



Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 12:30 AM JST

PDB ID : 8J22
EMDB ID : EMD-35942
Title : Cryo-EM structure of FFAR2 complex bound with TUG-1375
Authors : Tai, L.; Li, F.; Sun, X.; Tang, W.; Wang, J.
Deposited on : 2023-04-14
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

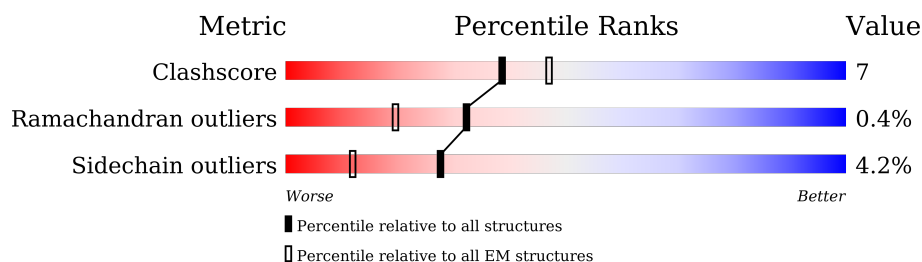
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	377	
2	B	354	
3	C	311	
4	D	71	
5	F	297	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	340	2610	1609	469	511	21	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP P62873
A	-11	HIS	-	expression tag	UNP P62873
A	-10	HIS	-	expression tag	UNP P62873
A	-9	HIS	-	expression tag	UNP P62873
A	-8	HIS	-	expression tag	UNP P62873
A	-7	HIS	-	expression tag	UNP P62873
A	-6	HIS	-	expression tag	UNP P62873
A	-5	GLY	-	expression tag	UNP P62873
A	-4	SER	-	expression tag	UNP P62873
A	-3	LEU	-	expression tag	UNP P62873
A	-2	LEU	-	expression tag	UNP P62873
A	-1	GLN	-	expression tag	UNP P62873
A	339	GLY	-	expression tag	UNP P62873
A	340	SER	-	expression tag	UNP P62873
A	341	SER	-	expression tag	UNP P62873
A	342	GLY	-	expression tag	UNP P62873
A	343	GLY	-	expression tag	UNP P62873
A	344	GLY	-	expression tag	UNP P62873
A	345	GLY	-	expression tag	UNP P62873
A	346	SER	-	expression tag	UNP P62873
A	347	GLY	-	expression tag	UNP P62873
A	348	GLY	-	expression tag	UNP P62873
A	349	GLY	-	expression tag	UNP P62873
A	350	GLY	-	expression tag	UNP P62873
A	351	SER	-	expression tag	UNP P62873
A	352	SER	-	expression tag	UNP P62873
A	353	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
A	354	VAL	-	expression tag	UNP P62873
A	355	SER	-	expression tag	UNP P62873
A	356	GLY	-	expression tag	UNP P62873
A	357	TRP	-	expression tag	UNP P62873
A	358	ARG	-	expression tag	UNP P62873
A	359	LEU	-	expression tag	UNP P62873
A	360	PHE	-	expression tag	UNP P62873
A	361	LYS	-	expression tag	UNP P62873
A	362	LYS	-	expression tag	UNP P62873
A	363	ILE	-	expression tag	UNP P62873
A	364	SER	-	expression tag	UNP P62873

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	215	Total	C	N	O	S	0	0
			1693	1081	283	317	12		

- Molecule 3 is a protein called Free fatty acid receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	285	Total	C	N	O	S	0	0
			2285	1527	377	370	11		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	THR	LEU	conflict	UNP O15552
C	35	VAL	ARG	conflict	UNP O15552
C	36	VAL	ILE	conflict	UNP O15552
C	80	ILE	VAL	variant	UNP O15552
C	86	GLY	SER	conflict	UNP O15552
C	158	ASN	SER	variant	UNP O15552
C	171	GLU	ASN	conflict	UNP O15552
C	208	THR	SER	conflict	UNP O15552
C	211	HIS	LEU	variant	UNP O15552
C	246	PHE	TYR	variant	UNP O15552
C	247	TYR	HIS	conflict	UNP O15552

