



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:06 AM UTC

PDB ID : 1XIU / pdb_00001xiu
Title : Crystal structure of the agonist-bound ligand-binding domain of Biomphalaria glabrata RXR
Authors : De Groot, A.; De Rosny, E.; Juillan-Binard, C.; Ferrer, J.-L.; Laudet, V.; Pebay-Peroula, E.; Fontecilla-Camps, J.-C.; Borel, F.
Deposited on : 2004-09-22
Resolution : 2.50 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

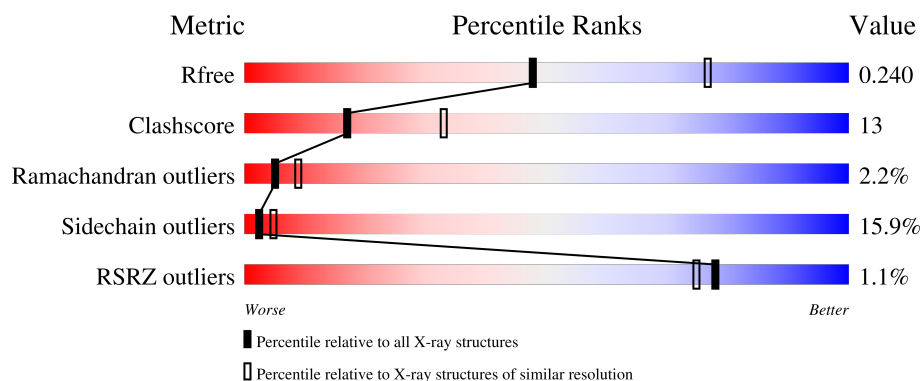
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

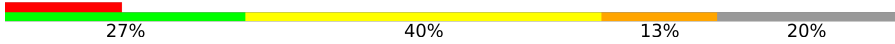
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	230	
1	B	230	
2	E	15	
2	F	15	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3782 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.

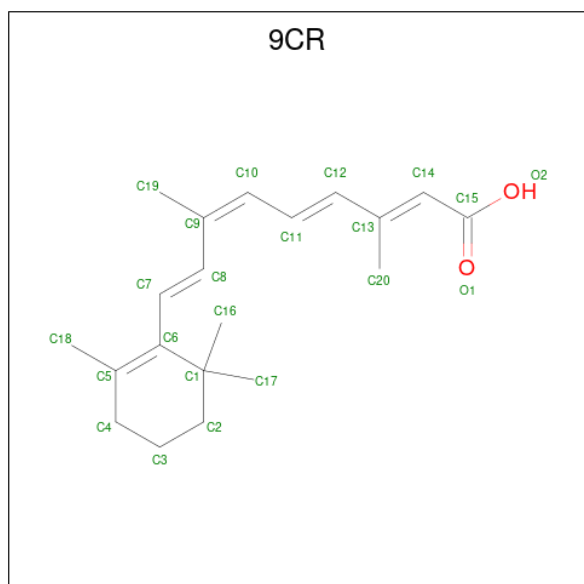
- Molecule 1 is a protein called RXR-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1748	1124	297	317	10			
1	B	224	Total	C	N	O	S	0	0	0
			1759	1132	300	317	10			

- Molecule 2 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	0	0	0
			100	63	21	16			
2	F	10	Total	C	N	O	0	0	0
			84	54	17	13			

- Molecule 3 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: C₂₀H₂₈O₂).



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

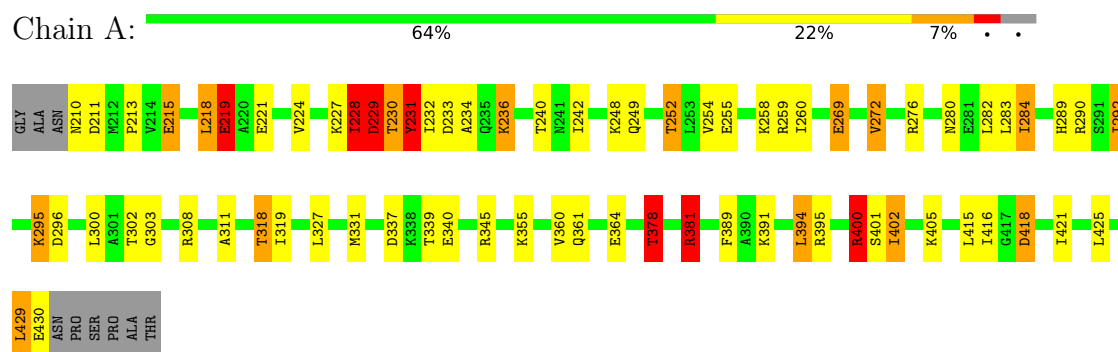
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	17	Total	O	0	0
			17	17		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		

