



wwPDB EM Validation Summary Report ⓘ

Jul 9, 2025 – 02:05 PM JST

PDB ID : 8XQN / pdb_00008xqn
EMDB ID : EMD-38582
Title : Structure of human class T GPCR TAS2R14-DNGi complex with Aristolochic acid A.
Authors : Hu, X.L.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on : 2024-01-05
Resolution : 3.05 Å(reported)

This is a wwPDB EM Validation Summary 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 Phenix2.0rc1
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) : 2.44

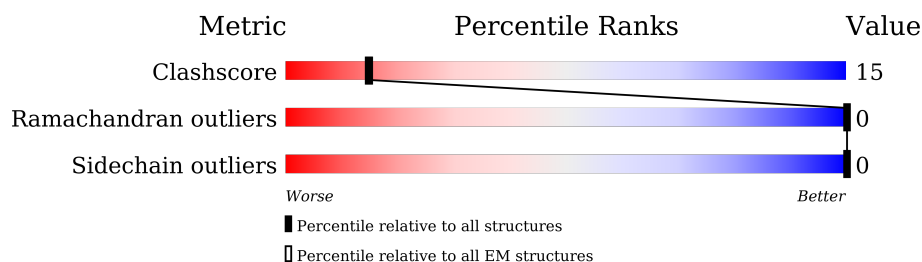
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

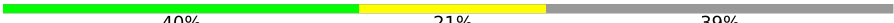




The reported resolution of this entry is 3.05 Å.

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	370	
2	B	366	
3	C	71	
4	S	286	
5	R	990	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8976 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	225	Total	C	N	O	S	0	0
			1813	1151	300	348	14		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P63096
A	-14	ASP	-	expression tag	UNP P63096
A	-13	TYR	-	expression tag	UNP P63096
A	-12	LYS	-	expression tag	UNP P63096
A	-11	ASP	-	expression tag	UNP P63096
A	-10	ASP	-	expression tag	UNP P63096
A	-9	ASP	-	expression tag	UNP P63096
A	-8	ASP	-	expression tag	UNP P63096
A	-7	LYS	-	expression tag	UNP P63096
A	-6	GLU	-	expression tag	UNP P63096
A	-5	ASN	-	expression tag	UNP P63096
A	-4	LEU	-	expression tag	UNP P63096
A	-3	TYR	-	expression tag	UNP P63096
A	-2	PHE	-	expression tag	UNP P63096
A	-1	GLN	-	expression tag	UNP P63096
A	0	SER	-	expression tag	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	326	SER	ALA	conflict	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	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	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	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	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	56	Total	C	N	O	S	0	0
			429	269	76	81	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	232	Total	C	N	O	S	0	0
			1783	1131	295	347	10		

- Molecule 5 is a protein called Exo-alpha-sialidase,Taste receptor type 2 member 14,LgBiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	284	Total	C	N	O	S	0	0
			2298	1548	373	366	11		

There are 50 discrepancies between the modelled and reference sequences:

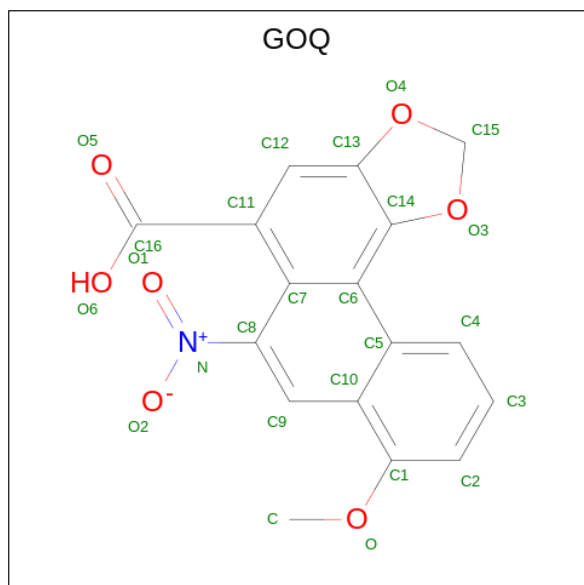
Chain	Residue	Modelled	Actual	Comment	Reference
R	-499	MET	-	initiating methionine	UNP Q59310
R	-498	LYS	-	expression tag	UNP Q59310
R	-497	THR	-	expression tag	UNP Q59310
R	-496	ILE	-	expression tag	UNP Q59310
R	-495	ILE	-	expression tag	UNP Q59310
R	-494	ALA	-	expression tag	UNP Q59310
R	-493	LEU	-	expression tag	UNP Q59310
R	-492	SER	-	expression tag	UNP Q59310
R	-491	TYR	-	expression tag	UNP Q59310
R	-490	ILE	-	expression tag	UNP Q59310
R	-489	PHE	-	expression tag	UNP Q59310
R	-488	CYS	-	expression tag	UNP Q59310
R	-487	LEU	-	expression tag	UNP Q59310
R	-486	VAL	-	expression tag	UNP Q59310
R	-485	PHE	-	expression tag	UNP Q59310
R	-484	ALA	-	expression tag	UNP Q59310
R	-483	ASP	-	expression tag	UNP Q59310
R	-482	TYR	-	expression tag	UNP Q59310
R	-481	LYS	-	expression tag	UNP Q59310
R	-480	ASP	-	expression tag	UNP Q59310
R	-479	ASP	-	expression tag	UNP Q59310
R	-478	ASP	-	expression tag	UNP Q59310
R	-477	ASP	-	expression tag	UNP Q59310
R	-476	ALA	-	expression tag	UNP Q59310
R	-475	HIS	-	expression tag	UNP Q59310
R	-474	HIS	-	expression tag	UNP Q59310
R	-473	HIS	-	expression tag	UNP Q59310
R	-472	HIS	-	expression tag	UNP Q59310
R	-471	HIS	-	expression tag	UNP Q59310
R	-470	HIS	-	expression tag	UNP Q59310
R	-469	HIS	-	expression tag	UNP Q59310
R	-468	HIS	-	expression tag	UNP Q59310
R	-467	HIS	-	expression tag	UNP Q59310
R	-466	HIS	-	expression tag	UNP Q59310
R	-465	GLU	-	expression tag	UNP Q59310
R	-464	ASN	-	expression tag	UNP Q59310
R	-463	LEU	-	expression tag	UNP Q59310

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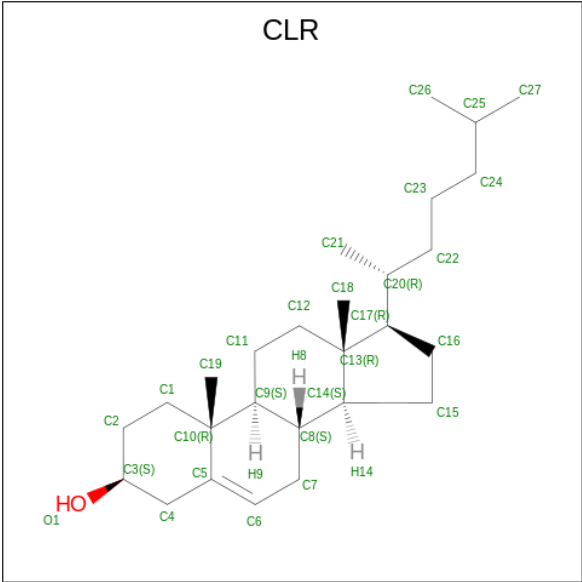
Chain	Residue	Modelled	Actual	Comment	Reference
R	-462	TYR	-	expression tag	UNP Q59310
R	-461	PHE	-	expression tag	UNP Q59310
R	-460	GLN	-	expression tag	UNP Q59310
R	-459	SER	-	expression tag	UNP Q59310
R	-458	GLY	-	expression tag	UNP Q59310
R	-457	ARG	-	expression tag	UNP Q59310
R	-456	ALA	-	expression tag	UNP Q59310
R	-305	SER	GLY	conflict	UNP Q59310
R	-3	GLY	-	linker	UNP Q59310
R	-2	SER	-	linker	UNP Q59310
R	-1	ALA	-	linker	UNP Q59310
R	0	GLY	-	linker	UNP Q59310
R	1	SER	-	linker	UNP Q59310