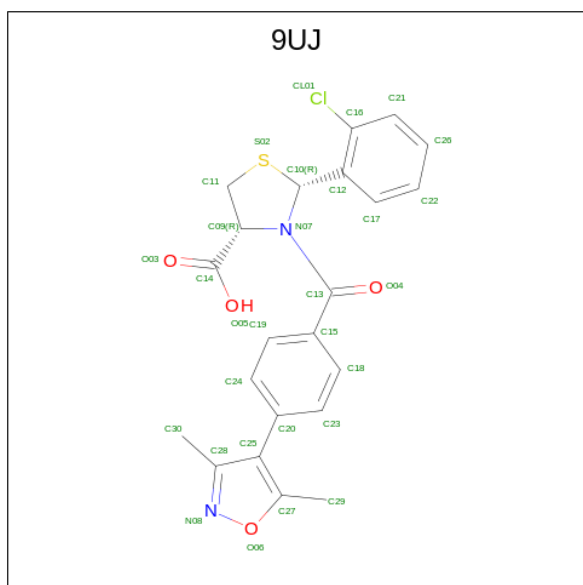
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	57	Total	C	N	O	S	0	0
			433	271	75	84	3		

- Molecule 5 is a protein called scFV16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	235	Total	C	N	O	S	0	0
			1805	1144	299	352	10		

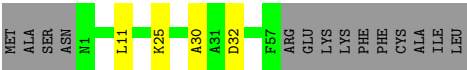
- Molecule 6 is (2R,4R)-2-(2-chlorophenyl)-3-[4-(3,5-dimethyl-1,2-oxazol-4-yl)phenyl]carbonyl-1,3-thiazolidine-4-carboxylic acid (three-letter code: 9UJ) (formula: C₂₂H₁₉ClN₂O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	Cl	N	O	S
			30	22	1	2	4	1
								0



● Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



● Molecule 5: scFV16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	836117	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9UJ