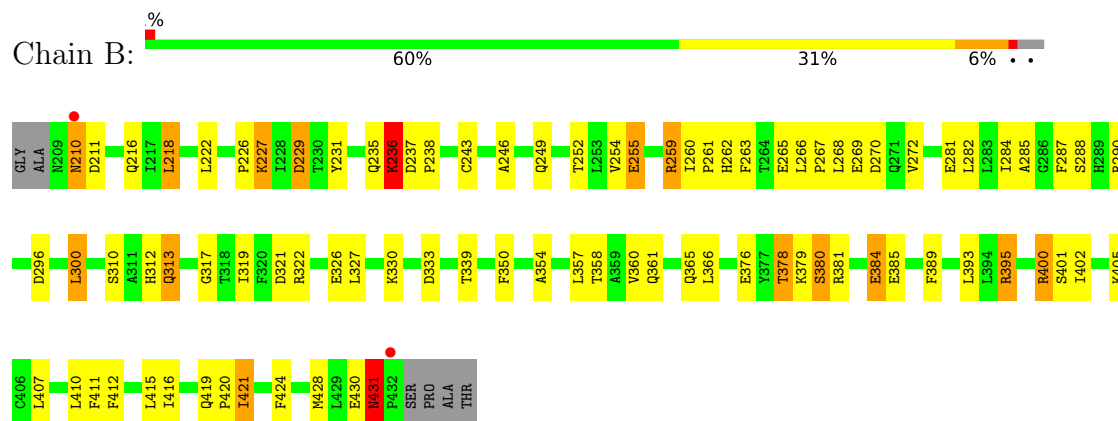
3 Residue-property plots

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.

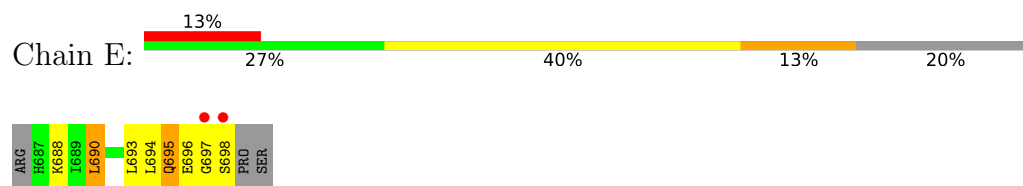
• Molecule 1: RXR-like protein



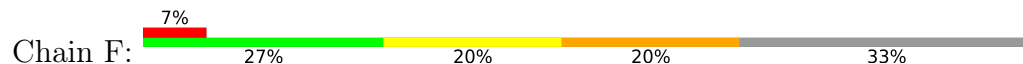
• Molecule 1: RXR-like protein



• Molecule 2: Nuclear receptor coactivator 1



• Molecule 2: Nuclear receptor coactivator 1



ARG	HIS	K688	I689	L690	H691	R692	L693	L694	G697	SER	PRO	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.10Å 87.10Å 320.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.40 – 2.50 24.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.40-2.50) 99.5 (24.40-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.193 , 0.243 0.190 , 0.240	Depositor DCC
R_{free} test set	1292 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3782	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: 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	1.71	20/1781 (1.1%)	1.56	21/2409 (0.9%)
1	B	1.58	10/1793 (0.6%)	1.52	19/2428 (0.8%)
2	E	1.48	1/101 (1.0%)	1.81	3/133 (2.3%)
2	F	1.52	0/84	1.84	2/110 (1.8%)
All	All	1.64	31/3759 (0.8%)	1.55	45/5080 (0.9%)

