



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:03 pm BST

PDB ID : 4NQA
Title : Crystal structure of liganded hRXR-alpha/hLXR-beta heterodimer on DNA
Authors : Lou, X.H.; Toresson, G.; Benod, C.; Suh, J.H.; Phillips, K.J.; Webb, P.; Gustafsson, J.A.
Deposited on : 2013-11-24
Resolution : 3.10 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 : 2.11
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

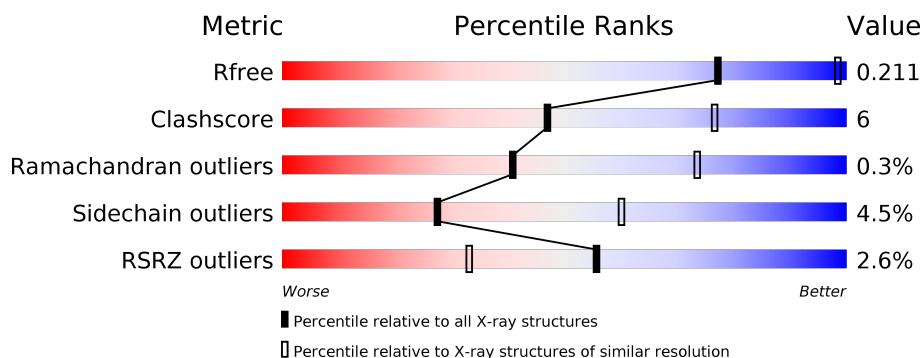
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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	365	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 65% 21% • 13% </div> </div>
1	H	365	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 69% 18% 13% </div> </div>
2	B	391	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 3% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 81% 13% 6% </div> </div>
2	I	391	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 3% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 79% 17% • • </div> </div>
3	C	13	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 69% 8% 23% </div> </div>
3	D	13	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 69% 23% 8% </div> </div>

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Mol	Chain	Length	Quality of chain
3	J	13	
3	K	13	
4	E	18	
4	L	18	
5	F	18	
5	M	18	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12978 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	317	Total	C	N	O	S	0	0	0
			2513	1581	449	461	22			
1	H	319	Total	C	N	O	S	0	0	0
			2528	1586	454	466	22			

- Molecule 2 is a protein called Liver X nuclear receptor beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	369	Total	C	N	O	S	0	0	0
			2934	1833	543	537	21			
2	I	385	Total	C	N	O	S	0	0	0
			3016	1878	557	560	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	MET	-	INITIATING METHIONINE	UNP F1D8P7
I	71	MET	-	INITIATING METHIONINE	UNP F1D8P7

- Molecule 3 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			89	57	19	13			
3	D	12	Total	C	N	O	0	0	0
			101	63	21	17			
3	J	12	Total	C	N	O	0	0	0
			101	63	21	17			
3	K	11	Total	C	N	O	0	0	0
			98	63	21	14			

- Molecule 4 is a DNA chain called 5'-D(*TP*AP*AP*GP*GP*TP*CP*AP*CP*TP*TP*CP

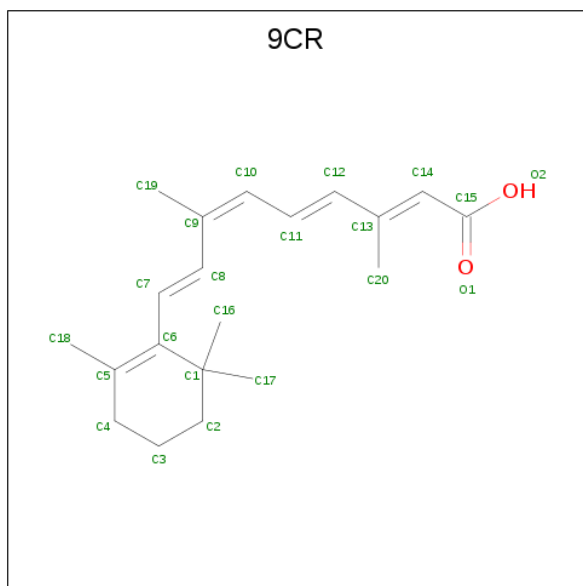
*AP*GP*GP*TP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			
4	L	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			

- Molecule 5 is a DNA chain called 5'-D(*TP*AP*TP*GP*AP*CP*CP*TP*GP*AP*AP*GP*TP*GP*AP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			
5	M	18	Total	C	N	O	P	0	0	0
			366	176	67	106	17			

- Molecule 6 is (9cis)-retinoic acid (three-letter code: 9CR) (formula: C₂₀H₂₈O₂).

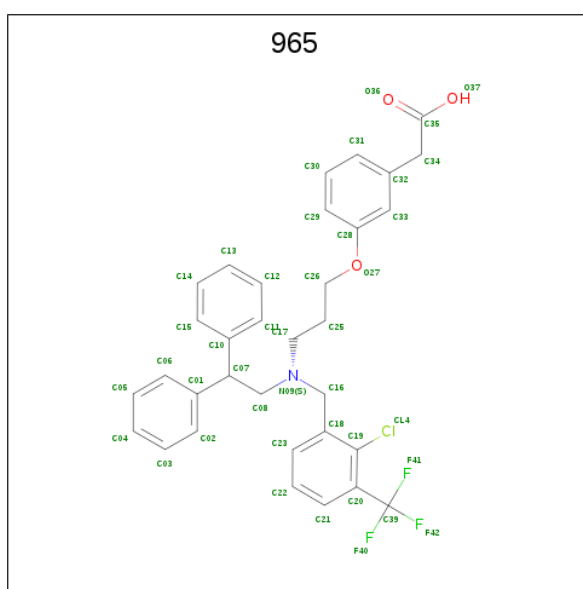


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			22	20	2		
6	H	1	Total	C	O	0	0
			22	20	2		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	2	Total Zn 2 2	0	0
7	B	2	Total Zn 2 2	0	0
7	A	2	Total Zn 2 2	0	0
7	I	2	Total Zn 2 2	0	0

- Molecule 8 is [3-(3-{[2-chloro-3-(trifluoromethyl)benzyl](2,2-diphenylethyl)amino}propoxy)phenyl]acetic acid (three-letter code: 965) (formula: C₃₃H₃₁ClF₃NO₃).

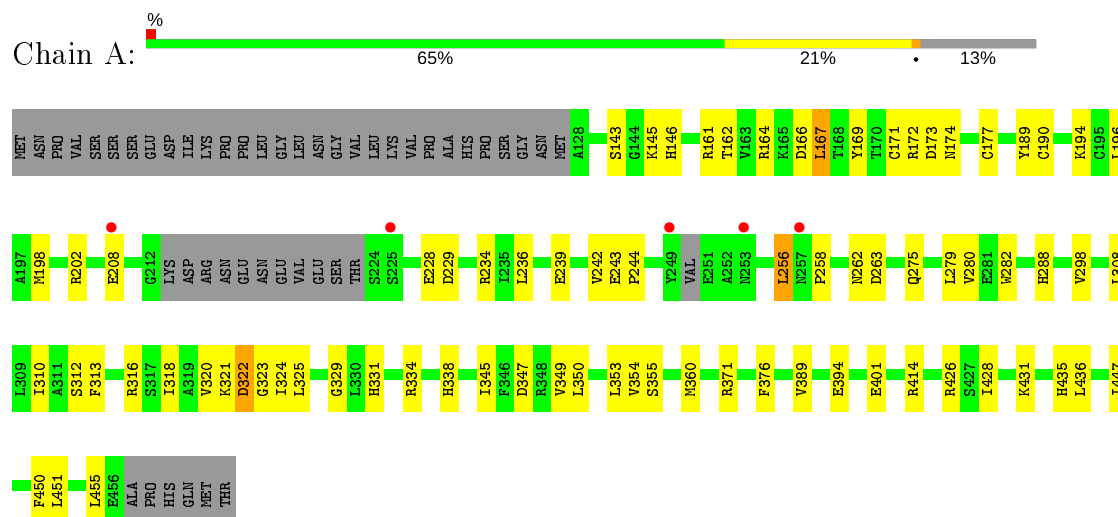


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	Cl	F	N	O	0	0
			41	33	1	3	1	3		
8	I	1	Total	C	Cl	F	N	O	0	0
			41	33	1	3	1	3		

