Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:43 pm BST

PDB ID	:	5Z12
Title	:	A structure of FXR/RXR
Authors	:	Lu, Y.; Li, Y.
Deposited on	:	2017-12-23
Resolution	:	2.75 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:

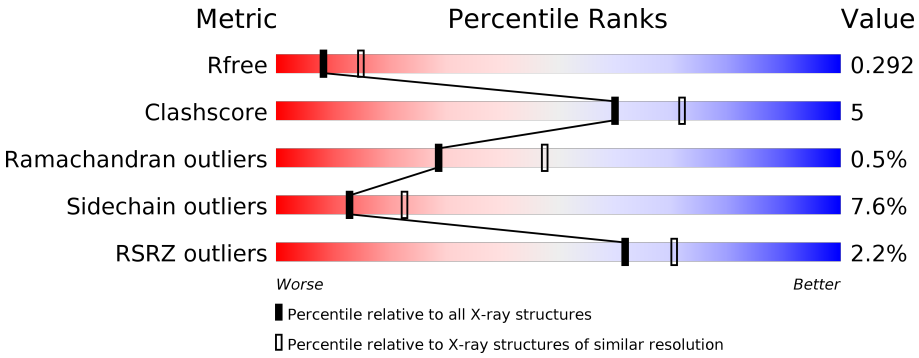
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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	228	85% 12%
1	D	228	5% 86% 11%
2	B	231	2% 82% 11% 6%
2	C	231	80% 8% 12%
3	F	9	44% 33% 22%
3	I	9	11% 44% 56%

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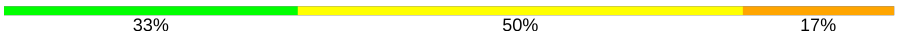
Mol	Chain	Length	Quality of chain
4	H	6	
4	J	6	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7405 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	223	Total	C	N	O	S	0	0	0
			1828	1172	304	341	11			
1	D	223	Total	C	N	O	S	0	0	0
			1816	1165	302	338	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	203	Total	C	N	O	S	0	0	0
			1596	1029	274	284	9			
2	B	217	Total	C	N	O	S	0	0	0
			1714	1099	293	312	10			

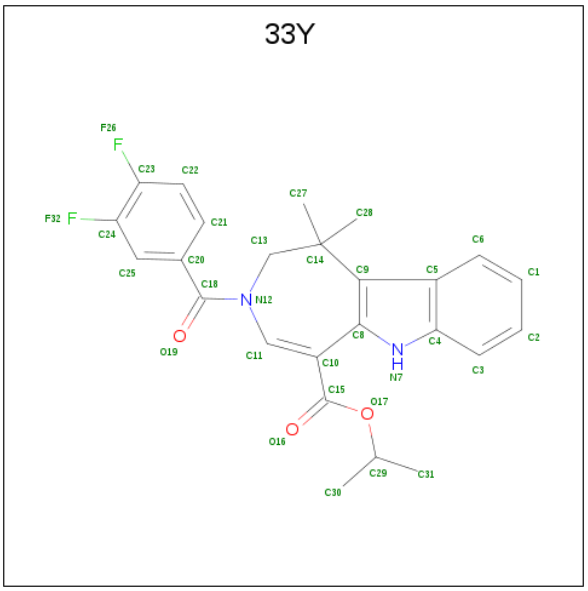
- Molecule 3 is a protein called Peptide from Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	9	Total	C	N	O	0	0	0
			81	53	18	10			
3	I	9	Total	C	N	O	0	0	0
			81	53	18	10			

- Molecule 4 is a protein called Peptide from Nuclear receptor coactivator 2.

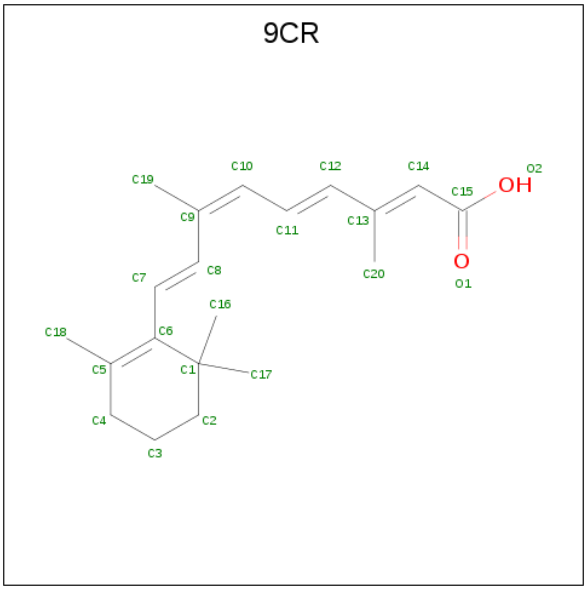
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	6	Total	C	N	O	0	0	0
			56	36	14	6			
4	H	6	Total	C	N	O	0	0	0
			56	36	14	6			

- Molecule 5 is 1-methylethyl 3-[(3,4-difluorophenyl)carbonyl]-1,1-dimethyl-1,2,3,6-tetrahydro azepino[4,5-b]indole-5-carboxylate (three-letter code: 33Y) (formula: $C_{25}H_{24}F_2N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			32	25	2	2	3		
5	D	1	Total	C	F	N	O	0	0
			32	25	2	2	3		

- Molecule 6 is (9cis)-retinoic acid (three-letter code: 9CR) (formula: $C_{20}H_{28}O_2$).



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

- Molecule 7 is water.

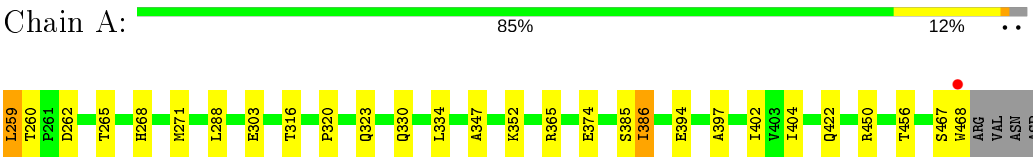
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	20	Total O 20 20	0	0
7	C	18	Total O 18 18	0	0
7	D	14	Total O 14 14	0	0
7	B	17	Total O 17 17	0	0

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.

