



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2025 – 02:05 pm BST

PDB ID : 9H65 / pdb\_00009h65  
Title : Steroidal Selective Modulators of FXR with Therapeutic Potential  
Authors : Kydd-Sinclair, D.; Watson, K.A.  
Deposited on : 2024-10-23  
Resolution : 3.10 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 Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

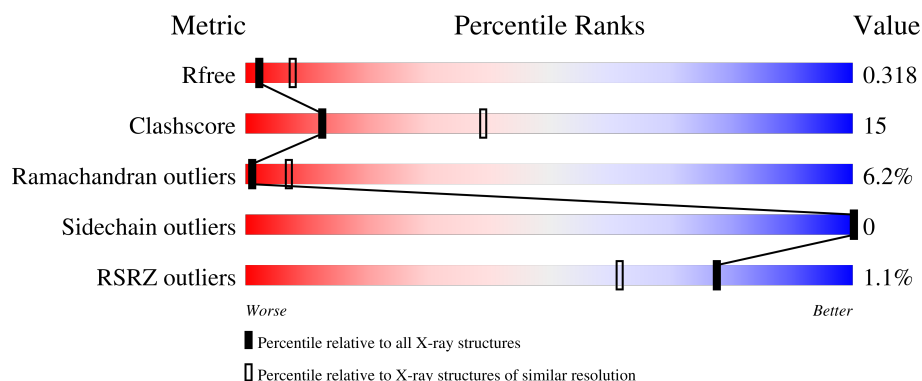
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




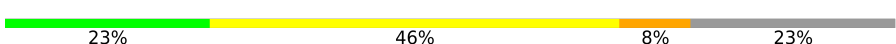
The reported resolution of this entry is 3.10 Å.

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))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	233	
1	B	233	
2	C	13	
2	D	13	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3482 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	229	Total	C	N	O	S	0	0	0
			1659	1063	281	305	10			
1	B	224	Total	C	N	O	S	0	0	0
			1547	984	265	287	11			

There are 12 discrepancies between the modelled and reference sequences:

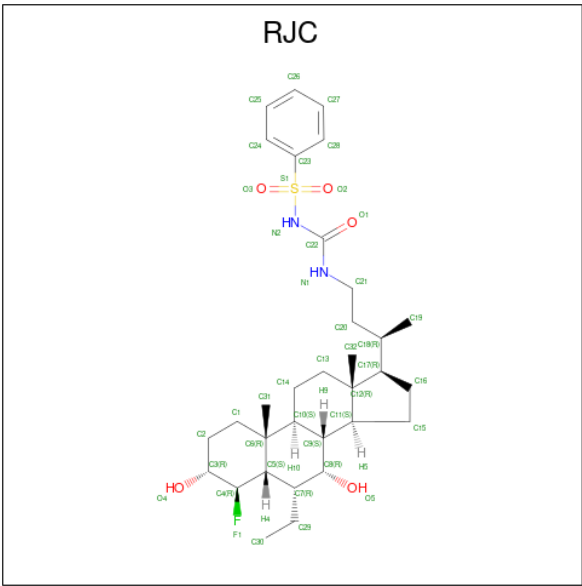
Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLY	-	expression tag	UNP Q96RI1
A	241	SER	-	expression tag	UNP Q96RI1
A	242	HIS	-	expression tag	UNP Q96RI1
A	243	MET	-	expression tag	UNP Q96RI1
A	277	ALA	GLU	engineered mutation	UNP Q96RI1
A	350	ALA	GLU	engineered mutation	UNP Q96RI1
B	240	GLY	-	expression tag	UNP Q96RI1
B	241	SER	-	expression tag	UNP Q96RI1
B	242	HIS	-	expression tag	UNP Q96RI1
B	243	MET	-	expression tag	UNP Q96RI1
B	277	ALA	GLU	engineered mutation	UNP Q96RI1
B	350	ALA	GLU	engineered mutation	UNP Q96RI1

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	0
			103	66	18	19			
2	D	10	Total	C	N	O	0	0	0
			73	47	11	15			

- Molecule 3 is 1-[(3R)-3-[(3R,4R,5S,6R,7R,8S,9S,10R,13R,14S,17R)-6-ethyl-4-fluoranyl-10,13-dimethyl-3,7-bis(oxidanyl)-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]butyl]-3-(phenylsulfonyl)urea (CCD ID: RJC) (formula:

C<sub>32</sub>H<sub>49</sub>FN<sub>2</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			41	32	1	2	5	1		
3	B	1	Total	C	F	N	O	S	0	0
			41	32	1	2	5	1		

