



Full wwPDB EM Validation Report ⓘ

Apr 26, 2026 – 12:20 AM JST

PDB ID : 9W0S / pdb_00009w0s
EMDB ID : EMD-65514
Title : CryoEM structure of T2R46 in complex with Artemisinin and heterotrimeric G protein complex
Authors : Tan, Q.; Yu, Y.; Han, X.; Zhao, Q.; Wu, B.
Deposited on : 2025-07-24
Resolution : 3.30 Å(reported)
Based on initial model : 7x9a

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

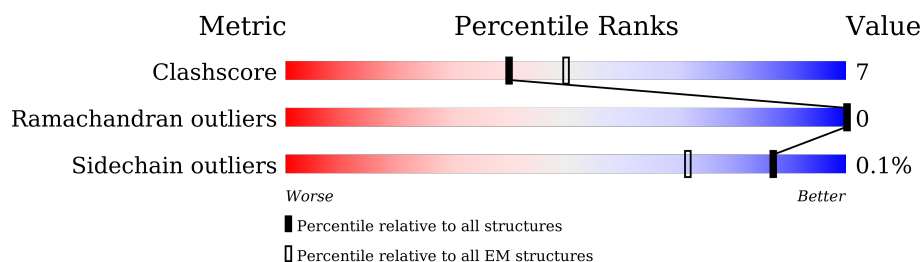
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	363	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6650 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	217	Total	C	N	O	S	0	0
			1680	1074	289	305	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ASP	GLU	engineered mutation	UNP P63096
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
			2461	1531	436	474	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP P62873
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
			371	237	65	66	3		

- Molecule 4 is a protein called Taste receptor type 2 member 46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	279	Total	C	N	O	S	0	0
			2118	1417	345	348	8		

There are 60 discrepancies between the modelled and reference sequences:

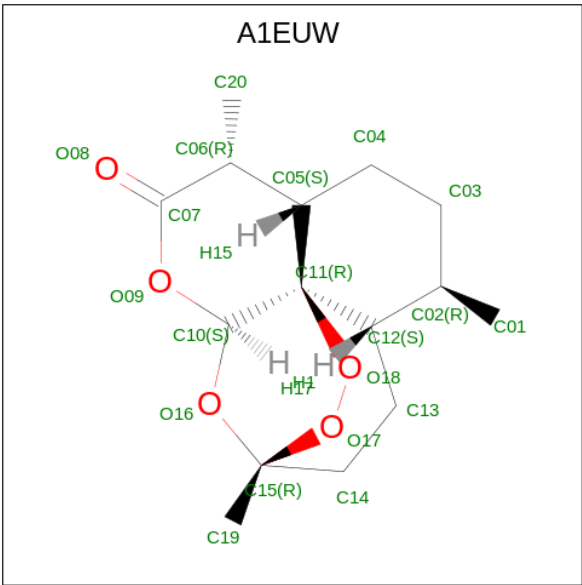
Chain	Residue	Modelled	Actual	Comment	Reference
R	-21	MET	-	initiating methionine	UNP P59540
R	-20	LYS	-	expression tag	UNP P59540
R	-19	THR	-	expression tag	UNP P59540
R	-18	ILE	-	expression tag	UNP P59540
R	-17	ILE	-	expression tag	UNP P59540
R	-16	ALA	-	expression tag	UNP P59540
R	-15	LEU	-	expression tag	UNP P59540
R	-14	SER	-	expression tag	UNP P59540
R	-13	TYR	-	expression tag	UNP P59540
R	-12	ILE	-	expression tag	UNP P59540
R	-11	PHE	-	expression tag	UNP P59540
R	-10	CYS	-	expression tag	UNP P59540
R	-9	LEU	-	expression tag	UNP P59540
R	-8	VAL	-	expression tag	UNP P59540
R	-7	PHE	-	expression tag	UNP P59540
R	-6	ALA	-	expression tag	UNP P59540
R	-5	ASP	-	expression tag	UNP P59540
R	-4	TYR	-	expression tag	UNP P59540
R	-3	LYS	-	expression tag	UNP P59540
R	-2	ASP	-	expression tag	UNP P59540
R	-1	ASP	-	expression tag	UNP P59540
R	0	ASP	-	expression tag	UNP P59540
R	63	LEU	VAL	conflict	UNP P59540

