



Full wwPDB EM Validation Report ⓘ

Apr 26, 2026 – 12:21 AM JST

PDB ID : 9W0P / pdb_00009w0p
EMDB ID : EMD-65511
Title : CryoEM structure of T2R14 in complex with chlorhexidine and heterotrimeric G protein complex
Authors : Tan, Q.; Yu, Y.; Han, X.; Zhao, Q.; Wu, B.
Deposited on : 2025-07-24
Resolution : 3.60 Å(reported)
Based on initial model : 4NXW

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

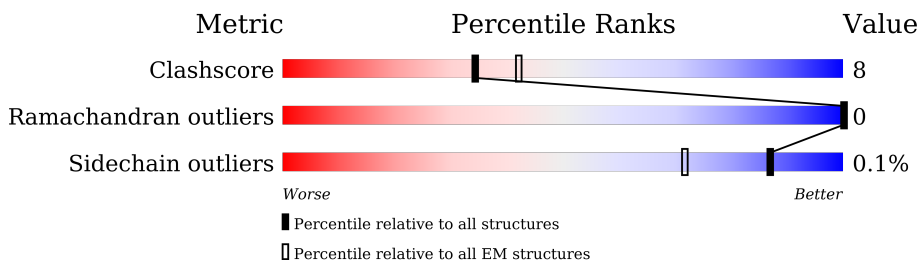
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	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	354	
2	B	351	
3	C	71	
4	R	483	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6721 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) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	215	Total	C	N	O	S	0	0
			1665	1061	282	310	12		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	202	THR	GLY	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- 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
			2501	1552	447	482	20		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	54	Total	C	N	O	S	0	0
			381	241	66	71	3		

- Molecule 4 is a protein called Soluble cytochrome b562,Taste receptor type 2 member 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	282	Total	C	N	O	S	0	0
			2140	1429	351	349	11		

There are 63 discrepancies between the modelled and reference sequences:

