Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:16 PM BST

PDB ID	:	5JI0
Title	:	PPARgamma-RXRalpha(S427F) heterodimer in complex with SRC-1, rosiglitazone, and 9-cis-retanoic acid
Authors	:	Bloudoff, K.; Larsen, N.A.
Deposited on	:	2016-04-21
Resolution	:	1.98 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:

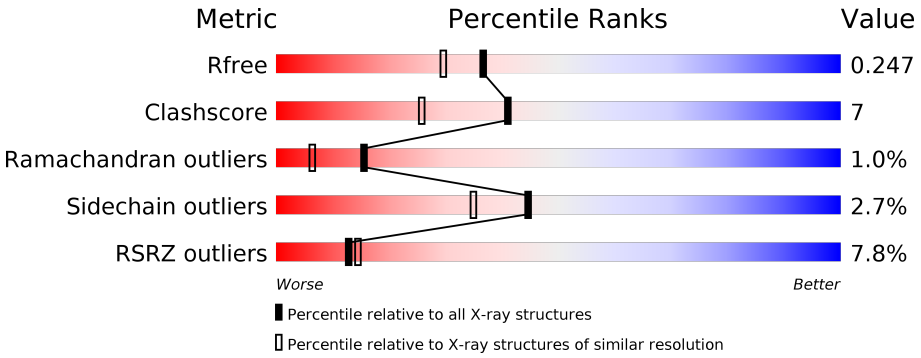
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	242	10%, 76%, 11%, ·, 11%
2	D	273	3%, 85%, 12%, ··
3	E	27	7%, 59%, 11%, 30%
3	F	27	22%, 22%, 7%, ·, 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	9CR	A	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4370 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1718	1104	293	311	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	GLY	-	expression tag	UNP P19793
A	222	MET	-	expression tag	UNP P19793
A	427	PHE	SER	engineered mutation	UNP P19793

- Molecule 2 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	269	Total	C	N	O	S	0	1	0
			2150	1386	349	405	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	205	GLY	-	expression tag	UNP P37231

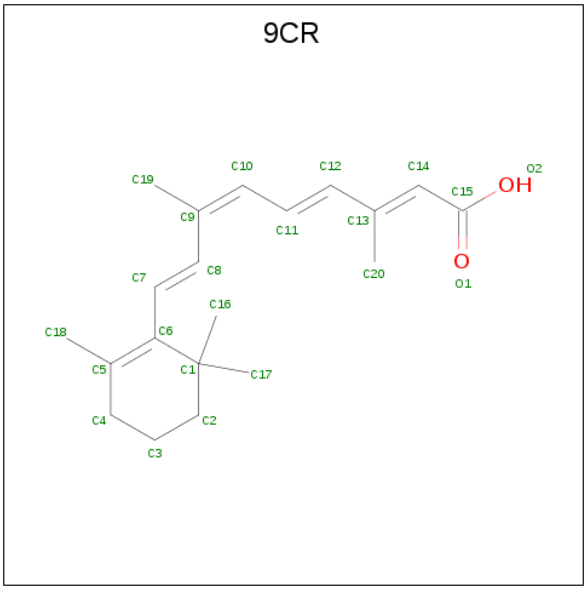
- Molecule 3 is a protein called Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	19	Total	C	N	O	0	0	0
			148	92	28	28			
3	F	9	Total	C	N	O	0	0	0
			76	49	15	12			

There are 4 discrepancies between the modelled and reference sequences:

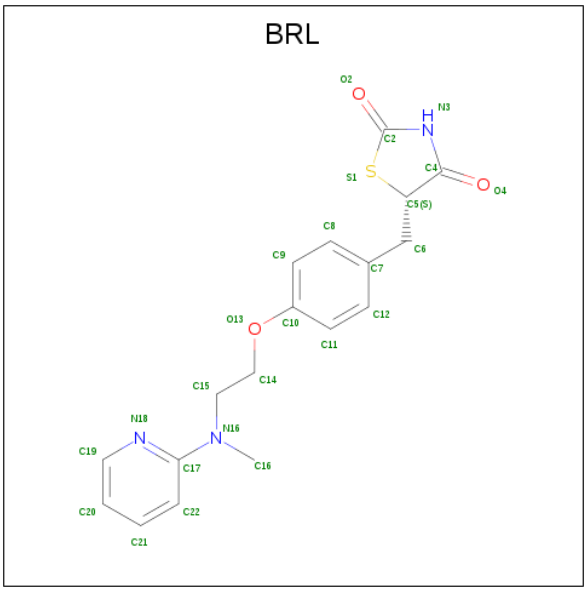
Chain	Residue	Modelled	Actual	Comment	Reference
E	675	ACE	-	acetylation	UNP Q15788
E	701	NH2	-	amidation	UNP Q15788
F	675	ACE	-	acetylation	UNP Q15788
F	701	NH2	-	amidation	UNP Q15788

- Molecule 4 is (9cis)-retinoic acid (three-letter code: 9CR) (formula: $C_{20}H_{28}O_2$).