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	0.24	0/2657	0.51	1/3602 (0.0%)
2	B	0.24	0/1722	0.43	0/2315
3	C	0.24	0/2349	0.51	2/3209 (0.1%)
4	D	0.25	0/439	0.42	0/594
5	F	0.25	0/1849	0.53	2/2506 (0.1%)
All	All	0.24	0/9016	0.50	5/12226 (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
5	F	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	73	PHE	C-N-CA	10.89	148.94	121.70
5	F	221	TYR	N-CA-C	6.81	129.39	111.00
1	A	234	PRO	CA-N-CD	-5.77	103.43	111.50
5	F	222	PRO	CB-CA-C	5.49	125.73	112.00
3	C	74	ARG	N-CA-C	-5.48	96.21	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	220	GLU	Peptide
5	F	221	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2610	0	2516	47	0
2	B	1693	0	1652	22	0
3	C	2285	0	2372	27	0
4	D	433	0	444	3	0
5	F	1805	0	1744	32	0
6	C	30	0	0	1	0
All	All	8856	0	8728	125	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 7.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:OE2	1:A:261:THR:OG1	2.03	0.75
3:C:149:TYR:HE1	3:C:161:GLU:HB2	1.53	0.73
1:A:318:VAL:HG22	1:A:325:VAL:HG22	1.73	0.69
3:C:74:ARG:HG3	3:C:75:TRP:H	1.58	0.69
5:F:218:HIS:HA	5:F:223:LEU:HD22	1.75	0.69
1:A:150:LEU:HD11	1:A:156:VAL:HG23	1.75	0.67
5:F:104:GLY:O	5:F:177:ARG:NH2	2.30	0.64
3:C:16:ILE:O	3:C:20:THR:OG1	2.17	0.63
2:B:8:GLU:OE2	5:F:106:SER:N	2.31	0.63
5:F:164:LEU:HB2	5:F:174:LEU:HD11	1.82	0.62
2:B:229:ASP:HB2	2:B:242:ARG:HB2	1.81	0.62
2:B:251:ASP:OD1	2:B:255:ASN:ND2	2.34	0.61
1:A:245:ASP:OD2	1:A:247:THR:HG22	2.01	0.60
1:A:28:LEU:HD13	4:D:30:ALA:HB1	1.82	0.60
1:A:116:ASP:N	1:A:116:ASP:OD1	2.35	0.59
5:F:109:ASP:N	5:F:109:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:GLU:HB2	2:B:258:TRP:HB3	1.85	0.58
1:A:254:ARG:NH2	4:D:32:ASP:OD2	2.36	0.57
1:A:96:SER:OG	1:A:96:SER:O	2.23	0.57
1:A:275:SER:HB3	1:A:316:LEU:HD23	1.86	0.56
5:F:163:PHE:HE2	5:F:216:MET:HG2	1.69	0.56
3:C:162:ILE:HG22	3:C:163:THR:H	1.70	0.56
3:C:72:ASN:HB2	3:C:75:TRP:CZ3	2.42	0.55
1:A:154:GLN:HB3	1:A:166:LEU:HD11	1.88	0.55
3:C:79:LYS:O	3:C:79:LYS:NZ	2.39	0.55
1:A:213:GLU:OE2	1:A:217:ARG:NH2	2.39	0.55
3:C:163:THR:HG21	6:C:401:9UJ:CL01	2.44	0.54
1:A:115:LEU:HB2	2:B:184:ILE:HD13	1.90	0.53
2:B:325:CYS:SG	2:B:326:ALA:N	2.81	0.53
2:B:52:GLN:NE2	2:B:328:ASP:O	2.42	0.53
3:C:169:THR:HG23	3:C:170:ASP:H	1.73	0.53
3:C:186:VAL:HG12	3:C:187:LEU:HD23	1.91	0.53
5:F:69:THR:HG23	5:F:82:GLN:HB3	1.91	0.53
5:F:52:SER:O	5:F:72:ARG:NH1	2.42	0.53
5:F:91:THR:HG23	5:F:118:THR:HA	1.91	0.53
3:C:74:ARG:CG	3:C:75:TRP:H	2.22	0.52
1:A:77:LEU:HD11	1:A:112:CYS:HB3	1.91	0.52
5:F:67:ARG:NH1	5:F:85:SER:O	2.42	0.52
2:B:223:PHE:HB3	2:B:266:LEU:HD12	1.91	0.52
3:C:148:GLN:HG2	3:C:162:ILE:HD13	1.93	0.51
1:A:73:GLN:O	1:A:96:SER:OG	2.27	0.50
3:C:148:GLN:O	3:C:152:THR:OG1	2.26	0.50
1:A:193:ASP:OD1	1:A:195:ARG:HB2	2.12	0.50
1:A:98:VAL:HA	1:A:114:GLY:HA3	1.92	0.50
5:F:216:MET:HE1	5:F:223:LEU:HD13	1.94	0.50
1:A:190:LEU:HD23	1:A:197:PHE:HB3	1.93	0.49
5:F:48:VAL:HG13	5:F:64:VAL:HG21	1.94	0.49
3:C:51:LEU:HD21	3:C:269:ASP:OD2	2.12	0.49
5:F:178:MET:HG2	5:F:178:MET:O	2.13	0.49
2:B:259:PHE:O	2:B:317:LYS:NZ	2.46	0.49
1:A:117:ASN:HA	1:A:144:LEU:HD23	1.94	0.49
1:A:147:CYS:O	1:A:148:ARG:NH1	2.46	0.49
2:B:293:SER:N	2:B:298:GLU:OE2	2.41	0.48
