



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:23 PM UTC

PDB ID : 6A5Z / pdb_00006a5z
Title : Crystal structure of human FXR/RXR-LBD heterodimer bound to HNC180 and 9cRA and SRC1
Authors : Wang, N.; Liu, J.
Deposited on : 2018-06-25
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

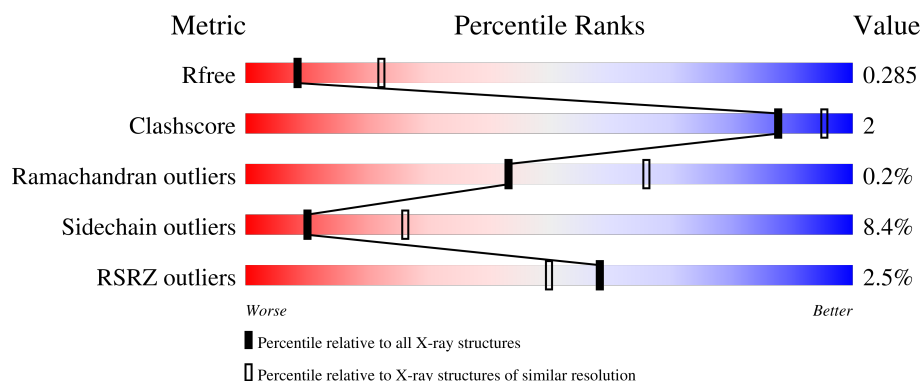
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



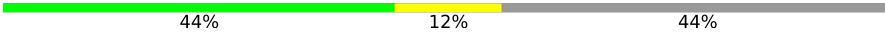
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	229	2% 85% 10% .
1	H	229	5% 86% 11% .
2	D	238	% 78% 10% . 11%
2	L	238	79% 8% 13%
3	E	16	6% 69% 25% 6%

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Mol	Chain	Length	Quality of chain
3	F	16	
3	G	16	
3	I	16	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7517 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 Bile acid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1808	1158	300	341	9			
1	H	224	Total	C	N	O	S	0	0	0
			1838	1174	307	348	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	GLU	CYS	engineered mutation	UNP Q96RI1
A	466	GLU	CYS	engineered mutation	UNP Q96RI1
H	432	GLU	CYS	engineered mutation	UNP Q96RI1
H	466	GLU	CYS	engineered mutation	UNP Q96RI1

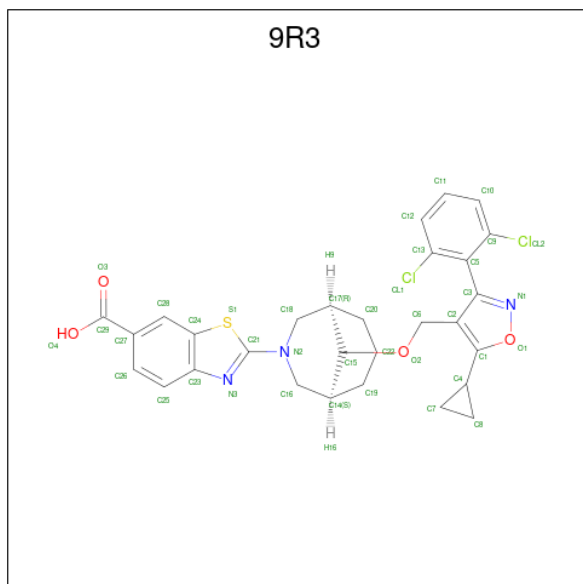
- Molecule 2 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	212	Total	C	N	O	S	0	1	0
			1684	1081	289	304	10			
2	L	208	Total	C	N	O	S	0	0	0
			1645	1058	282	295	10			

- Molecule 3 is a protein called Nuclear receptor coactivator 1.

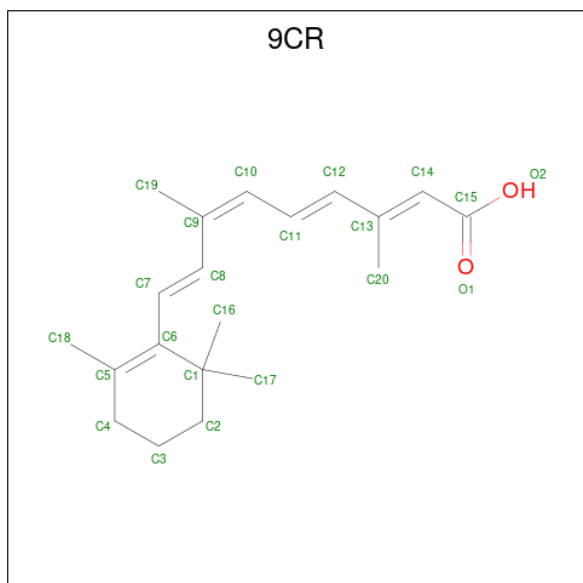
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	15	Total	C	N	O	0	0	0
			127	79	27	21			
3	F	11	Total	C	N	O	0	0	0
			94	60	20	14			
3	G	11	Total	C	N	O	0	0	0
			101	64	23	14			
3	I	9	Total	C	N	O	0	0	0
			81	53	18	10			

- Molecule 4 is 2-[(1R,5S)-9-[[3-[2,6-bis(chloranyl)phenyl]-5-cyclopropyl-1,2-oxazol-4-yl]methoxy]-3-azabicyclo[3.3.1]nonan-3-yl]-1,3-benzothiazole-6-carboxylic acid (CCD ID: 9R3) (formula: $C_{29}H_{27}Cl_2N_3O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			39	29	2	3	4	1		
4	H	1	Total	C	Cl	N	O	S	0	0
			39	29	2	3	4	1		

- Molecule 5 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: $C_{20}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			22	20	2		
5	L	1	Total	C	O	0	0
			22	20	2		

