Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:10 AM JST

PDB ID	:	8JPP
EMDB ID	:	EMD-36486
Title	:	Cryo-EM structure of succinate receptor bound to succinate acid coupling MiniGsq
Authors	:	Wang, T.X.; Tang, W.Q.; Li, F.H.; Wang, J.Y.
Deposited on	:	2023-06-12
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:

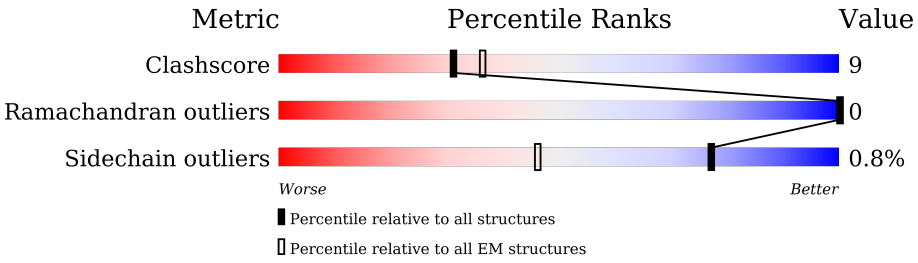
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	253	81% 13% 6%
2	B	377	73% 14% 12%
3	G	71	62% 7% 31%
4	R	658	36% 10% 54%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7137 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(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	237	1897	1203	334	353	7	0	0

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	ASP	GLY	conflict	UNP P63092
A	50	ASN	GLU	conflict	UNP P63092
A	196	GLY	-	insertion	UNP P63092
A	197	GLY	VAL	conflict	UNP P63092
A	198	SER	ASN	conflict	UNP P63092
A	200	GLY	PHE	conflict	UNP P63092
A	201	SER	ASN	conflict	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	SER	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	LYS	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	THR	deletion	UNP P63092
A	?	-	LYS	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	LYS	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	LYS	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	MET	deletion	UNP P63092
A	?	-	SER	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	PRO	deletion	UNP P63092
A	?	-	PRO	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	PRO	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	PHE	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	TYR	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	SER	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	MET	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	PRO	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	PHE	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	PHE	deletion	UNP P63092
A	?	-	PRO	deletion	UNP P63092
A	?	-	PRO	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	PHE	deletion	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	HIS	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	LYS	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	TRP	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	GLY	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	CYS	deletion	UNP P63092
A	?	-	TYR	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	SER	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	TYR	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	CYS	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	TYR	deletion	UNP P63092
A	?	-	PHE	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	LYS	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	LYS	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	ALA	deletion	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P63092
A	?	-	TYR	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	PRO	deletion	UNP P63092
A	?	-	SER	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	LEU	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	CYS	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	203	GLY	LEU	conflict	UNP P63092
A	249	ASP	ALA	conflict	UNP P63092
A	252	ASP	SER	conflict	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	MET	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	THR	deletion	UNP P63092
A	362	ALA	ILE	conflict	UNP P63092
A	365	ILE	VAL	conflict	UNP P63092
A	370	LYS	ARG	conflict	UNP P63092
A	374	LEU	GLN	conflict	UNP P63092
A	375	GLN	ARG	conflict	UNP P63092
A	377	ASN	HIS	conflict	UNP P63092
A	380	GLU	GLN	conflict	UNP P63092
A	382	ASN	GLU	conflict	UNP P63092
A	384	VAL	LEU	conflict	UNP P63092

- 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	331	Total	C	N	O	S	0	0
			2511	1556	455	480	20		

There are 38 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
B	1	GLN	-	expression tag	UNP P62873
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	G	49	Total	C	N	O	S	0	0
			376	237	64	72	3		