- Molecule 6 is 8-methoxy-6-nitro-naphtho[1,2-e][1,3]benzodioxole-5-carboxylic acid (CCD ID: GOQ) (formula: $C_{17}H_{11}NO_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			25	17	1	7	

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

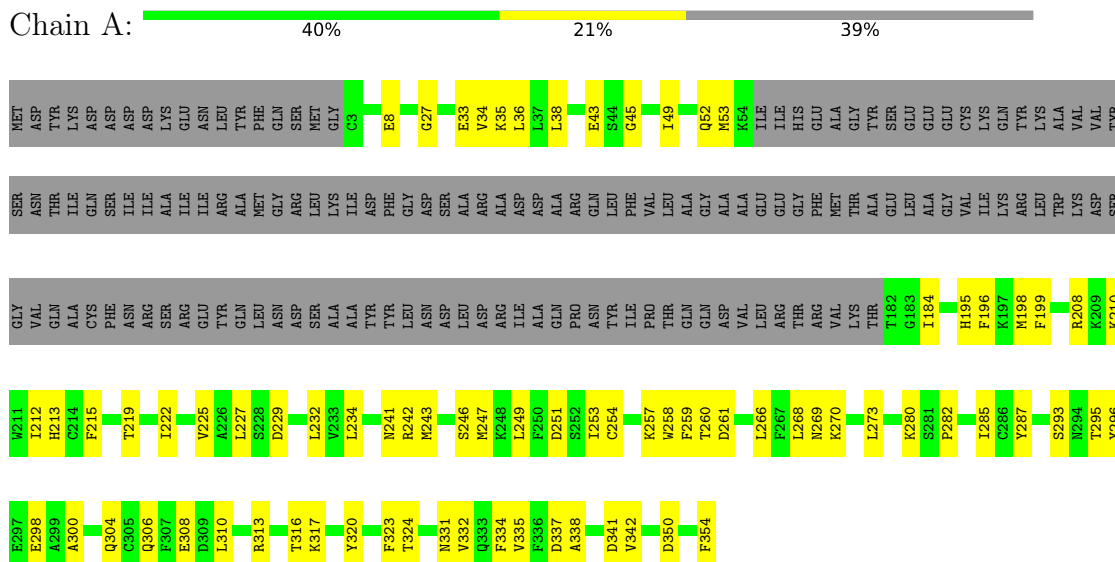


Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			28	27	1	

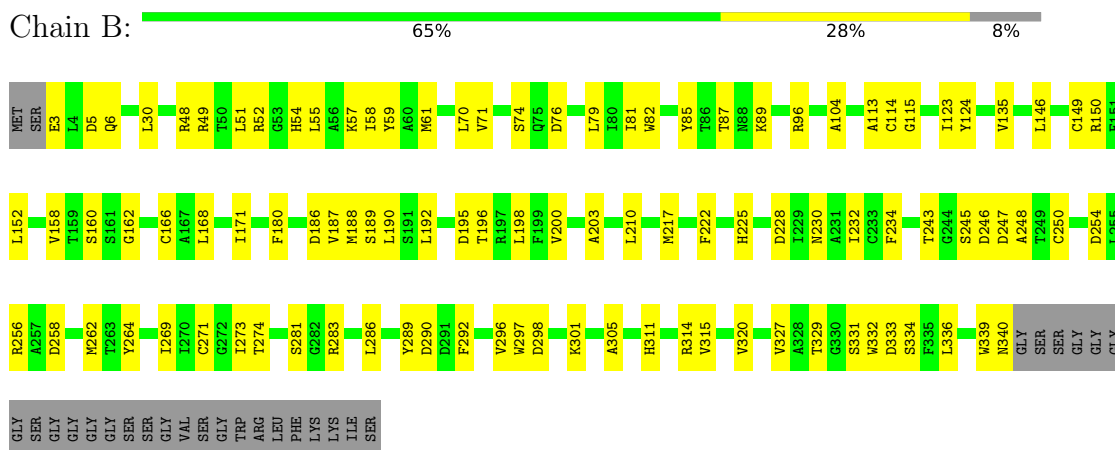
3 Residue-property plots [i](#)

