



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:30 PM UTC

PDB ID : 9H66 / pdb\_00009h66  
Title : Steroidal Selective Modulators of FXR with Therapeutic Potential  
Authors : Kydd-Sinclair, D.; Watson, K.A.  
Deposited on : 2024-10-23  
Resolution : 2.60 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

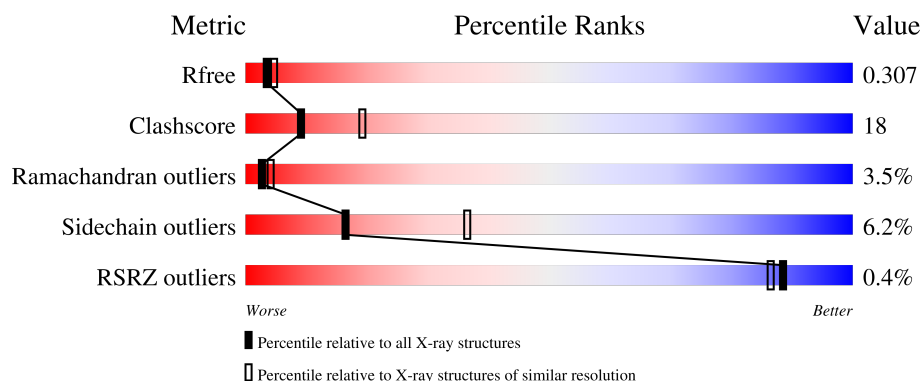
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.






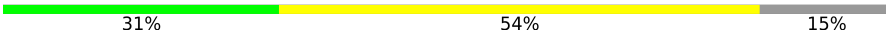

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	
1	C	233	
1	D	233	
2	E	13	

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Mol	Chain	Length	Quality of chain
2	F	13	 46% 38% 15%
2	G	13	 69% 31%
2	H	13	 54% 31% 15%
2	I	13	 31% 54% 15%
2	J	13	 69% 23% 8%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8038 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	228	Total	C	N	O	S	0	2	0
			1826	1165	308	342	11			
1	B	229	Total	C	N	O	S	0	1	0
			1835	1171	312	341	11			
1	C	227	Total	C	N	O	S	0	0	0
			1777	1137	298	331	11			
1	D	229	Total	C	N	O	S	0	1	0
			1790	1149	304	326	11			

There are 24 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
C	240	GLY	-	expression tag	UNP Q96RI1
C	241	SER	-	expression tag	UNP Q96RI1
C	242	HIS	-	expression tag	UNP Q96RI1
C	243	MET	-	expression tag	UNP Q96RI1
C	277	ALA	GLU	engineered mutation	UNP Q96RI1
C	350	ALA	GLU	engineered mutation	UNP Q96RI1
D	240	GLY	-	expression tag	UNP Q96RI1
D	241	SER	-	expression tag	UNP Q96RI1
D	242	HIS	-	expression tag	UNP Q96RI1

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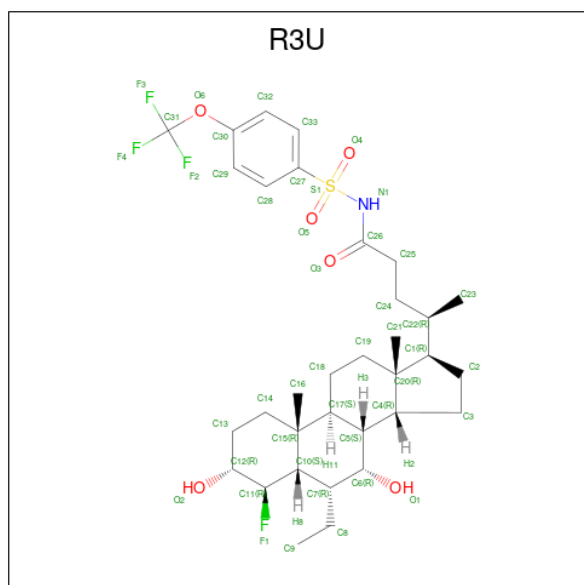
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Chain	Residue	Modelled	Actual	Comment	Reference
D	243	MET	-	expression tag	UNP Q96RI1
D	277	ALA	GLU	engineered mutation	UNP Q96RI1
D	350	ALA	GLU	engineered mutation	UNP Q96RI1

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	0	0	0
			98	63	17	18			
2	F	11	Total	C	N	O	0	0	0
			90	59	16	15			
2	G	13	Total	C	N	O	0	0	0
			107	68	18	21			
2	H	11	Total	C	N	O	0	0	0
			94	61	16	17			
2	I	11	Total	C	N	O	0	0	0
			77	52	11	14			
2	J	12	Total	C	N	O	0	0	0
			91	59	16	16			

- Molecule 3 is (4 {R})-4-[(3 {R},4 {R},5 {S},6 {R},7 {R},8 {S},9 {S},10 {R},13 {R},14 {R},17 {R})-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-1 {H}-cyclopenta[a]phenanthren-17-yl]-{N}-[4-(trifluoromethoxy)phenyl]sulfonyl-pentanamide (CCD ID: R3U) (formula: C<sub>33</sub>H<sub>47</sub>F<sub>4</sub>NO<sub>6</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
			45	33	4	1	6	1		
3	B	1	Total	C	F	N	O	S	0	0
			45	33	4	1	6	1		
3	C	1	Total	C	F	N	O	S	0	0
			45	33	4	1	6	1		
3	D	1	Total	C	F	N	O	S	0	0
			45	33	4	1	6	1		

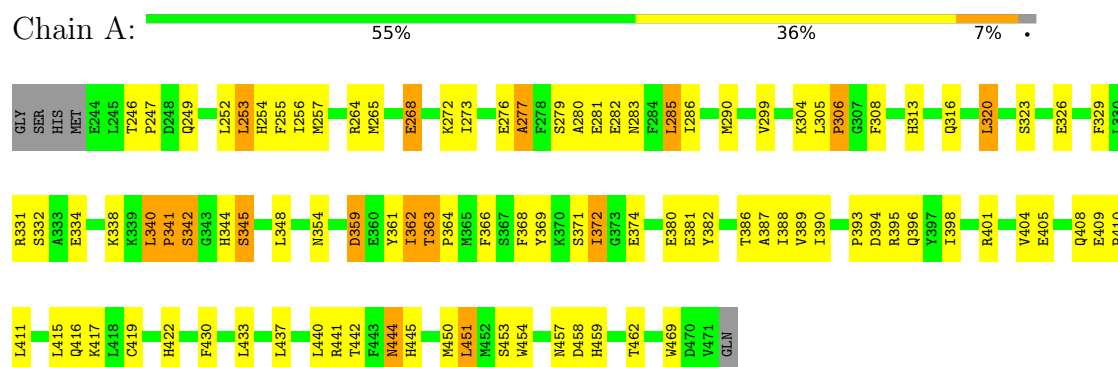
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	22	Total	O	0	0
			22	22		
4	C	9	Total	O	0	0
			9	9		
4	D	11	Total	O	0	0
			11	11		
4	F	3	Total	O	0	0
			3	3		
4	G	4	Total	O	0	0
			4	4		
4	H	2	Total	O	0	0
			2	2		

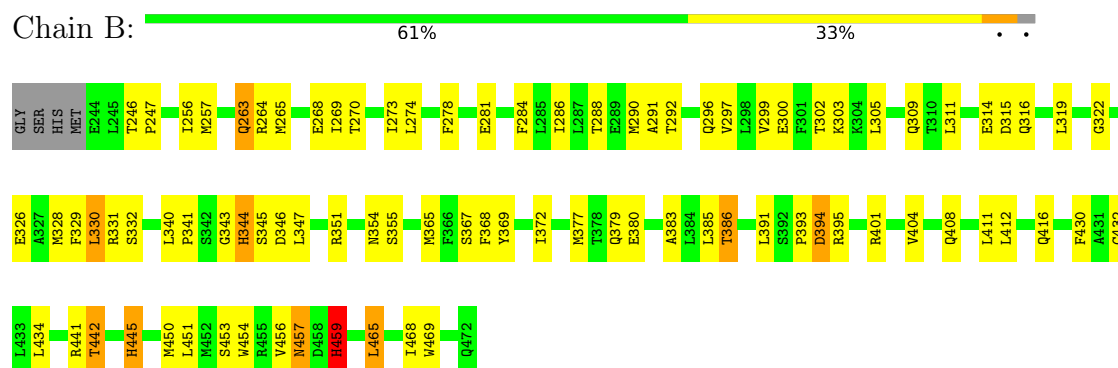
### 3 Residue-property plots [i](#)

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.