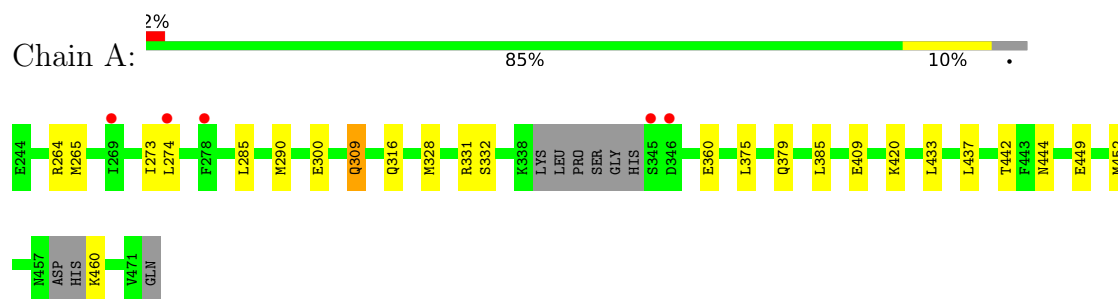
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	D	1	Total	O	0	0
			1	1		
6	H	8	Total	O	0	0
			8	8		
6	L	5	Total	O	0	0
			5	5		
6	I	1	Total	O	0	0
			1	1		

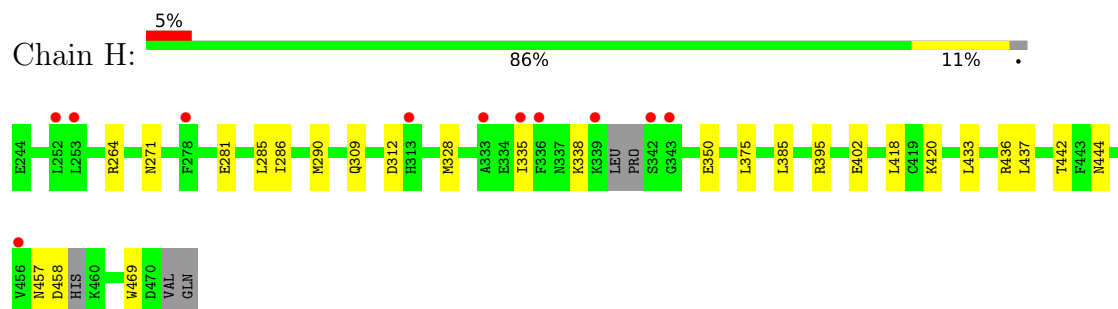
3 Residue-property plots [i](#)

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.

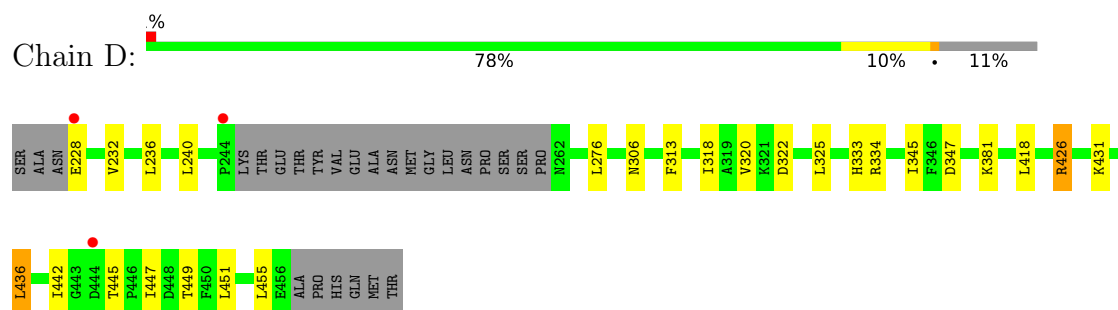
- Molecule 1: Bile acid receptor



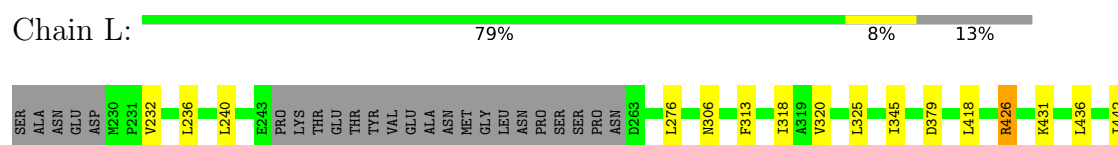
- Molecule 1: Bile acid receptor



- Molecule 2: Retinoic acid receptor RXR-alpha



- Molecule 2: Retinoic acid receptor RXR-alpha

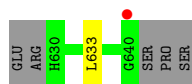




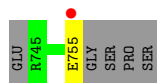
- Molecule 3: Nuclear receptor coactivator 1



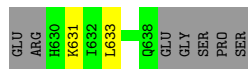
- Molecule 3: Nuclear receptor coactivator 1



- Molecule 3: Nuclear receptor coactivator 1



- Molecule 3: Nuclear receptor coactivator 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.53Å 96.13Å 114.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.55 – 2.95 73.55 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.3 (73.55-2.95) 97.3 (73.55-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.221 , 0.282 0.228 , 0.285	Depositor DCC
R_{free} test set	1070 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7517	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: 9R3, 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	0.69	0/1843	0.94	0/2488
1	H	0.66	0/1874	0.92	1/2528 (0.0%)
2	D	0.71	0/1721	0.94	0/2327
2	L	0.67	0/1677	0.94	0/2266
3	E	0.62	0/129	0.92	0/171
3	F	0.67	0/95	1.03	0/125
3	G	0.60	0/102	0.88	0/134
3	I	0.73	0/82	0.97	0/108
All	All	0.68	0/7523	0.94	1/10147 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	469	TRP	N-CA-C	-5.30	101.59	109.96

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	1808	0	1796	10	0
1	H	1838	0	1819	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1684	0	1716	5	0
2	L	1645	0	1686	3	0
3	E	127	0	131	1	0
3	F	94	0	100	0	0
3	G	101	0	110	0	0
3	I	81	0	91	0	0
4	A	39	0	0	2	0
4	H	39	0	0	3	0
5	D	22	0	23	3	0
5	L	22	0	23	2	0
6	A	2	0	0	0	0
6	D	1	0	0	0	0
6	H	8	0	0	0	0
6	I	1	0	0	0	0
6	L	5	0	0	0	0
All	All	7517	0	7495	30	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 2.