- Molecule 4 is a protein called Soluble cytochrome b562,Succinate receptor 1,Oplophorus-luciferin 2-monooxygenase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	305	Total	C	N	O	S	0	0
			2345	1565	375	394	11		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-162	MET	-	initiating methionine	UNP P0ABE7
R	-161	LYS	-	expression tag	UNP P0ABE7
R	-160	THR	-	expression tag	UNP P0ABE7
R	-159	ILE	-	expression tag	UNP P0ABE7
R	-158	ILE	-	expression tag	UNP P0ABE7
R	-157	ALA	-	expression tag	UNP P0ABE7
R	-156	LEU	-	expression tag	UNP P0ABE7
R	-155	SER	-	expression tag	UNP P0ABE7
R	-154	TYR	-	expression tag	UNP P0ABE7
R	-153	ILE	-	expression tag	UNP P0ABE7
R	-152	PHE	-	expression tag	UNP P0ABE7
R	-151	CYS	-	expression tag	UNP P0ABE7
R	-150	LEU	-	expression tag	UNP P0ABE7
R	-149	VAL	-	expression tag	UNP P0ABE7
R	-148	PHE	-	expression tag	UNP P0ABE7
R	-147	ALA	-	expression tag	UNP P0ABE7
R	-146	ASP	-	expression tag	UNP P0ABE7
R	-145	TYR	-	expression tag	UNP P0ABE7
R	-144	LYS	-	expression tag	UNP P0ABE7
R	-143	ASP	-	expression tag	UNP P0ABE7
R	-142	ASP	-	expression tag	UNP P0ABE7
R	-141	ASP	-	expression tag	UNP P0ABE7
R	-140	ASP	-	expression tag	UNP P0ABE7
R	-139	ALA	-	expression tag	UNP P0ABE7
R	-138	GLY	-	expression tag	UNP P0ABE7
R	-137	ARG	-	expression tag	UNP P0ABE7
R	-136	ALA	-	expression tag	UNP P0ABE7
R	-135	HIS	-	expression tag	UNP P0ABE7
R	-134	HIS	-	expression tag	UNP P0ABE7
R	-133	HIS	-	expression tag	UNP P0ABE7

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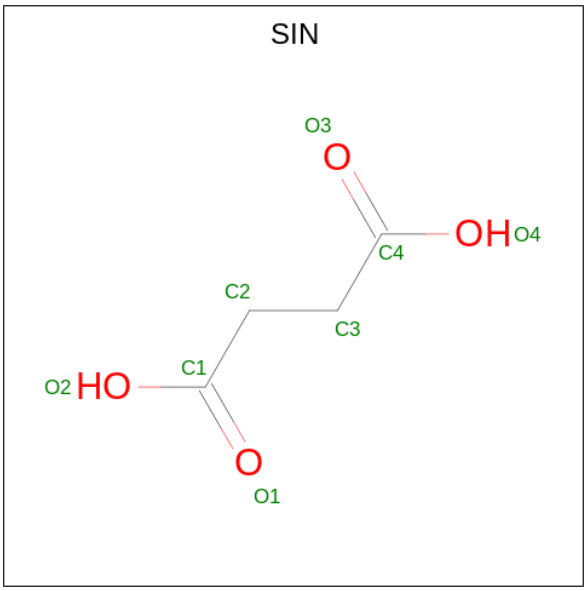
Chain	Residue	Modelled	Actual	Comment	Reference
R	-132	HIS	-	expression tag	UNP P0ABE7
R	-131	HIS	-	expression tag	UNP P0ABE7
R	-130	HIS	-	expression tag	UNP P0ABE7
R	-129	HIS	-	expression tag	UNP P0ABE7
R	-128	HIS	-	expression tag	UNP P0ABE7
R	-127	HIS	-	expression tag	UNP P0ABE7
R	-126	HIS	-	expression tag	UNP P0ABE7
R	-125	GLU	-	expression tag	UNP P0ABE7
R	-124	ASN	-	expression tag	UNP P0ABE7
R	-123	LEU	-	expression tag	UNP P0ABE7
R	-122	TYR	-	expression tag	UNP P0ABE7
R	-121	PHE	-	expression tag	UNP P0ABE7
R	-120	GLN	-	expression tag	UNP P0ABE7
R	-119	SER	-	expression tag	UNP P0ABE7
R	-118	GLY	-	expression tag	UNP P0ABE7
R	-117	ALA	-	expression tag	UNP P0ABE7
R	-116	PRO	-	expression tag	UNP P0ABE7
R	-109	TRP	MET	conflict	UNP P0ABE7
R	-14	ILE	HIS	conflict	UNP P0ABE7
R	-10	LEU	-	linker	UNP P0ABE7
R	-9	LEU	-	linker	UNP P0ABE7
R	-8	GLU	-	linker	UNP P0ABE7
R	-7	VAL	-	linker	UNP P0ABE7
R	-6	LEU	-	linker	UNP P0ABE7
R	-5	PHE	-	linker	UNP P0ABE7
R	-4	GLN	-	linker	UNP P0ABE7
R	-3	GLY	-	linker	UNP P0ABE7
R	-2	PRO	-	linker	UNP P0ABE7
R	-1	GLU	-	linker	UNP P0ABE7
R	0	PHE	-	linker	UNP P0ABE7
R	335	ALA	-	linker	UNP Q9BXA5
R	336	ALA	-	linker	UNP Q9BXA5
R	337	ALA	-	linker	UNP Q9BXA5
R	338	VAL	-	linker	UNP Q9BXA5

