



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:20 AM UTC

PDB ID : 9DT3 / pdb\_00009dt3  
Title : Crystal structure of the engineered sulfonyleurea repressor EsR (L11-C6), bound to ethametsulfuron-methyl  
Authors : Schreiter, E.R.; Leija, C.; Kakani, N.K.; McBride, K.E.; Looger, L.L.  
Deposited on : 2024-09-30  
Resolution : 2.80 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](mailto: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>.

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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

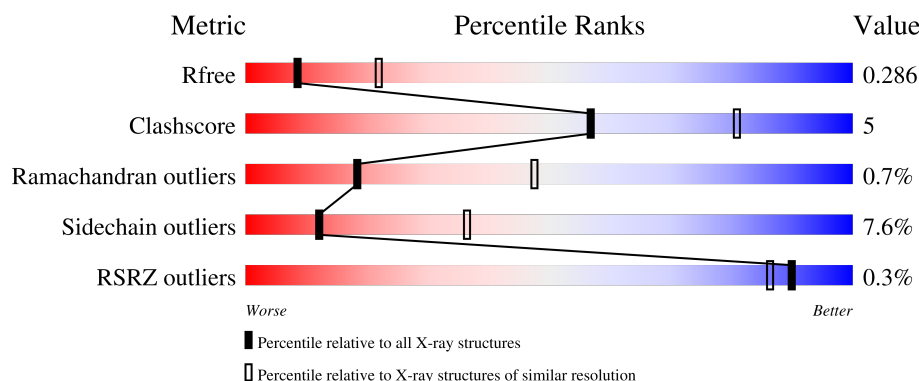
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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  $\geq 3$ , 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	207	 75% 16% • 5%
1	B	207	 74% 16% • 9%
1	C	207	 75% 17% • 6%
1	D	207	 75% 16% • 8%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RXF	C	301	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6169 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 Sulfonylurea repressor EsR (L11-C6).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1542	973	267	295	7			
1	B	188	Total	C	N	O	S	0	0	0
			1470	927	253	282	8			
1	C	195	Total	C	N	O	S	0	0	0
			1534	967	266	294	7			
1	D	191	Total	C	N	O	S	0	0	0
			1498	945	261	285	7			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	conflict	UNP P04483
A	55	MET	LEU	conflict	UNP P04483
A	64	ALA	HIS	conflict	UNP P04483
A	67	TYR	PHE	conflict	UNP P04483
A	68	SER	CYS	conflict	UNP P04483
A	72	ARG	GLY	conflict	UNP P04483
A	77	ASN	ASP	conflict	UNP P04483
A	86	MET	PHE	conflict	UNP P04483
A	88	ASN	CYS	conflict	UNP P04483
A	100	CYS	HIS	conflict	UNP P04483
A	104	GLY	ARG	conflict	UNP P04483
A	105	PHE	PRO	conflict	UNP P04483
A	108	GLN	LYS	conflict	UNP P04483
A	113	ALA	LEU	conflict	UNP P04483
A	116	SER	GLN	conflict	UNP P04483
A	121	THR	CYS	conflict	UNP P04483
A	134	MET	LEU	conflict	UNP P04483
A	135	GLN	SER	conflict	UNP P04483
A	139	ILE	HIS	conflict	UNP P04483
A	140	TYR	PHE	conflict	UNP P04483
A	147	LEU	GLU	conflict	UNP P04483

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Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LEU	HIS	conflict	UNP P04483
A	170	VAL	LEU	conflict	UNP P04483
A	174	VAL	ILE	conflict	UNP P04483
A	177	LYS	PHE	conflict	UNP P04483
A	195	ALA	CYS	conflict	UNP P04483
B	2	ALA	SER	conflict	UNP P04483
B	55	MET	LEU	conflict	UNP P04483
B	64	ALA	HIS	conflict	UNP P04483
B	67	TYR	PHE	conflict	UNP P04483
B	68	SER	CYS	conflict	UNP P04483
B	72	ARG	GLY	conflict	UNP P04483
B	77	ASN	ASP	conflict	UNP P04483
B	86	MET	PHE	conflict	UNP P04483
B	88	ASN	CYS	conflict	UNP P04483
B	100	CYS	HIS	conflict	UNP P04483
B	104	GLY	ARG	conflict	UNP P04483
B	105	PHE	PRO	conflict	UNP P04483
B	108	GLN	LYS	conflict	UNP P04483
B	113	ALA	LEU	conflict	UNP P04483
B	116	SER	GLN	conflict	UNP P04483
B	121	THR	CYS	conflict	UNP P04483
B	134	MET	LEU	conflict	UNP P04483
B	135	GLN	SER	conflict	UNP P04483
B	139	ILE	HIS	conflict	UNP P04483
B	140	TYR	PHE	conflict	UNP P04483
B	147	LEU	GLU	conflict	UNP P04483
B	151	LEU	HIS	conflict	UNP P04483
B	170	VAL	LEU	conflict	UNP P04483
B	174	VAL	ILE	conflict	UNP P04483
B	177	LYS	PHE	conflict	UNP P04483
B	195	ALA	CYS	conflict	UNP P04483
C	2	ALA	SER	conflict	UNP P04483
C	55	MET	LEU	conflict	UNP P04483
C	64	ALA	HIS	conflict	UNP P04483
C	67	TYR	PHE	conflict	UNP P04483
C	68	SER	CYS	conflict	UNP P04483
C	72	ARG	GLY	conflict	UNP P04483
C	77	ASN	ASP	conflict	UNP P04483
C	86	MET	PHE	conflict	UNP P04483
C	88	ASN	CYS	conflict	UNP P04483
C	100	CYS	HIS	conflict	UNP P04483
C	104	GLY	ARG	conflict	UNP P04483