All (30) 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:309:GLN:HA	1:A:316:GLN:NE2	2.18	0.59
1:A:309:GLN:HA	1:A:316:GLN:HE22	1.70	0.57
1:H:328:MET:CE	4:H:501:9R3:CL1	2.90	0.56
1:A:265:MET:HE3	1:A:290:MET:HE2	1.88	0.56
1:A:328:MET:HE2	4:A:501:9R3:CL2	2.44	0.54
1:H:328:MET:HE2	4:H:501:9R3:CL1	2.45	0.53
1:A:375:LEU:HD13	1:A:433:LEU:HD23	1.91	0.53
1:A:385:LEU:HD22	1:A:437:LEU:HD21	1.92	0.52
2:D:322:ASP:O	2:D:333[B]:HIS:ND1	2.44	0.51
1:H:436:ARG:NH2	2:L:379:ASP:OD2	2.44	0.51
1:H:385:LEU:HD22	1:H:437:LEU:HD21	1.93	0.51
5:L:501:9CR:H25	5:L:501:9CR:O1	2.11	0.50
1:H:328:MET:HE3	4:H:501:9R3:CL1	2.50	0.48
1:H:375:LEU:HD13	1:H:433:LEU:HD23	1.94	0.48
1:A:444:ASN:C	1:A:444:ASN:HD22	2.23	0.46
1:H:444:ASN:HD22	1:H:444:ASN:C	2.22	0.45
2:D:447:ILE:HG23	2:D:451:LEU:HD23	1.99	0.44
1:A:449:GLU:HA	1:A:452:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:286:ILE:HG22	1:H:290:MET:HE2	2.00	0.43
2:D:334:ARG:HD2	2:D:347:ASP:OD1	2.19	0.43
2:D:436:LEU:HD22	5:D:501:9CR:H16	2.01	0.43
2:L:447:ILE:HG23	2:L:451:LEU:HD23	2.00	0.42
3:E:754:GLN:HA	3:E:754:GLN:HE21	1.84	0.42
1:H:281:GLU:HG3	1:H:457:ASN:HD22	1.84	0.42
5:L:501:9CR:C8	5:L:501:9CR:H19	2.49	0.42
1:H:442:THR:CG2	2:L:426:ARG:HE	2.32	0.42
5:D:501:9CR:H13	5:D:501:9CR:H7	1.81	0.41
5:D:501:9CR:O2	5:D:501:9CR:H25	2.20	0.41
1:A:332:SER:HB3	4:A:501:9R3:C22	2.51	0.41
1:A:442:THR:CG2	2:D:426:ARG:HE	2.34	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	214/229 (93%)	201 (94%)	13 (6%)	0	100	100
1	H	218/229 (95%)	202 (93%)	16 (7%)	0	100	100
2	D	209/238 (88%)	202 (97%)	6 (3%)	1 (0%)	24	49
2	L	204/238 (86%)	198 (97%)	5 (2%)	1 (0%)	24	49
3	E	13/16 (81%)	9 (69%)	4 (31%)	0	100	100
3	F	9/16 (56%)	8 (89%)	1 (11%)	0	100	100
3	G	9/16 (56%)	7 (78%)	2 (22%)	0	100	100
3	I	7/16 (44%)	6 (86%)	1 (14%)	0	100	100
All	All	883/998 (88%)	833 (94%)	48 (5%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	445	THR
2	L	445	THR

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	202/212 (95%)	190 (94%)	12 (6%)	18	41
1	H	205/212 (97%)	192 (94%)	13 (6%)	16	38
2	D	184/205 (90%)	165 (90%)	19 (10%)	7	19
2	L	179/205 (87%)	162 (90%)	17 (10%)	8	22
3	E	14/15 (93%)	11 (79%)	3 (21%)	1	2
3	F	10/15 (67%)	9 (90%)	1 (10%)	7	20
3	G	11/15 (73%)	10 (91%)	1 (9%)	9	23
3	I	9/15 (60%)	7 (78%)	2 (22%)	1	2
All	All	814/894 (91%)	746 (92%)	68 (8%)	10	26

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ARG
1	A	273	ILE
1	A	274	LEU
1	A	285	LEU
1	A	300	GLU
1	A	309	GLN
1	A	331	ARG
1	A	360	GLU
1	A	379	GLN
1	A	409	GLU
1	A	420	LYS
1	A	460	LYS
2	D	228	GLU
2	D	232	VAL

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Mol	Chain	Res	Type
2	D	236	LEU
2	D	240	LEU
2	D	276	LEU
2	D	306	ASN
2	D	313	PHE
2	D	318	ILE
2	D	320	VAL
2	D	325	LEU
2	D	345	ILE
2	D	381	LYS
2	D	418	LEU
2	D	426	ARG
2	D	431	LYS
2	D	436	LEU
2	D	442	ILE
2	D	449	THR
2	D	455	LEU
1	H	264	ARG
1	H	271	ASN
1	H	285	LEU
1	H	309	GLN
1	H	312	ASP
1	H	335	ILE
1	H	338	LYS
1	H	350	GLU
1	H	395	ARG
1	H	402	GLU
1	H	418	LEU
1	H	420	LYS
1	H	458	ASP
2	L	232	VAL
2	L	236	LEU
2	L	240	LEU
2	L	276	LEU
2	L	306	ASN
2	L	313	PHE
2	L	318	ILE
2	L	320	VAL
2	L	325	LEU
2	L	345	ILE
2	L	418	LEU
2	L	426	ARG

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Mol	Chain	Res	Type
2	L	431	LYS
2	L	436	LEU
2	L	442	ILE
2	L	449	THR
2	L	455	LEU
3	E	745	ARG
3	E	747	LYS
3	E	757	SER
3	F	633	LEU
3	G	755	GLU
3	I	631	LYS
3	I	633	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	293	ASN
1	A	296	GLN
1	A	316	GLN
1	A	379	GLN
1	A	416	GLN
1	A	428	GLN
1	A	444	ASN
1	A	457	ASN
2	D	267	ASN
2	D	270	GLN
2	D	306	ASN
1	H	263	GLN
1	H	271	ASN
1	H	293	ASN
1	H	309	GLN
1	H	379	GLN
1	H	416	GLN
1	H	444	ASN
1	H	445	HIS
2	L	270	GLN
2	L	288	HIS
2	L	306	ASN
2	L	385	ASN
3	E	754	GLN
3	G	746	HIS