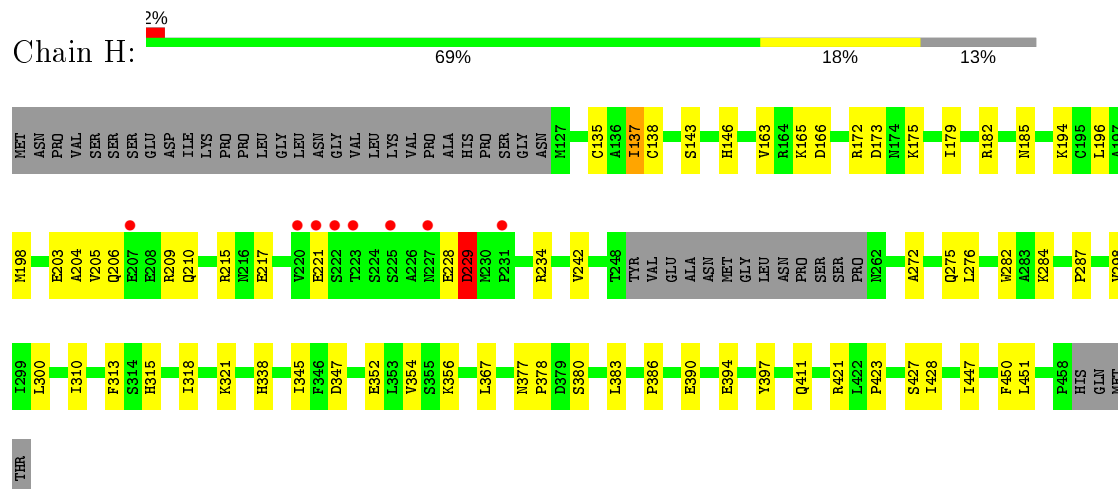
3 Residue-property plots

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 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.

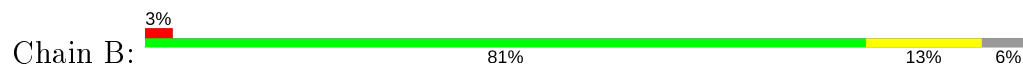
• Molecule 1: Retinoic acid receptor RXR-alpha

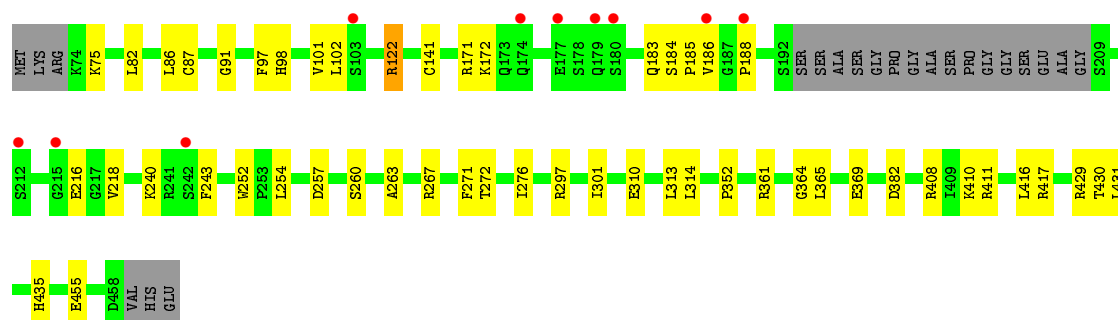


• Molecule 1: Retinoic acid receptor RXR-alpha

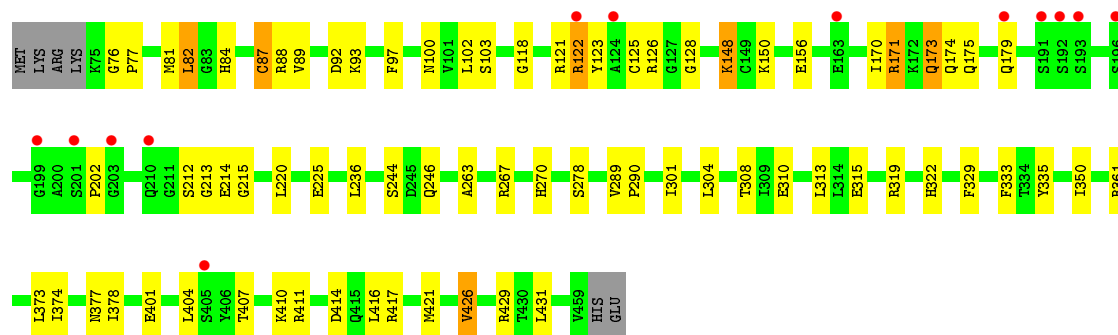
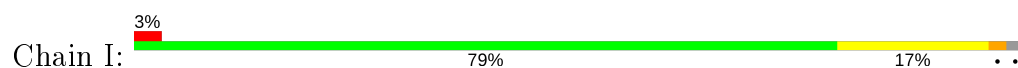


• Molecule 2: Liver X nuclear receptor beta





• Molecule 2: Liver X nuclear receptor beta



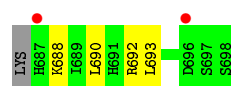
• Molecule 3: Nuclear receptor coactivator 2



• Molecule 3: Nuclear receptor coactivator 2

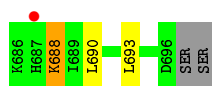


• Molecule 3: Nuclear receptor coactivator 2



• Molecule 3: Nuclear receptor coactivator 2





- Molecule 4: 5'-D(*TP*AP*AP*GP*GP*TP*CP*AP*CP*TP*TP*CP*AP*GP*GP*TP*CP*A)-3'

Chain E: 72% 28%



- Molecule 4: 5'-D(*TP*AP*AP*GP*GP*TP*CP*AP*CP*TP*TP*CP*AP*GP*GP*TP*CP*A)-3'

Chain L: 89% 11%



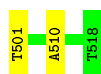
- Molecule 5: 5'-D(*TP*AP*TP*GP*AP*CP*CP*TP*GP*AP*AP*GP*TP*GP*AP*CP*CP*T)-3'

Chain F: 61% 39%



- Molecule 5: 5'-D(*TP*AP*TP*GP*AP*CP*CP*TP*GP*AP*AP*GP*TP*GP*AP*CP*CP*T)-3'

Chain M: 89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	85.78Å 85.78Å 238.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.10 37.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.6 (48.97-3.10) 82.6 (37.88-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.180 , 0.218 0.181 , 0.211	Depositor DCC
R_{free} test set	1313 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12978	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: 965, ZN, 9CR

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	0.21	0/2558	0.42	0/3440
1	H	0.22	0/2572	0.44	0/3460
2	B	0.22	0/2984	0.40	0/4005
2	I	0.22	0/3069	0.44	0/4125
3	C	0.18	0/90	0.34	0/119
3	D	0.19	0/102	0.38	0/135
3	J	0.19	0/102	0.38	0/135
3	K	0.19	0/99	0.34	0/130
4	E	0.42	0/410	0.99	0/631
4	L	0.42	0/410	0.96	0/631
5	F	0.42	0/410	1.06	0/631
5	M	0.42	0/410	1.04	0/631
All	All	0.25	0/13216	0.55	0/18073

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	H	0	3
2	B	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	216	GLU	Peptide
1	H	217	GLU	Peptide
1	H	221	GLU	Peptide
1	H	228	GLU	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	2513	0	2520	47	0
1	H	2528	0	2529	36	0
2	B	2934	0	2947	30	0
2	I	3016	0	3008	40	0
3	C	89	0	95	1	0
3	D	101	0	105	2	0
3	J	101	0	105	3	0
3	K	98	0	108	2	0
4	E	366	0	205	5	0
4	L	366	0	205	1	0
5	F	366	0	205	8	0
5	M	366	0	205	2	0
6	A	22	0	27	1	0
6	H	22	0	27	1	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	H	2	0	0	0	0
7	I	2	0	0	0	0
8	B	41	0	30	5	0
8	I	41	0	30	3	0
All	All	12978	0	12351	156	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 6.