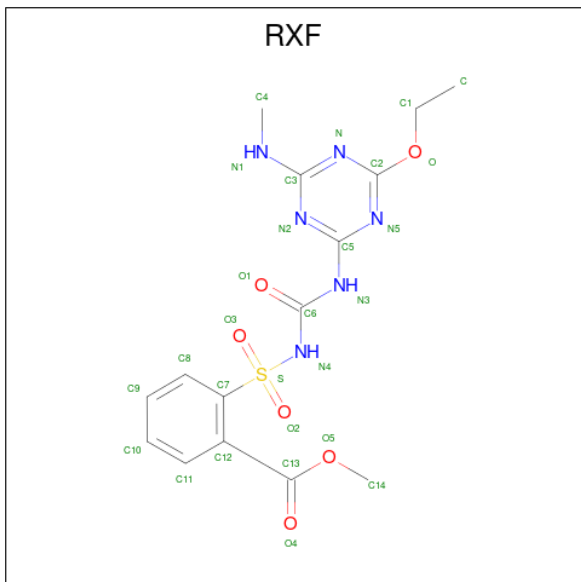
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Chain	Residue	Modelled	Actual	Comment	Reference
C	105	PHE	PRO	conflict	UNP P04483
C	108	GLN	LYS	conflict	UNP P04483
C	113	ALA	LEU	conflict	UNP P04483
C	116	SER	GLN	conflict	UNP P04483
C	121	THR	CYS	conflict	UNP P04483
C	134	MET	LEU	conflict	UNP P04483
C	135	GLN	SER	conflict	UNP P04483
C	139	ILE	HIS	conflict	UNP P04483
C	140	TYR	PHE	conflict	UNP P04483
C	147	LEU	GLU	conflict	UNP P04483
C	151	LEU	HIS	conflict	UNP P04483
C	170	VAL	LEU	conflict	UNP P04483
C	174	VAL	ILE	conflict	UNP P04483
C	177	LYS	PHE	conflict	UNP P04483
C	195	ALA	CYS	conflict	UNP P04483
D	2	ALA	SER	conflict	UNP P04483
D	55	MET	LEU	conflict	UNP P04483
D	64	ALA	HIS	conflict	UNP P04483
D	67	TYR	PHE	conflict	UNP P04483
D	68	SER	CYS	conflict	UNP P04483
D	72	ARG	GLY	conflict	UNP P04483
D	77	ASN	ASP	conflict	UNP P04483
D	86	MET	PHE	conflict	UNP P04483
D	88	ASN	CYS	conflict	UNP P04483
D	100	CYS	HIS	conflict	UNP P04483
D	104	GLY	ARG	conflict	UNP P04483
D	105	PHE	PRO	conflict	UNP P04483
D	108	GLN	LYS	conflict	UNP P04483
D	113	ALA	LEU	conflict	UNP P04483
D	116	SER	GLN	conflict	UNP P04483
D	121	THR	CYS	conflict	UNP P04483
D	134	MET	LEU	conflict	UNP P04483
D	135	GLN	SER	conflict	UNP P04483
D	139	ILE	HIS	conflict	UNP P04483
D	140	TYR	PHE	conflict	UNP P04483
D	147	LEU	GLU	conflict	UNP P04483
D	151	LEU	HIS	conflict	UNP P04483
D	170	VAL	LEU	conflict	UNP P04483
D	174	VAL	ILE	conflict	UNP P04483
D	177	LYS	PHE	conflict	UNP P04483
D	195	ALA	CYS	conflict	UNP P04483

- Molecule 2 is methyl 2-[[4-ethoxy-6-(methylamino)-1,3,5-triazin-2-yl]carbamoylsulfamo

yl]benzoate (CCD ID: RXF) (formula:  $C_{15}H_{18}N_6O_6S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	15	6	6	1		
2	B	1	Total	C	N	O	S	0	0
			28	15	6	6	1		
2	C	1	Total	C	N	O	S	0	0
			28	15	6	6	1		
2	D	1	Total	C	N	O	S	0	0
			28	15	6	6	1		

- Molecule 3 is water.

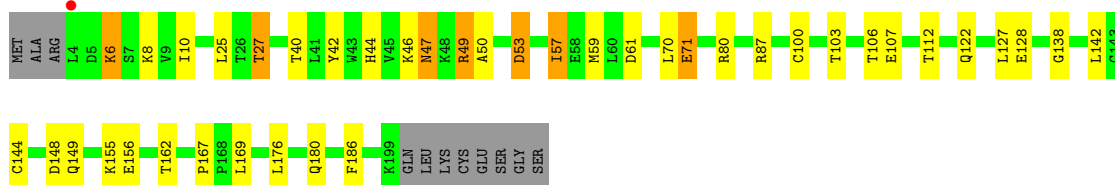
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	4	Total	O	0	0
			4	4		
3	C	1	Total	O	0	0
			1	1		
3	D	3	Total	O	0	0
			3	3		

### 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: Sulfonylurea repressor EsR (L11-C6)

Chain A: 





R158	M166 P167	V174 E175 L176	F186	L201	LYS CYS GLU SER GLY SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.82Å 71.02Å 90.53Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	29.84 – 2.80 29.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.84-2.80) 99.4 (29.84-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.190 , 0.278 0.201 , 0.286	Depositor DCC
$R_{free}$ test set	1073 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.1	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6169	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RXF

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	0.61	0/1567	1.22	7/2118 (0.3%)
1	B	0.59	0/1490	1.21	4/2010 (0.2%)
1	C	0.56	0/1559	1.22	5/2107 (0.2%)
1	D	0.56	0/1519	1.22	6/2050 (0.3%)
All	All	0.58	0/6135	1.22	22/8285 (0.3%)

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
1	B	0	1
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	11	ASN	CB-CA-C	7.00	124.95	110.31
1	C	80	ARG	CB-CA-C	-6.98	99.21	110.79
1	A	107	GLU	CB-CA-C	-6.68	99.33	110.68
1	B	156	GLU	CB-CA-C	-6.63	99.78	110.79
1	D	158	ARG	CB-CA-C	6.23	120.55	109.65
1	C	180	GLN	CB-CA-C	6.14	121.30	110.37
1	B	15	GLU	N-CA-CB	5.98	120.15	110.40
1	B	148	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	112	THR	CA-CB-OG1	-5.80	100.90	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	8	LYS	N-CA-CB	5.52	118.33	110.16
1	C	26	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	25	LEU	N-CA-CB	-5.43	102.51	110.49
1	A	40	THR	CA-CB-OG1	-5.37	101.55	109.60
1	D	95	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	158	ARG	N-CA-CB	-5.33	101.85	110.81
1	B	146	LEU	N-CA-CB	5.33	118.06	110.06
1	C	141	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	144	CYS	CB-CA-C	-5.28	102.02	110.79
1	D	175	GLU	CB-CG-CD	5.04	121.17	112.60
1	C	156	GLU	CB-CG-CD	5.04	121.16	112.60
1	D	76	GLN	N-CA-CB	5.02	117.58	110.06

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	ARG	Sidechain
1	B	87	ARG	Sidechain
1	C	65	THR	Peptide
1	C	80	ARG	Sidechain