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

- Molecule 5 is 2,4-THIAZOLIDIINEDIONE, 5-[[4-[2-(METHYL-2-PYRIDINYLAMINO)ETHOXY]PHENYL]METHYL]-(9CL) (three-letter code: BRL) (formula: $C_{18}H_{19}N_3O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			25	18	3	3	1		

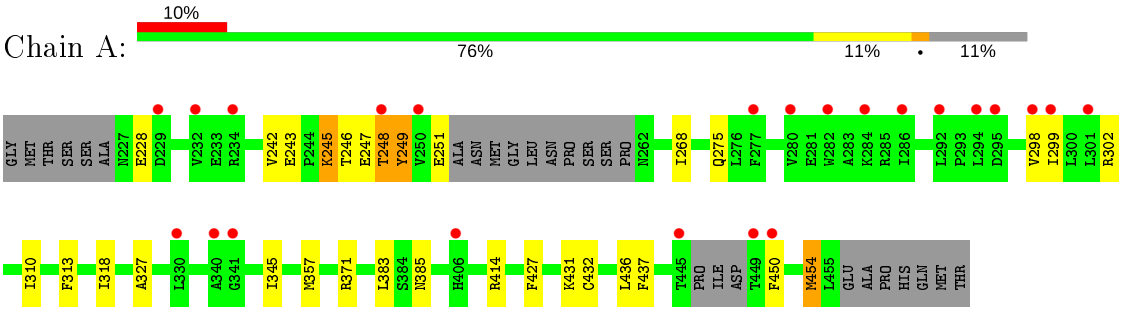
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	D	176	Total	O	0	0
			176	176		
6	E	7	Total	O	0	0
			7	7		

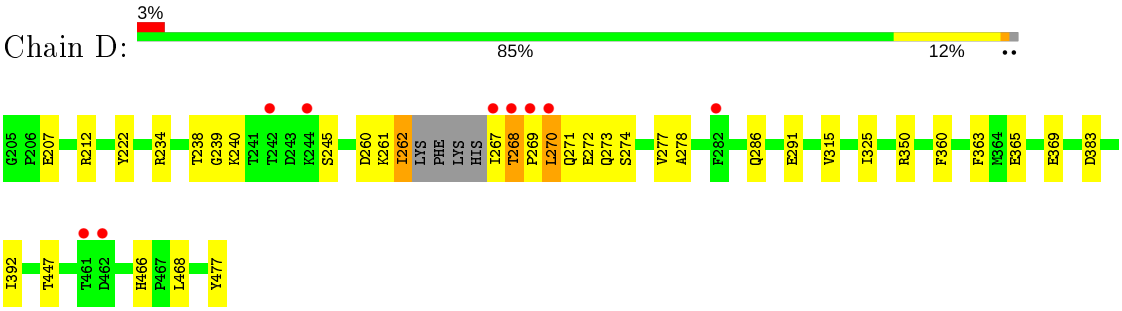
3 Residue-property plots

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: Retinoic acid receptor RXR-alpha

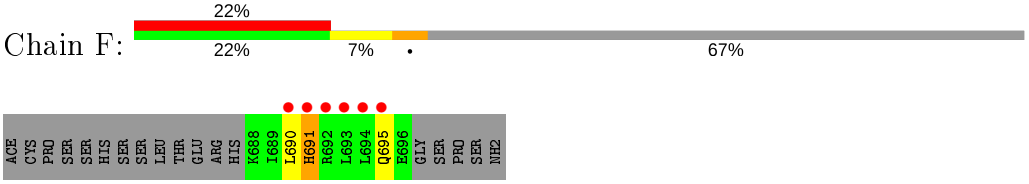


- Molecule 2: Peroxisome proliferator-activated receptor gamma



- Molecule 3: Nuclear receptor coactivator 1

- Molecule 3: Nuclear receptor coactivator 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.88Å 66.53Å 165.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.20 – 1.98 45.19 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.20-1.98) 93.5 (45.19-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.246 0.197 , 0.247	Depositor DCC
R_{free} test set	2141 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4370	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, BRL