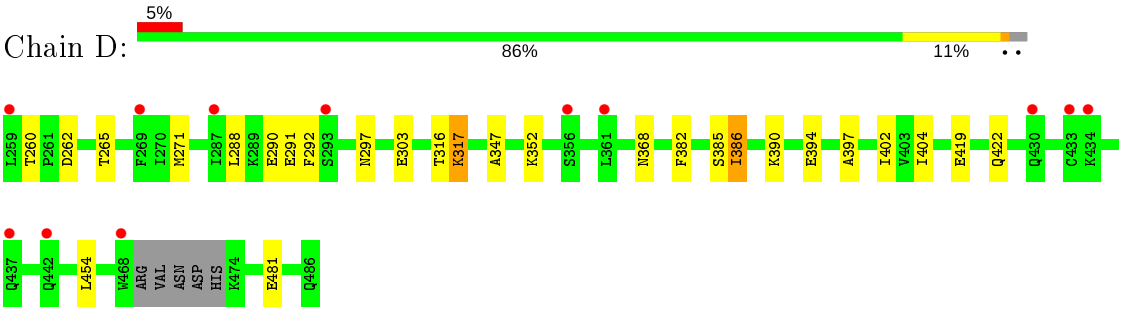
- Molecule 1: Bile acid receptor

Chain A:



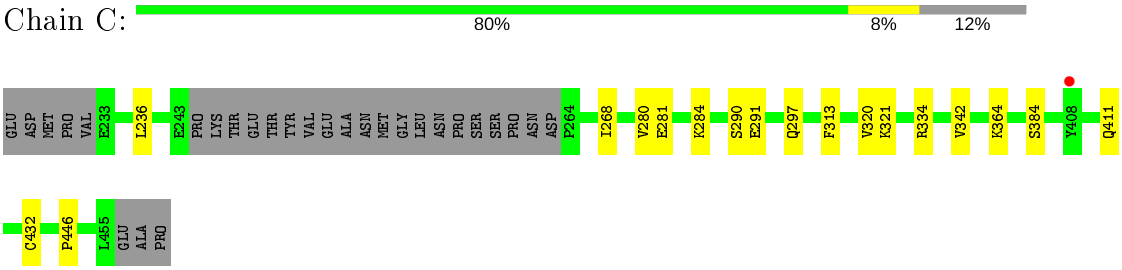
- Molecule 1: Bile acid receptor

Chain D:



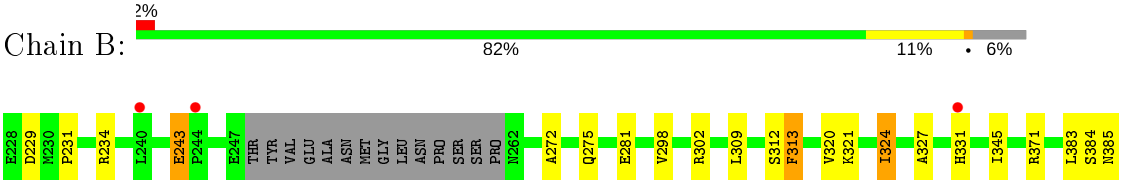
- Molecule 2: Retinoic acid receptor RXR-alpha

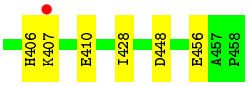
Chain C:



- Molecule 2: Retinoic acid receptor RXR-alpha

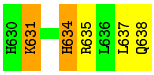
Chain B:





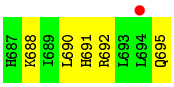
• Molecule 3: Peptide from Nuclear receptor coactivator 2

Chain F:



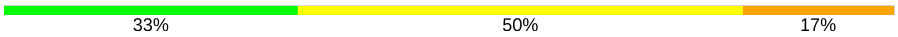
• Molecule 3: Peptide from Nuclear receptor coactivator 2

Chain I:



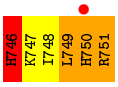
• Molecule 4: Peptide from Nuclear receptor coactivator 2

Chain J:



• Molecule 4: Peptide from Nuclear receptor coactivator 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.87Å 95.48Å 116.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 49.80 – 2.75	Depositor EDS
% Data completeness (in resolution range)	70.9 (50.00-2.75) 70.9 (49.80-2.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.50 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.230 , 0.290 0.230 , 0.292	Depositor DCC
R_{free} test set	968 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7405	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6786e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 9CR, 33Y