1:A:288:ASP:HA	1:A:312:ARG:HG3	1.96	0.48
1:A:329:SER:OG	1:A:330:TRP:N	2.46	0.48
1:A:25:ASP:OD2	4:D:25:LYS:HB3	2.13	0.48
5:F:47:TRP:HZ2	5:F:50:TYR:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:12:VAL:HG11	5:F:86:LEU:HD12	1.96	0.47
5:F:220:GLU:O	5:F:222:PRO:HB2	2.15	0.47
1:A:185:VAL:HA	1:A:201:ALA:HA	1.97	0.47
1:A:142:GLY:H	1:A:161:ASP:HB3	1.79	0.47
2:B:43:GLU:OE2	2:B:46:LYS:HB3	2.16	0.46
1:A:77:LEU:HD12	1:A:93:LEU:HD21	1.97	0.46
3:C:59:LEU:HD23	3:C:62:LEU:HD12	1.98	0.46
1:A:145:SER:HB2	1:A:186:MET:HA	1.98	0.46
5:F:166:ARG:HB2	5:F:169:GLN:HB2	1.98	0.46
1:A:187:SER:OG	1:A:230:ILE:HG22	2.16	0.46
2:B:351:CYS:HA	3:C:44:VAL:HG11	1.98	0.46
3:C:121:ARG:O	3:C:122:ARG:NE	2.48	0.46
1:A:64:ASP:OD1	1:A:64:ASP:N	2.47	0.45
1:A:229:ALA:HB3	1:A:274:VAL:HG23	1.99	0.45
5:F:174:LEU:HA	5:F:185:VAL:HG21	1.98	0.45
3:C:36:VAL:HG21	3:C:49:LEU:HD22	1.97	0.45
2:B:229:ASP:OD1	2:B:229:ASP:N	2.41	0.45
1:A:184:ASP:O	1:A:202:CYS:N	2.50	0.45
1:A:208:LEU:HD22	1:A:253:LEU:HD22	1.98	0.45
5:F:33:GLY:N	5:F:99:SER:O	2.50	0.45
3:C:249:ARG:HD3	3:C:249:ARG:HA	1.81	0.44
3:C:163:THR:HG23	3:C:166:GLU:HG3	1.98	0.44
1:A:93:LEU:HD13	1:A:98:VAL:HG11	2.00	0.44
5:F:40:ALA:HB3	5:F:43:LYS:HB2	1.99	0.44
5:F:108:PHE:HE1	5:F:218:HIS:HD2	1.66	0.44
1:A:227:ILE:HA	1:A:243:SER:HA	2.00	0.43
3:C:186:VAL:HA	3:C:190:ILE:HD12	2.00	0.43
5:F:188:ARG:NH2	5:F:209:ASP:OD2	2.51	0.43
1:A:81:ASP:OD2	1:A:84:THR:OG1	2.35	0.43
1:A:65:SER:O	1:A:65:SER:OG	2.35	0.43
1:A:186:MET:N	1:A:186:MET:SD	2.91	0.43
1:A:237:ASN:HA	1:A:253:LEU:HD12	2.01	0.43
1:A:321:ASP:N	1:A:321:ASP:OD1	2.47	0.43
5:F:205:LEU:HD23	5:F:205:LEU:HA	1.86	0.43
5:F:67:ARG:O	5:F:84:THR:OG1	2.31	0.43
3:C:276:SER:O	3:C:279:VAL:HG22	2.18	0.43
5:F:100:ILE:O	5:F:106:SER:HA	2.19	0.43
3:C:10:ILE:HD11	3:C:257:ILE:HG13	1.99	0.42
3:C:239:ASN:OD1	3:C:239:ASN:N	2.52	0.42
2:B:266:LEU:HD23	2:B:321:THR:HG23	2.01	0.42
1:A:43:MET:HG3	1:A:306:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:173:LEU:HD12	5:F:174:LEU:N	2.34	0.42
1:A:132:ARG:HG2	1:A:133:VAL:O	2.20	0.42
2:B:266:LEU:N	2:B:320:TYR:O	2.51	0.42
2:B:317:LYS:HB3	2:B:317:LYS:HE2	1.93	0.42
5:F:108:PHE:H	5:F:173:LEU:HD22	1.84	0.42
1:A:1:GLU:OE1	1:A:4:GLN:N	2.51	0.42
1:A:185:VAL:HG21	1:A:199:SER:HB2	2.02	0.42
5:F:68:PHE:CE1	5:F:83:MET:HB3	2.54	0.42
2:B:33:GLU:HG2	2:B:195:HIS:HB2	2.01	0.42
2:B:223:PHE:O	2:B:267:PHE:N	2.51	0.42
2:B:230:TYR:HH	2:B:281:SER:HG	1.64	0.42
5:F:12:VAL:HG22	5:F:18:ARG:HH11	1.85	0.42
5:F:217:GLN:HE21	5:F:224:THR:H	1.68	0.41
2:B:230:TYR:HB2	2:B:286:CYS:HB2	2.01	0.41
2:B:337:ASP:OD1	2:B:337:ASP:N	2.52	0.41
5:F:105:SER:HB3	5:F:177:ARG:CZ	2.50	0.41
1:A:59:MET:HG2	1:A:68:LEU:HD11	2.03	0.41
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.93	0.41
5:F:107:PRO:HA	5:F:161:TYR:HE2	1.84	0.41
1:A:233:PHE:HD2	1:A:235:ASN:HB3	1.85	0.41
2:B:257:LYS:H	2:B:257:LYS:HG2	1.62	0.41
1:A:148:ARG:HB3	1:A:190:LEU:HD12	2.03	0.40
3:C:11:LEU:HD22	3:C:70:ALA:HB2	2.02	0.40
3:C:62:LEU:O	3:C:66:ILE:HG13	2.21	0.40
1:A:41:ILE:HD13	1:A:282:LEU:HD11	2.03	0.40
3:C:18:PHE:CE1	3:C:22:LEU:HD22	2.57	0.40
3:C:62:LEU:N	3:C:63:PRO:HD2	2.37	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 PDB entries followed by that with respect to all EM entries.