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	0.73	0/1751	0.89	4/2365 (0.2%)
2	D	0.93	1/2189 (0.0%)	0.96	4/2953 (0.1%)
3	E	0.89	0/150	0.83	0/201
3	F	0.57	0/76	0.85	0/101
All	All	0.84	1/4166 (0.0%)	0.93	8/5620 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	222	TYR	CB-CG	-5.18	1.43	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	234	ARG	NE-CZ-NH2	-8.24	116.18	120.30
2	D	234	ARG	NE-CZ-NH1	8.15	124.38	120.30
2	D	212	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	371	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	248	THR	N-CA-C	-5.84	95.22	111.00
2	D	383	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	371	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	414	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	GLU	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	1718	0	1747	31	0
2	D	2150	0	2203	18	10
3	E	148	0	148	4	0
3	F	76	0	79	2	0
4	A	22	0	27	17	0
5	D	25	0	19	1	0
6	A	48	0	0	2	0
6	D	176	0	0	4	0
6	E	7	0	0	0	0
All	All	4370	0	4223	59	10

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 7.

All (59) 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:432:CYS:SG	4:A:501:9CR:H15	1.87	1.14
1:A:432:CYS:SG	4:A:501:9CR:C16	2.55	0.93
1:A:247:GLU:N	1:A:247:GLU:OE1	2.04	0.90
3:E:691:HIS:NE2	3:E:695:GLN:OE1	2.07	0.87
1:A:268:ILE:HD13	4:A:501:9CR:H21	1.58	0.85
1:A:298:VAL:HG13	3:F:690:LEU:HD23	1.59	0.84
1:A:302:ARG:HG2	1:A:454:MET:HE1	1.68	0.76
1:A:436:LEU:HD11	4:A:501:9CR:H23	1.71	0.71
4:A:501:9CR:H13	4:A:501:9CR:H8	1.71	0.71
5:D:501:BRL:H22	6:D:768:HOH:O	1.89	0.71
1:A:313:PHE:CD2	4:A:501:9CR:H26	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:691:HIS:CD2	3:E:695:GLN:OE1	2.47	0.66
2:D:466:HIS:HD2	2:D:468:LEU:H	1.44	0.64
4:A:501:9CR:H13	4:A:501:9CR:C8	2.28	0.63
1:A:454:MET:HA	1:A:454:MET:CE	2.30	0.62
2:D:466:HIS:HE1	6:D:753:HOH:O	1.83	0.61
1:A:454:MET:HA	1:A:454:MET:HE3	1.81	0.61
2:D:350:ARG:NH2	2:D:365:GLU:OE2	2.30	0.60
1:A:268:ILE:CD1	4:A:501:9CR:H21	2.32	0.59
1:A:242:VAL:HG23	6:A:641:HOH:O	2.02	0.59
1:A:427:PHE:CD1	2:D:447:THR:HG21	2.39	0.57
1:A:275:GLN:HG3	4:A:501:9CR:O2	2.05	0.56
4:A:501:9CR:H25	4:A:501:9CR:O1	2.04	0.56
1:A:318:ILE:HD11	1:A:357:MET:HB2	1.88	0.56
3:E:683:LEU:HD23	3:E:683:LEU:C	2.28	0.54
3:F:691:HIS:O	3:F:695:GLN:HG3	2.07	0.54
1:A:248:THR:OG1	1:A:249:TYR:N	2.41	0.52
1:A:432:CYS:CB	4:A:501:9CR:C16	2.89	0.51
1:A:242:VAL:CG2	6:A:641:HOH:O	2.58	0.51
1:A:251:GLU:N	1:A:251:GLU:OE2	2.44	0.51
2:D:447:THR:HG22	2:D:477:TYR:CD2	2.46	0.51
2:D:268:THR:O	2:D:268:THR:HG22	2.11	0.50
4:A:501:9CR:H16	4:A:501:9CR:C8	2.42	0.50
2:D:466:HIS:CD2	2:D:468:LEU:H	2.27	0.50
2:D:315:VAL:CG1	3:E:683:LEU:HD21	2.42	0.49
1:A:246:THR:OG1	1:A:247:GLU:OE1	2.31	0.49
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.50	0.47
2:D:286:GLN:OE1	6:D:601:HOH:O	2.20	0.47
1:A:318:ILE:HD11	1:A:357:MET:CB	2.45	0.46
2:D:360:PHE:O	2:D:363:PHE:HD1	1.99	0.46
2:D:267:ILE:CD1	6:D:746:HOH:O	2.63	0.46
1:A:345:ILE:HD13	1:A:431:LYS:HB2	1.98	0.46
1:A:432:CYS:HB3	4:A:501:9CR:H13	1.98	0.45
1:A:327:ALA:HB2	4:A:501:9CR:O2	2.15	0.45
1:A:299:ILE:HG21	1:A:383:LEU:HD12	2.00	0.44
4:A:501:9CR:H16	4:A:501:9CR:H8	2.00	0.44
2:D:270:LEU:HD13	2:D:271:GLN:HG2	2.00	0.44
2:D:272:GLU:O	2:D:272:GLU:HG2	2.18	0.43
2:D:466:HIS:HD2	2:D:468:LEU:N	2.14	0.43
2:D:260:ASP:C	2:D:262:ILE:H	2.22	0.43
1:A:302:ARG:HG2	1:A:454:MET:CE	2.45	0.42
1:A:245:LYS:CE	1:A:245:LYS:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:ILE:HB	2:D:291:GLU:OE1	2.19	0.42
4:A:501:9CR:H7	4:A:501:9CR:H19	1.85	0.42
1:A:245:LYS:CD	1:A:245:LYS:H	2.34	0.41
2:D:325:ILE:HD11	2:D:392:ILE:HG13	2.03	0.41
2:D:277:VAL:HG13	2:D:278:ALA:N	2.36	0.41
1:A:268:ILE:HG21	4:A:501:9CR:C18	2.51	0.40
1:A:302:ARG:HA	1:A:454:MET:HE1	2.03	0.40