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	0.52	0/1866	0.73	0/2519
1	D	0.51	0/1854	0.74	0/2505
2	B	0.54	0/1748	0.76	1/2364 (0.0%)
2	C	0.50	0/1627	0.75	0/2198
3	F	0.67	0/82	0.94	0/108
3	I	0.64	0/82	1.05	2/108 (1.9%)
4	H	0.75	0/57	1.38	1/74 (1.4%)
4	J	0.64	0/57	1.22	0/74
All	All	0.52	0/7373	0.76	4/9950 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	2
4	H	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	749	LEU	CA-CB-CG	5.61	128.21	115.30
3	I	692	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	B	371	ARG	NE-CZ-NH1	5.21	122.91	120.30
3	I	692	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	PRO	Peptide
2	C	320	VAL	Peptide
2	C	321	LYS	Peptide
4	H	746	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1828	0	1830	9	0
1	D	1816	0	1809	11	0
2	B	1714	0	1747	11	0
2	C	1596	0	1637	8	0
3	F	81	0	91	7	0
3	I	81	0	91	0	0
4	H	56	0	61	20	0
4	J	56	0	61	2	0
5	A	32	0	24	1	0
5	D	32	0	24	1	0
6	B	22	0	27	5	0
6	C	22	0	27	6	0
7	A	20	0	0	1	0
7	B	17	0	0	0	0
7	C	18	0	0	0	0
7	D	14	0	0	1	0
All	All	7405	0	7429	68	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 (68) 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)
4:H:746:HIS:HA	4:H:750:HIS:CD2	1.75	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:LEU:HB3	6:B:501:9CR:H27	1.54	0.87
4:H:746:HIS:HA	4:H:750:HIS:NE2	1.90	0.85
6:C:501:9CR:O2	6:C:501:9CR:H25	1.78	0.83
1:D:481:GLU:OE2	4:H:746:HIS:N	2.17	0.77
4:H:746:HIS:HA	4:H:750:HIS:HD2	1.49	0.71
6:B:501:9CR:O2	6:B:501:9CR:H25	1.90	0.70
4:H:746:HIS:CA	4:H:750:HIS:CD2	2.68	0.69
2:C:268:ILE:HG21	6:C:501:9CR:H13	1.78	0.65
4:H:746:HIS:CA	4:H:750:HIS:NE2	2.60	0.65
1:A:402:ILE:HG23	1:A:422:GLN:HE21	1.64	0.63
2:B:231:PRO:HG2	2:B:234:ARG:HB3	1.85	0.58
1:D:317:LYS:HD3	4:H:751:ARG:HB3	1.86	0.58
4:H:746:HIS:O	4:H:750:HIS:NE2	2.36	0.58
4:H:746:HIS:N	4:H:749:LEU:CB	2.68	0.57
4:H:746:HIS:CA	4:H:750:HIS:HE2	2.16	0.56
1:A:271:MET:HE1	1:A:397:ALA:HB3	1.87	0.56
2:B:272:ALA:HA	6:B:501:9CR:H26	1.90	0.54
1:D:402:ILE:HG23	1:D:422:GLN:HE21	1.72	0.54
3:F:631:LYS:O	3:F:634:HIS:CD2	2.61	0.54
1:D:347:ALA:HB1	1:D:386:ILE:HG12	1.90	0.54
1:D:271:MET:HE1	1:D:397:ALA:HB3	1.90	0.53
4:H:747:LYS:HG3	4:H:748:ILE:HG23	1.91	0.52
6:B:501:9CR:H8	6:B:501:9CR:H13	1.90	0.52
4:H:746:HIS:C	4:H:750:HIS:HE2	2.11	0.52
5:A:501:33Y:H6	5:A:501:33Y:H128	1.91	0.52
2:C:432:CYS:HB3	6:C:501:9CR:H7	1.90	0.52
2:C:280:VAL:HG13	3:F:637:LEU:HD22	1.92	0.51
4:H:746:HIS:N	4:H:749:LEU:H	2.10	0.50
1:A:334:LEU:HD13	4:J:749:LEU:HD11	1.94	0.49
1:D:271:MET:CE	1:D:394:GLU:HA	2.44	0.48
1:D:368:ASN:HB2	7:D:611:HOH:O	2.14	0.47
2:C:268:ILE:HD13	6:C:501:9CR:C16	2.45	0.47
1:D:382:PHE:CZ	1:D:454:LEU:HD13	2.49	0.47
4:H:746:HIS:N	4:H:749:LEU:N	2.62	0.47
2:B:298:VAL:O	2:B:302:ARG:HB2	2.14	0.47
1:A:347:ALA:HB1	1:A:386:ILE:HG12	1.96	0.47
1:D:290:GLU:O	1:D:292:PHE:CD2	2.68	0.46
1:A:271:MET:CE	1:A:394:GLU:HA	2.45	0.46
5:D:501:33Y:H6	5:D:501:33Y:H127	1.98	0.46
4:H:749:LEU:O	4:H:750:HIS:HB2	2.16	0.46
1:A:450:ARG:HD2	1:A:450:ARG:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:VAL:HG21	6:C:501:9CR:C3	2.46	0.46
4:H:746:HIS:N	4:H:749:LEU:HB2	2.30	0.45
2:B:302:ARG:NH2	2:B:456:GLU:O	2.51	0.44
1:D:316:THR:HG22	1:D:404:ILE:HG21	1.99	0.44
2:C:342:VAL:CG2	6:C:501:9CR:H4	2.48	0.44
2:B:313:PHE:CE1	2:B:324:ILE:HG12	2.53	0.43
2:B:345:ILE:HD11	2:B:428:ILE:HG23	2.00	0.43
2:B:313:PHE:CD1	2:B:313:PHE:C	2.93	0.42
4:H:746:HIS:N	4:H:749:LEU:HB3	2.34	0.42
4:H:749:LEU:HD12	4:H:751:ARG:HH21	1.84	0.42
3:F:634:HIS:HD2	3:F:635:ARG:N	2.17	0.42
3:F:634:HIS:CD2	3:F:635:ARG:N	2.87	0.42
3:F:637:LEU:O	3:F:638:GLN:HG2	2.20	0.42
2:B:275:GLN:NE2	2:B:327:ALA:HB1	2.34	0.42
2:B:275:GLN:HG3	6:B:501:9CR:O2	2.20	0.42
1:D:271:MET:HE1	1:D:394:GLU:HA	2.01	0.42
2:C:297:GLN:HB3	3:F:637:LEU:HD11	2.02	0.42
4:J:746:HIS:O	4:J:750:HIS:N	2.47	0.41
1:A:323:GLN:HA	1:A:330:GLN:HE22	1.86	0.41
2:C:290:SER:HA	2:C:297:GLN:NE2	2.36	0.41
4:H:746:HIS:C	4:H:750:HIS:NE2	2.74	0.41
1:A:316:THR:HG22	1:A:404:ILE:HG21	2.02	0.41
2:B:320:VAL:HG11	2:B:331:HIS:CD2	2.55	0.41
1:A:259:LEU:N	7:A:601:HOH:O	2.54	0.40
3:F:634:HIS:O	3:F:638:GLN:N	2.54	0.40
4:H:746:HIS:C	4:H:746:HIS:CD2	2.95	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	219/228 (96%)	215 (98%)	4 (2%)	0	100 100
1	D	219/228 (96%)	210 (96%)	8 (4%)	1 (0%)	29 47
2	B	213/231 (92%)	198 (93%)	14 (7%)	1 (0%)	29 47
2	C	199/231 (86%)	184 (92%)	14 (7%)	1 (0%)	29 47
3	F	7/9 (78%)	7 (100%)	0	0	100 100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
4	H	4/6 (67%)	2 (50%)	1 (25%)	1 (25%)	0 0
4	J	4/6 (67%)	2 (50%)	2 (50%)	0	100 100
All	All	872/948 (92%)	824 (94%)	44 (5%)	4 (0%)	29 47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	291	GLU
4	H	750	HIS
2	B	243	GLU
2	C	446	PRO

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	206/211 (98%)	190 (92%)	16 (8%)	12 22
1	D	203/211 (96%)	191 (94%)	12 (6%)	19 34
2	B	187/199 (94%)	173 (92%)	14 (8%)	13 23
2	C	172/199 (86%)	163 (95%)	9 (5%)	23 39
3	F	9/9 (100%)	7 (78%)	2 (22%)	1 1
3	I	9/9 (100%)	5 (56%)	4 (44%)	0 0
4	H	6/6 (100%)	4 (67%)	2 (33%)	0 0
4	J	6/6 (100%)	4 (67%)	2 (33%)	0 0
All	All	798/850 (94%)	737 (92%)	61 (8%)	13 23

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	260	THR
1	A	262	ASP
1	A	265	THR
1	A	268	HIS
1	A	288	LEU
1	A	303	GLU
1	A	352	LYS
1	A	365	ARG
1	A	374	GLU
1	A	385	SER
1	A	386	ILE
1	A	456	THR
1	A	467	SER
1	A	468	TRP
1	A	486	GLN
2	C	236	LEU
2	C	281	GLU
2	C	284	LYS
2	C	291	GLU
2	C	313	PHE
2	C	334	ARG
2	C	364	LYS
2	C	384	SER
2	C	411	GLN
3	F	631	LYS
3	F	634	HIS
4	J	746	HIS
4	J	747	LYS
1	D	260	THR
1	D	262	ASP
1	D	265	THR
1	D	288	LEU
1	D	297	ASN
1	D	303	GLU
1	D	317	LYS
1	D	352	LYS
1	D	385	SER
1	D	386	ILE
1	D	390	LYS
1	D	419	GLU
4	H	746	HIS

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Mol	Chain	Res	Type
4	H	751	ARG
2	B	229	ASP
2	B	243	GLU
2	B	281	GLU
2	B	312	SER
2	B	313	PHE
2	B	321	LYS
2	B	324	ILE
2	B	383	LEU
2	B	384	SER
2	B	385	ASN
2	B	406	HIS
2	B	407	LYS
2	B	410	GLU
2	B	448	ASP
3	I	688	LYS
3	I	690	LEU
3	I	691	HIS
3	I	695	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	A	443	HIS
2	C	335	ASN
2	C	411	GLN
3	F	634	HIS
1	D	277	GLN
1	D	443	HIS
4	H	746	HIS
2	B	331	HIS
2	B	333	HIS
2	B	335	ASN
2	B	385	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
6	9CR	B	501	-	19,22,22	0.59	0	26,30,30	2.41	9 (34%)
5	33Y	D	501	-	29,35,35	1.51	2 (6%)	37,53,53	1.68	6 (16%)
5	33Y	A	501	-	29,35,35	1.74	3 (10%)	37,53,53	2.40	11 (29%)
6	9CR	C	501	-	19,22,22	0.84	0	26,30,30	3.41	15 (57%)

