



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 08:41 am BST

PDB ID : 1PQ6  
Title : HUMAN LXR BETA HORMONE RECEPTOR / GW3965 COMPLEX  
Authors : Farnegardh, M.; Bonn, T.; Sun, S.; Ljunggren, J.; Ahola, H.; Wilhelmsson, A.; Gustafsson, J.-A.; Carlquist, M.  
Deposited on : 2003-06-18  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

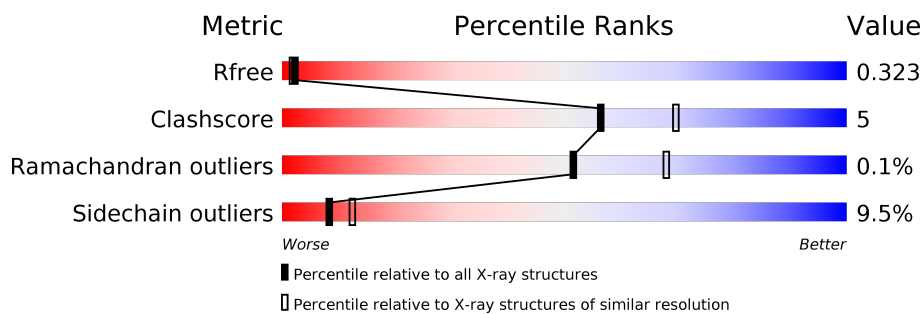
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	253	
1	B	253	
1	C	253	
1	D	253	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7673 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.

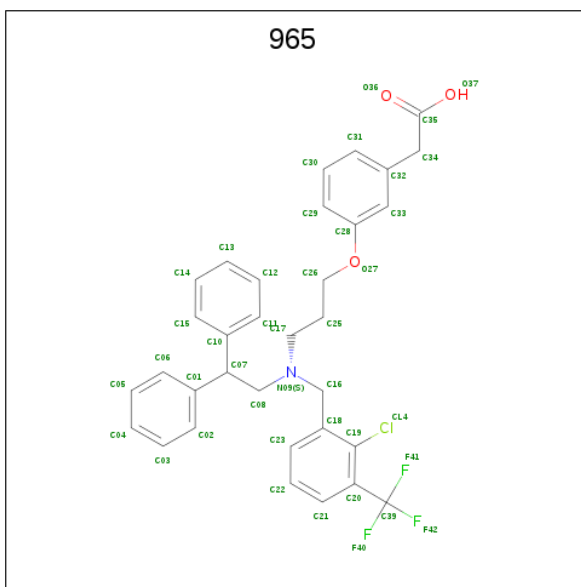
- Molecule 1 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1879	1203	330	339	7			
1	B	241	Total	C	N	O	S	0	0	0
			1950	1246	341	356	7			
1	C	208	Total	C	N	O	S	0	0	0
			1698	1082	300	309	7			
1	D	227	Total	C	N	O	S	0	0	0
			1848	1188	323	330	7			

There are 16 discrepancies between the modelled and reference sequences:

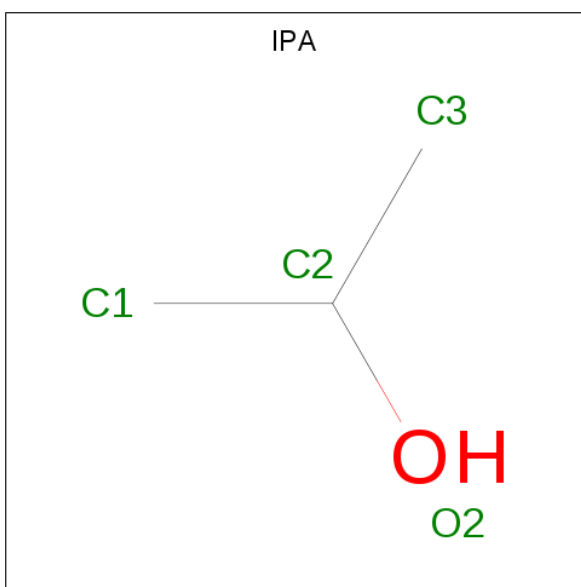
Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	CLONING ARTIFACT	UNP P55055
A	210	SER	-	CLONING ARTIFACT	UNP P55055
A	211	HIS	-	CLONING ARTIFACT	UNP P55055
A	212	MET	-	CLONING ARTIFACT	UNP P55055
B	209	GLY	-	CLONING ARTIFACT	UNP P55055
B	210	SER	-	CLONING ARTIFACT	UNP P55055
B	211	HIS	-	CLONING ARTIFACT	UNP P55055
B	212	MET	-	CLONING ARTIFACT	UNP P55055
C	209	GLY	-	CLONING ARTIFACT	UNP P55055
C	210	SER	-	CLONING ARTIFACT	UNP P55055
C	211	HIS	-	CLONING ARTIFACT	UNP P55055
C	212	MET	-	CLONING ARTIFACT	UNP P55055
D	209	GLY	-	CLONING ARTIFACT	UNP P55055
D	210	SER	-	CLONING ARTIFACT	UNP P55055
D	211	HIS	-	CLONING ARTIFACT	UNP P55055
D	212	MET	-	CLONING ARTIFACT	UNP P55055