All (10) 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)
2:D:238:THR:O	2:D:273:GLN:OE1[4_447]	1.52	0.68
2:D:239:GLY:CA	2:D:273:GLN:OE1[4_447]	1.57	0.63
2:D:239:GLY:O	2:D:273:GLN:CG[4_447]	1.73	0.47
2:D:239:GLY:N	2:D:273:GLN:OE1[4_447]	1.75	0.45
2:D:238:THR:C	2:D:273:GLN:OE1[4_447]	1.78	0.42
2:D:240:LYS:N	2:D:273:GLN:NE2[4_447]	1.78	0.42
2:D:239:GLY:C	2:D:273:GLN:NE2[4_447]	1.84	0.36
2:D:239:GLY:CA	2:D:273:GLN:CD[4_447]	1.87	0.33
2:D:239:GLY:C	2:D:273:GLN:CG[4_447]	2.06	0.14
2:D:239:GLY:O	2:D:273:GLN:CD[4_447]	2.14	0.06

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	210/242 (87%)	198 (94%)	11 (5%)	1 (0%)	29 16
2	D	266/273 (97%)	253 (95%)	9 (3%)	4 (2%)	10 2
3	E	17/27 (63%)	16 (94%)	1 (6%)	0	100 100
3	F	7/27 (26%)	7 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	500/569 (88%)	474 (95%)	21 (4%)	5 (1%)	15 6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	GLU
2	D	261	LYS
2	D	245	SER
2	D	268	THR
2	D	269	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	187/208 (90%)	181 (97%)	6 (3%)	39 28
2	D	241/245 (98%)	236 (98%)	5 (2%)	53 47
3	E	17/24 (71%)	17 (100%)	0	100 100
3	F	8/24 (33%)	7 (88%)	1 (12%)	4 1
All	All	453/501 (90%)	441 (97%)	12 (3%)	44 37

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LYS
1	A	249	TYR
1	A	385	ASN
1	A	437	PHE
1	A	450	PHE
1	A	454	MET
2	D	207	GLU
2	D	262	ILE
2	D	270	LEU
2	D	274	SER

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Mol	Chain	Res	Type
2	D	369	GLU
3	F	691	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	267	ASN
1	A	335	ASN
2	D	294	GLN
2	D	308	ASN
2	D	375	ASN
2	D	437	GLN
2	D	451	GLN
2	D	466	HIS
3	F	691	HIS