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
6	9CR	B	501	-	-	2/13/32/32	0/1/1/1
5	33Y	D	501	-	-	5/16/35/35	0/4/4/4
5	33Y	A	501	-	-	4/16/35/35	0/4/4/4
6	9CR	C	501	-	-	5/13/32/32	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	33Y	O17-C15	6.74	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	33Y	O17-C15	5.50	1.47	1.34
5	A	501	33Y	C8-C9	3.72	1.48	1.40
5	D	501	33Y	C8-C9	3.65	1.48	1.40
5	A	501	33Y	C14-C9	-3.34	1.49	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	33Y	O17-C15-C10	6.70	127.45	111.91
6	B	501	9CR	C7-C8-C9	-6.51	116.40	126.23
6	C	501	9CR	C8-C7-C6	-6.47	109.03	127.20
5	A	501	33Y	C20-C18-N12	6.27	124.64	118.38
6	C	501	9CR	C8-C9-C10	-6.09	109.59	118.94
6	C	501	9CR	C11-C10-C9	5.99	135.86	127.31
6	C	501	9CR	C19-C9-C8	5.51	126.76	118.08
6	B	501	9CR	C16-C1-C6	5.20	118.73	110.30
6	C	501	9CR	C10-C11-C12	-5.12	107.23	123.22
6	C	501	9CR	C20-C13-C12	-5.02	110.17	118.08
5	D	501	33Y	O17-C15-C10	4.84	123.12	111.91
5	A	501	33Y	O17-C15-O16	-4.63	114.49	123.32
5	A	501	33Y	C28-C14-C27	4.26	112.10	106.74
5	D	501	33Y	C13-C14-C9	-4.25	104.57	112.42
6	C	501	9CR	C16-C1-C6	4.14	117.01	110.30
5	A	501	33Y	C13-C14-C9	-4.07	104.91	112.42
5	A	501	33Y	C8-N7-C4	4.05	112.21	103.90
6	C	501	9CR	C11-C12-C13	3.97	137.56	126.42
6	C	501	9CR	C12-C13-C14	3.96	129.68	119.11
5	D	501	33Y	O16-C15-C10	-3.49	116.27	124.34
6	C	501	9CR	C2-C1-C6	-3.46	105.16	110.48
6	B	501	9CR	C10-C11-C12	-3.33	112.82	123.22
5	D	501	33Y	C27-C14-C9	3.26	115.83	110.55
6	B	501	9CR	C17-C1-C6	-3.25	105.02	110.30
6	B	501	9CR	C8-C9-C10	-3.25	113.95	118.94
6	C	501	9CR	C2-C3-C4	3.25	118.63	111.38
5	D	501	33Y	C8-N7-C4	3.23	110.54	103.90
6	C	501	9CR	C17-C1-C6	3.13	115.37	110.30
6	B	501	9CR	C1-C6-C7	3.01	124.29	115.78
5	A	501	33Y	O16-C15-C10	-2.73	118.03	124.34
5	A	501	33Y	O19-C18-C20	-2.63	115.11	120.23
6	C	501	9CR	C1-C6-C5	-2.59	118.96	122.61
5	A	501	33Y	O17-C29-C30	2.58	114.00	107.14
6	B	501	9CR	C7-C6-C5	-2.48	115.44	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	33Y	C20-C18-N12	2.35	120.73	118.38
5	A	501	33Y	C27-C14-C9	2.35	114.36	110.55
6	B	501	9CR	C18-C5-C6	-2.31	121.93	124.53
6	C	501	9CR	C18-C5-C6	-2.29	121.96	124.53
6	B	501	9CR	C19-C9-C8	2.25	121.63	118.08
6	C	501	9CR	C20-C13-C14	-2.23	119.98	124.64
5	A	501	33Y	C29-O17-C15	2.19	120.21	117.56

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	501	33Y	C20-C18-N12-C13
5	D	501	33Y	C20-C18-N12-C11
5	D	501	33Y	O19-C18-N12-C13
5	D	501	33Y	O19-C18-N12-C11
5	A	501	33Y	C10-C15-O17-C29
6	C	501	9CR	C11-C12-C13-C14
6	C	501	9CR	C11-C12-C13-C20
5	A	501	33Y	O16-C15-O17-C29
6	B	501	9CR	C7-C8-C9-C10
5	A	501	33Y	C30-C29-O17-C15
6	B	501	9CR	C7-C8-C9-C19
6	C	501	9CR	C1-C6-C7-C8
6	C	501	9CR	C5-C6-C7-C8
5	A	501	33Y	C31-C29-O17-C15
6	C	501	9CR	C7-C8-C9-C10
5	D	501	33Y	N12-C18-C20-C25

There are no ring outliers.

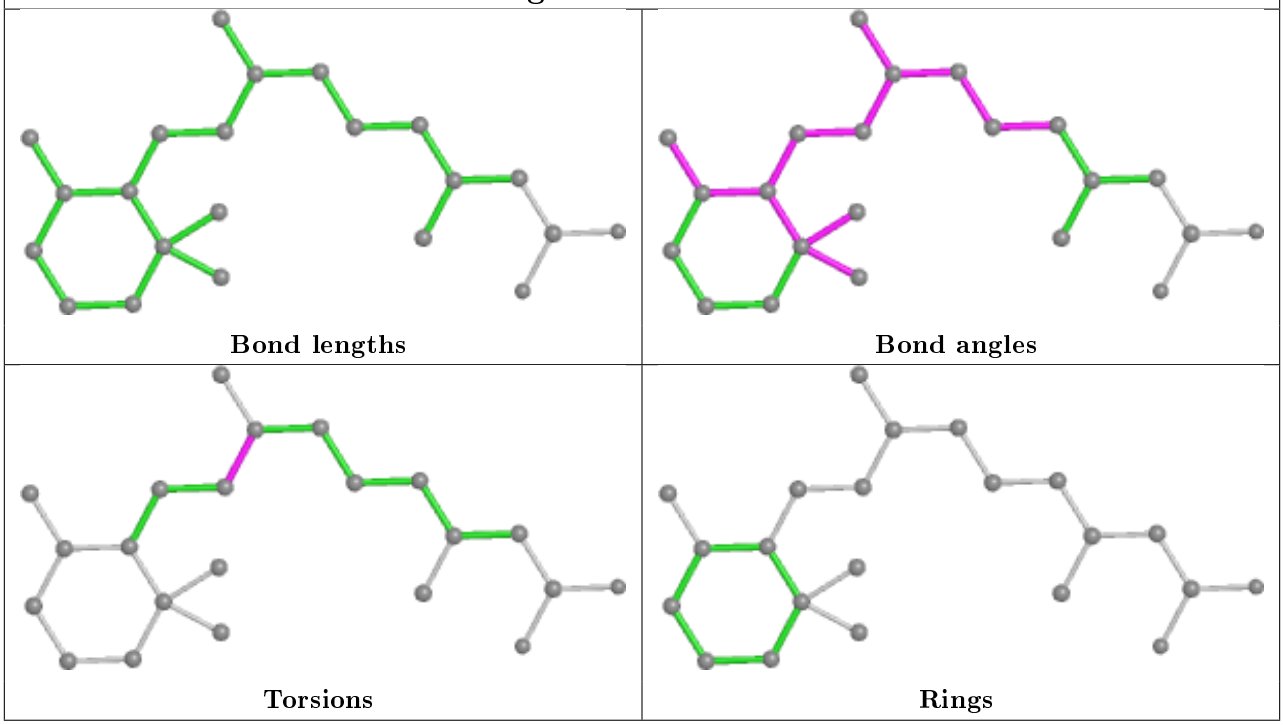
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	9CR	5	0
5	D	501	33Y	1	0
5	A	501	33Y	1	0
6	C	501	9CR	6	0