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Chain	Residue	Modelled	Actual	Comment	Reference
R	305	PHE	-	expression tag	UNP P59540
R	306	LEU	-	expression tag	UNP P59540
R	307	GLU	-	expression tag	UNP P59540
R	308	VAL	-	expression tag	UNP P59540
R	309	LEU	-	expression tag	UNP P59540
R	310	PHE	-	expression tag	UNP P59540
R	311	GLN	-	expression tag	UNP P59540
R	312	GLY	-	expression tag	UNP P59540
R	313	PRO	-	expression tag	UNP P59540
R	314	TRP	-	expression tag	UNP P59540
R	315	SER	-	expression tag	UNP P59540
R	316	HIS	-	expression tag	UNP P59540
R	317	PRO	-	expression tag	UNP P59540
R	318	GLN	-	expression tag	UNP P59540
R	319	PHE	-	expression tag	UNP P59540
R	320	GLU	-	expression tag	UNP P59540
R	321	LYS	-	expression tag	UNP P59540
R	322	GLY	-	expression tag	UNP P59540
R	323	GLY	-	expression tag	UNP P59540
R	324	GLY	-	expression tag	UNP P59540
R	325	SER	-	expression tag	UNP P59540
R	326	GLY	-	expression tag	UNP P59540
R	327	GLY	-	expression tag	UNP P59540
R	328	GLY	-	expression tag	UNP P59540
R	329	SER	-	expression tag	UNP P59540
R	330	GLY	-	expression tag	UNP P59540
R	331	GLY	-	expression tag	UNP P59540
R	332	SER	-	expression tag	UNP P59540
R	333	ALA	-	expression tag	UNP P59540
R	334	TRP	-	expression tag	UNP P59540
R	335	SER	-	expression tag	UNP P59540
R	336	HIS	-	expression tag	UNP P59540
R	337	PRO	-	expression tag	UNP P59540
R	338	GLN	-	expression tag	UNP P59540
R	339	PHE	-	expression tag	UNP P59540
R	340	GLU	-	expression tag	UNP P59540
R	341	LYS	-	expression tag	UNP P59540

- Molecule 5 is Artemisinin (CCD ID: A1EUW) (formula: $C_{15}H_{22}O_5$).