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	431	ASN	CA-C	8.40	1.63	1.52
1	A	229	ASP	CA-C	7.21	1.62	1.52
1	A	242	ILE	N-CA	-7.08	1.37	1.46
1	B	421	ILE	CA-CB	6.69	1.63	1.54
1	A	242	ILE	CA-CB	-6.68	1.45	1.54
1	A	229	ASP	CB-CG	6.63	1.68	1.52
1	B	254	VAL	CA-CB	-6.23	1.47	1.54
1	A	405	LYS	N-CA	-5.95	1.39	1.46
1	A	360	VAL	CA-CB	5.92	1.62	1.54
1	A	229	ASP	CA-CB	5.86	1.63	1.53
1	A	400	ARG	N-CA	-5.72	1.39	1.46
1	B	360	VAL	CA-CB	5.72	1.60	1.54
1	A	240	THR	C-O	5.67	1.30	1.24
2	E	695	GLN	N-CA	5.67	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ILE	N-CA	-5.52	1.39	1.46
1	A	311	ALA	N-CA	-5.49	1.39	1.46
1	B	354	ALA	CA-CB	-5.47	1.44	1.53
1	A	401	SER	CA-C	5.39	1.59	1.52
1	B	402	ILE	N-CA	-5.38	1.39	1.46
1	B	210	ASN	N-CA	5.37	1.53	1.46
1	B	421	ILE	N-CA	5.37	1.53	1.46
1	A	402	ILE	CA-CB	-5.36	1.47	1.54
1	A	231	TYR	N-CA	5.34	1.53	1.46
1	A	230	THR	N-CA	-5.33	1.39	1.46
1	A	260	ILE	CA-C	5.27	1.57	1.53
1	A	284	ILE	CA-CB	-5.27	1.47	1.54
1	A	254	VAL	CA-CB	-5.22	1.48	1.54
1	A	355	LYS	N-CA	5.19	1.52	1.46
1	B	381	ARG	C-O	-5.14	1.17	1.24
1	A	219	GLU	CG-CD	5.06	1.64	1.52
1	A	400	ARG	CZ-NH2	-5.03	1.26	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	PHE	N-CA-C	-9.92	100.55	111.36
2	E	696	GLU	N-CA-C	9.48	121.56	111.03
1	A	236	LYS	CA-C-N	-8.24	114.00	122.74
1	A	236	LYS	C-N-CA	-8.24	114.00	122.74
1	A	228	ILE	N-CA-C	8.14	120.92	107.24
2	E	695	GLN	N-CA-C	8.09	120.18	111.36
1	A	228	ILE	CA-C-N	7.25	135.38	121.54
1	A	228	ILE	C-N-CA	7.25	135.38	121.54
1	B	385	GLU	CA-C-N	-7.23	111.52	119.19
1	B	385	GLU	C-N-CA	-7.23	111.52	119.19
1	B	211	ASP	N-CA-CB	-7.11	99.46	111.20
1	A	331	MET	N-CA-C	-6.73	104.03	111.36
1	A	228	ILE	CB-CA-C	6.64	118.64	110.73
2	F	689	ILE	CB-CA-C	-6.57	100.52	111.29
1	B	384	GLU	CB-CA-C	-6.47	96.66	110.32
1	A	400	ARG	CG-CD-NE	-6.29	98.17	112.00
1	A	296	ASP	N-CA-C	5.89	119.56	111.54
1	A	276	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	A	227	LYS	CA-C-N	-5.83	115.07	123.11
1	A	227	LYS	C-N-CA	-5.83	115.07	123.11
1	B	380	SER	N-CA-C	5.77	118.44	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	CYS	CA-CB-SG	-5.73	101.23	114.40
1	A	391	LYS	N-CA-C	-5.67	105.10	111.28
1	B	358	THR	N-CA-C	-5.65	105.16	112.68
2	E	695	GLN	CB-CA-C	-5.57	101.38	110.85
1	B	400	ARG	NE-CZ-NH1	-5.54	115.97	121.50
1	B	395	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	229	ASP	N-CA-CB	-5.46	101.26	110.49
1	B	360	VAL	N-CA-CB	5.45	116.56	110.51
1	A	227	LYS	N-CA-C	-5.43	99.66	108.41
1	A	381	ARG	N-CA-C	5.38	119.46	113.01
1	A	378	THR	N-CA-C	5.37	116.82	111.07
1	B	330	LYS	CA-CB-CG	-5.36	103.38	114.10
1	B	326	GLU	N-CA-C	5.36	119.53	112.89
1	B	285	ALA	N-CA-C	-5.31	105.66	111.82
1	A	401	SER	N-CA-CB	-5.29	102.33	110.01
1	B	322	ARG	N-CA-C	-5.27	105.71	111.82
1	B	269	GLU	N-CA-C	-5.18	106.22	112.54
1	A	231	TYR	N-CA-CB	5.17	119.23	110.49
1	A	224	VAL	N-CA-C	5.13	117.04	112.17
1	B	360	VAL	N-CA-C	5.13	115.75	110.36
1	A	308	ARG	CG-CD-NE	-5.11	100.75	112.00
2	F	688	LYS	N-CA-C	-5.10	96.72	111.00
1	B	333	ASP	O-C-N	-5.05	116.76	122.12
1	B	288	SER	N-CA-C	-5.04	105.79	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ASP	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	1748	0	1786	42	1
1	B	1759	0	1792	43	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	100	0	105	4	0
2	F	84	0	93	5	0
3	A	22	0	27	2	0
3	B	22	0	27	7	0
4	A	28	0	0	11	0
4	B	17	0	0	3	0
4	E	1	0	0	0	0
4	F	1	0	0	2	0
All	All	3782	0	3830	96	1

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 13.