All (156) 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)
2:I:89:VAL:HG13	2:I:148:LYS:HB3	1.74	0.68
1:A:242:VAL:HG21	1:A:282:TRP:HB2	1.75	0.68
1:A:322:ASP:N	1:A:322:ASP:OD1	2.28	0.67
1:A:320:VAL:HG11	1:A:325:LEU:HD13	1.78	0.65
2:I:121:ARG:O	2:I:122:ARG:NH1	2.27	0.65
8:B:501:965:H07	8:B:501:965:H252	1.78	0.65
2:I:125:CYS:SG	2:I:126:ARG:N	2.70	0.65
1:H:163:VAL:HG11	1:H:203:GLU:HB3	1.79	0.65
2:B:172:LYS:NZ	5:F:511:DA:OP1	2.29	0.64
1:H:380:SER:HB2	1:H:383:LEU:HD21	1.80	0.62
1:A:321:LYS:NZ	1:A:350:LEU:O	2.33	0.62
2:B:97:PHE:HA	2:B:102:LEU:HA	1.80	0.61
1:A:318:ILE:HA	1:A:354:VAL:HG23	1.81	0.61
2:I:350:ILE:HG23	8:I:501:965:H13	1.82	0.61
2:B:382:ASP:OD2	2:B:429:ARG:NH1	2.31	0.60
1:H:318:ILE:HA	1:H:354:VAL:HG23	1.83	0.60
1:A:164:ARG:HH22	4:E:504:DG:H5''	1.67	0.60
2:B:87:CYS:HB3	2:B:91:GLY:H	1.65	0.59
4:E:509:DC:O2	5:F:512:DG:N2	2.27	0.59
1:A:338:HIS:NE2	1:A:347:ASP:OD2	2.36	0.58
2:B:297:ARG:H	2:B:297:ARG:HE	1.50	0.58
2:I:170:ILE:O	2:I:173:GLN:NE2	2.37	0.58
1:A:426:ARG:NH1	2:B:430:THR:OG1	2.36	0.58
1:A:325:LEU:HD12	1:A:331:HIS:HD2	1.69	0.57
2:I:150:LYS:NZ	2:I:156:GLU:OE2	2.37	0.57
1:A:360:MET:O	1:A:414:ARG:NH1	2.32	0.57
2:B:257:ASP:HB3	2:B:260:SER:HB2	1.87	0.57
2:B:98:HIS:N	2:B:101:VAL:O	2.31	0.56
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.41	0.56
1:A:228:GLU:O	2:B:122:ARG:NH1	2.39	0.56
2:B:365:LEU:HA	2:B:417:ARG:HH21	1.71	0.55
8:B:501:965:CL4	8:B:501:965:F40	2.51	0.55
2:I:87:CYS:HB2	2:I:103:SER:HA	1.89	0.55
1:H:229:ASP:HA	2:I:128:GLY:HA2	1.89	0.54
2:B:75:LYS:HE3	5:F:515:DA:H3'	1.89	0.54
2:I:322:HIS:HB2	2:I:361:ARG:HG2	1.91	0.54
1:A:177:CYS:HB2	1:A:190:CYS:SG	2.48	0.53
1:A:243:GLU:OE1	1:A:316:ARG:NH1	2.41	0.53
2:B:301:ILE:HG23	3:D:690:LEU:HD23	1.90	0.53
2:I:315:GLU:OE1	2:I:319:ARG:NH2	2.41	0.53
1:A:298:VAL:HG13	3:C:690:LEU:HD23	1.89	0.53
2:I:171:ARG:HG2	5:M:510:DA:H5''	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:338:HIS:NE2	1:H:347:ASP:OD2	2.42	0.52
2:I:319:ARG:NH1	8:I:501:965:O37	2.42	0.52
2:I:301:ILE:HG23	3:K:690:LEU:HD23	1.90	0.52
2:I:102:LEU:H	2:I:102:LEU:HD23	1.73	0.52
1:A:308:LEU:O	1:A:371:ARG:NH1	2.42	0.52
1:H:242:VAL:HG21	1:H:282:TRP:HB2	1.92	0.52
1:H:310:ILE:HA	1:H:313:PHE:CE2	2.45	0.52
2:I:118:GLY:O	2:I:122:ARG:NH1	2.38	0.52
1:A:349:VAL:HG13	1:A:353:LEU:HD12	1.92	0.52
2:I:121:ARG:NH2	5:M:501:DT:O5'	2.43	0.51
5:F:512:DG:H2'	5:F:513:DT:H71	1.92	0.51
1:A:279:LEU:HD21	1:A:308:LEU:HD13	1.93	0.51
1:A:323:GLY:O	1:A:331:HIS:NE2	2.43	0.51
2:I:310:GLU:OE1	2:I:377:ASN:ND2	2.39	0.51
1:H:423:PRO:HG3	2:I:426:VAL:HG12	1.93	0.51
1:A:229:ASP:O	1:A:288:HIS:NE2	2.44	0.50
2:B:252:TRP:HD1	2:B:254:LEU:HG	1.76	0.50
1:A:313:PHE:HE1	1:A:324:ILE:HG21	1.76	0.50
1:H:234:ARG:HB2	1:H:287:PRO:HG3	1.93	0.50
1:A:394:GLU:HB3	2:B:416:LEU:HD13	1.93	0.50
2:B:183:GLN:HB3	2:B:185:PRO:HD2	1.94	0.50
1:A:256:LEU:HD13	1:A:329:GLY:HA2	1.92	0.49
2:I:304:LEU:O	2:I:308:THR:OG1	2.19	0.49
1:A:173:ASP:HB3	1:A:174:ASN:HA	1.95	0.49
2:I:212:SER:OG	2:I:213:GLY:N	2.45	0.49
2:I:401:GLU:HA	2:I:404:LEU:HD12	1.93	0.49
2:B:102:LEU:HD23	2:B:102:LEU:H	1.77	0.49
2:I:244:SER:HA	2:I:246:GLN:HG2	1.94	0.48
2:I:278:SER:HB2	8:I:501:965:C33	2.43	0.48
1:H:275:GLN:HG3	6:H:501:9CR:O2	2.13	0.48
1:A:275:GLN:HG3	6:A:501:9CR:O2	2.14	0.48
1:H:137:ILE:HG13	1:H:138:CYS:N	2.28	0.48
2:I:92:ASP:OD1	2:I:93:LYS:N	2.40	0.48
2:B:352:PRO:HB2	2:B:431:LEU:HD11	1.96	0.48
1:H:143:SER:HG	1:H:146:HIS:HE2	1.61	0.47
1:H:194:LYS:O	1:H:198:MET:HG2	2.14	0.47
1:H:298:VAL:HG13	3:J:690:LEU:HD23	1.95	0.47
2:B:369:GLU:OE2	2:B:417:ARG:NH2	2.48	0.47
4:L:509:DC:H2'	4:L:510:DT:C6	2.50	0.47
8:B:501:965:H07	8:B:501:965:C25	2.43	0.47
1:H:300:LEU:HD22	1:H:377:ASN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:427:SER:OG	2:I:429:ARG:NH1	2.43	0.46
2:I:270:HIS:NE2	2:I:335:TYR:OH	2.48	0.46
2:I:410:LYS:HG3	2:I:411:ARG:HG2	1.97	0.46
2:I:76:GLY:N	2:I:77:PRO:HD3	2.31	0.46
2:I:407:THR:HG23	2:I:417:ARG:HD3	1.98	0.46
1:A:312:SER:HB2	1:A:371:ARG:NH1	2.30	0.46
1:H:378:PRO:HB3	1:H:390:GLU:HB2	1.98	0.46
1:H:185:ASN:HB2	2:I:81:MET:SD	2.55	0.46
2:B:410:LYS:HG2	2:B:411:ARG:HG2	1.98	0.46
5:F:501:DT:H2'	5:F:502:DA:C8	2.51	0.45
1:H:137:ILE:HD12	1:H:194:LYS:HD3	1.98	0.45
1:A:401:GLU:OE2	2:B:408:ARG:NH2	2.50	0.45
2:I:329:PHE:O	2:I:333:PHE:N	2.45	0.45
1:A:436:LEU:HD13	1:A:455:LEU:HD21	1.97	0.45
1:H:163:VAL:HG13	1:H:204:ALA:HB2	1.98	0.45
2:I:373:LEU:HD21	2:I:421:MET:HB3	1.98	0.45
1:A:431:LYS:HE3	1:A:435:HIS:HE1	1.82	0.45
4:E:511:DT:H3	5:F:510:DA:H61	1.64	0.45
1:H:138:CYS:HA	1:H:179:ILE:HG22	1.98	0.45
1:H:447:ILE:HG23	1:H:451:LEU:HD23	1.99	0.45
2:B:310:GLU:HA	2:B:313:LEU:HD12	1.99	0.44
1:A:376:PHE:HB3	1:A:389:VAL:HG13	1.99	0.44
1:H:352:GLU:O	1:H:421:ARG:NH1	2.51	0.44
1:H:315:HIS:CG	1:H:367:LEU:HD22	2.52	0.44
1:A:258:PRO:HD2	1:A:329:GLY:O	2.17	0.44
1:H:394:GLU:HB3	2:I:416:LEU:HD13	1.99	0.44
1:H:284:LYS:NZ	3:J:693:LEU:O	2.47	0.44
2:I:263:ALA:O	2:I:267:ARG:HG3	2.17	0.44
1:A:321:LYS:NZ	1:A:355:SER:OG	2.38	0.44
2:I:313:LEU:HD13	2:I:431:LEU:HB3	2.00	0.44
3:D:689:ILE:O	3:D:692:ARG:HG2	2.18	0.43
1:A:345:ILE:HD11	1:A:428:ILE:HG23	2.01	0.43
1:A:171:CYS:HB2	1:A:189:TYR:HB3	2.01	0.43
2:I:97:PHE:HA	2:I:102:LEU:HA	2.00	0.43
2:I:214:GLU:HA	2:I:215:GLY:HA3	1.69	0.42
1:H:234:ARG:NH2	1:H:287:PRO:HB3	2.34	0.42
2:I:81:MET:HB3	2:I:82:LEU:H	1.46	0.42
2:B:271:PHE:CD1	8:B:501:965:H172	2.54	0.42
2:B:172:LYS:HB3	5:F:510:DA:H5'	2.00	0.42
1:A:194:LYS:O	1:A:198:MET:HG2	2.20	0.42
1:H:135:CYS:SG	1:H:137:ILE:HG23	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ILE:HG23	1:A:451:LEU:HD23	2.01	0.42
1:A:145:LYS:NZ	4:E:502:DA:OP1	2.40	0.42
1:H:173:ASP:OD1	1:H:173:ASP:N	2.39	0.42
1:H:345:ILE:HB	1:H:428:ILE:HD11	2.02	0.42
1:H:165:LYS:HG3	1:H:166:ASP:H	1.85	0.42
1:A:262:ASN:HA	1:A:263:ASP:HA	1.65	0.41
1:A:239:GLU:OE2	1:A:282:TRP:NE1	2.54	0.41
2:B:272:THR:O	2:B:276:ILE:HG13	2.21	0.41
2:B:364:GLY:O	2:B:417:ARG:NH2	2.54	0.41
4:E:509:DC:H2'	4:E:510:DT:C6	2.56	0.41
2:I:289:VAL:HA	2:I:290:PRO:HD3	1.95	0.41
1:A:243:GLU:HA	1:A:244:PRO:HD2	1.97	0.41
1:A:162:THR:O	1:A:166:ASP:N	2.53	0.41
2:B:435:HIS:HE1	8:B:501:965:H21	1.86	0.41
1:A:167:LEU:HD13	1:A:169:TYR:CE1	2.56	0.41
2:I:374:ILE:O	2:I:378:ILE:HG13	2.20	0.41
3:J:688:LYS:O	3:J:692:ARG:HG2	2.21	0.41
2:B:82:LEU:HD12	2:B:82:LEU:HA	1.82	0.41
3:K:688:LYS:HE3	3:K:688:LYS:HB2	1.79	0.41
1:A:143:SER:OG	1:A:146:HIS:NE2	2.54	0.41
1:A:313:PHE:CE1	1:A:324:ILE:HD13	2.56	0.40
2:B:263:ALA:O	2:B:267:ARG:HG3	2.21	0.40
1:H:196:LEU:HB3	1:H:206:GLN:NE2	2.35	0.40
1:A:161:ARG:NH1	5:F:513:DT:OP2	2.55	0.40
2:B:365:LEU:HD23	2:B:417:ARG:HH21	1.87	0.40
1:H:383:LEU:HB2	1:H:386:PRO:HG3	2.03	0.40
1:H:394:GLU:O	1:H:397:TYR:HB2	2.22	0.40
1:H:272:ALA:O	1:H:276:LEU:HG	2.21	0.40
1:A:321:LYS:HA	1:A:322:ASP:HA	1.78	0.40
1:A:313:PHE:CE1	1:A:324:ILE:HG21	2.56	0.40
2:B:87:CYS:HB3	2:B:91:GLY:N	2.35	0.40
1:H:182:ARG:HD3	1:H:182:ARG:HA	1.60	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	311/365 (85%)	290 (93%)	21 (7%)	0	100	100
1	H	315/365 (86%)	291 (92%)	23 (7%)	1 (0%)	41	73
2	B	365/391 (93%)	344 (94%)	18 (5%)	3 (1%)	19	54
2	I	383/391 (98%)	352 (92%)	31 (8%)	0	100	100
3	C	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
3	D	10/13 (77%)	9 (90%)	1 (10%)	0	100	100
3	J	10/13 (77%)	8 (80%)	2 (20%)	0	100	100
3	K	9/13 (69%)	8 (89%)	1 (11%)	0	100	100
All	All	1411/1564 (90%)	1309 (93%)	98 (7%)	4 (0%)	41	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	186	VAL
1	H	229	ASP
2	B	218	VAL
2	B	188	PRO

