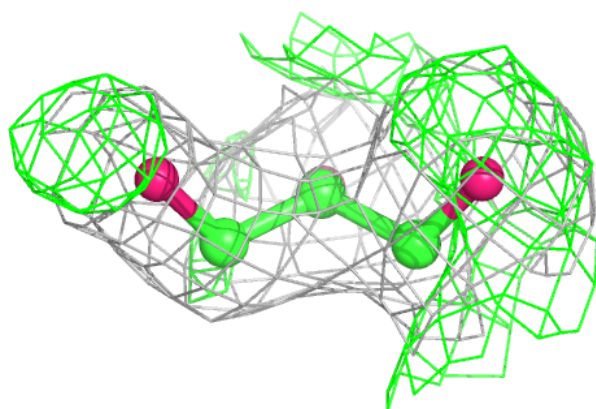
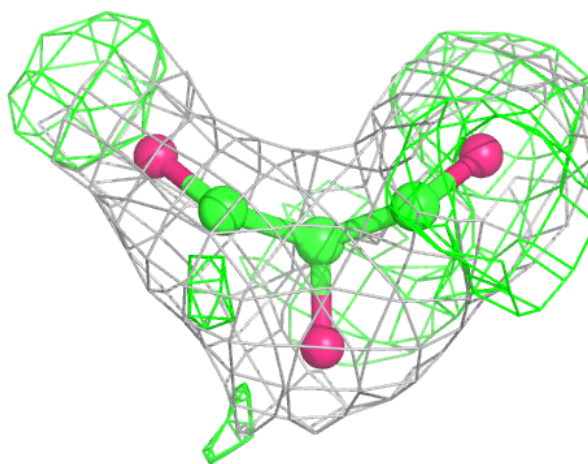
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	501	6/6	0.55	0.28	42,57,62,65	0
2	WZ6	A	500	36/36	0.74	0.31	87,115,167,172	0
3	GOL	C	501	6/6	0.88	0.14	48,55,57,62	0
2	WZ6	B	500	36/36	0.90	0.14	58,74,80,81	0
2	WZ6	C	500	36/36	0.93	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.

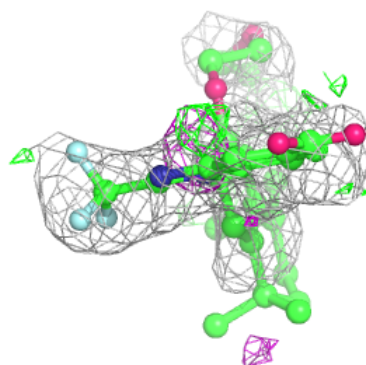
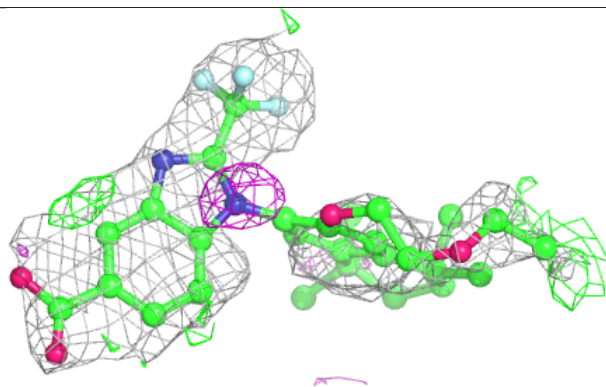
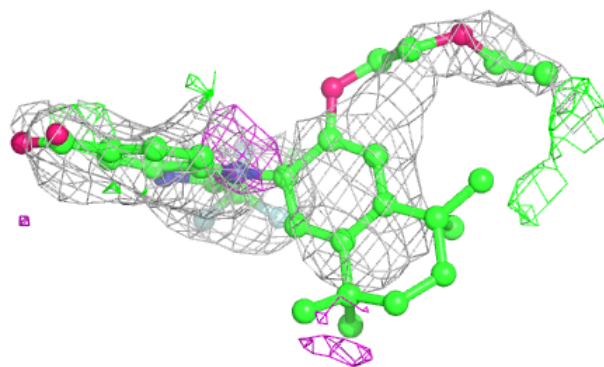
Electron density around GOL B 501:

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



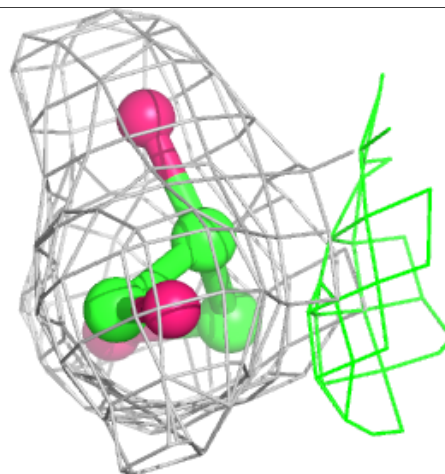
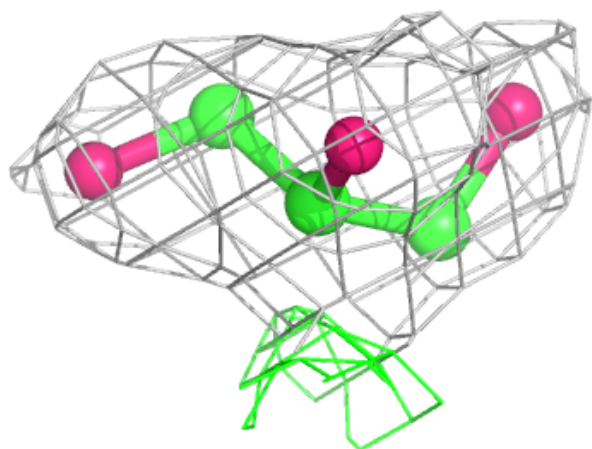
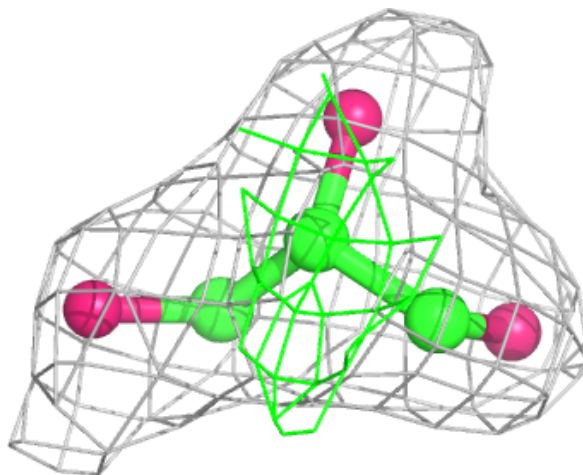
Electron density around WZ6 A 500:

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



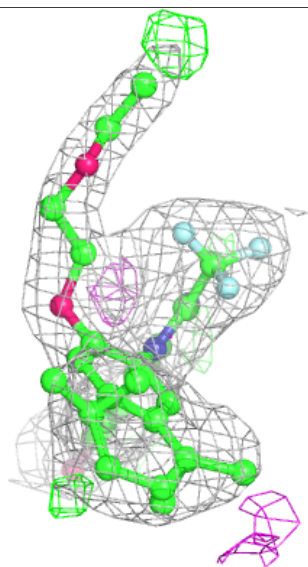
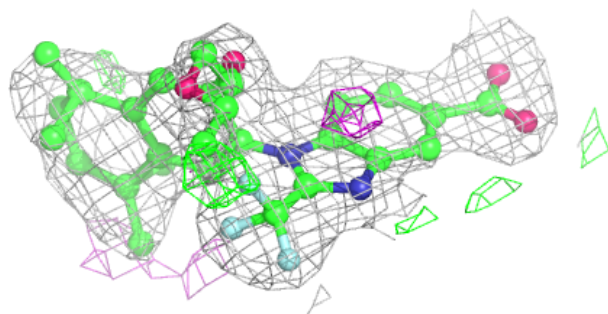
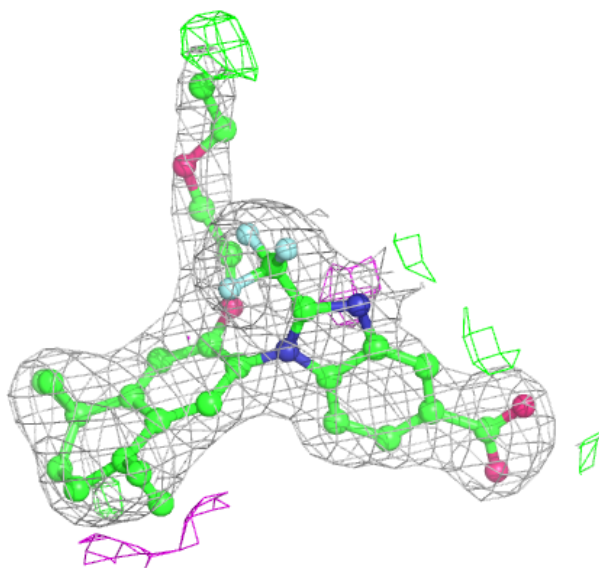
Electron density around GOL C 501:

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



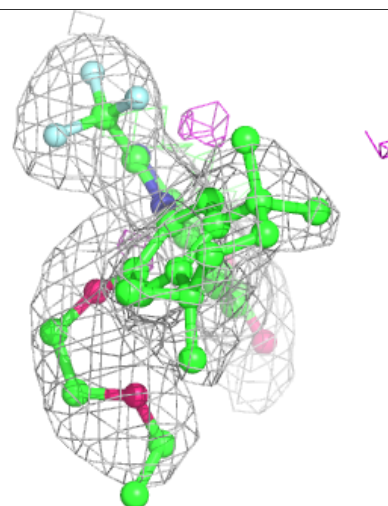
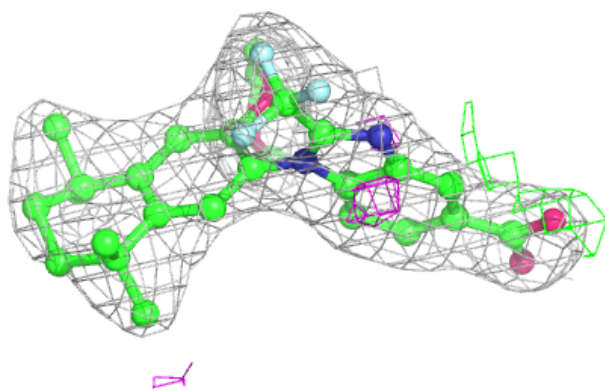
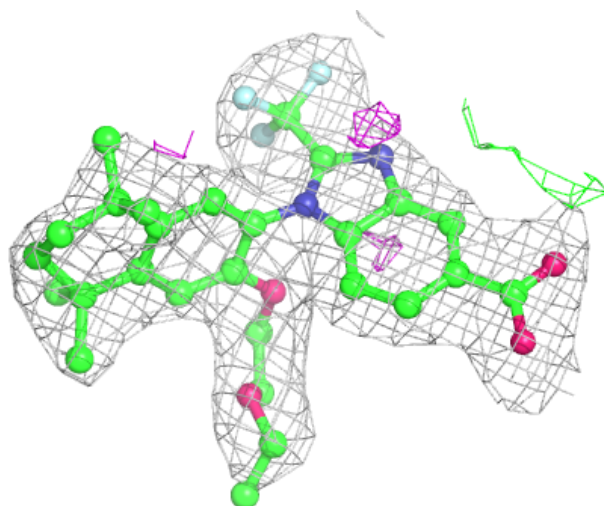
Electron density around WZ6 B 500:

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



Electron density around WZ6 C 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.