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Mol	Chain	Res	Type
3	I	638	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	9R3	A	501	-	45,45,45	1.94	7 (15%)	59,67,67	2.30	16 (27%)
5	9CR	D	501	-	22,22,22	4.43	9 (40%)	30,30,30	9.59	14 (46%)
5	9CR	L	501	-	22,22,22	4.05	7 (31%)	30,30,30	9.06	13 (43%)
4	9R3	H	501	-	45,45,45	2.09	7 (15%)	59,67,67	2.20	18 (30%)

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
4	9R3	A	501	-	-	1/21/45/45	0/8/7/7
5	9CR	D	501	-	-	9/15/32/32	0/1/1/1
5	9CR	L	501	-	-	8/15/32/32	0/1/1/1
4	9R3	H	501	-	-	5/21/45/45	0/8/7/7

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	501	9CR	C5-C6	12.60	1.55	1.34
5	D	501	9CR	C5-C6	12.06	1.54	1.34
4	H	501	9R3	C2-C1	10.92	1.47	1.34
5	D	501	9CR	C8-C9	-10.34	1.23	1.46
4	A	501	9R3	C2-C1	9.37	1.45	1.34
5	D	501	9CR	C12-C13	-8.30	1.28	1.46
5	L	501	9CR	C8-C9	-8.06	1.28	1.46
5	L	501	9CR	C12-C13	-7.61	1.29	1.46
5	D	501	9CR	C11-C10	-6.80	1.22	1.43
5	L	501	9CR	C11-C10	-6.19	1.24	1.43
5	D	501	9CR	C11-C12	-5.17	1.21	1.34
4	H	501	9R3	O1-N1	-4.24	1.34	1.42
4	A	501	9R3	O1-N1	-4.08	1.34	1.42
5	L	501	9CR	C11-C12	-4.01	1.24	1.34
5	D	501	9CR	C10-C9	-3.70	1.27	1.35
4	A	501	9R3	C9-CL2	2.72	1.80	1.73
4	H	501	9R3	C3-C2	2.66	1.50	1.42
5	L	501	9CR	C7-C6	2.64	1.54	1.45
4	A	501	9R3	C3-C2	2.64	1.49	1.42
4	A	501	9R3	C3-N1	2.59	1.36	1.31
5	D	501	9CR	C8-C7	-2.57	1.25	1.33
4	H	501	9R3	C3-N1	2.51	1.36	1.31
5	D	501	9CR	O2-C15	-2.49	1.24	1.30
4	A	501	9R3	C13-CL1	2.46	1.79	1.73
4	H	501	9R3	C21-N3	2.41	1.36	1.30
4	H	501	9R3	C13-CL1	2.38	1.79	1.73
4	H	501	9R3	C24-S1	-2.37	1.69	1.74
4	A	501	9R3	C21-N3	2.30	1.36	1.30
5	D	501	9CR	C7-C6	2.19	1.52	1.45
5	L	501	9CR	C10-C9	-2.14	1.30	1.35

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	501	9CR	C7-C8-C9	33.47	175.75	126.23
5	D	501	9CR	C11-C10-C9	31.76	171.82	127.28
5	D	501	9CR	C7-C8-C9	30.08	170.74	126.23
5	L	501	9CR	C11-C10-C9	25.62	163.21	127.28
5	D	501	9CR	C11-C12-C13	16.16	170.67	126.36
5	D	501	9CR	C10-C11-C12	15.69	168.65	123.20
5	L	501	9CR	C11-C12-C13	15.45	168.72	126.36
5	L	501	9CR	C10-C11-C12	13.28	161.68	123.20
5	D	501	9CR	C18-C5-C6	-13.10	110.19	124.48
5	L	501	9CR	C18-C5-C6	-11.45	111.99	124.48
5	L	501	9CR	C1-C6-C5	-7.34	112.61	122.64
4	A	501	9R3	C1-O1-N1	7.31	115.44	109.45
4	H	501	9R3	C7-C4-C1	-6.04	113.85	120.50
4	H	501	9R3	S1-C21-N2	5.98	127.22	119.32
4	A	501	9R3	C18-N2-C16	5.96	126.68	114.51
4	A	501	9R3	O1-C1-C2	-5.69	104.70	110.15
5	D	501	9CR	C1-C6-C5	-5.61	114.97	122.64
4	A	501	9R3	C5-C3-N1	5.49	127.48	119.67
4	A	501	9R3	C7-C4-C1	-5.44	114.52	120.50
5	D	501	9CR	C7-C6-C5	-5.13	109.74	121.56
4	H	501	9R3	C1-O1-N1	4.89	113.45	109.45
4	H	501	9R3	C5-C3-N1	4.87	126.60	119.67
5	L	501	9CR	C4-C5-C6	-4.83	116.17	122.70
5	D	501	9CR	C4-C5-C6	-4.58	116.52	122.70
4	H	501	9R3	O1-C1-C2	-4.51	105.83	110.15
4	H	501	9R3	C18-N2-C16	4.40	123.48	114.51
5	D	501	9CR	O2-C15-C14	4.36	126.37	113.40
5	D	501	9CR	O2-C15-O1	-4.10	114.36	122.70
5	L	501	9CR	C7-C6-C5	-3.95	112.45	121.56
4	A	501	9R3	C13-C5-C3	-3.66	117.65	121.58
5	D	501	9CR	C8-C9-C10	-3.31	113.81	119.01
5	D	501	9CR	C20-C13-C12	-3.21	113.18	118.09
5	L	501	9CR	C20-C13-C12	-3.13	113.30	118.09
4	A	501	9R3	O1-C1-C4	3.13	121.52	117.00
4	A	501	9R3	C5-C13-CL1	-3.08	115.65	119.62
4	H	501	9R3	O1-N1-C3	3.07	109.18	105.91
4	A	501	9R3	C18-N2-C21	-3.03	114.42	122.09
4	H	501	9R3	C16-C14-C15	2.96	114.58	109.60
5	L	501	9CR	C18-C5-C4	-2.92	107.38	113.60
4	A	501	9R3	C23-C24-S1	2.72	113.77	109.75
4	A	501	9R3	C16-C14-C15	2.70	114.15	109.60
4	H	501	9R3	S1-C21-N3	-2.69	112.89	116.92
5	D	501	9CR	C1-C6-C7	-2.57	108.69	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	9R3	C8-C4-C1	-2.51	117.74	120.50
4	H	501	9R3	C16-N2-C21	-2.50	115.76	122.09
4	A	501	9R3	S1-C21-N2	2.49	122.61	119.32
4	H	501	9R3	C19-C22-C20	2.46	119.94	113.00
4	A	501	9R3	C9-C5-C13	2.38	120.02	116.70
5	L	501	9CR	C16-C1-C6	2.36	113.95	110.24
4	H	501	9R3	C26-C27-C29	-2.34	115.74	120.37
4	H	501	9R3	C23-C24-S1	2.29	113.13	109.75
4	H	501	9R3	N2-C21-N3	-2.29	119.86	124.34
4	A	501	9R3	C5-C3-C2	-2.23	124.59	129.54
4	H	501	9R3	C8-C4-C1	-2.21	118.07	120.50
4	A	501	9R3	C12-C13-CL1	2.21	122.77	118.42
4	H	501	9R3	C14-C16-N2	2.19	116.02	111.86
5	L	501	9CR	O2-C15-O1	-2.18	118.27	122.70
5	D	501	9CR	C19-C9-C10	2.17	126.33	122.82
4	H	501	9R3	C20-C17-C15	2.13	113.55	109.91
5	L	501	9CR	C1-C6-C7	-2.08	110.01	115.65
4	H	501	9R3	O1-C1-C4	2.08	120.00	117.00