All (96) 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:229:ASP:HA	4:A:40:HOH:O	1.32	1.25
1:A:210:ASN:HB3	4:A:46:HOH:O	1.48	1.13
2:F:688:LYS:HB2	4:F:31:HOH:O	1.47	1.11
1:A:234:ALA:HB1	4:A:33:HOH:O	1.52	1.06
1:A:381:ARG:HG2	4:A:43:HOH:O	1.68	0.94
1:A:381:ARG:CG	4:A:43:HOH:O	2.20	0.90
1:A:210:ASN:CB	4:A:46:HOH:O	2.11	0.89
1:B:255:GLU:HA	1:B:255:GLU:OE2	1.73	0.87
1:A:255:GLU:HG3	4:A:38:HOH:O	1.78	0.83
1:B:431:ASN:O	1:B:431:ASN:ND2	2.14	0.81
3:B:202:9CR:C8	3:B:202:9CR:H19	2.13	0.77
2:F:690:LEU:HD13	2:F:694:LEU:HD12	1.67	0.76
1:B:236:LYS:O	1:B:238:PRO:HD3	1.86	0.75
1:B:227:LYS:NZ	1:B:227:LYS:HB3	2.04	0.73
1:A:228:ILE:HD13	1:A:229:ASP:N	2.04	0.72
3:B:202:9CR:H25	3:B:202:9CR:O2	1.89	0.71
1:A:295:LYS:HE2	1:A:295:LYS:H	1.56	0.70
1:B:259:ARG:HH11	1:B:259:ARG:HG3	1.57	0.69
1:A:400:ARG:NH1	4:A:15:HOH:O	2.25	0.69
2:E:690:LEU:HD22	2:E:694:LEU:CD1	2.23	0.69
1:B:281:GLU:OE1	1:B:400:ARG:HD3	1.95	0.66
1:B:235:GLN:O	1:B:236:LYS:O	2.13	0.66
1:B:266:LEU:O	1:B:267:PRO:C	2.40	0.64
1:A:318:THR:HG23	4:A:36:HOH:O	1.98	0.63
1:A:318:THR:CG2	4:A:36:HOH:O	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:690:LEU:HD13	2:F:694:LEU:CD1	2.29	0.62
1:B:361:GLN:OE1	1:B:361:GLN:HA	2.00	0.61
1:B:281:GLU:OE1	1:B:400:ARG:HA	2.01	0.61
1:A:228:ILE:HD13	1:A:228:ILE:C	2.27	0.60
1:A:230:THR:O	1:A:231:TYR:HB2	2.02	0.59
1:B:218:LEU:HG	1:B:339:THR:OG1	2.02	0.59
1:A:283:LEU:HB3	3:A:201:9CR:H11	1.86	0.58
1:B:236:LYS:O	1:B:238:PRO:CD	2.52	0.58
1:A:230:THR:O	1:A:231:TYR:CB	2.52	0.58
1:B:226:PRO:HD2	4:B:37:HOH:O	2.04	0.57
1:A:319:ILE:HD11	1:A:402:ILE:HG23	1.85	0.57
2:E:690:LEU:HD22	2:E:694:LEU:HD12	1.87	0.56
1:A:231:TYR:HA	1:A:303:GLY:O	2.06	0.55
1:B:227:LYS:HB3	1:B:227:LYS:HZ1	1.71	0.55
1:A:215:GLU:H	1:A:215:GLU:CD	2.16	0.54
1:B:378:THR:CG2	4:B:29:HOH:O	2.56	0.54
1:A:272:VAL:HB	2:E:690:LEU:HD13	1.90	0.53
1:A:228:ILE:C	1:A:228:ILE:CD1	2.81	0.53
1:B:312:HIS:HE1	1:B:321:ASP:OD1	1.91	0.52
1:B:431:ASN:HD22	1:B:431:ASN:C	2.14	0.52
1:A:421:ILE:HG23	1:A:425:LEU:HD23	1.91	0.52
1:A:280:ASN:O	1:A:284:ILE:HD12	2.11	0.51
1:A:415:LEU:O	1:A:416:ILE:C	2.53	0.51
1:A:289:HIS:O	1:A:292:ILE:HD12	2.11	0.50
