



Full wwPDB EM Validation Report ⓘ

May 31, 2026 – 12:10 AM JST

PDB ID : 9V0X / pdb_00009v0x
EMDB ID : EMD-64674
Title : Cryo-EM structure of Gq-coupled PrRPR in complex with GUB08248
Authors : Zhao, L.; Li, X.; Li, S.; Yuan, Q.; Xu, H.E.
Deposited on : 2025-05-19
Resolution : 2.66 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 : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

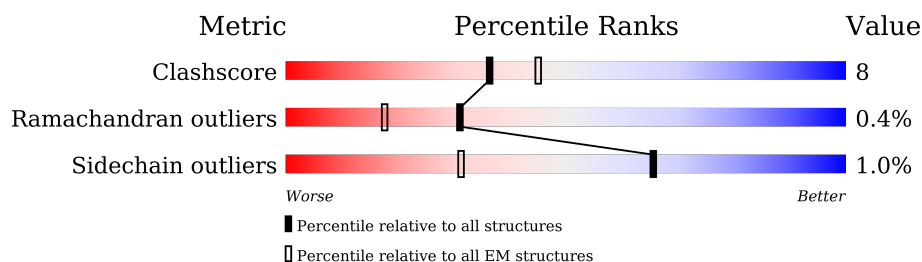
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.66 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	361	
2	B	371	
3	E	247	
4	G	70	
5	L	11	
6	R	370	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9126 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(324) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1885	1192	335	350	8		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	336	Total	C	N	O	S	0	0
			2583	1593	465	504	21		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P62873
B	2	GLY	-	expression tag	UNP P62873
B	3	SER	-	expression tag	UNP P62873
B	4	LEU	-	expression tag	UNP P62873
B	5	LEU	-	expression tag	UNP P62873
B	6	GLN	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	SER	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	GLY	-	expression tag	UNP P62873
B	357	GLY	-	expression tag	UNP P62873
B	358	SER	-	expression tag	UNP P62873
B	359	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	360	GLY	-	expression tag	UNP P62873
B	361	VAL	-	expression tag	UNP P62873
B	362	SER	-	expression tag	UNP P62873
B	363	GLY	-	expression tag	UNP P62873
B	364	TRP	-	expression tag	UNP P62873
B	365	ARG	-	expression tag	UNP P62873
B	366	LEU	-	expression tag	UNP P62873
B	367	PHE	-	expression tag	UNP P62873
B	368	LYS	-	expression tag	UNP P62873
B	369	LYS	-	expression tag	UNP P62873
B	370	ILE	-	expression tag	UNP P62873
B	371	SER	-	expression tag	UNP P62873

- Molecule 3 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	232	Total	C	N	O	S	0	0
			1782	1131	295	346	10		

- 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	G	53	Total	C	N	O	S	0	0
			400	251	69	77	3		

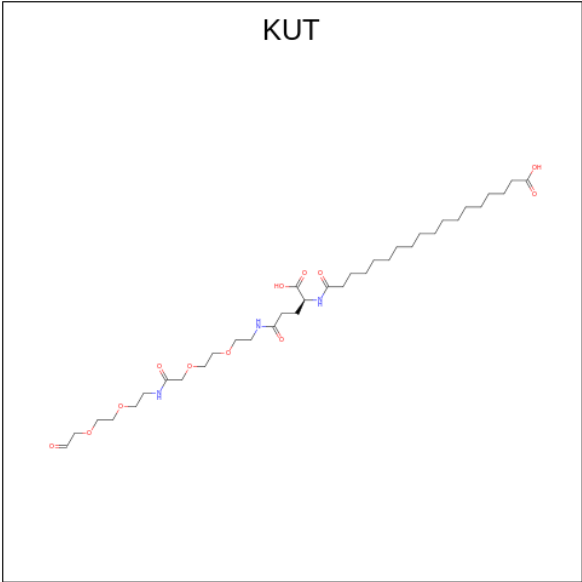
- Molecule 5 is a protein called GUB08248.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	11	Total	C	N	O	0	1
			82	50	21	11		

- Molecule 6 is a protein called Prolactin-releasing peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	292	Total	C	N	O	S	0	0
			2346	1558	405	372	11		

- Molecule 7 is KUT [2-(2-[2-(2-[2-(Octadecandioyl-gamma-Glu)amino]ethoxy)ethoxy]acetyl amino)ethoxy]ethoxy]acetyl] (CCD ID: KUT) (formula: C₃₅H₆₃N₃O₁₂) (labeled as "Ligand of Interest" by depositor).