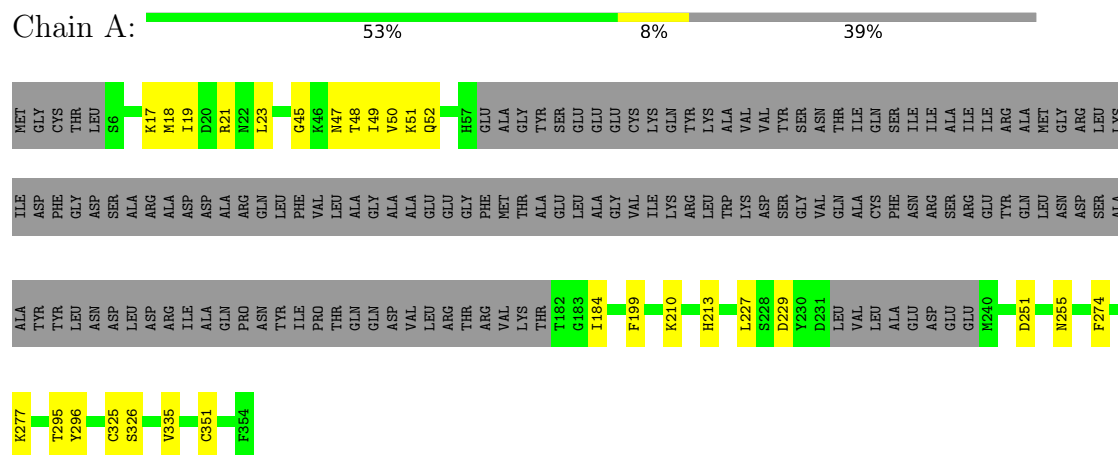


Mol	Chain	Residues	Atoms			AltConf
5	R	1	Total	C	O	0
			20	15	5	

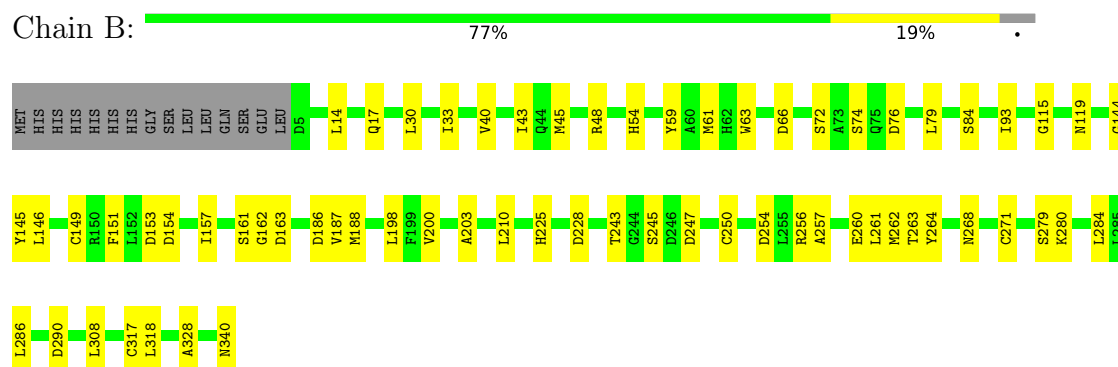
3 Residue-property plots [i](#)

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.

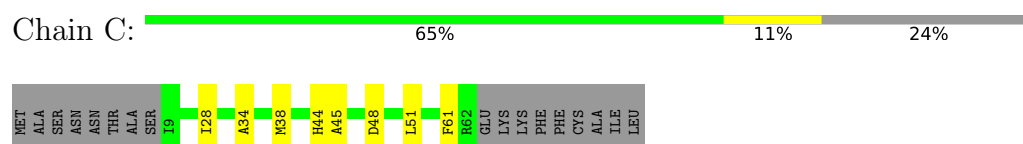
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



- 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: Taste receptor type 2 member 46





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1026223	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: A1EUW

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	0.10	0/1710	0.31	0/2305
2	B	0.07	0/2508	0.22	0/3417
3	C	0.13	0/377	0.28	0/517
4	R	0.12	0/2172	0.33	0/2975
All	All	0.10	0/6767	0.28	0/9214