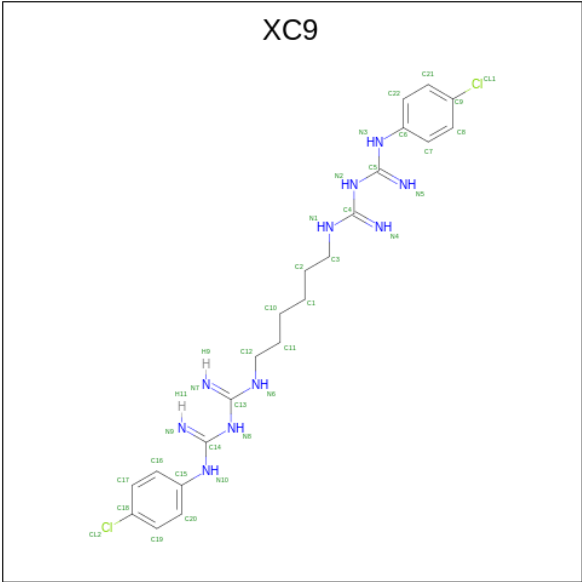
Chain	Residue	Modelled	Actual	Comment	Reference
R	-127	MET	-	initiating methionine	UNP P0ABE7
R	-126	LYS	-	expression tag	UNP P0ABE7
R	-125	THR	-	expression tag	UNP P0ABE7
R	-124	ILE	-	expression tag	UNP P0ABE7
R	-123	ILE	-	expression tag	UNP P0ABE7
R	-122	ALA	-	expression tag	UNP P0ABE7
R	-121	LEU	-	expression tag	UNP P0ABE7
R	-120	SER	-	expression tag	UNP P0ABE7
R	-119	TYR	-	expression tag	UNP P0ABE7
R	-118	ILE	-	expression tag	UNP P0ABE7
R	-117	PHE	-	expression tag	UNP P0ABE7
R	-116	CYS	-	expression tag	UNP P0ABE7
R	-115	LEU	-	expression tag	UNP P0ABE7
R	-114	VAL	-	expression tag	UNP P0ABE7
R	-113	PHE	-	expression tag	UNP P0ABE7
R	-112	ALA	-	expression tag	UNP P0ABE7
R	-111	ASP	-	expression tag	UNP P0ABE7
R	-110	TYR	-	expression tag	UNP P0ABE7
R	-109	LYS	-	expression tag	UNP P0ABE7
R	-108	ASP	-	expression tag	UNP P0ABE7
R	-107	ASP	-	expression tag	UNP P0ABE7
R	-106	ASP	-	expression tag	UNP P0ABE7
R	-99	TRP	MET	conflict	UNP P0ABE7
R	-4	ILE	HIS	conflict	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	0	LEU	ARG	conflict	UNP P0ABE7
R	318	GLU	-	expression tag	UNP Q9NYV8
R	319	PHE	-	expression tag	UNP Q9NYV8
R	320	LEU	-	expression tag	UNP Q9NYV8
R	321	GLU	-	expression tag	UNP Q9NYV8
R	322	VAL	-	expression tag	UNP Q9NYV8
R	323	LEU	-	expression tag	UNP Q9NYV8
R	324	PHE	-	expression tag	UNP Q9NYV8
R	325	GLN	-	expression tag	UNP Q9NYV8
R	326	GLY	-	expression tag	UNP Q9NYV8
R	327	PRO	-	expression tag	UNP Q9NYV8
R	328	TRP	-	expression tag	UNP Q9NYV8
R	329	SER	-	expression tag	UNP Q9NYV8
R	330	HIS	-	expression tag	UNP Q9NYV8
R	331	PRO	-	expression tag	UNP Q9NYV8
R	332	GLN	-	expression tag	UNP Q9NYV8
R	333	PHE	-	expression tag	UNP Q9NYV8
R	334	GLU	-	expression tag	UNP Q9NYV8
R	335	LYS	-	expression tag	UNP Q9NYV8
R	336	GLY	-	expression tag	UNP Q9NYV8
R	337	GLY	-	expression tag	UNP Q9NYV8
R	338	GLY	-	expression tag	UNP Q9NYV8
R	339	SER	-	expression tag	UNP Q9NYV8
R	340	GLY	-	expression tag	UNP Q9NYV8
R	341	GLY	-	expression tag	UNP Q9NYV8
R	342	GLY	-	expression tag	UNP Q9NYV8
R	343	SER	-	expression tag	UNP Q9NYV8
R	344	GLY	-	expression tag	UNP Q9NYV8
R	345	GLY	-	expression tag	UNP Q9NYV8
R	346	SER	-	expression tag	UNP Q9NYV8
R	347	ALA	-	expression tag	UNP Q9NYV8
R	348	TRP	-	expression tag	UNP Q9NYV8
R	349	SER	-	expression tag	UNP Q9NYV8
R	350	HIS	-	expression tag	UNP Q9NYV8
R	351	PRO	-	expression tag	UNP Q9NYV8
R	352	GLN	-	expression tag	UNP Q9NYV8
R	353	PHE	-	expression tag	UNP Q9NYV8
R	354	GLU	-	expression tag	UNP Q9NYV8
R	355	LYS	-	expression tag	UNP Q9NYV8

- Molecule 5 is 1-[6-[azanylidene-[[azanylidene-[[[(4-chlorophenyl)amino]methyl]-\$1^{\{4\}}\$-azanyl]methyl]-\$1^{\{4\}}\$-azanyl]hexyl]-3-[{N}-(4-chlorophenyl)carbamidoyl]guanidine (CCD ID: XC9) (formula: C₂₂H₃₀Cl₂N₁₀) (labeled as "Ligand of Interest" by depositor).