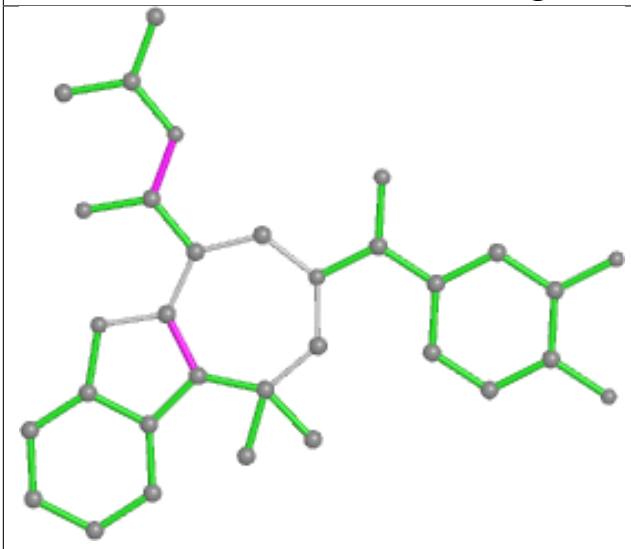
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

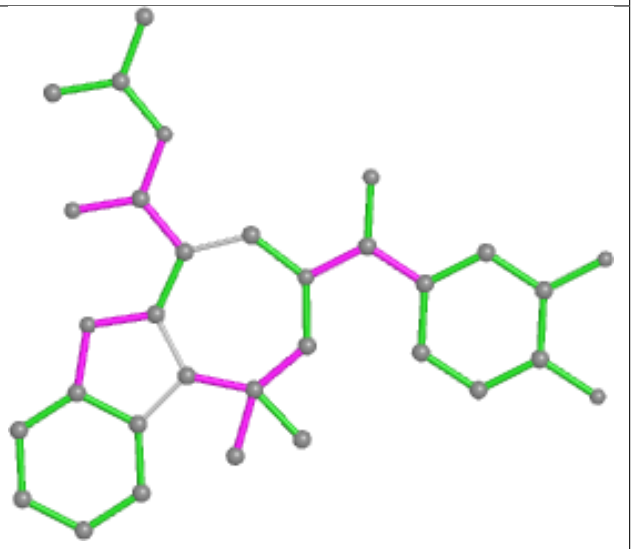
Ligand 9CR B 501



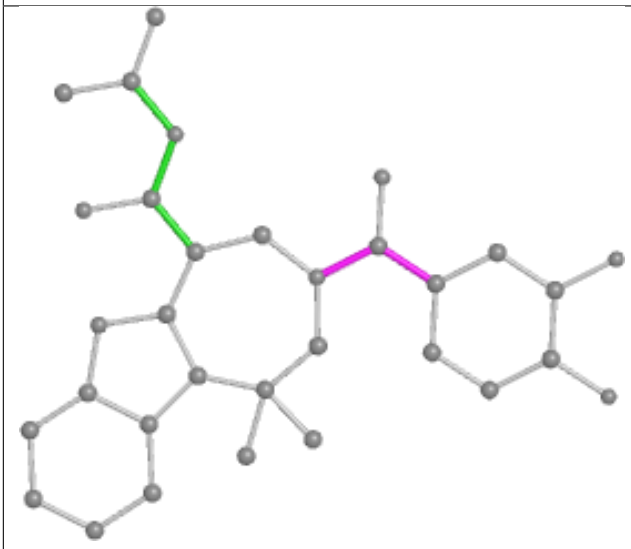
Ligand 33Y D 501



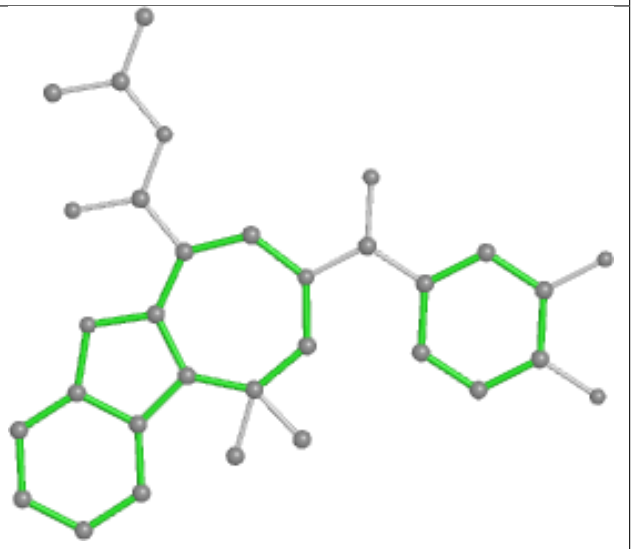
Bond lengths



Bond angles

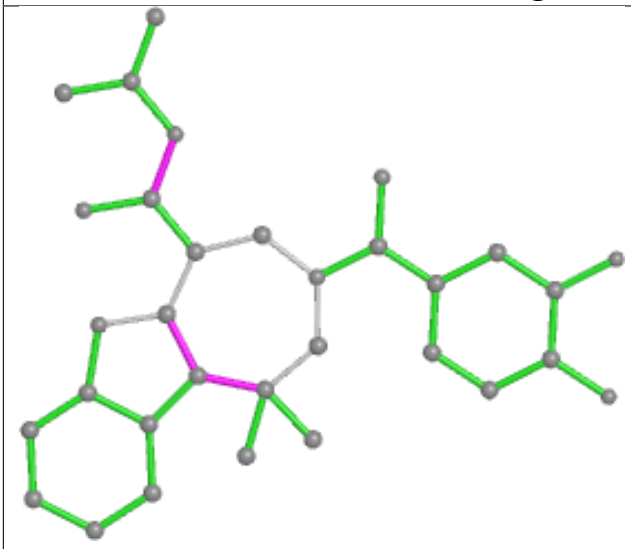


Torsions

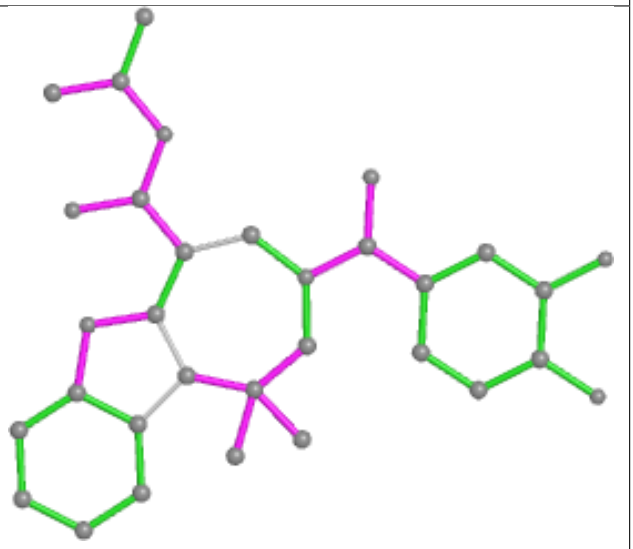


Rings

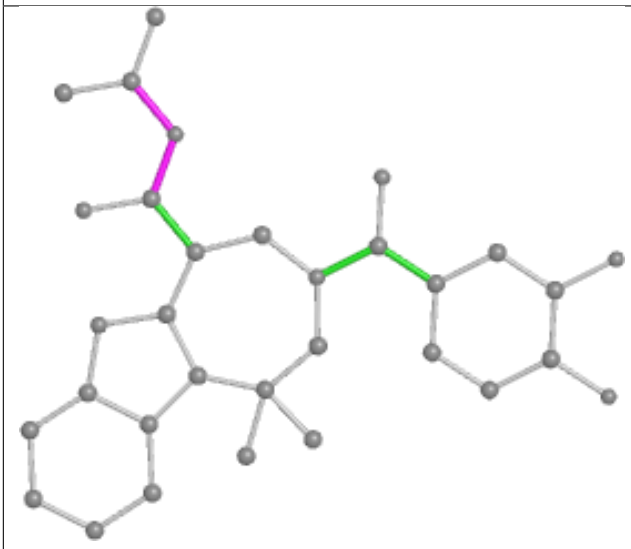
Ligand 33Y A 501



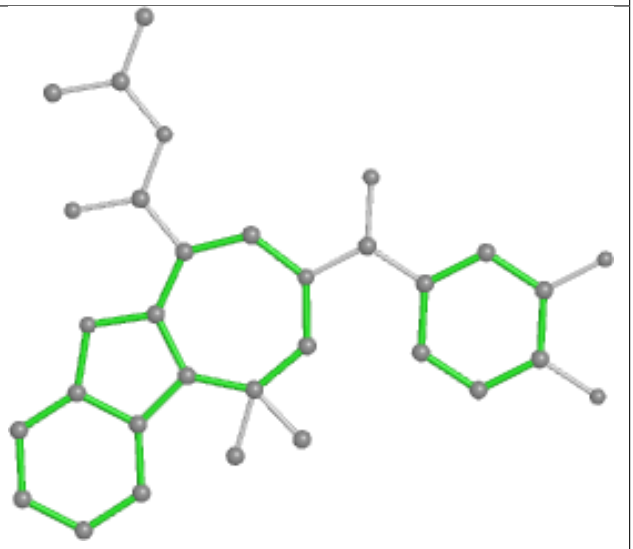
Bond lengths



Bond angles

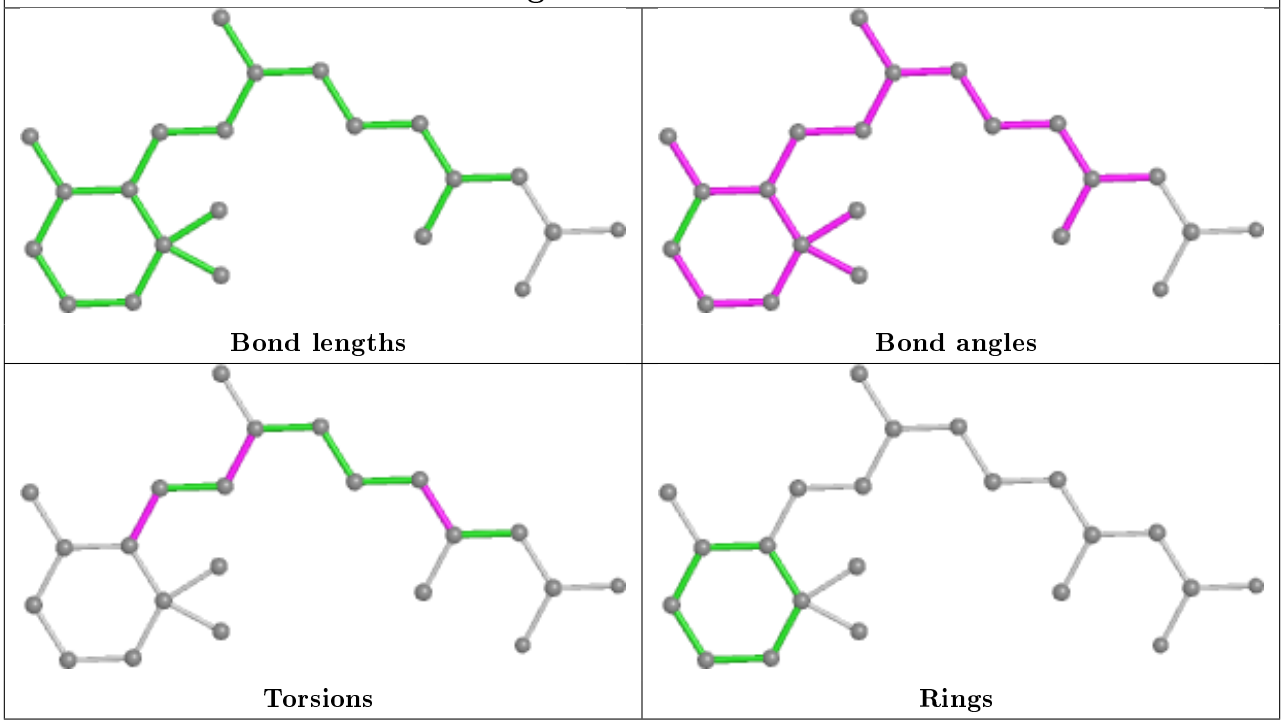


Torsions



Rings

Ligand 9CR C 501



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

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, 95^{th} 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	223/228 (97%)	-0.18	1 (0%) 92 95	13, 38, 69, 87	0