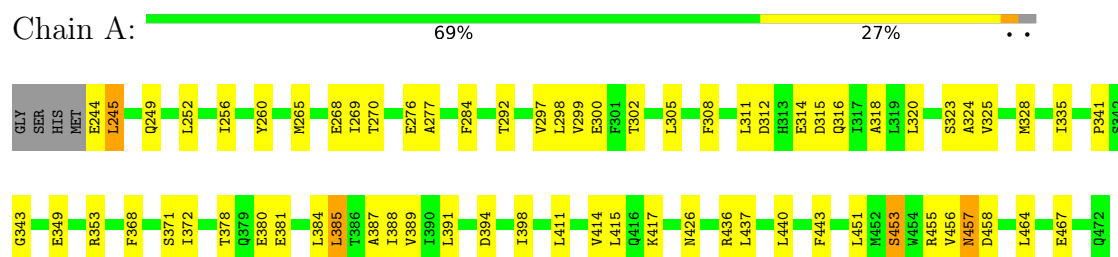
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	10	Total	O	0	0
			10	10		
4	C	1	Total	O	0	0
			1	1		

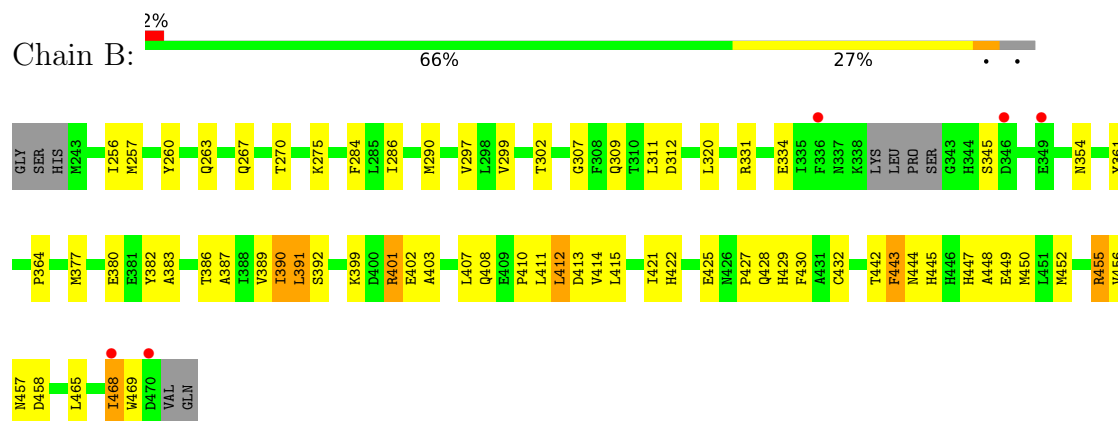
### 3 Residue-property plots

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.

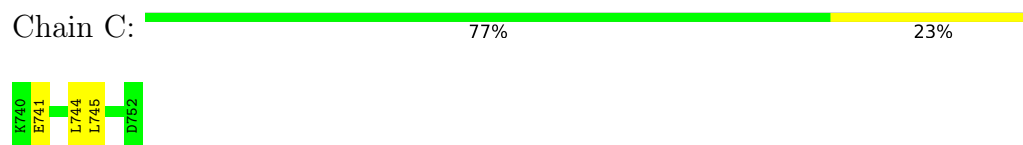
#### • Molecule 1: Bile acid receptor



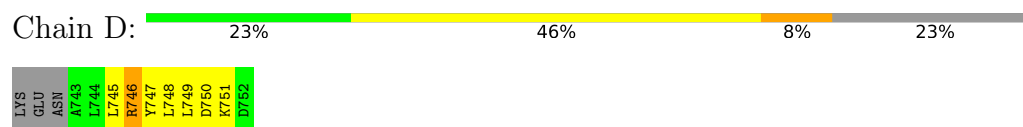
#### • Molecule 1: Bile acid receptor



#### • Molecule 2: Nuclear receptor coactivator 2



#### • Molecule 2: Nuclear receptor coactivator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.06Å 104.81Å 155.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.03 – 3.10 47.03 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.03-3.10) 99.8 (47.03-3.10)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.227 , 0.323 0.228 , 0.318	Depositor DCC
$R_{free}$ test set	713 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	124.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 113.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3482	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: RJC

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	0.46	0/1695	0.66	0/2321
1	B	0.43	0/1579	0.66	0/2164
2	C	0.40	0/103	0.45	0/138
2	D	0.31	0/73	0.79	0/98
All	All	0.44	0/3450	0.66	0/4721

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1659	0	1478	49	0
1	B	1547	0	1287	41	0
2	C	103	0	101	2	0
2	D	73	0	62	5	0
3	A	41	0	0	0	0
3	B	41	0	0	0	0
4	A	7	0	0	0	0
4	B	10	0	0	1	0
4	C	1	0	0	0	0
All	All	3482	0	2928	96	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 15.