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	338/377 (90%)	333 (98%)	5 (2%)	0	100	100
2	B	209/354 (59%)	209 (100%)	0	0	100	100
3	C	283/311 (91%)	266 (94%)	15 (5%)	2 (1%)	19	54
4	D	55/71 (78%)	55 (100%)	0	0	100	100
5	F	231/297 (78%)	222 (96%)	7 (3%)	2 (1%)	14	49
All	All	1116/1410 (79%)	1085 (97%)	27 (2%)	4 (0%)	32	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	73	PHE
3	C	74	ARG
5	F	221	TYR
5	F	222	PRO

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 PDB entries followed by that with respect to all EM entries.

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	282/308 (92%)	265 (94%)	17 (6%)	16	48
2	B	180/305 (59%)	174 (97%)	6 (3%)	33	64
3	C	249/270 (92%)	240 (96%)	9 (4%)	30	62
4	D	46/58 (79%)	45 (98%)	1 (2%)	47	73
5	F	199/239 (83%)	192 (96%)	7 (4%)	31	63
All	All	956/1180 (81%)	916 (96%)	40 (4%)	27	58

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	44	ARG
1	A	50	ARG
1	A	103	TYR

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Mol	Chain	Res	Type
1	A	132	ARG
1	A	150	LEU
1	A	186	MET
1	A	189	SER
1	A	231	CYS
1	A	232	PHE
1	A	237	ASN
1	A	244	ASP
1	A	245	ASP
1	A	265	ASP
1	A	275	SER
1	A	281	ARG
1	A	329	SER
2	B	9	ASP
2	B	209	LYS
2	B	229	ASP
2	B	261	ASP
2	B	274	PHE
2	B	309	ASP
3	C	30	ARG
3	C	56	LEU
3	C	149	TYR
3	C	216	ARG
3	C	219	ARG
3	C	230	ASN
3	C	239	ASN
3	C	263	SER
3	C	286	ARG
4	D	11	LEU
5	F	3	GLN
5	F	50	TYR
5	F	122	SER
5	F	144	SER
5	F	145	CYS
5	F	166	ARG
5	F	179	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	213	HIS
4	D	14	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 ⓘ

1 ligand is 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
6	9UJ	C	401	-	29,33,33	2.31	5 (17%)	41,48,48	2.57	19 (46%)

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
6	9UJ	C	401	-	-	6/20/33/33	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	9UJ	C09-N07	7.28	1.56	1.46
6	C	401	9UJ	C15-C13	5.62	1.59	1.50
6	C	401	9UJ	C09-C14	4.48	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	9UJ	C13-N07	4.20	1.43	1.35
6	C	401	9UJ	C12-C10	3.29	1.54	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	401	9UJ	C12-C10-N07	6.89	121.77	113.94
6	C	401	9UJ	C09-N07-C10	-5.96	111.19	116.60
6	C	401	9UJ	C15-C13-N07	5.05	127.17	118.47
6	C	401	9UJ	C19-C15-C18	-4.72	111.86	118.59
6	C	401	9UJ	C11-C09-N07	3.39	109.94	106.17
6	C	401	9UJ	C11-C09-C14	-3.12	105.52	111.14
6	C	401	9UJ	C24-C19-C15	3.08	124.36	120.78
6	C	401	9UJ	C17-C12-C16	-3.03	113.79	116.81
6	C	401	9UJ	O04-C13-N07	-2.97	117.62	122.38
6	C	401	9UJ	C23-C18-C15	2.85	124.09	120.78
6	C	401	9UJ	O04-C13-C15	-2.58	115.21	120.23
6	C	401	9UJ	C21-C16-CL01	-2.54	113.31	118.41
6	C	401	9UJ	S02-C10-N07	-2.43	101.56	104.01
6	C	401	9UJ	C12-C16-CL01	2.40	122.90	120.41
6	C	401	9UJ	C16-C12-C10	2.40	126.90	122.10
6	C	401	9UJ	C23-C20-C25	2.39	124.76	120.79
6	C	401	9UJ	C24-C20-C23	-2.33	112.95	117.59
6	C	401	9UJ	C18-C15-C13	2.21	125.90	120.29
6	C	401	9UJ	O03-C14-C09	-2.17	115.64	122.48

There are no chirality outliers.