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	274/317 (86%)	262 (96%)	12 (4%)	28	61
1	H	275/317 (87%)	263 (96%)	12 (4%)	28	61
2	B	317/332 (96%)	307 (97%)	10 (3%)	39	69
2	I	324/332 (98%)	305 (94%)	19 (6%)	19	50
3	C	10/13 (77%)	10 (100%)	0	100	100
3	D	12/13 (92%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	12/13 (92%)	12 (100%)	0	100	100
3	K	11/13 (85%)	9 (82%)	2 (18%)	1	7
All	All	1235/1350 (92%)	1180 (96%)	55 (4%)	27	60

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LEU
1	A	172	ARG
1	A	196	LEU
1	A	202	ARG
1	A	208	GLU
1	A	234	ARG
1	A	236	LEU
1	A	256	LEU
1	A	280	VAL
1	A	322	ASP
1	A	334	ARG
1	A	450	PHE
2	B	86	LEU
2	B	122	ARG
2	B	141	CYS
2	B	171	ARG
2	B	184	SER
2	B	240	LYS
2	B	243	PHE
2	B	314	LEU
2	B	361	ARG
2	B	455	GLU
1	H	137	ILE
1	H	172	ARG
1	H	175	LYS
1	H	205	VAL
1	H	209	ARG
1	H	210	GLN
1	H	215	ARG
1	H	229	ASP
1	H	321	LYS
1	H	356	LYS
1	H	411	GLN
1	H	450	PHE