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

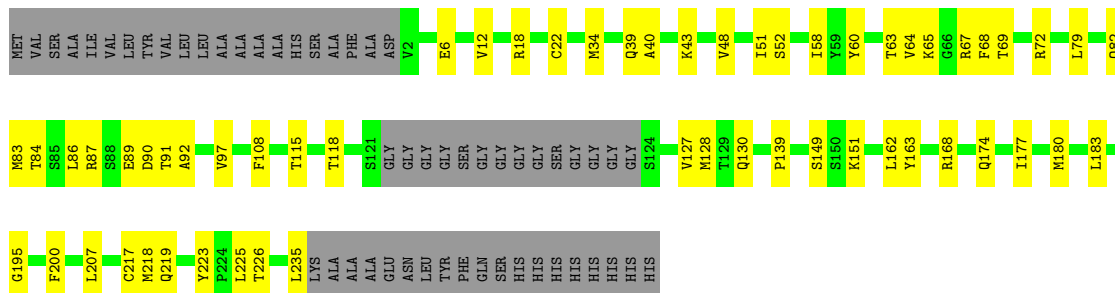


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



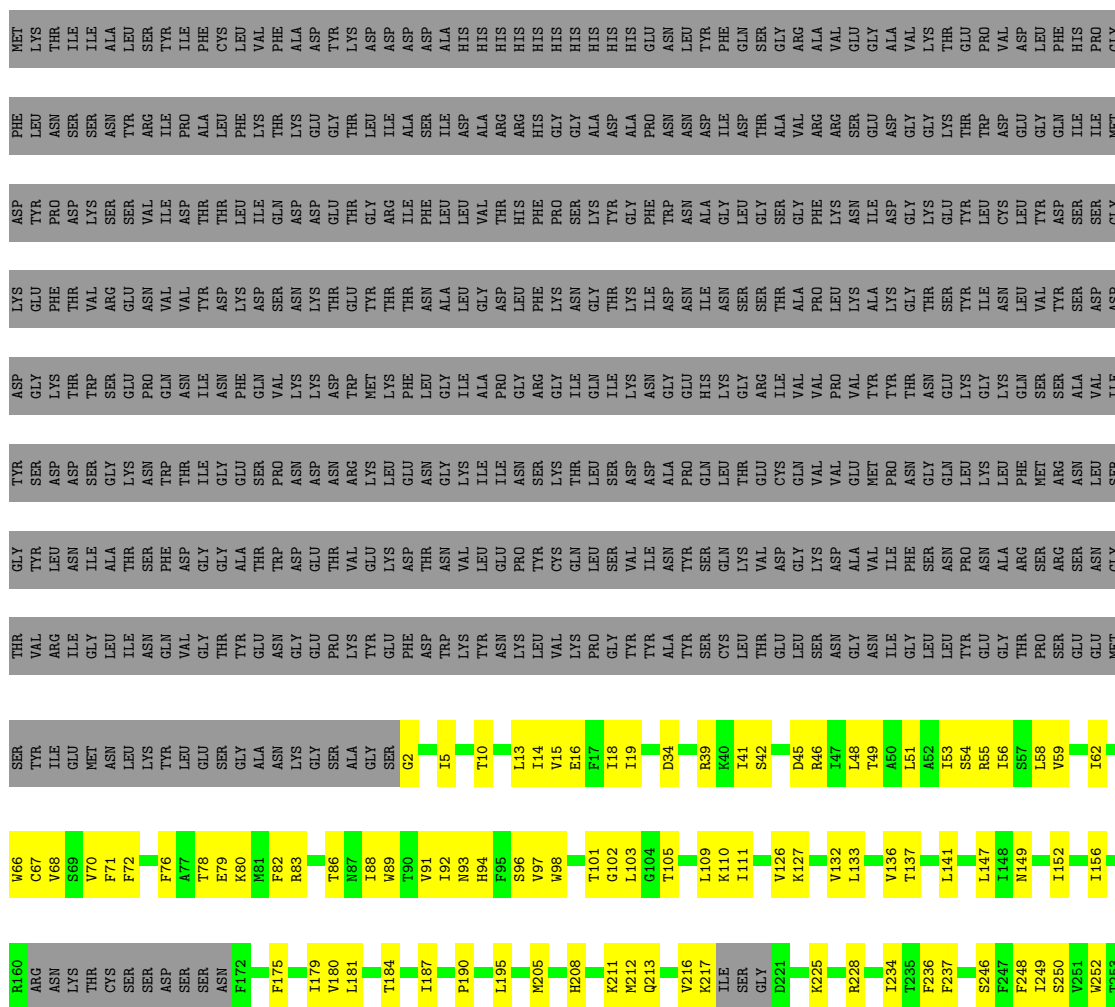
- Molecule 4: scFv16

Chain S:  61% 20% 19%



- Molecule 5: Exo-alpha-sialidase, Taste receptor type 2 member 14, LgBiT

Chain R: 19% 10% 71%



LEU	ALA	GLU	S254
TRP	GLN	GLN	
ASN	ILE	THR	I263
GLY	GLU	ALA	
ASN	GLU	ALA	H270
LYS	VAL	TYR	
ILE	PHE	ASN	P273
ILE	LYS	LEU	
ASP	VAL	ASP	V279
GLU	VAL	GLN	L280
ARG	TYR	VAL	
LEU	PRO	LEU	K285
ILE	VAL	LEU	P286
THR	ASP	GLN	L287
PRO	ASP	GLY	
ASP	HIS	GLY	P299
GLY	HIS	VAL	
SER	PHE	SER	TYR
MET	LYS	SER	THR
LEU	VAL	LEU	LYS
PHE	ILE	LEU	ASP
ARG	LEU	GLN	GLY
VAL	PRO	ASN	GLU
THR	TYR	LEU	PRO
ILE	GLY	ALA	SER
ASN	THR	VAL	GLY
SER	LEU	SER	HIS
	VAL	VAL	LYS
	ILE	THR	GLU
	ASP	PRO	GLU
	GLY	TYR	LEU
	LYS	GLY	GLU
	ILE	ASP	ASP
	ALA	VAL	PHE
	VAL	ILE	VAL
	PHE	ILE	SER
	ASP	PRO	THR
	GLY	TYR	THR
	LYS	GLY	GLY
	ILE	HIS	GLY
	ALA	VAL	SER
	VAL	ILE	SER
	PHE	ILE	SER
	ASP	PRO	SER
	GLY	TYR	GLY
	ILE	ASP	SER
	ALA	ASN	SER