- Molecule 5 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$) (labeled as "Ligand of Interest" by depositor).



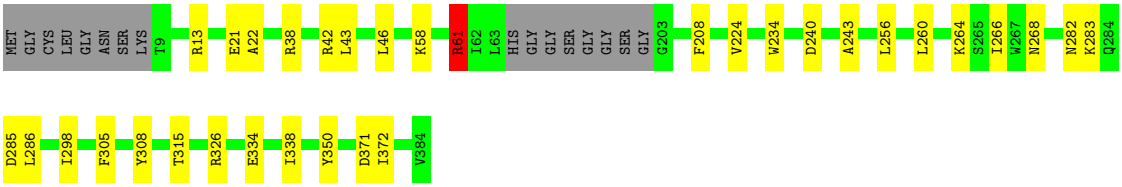
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	R	1	8	4	4	0

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.

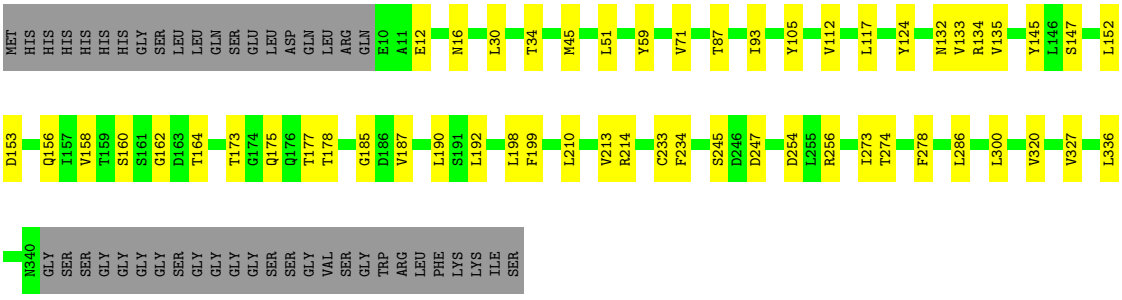
• Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain A:



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

Chain B:

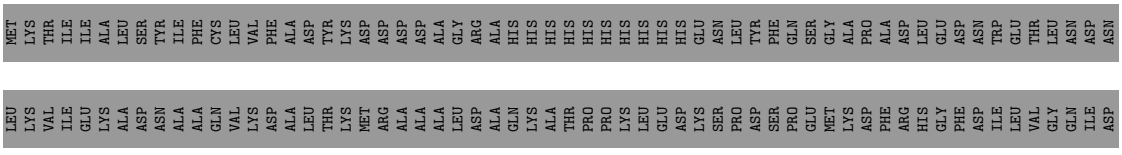


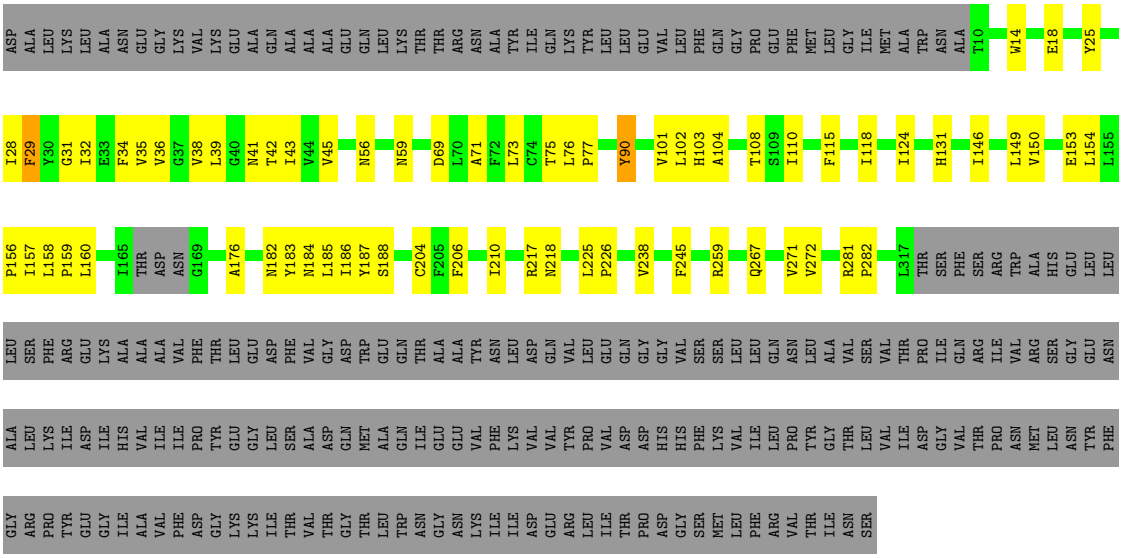
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

• Molecule 4: Soluble cytochrome b562,Succinate receptor 1,Oplophorus-luciferin 2-monooxygenase catalytic subunit

Chain R:




ASP ALA LEU LYS LEU ALA ASN GLU GLY LYS VAL LYS GLU ALA GLN ALA ALA ALA GLU GLN LEU LYS THR THR ARG ASN ALA TYR ILE GLN LYS TYR LEU LEU GLU VAL LEU PHE GLN GLY PRO GLU PHE MET LEU GLY ILE MET ALA TRP ASN ALA T10 W14 E18 Y25
I28 F29 Y30 G31 I32 E33 F34 V35 V36 G37 V38 L39 G40 N41 T42 I43 V44 V45 N56 N59 D69 L70 A71 F72 L73 C74 T75 L76 P77 Y90 V101 L102 H103 A104 T108 S109 I110 F115 I118 I124 H131 I146 L149 V150 E153 L154 L155
P156 I157 L158 P159 L160 I165 THR ASP ASN G169 A176 N182 Y183 N184 L185 I186 Y187 S188 C204 F205 F206 I210 R217 N218 L225 P226 V238 F245 R259 Q267 V271 V272 R281 P282 L317 THR SER PHE SER ARG TRP ALA HIS GLU LEU LEU
LEU SER PHE ARG GLU LYS ALA ALA ALA VAL PHE THR LEU GLU ASP PHE VAL GLY ASP TRP GLU GLN THR ALA ALA TYR ASN LEU ASP GLN VAL LEU GLU GLN GLY GLY VAL SER SER LEU LEU GLN ASN LEU ALA VAL SER VAL THR PRO ILE GLN ARG ILE VAL ARG SER GLY GLU ASN
ALA LEU LYS ILE ASP ILE HIS VAL ILE ILE PRO TYR GLU GLY LEU SER ALA ASP GLN MET ALA GLN ILE GLU GLU VAL PHE LYS VAL VAL TYR PRO VAL ASP ASP HIS HIS PHE LYS VAL ILE LEU PRO TYR GLY THR LEU VAL ILE ASP GLY VAL THR PRO ASN MET LEU ASN TYR PHE
GLY ARG PRO TYR GLU GLY ILE ALA VAL PHE ASP GLY LYS LYS ILE THR VAL THR GLY THR LEU TRP ASN GLY ASN LYS ILE ILE ASP GLU ARG LEU ILE THR PRO ASP GLY SER MET LEU PHE ARG VAL THR ILE ASN SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	239096	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 ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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: SIN