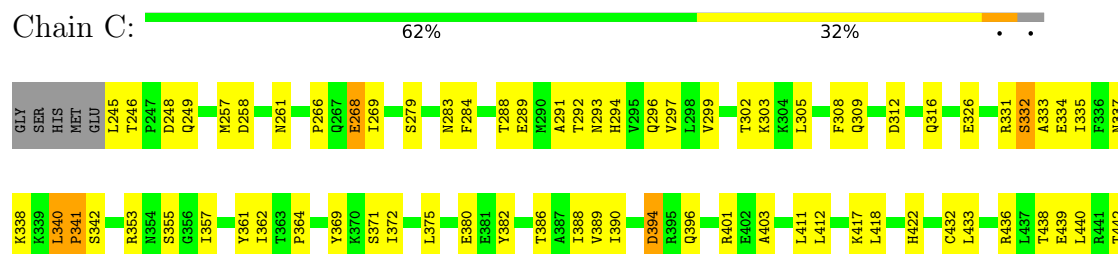
#### • Molecule 1: Bile acid receptor



#### • Molecule 1: Bile acid receptor

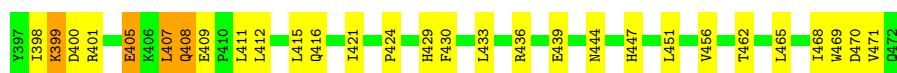


#### • Molecule 1: Bile acid receptor

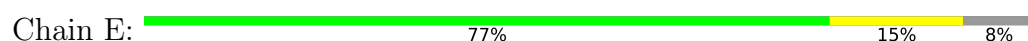




- Molecule 1: Bile acid receptor



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2







● Molecule 2: Nuclear receptor coactivator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.58Å 101.21Å 104.81Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	57.92 – 2.60 57.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.92-2.60) 99.5 (57.92-2.60)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.259 , 0.312 0.259 , 0.307	Depositor DCC
$R_{free}$ test set	2223 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 116.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k 0.015 for -h,-l,-k 0.156 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R3U

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/1867	0.75	0/2534
1	B	0.52	0/1876	0.73	1/2545 (0.0%)
1	C	0.33	0/1816	0.57	0/2467
1	D	0.34	0/1831	0.61	0/2487
2	E	0.21	0/98	0.38	0/131
2	F	0.29	0/90	0.71	0/120
2	G	0.29	0/107	0.45	0/143
2	H	0.19	0/94	0.38	0/125
2	I	0.26	0/77	0.49	0/105
2	J	0.24	0/91	0.43	0/123
All	All	0.43	0/7947	0.66	1/10780 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	CYS	CA-CB-SG	6.08	128.39	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	ARG	Sidechain

## 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	1826	0	1749	76	0
1	B	1835	0	1770	62	0
1	C	1777	0	1697	59	0
1	D	1790	0	1711	86	0
2	E	98	0	99	2	0
2	F	90	0	95	4	0
2	G	107	0	105	2	0
2	H	94	0	99	2	0
2	I	77	0	69	7	0
2	J	91	0	86	5	0
3	A	45	0	0	1	0
3	B	45	0	0	0	0
3	C	45	0	0	1	0
3	D	45	0	0	2	0
4	A	22	0	0	0	0
4	B	22	0	0	3	0
4	C	9	0	0	2	0
4	D	11	0	0	1	0
4	F	3	0	0	0	0
4	G	4	0	0	0	0
4	H	2	0	0	0	0
All	All	8038	0	7480	282	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 18.