	ARG	ASN	GLY
	PRO	ILE	SER
	MET	ARG	SER
	LEU	SER	GLY
	ASN	GLY	SER
	TYR	GLU	SER
	PHE	ASN	GLY
	GLY	ALA	SER
	ARG	LEU	GLY
	PRO	LYS	SER
	TYR	ILE	SER
	GLU	ASP	GLY
	GLY	ILE	SER
	ILE	HIS	GLY
	ALA	VAL	SER
	VAL	ILE	SER
	PHE	ILE	VAL
	ASP	PRO	PHE
	GLY	TYR	THR
	LYS	GLY	LEU
	ILE	GLY	GLU
	ASP	ALA	ASP
	VAL	VAL	GLY
	THR	THR	VAL
	THR	ASP	GLY
	GLY	GLN	ASP
	THR	MET	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	450989	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	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: GOQ, CLR

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	0.18	0/1843	0.32	0/2473
2	B	0.19	0/2647	0.33	0/3589
3	C	0.14	0/435	0.30	0/587
4	S	0.19	0/1827	0.33	0/2477
5	R	0.17	0/2355	0.35	0/3189
All	All	0.18	0/9107	0.33	0/12315

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	1813	0	1799	74	0
2	B	2600	0	2505	80	0
3	C	429	0	441	12	0
4	S	1783	0	1717	36	0
5	R	2298	0	2432	92	0
6	R	25	0	0	1	0
7	R	28	0	46	5	0
All	All	8976	0	8940	267	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 15.