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	0.29	0/1933	0.50	0/2611
2	B	0.27	0/2558	0.54	0/3473
3	G	0.26	0/382	0.45	0/517
4	R	0.31	0/2409	0.47	0/3304
All	All	0.29	0/7282	0.50	0/9905

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	ARG	Sidechain

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	1897	0	1822	26	0
2	B	2511	0	2404	39	0
3	G	376	0	378	6	0
4	R	2345	0	2268	55	0
5	R	8	0	4	1	0
All	All	7137	0	6876	121	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 9.

All (121) 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:45:MET:CE	3:G:50:LEU:HD22	2.19	0.72
3:G:47:GLU:N	3:G:47:GLU:OE2	2.24	0.71
4:R:41:ASN:O	4:R:45:VAL:HG22	1.90	0.71
4:R:75:THR:HG21	4:R:101:VAL:HG13	1.72	0.69
1:A:224:VAL:HG11	1:A:234:TRP:CH2	2.28	0.68
2:B:173:THR:HG23	2:B:175:GLN:OE1	1.94	0.67
4:R:32:ILE:O	4:R:36:VAL:HG23	1.95	0.67
4:R:34:PHE:HA	4:R:73:LEU:HD12	1.78	0.66
1:A:234:TRP:HB2	2:B:117:LEU:HD21	1.78	0.65
4:R:110:ILE:HD11	4:R:245:PHE:CE1	2.32	0.64
2:B:213:VAL:HG23	2:B:214:ARG:HD2	1.79	0.64
1:A:308:TYR:O	1:A:326:ARG:NH1	2.32	0.63
1:A:61:ARG:NE	1:A:208:PHE:CZ	2.67	0.62
4:R:267:GLN:O	4:R:271:VAL:HG23	1.99	0.61
4:R:34:PHE:O	4:R:38:VAL:HG22	2.00	0.61
4:R:176:ALA:O	4:R:259:ARG:NH1	2.33	0.61
4:R:39:LEU:O	4:R:43:ILE:HG13	2.01	0.60
4:R:118:ILE:HD13	4:R:206:PHE:CD2	2.37	0.60
4:R:185:LEU:O	4:R:186:ILE:C	2.40	0.60
1:A:315:THR:O	1:A:315:THR:HG23	2.02	0.59
1:A:282:ASN:OD1	1:A:283:LYS:N	2.37	0.58
2:B:34:THR:HG21	2:B:300:LEU:O	2.03	0.58
2:B:175:GLN:OE1	2:B:175:GLN:N	2.36	0.58
2:B:245:SER:OG	2:B:247:ASP:OD1	2.22	0.57
2:B:286:LEU:HD22	2:B:327:VAL:HG11	1.85	0.57
2:B:233:CYS:SG	2:B:278:PHE:CE2	2.98	0.56
2:B:71:VAL:HG21	2:B:112:VAL:HG11	1.88	0.56
2:B:147:SER:OG	2:B:187:VAL:O	2.23	0.56
1:A:264:LYS:O	1:A:268:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:TYR:CE2	2:B:135:VAL:HG22	2.42	0.55
2:B:87:THR:O	2:B:87:THR:HG22	2.06	0.55
4:R:217:ARG:NH2	4:R:225:LEU:O	2.40	0.54
2:B:132:ASN:O	2:B:134:ARG:NH1	2.41	0.54
4:R:182:ASN:O	4:R:186:ILE:HG23	2.07	0.53
4:R:90:TYR:N	4:R:90:TYR:CD1	2.77	0.53
4:R:118:ILE:HD13	4:R:206:PHE:CE2	2.44	0.53
1:A:46:LEU:HD13	1:A:266:ILE:HD11	1.91	0.53