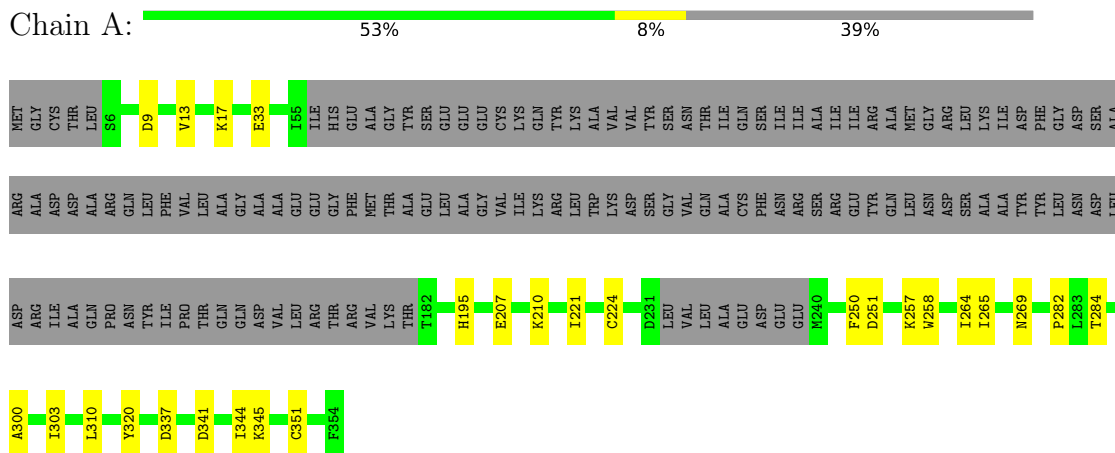


Mol	Chain	Residues	Atoms				AltConf
			Total	C	Cl	N	
5	R	1	34	22	2	10	0

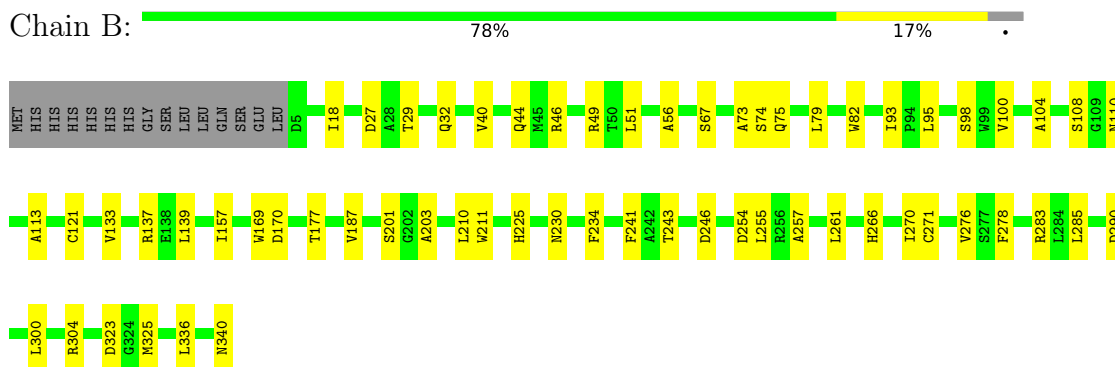
3 Residue-property plots [i](#)

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.

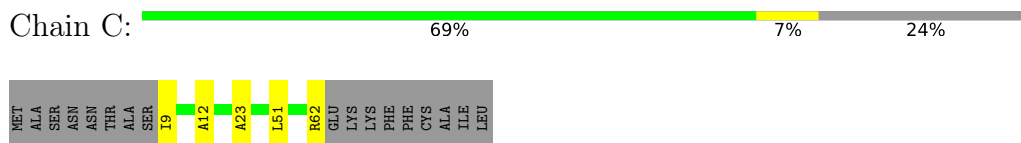
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



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



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: Soluble cytochrome b562, Taste receptor type 2 member 14





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2067338	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: XC9

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	0.09	0/1693	0.25	0/2281
2	B	0.06	0/2548	0.20	0/3466
3	C	0.13	0/387	0.24	0/530
4	R	0.15	0/2189	0.48	1/2976 (0.0%)
All	All	0.11	0/6817	0.33	1/9253 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	76	PHE	CA-C-O	-5.14	116.22	122.64