The worst 5 of 267 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:329:THR:HG22	2:B:339:TRP:HE1	1.15	1.06
5:R:13:LEU:HD22	5:R:263:ILE:HD11	1.41	0.98
1:A:337:ASP:HB3	5:R:212:MET:SD	2.13	0.89
2:B:311:HIS:NE2	2:B:329:THR:HG23	1.88	0.88
1:A:337:ASP:OD2	5:R:212:MET:HE1	1.73	0.88

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	221/370 (60%)	213 (96%)	8 (4%)	0	100	100
2	B	336/366 (92%)	319 (95%)	17 (5%)	0	100	100
3	C	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
4	S	228/286 (80%)	219 (96%)	9 (4%)	0	100	100
5	R	278/990 (28%)	274 (99%)	4 (1%)	0	100	100
All	All	1117/2083 (54%)	1077 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	201/322 (62%)	201 (100%)	0	100	100
2	B	281/298 (94%)	281 (100%)	0	100	100
3	C	45/58 (78%)	45 (100%)	0	100	100
4	S	197/229 (86%)	197 (100%)	0	100	100
5	R	257/864 (30%)	257 (100%)	0	100	100
All	All	981/1771 (55%)	981 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	333	GLN
2	B	340	ASN
4	S	155	HIS
5	R	260	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 ⓘ

2 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	$\# Z > 2$
6	GOQ	R	501	-	27,28,28	0.83	0	34,42,42	1.02	2 (5%)
7	CLR	R	502	-	31,31,31	0.46	0	48,48,48	1.16	6 (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
6	GOQ	R	501	-	-	6/8/16/16	0/4/4/4
7	CLR	R	502	-	-	6/10/68/68	0/4/4/4

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	GOQ	C1-C10-C5	2.61	120.65	118.90
7	R	502	CLR	C22-C20-C17	-2.52	105.09	110.28
7	R	502	CLR	C21-C20-C17	2.51	116.76	112.92
6	R	501	GOQ	C14-C6-C5	-2.44	121.09	124.06
7	R	502	CLR	C1-C2-C3	2.38	113.53	110.47