2:B:93:ILE:HG13	2:B:133:VAL:HG21	1.90	0.52
4:R:185:LEU:O	4:R:187:TYR:N	2.42	0.52
4:R:160:LEU:HD21	4:R:184:ASN:HA	1.90	0.52
2:B:51:LEU:HD23	2:B:87:THR:HG23	1.92	0.52
4:R:108:THR:HG23	4:R:150:VAL:HG11	1.92	0.52
4:R:184:ASN:HD22	4:R:259:ARG:NH1	2.08	0.52
2:B:45:MET:HE2	3:G:50:LEU:HD22	1.91	0.51
4:R:184:ASN:HD22	4:R:259:ARG:HH12	1.58	0.51
4:R:124:ILE:HD12	4:R:210:ILE:HG23	1.93	0.50
1:A:13:ARG:N	1:A:13:ARG:HD2	2.27	0.50
1:A:61:ARG:NE	1:A:208:PHE:CE2	2.80	0.50
1:A:61:ARG:NH1	1:A:208:PHE:CZ	2.78	0.50
4:R:118:ILE:CD1	4:R:206:PHE:CE2	2.94	0.49
2:B:254:ASP:OD1	2:B:256:ARG:N	2.45	0.49
4:R:31:GLY:O	4:R:35:VAL:HG23	2.12	0.49
2:B:198:LEU:HD13	2:B:210:LEU:HD11	1.93	0.49
4:R:103:HIS:HB3	4:R:154:LEU:HD21	1.94	0.49
4:R:281:ARG:NE	5:R:501:SIN:O1	2.46	0.48
4:R:71:ALA:O	4:R:75:THR:HG23	2.13	0.48
4:R:39:LEU:O	4:R:42:THR:OG1	2.26	0.48
1:A:260:LEU:CD2	1:A:334:GLU:HB3	2.44	0.48
2:B:153:ASP:OD1	2:B:156:GLN:N	2.47	0.47
4:R:69:ASP:O	4:R:73:LEU:HD23	2.14	0.47
1:A:256:LEU:HG	1:A:260:LEU:CD1	2.44	0.47
4:R:76:LEU:N	4:R:77:PRO:CD	2.78	0.47
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.97	0.46
2:B:12:GLU:O	2:B:16:ASN:ND2	2.48	0.46
4:R:185:LEU:C	4:R:187:TYR:N	2.67	0.46
1:A:298:ILE:HG23	1:A:305:PHE:CD2	2.50	0.46
2:B:117:LEU:HD23	2:B:145:TYR:HB3	1.97	0.45
2:B:336:LEU:O	2:B:336:LEU:HD23	2.15	0.45
4:R:29:PHE:CD2	4:R:282:PRO:HB2	2.51	0.45
4:R:204:CYS:SG	4:R:238:VAL:HG21	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLU:HA	1:A:334:GLU:OE1	2.15	0.45
1:A:58:LYS:HA	1:A:61:ARG:HB2	1.99	0.44
1:A:350:TYR:OH	1:A:371:ASP:OD1	2.28	0.44
1:A:240:ASP:OD1	1:A:240:ASP:C	2.56	0.44
4:R:14:TRP:CD2	4:R:272:VAL:HG22	2.53	0.44
4:R:218:ASN:ND2	4:R:226:PRO:O	2.51	0.43
1:A:243:ALA:HB2	1:A:372:ILE:HD13	2.00	0.43
2:B:164:THR:HG22	2:B:185:GLY:C	2.37	0.43
4:R:160:LEU:HD21	4:R:184:ASN:CA	2.48	0.43
2:B:30:LEU:O	2:B:34:THR:HG23	2.18	0.43
4:R:183:TYR:HA	4:R:186:ILE:HG12	1.99	0.43
2:B:51:LEU:HD12	2:B:336:LEU:HD22	2.00	0.43
2:B:30:LEU:HD13	3:G:34:ALA:HB1	2.01	0.43
4:R:25:TYR:HA	4:R:28:ILE:HD11	1.99	0.42
4:R:102:LEU:C	4:R:102:LEU:HD23	2.40	0.42
4:R:182:ASN:H	4:R:182:ASN:HD22	1.66	0.42