1	D	223/228 (97%)	0.12	12 (5%) 25 31	22, 47, 86, 109	0
2	B	217/231 (93%)	-0.13	4 (1%) 68 76	16, 41, 72, 103	0
2	C	203/231 (87%)	-0.11	1 (0%) 91 94	18, 43, 72, 98	0
3	F	9/9 (100%)	0.19	0 100 100	41, 46, 60, 60	0
3	I	9/9 (100%)	0.24	1 (11%) 5 6	45, 55, 67, 76	0
4	H	6/6 (100%)	1.28	1 (16%) 1 1	65, 84, 87, 99	0
4	J	6/6 (100%)	0.36	0 100 100	48, 63, 69, 75	0
All	All	896/948 (94%)	-0.06	20 (2%) 62 70	13, 43, 75, 109	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	356	SER	5.7
1	D	434	LYS	3.6
1	D	468	TRP	3.4
2	B	407	LYS	3.4
2	C	408	TYR	3.2
1	D	430	GLN	3.0
3	I	694	LEU	2.8
1	D	259	LEU	2.8
2	B	240	LEU	2.7
1	A	468	TRP	2.6
1	D	269	PHE	2.6
1	D	437	GLN	2.4
1	D	287	ILE	2.3
4	H	750	HIS	2.3
1	D	293	SER	2.2
2	B	244	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	442	GLN	2.1
1	D	433	CYS	2.1
1	D	361	LEU	2.0
2	B	331	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