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 monosaccharides 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	$\#\|Z\|>2$
5	BRL	D	501	-	27,27,27	2.20	7 (25%)	36,36,36	3.20	15 (41%)
4	9CR	A	501	-	19,22,22	6.05	14 (73%)	26,30,30	2.93	8 (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
5	BRL	D	501	-	-	0/14/26/26	0/3/3/3
4	9CR	A	501	-	-	4/13/32/32	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	9CR	C14-C13	15.33	1.52	1.35
4	A	501	9CR	C10-C9	10.91	1.50	1.35
4	A	501	9CR	C1-C6	-9.96	1.40	1.53
5	D	501	BRL	C5-C4	-8.06	1.47	1.52
4	A	501	9CR	C11-C12	7.16	1.53	1.34
4	A	501	9CR	C8-C7	6.26	1.52	1.33
4	A	501	9CR	C18-C5	-6.24	1.40	1.50
4	A	501	9CR	C4-C5	-5.88	1.39	1.51
4	A	501	9CR	C5-C6	3.96	1.41	1.34
5	D	501	BRL	C19-N18	3.85	1.42	1.34
4	A	501	9CR	C16-C1	-3.66	1.46	1.53
4	A	501	9CR	C12-C13	3.30	1.53	1.45
4	A	501	9CR	C17-C1	3.25	1.60	1.53
5	D	501	BRL	C2-N3	-3.09	1.32	1.36
5	D	501	BRL	C6-C7	-2.97	1.44	1.51
5	D	501	BRL	C4-N3	-2.74	1.34	1.37
4	A	501	9CR	C2-C3	-2.55	1.46	1.52
4	A	501	9CR	C8-C9	2.53	1.51	1.45
4	A	501	9CR	C11-C10	2.32	1.50	1.43
5	D	501	BRL	C15-N16	2.08	1.53	1.46
5	D	501	BRL	C17-N16	-2.03	1.32	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	BRL	C5-C4-N3	9.50	120.27	112.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	9CR	C8-C9-C10	8.40	131.82	118.94
5	D	501	BRL	O4-C4-N3	-7.43	115.94	124.94
4	A	501	9CR	C19-C9-C10	-7.36	112.62	122.92
5	D	501	BRL	C4-C5-S1	-6.76	100.12	105.90
5	D	501	BRL	C21-C22-C17	6.71	126.76	117.66
5	D	501	BRL	C4-N3-C2	-5.36	114.62	118.24
4	A	501	9CR	C2-C1-C6	5.22	118.52	110.48
5	D	501	BRL	C15-N16-C17	4.65	125.83	120.94
4	A	501	9CR	C1-C6-C5	-4.16	116.76	122.61
4	A	501	9CR	C10-C11-C12	-3.54	112.16	123.22
5	D	501	BRL	N18-C17-N16	3.37	120.67	116.39
4	A	501	9CR	C3-C4-C5	-3.28	108.22	114.08
5	D	501	BRL	C20-C21-C22	-2.97	115.67	120.19
5	D	501	BRL	C5-S1-C2	2.88	94.41	92.86
5	D	501	BRL	C14-C15-N16	-2.86	106.74	112.32
5	D	501	BRL	C22-C17-N18	-2.80	118.27	123.41
5	D	501	BRL	C7-C6-C5	-2.51	109.73	113.32
5	D	501	BRL	O2-C2-N3	-2.35	123.34	125.76
5	D	501	BRL	C11-C10-C9	-2.31	116.62	120.18
5	D	501	BRL	C6-C5-S1	2.31	115.43	113.04
4	A	501	9CR	C2-C3-C4	-2.30	106.24	111.38
4	A	501	9CR	C11-C10-C9	2.10	130.30	127.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	9CR	C7-C8-C9-C19
4	A	501	9CR	C7-C8-C9-C10
4	A	501	9CR	C11-C10-C9-C19
4	A	501	9CR	C11-C10-C9-C8

There are no ring outliers.

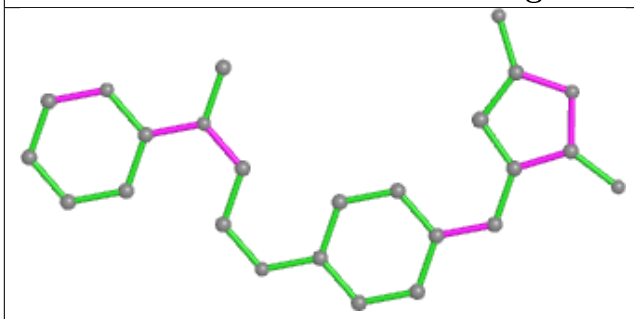
2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	BRL	1	0
4	A	501	9CR	17	0

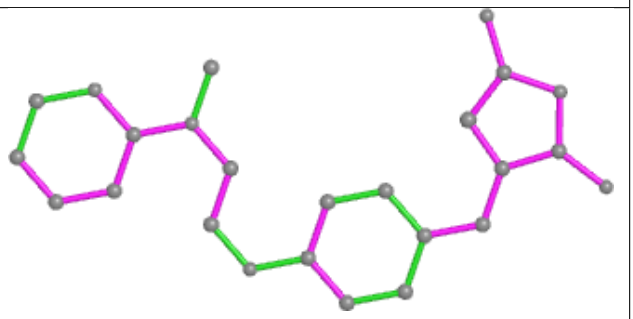
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