## 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	1542	0	1548	19	0
1	B	1470	0	1484	15	0
1	C	1534	0	1537	12	0
1	D	1498	0	1515	18	0
2	A	28	0	0	1	0
2	B	28	0	0	1	0
2	C	28	0	0	0	0
2	D	28	0	0	0	0
3	A	5	0	0	1	0
3	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	3	0	0	0	0
All	All	6169	0	6084	56	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 (56) 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:C:164:ASP:O	1:C:166:MET:N	2.24	0.70
1:C:169:LEU:HB2	1:D:114:GLU:OE1	1.95	0.67
1:A:70:LEU:O	1:A:71:GLU:CB	2.44	0.66
1:A:46:LYS:O	1:A:47:ASN:O	2.15	0.65
1:B:86:MET:HE1	1:B:138:GLY:HA2	1.79	0.63
1:D:166:MET:HE1	1:D:174:VAL:HG11	1.80	0.62
1:C:37:GLU:O	1:C:40:THR:OG1	2.18	0.61
1:B:42:TYR:CD2	1:D:39:PRO:HG2	2.37	0.59
1:A:70:LEU:O	1:A:71:GLU:HB2	2.03	0.59
1:D:77:ASN:OD1	1:D:80:ARG:NH1	2.37	0.57
1:C:64:ALA:O	1:C:65:THR:C	2.47	0.57
1:D:201:LEU:HD12	1:D:201:LEU:C	2.33	0.54
1:D:63:HIS:O	1:D:85:SER:OG	2.25	0.53
1:A:49:ARG:NH2	3:A:401:HOH:O	2.36	0.53
1:A:46:LYS:O	1:A:50:ALA:HB3	2.09	0.52
1:B:38:GLN:N	1:B:39:PRO:HD2	2.25	0.52
1:B:16:LEU:HD23	1:B:25:LEU:HD12	1.90	0.52
1:A:57:ILE:O	1:A:61:ASP:HB2	2.10	0.52
1:B:61:ASP:O	1:B:62:ARG:C	2.53	0.52
1:C:57:ILE:HD13	1:C:109:GLN:HG2	1.91	0.52
1:C:173:ALA:HB1	1:D:131:LEU:HG	1.92	0.51
1:C:164:ASP:O	1:C:165:SER:C	2.55	0.49
1:A:128:GLU:HG3	1:B:176:LEU:HD21	1.94	0.48
1:A:27:THR:HG21	1:A:42:TYR:OH	2.13	0.48
1:C:39:PRO:HA	1:C:42:TYR:HD2	1.80	0.47
1:D:87:ARG:HD2	1:D:186:PHE:CE2	2.50	0.47
1:A:53:ASP:OD2	1:B:158:ARG:HD2	2.14	0.47
1:B:127:LEU:C	1:B:127:LEU:HD23	2.40	0.47
1:A:167:PRO:HB2	1:B:114:GLU:OE1	2.15	0.46
1:D:6:LYS:O	1:D:7:SER:C	2.59	0.46
1:A:169:LEU:HD22	1:B:127:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LEU:HD21	1:D:40:THR:HG22	1.97	0.46
1:B:121:THR:HA	1:B:125:PHE:O	2.16	0.45
1:C:28:ARG:NH1	1:C:32:GLN:OE1	2.49	0.45
1:A:49:ARG:O	1:A:49:ARG:HD3	2.16	0.45
1:C:38:GLN:HB2	1:C:39:PRO:HD3	2.00	0.44
1:C:188:PHE:O	1:C:192:LEU:HG	2.18	0.44
1:A:148:ASP:O	1:A:149:GLN:C	2.60	0.44
1:A:103:THR:HA	1:A:106:THR:HG23	1.99	0.43
1:D:21:GLY:HA2	1:D:94:ARG:HD2	1.98	0.43
1:C:183:GLU:N	1:C:184:PRO:CD	2.82	0.43
1:D:109:GLN:O	1:D:110:TYR:C	2.63	0.42
1:B:42:TYR:CE2	1:D:39:PRO:HG2	2.54	0.42
1:D:92:SER:OG	1:D:93:HIS:ND1	2.53	0.42
1:D:201:LEU:C	1:D:201:LEU:CD1	2.93	0.41
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.99	0.41
1:D:20:VAL:HG22	1:D:20:VAL:O	2.20	0.41
1:A:138:GLY:HA3	2:A:301:RXF:O4	2.21	0.41
1:B:119:PHE:CZ	1:B:123:GLN:NE2	2.89	0.41
1:B:177:LYS:C	1:B:179:HIS:H	2.29	0.41
1:A:87:ARG:HD3	1:A:186:PHE:CE2	2.56	0.41
1:A:6:LYS:HD2	1:A:10:ILE:CD1	2.51	0.40
1:D:135:GLN:NE2	1:D:135:GLN:HA	2.36	0.40
1:A:6:LYS:HD2	1:A:10:ILE:HD11	2.02	0.40
1:A:59:MET:HE2	1:A:100:CYS:SG	2.60	0.40
1:B:102:GLY:HA2	2:B:301:RXF:O1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/207 (94%)	186 (96%)	6 (3%)	2 (1%)	12	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	184/207 (89%)	170 (92%)	13 (7%)	1 (0%)	24	55
1	C	193/207 (93%)	179 (93%)	12 (6%)	2 (1%)	12	38
1	D	187/207 (90%)	180 (96%)	7 (4%)	0	100	100
All	All	758/828 (92%)	715 (94%)	38 (5%)	5 (1%)	18	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	B	61	ASP
1	C	165	SER
1	A	71	GLU
1	C	164	ASP

### 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	165/174 (95%)	152 (92%)	13 (8%)	11	35
1	B	158/174 (91%)	147 (93%)	11 (7%)	14	40
1	C	164/174 (94%)	148 (90%)	16 (10%)	7	25
1	D	160/174 (92%)	151 (94%)	9 (6%)	19	50
All	All	647/696 (93%)	598 (92%)	49 (8%)	12	36

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	27	THR
1	A	44	HIS
1	A	49	ARG
1	A	57	ILE
1	A	122	GLN

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Mol	Chain	Res	Type
1	A	127	LEU
1	A	142	LEU
1	A	155	LYS
1	A	156	GLU
1	A	162	THR
1	A	176	LEU
1	A	180	GLN
1	B	15	GLU
1	B	20	VAL
1	B	33	LYS
1	B	40	THR
1	B	49	ARG
1	B	57	ILE
1	B	128	GLU
1	B	142	LEU
1	B	183	GLU
1	B	184	PRO
1	B	194	ILE
1	C	8	LYS
1	C	20	VAL
1	C	25	LEU
1	C	27	THR
1	C	30	LEU
1	C	46	LYS
1	C	49	ARG
1	C	58	GLU
1	C	65	THR
1	C	79	LEU
1	C	131	LEU
1	C	153	VAL
1	C	155	LYS
1	C	162	THR
1	C	163	THR
1	C	178	ASP
1	D	11	ASN
1	D	45	VAL
1	D	49	ARG
1	D	65	THR
1	D	94	ARG
1	D	131	LEU
1	D	146	LEU
1	D	167	PRO