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1680	0	1627	19	0
2	B	2461	0	2298	39	0
3	C	371	0	350	7	0
4	R	2118	0	2107	34	0
5	R	20	0	0	0	0
All	All	6650	0	6382	93	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 (93) 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)
2:B:286:LEU:HB3	2:B:318:LEU:HD21	1.71	0.73
1:A:47:ASN:HA	1:A:51:LYS:HB2	1.72	0.72
1:A:184:ILE:HD11	1:A:199:PHE:HB3	1.75	0.69
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.75	0.69
2:B:119:ASN:ND2	2:B:144:GLY:O	2.27	0.67
2:B:145:TYR:OH	2:B:188:MET:SD	2.56	0.63
4:R:41:ILE:HD12	4:R:45:ASP:HB3	1.79	0.63
4:R:291:LEU:HD13	4:R:294:LEU:HD21	1.80	0.62
1:A:229:ASP:O	1:A:277:LYS:NZ	2.32	0.62
2:B:79:LEU:HD23	2:B:93:ILE:HD13	1.81	0.62
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.82	0.61
2:B:151:PHE:HE1	2:B:157:ILE:HD12	1.65	0.60
1:A:227:LEU:HB3	1:A:274:PHE:HB2	1.84	0.60
4:R:90:VAL:HG23	4:R:140:LEU:HD21	1.84	0.59
3:C:34:ALA:O	3:C:38:MET:HG3	2.03	0.59
2:B:30:LEU:HD13	3:C:34:ALA:HB1	1.84	0.58
2:B:115:GLY:HA3	2:B:146:LEU:HD23	1.86	0.57
2:B:84:SER:HB3	3:C:61:PHE:HE1	1.70	0.56
2:B:161:SER:OG	2:B:163:ASP:OD1	2.23	0.55
2:B:245:SER:OG	2:B:247:ASP:OD1	2.21	0.55
2:B:54:HIS:NE2	2:B:72:SER:OG	2.34	0.54
2:B:40:VAL:HG22	2:B:43:ILE:HD11	1.89	0.53
4:R:173:TYR:O	4:R:177:THR:OG1	2.26	0.53
2:B:145:TYR:O	2:B:162:GLY:N	2.41	0.53
1:A:19:ILE:O	1:A:23:LEU:HG	2.08	0.52
3:C:44:HIS:O	3:C:48:ASP:HB2	2.09	0.52
4:R:192:LEU:HD12	4:R:235:LEU:HD11	1.92	0.52
1:A:49:ILE:HG23	1:A:50:VAL:H	1.75	0.51
4:R:35:TRP:CZ3	4:R:41:ILE:HG12	2.46	0.50
1:A:49:ILE:HG13	1:A:335:VAL:HG21	1.93	0.50
2:B:48:ARG:HG3	2:B:340:ASN:HB3	1.94	0.50
3:C:45:ALA:HB1	3:C:51:LEU:HG	1.93	0.50
1:A:325:CYS:SG	1:A:326:SER:N	2.84	0.50
4:R:137:LEU:HD13	4:R:140:LEU:HD23	1.94	0.50
2:B:256:ARG:HB3	3:C:28:ILE:HG12	1.94	0.49
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.45	0.49
2:B:43:ILE:HD12	2:B:43:ILE:H	1.78	0.49
2:B:198:LEU:HD12	2:B:210:LEU:HD21	1.94	0.49
4:R:68:ALA:HB1	4:R:75:PHE:CG	2.48	0.49
1:A:47:ASN:HB2	1:A:52:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:NZ	2:B:228:ASP:OD2	2.39	0.48
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.31	0.48
4:R:195:PHE:CE2	4:R:234:PHE:HD2	2.33	0.47
4:R:252:PHE:CG	4:R:253:GLU:N	2.83	0.47
3:C:45:ALA:HA	3:C:48:ASP:HB2	1.96	0.46
4:R:276:PRO:O	4:R:280:ILE:HG12	2.16	0.46
4:R:248:SER:O	4:R:252:PHE:N	2.46	0.46
2:B:261:LEU:HB3	2:B:262:MET:HE3	1.99	0.45
4:R:77:SER:HB3	4:R:80:VAL:HG22	1.97	0.45
4:R:15:VAL:HA	4:R:18:VAL:HG22	1.98	0.45
4:R:241:TYR:O	4:R:245:ILE:HG12	2.17	0.45
1:A:213:HIS:ND1	2:B:59:TYR:OH	2.40	0.45
1:A:277:LYS:HE2	1:A:277:LYS:HB3	1.67	0.45
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.39	0.45
2:B:200:VAL:HG12	2:B:210:LEU:HA	1.99	0.45
1:A:45:GLY:O	1:A:48:THR:OG1	2.21	0.44
2:B:66:ASP:OD1	2:B:66:ASP:N	2.48	0.44
4:R:83:THR:HA	4:R:86:ASN:ND2	2.32	0.44
4:R:119:LEU:HB3	4:R:123:ARG:HH12	1.82	0.44
2:B:254:ASP:HB3	2:B:257:ALA:HB3	1.98	0.44
4:R:176:ASN:OD1	4:R:177:THR:N	2.50	0.44
4:R:83:THR:HA	4:R:86:ASN:HD21	1.81	0.44
4:R:97:TRP:CE2	4:R:187:PRO:HG3	2.53	0.44
2:B:63:TRP:HE1	2:B:328:ALA:HB3	1.83	0.44
4:R:33:ILE:O	4:R:37:LYS:HG3	2.18	0.44
4:R:108:LEU:HD11	4:R:128:VAL:HG11	2.00	0.44
2:B:45:MET:HB2	2:B:308:LEU:HD11	2.00	0.44
2:B:149:CYS:HB2	2:B:157:ILE:HD11	2.00	0.44
4:R:107:LEU:HD22	4:R:194:SER:HA	2.00	0.44
1:A:17:LYS:HD2	1:A:17:LYS:HA	1.73	0.43
4:R:110:ILE:HG22	4:R:110:ILE:O	2.19	0.43
4:R:265:GLU:O	4:R:269:PHE:HD1	2.00	0.43
1:A:351:CYS:SG	4:R:109:LYS:HD2	2.57	0.43
2:B:186:ASP:OD1	2:B:186:ASP:N	2.52	0.43
1:A:49:ILE:HG23	1:A:50:VAL:N	2.34	0.43
4:R:51:LEU:HG	4:R:55:ARG:HE	1.84	0.42
4:R:128:VAL:O	4:R:132:ILE:HG12	2.19	0.42
2:B:61:MET:HG3	2:B:317:CYS:HB2	2.02	0.42
2:B:30:LEU:HD12	2:B:33:ILE:HB	2.02	0.41
2:B:74:SER:OG	2:B:76:ASP:OD1	2.28	0.41
2:B:187:VAL:HA	2:B:203:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:93:HIS:CD2	4:R:140:LEU:HD22	2.55	0.41
4:R:283:ASN:HB3	4:R:286:LEU:HB3	2.01	0.41
2:B:14:LEU:HA	2:B:17:GLN:HG2	2.01	0.41
2:B:153:ASP:OD1	2:B:154:ASP:N	2.42	0.41
1:A:18:MET:HE2	1:A:21:ARG:HH21	1.86	0.41
4:R:53:VAL:HA	4:R:56:VAL:HG12	2.03	0.41
4:R:124:ARG:H	4:R:124:ARG:HG2	1.75	0.41
2:B:279:SER:OG	2:B:280:LYS:N	2.54	0.41
1:A:295:THR:HG22	1:A:296:TYR:N	2.35	0.41
4:R:287:LYS:O	4:R:291:LEU:HD23	2.21	0.40
2:B:40:VAL:HG21	2:B:284:LEU:HD11	2.03	0.40
4:R:107:LEU:HA	4:R:198:LEU:HD12	2.03	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	211/354 (60%)	200 (95%)	11 (5%)	0	100	100
2	B	334/351 (95%)	326 (98%)	8 (2%)	0	100	100
3	C	52/71 (73%)	51 (98%)	1 (2%)	0	100	100
4	R	275/363 (76%)	262 (95%)	13 (5%)	0	100	100
All	All	872/1139 (77%)	839 (96%)	33 (4%)	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	249/293 (85%)	248 (100%)	1 (0%)	84	84
3	C	32/58 (55%)	32 (100%)	0	100	100
4	R	219/325 (67%)	219 (100%)	0	100	100
All	All	674/982 (69%)	673 (100%)	1 (0%)	87	90