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Mol	Chain	Res	Type
2	I	82	LEU
2	I	84	HIS
2	I	87	CYS
2	I	88	ARG
2	I	100	ASN
2	I	122	ARG
2	I	123	TYR
2	I	148	LYS
2	I	171	ARG
2	I	173	GLN
2	I	174	GLN
2	I	175	GLN
2	I	179	GLN
2	I	202	PRO
2	I	220	LEU
2	I	225	GLU
2	I	236	LEU
2	I	414	ASP
2	I	426	VAL
3	K	688	LYS
3	K	693	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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$
8	965	I	501	-	39,44,44	1.10	2 (5%)	53,60,60	1.11	3 (5%)
6	9CR	A	501	-	19,22,22	0.84	0	26,30,30	2.31	8 (30%)
8	965	B	501	-	39,44,44	1.11	2 (5%)	53,60,60	1.16	4 (7%)
6	9CR	H	501	-	19,22,22	0.76	0	26,30,30	2.17	6 (23%)

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
8	965	I	501	-	-	5/31/33/33	0/4/4/4
6	9CR	A	501	-	-	4/13/32/32	0/1/1/1
8	965	B	501	-	-	7/31/33/33	0/4/4/4
6	9CR	H	501	-	-	3/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	965	C16-C18	3.02	1.56	1.51
8	I	501	965	C16-C18	2.99	1.56	1.51
8	B	501	965	O27-C28	2.95	1.44	1.37
8	I	501	965	O27-C28	2.88	1.44	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	9CR	C7-C8-C9	-5.94	117.26	126.23
6	H	501	9CR	C3-C4-C5	-5.80	103.73	114.08
6	A	501	9CR	C19-C9-C10	-5.50	115.22	122.92
6	H	501	9CR	C19-C9-C10	-4.74	116.28	122.92
6	H	501	9CR	C8-C9-C10	4.01	125.10	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	501	9CR	C8-C9-C10	3.87	124.87	118.94
6	H	501	9CR	C7-C8-C9	-3.85	120.41	126.23
8	B	501	965	C23-C18-C19	3.52	119.92	117.43
8	I	501	965	C23-C18-C19	3.41	119.84	117.43
6	A	501	9CR	C1-C6-C5	-3.34	117.91	122.61
8	B	501	965	C39-C20-C19	-3.10	119.67	121.78
8	I	501	965	C21-C20-C19	2.90	120.00	116.66
8	B	501	965	C21-C20-C19	2.87	119.97	116.66
6	H	501	9CR	C2-C1-C6	2.78	114.77	110.48
8	I	501	965	C39-C20-C19	-2.60	120.01	121.78
6	A	501	9CR	C10-C11-C12	-2.57	115.20	123.22
6	A	501	9CR	C17-C1-C6	-2.56	106.15	110.30
6	H	501	9CR	C4-C5-C6	-2.38	119.27	122.73
6	A	501	9CR	C18-C5-C4	2.12	117.69	113.62
8	B	501	965	C16-N09-C08	-2.11	108.49	110.95
6	A	501	9CR	C18-C5-C6	-2.07	122.21	124.53

There are no chirality outliers.

All (19) torsion outliers are listed below:

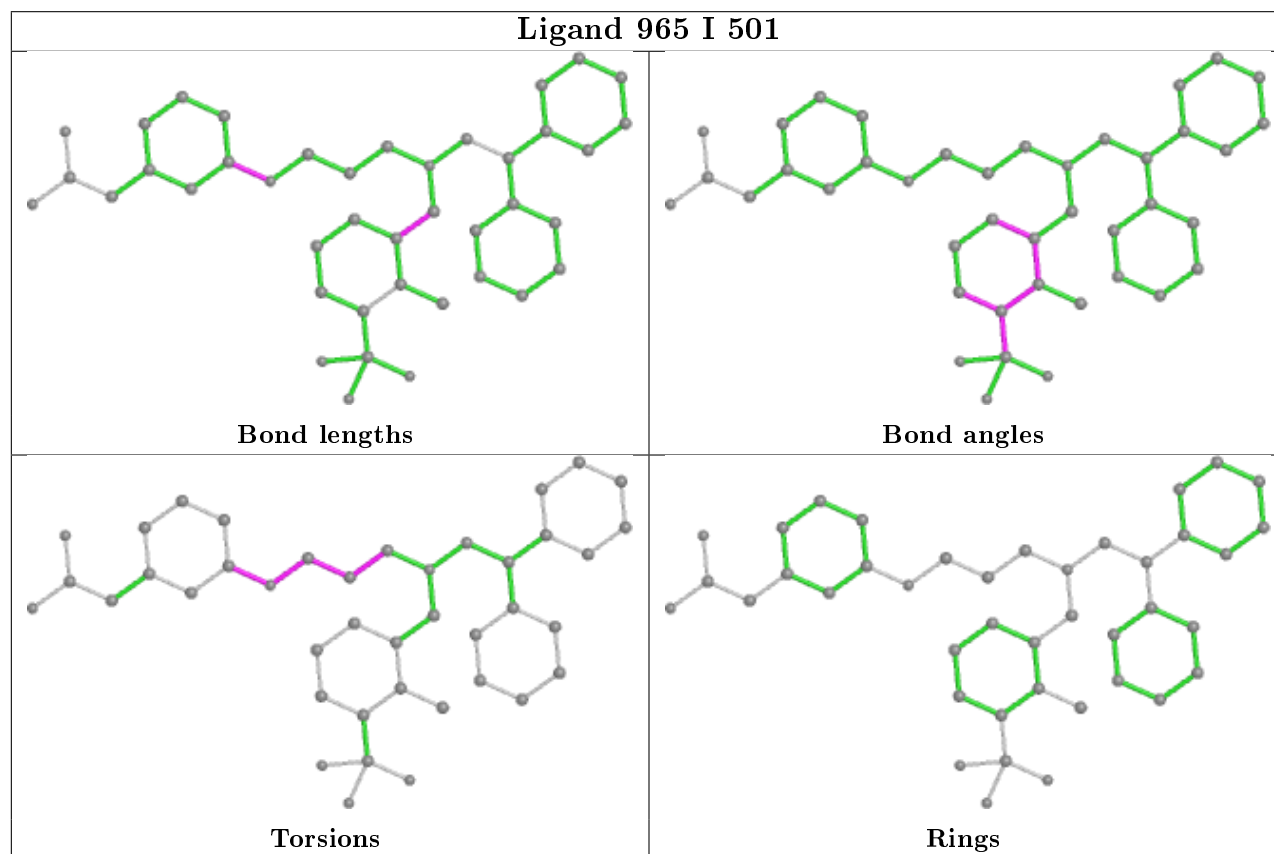
Mol	Chain	Res	Type	Atoms
8	B	501	965	C19-C20-C39-F41
8	B	501	965	C19-C20-C39-F40
8	B	501	965	C19-C20-C39-F42
6	H	501	9CR	C5-C6-C7-C8
6	A	501	9CR	C5-C6-C7-C8
8	I	501	965	C33-C28-O27-C26
8	I	501	965	C29-C28-O27-C26
8	B	501	965	C25-C26-O27-C28
8	I	501	965	N09-C17-C25-C26
8	I	501	965	C25-C26-O27-C28
8	B	501	965	C17-C25-C26-O27
8	B	501	965	C33-C28-O27-C26
6	H	501	9CR	C11-C10-C9-C19
6	A	501	9CR	C11-C10-C9-C19
6	H	501	9CR	C11-C10-C9-C8
6	A	501	9CR	C11-C10-C9-C8
8	B	501	965	C29-C28-O27-C26
6	A	501	9CR	C7-C8-C9-C10
8	I	501	965	C17-C25-C26-O27

There are no ring outliers.