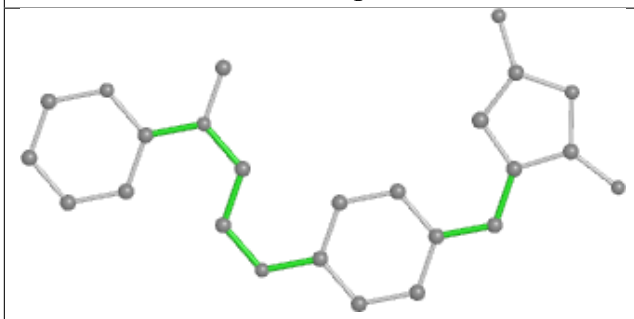
Ligand BRL D 501



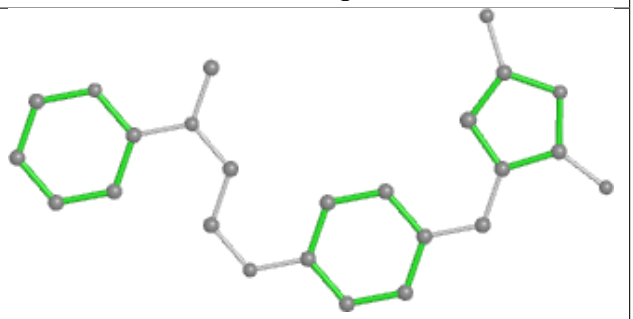
Bond lengths



Bond angles

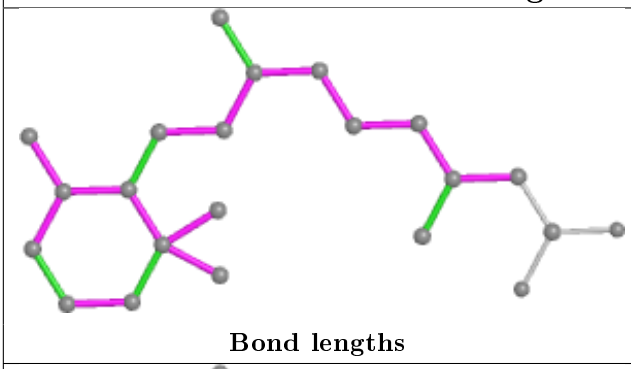


Torsions

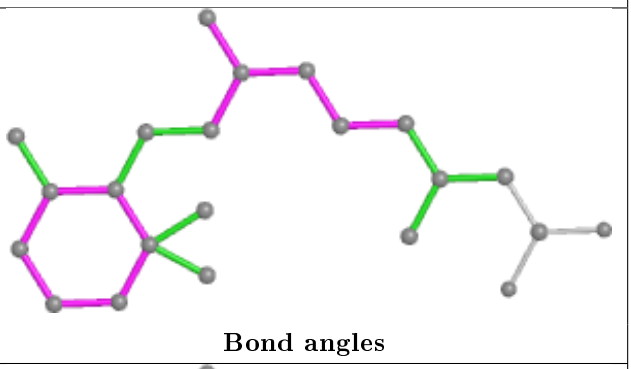


Rings

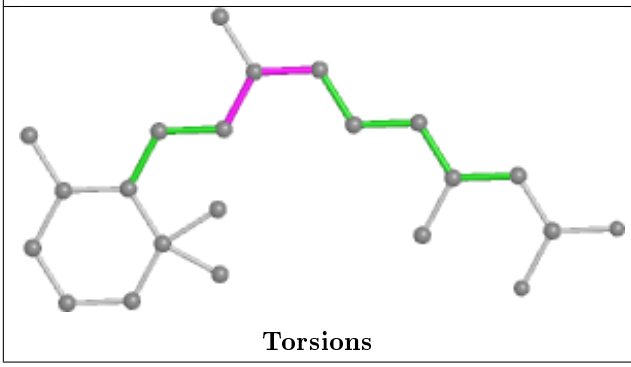
Ligand 9CR A 501



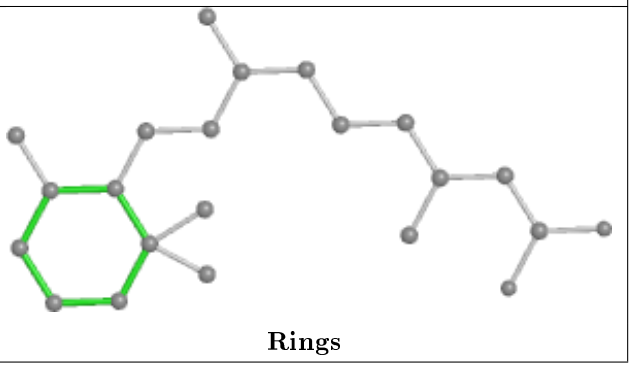
Bond lengths



Bond angles



Torsions



Rings

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	216/242 (89%)	0.56	23 (10%) 6 7	31, 53, 78, 113	0
2	D	269/273 (98%)	0.19	9 (3%) 46 49	21, 33, 88, 140	0
3	E	19/27 (70%)	0.41	2 (10%) 6 7	29, 40, 70, 71	0
3	F	9/27 (33%)	2.98	6 (66%) 0 0	67, 76, 94, 97	0
All	All	513/569 (90%)	0.40	40 (7%) 13 14	21, 43, 80, 140	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	10.1
3	F	694	LEU	5.9
3	F	690	LEU	5.4
2	D	267	ILE	5.3
1	A	294	LEU	4.5