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:B:345:SER:O	4:B:901:HOH:O	1.93	0.86
1:A:385:LEU:O	1:A:389:VAL:HG23	1.88	0.73
1:B:401:ARG:O	1:B:403:ALA:N	2.23	0.72
1:B:267:GLN:HA	1:B:270:THR:HB	1.74	0.69
1:A:394:ASP:HA	1:A:398:ILE:HD13	1.77	0.66
1:B:263:GLN:HB3	1:B:297:VAL:HG13	1.78	0.66
1:B:468:ILE:HG23	1:B:469:TRP:H	1.61	0.64
1:A:298:LEU:O	1:A:302:THR:OG1	2.14	0.64
1:A:312:ASP:OD1	1:A:314:GLU:N	2.31	0.63
2:D:745:LEU:O	2:D:747:TYR:N	2.32	0.62
1:A:440:LEU:HD12	1:A:443:PHE:HD2	1.66	0.61
1:A:297:VAL:O	1:A:300:GLU:HG3	2.02	0.60
1:A:378:THR:HB	1:A:381:GLU:H	1.67	0.60
1:B:387:ALA:HB1	1:B:411:LEU:HD13	1.84	0.59
1:A:368:PHE:CE2	1:A:372:ILE:HD11	2.38	0.59
1:A:456:VAL:O	1:A:458:ASP:N	2.35	0.59
1:B:391:LEU:HD13	1:B:407:LEU:HB3	1.85	0.59
1:A:455:ARG:HH12	1:A:458:ASP:H	1.51	0.58
1:A:378:THR:HG22	1:A:380:GLU:H	1.69	0.57
1:B:361:TYR:O	1:B:364:PRO:HD2	2.05	0.56
1:B:449:GLU:HA	1:B:452:MET:HE2	1.86	0.56
1:B:429:HIS:O	1:B:432:CYS:N	2.39	0.55
1:A:315:ASP:O	1:A:318:ALA:N	2.39	0.55
1:A:299:VAL:HG22	1:A:320:LEU:HD13	1.87	0.55
1:B:465:LEU:O	1:B:468:ILE:HG22	2.06	0.54
2:D:749:LEU:HD13	2:D:751:LYS:HB2	1.90	0.53
1:B:455:ARG:HH11	1:B:455:ARG:HG3	1.74	0.53
1:B:257:MET:O	1:B:260:TYR:N	2.41	0.53
1:B:427:PRO:C	1:B:429:HIS:H	2.16	0.53
1:A:384:LEU:HD22	1:A:415:LEU:HB2	1.90	0.52
1:A:371:SER:HB3	1:A:436:ARG:HH22	1.75	0.51
2:D:746:ARG:O	2:D:748:LEU:N	2.44	0.50
1:A:384:LEU:C	1:A:388:ILE:HD12	2.36	0.50
1:A:385:LEU:HD22	1:A:437:LEU:HD21	1.93	0.50
1:A:368:PHE:CZ	1:A:372:ILE:HD11	2.47	0.49
1:A:384:LEU:O	1:A:387:ALA:N	2.45	0.49
1:B:403:ALA:O	1:B:407:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LEU:O	1:B:415:LEU:N	2.46	0.49
2:D:750:ASP:OD1	2:D:750:ASP:N	2.42	0.49
1:A:252:LEU:HD21	1:A:411:LEU:HD23	1.96	0.48
1:B:442:THR:O	1:B:444:ASN:N	2.47	0.48
1:B:455:ARG:HG3	1:B:455:ARG:NH1	2.29	0.47
1:B:331:ARG:NH1	1:B:334:GLU:OE1	2.47	0.47
1:B:389:VAL:O	1:B:392:SER:HB2	2.14	0.47
1:A:384:LEU:O	1:A:388:ILE:HD12	2.13	0.47
1:A:256:ILE:O	1:A:260:TYR:N	2.47	0.47
1:B:257:MET:SD	1:B:380:GLU:HA	2.55	0.47
1:A:384:LEU:O	1:A:385:LEU:C	2.58	0.46
1:A:325:VAL:O	1:A:328:MET:HB3	2.15	0.46
1:A:414:VAL:O	1:A:417:LYS:N	2.49	0.46
1:A:467:GLU:OE1	2:C:744:LEU:HB2	2.15	0.46