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	1665	0	1607	17	0
2	B	2501	0	2362	39	0
3	C	381	0	360	4	0
4	R	2140	0	2140	53	0
5	R	34	0	0	1	0
All	All	6721	0	6469	107	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 (107) 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)
4:R:55:ARG:NE	4:R:96:SER:OG	2.24	0.71
1:A:224:CYS:SG	1:A:269:ASN:ND2	2.63	0.71
4:R:231:LYS:HA	4:R:234:ILE:HG12	1.72	0.70
4:R:27:ILE:HG23	4:R:286:LYS:HE3	1.77	0.67
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.75	0.67
4:R:149:ASN:O	4:R:153:ASN:ND2	2.27	0.66
1:A:341:ASP:HB2	4:R:212:MET:HE1	1.78	0.65
4:R:289:GLN:HA	4:R:292:LEU:HG	1.80	0.63
2:B:325:MET:O	2:B:340:ASN:ND2	2.32	0.62
4:R:108:PHE:HA	4:R:201:LEU:HD12	1.82	0.61
2:B:108:SER:OG	2:B:110:ASN:ND2	2.35	0.60
2:B:234:PHE:HD1	2:B:241:PHE:HB3	1.65	0.60
1:A:320:TYR:OH	1:A:341:ASP:OD2	2.18	0.59
2:B:187:VAL:HA	2:B:203:ALA:HA	1.85	0.58
4:R:198:PHE:HZ	4:R:233:VAL:HG12	1.69	0.57
4:R:276:HIS:CD2	4:R:280:LEU:HD13	2.40	0.57
4:R:55:ARG:HH11	4:R:273:PRO:HA	1.71	0.56
2:B:121:CYS:HB3	2:B:139:LEU:HB2	1.87	0.56
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.86	0.56
4:R:228:ARG:HA	4:R:231:LYS:HE3	1.86	0.55
4:R:16:GLU:HB2	4:R:270:MET:HE1	1.88	0.55
2:B:29:THR:OG1	2:B:32:GLN:OE1	2.22	0.55
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.32	0.55
2:B:283:ARG:HG2	3:C:51:LEU:HD11	1.89	0.55
4:R:211:LYS:HG3	4:R:212:MET:HG3	1.88	0.55
1:A:250:PHE:HE1	1:A:264:ILE:HG21	1.72	0.55
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.89	0.54
1:A:13:VAL:O	1:A:17:LYS:HG2	2.08	0.53
2:B:44:GLN:OE1	2:B:46:ARG:NH1	2.41	0.53
4:R:229:GLY:O	4:R:233:VAL:HG23	2.09	0.53
4:R:91:VAL:HA	4:R:141:LEU:HD11	1.90	0.52
4:R:78:THR:HG22	4:R:79:GLU:N	2.25	0.52
4:R:174:ARG:O	4:R:177:SER:OG	2.25	0.52
2:B:278:PHE:HE1	2:B:285:LEU:HD13	1.74	0.51
4:R:94:HIS:CG	4:R:141:LEU:HD12	2.45	0.51
1:A:251:ASP:HB2	1:A:310:LEU:HD11	1.93	0.51
4:R:94:HIS:NE2	4:R:137:THR:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:HD11	4:R:113:ASN:HD21	1.77	0.50
2:B:18:ILE:HD11	3:C:23:ALA:HA	1.94	0.50
2:B:73:ALA:HB2	2:B:79:LEU:HD12	1.93	0.50
2:B:95:LEU:HD13	2:B:100:VAL:HG11	1.94	0.49
4:R:270:MET:O	4:R:273:PRO:HD2	2.12	0.49
2:B:104:ALA:HB3	2:B:113:ALA:HB3	1.94	0.49
1:A:300:ALA:O	1:A:303:ILE:HG22	2.12	0.49
4:R:286:LYS:HA	4:R:289:GLN:NE2	2.28	0.48
2:B:157:ILE:HG23	2:B:169:TRP:HB2	1.95	0.48
2:B:201:SER:OG	2:B:211:TRP:NE1	2.46	0.48
4:R:55:ARG:HD2	4:R:273:PRO:HB3	1.96	0.48
1:A:345:LYS:HD2	1:A:345:LYS:HA	1.71	0.47
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.47	0.47
4:R:268:MET:HE3	4:R:268:MET:O	2.15	0.47
1:A:9:ASP:N	1:A:9:ASP:OD1	2.46	0.47
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.97	0.47
2:B:170:ASP:OD2	2:B:177:THR:OG1	2.32	0.46
2:B:27:ASP:N	2:B:27:ASP:OD1	2.48	0.46
4:R:55:ARG:HE	4:R:96:SER:HG	1.56	0.46