1	A	298	VAL	4.5
2	D	268	THR	4.4
3	F	691	HIS	4.4
2	D	270	LEU	4.1
1	A	232	VAL	4.1
2	D	462	ASP	4.0
1	A	406	HIS	3.6
1	A	450	PHE	3.6
1	A	277	PHE	3.6
3	F	693	LEU	3.5
3	E	682	SER	3.3
2	D	269	PRO	3.1
1	A	248	THR	3.0
1	A	299	ILE	3.0
1	A	449	THR	2.8
1	A	330	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	340	ALA	2.6
1	A	295	ASP	2.5
2	D	282	PHE	2.5
1	A	284	LYS	2.5
3	F	692	ARG	2.5
2	D	461	THR	2.4
1	A	282	TRP	2.4
1	A	234	ARG	2.3
2	D	242	THR	2.3
1	A	292	LEU	2.3
3	E	683	LEU	2.2
1	A	301	LEU	2.2
1	A	280	VAL	2.2
2	D	244	LYS	2.2
1	A	445	THR	2.1
1	A	229	ASP	2.1
1	A	341	GLY	2.1
1	A	286	ILE	2.0
3	F	695	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.

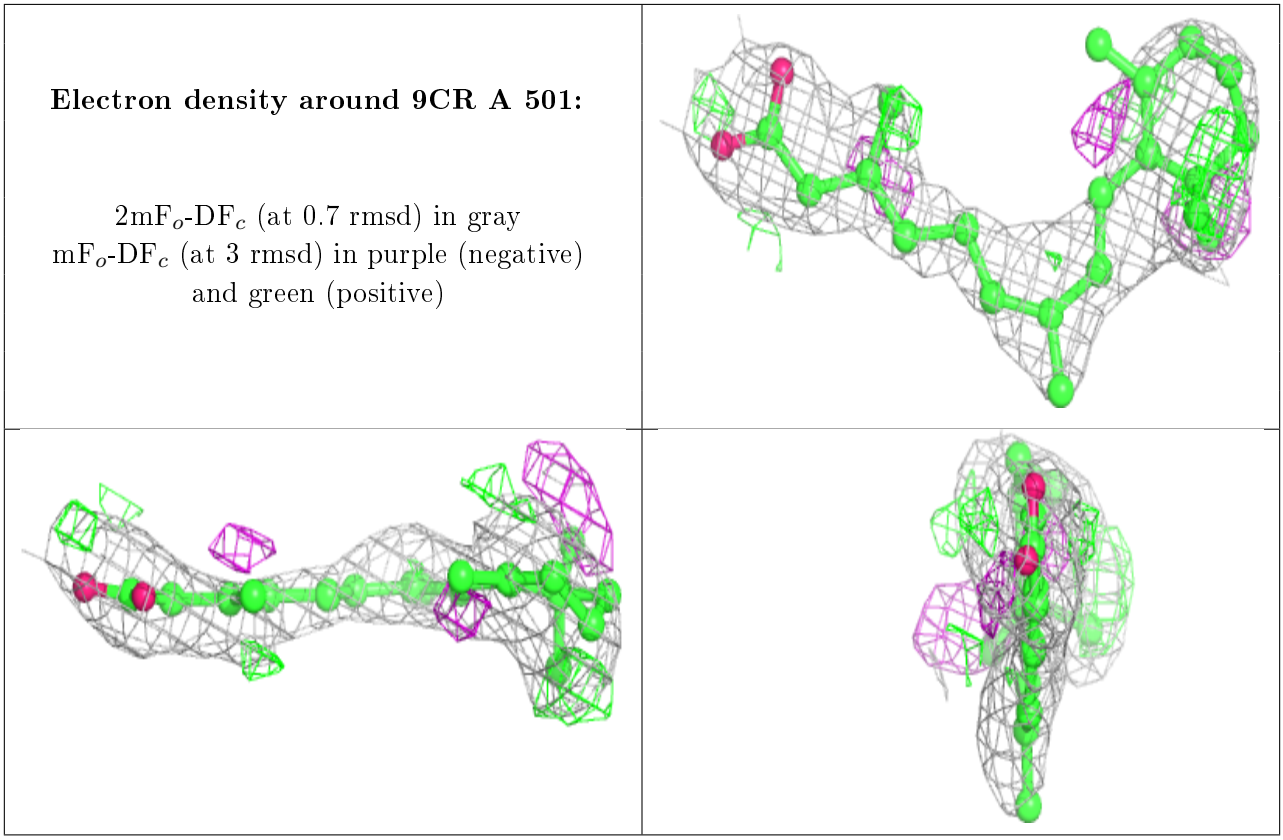
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	9CR	A	501	22/22	0.80	0.33	52,62,85,97	0
5	BRL	D	501	25/25	0.97	0.08	29,32,38,39	0