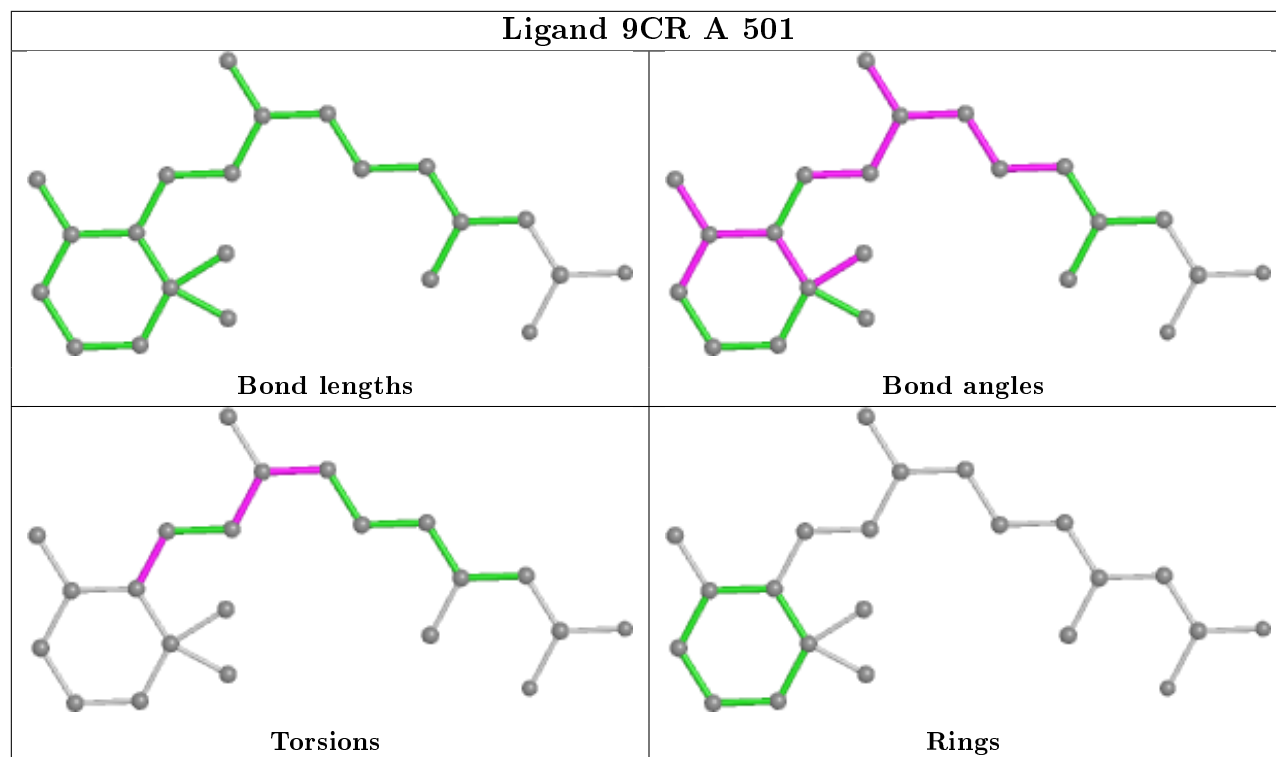
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	501	965	3	0
6	A	501	9CR	1	0
8	B	501	965	5	0
6	H	501	9CR	1	0

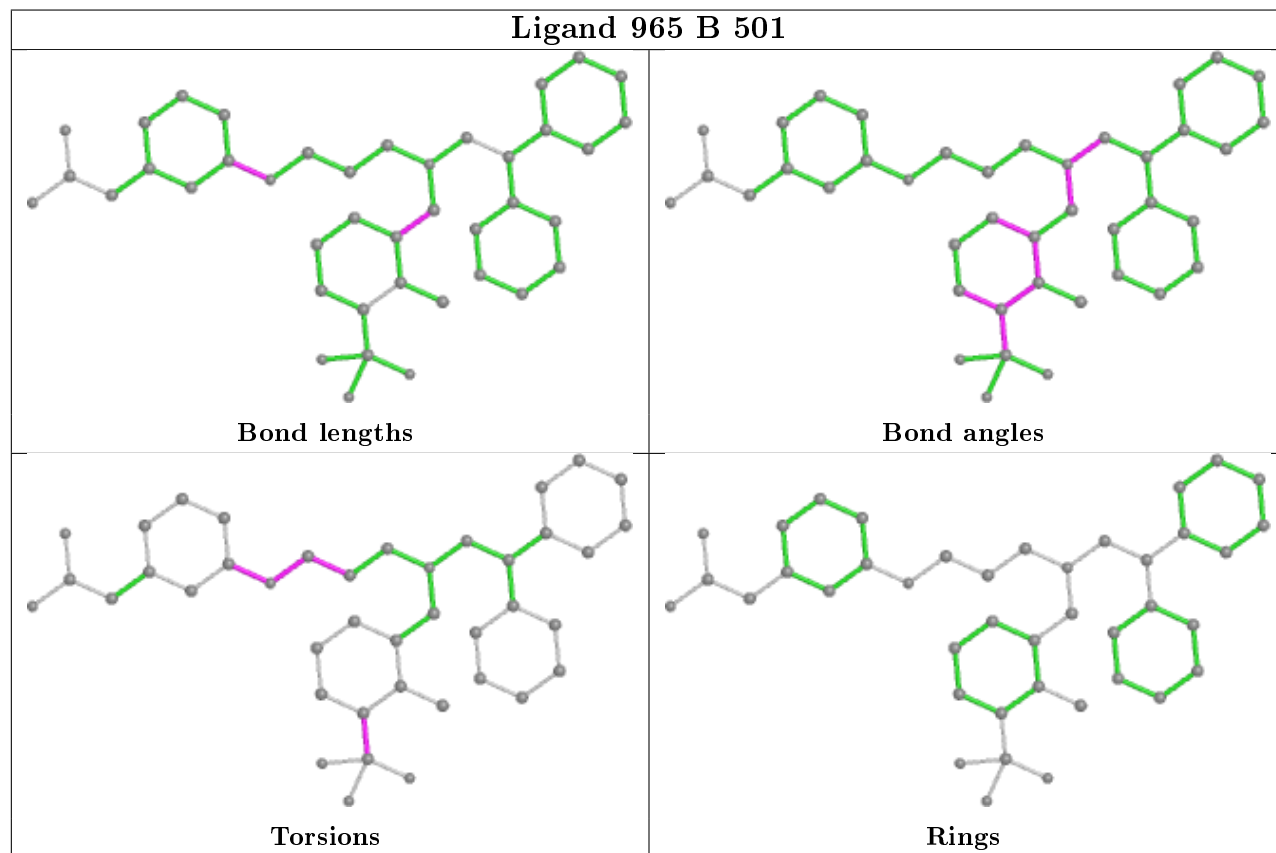
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