- Molecule 2 is [3-(3-{[2-chloro-3-(trifluoromethyl)benzyl](2,2-diphenylethyl)amino}propoxy)phenyl]acetic acid (three-letter code: 965) (formula: C<sub>33</sub>H<sub>31</sub>ClF<sub>3</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 41	C 33	Cl 1	F 3	N 1	O 3	0	0
2	B	1	Total 41	C 33	Cl 1	F 3	N 1	O 3	0	0
2	D	1	Total 41	C 33	Cl 1	F 3	N 1	O 3	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $\text{C}_3\text{H}_8\text{O}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	3	1		

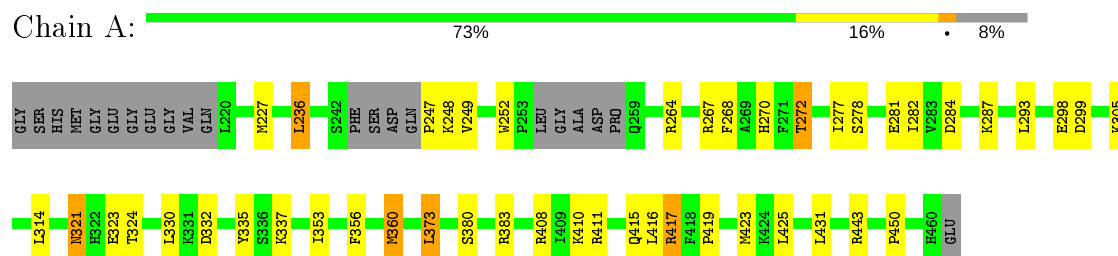
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	69	Total	O	0	0
			69	69		
4	C	19	Total	O	0	0
			19	19		
4	D	28	Total	O	0	0
			28	28		

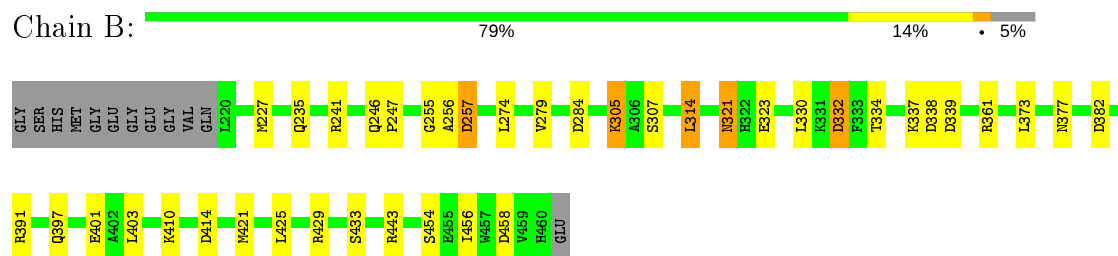
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

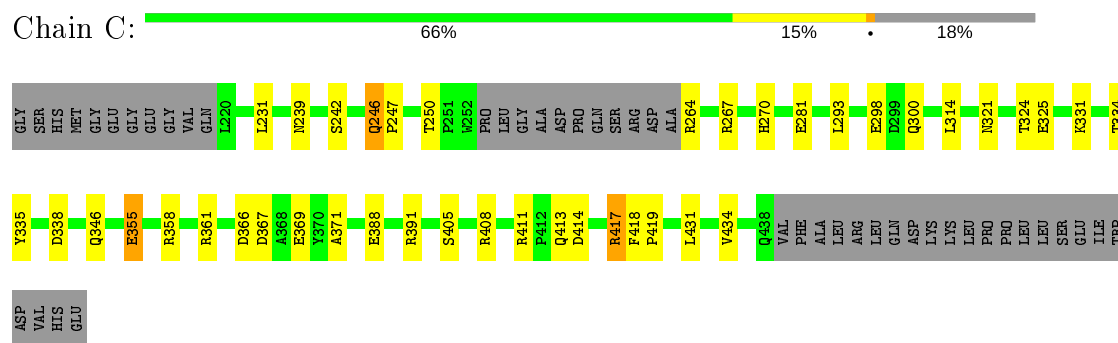
#### • Molecule 1: Oxysterols receptor LXR-beta



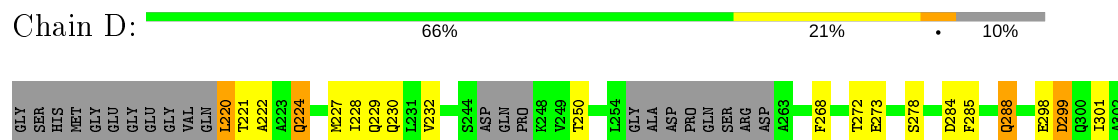
#### • Molecule 1: Oxysterols receptor LXR-beta

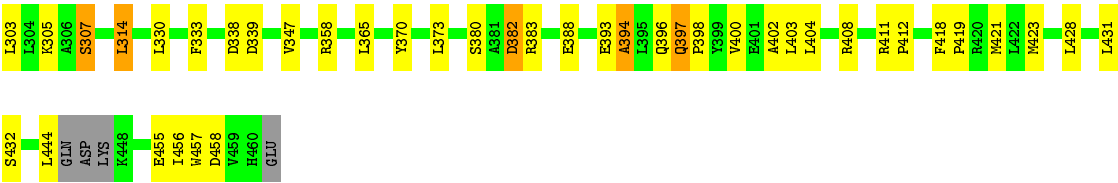


#### • Molecule 1: Oxysterols receptor LXR-beta



#### • Molecule 1: Oxysterols receptor LXR-beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.72Å 98.93Å 175.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.40 55.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (87.71-2.40) 98.4 (55.69-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.18 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.207 , 0.262 0.282 , 0.323	Depositor DCC
$R_{free}$ test set	2021 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 965, IPA