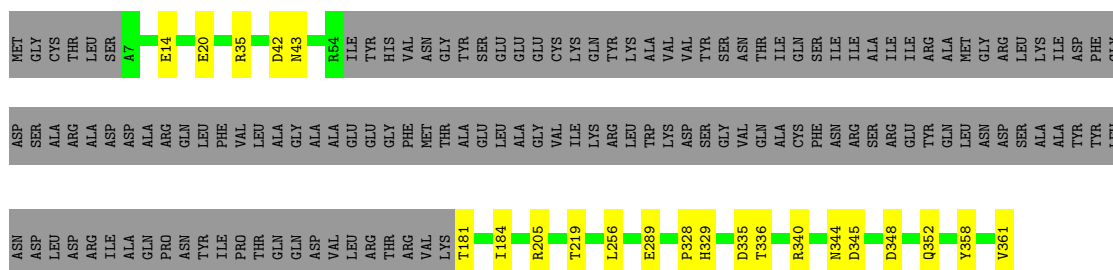
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	L	1	48	35	3	10	0

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. 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. 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: Guanine nucleotide-binding protein G(324) subunit alpha

Chain A: 



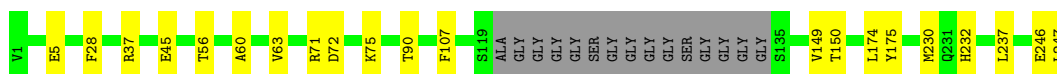
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 



- Molecule 3: scFv16

Chain E: 



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

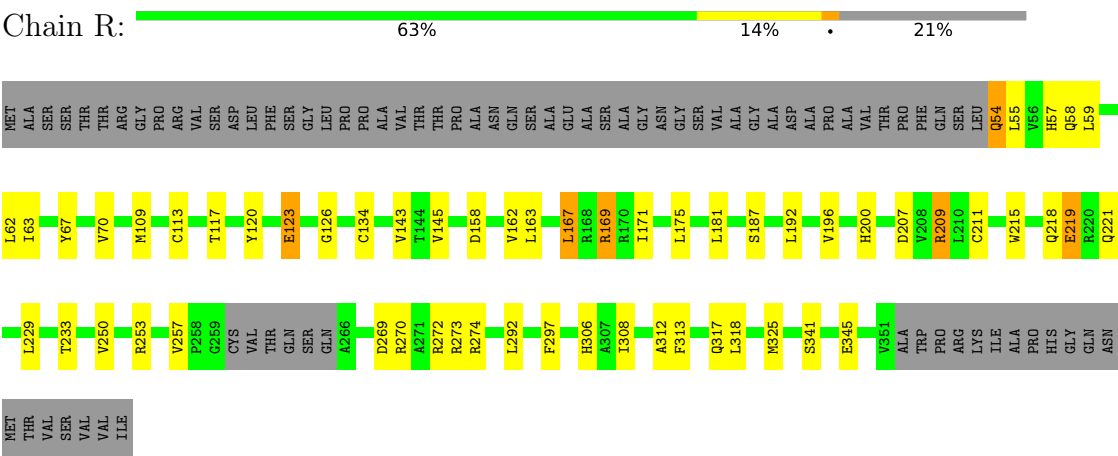
Chain G: 



● Molecule 5: GUB08248



● Molecule 6: Prolactin-releasing peptide receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	518909	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	18000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: KUT

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	0.11	0/1919	0.24	0/2583
2	B	0.09	0/2630	0.25	0/3566
3	E	0.10	0/1826	0.20	0/2476
4	G	0.11	0/406	0.17	0/550
5	L	0.69	0/83	0.87	0/108
6	R	0.23	0/2408	0.52	0/3297
All	All	0.16	0/9272	0.34	0/12580

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

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	1885	0	1878	20	0
2	B	2583	0	2488	36	0
3	E	1782	0	1724	16	0
4	G	400	0	398	4	0
5	L	82	0	90	25	0
6	R	2346	0	2448	52	0
7	L	48	0	0	18	0
All	All	9126	0	9026	140	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 8.