All (282) 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:264:ARG:NH2	4:B:3201:HOH:O	2.07	0.85
1:A:249:GLN:OE1	1:A:417:LYS:NZ	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:LEU:O	1:D:409:GLU:N	2.19	0.76
1:C:396:GLN:NE2	4:C:4201:HOH:O	2.19	0.74
1:B:256:ILE:HD11	1:B:411:LEU:HD11	1.74	0.70
1:C:337:ASN:ND2	1:C:369:TYR:O	2.24	0.69
1:D:330:LEU:HD11	1:D:385:LEU:HD23	1.72	0.69
1:D:359:ASP:HA	1:D:362:ILE:HD12	1.75	0.69
1:D:257:MET:CE	1:D:380:GLU:HA	2.23	0.68
1:D:375:LEU:HD12	1:D:429:HIS:CE1	2.28	0.68
1:A:396:GLN:HG3	1:B:401:ARG:CZ	2.24	0.68
1:D:330:LEU:HD21	1:D:385:LEU:HB3	1.76	0.67
1:D:357:ILE:O	1:D:362:ILE:HD11	1.95	0.67
1:B:408:GLN:HE21	1:B:412:LEU:HD11	1.59	0.66
1:D:395:ARG:O	1:D:398:ILE:HG12	1.94	0.66
1:D:447:HIS:O	1:D:451:LEU:HD22	1.95	0.66
1:C:293:ASN:O	1:C:297:VAL:HG23	1.96	0.66
1:D:436:ARG:NH1	1:D:439:GLU:OE2	2.29	0.66
1:C:326:GLU:HG2	1:C:440:LEU:HB3	1.77	0.65
1:C:450:MET:O	1:C:454:TRP:N	2.29	0.65
1:D:286:ILE:O	1:D:290:MET:HG3	1.94	0.65
1:A:264:ARG:HH12	1:A:338:LYS:NZ	1.95	0.65
1:D:257:MET:HE2	1:D:380:GLU:HA	1.78	0.65
1:C:299:VAL:O	1:C:303:LYS:HG2	1.97	0.65
1:A:338:LYS:HB3	1:A:340:LEU:HB2	1.78	0.64
1:C:246:THR:HG23	1:C:249:GLN:HE21	1.63	0.64
1:A:264:ARG:HH22	1:A:338:LYS:NZ	1.95	0.64
1:D:462:THR:HG23	1:D:465:LEU:H	1.62	0.64
1:C:462:THR:HG23	1:C:465:LEU:HB2	1.78	0.63
1:D:246:THR:HG22	1:D:247:PRO:HD2	1.79	0.63
1:D:279:SER:O	1:D:281:GLU:N	2.31	0.63
1:A:368:PHE:CZ	1:A:372:ILE:HD11	2.34	0.63
1:A:326:GLU:HG2	1:A:440:LEU:HB3	1.82	0.62
1:A:340:LEU:HD21	1:A:344[A]:HIS:HB3	1.82	0.62
1:A:396:GLN:HG3	1:B:401:ARG:NH1	2.15	0.62
1:B:284:PHE:O	1:B:288:THR:HG23	2.00	0.62
1:C:334:GLU:HG3	1:C:382:TYR:CD2	2.35	0.62
1:B:263:GLN:CD	1:B:297:VAL:HG13	2.25	0.61
1:B:281:GLU:HA	1:B:456:VAL:HG11	1.82	0.61
1:C:309:GLN:HA	1:C:316:GLN:NE2	2.15	0.61
1:B:330:LEU:HD21	1:B:385:LEU:HG	1.83	0.61
1:A:393:PRO:O	1:A:401:ARG:HG2	2.00	0.61
1:C:394:ASP:HB3	1:D:394:ASP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:HIS:O	1:B:346:ASP:N	2.29	0.60
1:A:462:THR:OG1	2:F:4007:LEU:O	2.18	0.60
1:C:266:PRO:HG2	1:C:269:ILE:HD11	1.85	0.59
1:D:291:ALA:HB3	1:D:465:LEU:HD11	1.83	0.59
1:C:457:ASN:O	1:C:458:ASP:HB2	2.01	0.59
1:D:292:THR:OG1	1:D:462:THR:HG21	2.02	0.59
1:B:394:ASP:HB2	1:B:441:ARG:HH12	1.68	0.58
1:A:415:LEU:HD21	1:A:433:LEU:HD23	1.85	0.58
1:A:290:MET:HE1	1:A:348:LEU:HD13	1.85	0.58
1:C:331:ARG:NH1	1:C:335:ILE:HD11	2.18	0.58
1:D:265:MET:HE3	3:D:3101:R3U:N1	2.18	0.58
1:D:325:VAL:HG21	1:D:447:HIS:CD2	2.38	0.58
1:B:278:PHE:HE1	1:B:354:ASN:HD22	1.51	0.57
1:C:291:ALA:O	1:C:294:HIS:HB3	2.02	0.57
1:A:450:MET:HE3	1:A:454:TRP:HB2	1.85	0.57
1:A:451:LEU:HD21	1:A:469:TRP:HE3	1.70	0.57
1:B:368:PHE:CZ	1:B:372:ILE:HD11	2.39	0.57
1:C:340:LEU:H	1:C:341:PRO:HD2	1.68	0.57
1:A:281:GLU:O	1:A:282:GLU:HB3	2.05	0.56
1:D:363:THR:O	1:D:367:SER:OG	2.23	0.56
1:A:282:GLU:O	1:A:286:ILE:HG13	2.05	0.56
1:A:329:PHE:O	1:A:332:SER:HB2	2.05	0.56
1:D:388:ILE:HD11	1:D:411:LEU:HB2	1.87	0.56
1:C:333:ALA:HB2	1:C:369:TYR:HD1	1.70	0.56
1:C:284:PHE:O	1:C:288:THR:HG23	2.05	0.56
1:C:332:SER:HB3	1:C:369:TYR:CZ	2.40	0.56
1:D:329:PHE:HZ	1:D:447:HIS:HB2	1.71	0.56
1:A:409:GLU:HG3	4:B:3210:HOH:O	2.06	0.56
1:D:349:GLU:HA	1:D:352:ILE:HD12	1.87	0.55
1:D:415:LEU:HD21	1:D:433:LEU:HD23	1.89	0.55
1:C:292:THR:OG1	1:C:462:THR:HG21	2.06	0.55
1:B:268:GLU:HG2	1:B:269:ILE:N	2.20	0.55
1:A:361:TYR:O	1:A:364:PRO:HD2	2.06	0.55
1:C:288:THR:O	1:C:292:THR:OG1	2.23	0.55
1:D:351:ARG:O	1:D:355:SER:HB3	2.07	0.55
1:D:366:PHE:O	1:D:370:LYS:HG3	2.06	0.55
1:A:359[A]:ASP:OD1	1:A:359[A]:ASP:N	2.40	0.54
1:C:357:ILE:HB	1:C:362:ILE:HD11	1.89	0.54
1:D:326:GLU:HG3	1:D:444:ASN:HD22	1.73	0.54
1:B:305:LEU:HD13	1:B:391:LEU:HD11	1.90	0.54
2:H:3008:LEU:HD21	2:I:4003:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:GLN:HG3	1:D:430:PHE:CD2	2.42	0.54
1:A:340:LEU:HD23	1:A:341:PRO:HD2	1.90	0.54
1:A:340:LEU:HD22	1:A:345:SER:HB3	1.90	0.53
1:B:263:GLN:CG	1:B:297:VAL:HG13	2.38	0.53
1:C:289:GLU:OE2	2:I:4008:LEU:HD21	2.08	0.53
1:C:468:ILE:HG23	1:C:469:TRP:CD1	2.43	0.53
1:B:263:GLN:HG2	1:B:297:VAL:HG13	1.89	0.53
1:A:255:PHE:HE2	1:A:304:LYS:O	1.92	0.53
1:B:450:MET:HE3	1:B:454:TRP:HB2	1.91	0.53
1:B:468:ILE:HD11	2:G:3005:LEU:HD13	1.90	0.52
1:C:401:ARG:NE	1:D:396:GLN:HG3	2.24	0.52
1:A:264:ARG:HH22	1:A:338:LYS:HZ2	1.57	0.52
1:D:317:ILE:HG23	2:J:3005:LEU:HD22	1.91	0.52
1:B:416:GLN:HB2	1:B:430:PHE:CE1	2.44	0.52
1:B:365:MET:HE3	1:B:369:TYR:CE1	2.44	0.52
1:B:315:ASP:O	1:B:319:LEU:HG	2.10	0.52
2:F:4005:ARG:NH2	2:I:4002:ALA:O	2.43	0.52
1:A:277:ALA:HB3	1:A:282:GLU:HG2	1.93	0.51
1:C:246:THR:HG23	1:C:249:GLN:NE2	2.24	0.51
1:C:333:ALA:HB1	1:C:372:ILE:HG21	1.92	0.51
1:A:386:THR:O	1:A:389:VAL:HG12	2.10	0.51
1:C:388:ILE:HD13	1:C:412:LEU:HD23	1.91	0.51
1:A:416:GLN:HB2	1:A:430:PHE:CZ	2.46	0.51
1:B:456:VAL:O	1:B:459:HIS:HB2	2.11	0.51
1:D:377:MET:HE1	1:D:385:LEU:HD22	1.92	0.51
1:D:384:LEU:O	1:D:388:ILE:HG12	2.11	0.51
1:A:276:GLU:HG3	1:A:277:ALA:N	2.25	0.51
1:C:456:VAL:HG23	1:C:457:ASN:O	2.11	0.51
1:A:401:ARG:HG3	1:A:401:ARG:HH11	1.76	0.50
1:C:371:SER:HB2	1:C:436:ARG:HH22	1.76	0.50
1:B:347:LEU:O	1:B:351:ARG:HG3	2.12	0.50
1:D:280:ALA:HA	1:D:283:ASN:HB2	1.94	0.50
1:A:409:GLU:HB3	1:A:410:PRO:HD3	1.93	0.50
1:C:333:ALA:HB2	1:C:369:TYR:CD1	2.46	0.50
1:D:280:ALA:HB2	1:D:354:ASN:OD1	2.11	0.50
1:A:450:MET:O	1:A:450:MET:HG2	2.12	0.50
1:D:265:MET:HE2	1:D:265:MET:HA	1.94	0.50
1:D:468:ILE:HD13	2:J:3005:LEU:HD12	1.94	0.50
1:A:268:GLU:OE1	2:F:4000:GLU:HA	2.13	0.49
1:C:249:GLN:HE22	1:C:417:LYS:NZ	2.09	0.49
1:B:430:PHE:CZ	1:B:434:LEU:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ARG:C	1:C:403:ALA:H	2.19	0.49
1:B:416:GLN:HB2	1:B:430:PHE:CZ	2.48	0.49
1:C:258:ASP:O	1:C:261:ASN:N	2.46	0.49
2:F:4000:GLU:O	2:F:4005:ARG:HG2	2.13	0.49
1:D:291:ALA:O	1:D:295:VAL:HG23	2.12	0.49
1:B:442:THR:HA	1:B:445[A]:HIS:CE1	2.48	0.49
1:B:330:LEU:HD23	1:B:386:THR:HA	1.94	0.49
1:A:276:GLU:HG2	1:A:282:GLU:OE2	2.12	0.49
1:C:386:THR:O	1:C:389:VAL:HG12	2.13	0.49
1:D:347:LEU:O	1:D:351:ARG:HG3	2.13	0.49
1:A:442:THR:O	1:A:445:HIS:ND1	2.43	0.48
1:B:351:ARG:O	1:B:355:SER:HB3	2.13	0.48
1:B:326:GLU:O	1:B:329:PHE:HB2	2.13	0.48
2:E:3007:TYR:HB2	2:H:3007:TYR:HB2	1.95	0.48
1:B:383:ALA:O	1:B:386:THR:HB	2.14	0.48
2:I:4003:LEU:O	2:I:4007:LEU:HG	2.14	0.48
1:A:395:ARG:O	1:A:398:ILE:HG12	2.13	0.48
1:C:268:GLU:OE2	2:I:4000:GLU:N	2.38	0.48
1:B:299:VAL:HG12	1:B:303:LYS:HD2	1.96	0.48
1:C:450:MET:HE2	1:C:450:MET:HB3	1.72	0.48