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.

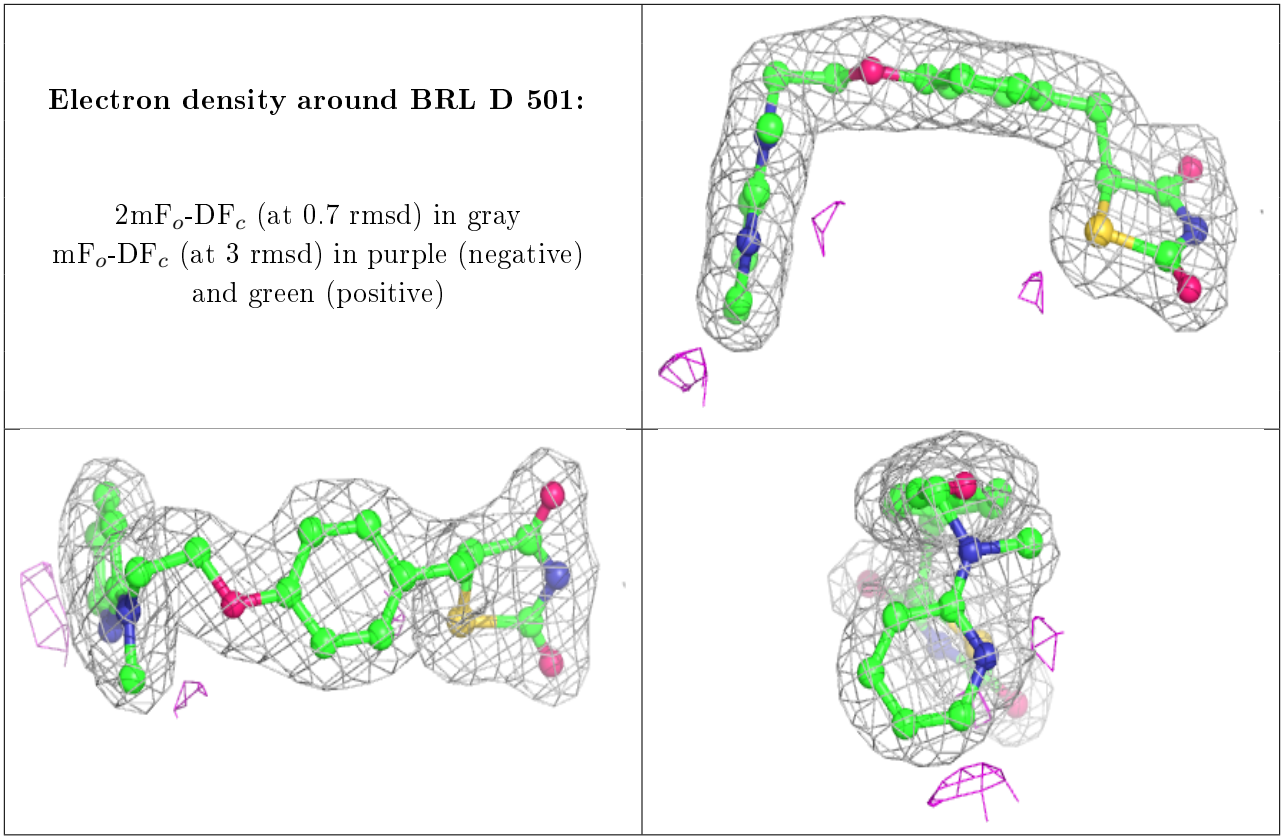
Electron density around 9CR A 501:

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



Electron density around BRL 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.