All (140) 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)
6:R:134:CYS:SG	6:R:211:CYS:CB	2.29	1.21
6:R:134:CYS:SG	6:R:211:CYS:SG	1.21	1.19
5:L:4:LYS:NZ	7:L:401:KUT:O9	1.81	1.12
5:L:4:LYS:NZ	7:L:401:KUT:C33	2.23	1.00
5:L:4:LYS:HZ1	7:L:401:KUT:C33	1.76	0.98
5:L:3:GLY:O	7:L:401:KUT:C10	2.13	0.97
2:B:160:ASN:ND2	2:B:175:ASP:OD1	2.05	0.89
5:L:4:LYS:NZ	7:L:401:KUT:C32	2.36	0.88
6:R:229:LEU:O	6:R:233:THR:OG1	1.90	0.87
2:B:30:CYS:SG	2:B:264:GLN:NE2	2.49	0.84
5:L:4:LYS:HZ2	7:L:401:KUT:C32	1.91	0.83
3:E:72:ASP:OD2	3:E:75:LYS:NZ	2.14	0.80
1:A:35:ARG:O	1:A:219:THR:OG1	2.05	0.75
5:L:4:LYS:HD2	5:L:6:PRO:HG3	1.68	0.74
6:R:67:TYR:HA	6:R:70:VAL:HG12	1.69	0.74
5:L:4:LYS:O	7:L:401:KUT:C11	2.36	0.74
5:L:4:LYS:HZ2	7:L:401:KUT:C33	1.99	0.73
2:B:286:SER:OG	4:G:47:ASP:OD2	2.08	0.72
6:R:67:TYR:O	6:R:70:VAL:HG12	1.91	0.70
5:L:4:LYS:HA	7:L:401:KUT:C11	2.22	0.70
2:B:27:ARG:O	2:B:264:GLN:NE2	2.26	0.69
6:R:134:CYS:SG	6:R:211:CYS:HB2	2.32	0.68
2:B:101:ARG:NH1	2:B:143:GLU:OE2	2.27	0.67
5:L:4:LYS:O	5:L:5:ARG:C	2.39	0.66
2:B:170:THR:OG1	2:B:185:PHE:O	2.04	0.65
6:R:257:VAL:HG21	6:R:273:ARG:HH21	1.62	0.64
1:A:20:GLU:OE2	2:B:94:LYS:NZ	2.21	0.64
2:B:281:VAL:HG13	2:B:290:LEU:HD21	1.81	0.62
6:R:221:GLN:OE1	6:R:221:GLN:N	2.32	0.62
1:A:348:ASP:O	1:A:352:GLN:NE2	2.32	0.61
3:E:5:GLU:N	3:E:5:GLU:OE1	2.34	0.60
1:A:340:ARG:HG3	1:A:344:ASN:ND2	2.17	0.60
2:B:336:SER:OG	2:B:338:ASP:OD1	2.20	0.59
2:B:80:GLN:OE1	2:B:104:TRP:HA	2.03	0.58
6:R:67:TYR:CA	6:R:70:VAL:HG12	2.34	0.58
5:L:2:ARG:C	5:L:4:LYS:H	2.11	0.57
6:R:67:TYR:HA	6:R:70:VAL:CG1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:67:TYR:C	6:R:70:VAL:HG12	2.30	0.57
5:L:4:LYS:HD2	5:L:6:PRO:CG	2.33	0.56
5:L:4:LYS:C	7:L:401:KUT:C10	2.78	0.56
2:B:157:LEU:HD23	2:B:197:LEU:HD13	1.87	0.56
3:E:246:GLU:N	3:E:246:GLU:OE1	2.40	0.54
6:R:67:TYR:O	6:R:70:VAL:CG1	2.55	0.54
2:B:338:ASP:O	2:B:339:SER:OG	2.19	0.54
1:A:184:ILE:HD11	2:B:122:LEU:CB	2.38	0.54
6:R:207:ASP:O	6:R:209:ARG:NH2	2.41	0.53
3:E:107:PHE:CZ	3:E:230:MET:HE1	2.44	0.53
2:B:82:GLY:O	2:B:100:LEU:N	2.38	0.52
2:B:32:ASP:OD1	2:B:33:ALA:N	2.43	0.52
2:B:220:GLU:N	2:B:220:GLU:OE1	2.41	0.52