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Mol	Chain	Res	Type
1	D	176	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	63	HIS
1	A	109	GLN
1	A	123	GLN
1	A	149	GLN
1	A	152	GLN
1	B	93	HIS
1	B	109	GLN
1	B	123	GLN
1	C	77	ASN
1	D	11	ASN
1	D	38	GLN
1	D	63	HIS
1	D	82	ASN
1	D	109	GLN
1	D	123	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
2	RXF	C	301	-	29,29,29	2.06	7 (24%)	38,40,40	4.01	23 (60%)
2	RXF	D	301	-	29,29,29	2.29	7 (24%)	38,40,40	3.15	14 (36%)
2	RXF	B	301	-	29,29,29	2.39	7 (24%)	38,40,40	3.55	17 (44%)
2	RXF	A	301	-	29,29,29	2.13	5 (17%)	38,40,40	3.45	15 (39%)

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
2	RXF	C	301	-	-	9/26/26/26	0/2/2/2
2	RXF	D	301	-	-	9/26/26/26	0/2/2/2
2	RXF	B	301	-	-	7/26/26/26	0/2/2/2
2	RXF	A	301	-	-	8/26/26/26	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	RXF	O2-S	8.53	1.53	1.43
2	D	301	RXF	O2-S	7.34	1.52	1.43
2	A	301	RXF	O2-S	6.69	1.51	1.43
2	A	301	RXF	O3-S	6.52	1.51	1.43
2	C	301	RXF	O2-S	6.49	1.51	1.43
2	B	301	RXF	O3-S	6.36	1.50	1.43
2	D	301	RXF	C7-S	-5.23	1.70	1.77
2	D	301	RXF	O3-S	5.12	1.49	1.43
2	C	301	RXF	O-C2	4.15	1.39	1.34
2	C	301	RXF	O3-S	3.81	1.48	1.43
2	C	301	RXF	C3-N1	-3.57	1.31	1.34
2	B	301	RXF	C3-N1	-3.53	1.31	1.34
2	A	301	RXF	O-C2	3.29	1.37	1.34
2	B	301	RXF	C6-N4	-3.26	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	RXF	C7-S	-3.19	1.73	1.77
2	D	301	RXF	C5-N3	-2.93	1.35	1.38
2	D	301	RXF	O-C2	2.68	1.37	1.34
2	D	301	RXF	C4-N1	2.50	1.49	1.45
2	C	301	RXF	O-C1	2.39	1.51	1.43
2	B	301	RXF	C12-C7	-2.36	1.38	1.40
2	A	301	RXF	C4-N1	2.31	1.48	1.45
2	A	301	RXF	C6-N4	-2.29	1.34	1.39
2	B	301	RXF	C5-N3	-2.20	1.35	1.38
2	B	301	RXF	S-N4	-2.19	1.58	1.64
2	C	301	RXF	C6-N4	-2.18	1.34	1.39
2	D	301	RXF	C3-N1	-2.01	1.32	1.34

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RXF	C2-N5-C5	12.22	122.83	112.86
2	C	301	RXF	O2-S-O3	-11.73	105.27	119.52
2	C	301	RXF	C2-N5-C5	11.24	122.03	112.86
2	D	301	RXF	C2-N-C3	10.15	121.15	112.86
2	C	301	RXF	C2-N-C3	9.87	120.92	112.86
2	B	301	RXF	C2-N5-C5	9.13	120.31	112.86
2	B	301	RXF	C2-N-C3	8.83	120.07	112.86
2	B	301	RXF	O2-S-O3	-8.66	109.00	119.52
2	A	301	RXF	C2-N-C3	8.40	119.72	112.86
2	D	301	RXF	C2-N5-C5	7.99	119.38	112.86
2	B	301	RXF	C4-N1-C3	-7.33	114.75	123.59
2	D	301	RXF	O2-S-O3	-6.96	111.07	119.52
2	B	301	RXF	C5-N3-C6	-6.42	123.73	130.34
2	B	301	RXF	N1-C3-N2	5.95	122.68	116.96
2	A	301	RXF	C5-N3-C6	-5.82	124.35	130.34
2	C	301	RXF	N5-C2-N	-5.75	117.19	127.65
2	A	301	RXF	O2-S-O3	-5.68	112.63	119.52
2	C	301	RXF	O-C1-C	5.04	123.78	108.04
2	A	301	RXF	N5-C2-N	-5.04	118.49	127.65
2	A	301	RXF	N5-C5-N2	-4.92	118.19	126.26
2	A	301	RXF	C14-O5-C13	-4.87	106.44	115.81
2	A	301	RXF	C11-C12-C7	4.78	123.16	118.01
2	C	301	RXF	N1-C3-N2	4.61	121.39	116.96
2	D	301	RXF	N5-C2-N	-4.61	119.28	127.65
2	D	301	RXF	N1-C3-N2	4.47	121.26	116.96
2	C	301	RXF	N5-C5-N2	-4.21	119.36	126.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RXF	N5-C2-N	-4.04	120.31	127.65
2	D	301	RXF	N5-C5-N2	-3.99	119.72	126.26
2	C	301	RXF	C4-N1-C3	-3.99	118.78	123.59
2	C	301	RXF	C9-C10-C11	-3.98	115.33	120.24
2	C	301	RXF	O5-C13-C12	3.98	118.91	112.31
2	D	301	RXF	C14-O5-C13	-3.88	108.36	115.81
2	D	301	RXF	N2-C3-N	-3.85	119.95	126.26
2	D	301	RXF	C5-N2-C3	3.72	120.52	113.85
2	D	301	RXF	C5-N3-C6	-3.55	126.69	130.34
2	B	301	RXF	O3-S-C7	3.55	113.53	107.68
2	C	301	RXF	C7-C12-C13	-3.50	119.57	124.25
2	B	301	RXF	N5-C5-N2	-3.39	120.70	126.26
2	C	301	RXF	O3-S-C7	3.38	113.25	107.68
2	D	301	RXF	O-C1-C	3.33	118.44	108.04
2	A	301	RXF	N3-C5-N2	3.31	126.06	116.44
2	B	301	RXF	N3-C5-N2	3.22	125.80	116.44
2	B	301	RXF	C11-C12-C7	3.22	121.48	118.01
2	B	301	RXF	N2-C3-N	-3.01	121.33	126.26
2	C	301	RXF	C5-N3-C6	-2.80	127.45	130.34
2	C	301	RXF	C8-C7-S	2.74	121.45	117.51
2	A	301	RXF	C5-N2-C3	2.69	118.67	113.85
2	C	301	RXF	O2-S-C7	2.64	112.05	107.68
2	A	301	RXF	N2-C3-N	-2.59	122.01	126.26
2	C	301	RXF	N3-C5-N2	2.54	123.83	116.44
2	D	301	RXF	C7-S-N4	2.52	109.09	105.96
2	C	301	RXF	C5-N2-C3	2.46	118.26	113.85
2	C	301	RXF	N2-C3-N	-2.45	122.24	126.26
2	C	301	RXF	C8-C7-C12	-2.43	118.41	121.25
2	B	301	RXF	C8-C7-C12	-2.37	118.48	121.25
2	B	301	RXF	C14-O5-C13	-2.36	111.28	115.81
2	A	301	RXF	C8-C7-C12	-2.32	118.54	121.25
2	A	301	RXF	N1-C3-N2	2.32	119.19	116.96
2	C	301	RXF	C14-O5-C13	-2.31	111.37	115.81
2	C	301	RXF	O5-C13-O4	-2.27	119.05	123.46
2	A	301	RXF	O-C2-N	2.24	123.27	116.17
2	B	301	RXF	O-C2-N	2.21	123.18	116.17
2	D	301	RXF	C4-N1-C3	-2.21	120.92	123.59
2	B	301	RXF	O2-S-N4	2.17	112.97	106.77
2	C	301	RXF	C10-C9-C8	2.13	122.86	120.24
2	D	301	RXF	O3-S-N4	2.11	112.81	106.77
2	A	301	RXF	O2-S-C7	2.11	111.16	107.68
2	C	301	RXF	C11-C12-C7	2.08	120.25	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RXF	C11-C12-C13	-2.02	114.56	118.66