1:A:426:ASN:N	1:A:426:ASN:OD1	2.49	0.46
1:A:312:ASP:OD1	1:A:312:ASP:C	2.59	0.46
1:B:429:HIS:O	1:B:432:CYS:HB3	2.16	0.45
1:B:445:HIS:O	1:B:448:ALA:HB3	2.17	0.45
1:B:307:GLY:C	1:B:407:LEU:HD11	2.42	0.45
1:B:429:HIS:O	1:B:430:PHE:C	2.59	0.45
1:B:408:GLN:HG2	1:B:412:LEU:HD12	1.98	0.45
1:B:444:ASN:HA	1:B:447:HIS:HB3	2.00	0.44
1:B:377:MET:HB2	1:B:382:TYR:CE2	2.53	0.44
1:A:368:PHE:O	1:A:372:ILE:HD12	2.17	0.43
1:B:410:PRO:O	1:B:414:VAL:HG23	2.18	0.43
2:D:748:LEU:C	2:D:748:LEU:HD13	2.43	0.43
1:A:268:GLU:C	1:A:270:THR:H	2.26	0.43
1:A:265:MET:HG3	1:A:297:VAL:HG21	2.01	0.43
1:A:451:LEU:C	1:A:453:SER:H	2.27	0.43
1:B:427:PRO:O	1:B:429:HIS:N	2.47	0.43
1:A:323:SER:O	1:A:324:ALA:C	2.61	0.42
1:A:292:THR:HG23	1:A:464:LEU:HD23	2.00	0.42
1:A:455:ARG:NH1	1:A:458:ASP:H	2.13	0.42
1:A:349:GLU:O	1:A:353:ARG:HG2	2.19	0.42
1:B:284:PHE:HB3	1:B:456:VAL:HG11	2.02	0.42
1:B:442:THR:OG1	1:B:443:PHE:N	2.52	0.42
1:A:456:VAL:O	1:A:457:ASN:C	2.63	0.42
1:A:244:GLU:O	1:A:245:LEU:HB2	2.19	0.42
1:B:361:TYR:CE2	1:B:450:MET:HE2	2.55	0.42
1:B:256:ILE:HG22	1:B:383:ALA:HB1	2.01	0.41
1:B:286:ILE:O	1:B:290:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:THR:OG1	1:B:320:LEU:HD21	2.20	0.41
1:A:311:LEU:O	1:A:312:ASP:C	2.63	0.41
1:A:378:THR:HB	1:A:381:GLU:N	2.34	0.41
1:B:427:PRO:C	1:B:429:HIS:N	2.79	0.41
1:B:299:VAL:HG22	1:B:320:LEU:HD13	2.03	0.41
1:B:386:THR:O	1:B:390:ILE:HG13	2.20	0.41
1:B:390:ILE:O	1:B:392:SER:N	2.47	0.41
1:A:437:LEU:HD13	1:A:437:LEU:HA	1.83	0.41
1:A:284:PHE:CD1	1:A:284:PHE:C	2.97	0.41
1:A:315:ASP:O	1:A:316:GLN:C	2.63	0.41
2:C:745:LEU:HD12	2:C:745:LEU:O	2.21	0.41
1:A:249:GLN:HG2	1:A:414:VAL:HG22	2.03	0.41
1:A:305:LEU:HD13	1:A:391:LEU:HD11	2.03	0.40
1:B:311:LEU:O	1:B:312:ASP:C	2.64	0.40
1:A:245:LEU:HD23	1:A:249:GLN:HB3	2.03	0.40
1:A:276:GLU:HG3	1:A:277:ALA:N	2.36	0.40
1:A:245:LEU:HD23	1:A:249:GLN:OE1	2.21	0.40
1:A:335:ILE:HG21	1:A:335:ILE:HD13	1.82	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	227/233 (97%)	182 (80%)	37 (16%)	8 (4%)	3	16
1	B	220/233 (94%)	172 (78%)	29 (13%)	19 (9%)	0	4
2	C	11/13 (85%)	9 (82%)	1 (9%)	1 (9%)	0	3
2	D	8/13 (62%)	4 (50%)	3 (38%)	1 (12%)	0	1
All	All	466/492 (95%)	367 (79%)	70 (15%)	29 (6%)	1	7