1:A:181:THR:O	2:B:124:ASN:ND2	2.43	0.52
1:A:361:VAL:HG12	6:R:272:ARG:HD3	1.93	0.51
1:A:14:GLU:OE2	3:E:56:THR:OG1	2.23	0.51
5:L:1:SER:C	5:L:3:GLY:H	2.18	0.51
5:L:4:LYS:C	7:L:401:KUT:C11	2.84	0.51
2:B:232:SER:OG	2:B:250:SER:OG	2.22	0.50
1:A:289:GLU:N	1:A:289:GLU:OE1	2.42	0.50
6:R:257:VAL:CG2	6:R:273:ARG:NH2	2.75	0.50
1:A:256:LEU:HB3	1:A:328:PRO:HA	1.93	0.50
6:R:162:VAL:HG13	6:R:163:LEU:HD13	1.94	0.50
6:R:55:LEU:HD23	6:R:312:ALA:HA	1.94	0.49
2:B:84:LEU:HD11	2:B:119:CYS:HB3	1.93	0.49
3:E:90:THR:O	3:E:90:THR:HG23	2.13	0.49
6:R:162:VAL:HG13	6:R:163:LEU:CD1	2.43	0.49
6:R:341:SER:O	6:R:345:GLU:HG2	2.12	0.49
3:E:247:LEU:H	3:E:247:LEU:HD23	1.78	0.48
6:R:297:PHE:CZ	6:R:317:GLN:HB2	2.49	0.48
5:L:3:GLY:O	7:L:401:KUT:C	2.62	0.48
6:R:308:ILE:HG23	6:R:313:PHE:HD2	1.79	0.48
2:B:92:THR:HG22	2:B:92:THR:O	2.13	0.47
6:R:257:VAL:CG2	6:R:273:ARG:HH21	2.27	0.47
1:A:184:ILE:HD11	2:B:122:LEU:HB3	1.96	0.47
2:B:80:GLN:OE1	2:B:104:TRP:CE3	2.68	0.47
1:A:340:ARG:HG3	1:A:344:ASN:HD21	1.79	0.47
2:B:284:SER:OG	4:G:47:ASP:OD2	2.27	0.47
6:R:113:CYS:O	6:R:117:THR:OG1	2.29	0.47
5:L:2:ARG:O	5:L:4:LYS:N	2.48	0.47
1:A:335:ASP:OD1	1:A:336:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:120:TYR:CD1	6:R:126:GLY:O	2.69	0.46
6:R:270:ARG:CD	6:R:274:ARG:HE	2.29	0.46
3:E:232:HIS:O	3:E:232:HIS:ND1	2.47	0.46
6:R:218:GLN:O	6:R:219:GLU:HB3	2.16	0.46
5:L:4:LYS:HA	7:L:401:KUT:C10	2.46	0.46
5:L:3:GLY:O	7:L:401:KUT:C1	2.64	0.46
2:B:39:THR:O	2:B:39:THR:HG22	2.16	0.45
3:E:230:MET:CE	3:E:237:LEU:HD13	2.46	0.45
6:R:270:ARG:NE	6:R:274:ARG:HE	2.14	0.45
6:R:269:ASP:O	6:R:273:ARG:HG3	2.17	0.45
7:L:401:KUT:O2	6:R:57:HIS:NE2	2.50	0.45
6:R:209:ARG:HB2	6:R:209:ARG:HH11	1.82	0.45
4:G:25:ASP:OD1	4:G:26:ARG:N	2.50	0.45
6:R:192:LEU:O	6:R:196:VAL:HG23	2.18	0.44
6:R:270:ARG:HD2	6:R:274:ARG:HE	1.82	0.44
5:L:4:LYS:HE3	5:L:4:LYS:HB3	1.77	0.44
2:B:88:ASP:O	2:B:92:THR:N	2.49	0.44
3:E:174:LEU:HD13	3:E:175:TYR:N	2.33	0.44
6:R:200:HIS:CE1	6:R:209:ARG:HG2	2.52	0.43
6:R:54:GLN:O	6:R:55:LEU:HB3	2.17	0.43
2:B:168:ASP:O	2:B:169:THR:OG1	2.25	0.43
3:E:37:ARG:O	3:E:45:GLU:N	2.51	0.43
2:B:80:GLN:OE1	2:B:104:TRP:HE3	2.01	0.43