There are no chirality outliers.

All (33) torsion outliers are listed below:

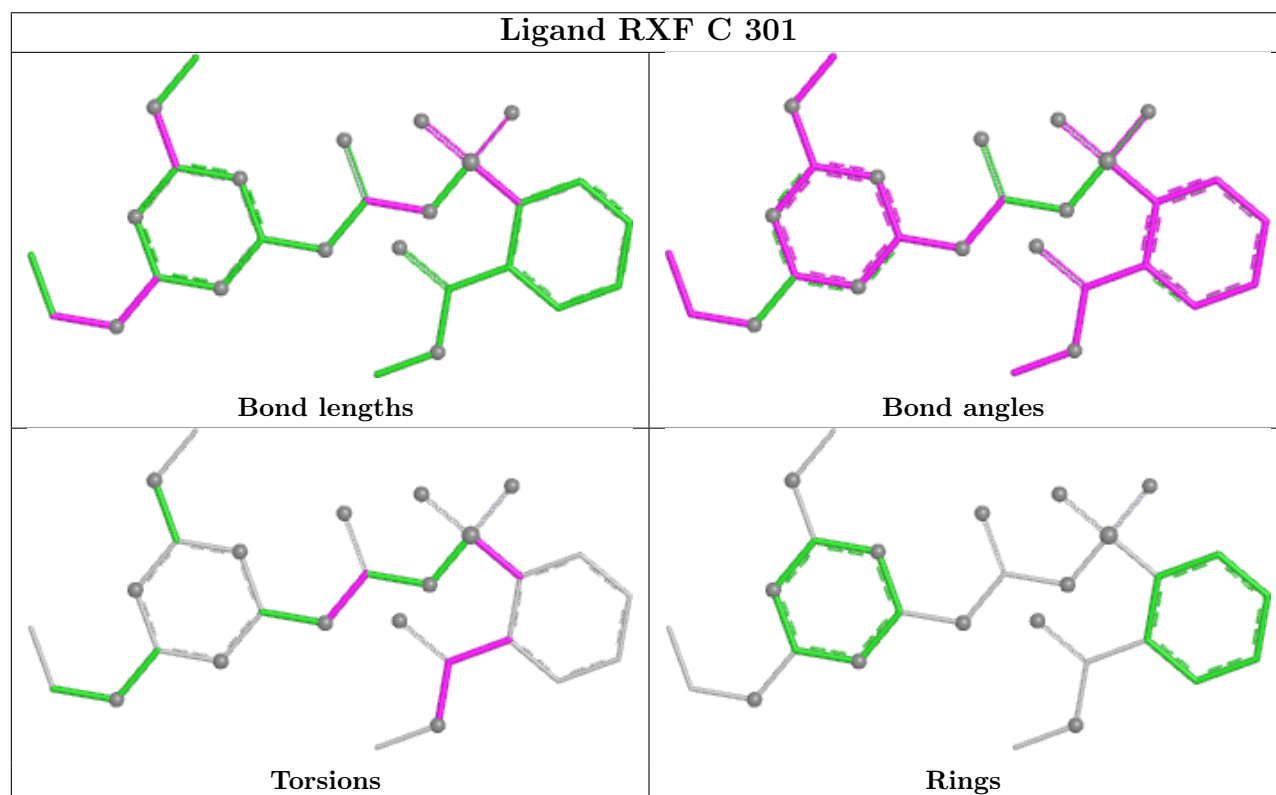
Mol	Chain	Res	Type	Atoms
2	C	301	RXF	C12-C13-O5-C14
2	C	301	RXF	O4-C13-O5-C14
2	B	301	RXF	C12-C7-S-O3
2	C	301	RXF	C12-C7-S-O3
2	D	301	RXF	C12-C7-S-O3
2	D	301	RXF	C12-C7-S-N4
2	A	301	RXF	N-C2-O-C1
2	A	301	RXF	N5-C2-O-C1
2	D	301	RXF	C8-C7-S-O3
2	D	301	RXF	C11-C12-C13-O5
2	B	301	RXF	C11-C12-C13-O5
2	C	301	RXF	C11-C12-C13-O5
2	A	301	RXF	C11-C12-C13-O5
2	A	301	RXF	C12-C7-S-O3
2	B	301	RXF	C-C1-O-C2
2	A	301	RXF	C7-C12-C13-O5
2	C	301	RXF	C7-C12-C13-O5
2	B	301	RXF	C7-C12-C13-O5
2	B	301	RXF	C7-C12-C13-O4
2	C	301	RXF	C7-C12-C13-O4
2	D	301	RXF	C7-C12-C13-O4
2	D	301	RXF	C7-C12-C13-O5
2	D	301	RXF	N-C2-O-C1
2	A	301	RXF	C7-C12-C13-O4
2	B	301	RXF	C11-C12-C13-O4
2	C	301	RXF	C11-C12-C13-O4
2	D	301	RXF	C11-C12-C13-O4
2	A	301	RXF	C11-C12-C13-O4
2	A	301	RXF	N4-C6-N3-C5
2	B	301	RXF	N4-C6-N3-C5
2	C	301	RXF	N4-C6-N3-C5
2	D	301	RXF	N4-C6-N3-C5
2	C	301	RXF	C8-C7-S-O3

There are no ring outliers.