1:A:451:LEU:HD21	1:A:469:TRP:CE3	2.48	0.48
1:B:326:GLU:HA	1:B:329:PHE:CD2	2.49	0.48
1:A:246:THR:HG23	1:A:417:LYS:NZ	2.29	0.48
1:B:393:PRO:HB3	1:B:404:VAL:HB	1.96	0.48
1:A:273:ILE:HD11	1:A:290:MET:HE3	1.96	0.47
1:A:393:PRO:HB3	1:A:404:VAL:HB	1.96	0.47
1:C:302:THR:HG23	1:C:390:ILE:HG21	1.95	0.47
1:C:334:GLU:HG3	1:C:382:TYR:CE2	2.48	0.47
1:D:259:SER:HB3	1:D:304:LYS:HE2	1.96	0.47
1:B:302:THR:HA	1:B:305:LEU:HG	1.97	0.47
1:A:405:GLU:OE1	1:B:445[A]:HIS:NE2	2.48	0.47
2:I:4006:TYR:C	2:I:4008:LEU:H	2.23	0.46
1:A:252:LEU:O	1:A:252:LEU:HD12	2.15	0.46
1:A:366:PHE:HA	1:A:369:TYR:CD2	2.49	0.46
1:B:257:MET:HE2	1:B:380:GLU:HG2	1.96	0.46
1:A:282:GLU:HA	1:A:285:LEU:HB2	1.97	0.46
1:D:325:VAL:HG12	1:D:329:PHE:CE2	2.50	0.46
1:D:326:GLU:HA	1:D:329:PHE:HD2	1.80	0.46
1:A:326:GLU:OE2	1:A:441:ARG:HG3	2.14	0.46
1:C:332:SER:HB3	1:C:369:TYR:CE1	2.50	0.46
1:D:309:GLN:HA	1:D:316:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:PHE:HA	1:D:369:TYR:CD2	2.50	0.46
4:C:4201:HOH:O	1:D:399:LYS:HA	2.14	0.46
1:D:345:SER:O	1:D:347:LEU:N	2.41	0.46
1:A:280:ALA:HA	1:A:354:ASN:O	2.15	0.46
1:B:292:THR:O	1:B:296:GLN:HG3	2.16	0.46
1:A:441:ARG:O	1:A:444:ASN:HB2	2.15	0.46
1:D:246:THR:HB	1:D:249:GLN:H	1.81	0.46
1:D:379:GLN:HE21	1:D:379:GLN:HB2	1.57	0.46
1:C:331:ARG:HH11	1:C:335:ILE:HD11	1.79	0.45
1:B:377:MET:HE1	1:B:385:LEU:HD22	1.99	0.45
1:D:321:LYS:NZ	2:J:3002:ASN:HD21	2.13	0.45
1:D:331:ARG:NH2	3:D:3101:R3U:O4	2.49	0.45
1:B:278:PHE:CE2	1:B:351:ARG:HG2	2.52	0.45
1:C:418:LEU:HG	1:C:422:HIS:CD2	2.52	0.45
1:A:388:ILE:HG23	1:A:408:GLN:HE21	1.82	0.45
1:B:263:GLN:HE21	1:B:300:GLU:HB2	1.81	0.45
1:D:280:ALA:HA	1:D:283:ASN:HD22	1.82	0.45
1:B:322:GLY:O	1:B:395:ARG:CZ	2.65	0.45
1:D:465:LEU:HD22	1:D:469:TRP:CE2	2.51	0.45
1:A:283:ASN:HA	1:A:286:ILE:HD12	1.99	0.45
1:A:381:GLU:OE2	1:A:422:HIS:HD2	2.00	0.45
1:A:387:ALA:HB1	1:A:411:LEU:HD13	1.99	0.45
1:A:264:ARG:HH22	1:A:338:LYS:HZ1	1.65	0.44
1:A:305:LEU:O	1:A:306:PRO:C	2.60	0.44
1:C:334:GLU:HG3	1:C:382:TYR:CG	2.53	0.44
1:D:282:GLU:O	1:D:286:ILE:HG13	2.17	0.44
1:D:312:ASP:HB3	1:D:315:ASP:OD2	2.16	0.44
1:D:421:ILE:O	1:D:424:PRO:HD3	2.18	0.44
1:D:308:PHE:C	1:D:310:THR:H	2.25	0.44
1:C:305:LEU:HB2	1:C:308:PHE:HB2	2.00	0.44
2:E:3011:LYS:HE2	2:E:3011:LYS:HB2	1.77	0.44
1:B:341:PRO:C	1:B:343:GLY:H	2.26	0.44
1:D:334:GLU:O	1:D:338:LYS:HG3	2.17	0.44
1:A:264:ARG:HD3	3:A:4101:R3U:O4	2.17	0.44
1:A:273:ILE:HD11	1:A:290:MET:CE	2.48	0.44
1:B:331:ARG:O	1:B:332:SER:C	2.60	0.44
1:C:279:SER:O	1:C:283:ASN:HB2	2.18	0.44
1:C:465:LEU:HD12	1:C:469:TRP:CZ3	2.53	0.44
1:D:326:GLU:O	1:D:329:PHE:N	2.51	0.44
1:C:312:ASP:OD2	1:C:312:ASP:C	2.60	0.43
1:B:465:LEU:HD13	1:B:465:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:SER:HA	1:A:374:GLU:CG	2.48	0.43
1:B:286:ILE:O	1:B:290:MET:HG3	2.17	0.43
1:A:334:GLU:HB2	1:A:382:TYR:CE1	2.54	0.43
1:B:326:GLU:HA	1:B:329:PHE:HD2	1.82	0.43
1:C:296:GLN:OE1	2:I:4003:LEU:HD23	2.18	0.43
1:D:447:HIS:NE2	1:D:451:LEU:HD21	2.34	0.43
1:A:299:VAL:HA	1:A:320:LEU:HD11	2.01	0.43
1:B:457:ASN:OD1	1:B:457:ASN:O	2.37	0.43
1:A:246:THR:HB	1:A:247:PRO:HD2	2.01	0.43
1:C:249:GLN:HE22	1:C:417:LYS:HZ3	1.66	0.43
1:C:401:ARG:CD	1:D:396:GLN:HG3	2.49	0.43
1:A:396:GLN:CD	1:B:401:ARG:HD2	2.44	0.43
1:B:246:THR:HB	1:B:247:PRO:HD2	2.01	0.43
1:B:377:MET:HE1	1:B:385:LEU:CD2	2.48	0.43
1:C:375:LEU:HD23	1:C:433:LEU:HD23	2.01	0.43
1:D:468:ILE:CD1	2:J:3005:LEU:HD12	2.48	0.43
1:A:290:MET:HE1	1:A:348:LEU:CD1	2.49	0.42
1:B:273:ILE:O	1:B:347:LEU:HD23	2.19	0.42
1:D:309:GLN:HA	1:D:316:GLN:HE22	1.83	0.42
1:D:325:VAL:O	1:D:328:MET:HB3	2.20	0.42
1:D:345:SER:C	1:D:347:LEU:H	2.25	0.42
1:A:374:GLU:H	1:A:374:GLU:HG2	1.69	0.42
1:C:394:ASP:HB3	1:D:394:ASP:CB	2.49	0.42
1:C:439:GLU:O	1:C:442:THR:N	2.52	0.42
1:D:367:SER:HA	1:D:370:LYS:HG3	2.01	0.42
1:A:272:LYS:O	1:A:276:GLU:HB3	2.19	0.42
1:A:323:SER:CB	1:A:390:ILE:HA	2.50	0.42
1:B:459:HIS:HA	4:B:3218:HOH:O	2.19	0.42
1:B:330:LEU:HD11	1:B:385:LEU:HD23	2.00	0.42
1:C:361:TYR:C	1:C:364:PRO:HD2	2.44	0.42
1:D:280:ALA:H	1:D:283:ASN:ND2	2.16	0.42
1:A:341:PRO:HB2	1:A:342:SER:H	1.58	0.42
1:B:274:LEU:HD21	1:B:344:HIS:HB3	2.02	0.42
1:A:257:MET:SD	1:A:380:GLU:HA	2.60	0.42
1:D:302:THR:HG21	1:D:320:LEU:HD21	2.01	0.42
1:D:264:ARG:NH1	4:D:3201:HOH:O	2.17	0.42
2:G:3000:LYS:O	2:G:3002:ASN:N	2.46	0.42
1:A:359[A]:ASP:HA	1:A:362:ILE:HB	2.01	0.42
1:D:302:THR:OG1	1:D:390:ILE:HD13	2.20	0.42
1:D:401:ARG:O	1:D:405:GLU:HG2	2.20	0.42
1:A:320:LEU:HD23	1:A:320:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:LEU:HD11	1:D:390:ILE:HD11	2.02	0.41
1:A:264:ARG:HH12	1:A:338:LYS:HZ3	1.66	0.41
1:B:328:MET:HB3	1:B:328:MET:HE3	1.74	0.41
1:C:418:LEU:O	1:C:422:HIS:HB2	2.19	0.41
1:A:457:ASN:O	1:A:457:ASN:CG	2.63	0.41
1:C:257:MET:SD	1:C:380:GLU:HA	2.60	0.41
1:D:270:THR:O	1:D:273:ILE:HB	2.20	0.41
1:D:279:SER:O	1:D:279:SER:OG	2.27	0.41
1:D:408:GLN:O	1:D:412:LEU:HD12	2.20	0.41
1:B:368:PHE:CE1	1:B:372:ILE:HD11	2.55	0.41
1:D:386:THR:O	1:D:389:VAL:HG12	2.19	0.41
1:A:405:GLU:OE1	1:B:445[A]:HIS:CD2	2.74	0.41
1:C:245:LEU:HA	1:C:417:LYS:HZ3	1.84	0.41
1:D:317:ILE:HD13	2:J:3009:LEU:HD13	2.02	0.41
1:D:379:GLN:O	1:D:379:GLN:HG3	2.19	0.41
1:D:436:ARG:O	1:D:439:GLU:HB2	2.21	0.41
1:A:338:LYS:C	1:A:340:LEU:N	2.78	0.41
1:A:265:MET:CE	1:A:290:MET:HG2	2.50	0.41
1:A:359[A]:ASP:O	1:A:363:THR:HB	2.20	0.41
1:C:353:ARG:HH11	1:C:353:ARG:HG2	1.86	0.41
1:D:347:LEU:O	1:D:350:ALA:HB3	2.20	0.41
1:B:311:LEU:O	1:B:316:GLN:NE2	2.52	0.41
1:B:450:MET:HE2	1:B:451:LEU:N	2.36	0.41
1:C:331:ARG:NH1	3:C:4101:R3U:N1	2.69	0.41
1:D:246:THR:CG2	1:D:247:PRO:HD2	2.50	0.41
1:D:293:ASN:O	1:D:297:VAL:HG23	2.20	0.41
1:D:302:THR:HG23	1:D:390:ILE:HG21	2.02	0.41
1:A:253:LEU:O	1:A:254:HIS:C	2.63	0.40
1:D:265:MET:HB3	1:D:270:THR:HG23	2.04	0.40
1:D:451:LEU:HD11	1:D:469:TRP:CE3	2.56	0.40
1:B:468:ILE:HG22	1:B:469:TRP:CD1	2.56	0.40
1:B:265:MET:HG2	1:B:270:THR:CG2	2.51	0.40
1:D:436:ARG:HA	1:D:439:GLU:HB2	2.03	0.40
1:A:308:PHE:CE2	1:A:316:GLN:HG2	2.56	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	228/233 (98%)	195 (86%)	27 (12%)	6 (3%)	4	7
1	B	228/233 (98%)	201 (88%)	19 (8%)	8 (4%)	3	4
1	C	225/233 (97%)	194 (86%)	21 (9%)	10 (4%)	2	2
1	D	228/233 (98%)	193 (85%)	28 (12%)	7 (3%)	3	5
2	E	10/13 (77%)	10 (100%)	0	0	100	100
2	F	9/13 (69%)	7 (78%)	0	2 (22%)	0	0
2	G	11/13 (85%)	9 (82%)	1 (9%)	1 (9%)	0	0
2	H	9/13 (69%)	9 (100%)	0	0	100	100
2	I	9/13 (69%)	7 (78%)	2 (22%)	0	100	100
2	J	10/13 (77%)	9 (90%)	1 (10%)	0	100	100
All	All	967/1010 (96%)	834 (86%)	99 (10%)	34 (4%)	3	4