2:B:233:CYS:HG	2:B:278:PHE:HD2	1.57	0.42
4:R:104:ALA:O	4:R:108:THR:HG23	2.19	0.42
4:R:187:TYR:CD1	4:R:187:TYR:C	2.93	0.42
2:B:192:LEU:HD13	2:B:199:PHE:HB3	2.02	0.42
2:B:160:SER:HB3	2:B:190:LEU:HD23	2.02	0.42
4:R:183:TYR:O	4:R:183:TYR:CD1	2.72	0.42
1:A:21:GLU:OE1	1:A:22:ALA:N	2.52	0.42
1:A:260:LEU:O	1:A:338:ILE:HD13	2.20	0.42
2:B:177:THR:HG22	2:B:178:THR:HG23	2.02	0.42
4:R:131:HIS:O	4:R:131:HIS:CG	2.72	0.42
2:B:51:LEU:CD2	2:B:87:THR:HG23	2.49	0.42
4:R:18:GLU:OE1	4:R:271:VAL:HG13	2.20	0.42
4:R:182:ASN:HD22	4:R:182:ASN:N	2.18	0.42
4:R:25:TYR:O	4:R:28:ILE:HG12	2.20	0.41
4:R:184:ASN:O	4:R:188:SER:HB2	2.20	0.41
2:B:233:CYS:SG	2:B:278:PHE:CD2	3.06	0.41
2:B:152:LEU:HD13	2:B:158:VAL:HG23	2.02	0.41
2:B:145:TYR:O	2:B:162:GLY:N	2.45	0.41
1:A:42:ARG:O	1:A:43:LEU:HD12	2.21	0.41
1:A:38:ARG:HG3	1:A:38:ARG:HH11	1.85	0.41
2:B:152:LEU:CD1	2:B:158:VAL:HG23	2.51	0.41
4:R:56:ASN:OD1	4:R:59:ASN:ND2	2.51	0.41
4:R:75:THR:HG21	4:R:101:VAL:CG1	2.47	0.41
1:A:285:ASP:OD1	1:A:286:LEU:N	2.53	0.40
2:B:34:THR:HG22	3:G:38:MET:CE	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:154:LEU:O	4:R:157:ILE:HG22	2.22	0.40
4:R:158:LEU:HB2	4:R:159:PRO:HD3	2.04	0.40
3:G:58:GLU:OE2	3:G:58:GLU:N	2.50	0.40
4:R:281:ARG:HB2	4:R:282:PRO:HD3	2.04	0.40
4:R:149:LEU:HD21	4:R:153:GLU:OE1	2.21	0.40
4:R:156:PRO:HB2	4:R:187:TYR:CE2	2.57	0.40
1:A:61:ARG:HE	1:A:208:PHE:HZ	1.63	0.40
1:A:260:LEU:HD21	1:A:334:GLU:HB3	2.04	0.40
2:B:273:ILE:HG22	2:B:274:THR:N	2.36	0.40
4:R:115:PHE:CD2	4:R:146:ILE:HD11	2.56	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	233/253 (92%)	224 (96%)	9 (4%)	0	100	100
2	B	329/377 (87%)	310 (94%)	19 (6%)	0	100	100
3	G	47/71 (66%)	47 (100%)	0	0	100	100
4	R	301/658 (46%)	287 (95%)	14 (5%)	0	100	100
All	All	910/1359 (67%)	868 (95%)	42 (5%)	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	196/222 (88%)	195 (100%)	1 (0%)	86 93
2	B	263/308 (85%)	260 (99%)	3 (1%)	70 86
3	G	40/58 (69%)	40 (100%)	0	100 100
4	R	238/576 (41%)	236 (99%)	2 (1%)	79 90
All	All	737/1164 (63%)	731 (99%)	6 (1%)	77 90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
2	B	59	TYR
2	B	105	TYR
2	B	234	PHE
4	R	29	PHE
4	R	90	TYR