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	501	9CR	C11-C10-C9-C8
5	D	501	9CR	C11-C10-C9-C19
5	D	501	9CR	C10-C11-C12-C13
5	L	501	9CR	C10-C11-C12-C13
4	H	501	9R3	C26-C27-C29-O3
4	H	501	9R3	C28-C27-C29-O3
4	H	501	9R3	C28-C27-C29-O4
4	H	501	9R3	C26-C27-C29-O4
5	D	501	9CR	C9-C10-C11-C12
5	L	501	9CR	C9-C10-C11-C12
5	D	501	9CR	C11-C12-C13-C20
5	D	501	9CR	C11-C12-C13-C14
5	L	501	9CR	C1-C6-C7-C8
5	L	501	9CR	C11-C10-C9-C19
5	D	501	9CR	C7-C8-C9-C19
5	L	501	9CR	C6-C7-C8-C9
5	L	501	9CR	C7-C8-C9-C19
5	D	501	9CR	C7-C8-C9-C10
5	L	501	9CR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	L	501	9CR	C11-C10-C9-C8
5	D	501	9CR	C5-C6-C7-C8
4	A	501	9R3	C3-C2-C6-O2
4	H	501	9R3	C3-C2-C6-O2

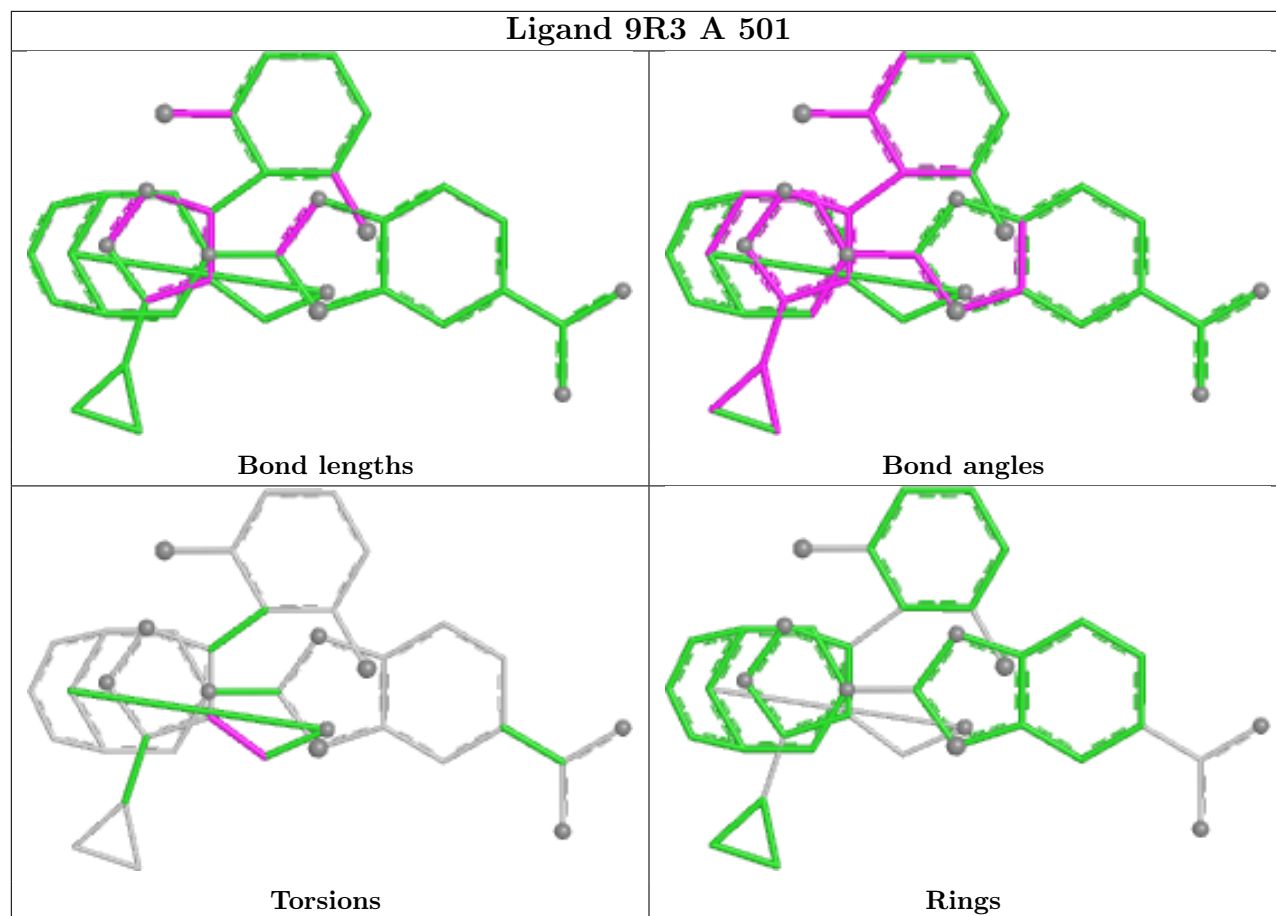
There are no ring outliers.