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	0.68	1/1914 (0.1%)	0.81	2/2587 (0.1%)
1	B	0.64	0/1989	0.85	9/2693 (0.3%)
1	C	0.56	1/1729 (0.1%)	0.75	4/2334 (0.2%)
1	D	0.89	6/1882 (0.3%)	0.92	7/2542 (0.3%)
All	All	0.71	8/7514 (0.1%)	0.84	22/10156 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	299	ASP	CG-OD2	21.94	1.75	1.25
1	D	299	ASP	CG-OD1	9.55	1.47	1.25
1	D	222	ALA	C-O	8.32	1.39	1.23
1	D	229	GLN	C-O	6.54	1.35	1.23
1	D	299	ASP	CB-CG	6.44	1.65	1.51
1	D	394	ALA	C-O	5.96	1.34	1.23
1	A	360	MET	SD-CE	-5.65	1.46	1.77
1	C	325	GLU	C-O	5.04	1.32	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	299	ASP	CB-CG-OD1	-21.07	99.34	118.30
1	D	299	ASP	CB-CG-OD2	12.24	129.32	118.30
1	D	358	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	A	284	ASP	CB-CG-OD2	8.24	125.71	118.30
1	D	358	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	339	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	391	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	C	366	ASP	CB-CG-OD2	6.19	123.88	118.30
1	D	284	ASP	CB-CG-OD2	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	LEU	CA-CB-CG	5.62	128.21	115.30
1	B	382	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	284	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	332	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	367	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	382	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	414	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	338	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	299	ASP	CB-CG-OD2	5.15	122.93	118.30
1	D	339	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	414	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	458	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	338	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1879	0	1902	21	0
1	B	1950	0	1968	20	0
1	C	1698	0	1716	11	0
1	D	1848	0	1883	24	0
2	A	41	0	30	1	0
2	B	41	0	30	1	0
2	D	41	0	30	1	0
3	A	4	0	8	2	0
3	B	4	0	8	0	0
4	A	51	0	0	0	0
4	B	69	0	0	1	0
4	C	19	0	0	0	0
4	D	28	0	0	0	0
All	All	7673	0	7575	76	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 (76) 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:D:299:ASP:OD2	1:D:299:ASP:CG	1.75	1.25
1:C:242:SER:OG	1:C:281:GLU:OE2	1.97	0.82
1:A:415:GLN:NE2	1:B:401:GLU:OE1	2.20	0.73
1:A:356:PHE:CZ	1:A:360:MET:CE	2.72	0.73
1:D:303:LEU:O	1:D:307:SER:HB2	1.95	0.67
1:A:419:PRO:O	1:A:423:MET:HG2	1.94	0.65
1:A:270:HIS:NE2	1:A:335:TYR:OH	2.25	0.65
1:B:321:ASN:C	1:B:321:ASN:HD22	2.04	0.61
1:A:356:PHE:CZ	1:A:360:MET:HE2	2.37	0.59
1:B:403:LEU:HD21	1:B:421:MET:HE2	1.82	0.59
1:D:228:ILE:O	1:D:232:VAL:HG23	2.02	0.58
1:D:419:PRO:O	1:D:423:MET:HG2	2.03	0.58
1:B:279:VAL:HG11	1:B:456:ILE:HD11	1.85	0.58
1:A:278:SER:HB2	2:A:1500:965:C32	2.35	0.57
1:A:321:ASN:HD22	1:A:324:THR:H	1.53	0.56
1:C:369:GLU:OE1	1:C:417:ARG:NH2	2.38	0.56
1:B:403:LEU:HD11	1:B:421:MET:HE1	1.87	0.55
1:A:272:THR:HG23	1:A:450:PRO:HG3	1.87	0.55
1:B:307:SER:HB2	1:B:377:ASN:ND2	2.22	0.54
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.89	0.54
1:D:224:GLN:HG2	1:D:402:ALA:HB2	1.88	0.54
1:B:321:ASN:ND2	1:B:323:GLU:H	2.06	0.53
1:C:250:THR:O	1:C:270:HIS:ND1	2.42	0.53
1:D:268:PHE:O	1:D:272:THR:HG23	2.10	0.52
1:A:380:SER:O	1:A:383:ARG:HG2	2.10	0.52
1:B:321:ASN:HD22	1:B:323:GLU:H	1.57	0.51
1:D:250:THR:OG1	1:D:273:GLU:OE2	2.28	0.51
1:B:274:LEU:HD22	1:B:330:LEU:HD11	1.93	0.51
1:C:388:GLU:OE1	1:C:391:ARG:HD2	2.11	0.51
1:D:314:LEU:HD13	1:D:428:LEU:HD11	1.93	0.50
1:D:403:LEU:HD11	1:D:421:MET:HE1	1.94	0.49
1:B:255:GLY:C	1:B:257:ASP:N	2.66	0.49
1:D:299:ASP:OD2	1:D:388:GLU:OE1	2.31	0.49
1:C:231:LEU:HB3	1:C:371:ALA:HB1	1.96	0.48
1:D:394:ALA:O	1:D:398:PRO:CD	2.61	0.48
1:A:281:GLU:HB3	3:A:1501:IPA:H31	1.96	0.48
1:A:287:LYS:HD2	1:A:293:LEU:HD21	1.96	0.47
1:D:220:LEU:HD22	1:D:224:GLN:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ALA:O	1:D:398:PRO:HD3	2.15	0.46
1:A:277:ILE:HG21	1:A:330:LEU:HD21	1.99	0.45
1:B:255:GLY:C	1:B:257:ASP:H	2.19	0.45
1:D:285:PHE:O	1:D:288:GLN:HG2	2.17	0.44
1:B:373:LEU:HD22	1:B:425:LEU:HD21	1.98	0.44
1:B:257:ASP:CG	1:B:257:ASP:O	2.56	0.44
1:C:246:GLN:N	1:C:247:PRO:CD	2.81	0.44
1:B:246:GLN:HE22	1:B:332:ASP:HB2	1.83	0.44
1:A:287:LYS:CD	1:A:293:LEU:HD21	2.47	0.44
2:B:2500:965:H251	2:B:2500:965:H161	1.87	0.44
1:D:397:GLN:HB3	1:D:398:PRO:HD3	1.99	0.44
1:D:404:LEU:HD13	1:D:418:PHE:CD2	2.53	0.43
1:C:270:HIS:NE2	1:C:335:TYR:OH	2.51	0.43
1:B:307:SER:HB2	1:B:377:ASN:HD22	1.84	0.43
1:A:282:ILE:HA	3:A:1501:IPA:H33	2.00	0.43
1:A:411:ARG:HD3	1:A:417:ARG:HG3	2.00	0.43
1:D:330:LEU:HD12	1:D:333:PHE:CE1	2.54	0.43
1:D:365:LEU:HB2	1:D:370:TYR:CE1	2.54	0.42
1:D:298:GLU:HA	1:D:301:ILE:HD12	2.02	0.42
1:A:236:LEU:HD12	1:A:236:LEU:O	2.20	0.42
1:B:257:ASP:OD2	1:B:257:ASP:O	2.38	0.42
1:D:418:PHE:HB3	1:D:419:PRO:HD3	2.01	0.42
1:B:305:LYS:NZ	4:B:57:HOH:O	2.52	0.41
2:D:3500:965:F42	2:D:3500:965:CL4	2.65	0.41
1:D:365:LEU:HD13	1:D:421:MET:HE3	2.03	0.41
1:D:456:ILE:HG22	1:D:457:TRP:CD1	2.55	0.41
1:C:293:LEU:HA	1:C:300:GLN:NE2	2.36	0.41
1:C:355:GLU:HG3	1:C:358:ARG:NH1	2.36	0.41
1:A:416:LEU:CD1	1:B:397:GLN:HG3	2.51	0.41
1:D:396:GLN:O	1:D:400:VAL:HG23	2.21	0.41
1:A:268:PHE:O	1:A:272:THR:HB	2.21	0.41
1:C:321:ASN:ND2	1:C:324:THR:HG23	2.36	0.41
1:A:247:PRO:HD2	1:A:277:ILE:HD12	2.03	0.40
1:A:373:LEU:HD22	1:A:425:LEU:HD21	2.03	0.40
1:D:380:SER:O	1:D:383:ARG:HG2	2.21	0.40
1:A:252:TRP:CH2	1:A:267:ARG:HD3	2.56	0.40
1:B:246:GLN:N	1:B:247:PRO:CD	2.83	0.40
1:B:429:ARG:HD3	1:B:429:ARG:HA	1.92	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	226/253 (89%)	221 (98%)	5 (2%)	0	100	100
1	B	239/253 (94%)	232 (97%)	6 (2%)	1 (0%)	34	48
1	C	204/253 (81%)	199 (98%)	5 (2%)	0	100	100
1	D	219/253 (87%)	209 (95%)	10 (5%)	0	100	100
All	All	888/1012 (88%)	861 (97%)	26 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	256	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	203/222 (91%)	183 (90%)	20 (10%)	8	11
1	B	212/222 (96%)	198 (93%)	14 (7%)	16	26
1	C	185/222 (83%)	167 (90%)	18 (10%)	8	12
1	D	201/222 (90%)	177 (88%)	24 (12%)	5	6
All	All	801/888 (90%)	725 (90%)	76 (10%)	8	12