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	GLU
1	C	340	LEU
1	C	341	PRO
1	C	454	TRP
1	D	400	ASP
1	D	408	GLN
2	F	4006	TYR
1	A	277	ALA
1	A	341	PRO
1	C	458	ASP
1	C	459	HIS
1	D	399	LYS
1	D	471	VAL
2	F	4001	ASN

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Mol	Chain	Res	Type
1	A	459	HIS
1	B	345	SER
1	C	338	LYS
1	C	342	SER
1	C	355	SER
1	C	455	ARG
1	D	245	LEU
1	D	280	ALA
1	D	470	ASP
2	G	3010	ASP
1	B	291	ALA
1	B	340	LEU
1	B	457	ASN
1	B	459	HIS
1	C	394	ASP
1	A	253	LEU
1	A	306	PRO
1	B	344	HIS
1	B	386	THR
1	A	340	LEU

### 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	196/213 (92%)	176 (90%)	20 (10%)	7	15
1	B	198/213 (93%)	186 (94%)	12 (6%)	17	37
1	C	187/213 (88%)	179 (96%)	8 (4%)	26	51
1	D	186/213 (87%)	176 (95%)	10 (5%)	20	42
2	E	10/12 (83%)	10 (100%)	0	100	100
2	F	9/12 (75%)	9 (100%)	0	100	100
2	G	11/12 (92%)	11 (100%)	0	100	100
2	H	10/12 (83%)	8 (80%)	2 (20%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	6/12 (50%)	5 (83%)	1 (17%)	2	4
2	J	8/12 (67%)	8 (100%)	0	100	100
All	All	821/924 (89%)	768 (94%)	53 (6%)	16	35

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	ILE
1	A	268	GLU
1	A	279	SER
1	A	285	LEU
1	A	313	HIS
1	A	320	LEU
1	A	342	SER
1	A	345	SER
1	A	359[A]	ASP
1	A	359[B]	ASP
1	A	362	ILE
1	A	363	THR
1	A	372	ILE
1	A	394	ASP
1	A	419	CYS
1	A	437	LEU
1	A	444	ASN
1	A	451	LEU
1	A	453	SER
1	A	458	ASP
1	B	263	GLN
1	B	309	GLN
1	B	330	LEU
1	B	367	SER
1	B	379	GLN
1	B	394	ASP
1	B	442	THR
1	B	445[A]	HIS
1	B	445[B]	HIS
1	B	453	SER
1	B	459	HIS
1	B	465	LEU
1	C	248	ASP
1	C	268	GLU

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Mol	Chain	Res	Type
1	C	332	SER
1	C	411	LEU
1	C	432	CYS
1	C	438	THR
1	C	462	THR
1	C	468	ILE
1	D	300	GLU
1	D	335	ILE
1	D	363	THR
1	D	367	SER
1	D	371	SER
1	D	378	THR
1	D	379	GLN
1	D	405	GLU
1	D	407	LEU
1	D	456	VAL
2	H	3001	GLU
2	H	3004	LEU
2	I	4004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	337	ASN
1	A	422	HIS
1	B	263	GLN
1	B	296	GLN
1	B	408	GLN
1	B	429	HIS
1	B	444	ASN
1	C	249	GLN
1	C	267	GLN
1	C	446	HIS
1	D	267	GLN
1	D	396	GLN
1	D	423	GLN
1	D	429	HIS
1	D	444	ASN
2	J	3002	ASN

### 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$
3	R3U	A	4101	-	49,49,49	0.53	0	72,78,78	1.40	9 (12%)
3	R3U	B	3101	-	49,49,49	0.55	0	72,78,78	1.37	7 (9%)
3	R3U	C	4101	-	49,49,49	0.56	0	72,78,78	1.61	9 (12%)
3	R3U	D	3101	-	49,49,49	0.53	0	72,78,78	1.45	9 (12%)

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	R3U	A	4101	-	-	5/27/96/96	0/5/5/5
3	R3U	B	3101	-	-	4/27/96/96	0/5/5/5
3	R3U	C	4101	-	-	9/27/96/96	0/5/5/5
3	R3U	D	3101	-	-	14/27/96/96	0/5/5/5



There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4101	R3U	C20-C4-C5	6.36	121.97	113.93
3	D	3101	R3U	C20-C4-C5	6.10	121.65	113.93
3	B	3101	R3U	C20-C4-C5	5.30	120.63	113.93
3	A	4101	R3U	C20-C4-C5	5.27	120.59	113.93
3	C	4101	R3U	C17-C5-C4	4.87	116.55	109.75
3	C	4101	R3U	C3-C4-C20	4.46	109.08	103.84
3	B	3101	R3U	C4-C5-C6	4.38	116.02	112.21
3	D	3101	R3U	C17-C5-C4	4.30	115.75	109.75
3	B	3101	R3U	C17-C5-C4	4.27	115.71	109.75
3	A	4101	R3U	C17-C5-C4	4.13	115.51	109.75
3	D	3101	R3U	C3-C4-C20	4.00	108.55	103.84
3	C	4101	R3U	C20-C1-C22	3.97	125.63	119.50
3	D	3101	R3U	C20-C1-C22	3.90	125.51	119.50
3	C	4101	R3U	C15-C17-C5	-3.61	107.81	111.84
3	A	4101	R3U	C4-C5-C6	3.59	115.34	112.21
3	A	4101	R3U	C3-C4-C20	3.50	107.95	103.84
3	C	4101	R3U	C18-C17-C15	3.45	117.79	113.91
3	B	3101	R3U	C3-C4-C20	3.31	107.73	103.84
3	B	3101	R3U	C1-C20-C4	3.16	103.72	100.10
3	D	3101	R3U	C15-C17-C5	-3.12	108.36	111.84
3	A	4101	R3U	C1-C20-C4	3.11	103.67	100.10
3	B	3101	R3U	C3-C4-C5	2.78	122.17	118.36
3	A	4101	R3U	C24-C25-C26	2.44	118.50	113.06
3	D	3101	R3U	C18-C17-C15	2.39	116.60	113.91
3	A	4101	R3U	C3-C4-C5	2.39	121.63	118.36
3	A	4101	R3U	C25-C24-C22	-2.38	110.02	114.46
3	C	4101	R3U	C23-C22-C1	2.25	116.26	112.88
3	D	3101	R3U	C2-C3-C4	-2.20	100.85	105.14
3	A	4101	R3U	O3-C26-C25	2.18	125.97	122.02
3	C	4101	R3U	C8-C7-C10	2.11	116.94	113.62
3	D	3101	R3U	C4-C5-C6	2.08	114.02	112.21
3	C	4101	R3U	C7-C6-C5	-2.05	109.79	112.07
3	B	3101	R3U	O3-C26-C25	2.01	125.67	122.02
3	D	3101	R3U	C1-C20-C4	2.01	102.41	100.10