4 monomers are involved in 10 short contacts:

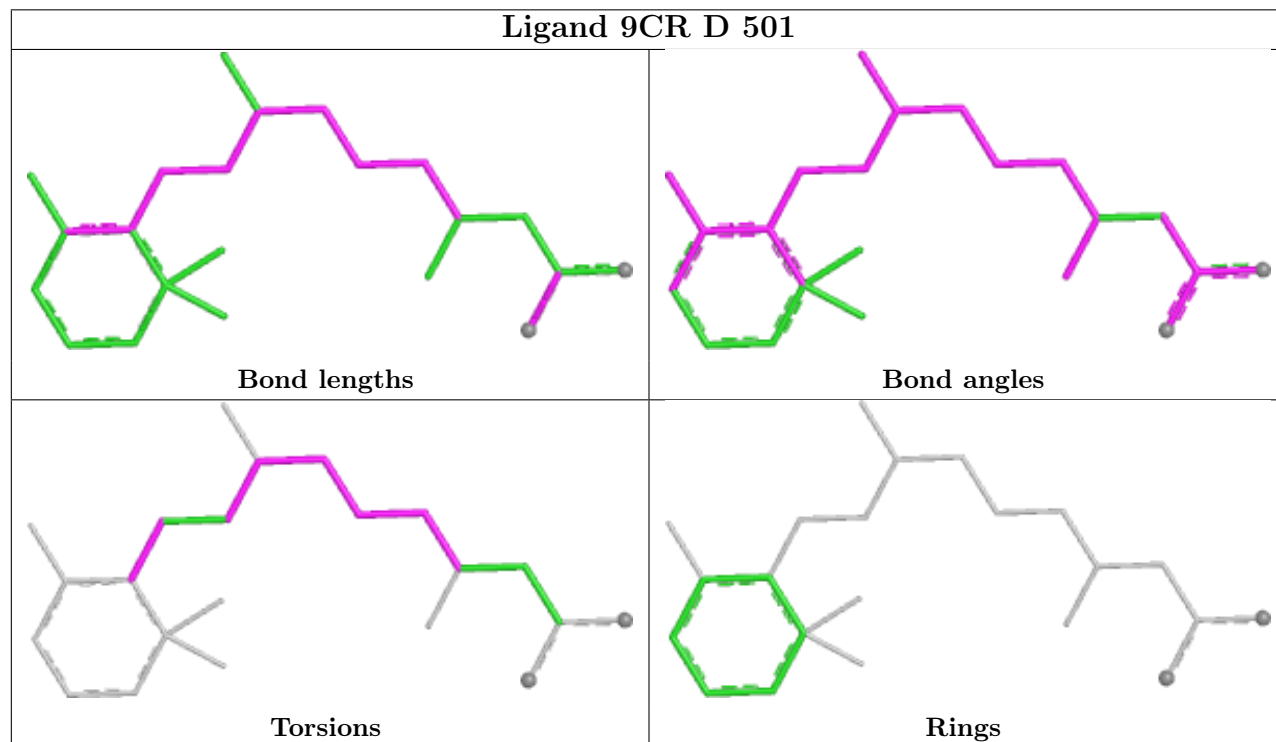
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	9R3	2	0
5	D	501	9CR	3	0
5	L	501	9CR	2	0
4	H	501	9R3	3	0

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.