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	MET
1	A	236	LEU
1	A	248	LYS
1	A	249	VAL
1	A	264	ARG
1	A	272	THR
1	A	298	GLU
1	A	305	LYS
1	A	314	LEU
1	A	321	ASN
1	A	323	GLU
1	A	332	ASP
1	A	337	LYS
1	A	353	ILE
1	A	373	LEU
1	A	408	ARG
1	A	410	LYS
1	A	417	ARG
1	A	431	LEU
1	A	443	ARG
1	B	227	MET
1	B	235	GLN
1	B	241	ARG
1	B	257	ASP
1	B	305	LYS
1	B	314	LEU
1	B	321	ASN
1	B	334	THR
1	B	337	LYS
1	B	361	ARG
1	B	410	LYS
1	B	433	SER
1	B	443	ARG
1	B	454	SER
1	C	239	ASN
1	C	246	GLN
1	C	264	ARG
1	C	267	ARG
1	C	298	GLU
1	C	314	LEU
1	C	331	LYS
1	C	334	THR
1	C	346	GLN

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Mol	Chain	Res	Type
1	C	355	GLU
1	C	361	ARG
1	C	405	SER
1	C	408	ARG
1	C	411	ARG
1	C	413	GLN
1	C	417	ARG
1	C	431	LEU
1	C	434	VAL
1	D	220	LEU
1	D	221	THR
1	D	224	GLN
1	D	227	MET
1	D	230	GLN
1	D	278	SER
1	D	288	GLN
1	D	305	LYS
1	D	307	SER
1	D	314	LEU
1	D	338	ASP
1	D	347	VAL
1	D	373	LEU
1	D	382	ASP
1	D	393	GLU
1	D	397	GLN
1	D	408	ARG
1	D	411	ARG
1	D	412	PRO
1	D	431	LEU
1	D	432	SER
1	D	444	LEU
1	D	455	GLU
1	D	458	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	265	GLN
1	A	300	GLN
1	A	321	ASN
1	A	377	ASN