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4101	R3U	C25-C26-N1-S1

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Mol	Chain	Res	Type	Atoms
3	C	4101	R3U	O3-C26-N1-S1
3	C	4101	R3U	C26-N1-S1-C27
3	C	4101	R3U	C26-N1-S1-O4
3	C	4101	R3U	C26-N1-S1-O5
3	D	3101	R3U	C26-N1-S1-C27
3	D	3101	R3U	C26-N1-S1-O4
3	D	3101	R3U	C26-N1-S1-O5
3	D	3101	R3U	F4-C31-O6-C30
3	D	3101	R3U	C20-C1-C22-C24
3	D	3101	R3U	C2-C1-C22-C24
3	C	4101	R3U	C20-C1-C22-C24
3	C	4101	R3U	C2-C1-C22-C24
3	D	3101	R3U	C33-C27-S1-O5
3	D	3101	R3U	F2-C31-O6-C30
3	D	3101	R3U	C28-C27-S1-O5
3	C	4101	R3U	C2-C1-C22-C23
3	D	3101	R3U	C2-C1-C22-C23
3	D	3101	R3U	F3-C31-O6-C30
3	D	3101	R3U	C33-C27-S1-N1
3	A	4101	R3U	C33-C27-S1-O5
3	D	3101	R3U	C28-C27-S1-N1
3	A	4101	R3U	C28-C27-S1-O5
3	C	4101	R3U	C1-C22-C24-C25
3	B	3101	R3U	C28-C27-S1-O5
3	B	3101	R3U	C33-C27-S1-O5
3	D	3101	R3U	C23-C22-C24-C25
3	A	4101	R3U	C33-C27-S1-N1
3	A	4101	R3U	C28-C27-S1-N1
3	A	4101	R3U	C23-C22-C24-C25
3	B	3101	R3U	C33-C27-S1-N1
3	B	3101	R3U	C28-C27-S1-N1

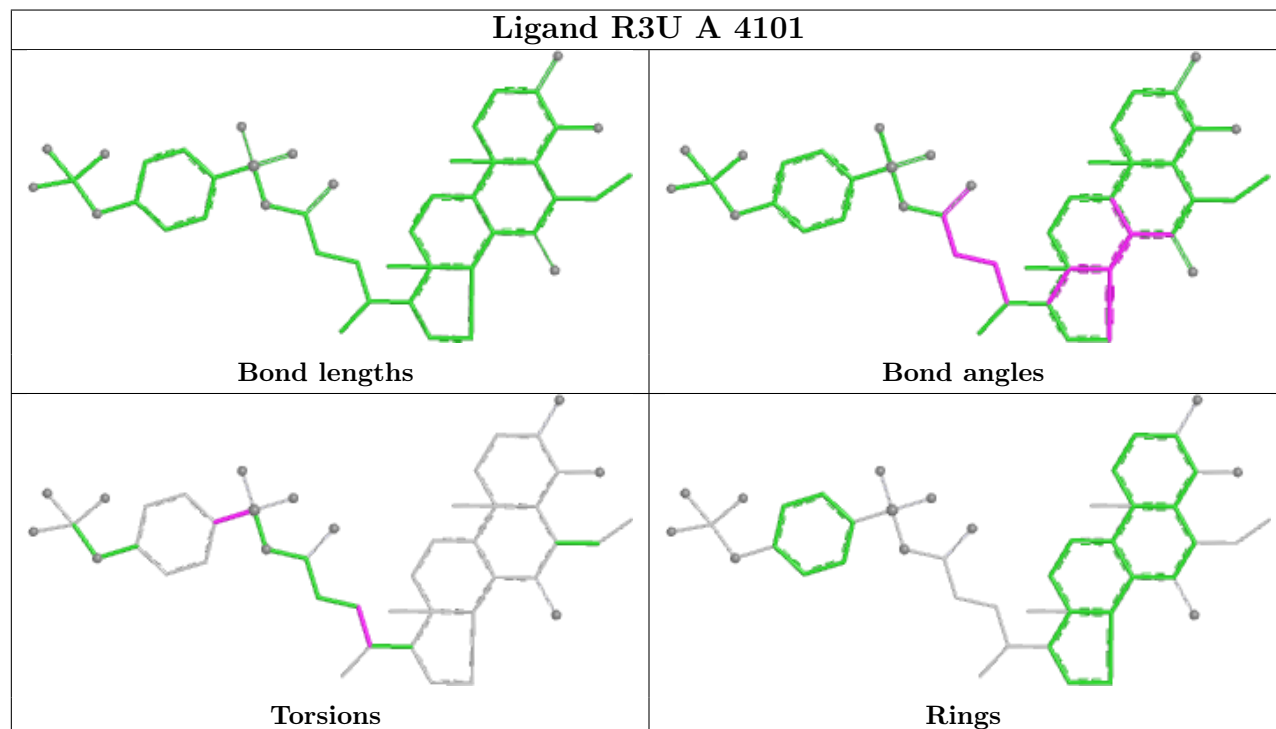
There are no ring outliers.

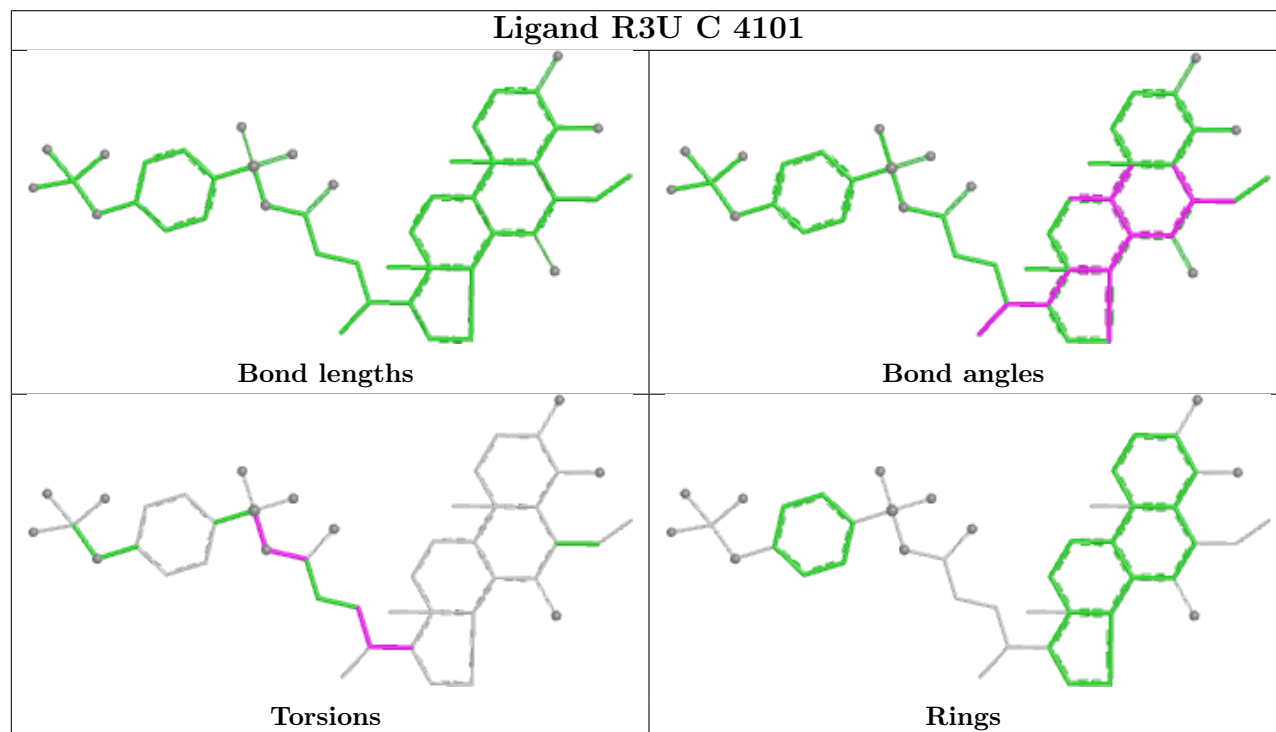
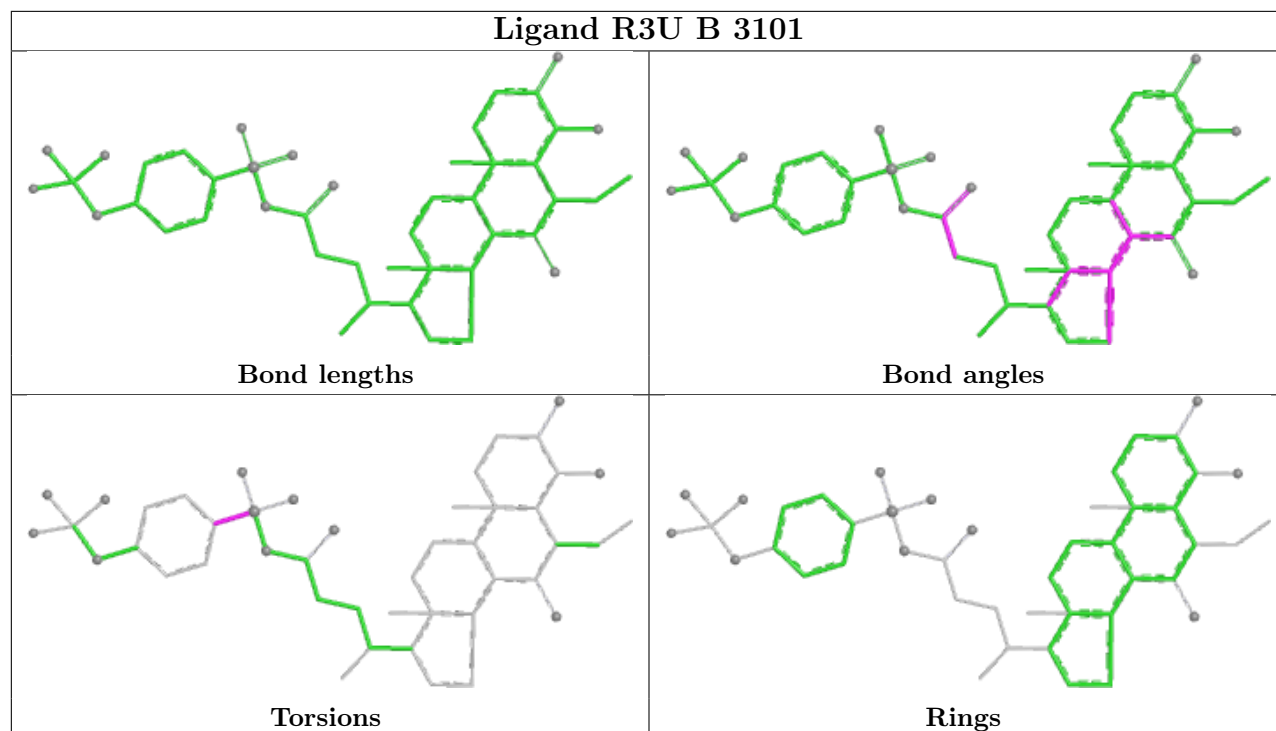
3 monomers are involved in 4 short contacts:

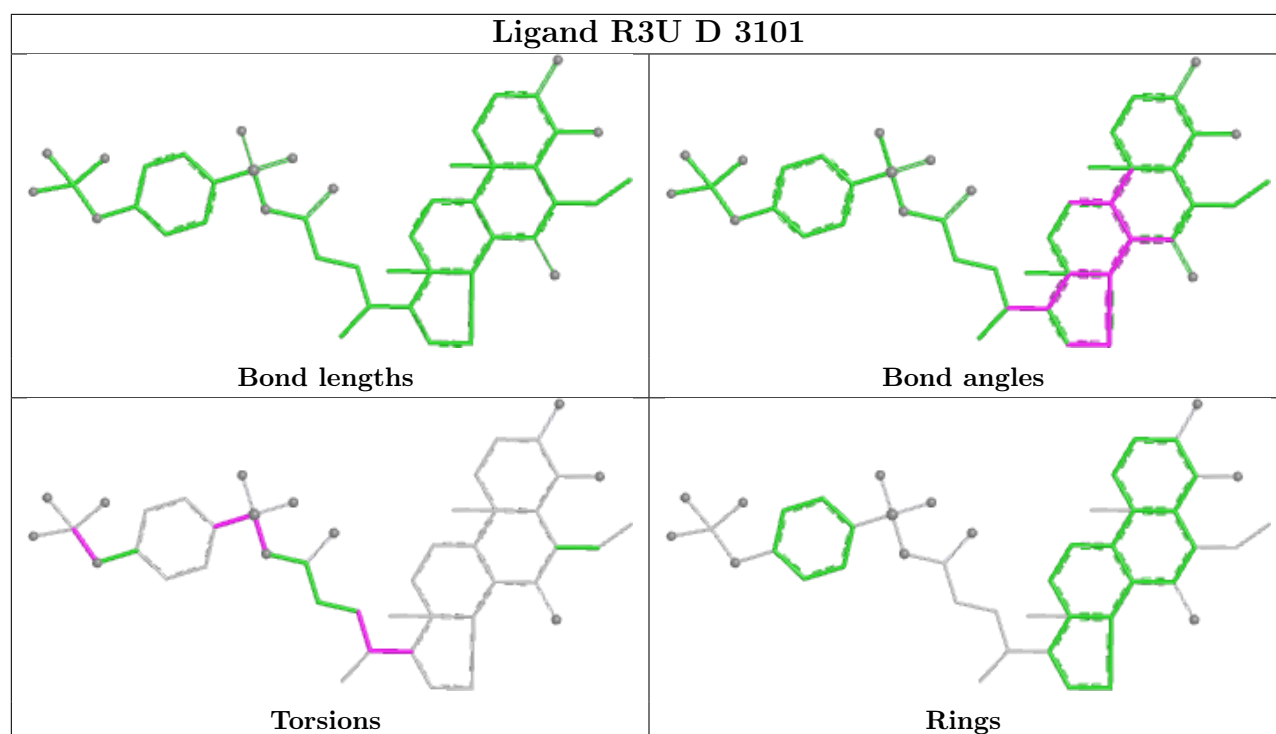
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4101	R3U	1	0
3	C	4101	R3U	1	0
3	D	3101	R3U	2	0

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 [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	228/233 (97%)	-0.84	0 <a href="#">100</a> <a href="#">100</a>	31, 60, 95, 127	5 (2%)
1	B	229/233 (98%)	-0.79	0 <a href="#">100</a> <a href="#">100</a>	29, 62, 104, 159	3 (1%)
1	C	227/233 (97%)	-0.68	0 <a href="#">100</a> <a href="#">100</a>	51, 86, 129, 166	4 (1%)
1	D	229/233 (98%)	-0.55	4 (1%) <a href="#">69</a> <a href="#">64</a>	42, 94, 136, 158	5 (2%)
2	E	12/13 (92%)	-0.04	0 <a href="#">100</a> <a href="#">100</a>	63, 73, 107, 135	8 (66%)
2	F	11/13 (84%)	0.09	0 <a href="#">100</a> <a href="#">100</a>	89, 114, 170, 174	4 (36%)
2	G	13/13 (100%)	-0.65	0 <a href="#">100</a> <a href="#">100</a>	61, 79, 127, 127	7 (53%)
2	H	11/13 (84%)	0.11	0 <a href="#">100</a> <a href="#">100</a>	69, 76, 112, 115	7 (63%)
2	I	11/13 (84%)	-0.05	0 <a href="#">100</a> <a href="#">100</a>	111, 131, 167, 171	2 (18%)
2	J	12/13 (92%)	-0.41	0 <a href="#">100</a> <a href="#">100</a>	92, 107, 150, 161	4 (33%)
All	All	983/1010 (97%)	-0.68	4 (0%) <a href="#">88</a> <a href="#">86</a>	29, 76, 129, 174	49 (4%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	342	SER	6.1
1	D	343	GLY	2.9
1	D	393	PRO	2.1
1	D	344	HIS	2.0