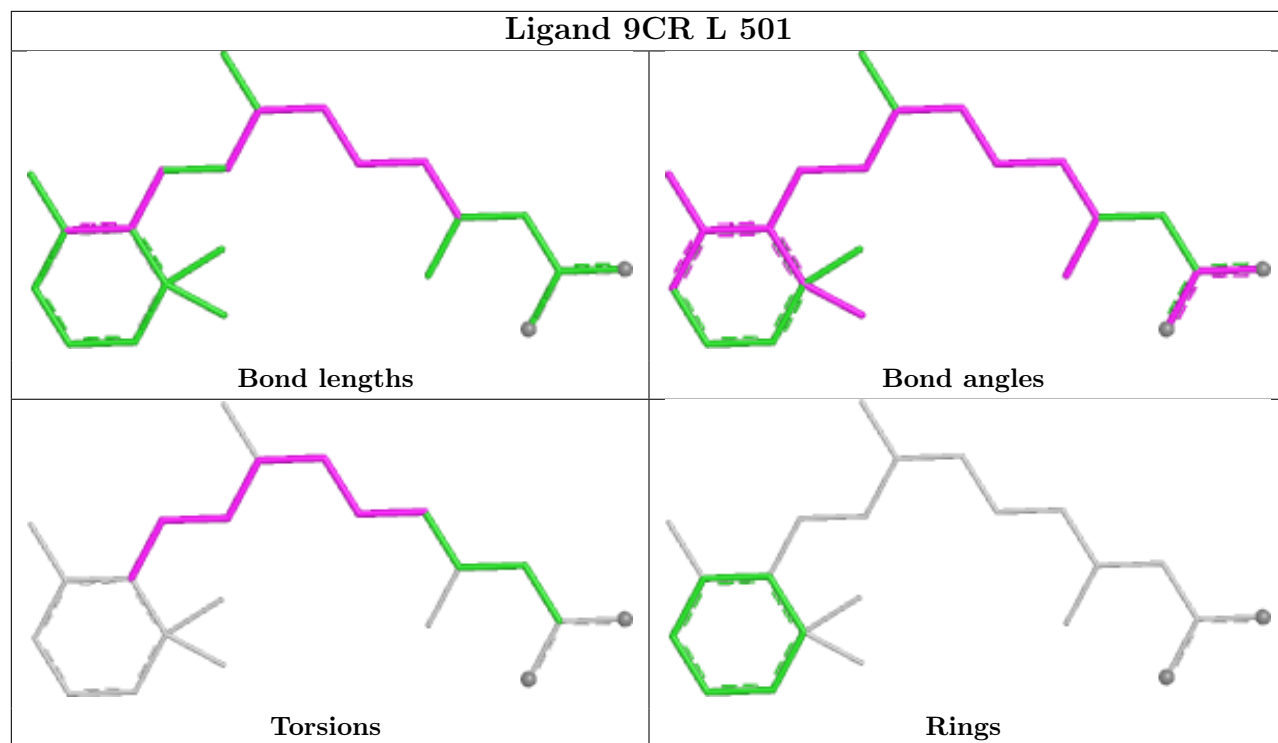
Ligand 9R3 A 501



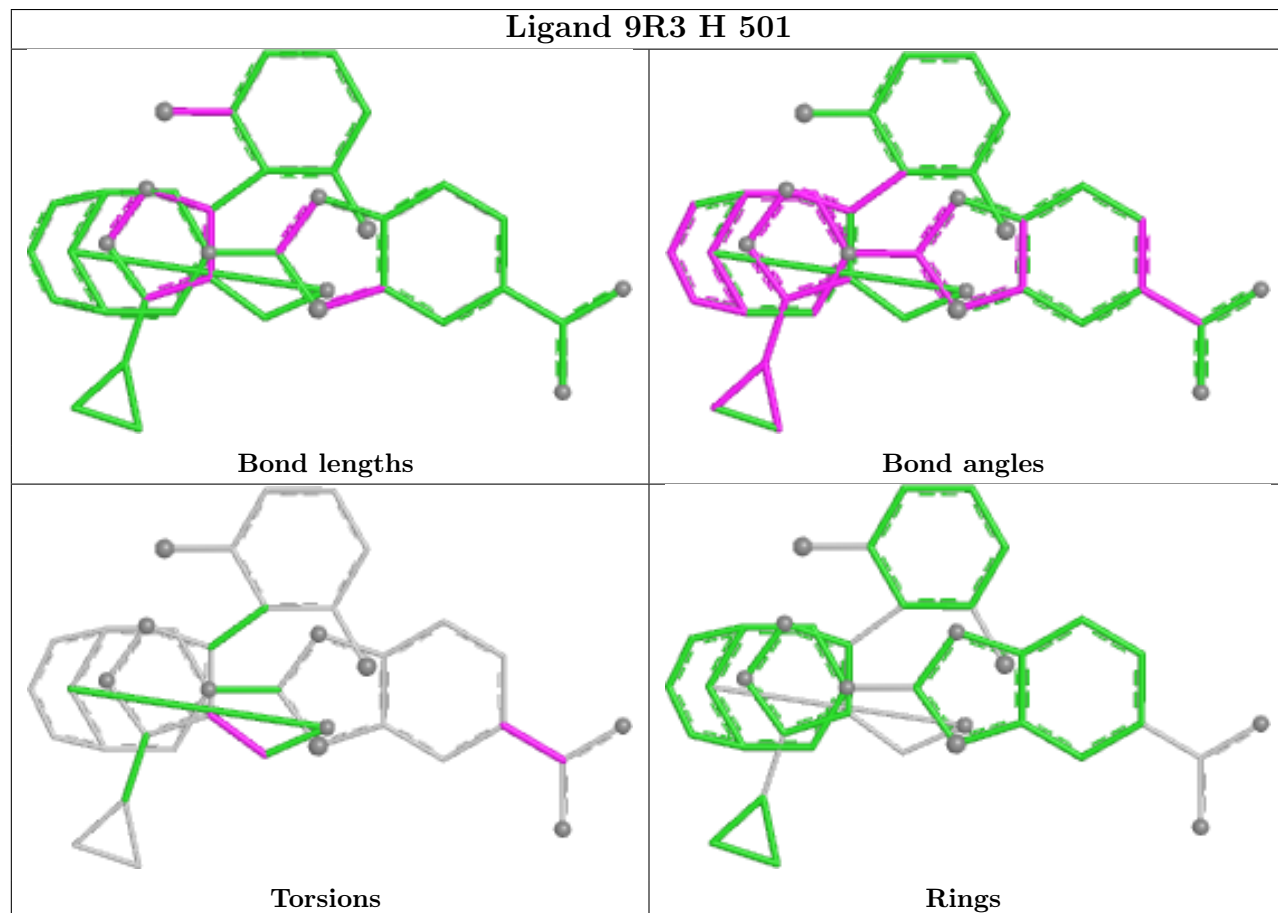
Ligand 9CR D 501



Ligand 9CR L 501



Ligand 9R3 H 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	220/229 (96%)	0.27	5 (2%) 61 53	24, 51, 102, 124	0
1	H	224/229 (97%)	0.73	11 (4%) 35 29	39, 71, 112, 133	0
2	D	212/238 (89%)	-0.09	3 (1%) 73 67	16, 37, 62, 97	1 (0%)
2	L	208/238 (87%)	0.03	1 (0%) 87 83	29, 44, 66, 89	0
3	E	15/16 (93%)	0.52	1 (6%) 24 20	46, 58, 96, 97	0
3	F	11/16 (68%)	0.39	1 (9%) 15 13	37, 47, 99, 109	0
3	G	11/16 (68%)	1.33	1 (9%) 15 13	79, 91, 113, 118	0
3	I	9/16 (56%)	-0.39	0 100 100	32, 40, 53, 57	0
All	All	910/998 (91%)	0.26	23 (2%) 58 50	16, 50, 102, 133	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	333	ALA	4.0
2	D	244	PRO	3.6
1	H	335	ILE	3.2
1	A	274	LEU	3.2
1	H	343	GLY	3.2
3	F	640	GLY	3.1
1	H	342	SER	3.1
1	H	253	LEU	3.0
1	H	336	PHE	2.8
1	A	345	SER	2.8
3	G	755	GLU	2.6
1	H	252	LEU	2.6
2	D	228	GLU	2.5
3	E	758	PRO	2.5
1	H	278	PHE	2.4
1	H	313	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	339	LYS	2.3
2	D	444	ASP	2.3
1	A	346	ASP	2.2
2	L	444	ASP	2.2
1	A	278	PHE	2.2
1	H	456	VAL	2.1
1	A	269	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