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Mol	Chain	Res	Type
1	A	415	GLN
1	B	230	GLN
1	B	321	ASN
1	B	346	GLN
1	B	377	ASN
1	B	445	GLN
1	C	246	GLN
1	C	266	GLN
1	C	300	GLN
1	C	321	ASN
1	C	387	GLN
1	C	397	GLN
1	D	237	GLN
1	D	300	GLN

### 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 carbohydrates 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
3	IPA	A	1501	-	3,3,3	0.42	0	3,3,3	0.40	0
2	965	A	1500	-	39,44,44	1.39	2 (5%)	53,60,60	1.67	8 (15%)
3	IPA	B	2501	-	3,3,3	0.35	0	3,3,3	0.40	0
2	965	D	3500	-	39,44,44	1.33	2 (5%)	53,60,60	1.84	7 (13%)
2	965	B	2500	-	39,44,44	1.52	2 (5%)	53,60,60	1.70	8 (15%)

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	965	A	1500	-	-	6/31/33/33	0/4/4/4
2	965	D	3500	-	-	10/31/33/33	0/4/4/4
2	965	B	2500	-	-	5/31/33/33	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2500	965	C19-C18	8.20	1.48	1.39
2	A	1500	965	C19-C18	7.30	1.47	1.39
2	D	3500	965	C19-C18	7.06	1.46	1.39
2	B	2500	965	C19-CL4	3.83	1.81	1.72
2	A	1500	965	C19-CL4	2.79	1.78	1.72
2	D	3500	965	C19-CL4	2.62	1.78	1.72

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2500	965	C16-N09-C08	7.69	119.88	110.95
2	D	3500	965	C16-N09-C08	7.33	119.46	110.95
2	A	1500	965	C16-N09-C08	7.16	119.27	110.95
2	D	3500	965	C17-N09-C08	5.50	125.06	111.96
2	D	3500	965	C39-C20-C19	-4.71	118.57	121.78
2	B	2500	965	C18-C16-N09	4.39	120.43	112.75
2	A	1500	965	C39-C20-C19	-4.33	118.83	121.78
2	D	3500	965	F41-C39-C20	-3.96	105.81	112.70
2	B	2500	965	C39-C20-C19	-3.61	119.32	121.78
2	A	1500	965	C17-N09-C08	3.50	120.30	111.96
2	A	1500	965	C16-N09-C17	3.29	118.23	111.29
2	A	1500	965	F41-C39-C20	-3.16	107.20	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2500	965	F41-C39-C20	-3.05	107.38	112.70
2	D	3500	965	C25-C17-N09	-2.99	106.30	113.84
2	A	1500	965	C21-C20-C39	2.93	123.98	118.12
2	D	3500	965	C21-C20-C39	2.84	123.79	118.12
2	A	1500	965	C23-C18-C19	2.80	119.41	117.43
2	B	2500	965	C17-N09-C08	2.69	118.38	111.96
2	B	2500	965	C16-N09-C17	2.68	116.94	111.29
2	B	2500	965	F42-C39-C20	-2.32	108.66	112.70
2	D	3500	965	C16-C18-C19	-2.30	117.91	121.73
2	A	1500	965	C16-C18-C19	-2.20	118.07	121.73
2	B	2500	965	C21-C20-C19	2.15	119.14	116.66

There are no chirality outliers.

All (21) torsion outliers are listed below:

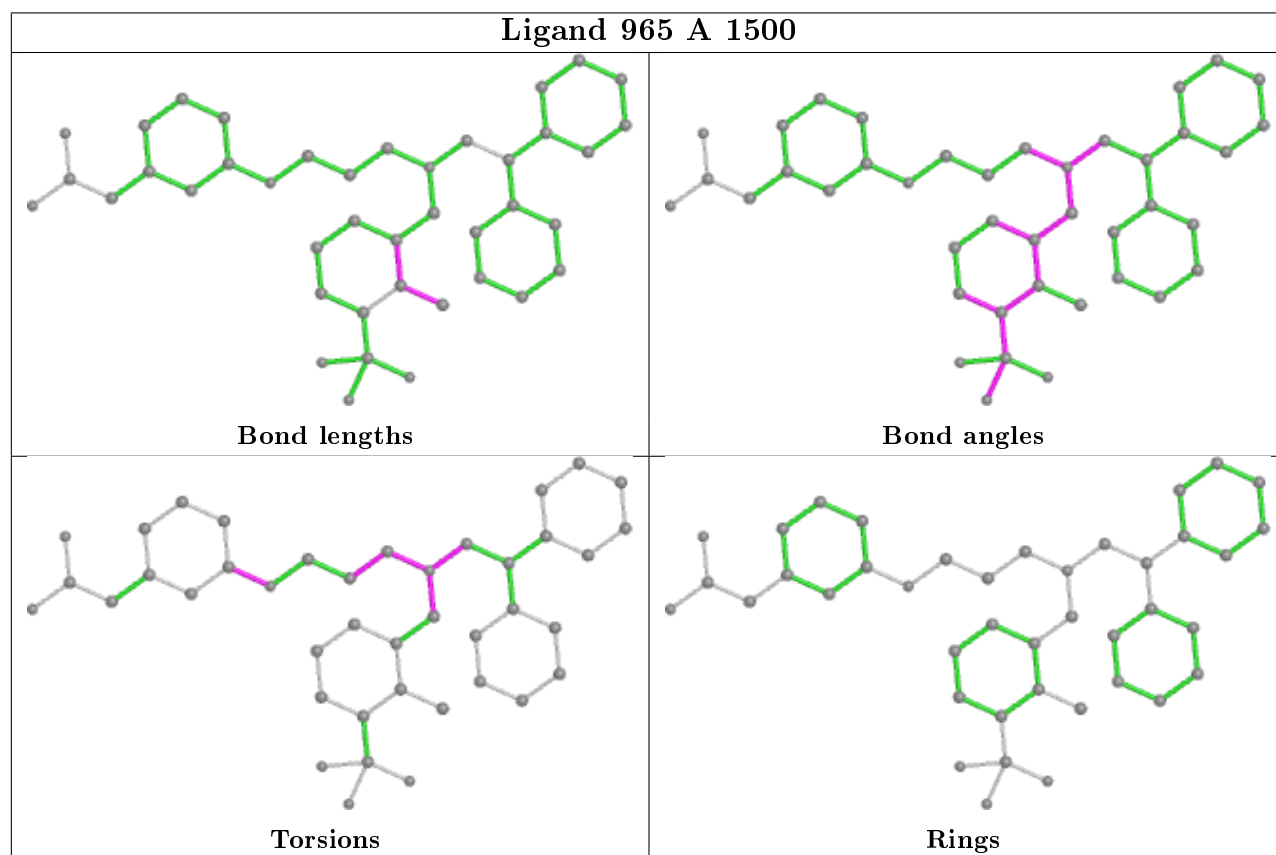
Mol	Chain	Res	Type	Atoms
2	D	3500	965	C07-C08-N09-C17
2	D	3500	965	C19-C20-C39-F40
2	D	3500	965	C19-C20-C39-F42
2	A	1500	965	C33-C28-O27-C26
2	A	1500	965	C29-C28-O27-C26
2	D	3500	965	C33-C28-O27-C26
2	D	3500	965	C25-C17-N09-C08
2	D	3500	965	C29-C28-O27-C26
2	D	3500	965	C19-C20-C39-F41
2	B	2500	965	C19-C20-C39-F41
2	A	1500	965	N09-C17-C25-C26
2	A	1500	965	C07-C08-N09-C17
2	D	3500	965	C25-C26-O27-C28
2	B	2500	965	C19-C20-C39-F40
2	B	2500	965	C19-C20-C39-F42
2	D	3500	965	C18-C16-N09-C17
2	D	3500	965	C10-C07-C08-N09
2	B	2500	965	C17-C25-C26-O27
2	A	1500	965	C18-C16-N09-C17
2	A	1500	965	C25-C17-N09-C16
2	B	2500	965	C25-C17-N09-C16

There are no ring outliers.

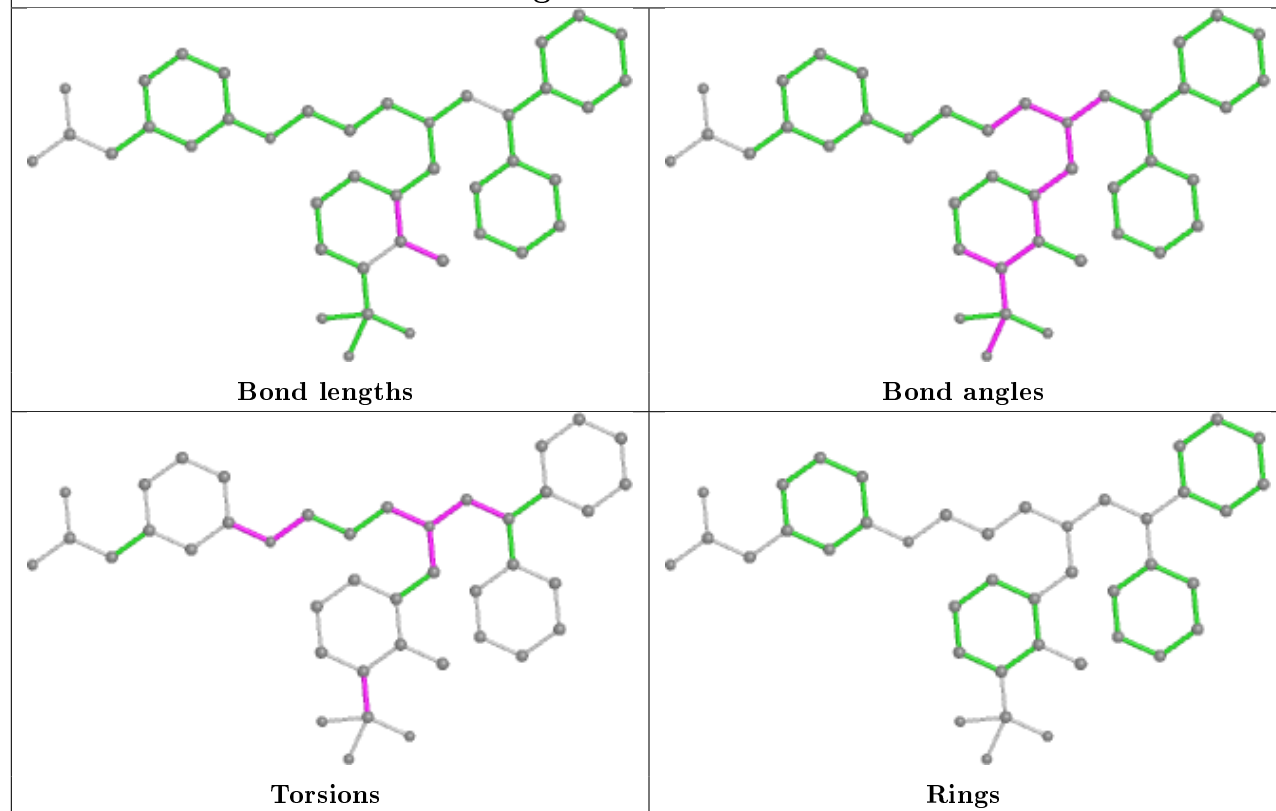
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	IPA	2	0
2	A	1500	965	1	0
2	D	3500	965	1	0
2	B	2500	965	1	0