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	ASN
1	B	401	ARG
1	B	402	GLU
1	B	425	GLU
2	D	746	ARG
1	A	308	PHE
1	A	453	SER
1	B	422	HIS
1	B	458	ASP
2	C	741	GLU
1	A	245	LEU
1	A	269	ILE
1	B	309	GLN
1	B	443	PHE
1	B	457	ASN
1	A	341	PRO
1	B	354	ASN
1	B	399	LYS
1	B	428	GLN
1	B	455	ARG
1	A	385	LEU
1	B	275	LYS
1	B	412	LEU
1	B	421	ILE
1	A	343	GLY
1	B	391	LEU
1	B	413	ASP
1	B	468	ILE
1	B	390	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	153/213 (72%)	153 (100%)	0	100	100
1	B	128/213 (60%)	128 (100%)	0	100	100
2	C	10/12 (83%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	6/12 (50%)	6 (100%)	0	100	100
All	All	297/450 (66%)	297 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	408	GLN
1	B	261	ASN
1	B	416	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	RJC	A	801	-	44,45,45	6.30	20 (45%)	64,70,70	2.01	18 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	RJC	B	801	-	44,45,45	6.14	23 (52%)	64,70,70	2.22	23 (35%)

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	RJC	A	801	-	-	6/23/92/92	0/5/5/5
3	RJC	B	801	-	-	9/23/92/92	0/5/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	RJC	O3-S1	22.75	1.69	1.43
3	A	801	RJC	O2-S1	22.55	1.69	1.43
3	B	801	RJC	O3-S1	22.24	1.68	1.43
3	B	801	RJC	O2-S1	21.55	1.68	1.43
3	B	801	RJC	C15-C11	-12.47	1.28	1.54
3	A	801	RJC	C12-C17	-12.26	1.31	1.55
3	B	801	RJC	C12-C17	-12.24	1.31	1.55
3	A	801	RJC	C15-C11	-12.05	1.29	1.54
3	A	801	RJC	C14-C10	8.65	1.68	1.53
3	B	801	RJC	C12-C11	8.62	1.71	1.55
3	A	801	RJC	C12-C11	8.29	1.70	1.55
3	B	801	RJC	C7-C8	7.33	1.61	1.53
3	A	801	RJC	C7-C8	6.93	1.60	1.53
3	B	801	RJC	C14-C10	6.47	1.64	1.53
3	A	801	RJC	C22-N1	6.40	1.48	1.35
3	B	801	RJC	C22-N1	6.20	1.48	1.35
3	A	801	RJC	C23-S1	6.10	1.85	1.76
3	B	801	RJC	C23-S1	5.60	1.85	1.76
3	A	801	RJC	C4-C3	4.43	1.57	1.52
3	A	801	RJC	S1-N2	4.31	1.73	1.64
3	B	801	RJC	C18-C17	4.22	1.61	1.54
3	A	801	RJC	O4-C3	-4.05	1.34	1.43
3	A	801	RJC	C18-C17	3.95	1.61	1.54
3	B	801	RJC	S1-N2	3.66	1.72	1.64
3	A	801	RJC	C22-N2	3.42	1.47	1.39
3	B	801	RJC	C16-C17	3.39	1.61	1.54
3	A	801	RJC	C13-C12	3.38	1.60	1.54
3	B	801	RJC	O4-C3	-3.38	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	RJC	C22-N2	3.34	1.47	1.39
3	A	801	RJC	C9-C10	3.07	1.59	1.53
3	B	801	RJC	C9-C10	3.05	1.59	1.53