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

Mol	Chain	Res	Type
2	B	268	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	HIS
3	C	18	GLN
3	C	44	HIS
4	R	24	ASN
4	R	93	HIS
4	R	96	ASN
4	R	257	ASN

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
5	A1EUW	R	401	-	23,23,23	5.62	9 (39%)	38,38,38	4.72	18 (47%)

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	A1EUW	R	401	-	-	-	0/5/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	401	A1EUW	O18-O17	-19.07	1.21	1.47
5	R	401	A1EUW	O18-C11	-13.09	1.29	1.46
5	R	401	A1EUW	O17-C15	-11.01	1.24	1.41
5	R	401	A1EUW	C11-C10	3.54	1.60	1.53
5	R	401	A1EUW	O16-C10	3.44	1.47	1.41
5	R	401	A1EUW	C14-C13	3.29	1.59	1.53
5	R	401	A1EUW	O16-C15	-3.07	1.38	1.44
5	R	401	A1EUW	C14-C15	2.69	1.59	1.53
5	R	401	A1EUW	C11-C12	-2.25	1.50	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	401	A1EUW	O18-O17-C15	14.05	120.88	108.55
5	R	401	A1EUW	O18-C11-C12	12.03	119.37	106.10
5	R	401	A1EUW	O18-C11-C10	-11.87	91.32	110.42
5	R	401	A1EUW	O17-O18-C11	9.83	120.12	111.67
5	R	401	A1EUW	C13-C12-C02	-7.85	103.45	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	401	A1EUW	C04-C05-C06	-5.66	105.19	114.12
5	R	401	A1EUW	O17-C15-C14	-5.18	108.02	112.44
5	R	401	A1EUW	O18-C11-C05	-3.94	99.43	104.45
5	R	401	A1EUW	C11-C05-C06	3.67	114.29	110.00
5	R	401	A1EUW	O16-C15-C14	3.64	114.50	110.14
5	R	401	A1EUW	C10-C11-C05	3.61	114.49	110.57
5	R	401	A1EUW	O09-C07-O08	3.50	123.57	118.47
5	R	401	A1EUW	O17-C15-C19	3.42	108.66	104.53
5	R	401	A1EUW	C19-C15-C14	-3.29	109.12	114.02
5	R	401	A1EUW	C20-C06-C05	-3.21	108.82	113.98
5	R	401	A1EUW	C20-C06-C07	-2.79	106.73	110.67
5	R	401	A1EUW	C01-C02-C12	-2.11	108.03	112.09
5	R	401	A1EUW	O16-C10-O09	-2.02	102.28	106.69