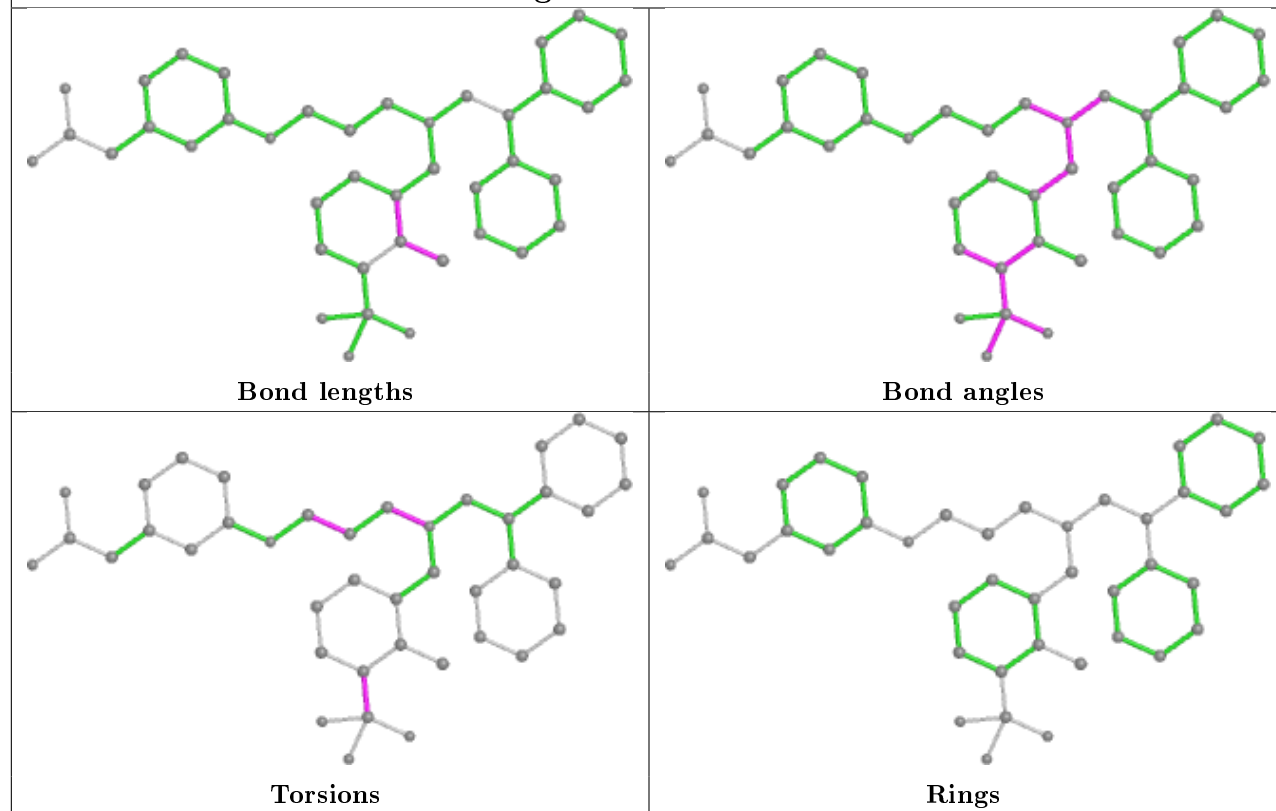
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 965 D 3500