2:B:148:THR:N	2:B:168:ASP:OD2	2.52	0.43
2:B:202:ARG:C	2:B:203:LEU:HD12	2.43	0.43
6:R:171:ILE:HB	6:R:175:LEU:HD23	1.99	0.43
1:A:205:ARG:NE	2:B:191:ASP:OD1	2.47	0.43
1:A:358:TYR:CE2	6:R:162:VAL:HG11	2.54	0.43
5:L:4:LYS:CA	7:L:401:KUT:C11	2.95	0.43
1:A:329:HIS:NE2	1:A:345:ASP:OD2	2.52	0.43
1:A:358:TYR:CZ	6:R:162:VAL:HG11	2.54	0.43
2:B:128:ILE:O	2:B:141:SER:N	2.52	0.43
5:L:4:LYS:CE	7:L:401:KUT:C32	2.96	0.43
6:R:143:VAL:HA	6:R:187:SER:OG	2.19	0.43
3:E:107:PHE:CE2	3:E:230:MET:HE1	2.54	0.42
6:R:181:LEU:C	6:R:181:LEU:HD23	2.44	0.42
5:L:2:ARG:C	5:L:4:LYS:N	2.74	0.42
3:E:28:PHE:O	3:E:71:ARG:NH2	2.53	0.42
6:R:158:ASP:O	6:R:162:VAL:HG12	2.20	0.42
6:R:308:ILE:HG23	6:R:313:PHE:CD2	2.55	0.42
4:G:27:ILE:C	4:G:27:ILE:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:LEU:HD13	2:B:260:LEU:HD22	2.01	0.41
3:E:60:ALA:HB3	3:E:63:VAL:HG22	2.02	0.41
3:E:149:VAL:HG22	3:E:150:THR:N	2.36	0.41
3:E:149:VAL:HG22	3:E:150:THR:H	1.84	0.41
1:A:184:ILE:HD11	2:B:122:LEU:HB2	2.01	0.41
5:L:4:LYS:CA	7:L:401:KUT:C10	2.98	0.41
6:R:167:LEU:H	6:R:167:LEU:HD12	1.85	0.41
6:R:292:LEU:C	6:R:292:LEU:HD13	2.45	0.41
2:B:11:GLN:N	2:B:11:GLN:OE1	2.54	0.41
6:R:63:ILE:HG21	6:R:318:LEU:HD23	2.02	0.41
6:R:123:GLU:HG3	6:R:126:GLY:H	1.85	0.41
2:B:291:LEU:HG	2:B:301:VAL:HG12	2.03	0.41
6:R:325:MET:HA	6:R:325:MET:HE3	2.02	0.41
1:A:42:ASP:OD1	1:A:43:ASN:N	2.54	0.40
1:A:361:VAL:HG12	6:R:272:ARG:CD	2.51	0.40
6:R:59:LEU:HD22	6:R:62:LEU:HD12	2.03	0.40
2:B:201:THR:O	2:B:201:THR:HG22	2.20	0.40
6:R:109:MET:SD	6:R:145:VAL:HG22	2.60	0.40
6:R:250:VAL:HA	6:R:253:ARG:HE	1.87	0.40
6:R:181:LEU:HD23	6:R:181:LEU:O	2.22	0.40
6:R:169:ARG:HE	6:R:169:ARG:HB2	1.39	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	225/361 (62%)	225 (100%)	0	0	100	100
2	B	334/371 (90%)	331 (99%)	3 (1%)	0	100	100
3	E	228/247 (92%)	226 (99%)	2 (1%)	0	100	100
4	G	51/70 (73%)	51 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	9/11 (82%)	5 (56%)	2 (22%)	2 (22%)	0	0
6	R	288/370 (78%)	271 (94%)	15 (5%)	2 (1%)	18	30
All	All	1135/1430 (79%)	1109 (98%)	22 (2%)	4 (0%)	31	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	R	58	GLN
6	R	219	GLU
5	L	3	GLY
5	L	5	ARG