1:A:295:LYS:HE2	1:A:295:LYS:N	2.25	0.50
1:B:312:HIS:CD2	1:B:317:GLY:HA3	2.47	0.50
2:E:690:LEU:HD22	2:E:694:LEU:HD11	1.93	0.49
1:B:424:PHE:HZ	2:F:690:LEU:HD23	1.76	0.49
1:A:290:ARG:HH22	3:A:201:9CR:C15	2.27	0.48
1:A:378:THR:HG21	1:A:389:PHE:HB2	1.95	0.48
1:B:378:THR:HG22	1:B:379:LYS:N	2.28	0.48
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.15	0.47
1:A:213:PRO:HB2	1:A:215:GLU:OE2	2.16	0.46
1:B:235:GLN:C	1:B:236:LYS:O	2.57	0.46
1:B:412:PHE:CE1	1:B:416:ILE:HD11	2.51	0.46
1:B:259:ARG:HG3	1:B:259:ARG:NH1	2.29	0.46
1:B:260:ILE:O	1:B:261:PRO:C	2.59	0.46
1:A:249:GLN:HA	1:A:252:THR:HG23	1.98	0.45
3:B:202:9CR:C8	3:B:202:9CR:C18	2.89	0.45
1:A:318:THR:HG22	4:A:36:HOH:O	2.14	0.45
1:B:389:PHE:CZ	1:B:393:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:O	1:A:231:TYR:CD2	2.70	0.44
1:B:236:LYS:HD2	4:B:32:HOH:O	2.17	0.44
1:A:337:ASP:OD2	1:A:340:GLU:HG3	2.17	0.44
1:B:262:HIS:O	1:B:263:PHE:C	2.60	0.44
1:B:350:PHE:CE2	1:B:366:LEU:HD13	2.52	0.44
1:A:210:ASN:HB3	1:A:211:ASP:H	1.66	0.44
1:A:429:LEU:O	1:A:430:GLU:HB2	2.17	0.44
1:B:287:PHE:C	1:B:287:PHE:CD1	2.96	0.44
1:B:300:LEU:CD1	1:B:300:LEU:N	2.80	0.43
1:A:269:GLU:OE1	1:A:269:GLU:HA	2.19	0.43
1:A:210:ASN:O	1:A:211:ASP:CB	2.66	0.43
1:A:218:LEU:HG	1:A:339:THR:OG1	2.19	0.43
1:B:412:PHE:CE1	1:B:416:ILE:CD1	3.02	0.42
3:B:202:9CR:H8	3:B:202:9CR:H10	1.78	0.42
1:B:268:LEU:O	1:B:272:VAL:HG23	2.20	0.42
1:B:249:GLN:HG3	3:B:202:9CR:O1	2.20	0.42
1:A:394:LEU:HD12	1:A:394:LEU:HA	1.90	0.42
2:F:691:HIS:ND1	4:F:31:HOH:O	2.37	0.41
1:A:221:GLU:OE2	1:A:345:ARG:NH1	2.47	0.41
1:B:284:ILE:HA	1:B:287:PHE:CE2	2.55	0.41
1:B:237:ASP:HA	1:B:238:PRO:HD2	1.83	0.41
1:B:313:GLN:HE21	1:B:313:GLN:HB2	1.60	0.41
1:B:365:GLN:HE21	1:B:365:GLN:HB2	1.63	0.41
1:B:267:PRO:O	1:B:270:ASP:HB2	2.21	0.41
1:B:290:ARG:HH22	3:B:202:9CR:C15	2.33	0.41
1:A:415:LEU:O	1:A:418:ASP:HB2	2.22	0.40
1:B:400:ARG:HD3	1:B:400:ARG:HH11	1.51	0.40
1:B:246:ALA:HB2	3:B:202:9CR:C12	2.52	0.40
1:B:410:LEU:HD23	1:B:410:LEU:HA	1.80	0.40
1:B:229:ASP:OD2	1:B:229:ASP:N	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:O	1:B:231:TYR:O[6_655]	2.07	0.13