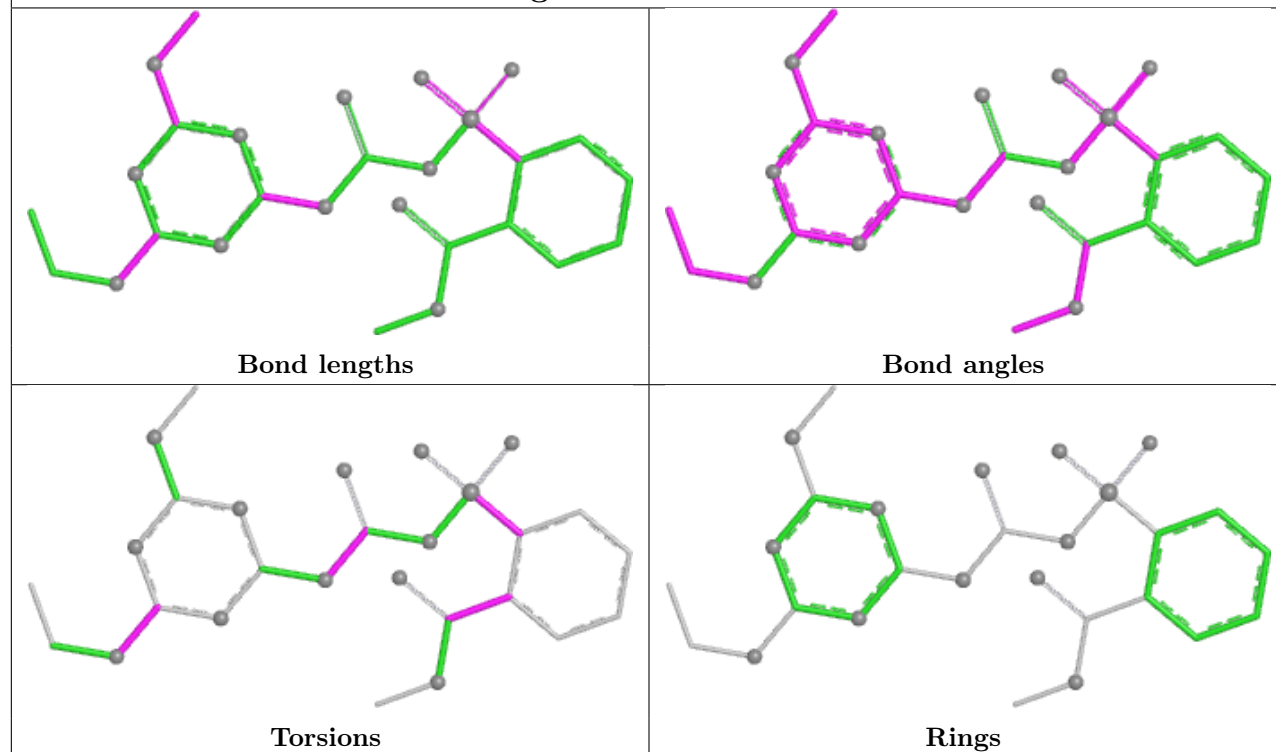
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	RXF	1	0
2	A	301	RXF	1	0

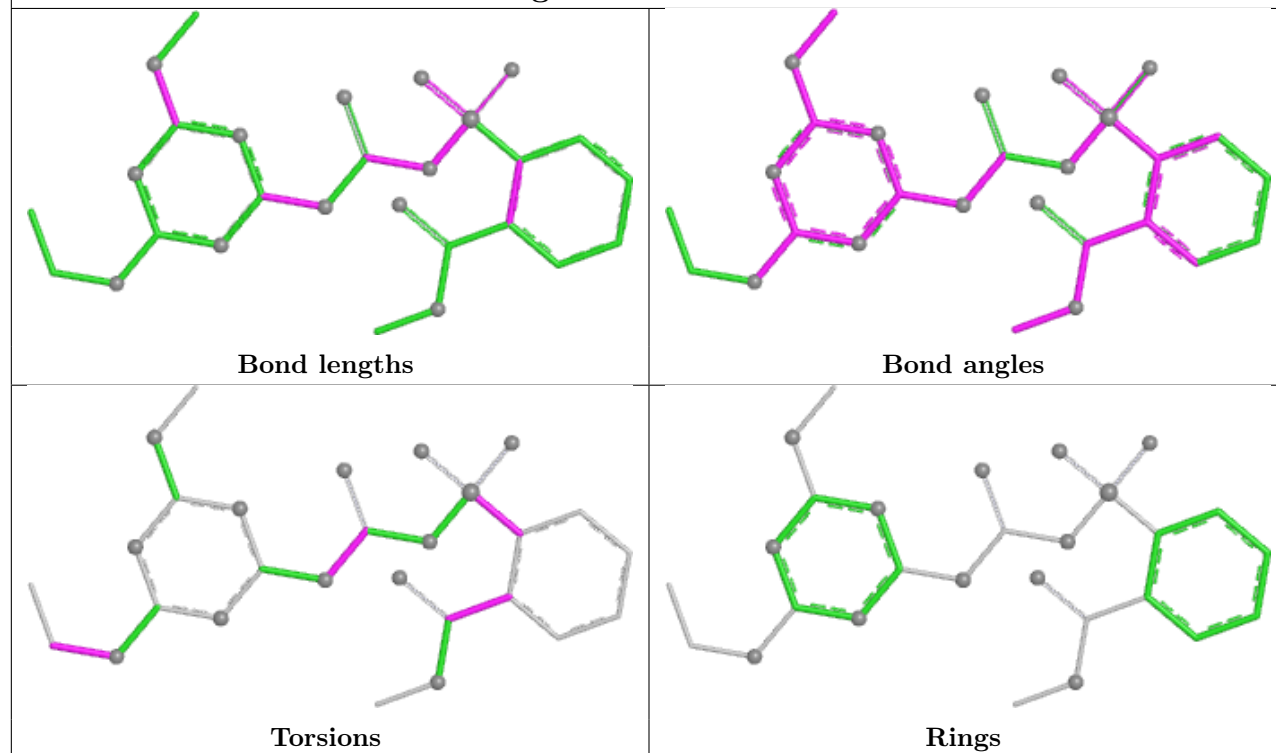
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