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	206/315 (65%)	206 (100%)	0	100	100
2	B	279/302 (92%)	278 (100%)	1 (0%)	84	93
3	E	196/198 (99%)	196 (100%)	0	100	100
4	G	41/57 (72%)	41 (100%)	0	100	100
5	L	8/8 (100%)	6 (75%)	2 (25%)	0	0
6	R	255/317 (80%)	248 (97%)	7 (3%)	39	61
All	All	985/1197 (82%)	975 (99%)	10 (1%)	65	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	239	PHE
5	L	4	LYS
5	L	9	ARG
6	R	54	GLN
6	R	123	GLU
6	R	167	LEU

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Mol	Chain	Res	Type
6	R	169	ARG
6	R	209	ARG
6	R	215	TRP
6	R	306	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	A	352	GLN
1	A	359	ASN
2	B	264	GLN
6	R	200	HIS
6	R	339	HIS

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](#)

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
7	KUT	L	401	-	47,47,49	1.55	6 (12%)	51,51,54	1.19	4 (7%)

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
7	KUT	L	401	-	-	23/50/51/53	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	401	KUT	C17-N	5.44	1.45	1.34
7	L	401	KUT	C27-N2	5.36	1.45	1.33
7	L	401	KUT	C21-N1	5.34	1.45	1.33
7	L	401	KUT	O2-C17	-2.13	1.18	1.23
7	L	401	KUT	O3-C21	-2.12	1.19	1.23
7	L	401	KUT	O6-C27	-2.03	1.19	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	401	KUT	C16-C17-N	2.48	120.13	115.83
7	L	401	KUT	O9-C33-C32	-2.37	119.24	126.39
7	L	401	KUT	C20-C21-N1	2.26	120.23	116.42
7	L	401	KUT	C26-C27-N2	2.13	120.11	116.58

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	401	KUT	C30-C31-O8-C32
7	L	401	KUT	N2-C28-C29-O7
7	L	401	KUT	C25-C24-O4-C23
7	L	401	KUT	O4-C24-C25-O5
7	L	401	KUT	C15-C16-C17-N
7	L	401	KUT	C15-C16-C17-O2
7	L	401	KUT	C14-C15-C16-C17
7	L	401	KUT	C10-C11-C12-C13
7	L	401	KUT	O5-C26-C27-O6

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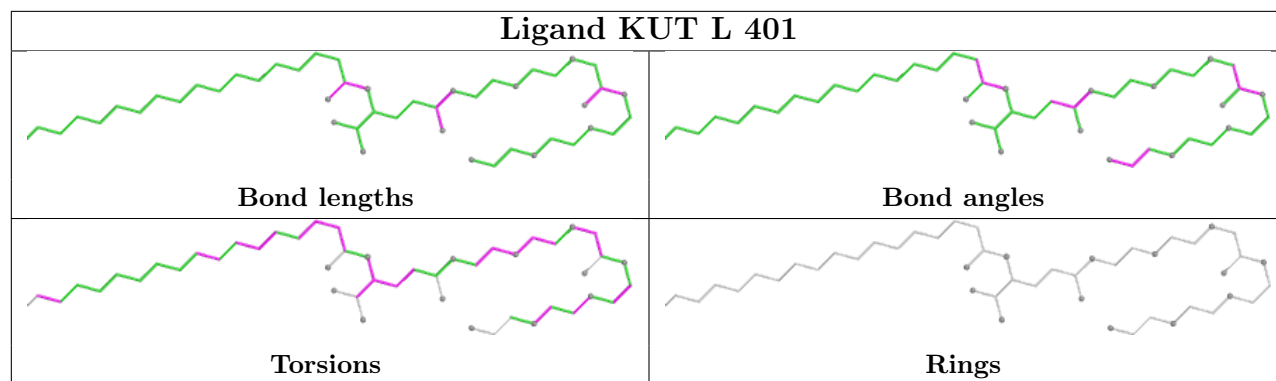
Mol	Chain	Res	Type	Atoms
7	L	401	KUT	O5-C26-C27-N2
7	L	401	KUT	C13-C14-C15-C16
7	L	401	KUT	C18-C19-C20-C21
7	L	401	KUT	C6-C7-C8-C9
7	L	401	KUT	N-C18-C34-O10
7	L	401	KUT	N-C18-C34-O11
7	L	401	KUT	C22-C23-O4-C24
7	L	401	KUT	C11-C12-C13-C14
7	L	401	KUT	N1-C22-C23-O4
7	L	401	KUT	C31-C30-O7-C29
7	L	401	KUT	C1-C-C10-C11
7	L	401	KUT	C34-C18-C19-C20
7	L	401	KUT	C27-C26-O5-C25
7	L	401	KUT	C34-C18-N-C17

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	401	KUT	18	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.