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

Mol	Chain	Res	Type
4	R	182	ASN
4	R	184	ASN

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	$\#\|Z\| > 2$
5	SIN	R	501	-	7,7,7	1.14	0	8,8,8	1.50	0

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	SIN	R	501	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	501	SIN	O1-C1-C2-C3
5	R	501	SIN	O2-C1-C2-C3

There are no ring outliers.

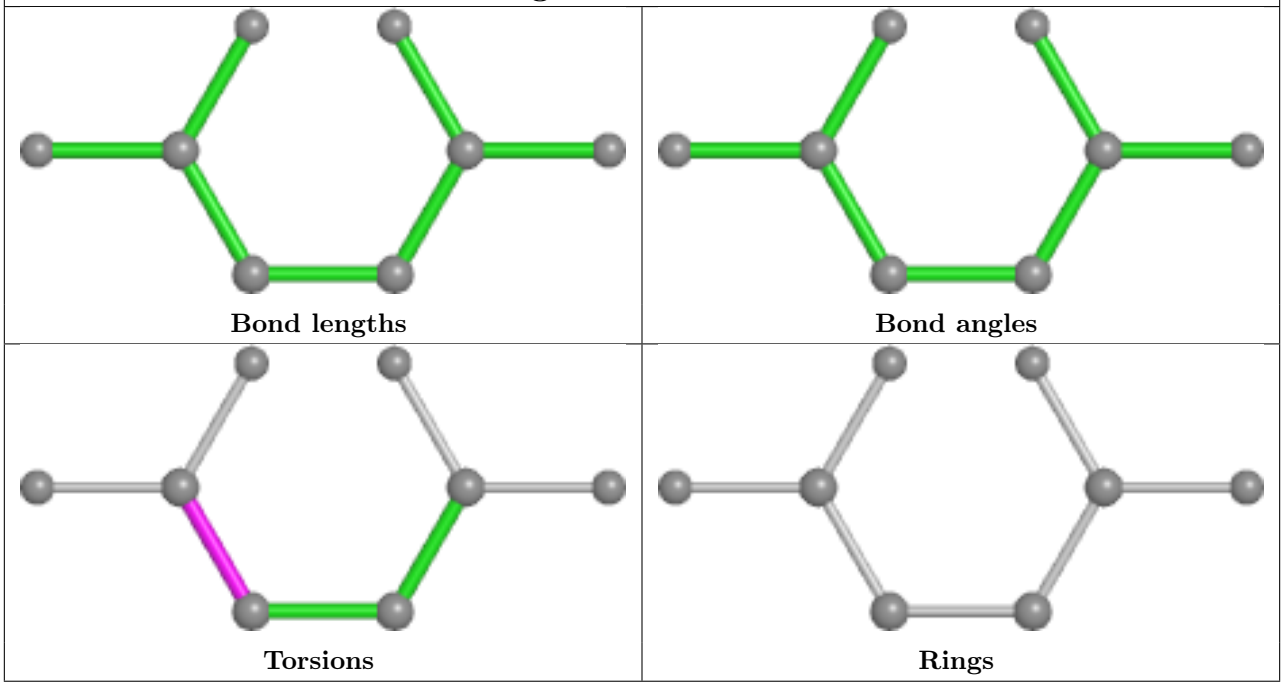
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	501	SIN	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 then 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.

Ligand SIN R 501



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.