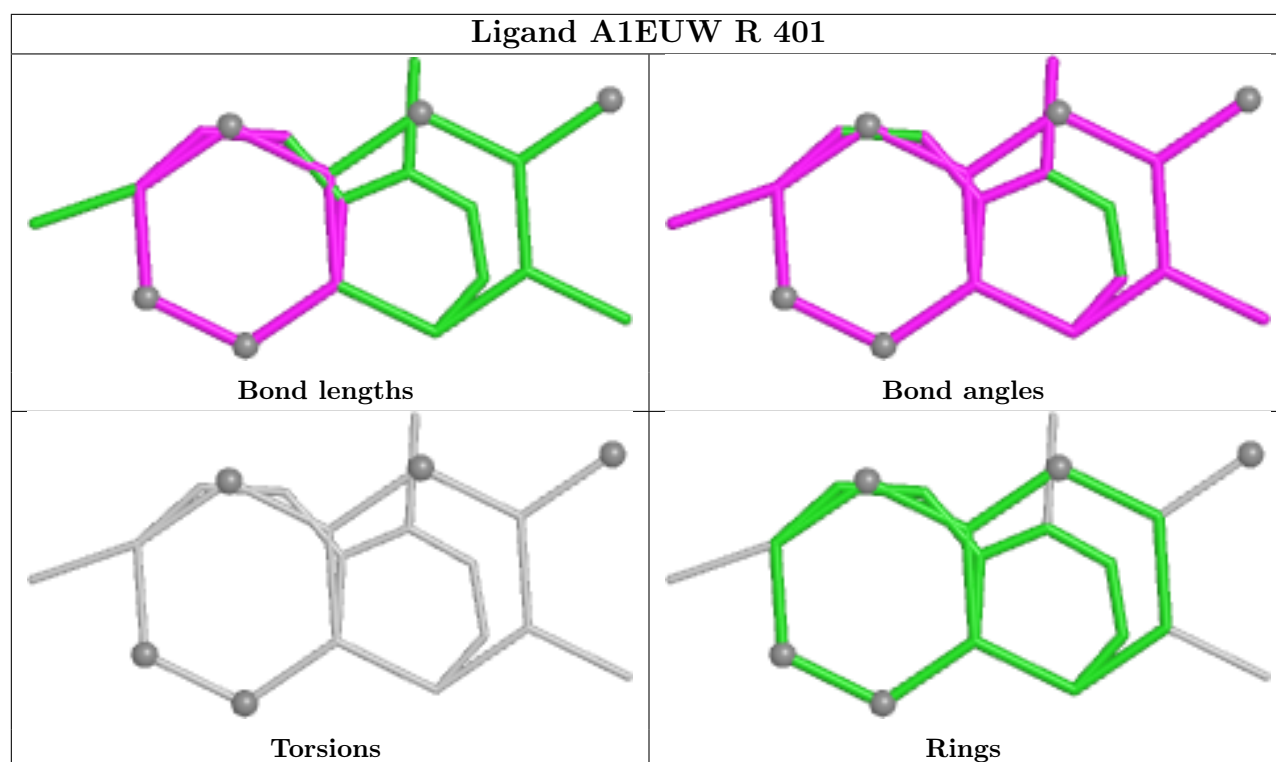
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.