2:B:49:ARG:HH12	3:C:62:ARG:HB2	1.81	0.45
2:B:79:LEU:HB3	2:B:93:ILE:HB	1.97	0.45
4:R:31:ASN:ND2	4:R:49:THR:OG1	2.43	0.45
4:R:79:GLU:HB2	4:R:156:ILE:HG21	1.98	0.45
4:R:16:GLU:HA	4:R:19:ILE:HG22	1.96	0.45
4:R:202:ILE:HD13	4:R:234:ILE:HG21	1.99	0.45
2:B:323:ASP:OD1	2:B:323:ASP:N	2.50	0.45
4:R:116:ASN:HB3	4:R:120:LEU:HD23	1.98	0.45
1:A:257:LYS:HE2	1:A:258:TRP:CZ2	2.51	0.45
2:B:266:HIS:CD2	2:B:304:ARG:HH22	2.35	0.45
1:A:351:CYS:SG	4:R:110:LYS:NZ	2.74	0.45
2:B:79:LEU:HD23	2:B:93:ILE:HD12	1.99	0.45
1:A:207:GLU:HB3	1:A:210:LYS:HG2	1.97	0.44
2:B:75:GLN:O	2:B:98:SER:OG	2.35	0.44
4:R:236:PHE:HA	4:R:279:VAL:HG21	1.99	0.44
4:R:94:HIS:ND1	4:R:141:LEU:HD12	2.33	0.44
4:R:216:VAL:HG12	4:R:217:LYS:H	1.82	0.44
2:B:254:ASP:HB3	2:B:257:ALA:HB3	2.00	0.44
4:R:117:SER:C	4:R:119:PHE:H	2.26	0.44
4:R:62:ILE:HG21	4:R:270:MET:HG2	2.00	0.43
2:B:40:VAL:HG23	2:B:283:ARG:HH21	1.82	0.43
4:R:98:TRP:CZ2	4:R:190:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:178:LEU:HD12	4:R:179:ILE:N	2.34	0.43
4:R:78:THR:HG22	4:R:79:GLU:H	1.84	0.43
4:R:276:HIS:HD2	4:R:280:LEU:HD13	1.84	0.43
4:R:262:ILE:O	4:R:266:GLN:HG3	2.18	0.43
2:B:283:ARG:HH12	2:B:300:LEU:HD22	1.84	0.42
1:A:221:ILE:O	1:A:265:ILE:N	2.39	0.42
4:R:98:TRP:HA	4:R:101:THR:HG22	2.00	0.42
1:A:282:PRO:HB2	1:A:284:THR:HG22	2.01	0.42
4:R:53:ILE:HA	4:R:56:ILE:HG22	2.00	0.42
4:R:216:VAL:HG12	4:R:217:LYS:N	2.34	0.42
1:A:337:ASP:HB3	4:R:212:MET:HE3	2.00	0.42
2:B:270:ILE:HD12	2:B:270:ILE:HA	1.94	0.42
4:R:42:SER:OG	4:R:43:SER:N	2.53	0.42
4:R:212:MET:HB3	4:R:216:VAL:HG23	2.02	0.42
2:B:51:LEU:HB3	2:B:82:TRP:CE3	2.54	0.42
5:R:401:XC9:N4	5:R:401:XC9:C6	2.83	0.42
2:B:67:SER:O	2:B:67:SER:OG	2.36	0.41
4:R:204:SER:HA	4:R:207:LYS:NZ	2.35	0.41
2:B:137:ARG:HD3	2:B:137:ARG:HA	1.93	0.41
4:R:175:PHE:O	4:R:179:ILE:HG22	2.21	0.41
4:R:198:PHE:CZ	4:R:233:VAL:HG12	2.51	0.41
2:B:276:VAL:HG13	2:B:285:LEU:HD11	2.02	0.41
1:A:33:GLU:CD	1:A:195:HIS:HD1	2.29	0.41
2:B:56:ALA:HB3	2:B:74:SER:HB2	2.02	0.41
4:R:41:ILE:HD13	4:R:41:ILE:HA	1.92	0.40
3:C:9:ILE:HG23	3:C:12:ALA:H	1.87	0.40
4:R:16:GLU:CB	4:R:270:MET:HE1	2.51	0.40
4:R:55:ARG:HA	4:R:55:ARG:HD3	1.72	0.40
2:B:93:ILE:HG12	2:B:133:VAL:HG11	2.04	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 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	209/354 (59%)	206 (99%)	3 (1%)	0	100	100
2	B	334/351 (95%)	326 (98%)	8 (2%)	0	100	100
3	C	52/71 (73%)	52 (100%)	0	0	100	100
4	R	278/483 (58%)	263 (95%)	15 (5%)	0	100	100
All	All	873/1259 (69%)	847 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	174/306 (57%)	174 (100%)	0	100	100
2	B	258/293 (88%)	258 (100%)	0	100	100
3	C	35/58 (60%)	35 (100%)	0	100	100
4	R	218/421 (52%)	217 (100%)	1 (0%)	81	80
All	All	685/1078 (64%)	684 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	76	PHE