3	B	801	RJC	O5-C8	-3.03	1.35	1.43
3	B	801	RJC	C2-C3	3.01	1.56	1.52
3	A	801	RJC	C16-C17	2.91	1.60	1.54
3	A	801	RJC	C16-C15	2.84	1.61	1.54
3	B	801	RJC	C6-C10	-2.82	1.50	1.56
3	B	801	RJC	C13-C12	2.82	1.59	1.54
3	B	801	RJC	C16-C15	2.74	1.61	1.54
3	A	801	RJC	O5-C8	-2.70	1.36	1.43
3	B	801	RJC	C4-C3	2.54	1.55	1.52
3	B	801	RJC	F1-C4	-2.50	1.34	1.40
3	B	801	RJC	C1-C2	2.45	1.58	1.53
3	A	801	RJC	O1-C22	-2.01	1.19	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	RJC	O3-S1-O2	-7.32	110.56	119.55
3	A	801	RJC	C15-C11-C9	-6.38	109.41	118.33
3	B	801	RJC	F1-C4-C3	-6.19	100.57	108.39
3	B	801	RJC	C15-C11-C9	-5.41	110.76	118.33
3	B	801	RJC	O3-S1-O2	-5.16	113.21	119.55
3	B	801	RJC	C14-C10-C6	-4.50	108.72	113.91
3	B	801	RJC	C16-C15-C11	-4.01	97.18	105.13
3	B	801	RJC	C1-C6-C10	3.91	117.50	111.35
3	A	801	RJC	N2-C22-N1	3.74	121.09	114.25
3	B	801	RJC	C31-C6-C10	-3.58	106.25	111.18
3	A	801	RJC	C16-C17-C18	-3.55	106.66	112.15
3	B	801	RJC	C19-C18-C20	-3.47	104.92	110.36
3	B	801	RJC	C7-C8-C9	-3.40	105.36	111.41
3	A	801	RJC	C22-N2-S1	-3.38	113.95	123.62
3	B	801	RJC	C29-C7-C8	3.37	119.84	112.10
3	A	801	RJC	C1-C6-C10	3.30	116.55	111.35
3	A	801	RJC	C11-C9-C8	-3.27	108.48	112.76
3	B	801	RJC	O5-C8-C7	3.23	116.74	110.05
3	B	801	RJC	C17-C12-C11	-3.18	96.31	100.07
3	A	801	RJC	C31-C6-C10	-3.16	106.83	111.18
3	A	801	RJC	C16-C15-C11	-2.77	99.64	105.13
3	B	801	RJC	O4-C3-C4	-2.71	104.41	109.72
3	B	801	RJC	C23-S1-N2	2.55	109.84	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	RJC	C31-C6-C5	-2.55	107.64	111.91
3	A	801	RJC	C7-C8-C9	-2.54	106.89	111.41
3	B	801	RJC	C31-C6-C1	-2.46	104.29	108.26
3	B	801	RJC	C11-C9-C8	-2.44	109.57	112.76
3	B	801	RJC	C20-C21-N1	-2.42	104.88	111.87
3	B	801	RJC	C22-N2-S1	-2.41	116.72	123.62
3	B	801	RJC	C1-C2-C3	2.35	116.28	111.72
3	A	801	RJC	C23-S1-N2	2.33	109.50	105.97
3	B	801	RJC	C13-C12-C11	2.32	110.88	107.27
3	A	801	RJC	C20-C18-C17	-2.31	105.52	110.28
3	A	801	RJC	C32-C12-C11	-2.23	107.56	111.71
3	A	801	RJC	O4-C3-C2	-2.23	104.63	109.96
3	A	801	RJC	C29-C7-C8	2.14	117.02	112.10
3	B	801	RJC	C13-C12-C17	2.13	119.76	116.57
3	B	801	RJC	O2-S1-C23	2.12	110.58	107.97
3	B	801	RJC	C29-C7-C5	-2.06	109.84	113.63
3	A	801	RJC	F1-C4-C3	2.02	110.93	108.39
3	A	801	RJC	O5-C8-C7	2.01	114.21	110.05