## Ligand 965 B 2500



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

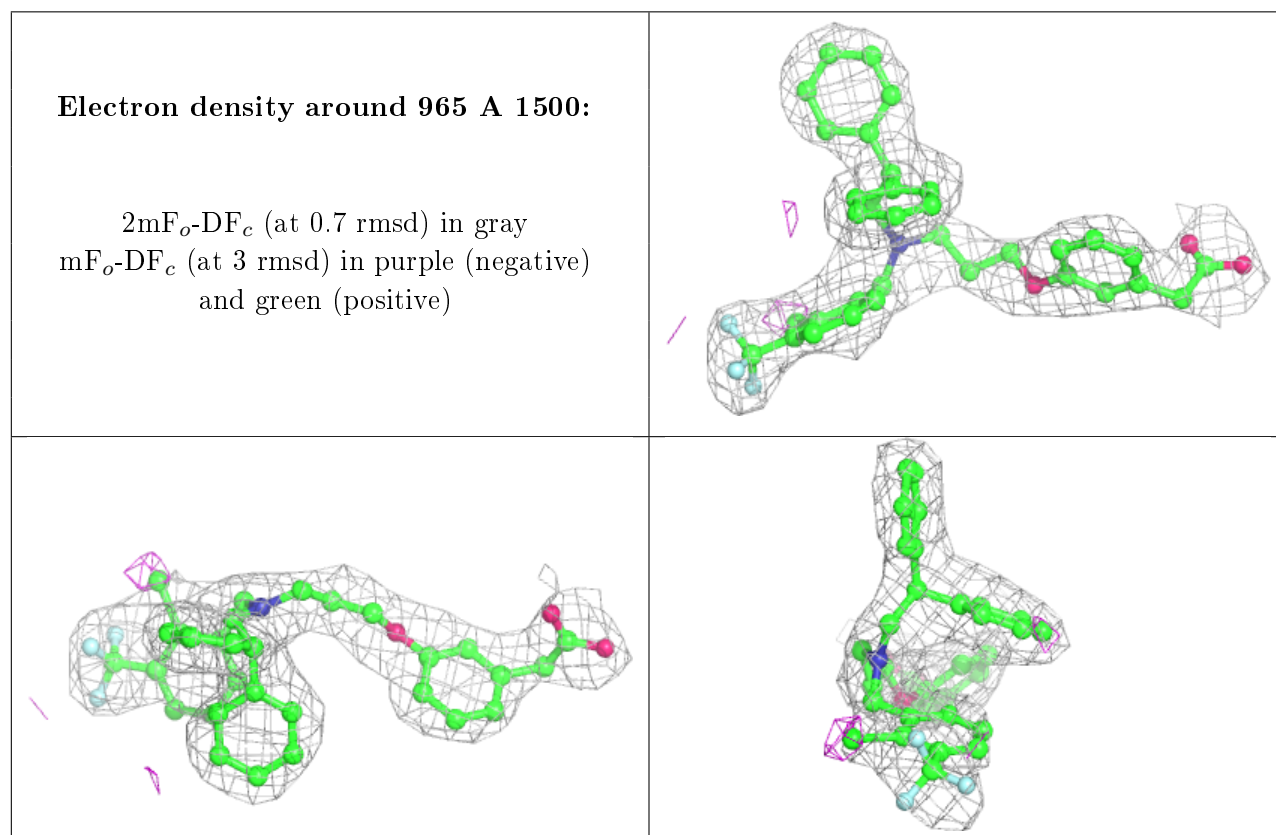
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

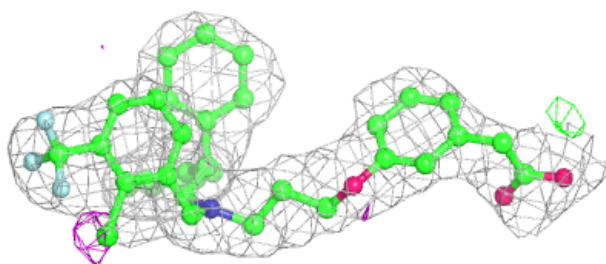
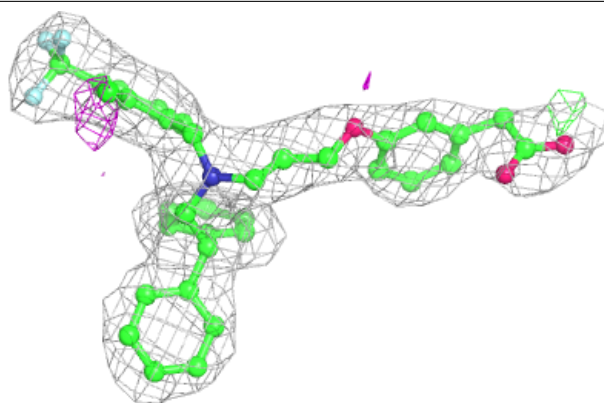
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

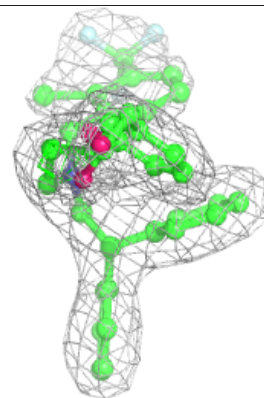
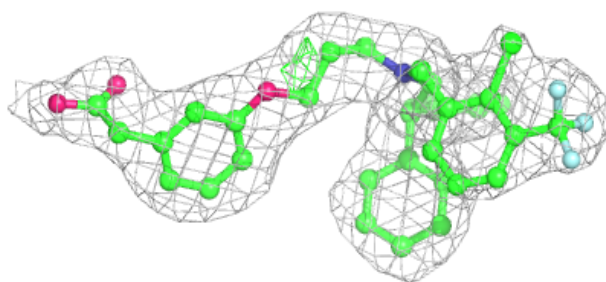
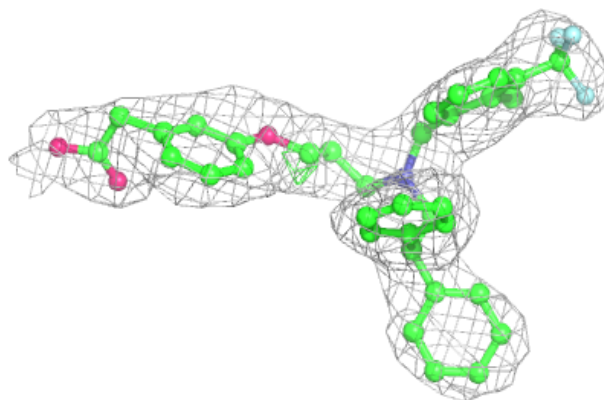


**Electron density around 965 D 3500:**

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

**Electron density around 965 B 2500:**

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



## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.