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	35	ASN
2	B	110	ASN

5.3.3 RNA ⓘ

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	$\# Z > 2$
5	XC9	R	401	-	29,35,35	3.19	10 (34%)	42,44,44	1.37	5 (11%)

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
5	XC9	R	401	-	-	9/27/27/27	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	401	XC9	C5-N3	8.36	1.48	1.37
5	R	401	XC9	C14-N10	7.91	1.47	1.37
5	R	401	XC9	C4-N4	6.11	1.46	1.29
5	R	401	XC9	C13-N7	6.07	1.46	1.29
5	R	401	XC9	C5-N5	5.76	1.45	1.29
5	R	401	XC9	C14-N9	5.38	1.44	1.29
5	R	401	XC9	C15-N10	2.71	1.47	1.41
5	R	401	XC9	C6-N3	2.23	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	401	XC9	C9-CL1	2.03	1.78	1.74
5	R	401	XC9	C18-CL2	2.00	1.78	1.74

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	401	XC9	C5-N2-C4	5.91	135.62	125.27
5	R	401	XC9	C15-N10-C14	-2.44	119.77	126.57
5	R	401	XC9	C12-N6-C13	-2.07	119.73	123.50
5	R	401	XC9	N1-C4-N4	-2.03	116.45	120.26
5	R	401	XC9	N3-C5-N5	-2.01	114.67	121.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	401	XC9	C1-C2-C3-N1
5	R	401	XC9	C10-C1-C2-C3
5	R	401	XC9	C10-C11-C12-N6
5	R	401	XC9	C1-C10-C11-C12
5	R	401	XC9	C2-C1-C10-C11
5	R	401	XC9	C7-C6-N3-C5
5	R	401	XC9	C22-C6-N3-C5
5	R	401	XC9	C16-C15-N10-C14
5	R	401	XC9	C20-C15-N10-C14

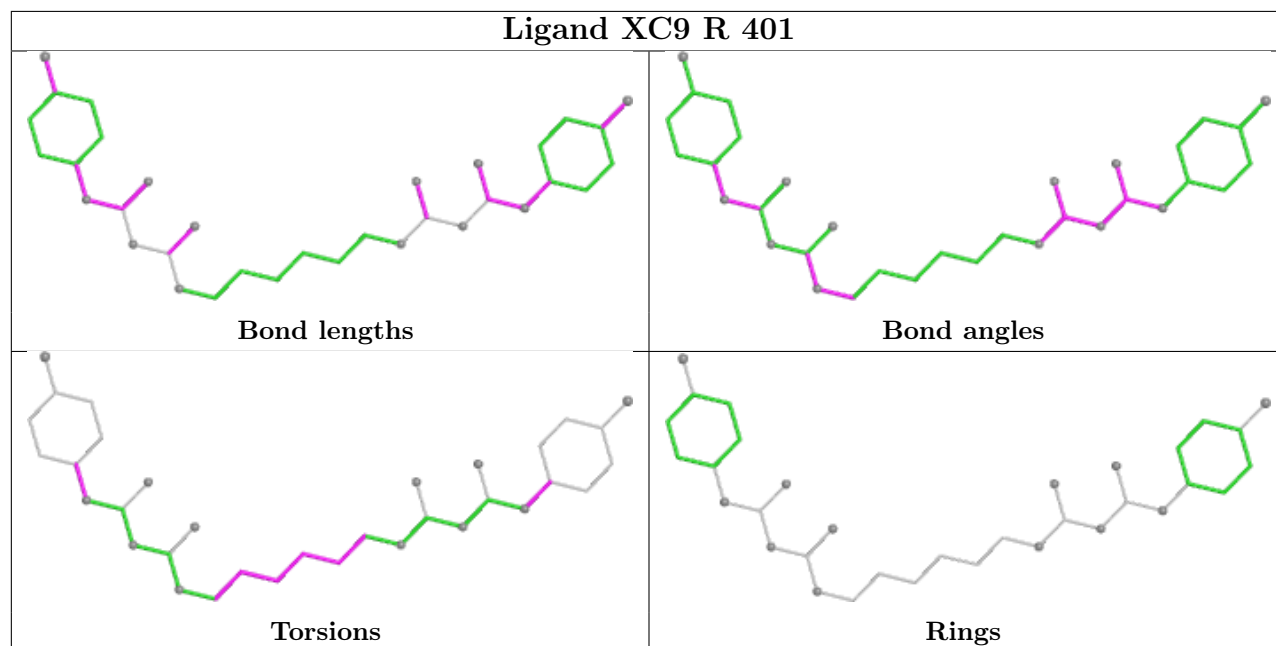
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	401	XC9	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.