There are no chirality outliers.

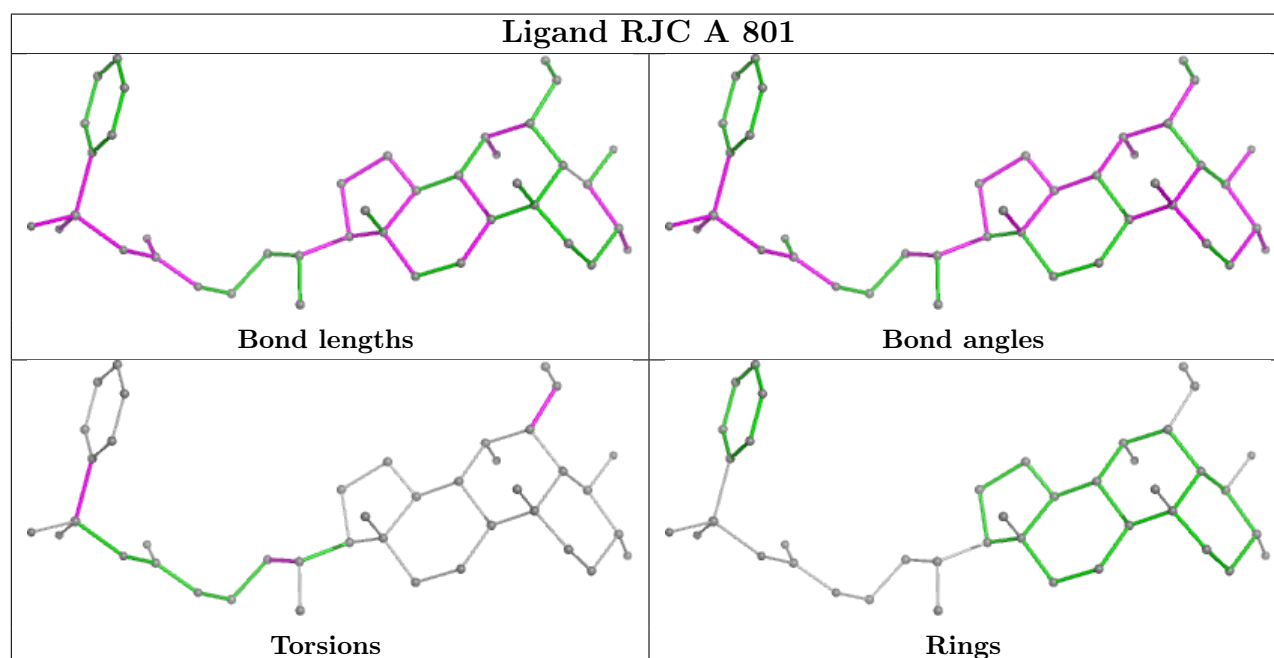
All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	RJC	C30-C29-C7-C5
3	A	801	RJC	C30-C29-C7-C8
3	B	801	RJC	C30-C29-C7-C5
3	B	801	RJC	C30-C29-C7-C8
3	A	801	RJC	C19-C18-C20-C21
3	B	801	RJC	C24-C23-S1-O2
3	B	801	RJC	C28-C23-S1-O2
3	B	801	RJC	C22-N2-S1-O2
3	B	801	RJC	C22-N2-S1-O3
3	B	801	RJC	C22-N2-S1-C23
3	B	801	RJC	C24-C23-S1-N2
3	A	801	RJC	C24-C23-S1-O2
3	B	801	RJC	C28-C23-S1-N2
3	A	801	RJC	C28-C23-S1-O2
3	A	801	RJC	C17-C18-C20-C21

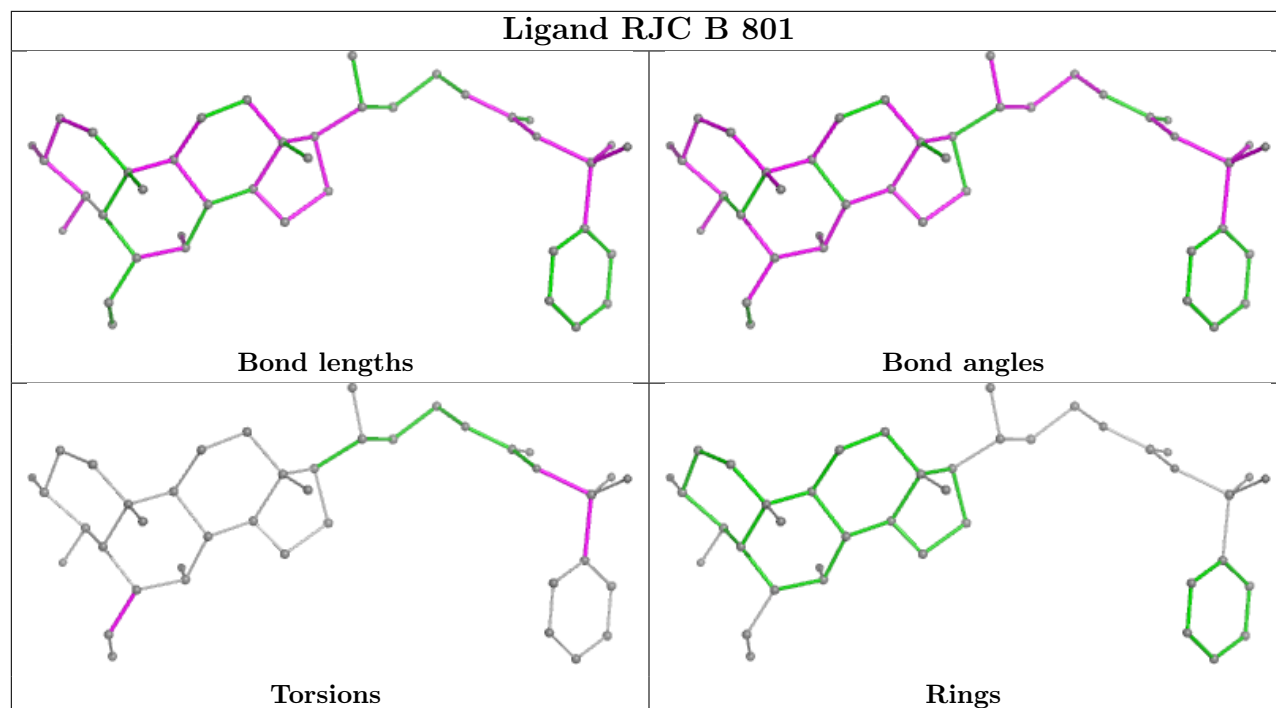
There are no ring outliers.