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	219/230 (95%)	205 (94%)	11 (5%)	3 (1%)	9	17
1	B	222/230 (96%)	206 (93%)	11 (5%)	5 (2%)	5	8
2	E	10/15 (67%)	9 (90%)	0	1 (10%)	0	0
2	F	8/15 (53%)	5 (62%)	2 (25%)	1 (12%)	0	0
All	All	459/490 (94%)	425 (93%)	24 (5%)	10 (2%)	5	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ASP
1	B	236	LYS
1	B	420	PRO
2	F	689	ILE
1	A	231	TYR
2	E	697	GLY
1	B	431	ASN
1	A	418	ASP
1	B	296	ASP
1	B	421	ILE

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	188/197 (95%)	161 (86%)	27 (14%)	3	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	188/197 (95%)	159 (85%)	29 (15%)	2	5
2	E	11/14 (79%)	6 (54%)	5 (46%)	0	0
2	F	9/14 (64%)	7 (78%)	2 (22%)	1	2
All	All	396/422 (94%)	333 (84%)	63 (16%)	2	5

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	GLU
1	A	218	LEU
1	A	219	GLU
1	A	228	ILE
1	A	232	ILE
1	A	236	LYS
1	A	248	LYS
1	A	252	THR
1	A	258	LYS
1	A	259	ARG
1	A	269	GLU
1	A	272	VAL
1	A	282	LEU
1	A	292	ILE
1	A	295	LYS
1	A	300	LEU
1	A	302	THR
1	A	318	THR
1	A	327	LEU
1	A	361	GLN
1	A	364	GLU
1	A	378	THR
1	A	381	ARG
1	A	394	LEU
1	A	395	ARG
1	A	400	ARG
1	A	429	LEU
1	B	210	ASN
1	B	216	GLN
1	B	218	LEU
1	B	222	LEU
1	B	227	LYS
1	B	229	ASP

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Mol	Chain	Res	Type
1	B	236	LYS
1	B	252	THR
1	B	255	GLU
1	B	259	ARG
1	B	265	GLU
1	B	282	LEU
1	B	300	LEU
1	B	310	SER
1	B	313	GLN
1	B	327	LEU
1	B	357	LEU
1	B	376	GLU
1	B	378	THR
1	B	380	SER
1	B	384	GLU
1	B	395	ARG
1	B	401	SER
1	B	405	LYS
1	B	407	LEU
1	B	415	LEU
1	B	419	GLN
1	B	428	MET
1	B	430	GLU
2	E	688	LYS
2	E	690	LEU
2	E	693	LEU
2	E	695	GLN
2	E	698	SER
2	F	690	LEU
2	F	692	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	A	312	HIS
1	B	209	ASN
1	B	312	HIS
1	B	313	GLN
1	B	365	GLN
1	B	409	HIS
1	B	419	GLN

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Mol	Chain	Res	Type
2	E	695	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	9CR	B	202	-	22,22,22	2.17	8 (36%)	30,30,30	3.08	12 (40%)
3	9CR	A	201	-	22,22,22	2.20	6 (27%)	30,30,30	2.58	11 (36%)

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
3	9CR	B	202	-	-	7/15/32/32	0/1/1/1
3	9CR	A	201	-	-	10/15/32/32	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	9CR	C5-C6	5.53	1.43	1.34
3	B	202	9CR	C11-C12	4.76	1.47	1.34
3	A	201	9CR	C11-C12	4.72	1.47	1.34
3	A	201	9CR	C8-C7	4.33	1.46	1.33
3	B	202	9CR	C8-C7	4.21	1.45	1.33
3	B	202	9CR	C1-C6	-4.07	1.48	1.53
3	B	202	9CR	C10-C9	3.71	1.44	1.35
3	A	201	9CR	C14-C13	3.41	1.40	1.35
3	B	202	9CR	C14-C13	2.97	1.39	1.35
3	A	201	9CR	O1-C15	2.87	1.30	1.23
3	B	202	9CR	O1-C15	2.85	1.30	1.23
3	A	201	9CR	C10-C9	2.78	1.42	1.35
3	B	202	9CR	C5-C6	2.29	1.38	1.34
3	B	202	9CR	O2-C15	-2.11	1.25	1.30

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	9CR	C11-C10-C9	-8.27	115.68	127.28
3	A	201	9CR	C11-C10-C9	-7.64	116.56	127.28
3	B	202	9CR	C18-C5-C6	-6.13	117.80	124.48
3	B	202	9CR	C7-C8-C9	-6.11	117.19	126.23
3	A	201	9CR	C7-C8-C9	-6.01	117.35	126.23
3	B	202	9CR	C15-C14-C13	-5.57	120.11	128.40
3	B	202	9CR	C19-C9-C8	5.22	126.06	118.09
3	A	201	9CR	C19-C9-C8	4.39	124.80	118.09
3	A	201	9CR	C19-C9-C10	-4.16	116.08	122.82
3	B	202	9CR	C17-C1-C6	-4.14	103.74	110.24
3	A	201	9CR	C17-C1-C6	-3.46	104.82	110.24
3	B	202	9CR	C10-C11-C12	-3.27	113.74	123.20
3	B	202	9CR	C19-C9-C10	-3.06	117.86	122.82
3	A	201	9CR	C10-C11-C12	-2.81	115.05	123.20
3	B	202	9CR	C16-C1-C6	-2.74	105.94	110.24
3	A	201	9CR	C12-C13-C14	-2.64	111.84	119.15
3	B	202	9CR	C3-C4-C5	-2.37	109.84	114.06
3	A	201	9CR	C2-C3-C4	2.33	116.40	111.28
3	A	201	9CR	C20-C13-C12	2.27	121.56	118.09
3	B	202	9CR	C20-C13-C12	2.22	121.48	118.09
3	A	201	9CR	C11-C12-C13	-2.07	120.67	126.36
3	A	201	9CR	C8-C7-C6	-2.07	121.48	127.00
3	B	202	9CR	C8-C7-C6	-2.02	121.61	127.00

There are no chirality outliers.