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

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

### 6.3 Carbohydrates [i](#)

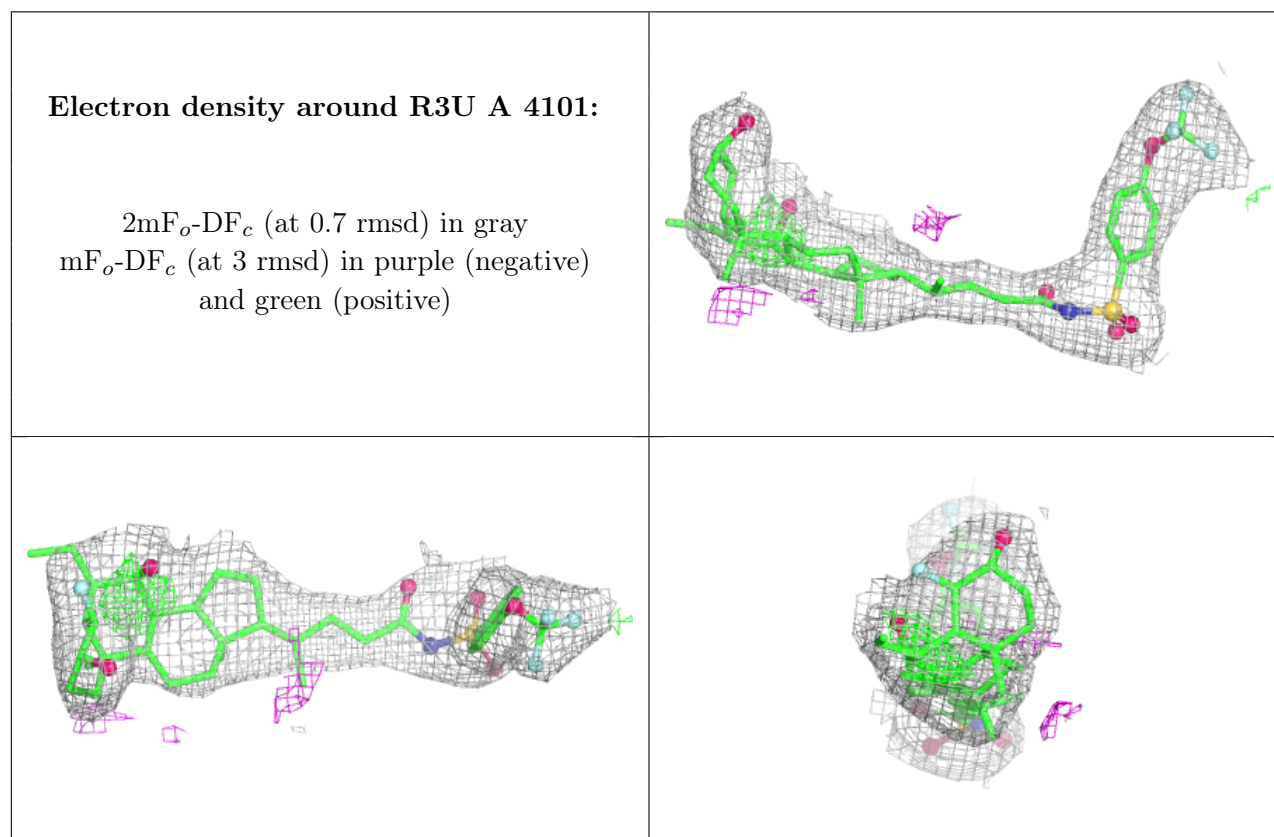
There are no oligosaccharides in this entry.

## 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.

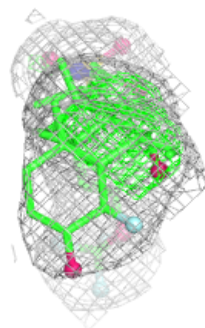
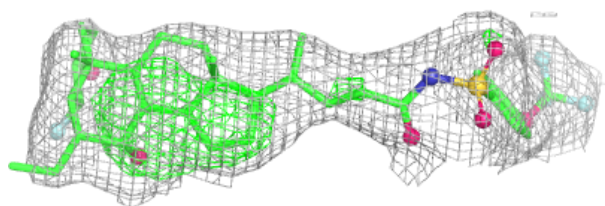
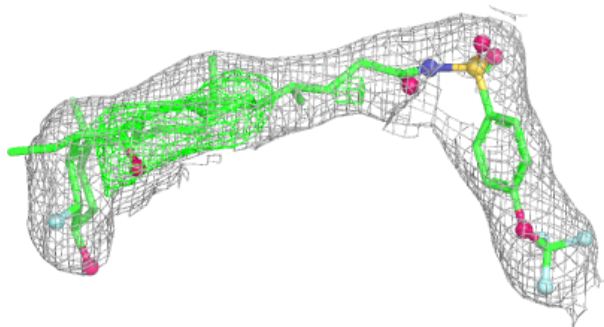
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	R3U	A	4101	45/45	0.99	0.09	53,62,73,118	45
3	R3U	B	3101	45/45	0.99	0.08	49,62,82,118	45
3	R3U	C	4101	45/45	0.99	0.09	69,87,96,103	45
3	R3U	D	3101	45/45	0.99	0.08	72,87,106,120	45

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.

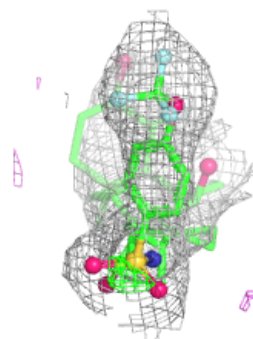
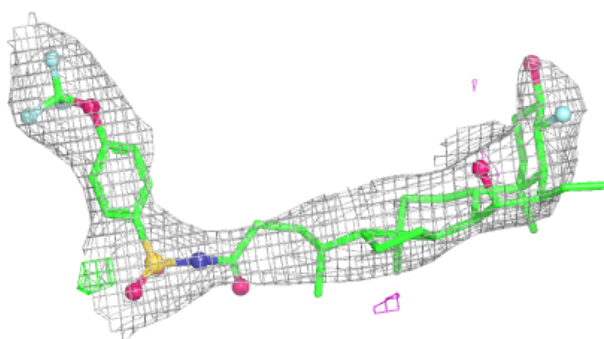


**Electron density around R3U B 3101:**

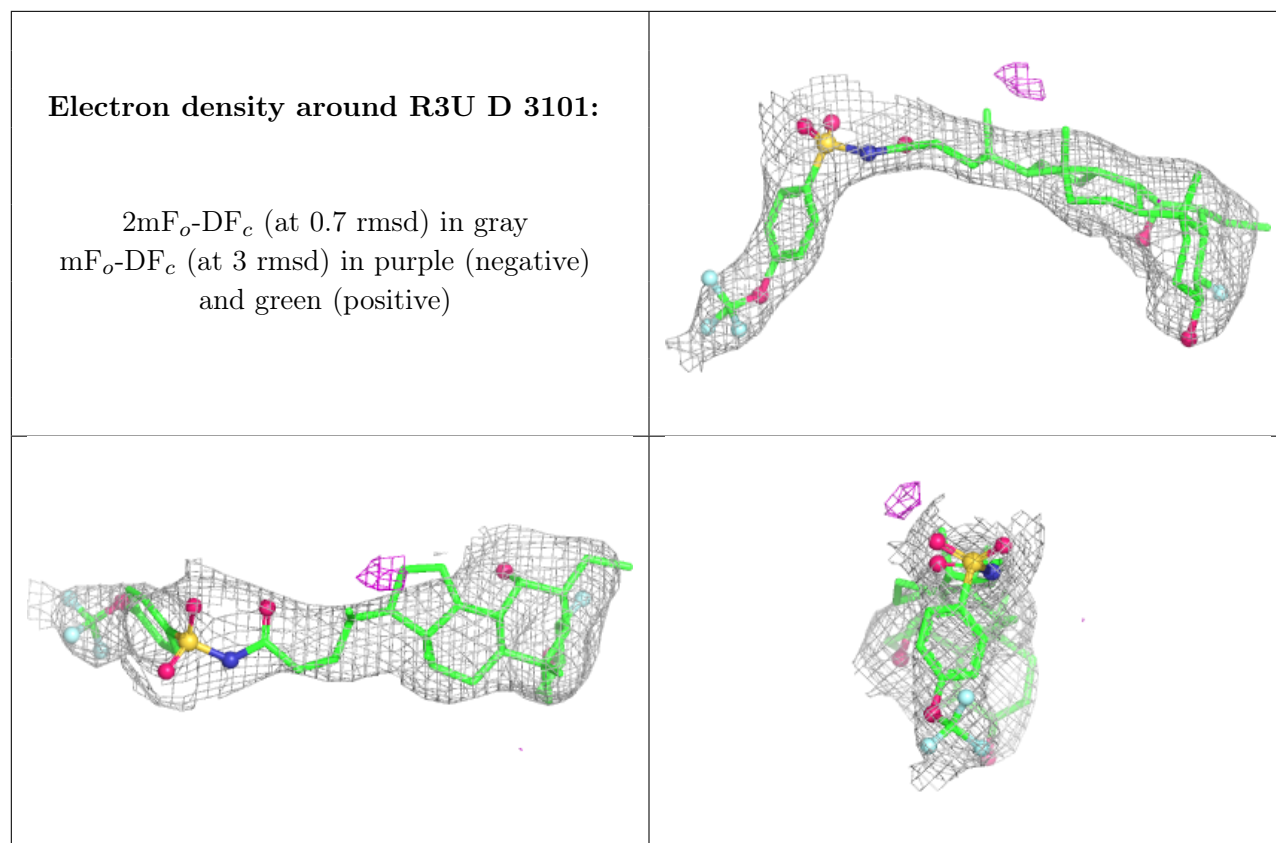
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around R3U C 4101:**

$2mF_o-DF_c$  (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.