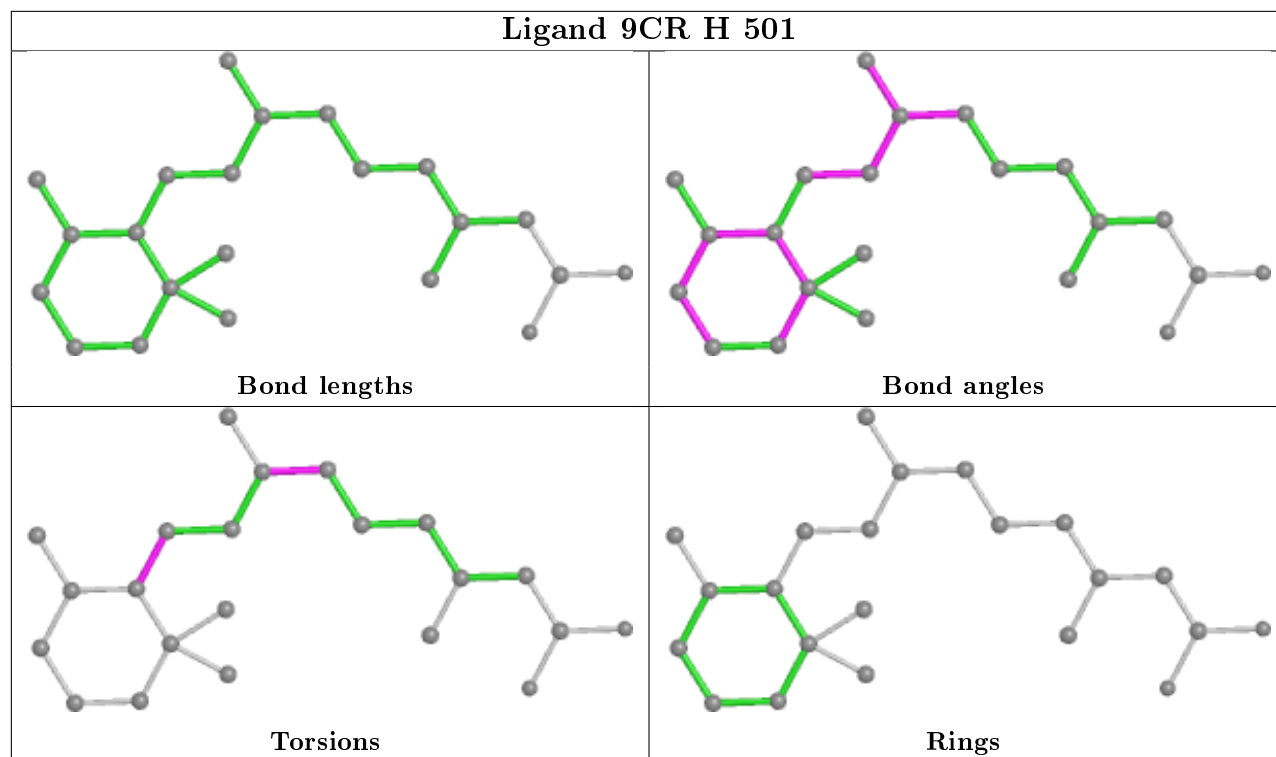


Ligand 9CR A 501



Ligand 965 B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	317/365 (86%)	-0.21	5 (1%) 72 51	16, 57, 114, 152	0
1	H	319/365 (87%)	-0.06	8 (2%) 57 34	19, 71, 128, 152	0
2	B	369/391 (94%)	-0.08	10 (2%) 54 31	21, 73, 128, 161	0
2	I	385/391 (98%)	0.02	13 (3%) 45 24	16, 79, 129, 162	0
3	C	10/13 (76%)	0.10	0 100 100	42, 70, 109, 126	0
3	D	12/13 (92%)	-0.23	0 100 100	67, 82, 122, 128	0
3	J	12/13 (92%)	0.01	2 (16%) 1 1	36, 65, 105, 131	0
3	K	11/13 (84%)	0.02	1 (9%) 9 3	67, 85, 129, 166	0
4	E	18/18 (100%)	-0.55	0 100 100	40, 61, 81, 85	0
4	L	18/18 (100%)	-0.58	0 100 100	49, 67, 97, 119	0
5	F	18/18 (100%)	-0.59	0 100 100	43, 59, 79, 93	0
5	M	18/18 (100%)	-0.54	0 100 100	41, 60, 99, 103	0
All	All	1507/1636 (92%)	-0.10	39 (2%) 56 33	16, 70, 126, 166	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	192	SER	6.3
1	H	220	VAL	4.4
2	B	179	GLN	3.9
1	A	225	SER	3.8
1	H	222	SER	3.8
2	I	191	SER	3.3
2	B	174	GLN	3.3
1	H	223	THR	3.1
3	J	696	ASP	3.0
2	B	242	SER	3.0
2	I	201	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	124	ALA	2.9
2	I	179	GLN	2.9
2	I	199	GLY	2.9
2	B	186	VAL	2.8
2	I	163	GLU	2.8
2	I	405	SER	2.8
2	I	122	ARG	2.8
2	I	196	SER	2.8
2	B	177	GLU	2.7
1	H	207	GLU	2.6
2	I	193	SER	2.6
2	B	215	GLY	2.5
1	H	227	ASN	2.5
3	J	687	HIS	2.5
1	A	249	TYR	2.4
2	B	180	SER	2.4
1	A	253	ASN	2.2
1	H	231	PRO	2.2
3	K	687	HIS	2.2
1	H	221	GLU	2.2
1	A	257	ASN	2.2
2	I	203	GLY	2.2
1	H	225	SER	2.1
2	B	212	SER	2.1
2	B	188	PRO	2.1
2	B	103	SER	2.1
1	A	208	GLU	2.0
2	I	210	GLN	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 carbohydrates in this entry.

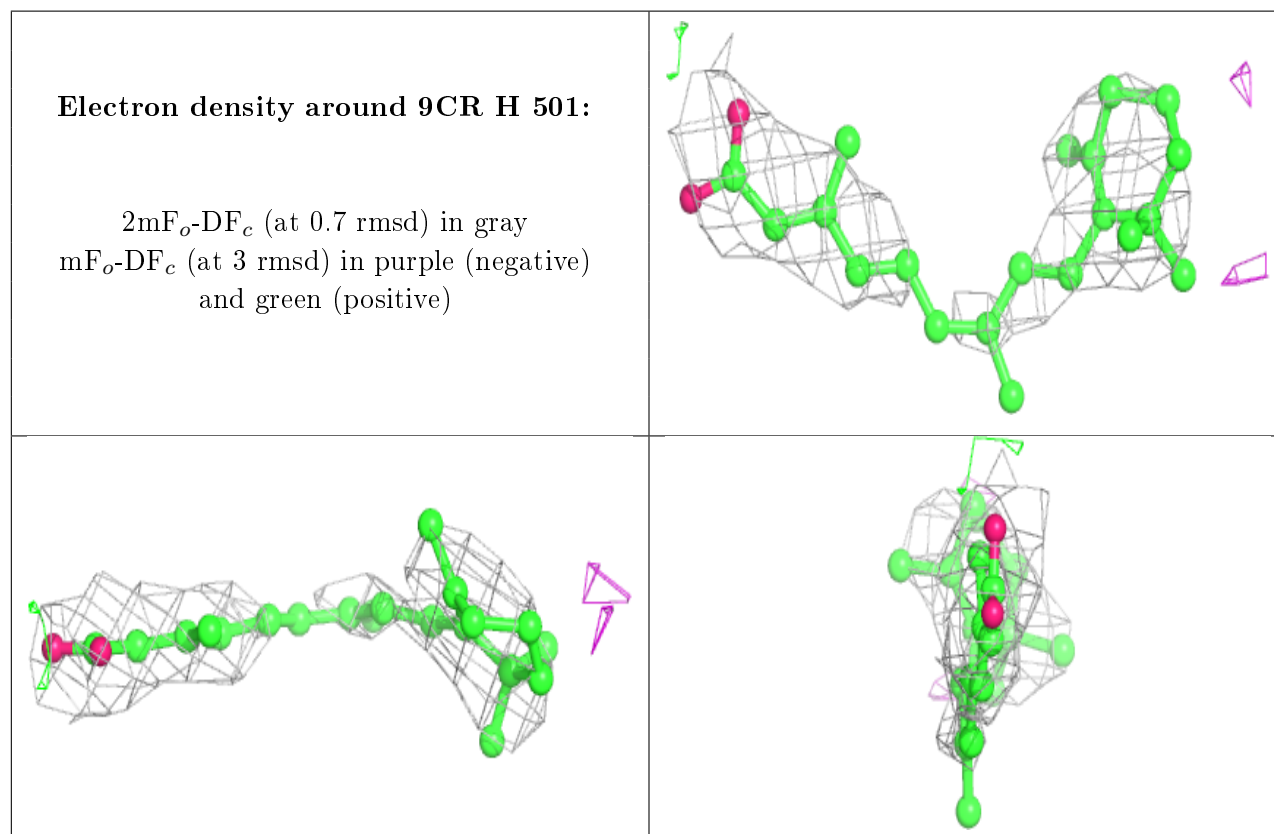
6.4 Ligands [i](#)

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.