All (17) torsion outliers are listed below:

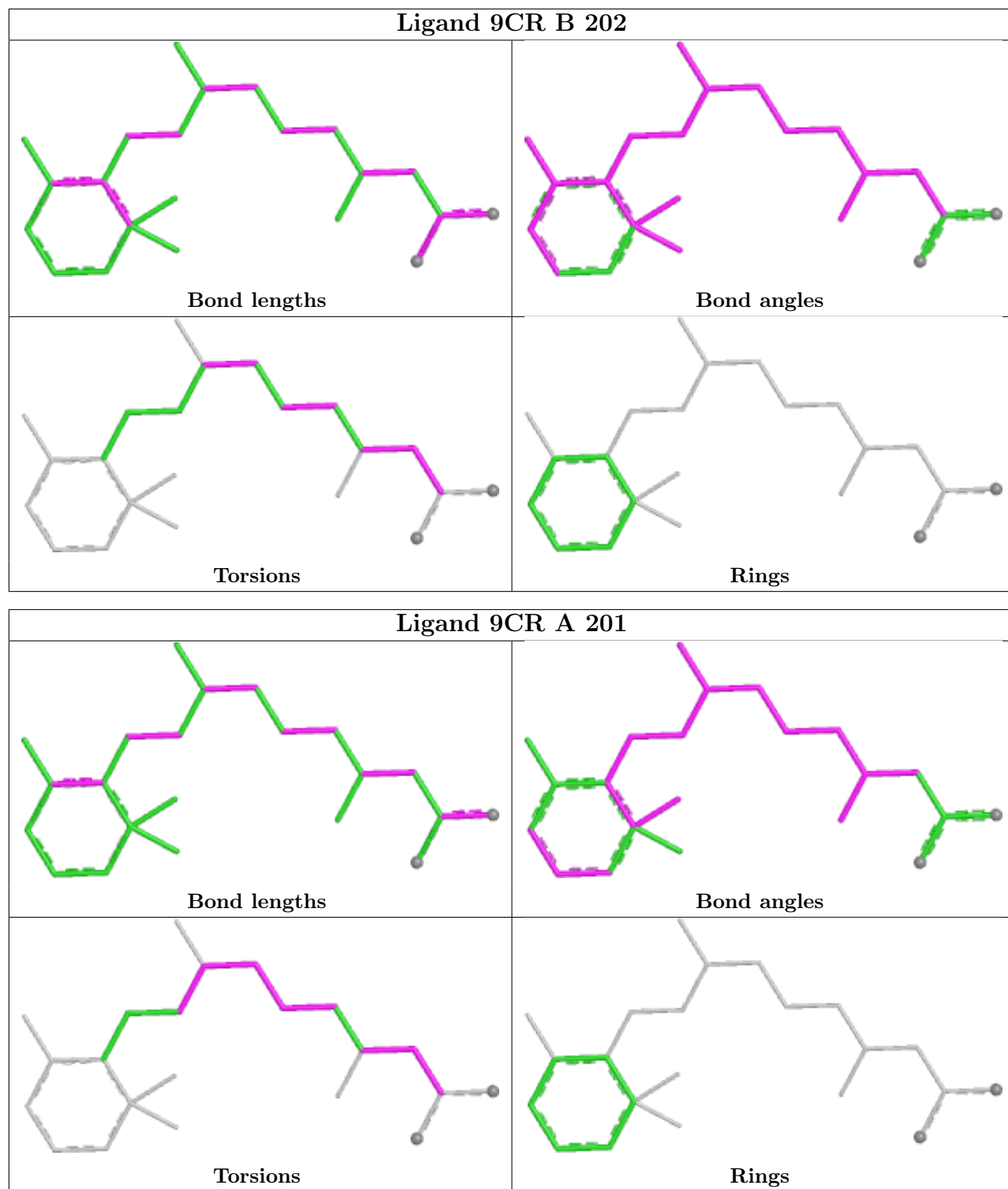
Mol	Chain	Res	Type	Atoms
3	A	201	9CR	C7-C8-C9-C10
3	A	201	9CR	C12-C13-C14-C15
3	A	201	9CR	C20-C13-C14-C15
3	A	201	9CR	C13-C14-C15-O1
3	A	201	9CR	C13-C14-C15-O2
3	A	201	9CR	C7-C8-C9-C19
3	B	202	9CR	C11-C10-C9-C19
3	A	201	9CR	C11-C10-C9-C8
3	B	202	9CR	C11-C10-C9-C8
3	B	202	9CR	C10-C11-C12-C13
3	B	202	9CR	C13-C14-C15-O1
3	B	202	9CR	C13-C14-C15-O2
3	A	201	9CR	C11-C10-C9-C19
3	B	202	9CR	C12-C13-C14-C15
3	B	202	9CR	C20-C13-C14-C15
3	A	201	9CR	C10-C11-C12-C13
3	A	201	9CR	C9-C10-C11-C12