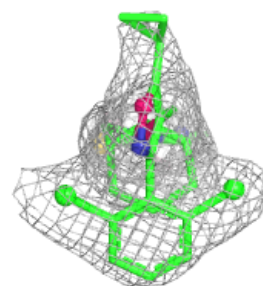
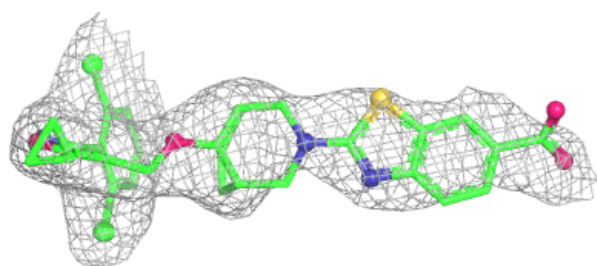
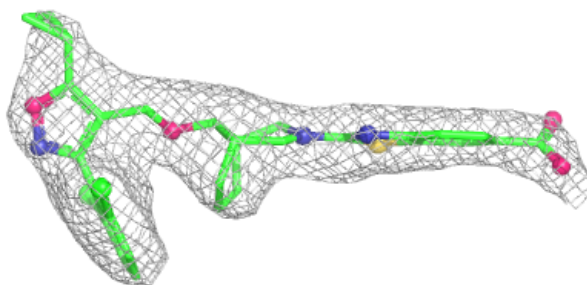
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	9R3	H	501	39/39	0.89	0.12	46,54,76,83	0
4	9R3	A	501	39/39	0.92	0.09	33,37,51,52	0
5	9CR	L	501	22/22	0.93	0.10	28,31,38,39	0
5	9CR	D	501	22/22	0.94	0.11	30,34,36,37	0

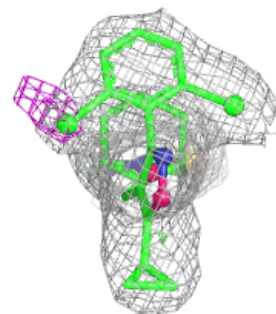
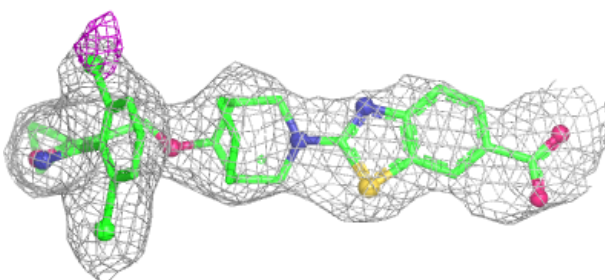
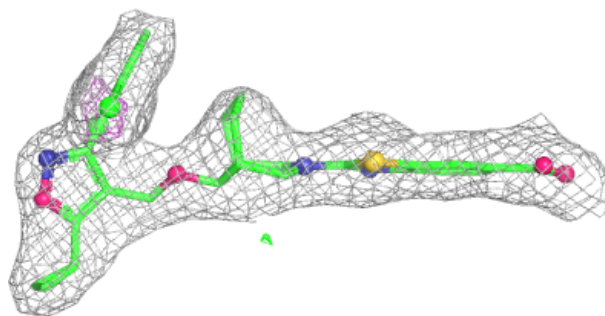
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9R3 H 501:

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

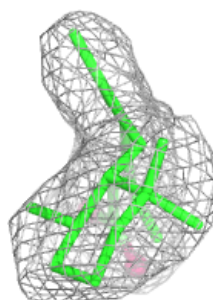
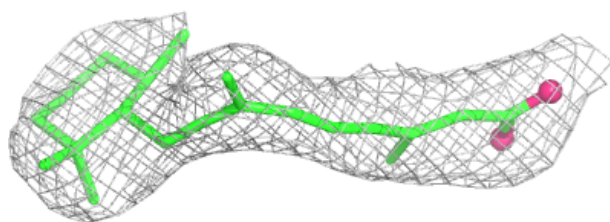
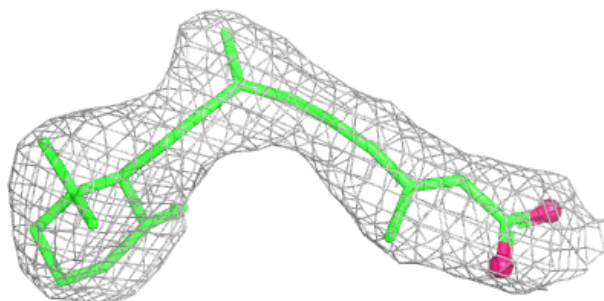
**Electron density around 9R3 A 501:**

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

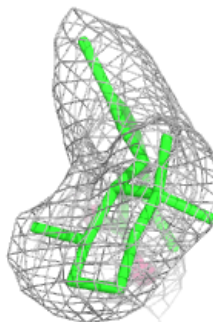
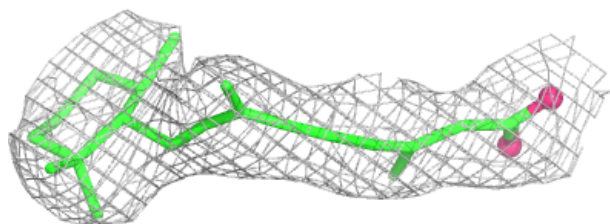
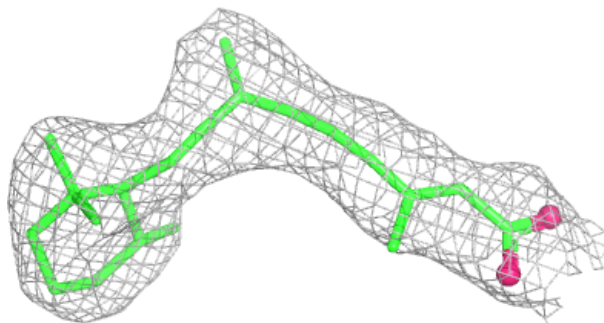


Electron density around 9CR L 501:

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

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

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



6.5 Other polymers [i](#)

There are no such residues in this entry.