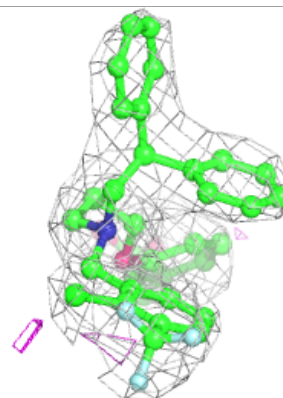
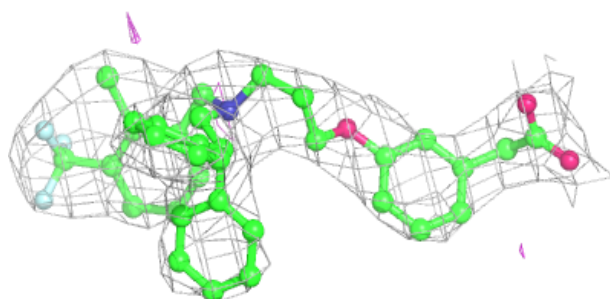
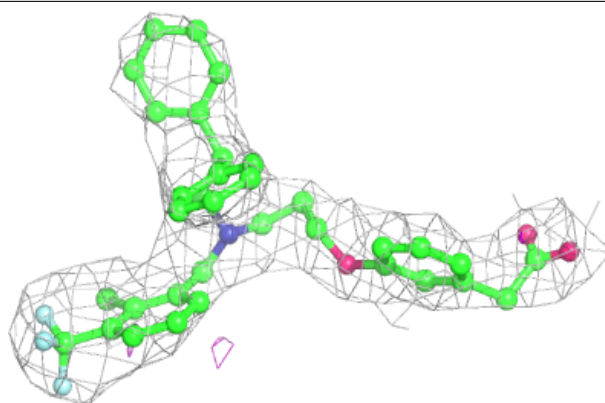
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	ZN	I	503	1/1	0.88	0.06	179,179,179,179	0
6	9CR	H	501	22/22	0.93	0.49	88,88,88,88	0
8	965	B	501	41/41	0.94	0.32	66,66,66,66	0
7	ZN	H	503	1/1	0.95	0.07	122,122,122,122	0
7	ZN	B	503	1/1	0.97	0.11	154,154,154,154	0
6	9CR	A	501	22/22	0.97	0.33	46,46,46,46	0
8	965	I	501	41/41	0.97	0.29	59,59,59,59	0
7	ZN	I	502	1/1	0.97	0.14	73,73,73,73	0
7	ZN	A	503	1/1	0.98	0.10	83,83,83,83	0
7	ZN	H	502	1/1	0.98	0.10	48,48,48,48	0
7	ZN	B	502	1/1	0.99	0.13	68,68,68,68	0
7	ZN	A	502	1/1	0.99	0.12	53,53,53,53	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.

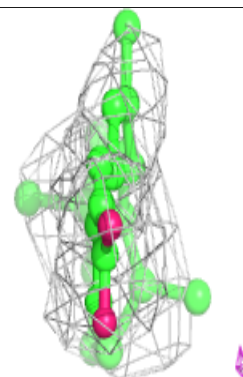
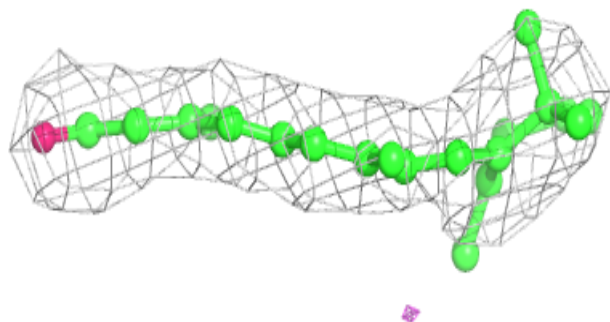
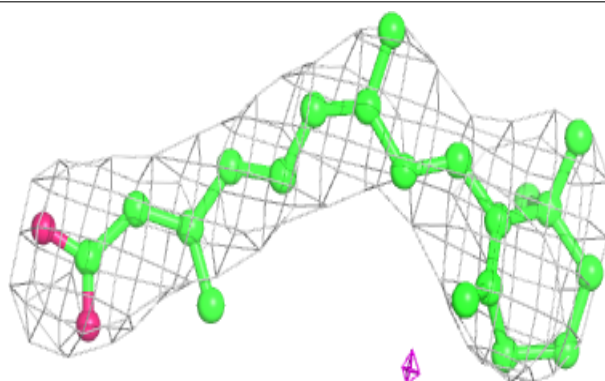


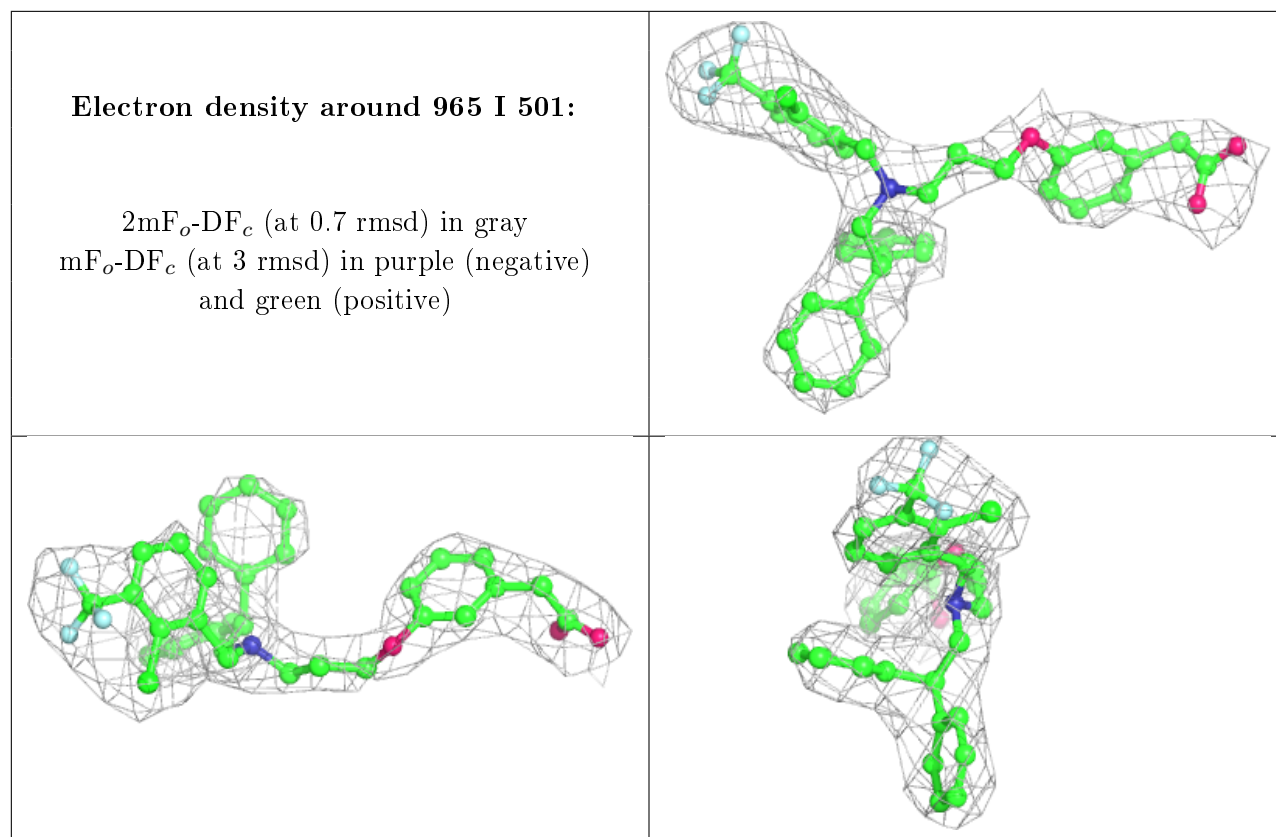
Electron density around 965 B 501:

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

**Electron density around 9CR A 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.