No monomer is involved in short contacts.

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 [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	229/233 (98%)	-0.38	0 <span>100</span> <span>100</span>	75, 97, 141, 167	0
1	B	224/233 (96%)	-0.23	5 (2%) <span>62</span> <span>42</span>	71, 94, 145, 183	0
2	C	13/13 (100%)	-0.39	0 <span>100</span> <span>100</span>	91, 104, 136, 146	0
2	D	10/13 (76%)	0.81	0 <span>100</span> <span>100</span>	134, 148, 166, 174	0
All	All	476/492 (96%)	-0.28	5 (1%) <span>77</span> <span>61</span>	71, 96, 146, 183	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	GLU	4.0
1	B	336	PHE	3.3
1	B	470	ASP	2.7
1	B	468	ILE	2.4
1	B	346	ASP	2.2

### 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,

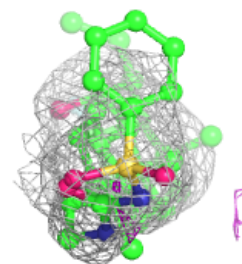
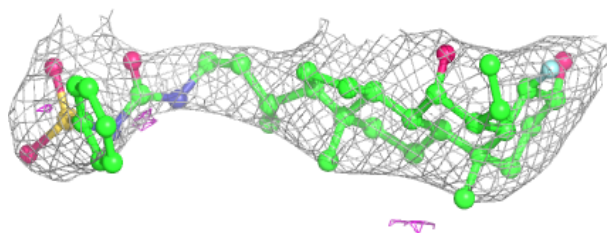
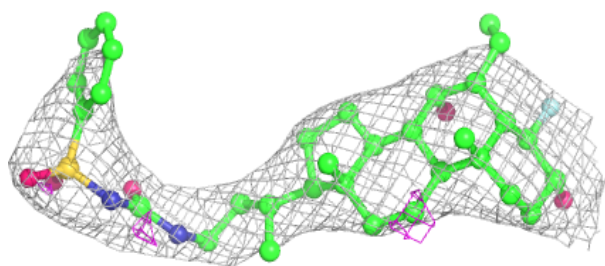
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	RJC	A	801	41/41	0.95	0.11	65,76,116,132	0
3	RJC	B	801	41/41	0.95	0.13	64,76,117,125	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.

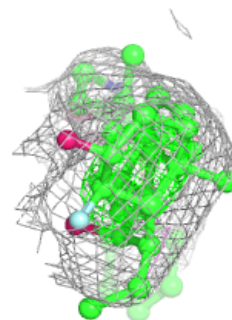
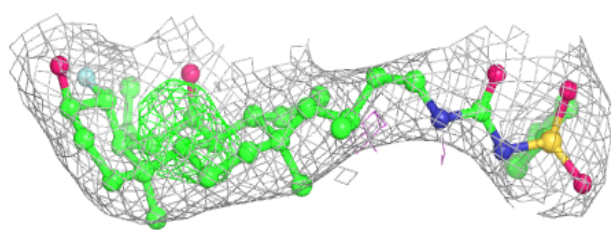
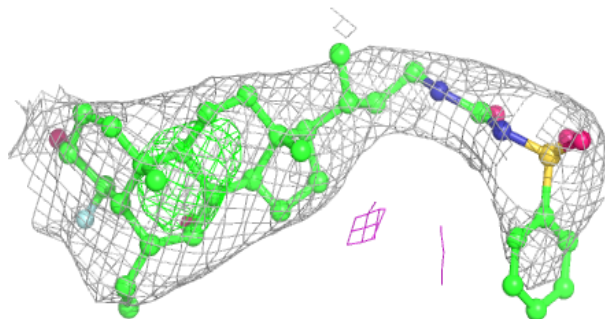
**Electron density around RJC A 801:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around RJC B 801:**

$2mF_o-DF_c$  (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.