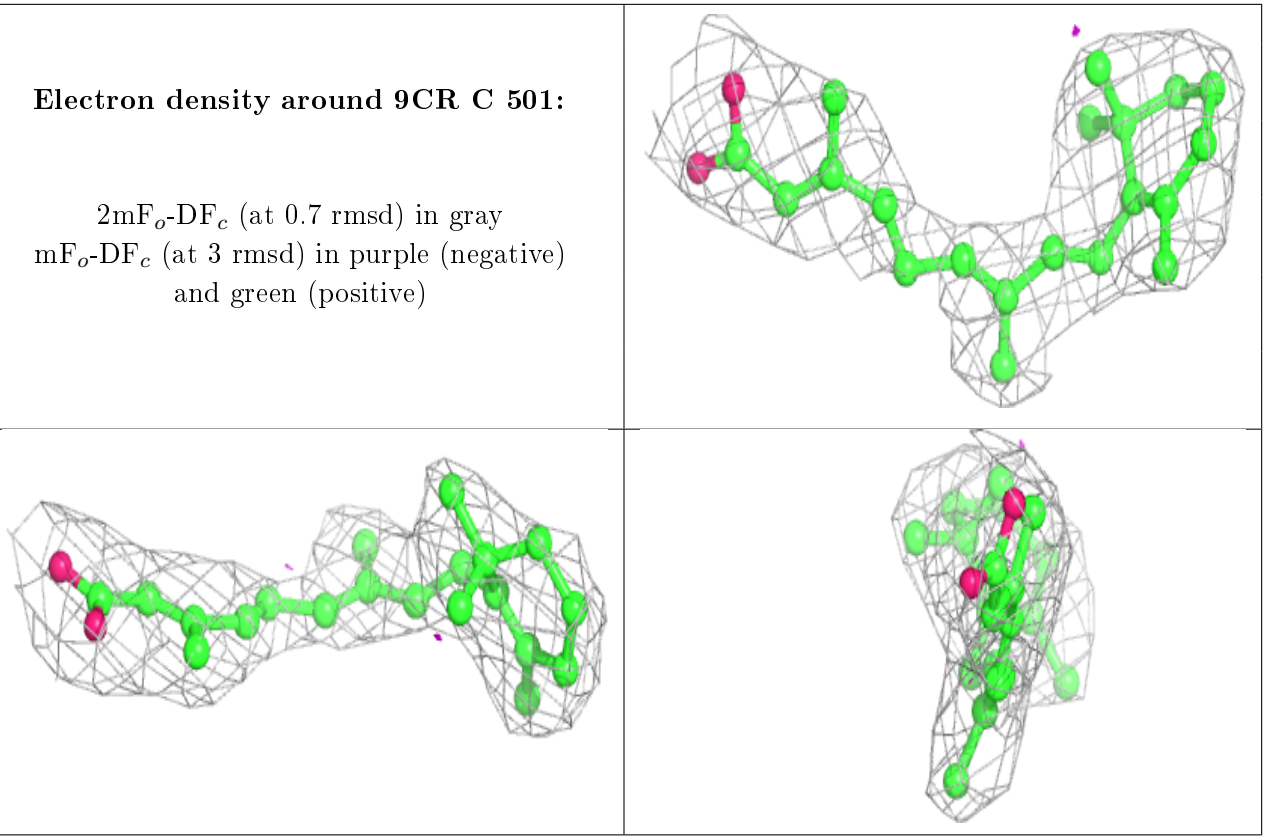
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	9CR	C	501	22/22	0.93	0.21	26,31,33,33	0
5	33Y	D	501	32/32	0.94	0.17	25,30,34,40	0
5	33Y	A	501	32/32	0.95	0.16	17,19,24,26	0
6	9CR	B	501	22/22	0.95	0.21	26,30,33,33	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.

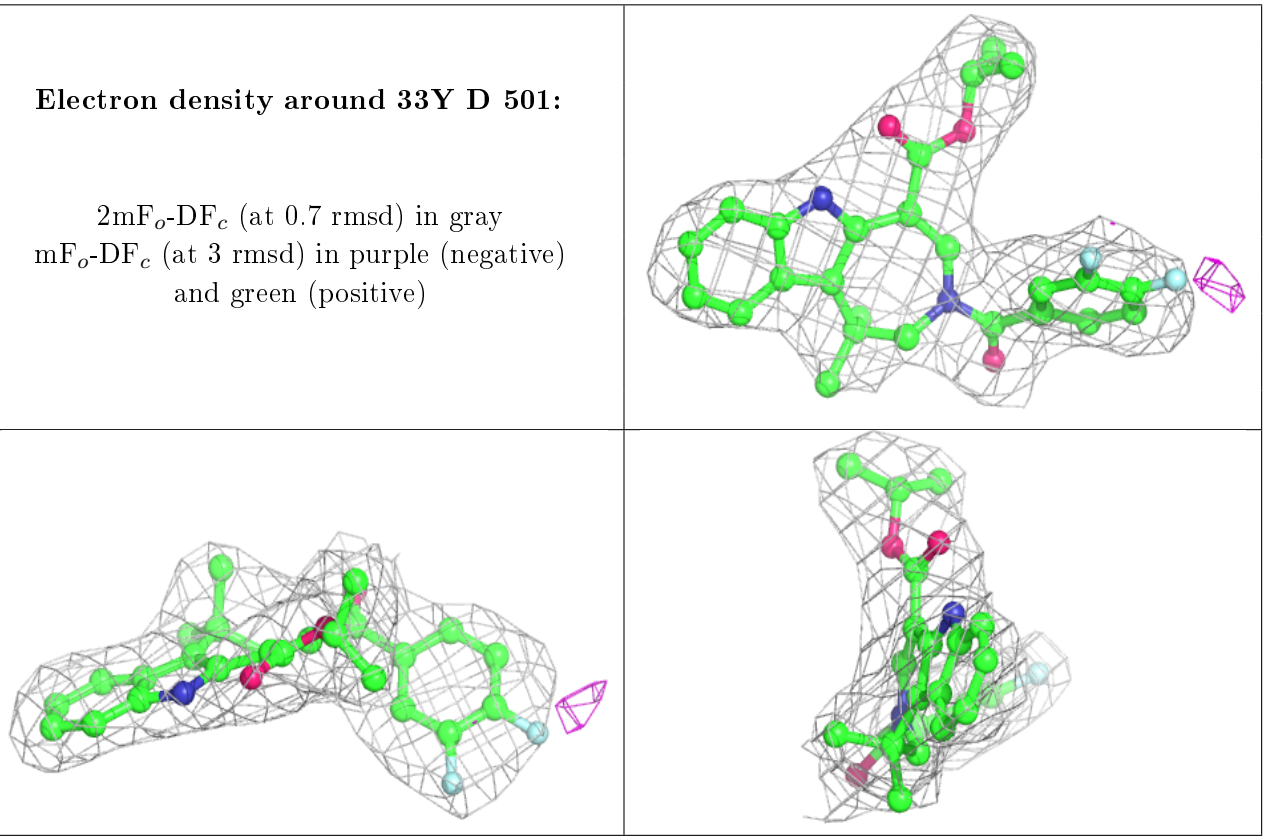
Electron density around 9CR C 501:

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



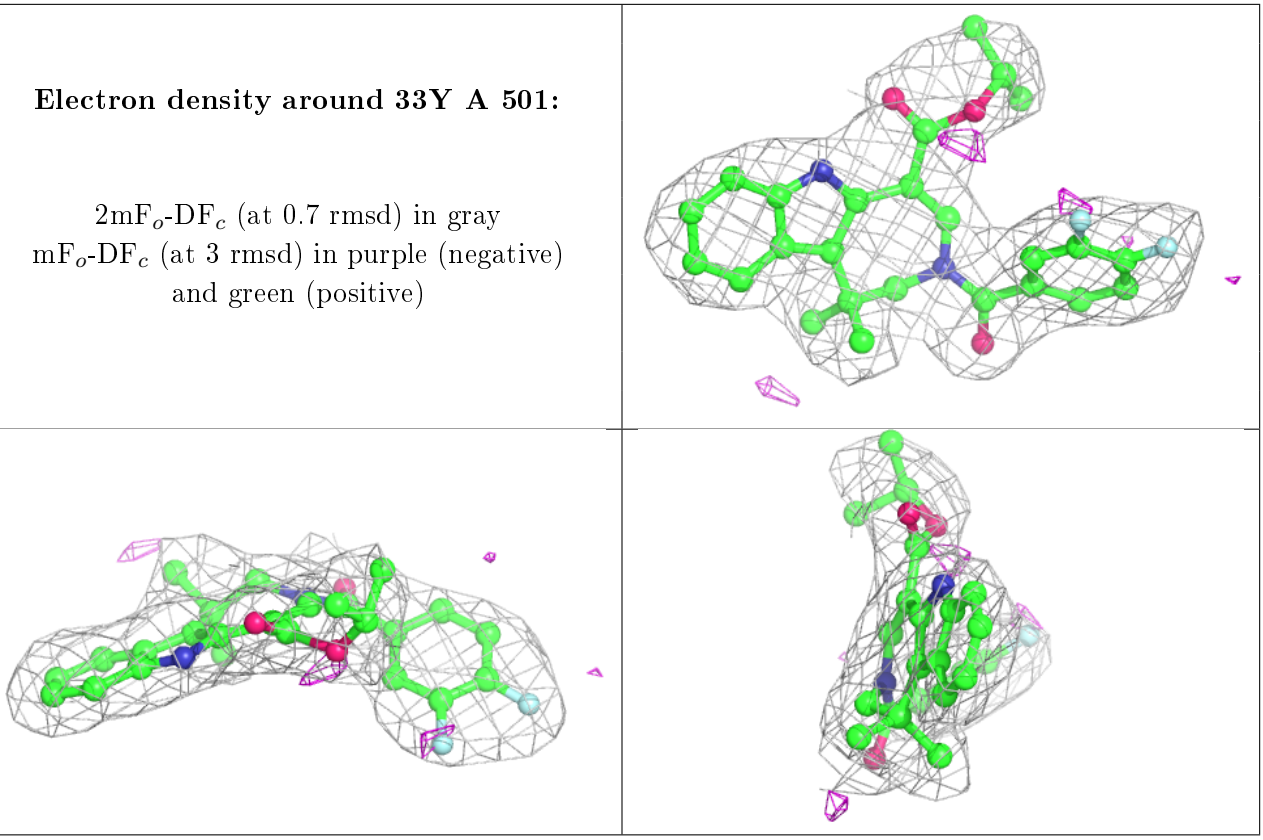
Electron density around 33Y D 501:

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



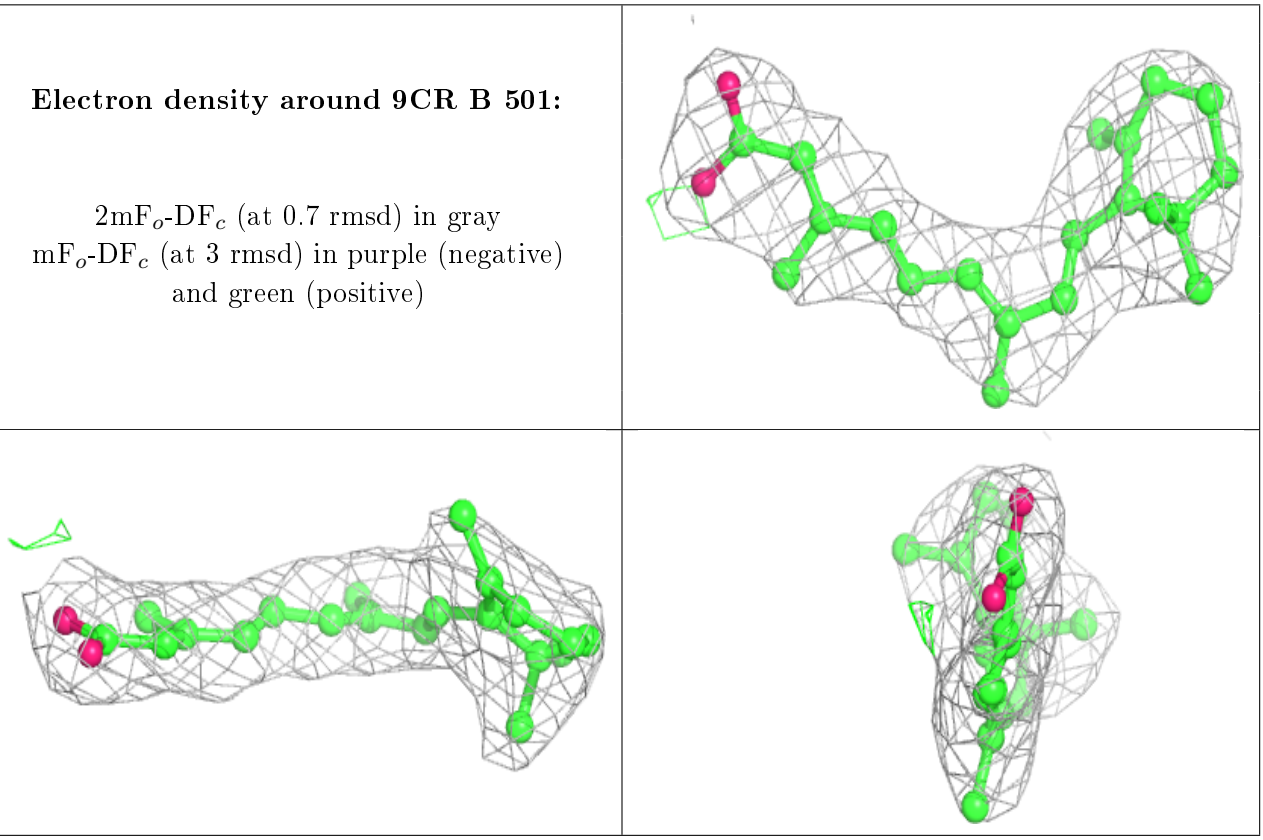
Electron density around 33Y A 501:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.