All (6) torsion outliers are listed below:

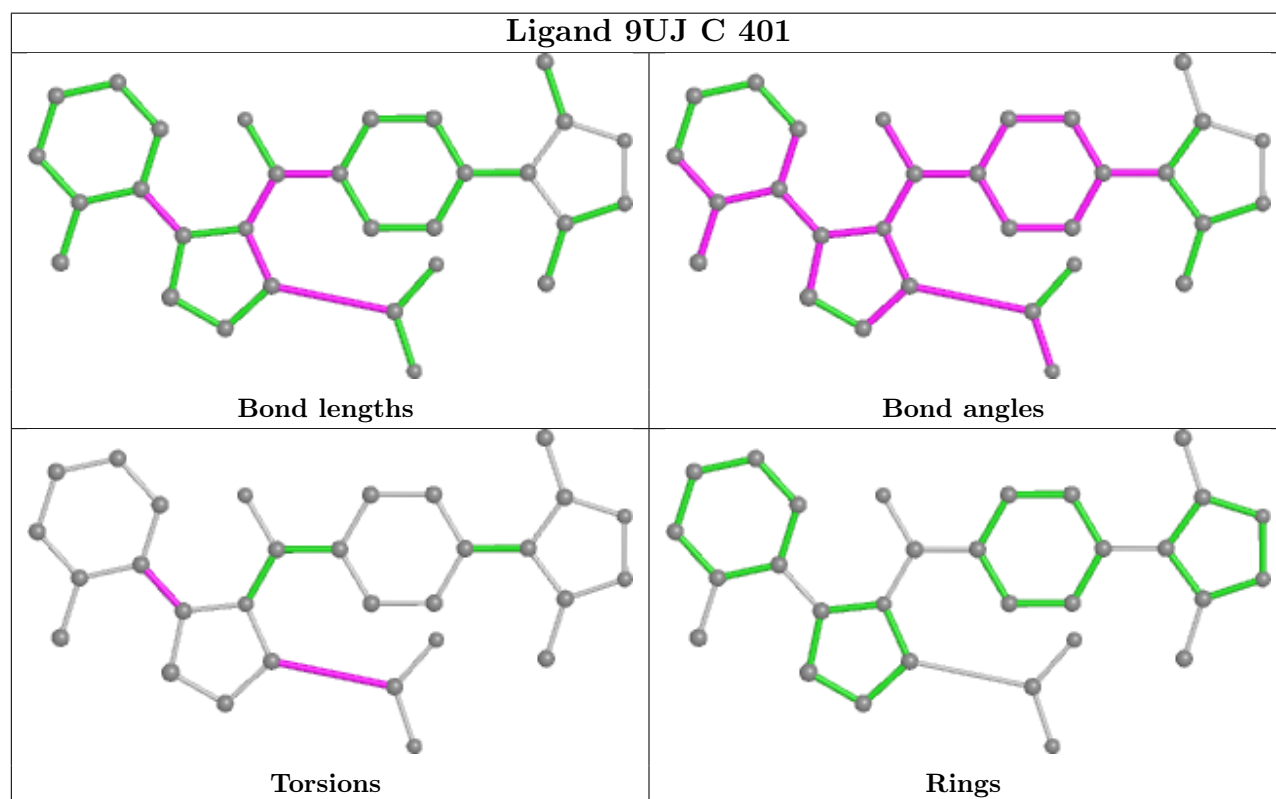
Mol	Chain	Res	Type	Atoms
6	C	401	9UJ	N07-C10-C12-C16
6	C	401	9UJ	N07-C10-C12-C17
6	C	401	9UJ	N07-C09-C14-O03
6	C	401	9UJ	N07-C09-C14-O05
6	C	401	9UJ	S02-C10-C12-C17
6	C	401	9UJ	S02-C10-C12-C16

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	9UJ	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.



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.