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

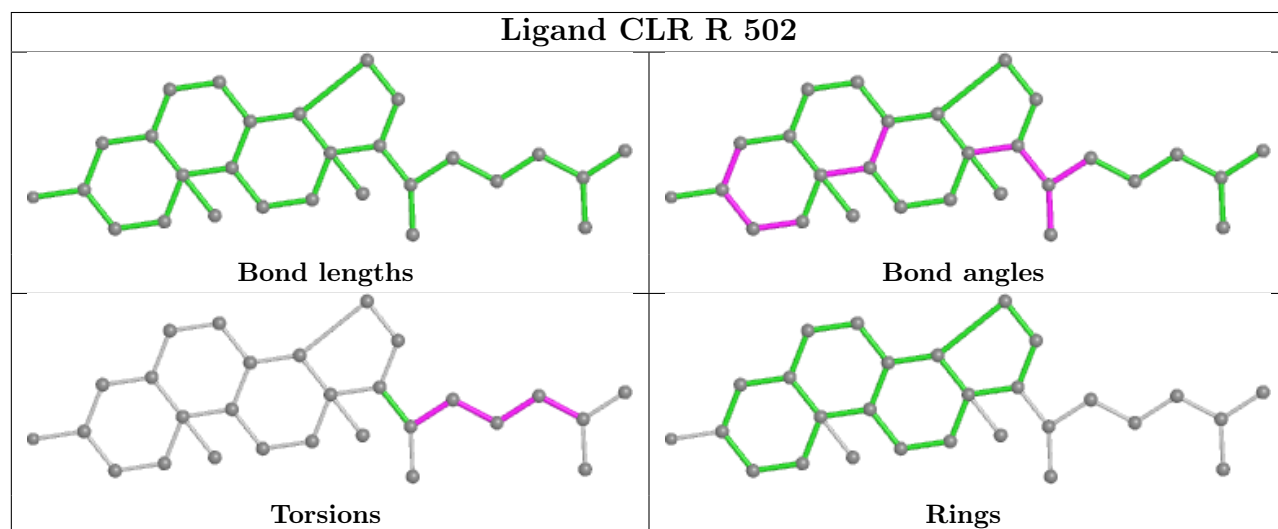
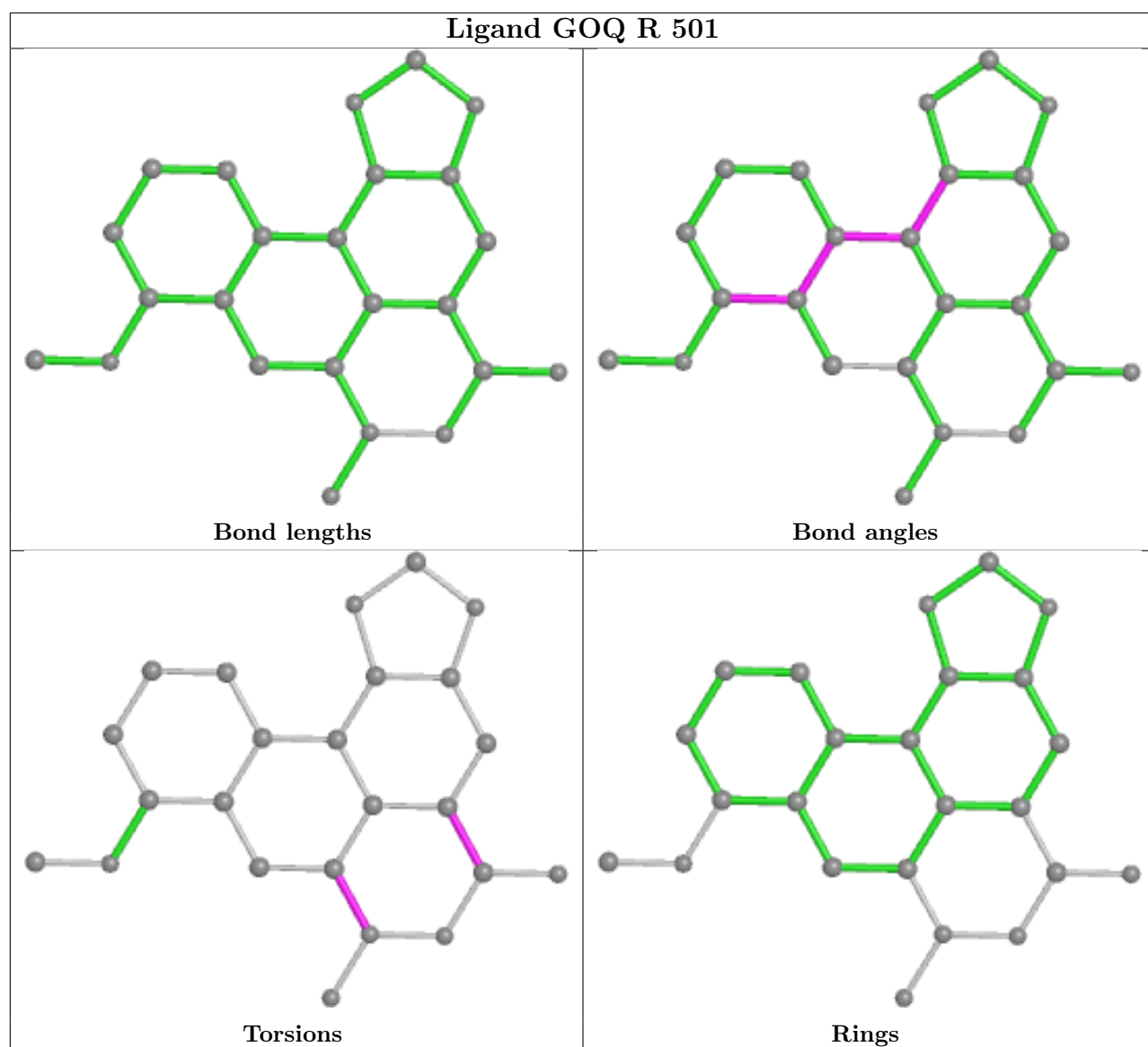
Mol	Chain	Res	Type	Atoms
7	R	502	CLR	C21-C20-C22-C23
7	R	502	CLR	C20-C22-C23-C24
6	R	501	GOQ	C9-C8-N-O1
6	R	501	GOQ	C12-C11-C16-O6
7	R	502	CLR	C17-C20-C22-C23

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	501	GOQ	1	0
7	R	502	CLR	5	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.