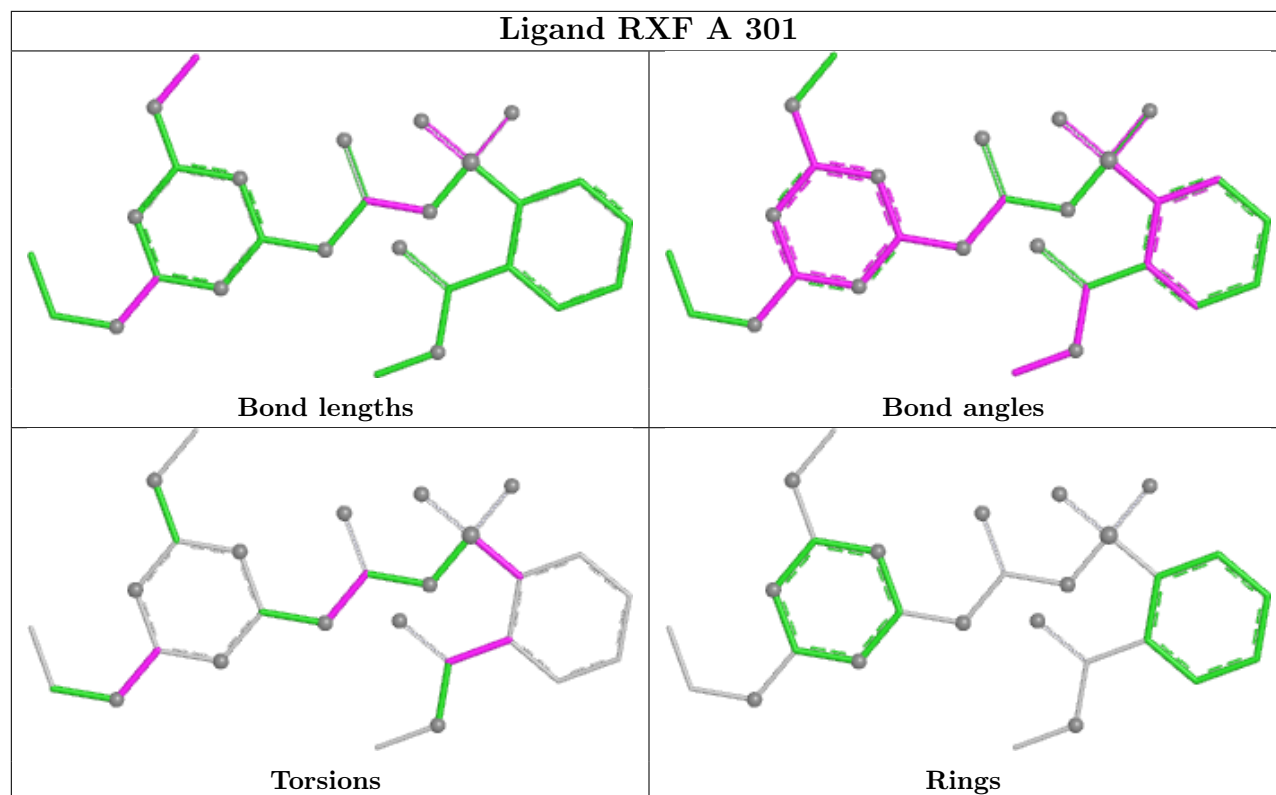


## Ligand RXF D 301



## Ligand RXF B 301





## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	196/207 (94%)	-0.39	1 (0%) 87 82	37, 55, 93, 107	0
1	B	188/207 (90%)	-0.27	0 100 100	33, 60, 93, 111	0
1	C	195/207 (94%)	-0.35	1 (0%) 87 82	41, 60, 89, 115	0
1	D	191/207 (92%)	-0.35	0 100 100	41, 62, 83, 96	0
All	All	770/828 (92%)	-0.34	2 (0%) 90 86	33, 60, 90, 115	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	2.8
1	C	42	TYR	2.3

### 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](#)

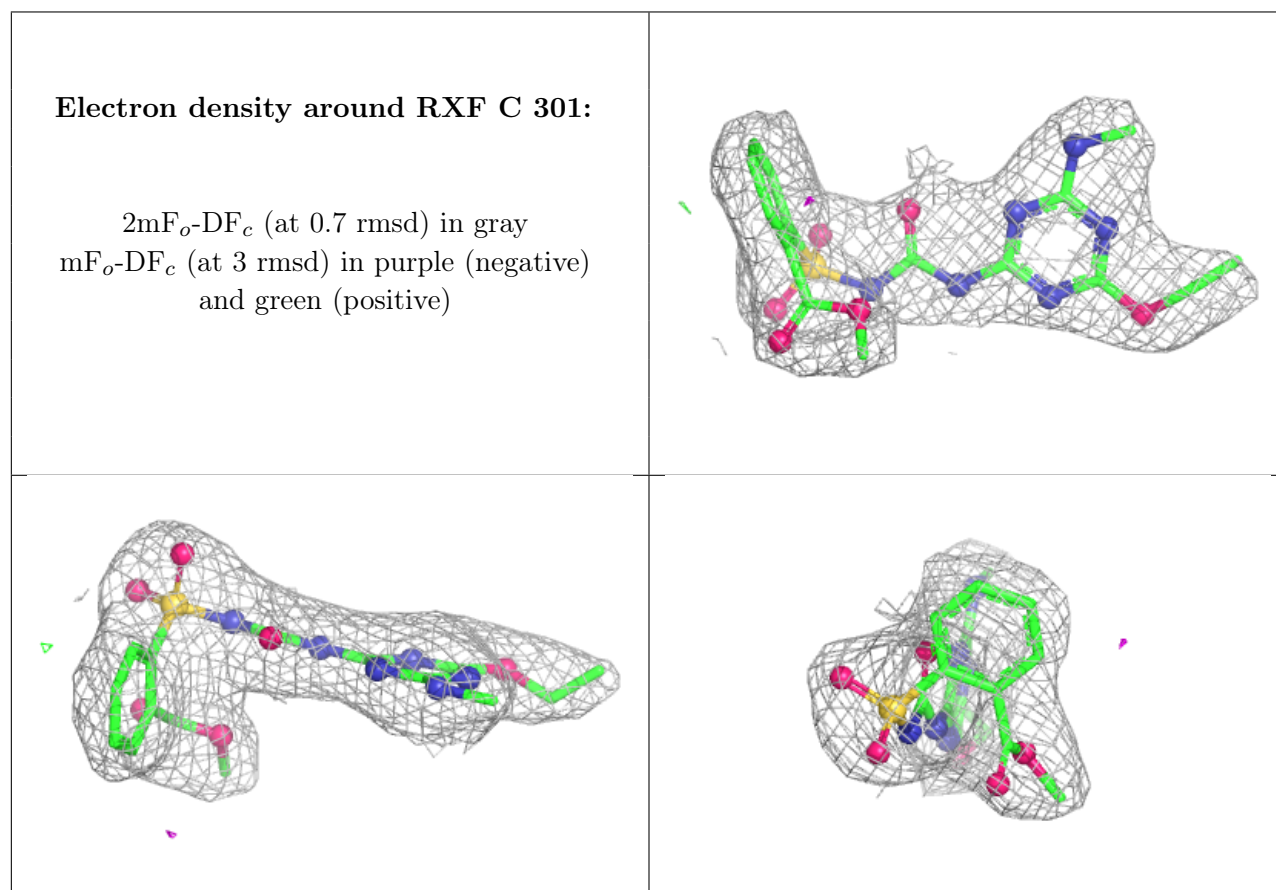
There are no oligosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