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	9CR	7	0
3	A	201	9CR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	221/230 (96%)	-0.51	0 100 100	30, 42, 59, 77	0
1	B	224/230 (97%)	-0.48	2 (0%) 81 78	32, 45, 63, 85	0
2	E	12/15 (80%)	0.75	2 (16%) 4 3	54, 66, 95, 99	0
2	F	10/15 (66%)	0.87	1 (10%) 12 10	66, 70, 91, 94	0
All	All	467/490 (95%)	-0.43	5 (1%) 78 75	30, 44, 68, 99	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	698	SER	4.4
1	B	432	PRO	2.8
2	F	688	LYS	2.5
2	E	697	GLY	2.5
1	B	210	ASN	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 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,

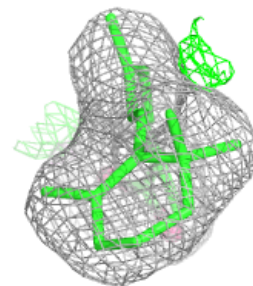
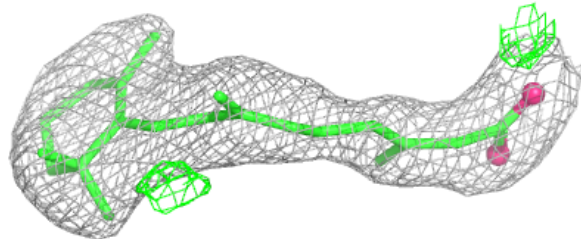
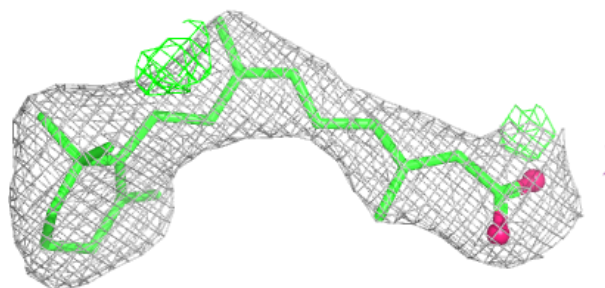
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	9CR	A	201	22/22	0.95	0.07	39,43,48,51	0
3	9CR	B	202	22/22	0.96	0.07	38,42,49,52	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.

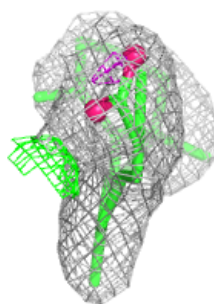
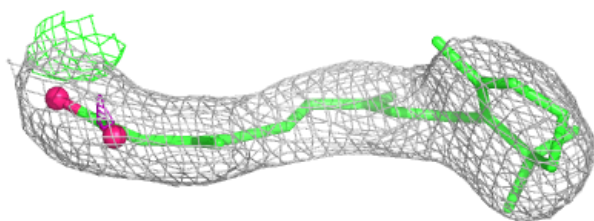
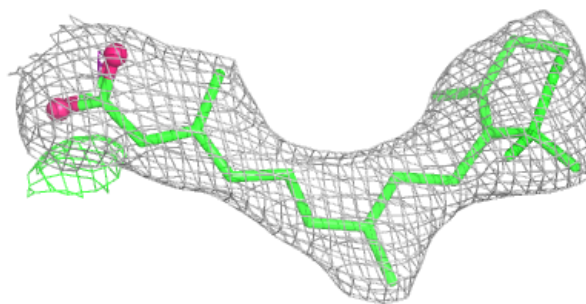
Electron density around 9CR A 201:

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 202:

$2mF_o-DF_c$ (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.