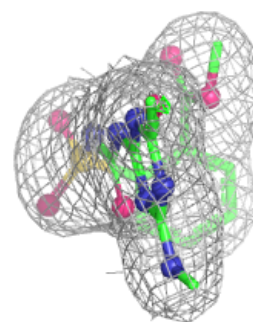
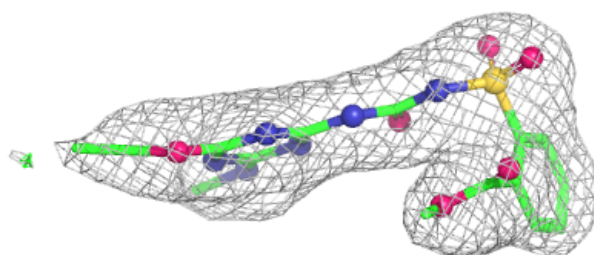
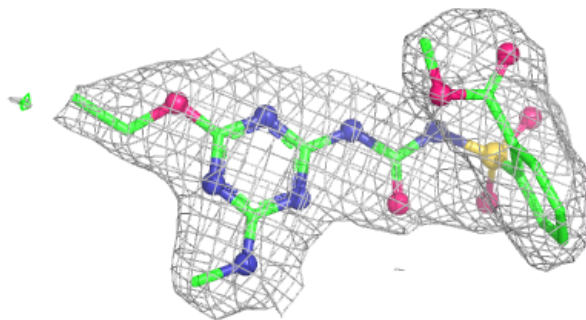
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RXF	C	301	28/28	0.97	0.06	35,48,63,66	0
2	RXF	D	301	28/28	0.97	0.06	38,49,71,74	0
2	RXF	A	301	28/28	0.98	0.06	28,38,69,77	0
2	RXF	B	301	28/28	0.98	0.05	38,45,52,55	0

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.

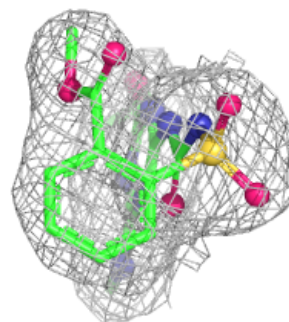
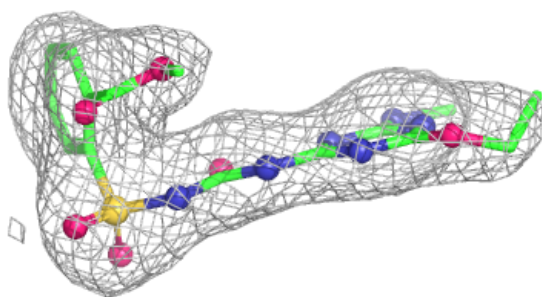
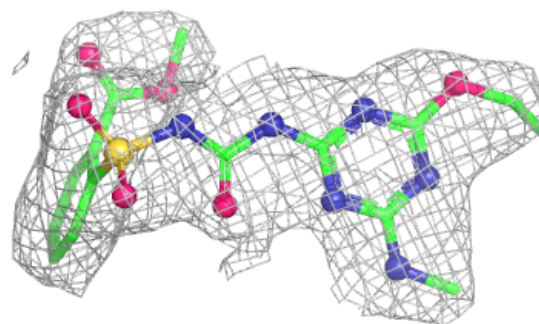


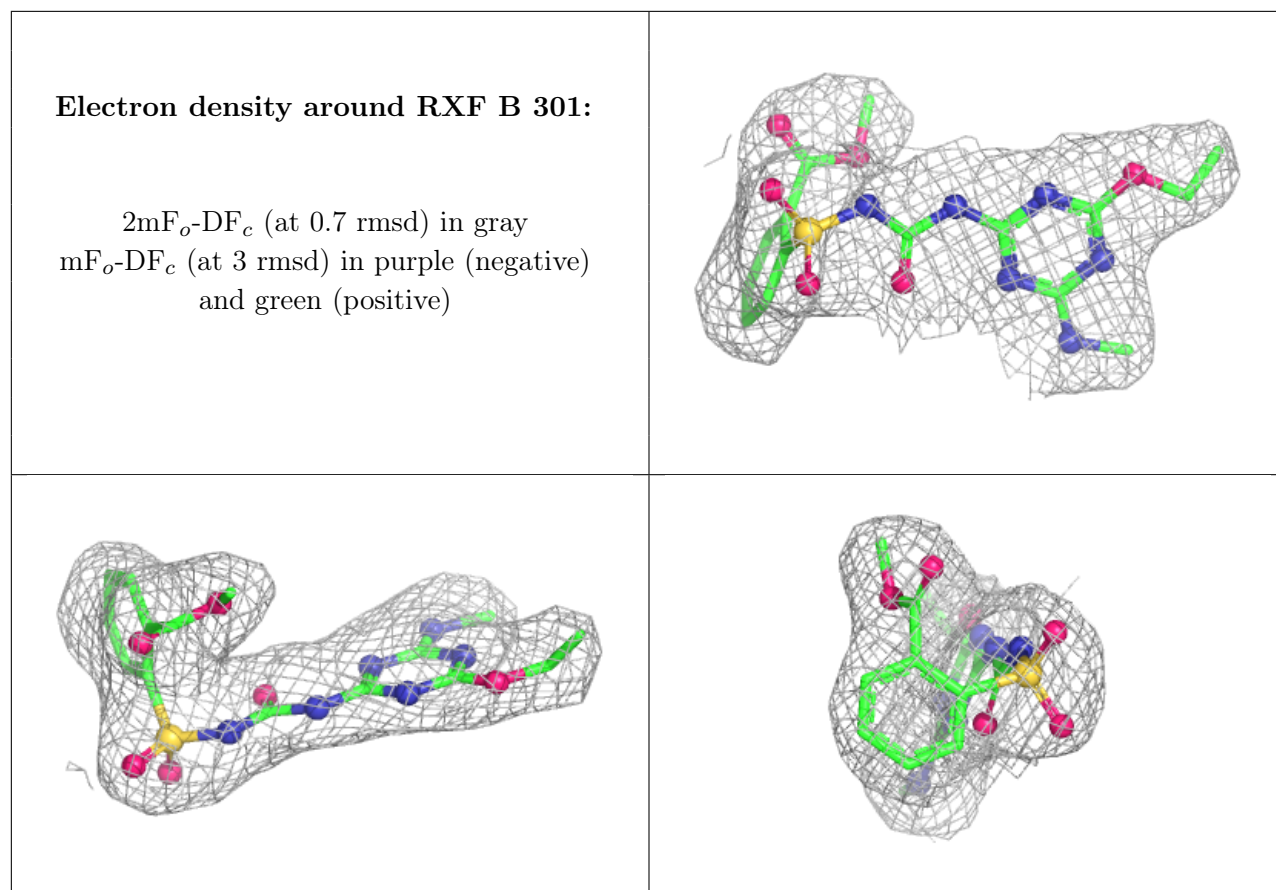
**Electron density around RXF D 301:**

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

**Electron density around RXF A 301:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.