Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 12:21 AM JST

PDB ID	:	8JPN
EMDB ID	:	EMD-36484
Title	:	Cryo-EM structure of succinate receptor bound to cis-epoxysuccinic acid coupling to Gi
Authors	:	Wang, T.X.; Tang, W.Q.; Li, F.H.; Wang, J.Y.
Deposited on	:	2023-06-12
Resolution	:	2.90 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:

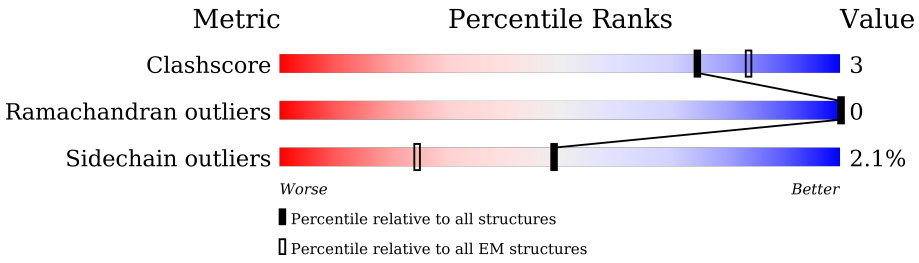
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	354	63% · 36%
2	B	377	84% 7% 9%
3	C	71	80% · 18%
4	R	658	38% 7% 55%
5	S	286	76% 5% 18%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8557 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
			Total	C	N	O	S		
1	A	227	1713	1098	288	316	11	0	0

- 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
			Total	C	N	O	S		
2	B	342	2528	1563	445	499	21	0	0

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	58	Total	C	N	O	S	0	0
			397	250	69	76	2		

- 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	296	Total	C	N	O	S	0	0
			2187	1454	356	369	8		

There are 102 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	46	PHE	TYR	conflict	UNP Q9BXA5
R	49	LEU	ILE	conflict	UNP Q9BXA5
R	51	CYS	SER	conflict	UNP Q9BXA5
R	67	ILE	VAL	conflict	UNP Q9BXA5
R	175	TYR	PHE	conflict	UNP Q9BXA5
R	221	LEU	VAL	conflict	UNP Q9BXA5
R	304	GLU	ASP	conflict	UNP Q9BXA5
R	309	LYS	GLN	conflict	UNP Q9BXA5
R	321	ARG	SER	conflict	UNP Q9BXA5
R	335	ALA	-	linker	UNP Q9BXA5
R	336	ALA	-	linker	UNP Q9BXA5
R	337	ALA	-	linker	UNP Q9BXA5
R	338	VAL	-	linker	UNP Q9BXA5
R	342	GLU	ALA	conflict	UNP Q9GV45
R	349	GLU	GLN	conflict	UNP Q9GV45
R	353	ALA	GLY	conflict	UNP Q9GV45
R	356	LEU	GLN	conflict	UNP Q9GV45
R	365	VAL	LEU	conflict	UNP Q9GV45
R	369	LEU	PHE	conflict	UNP Q9GV45
R	371	ASN	ALA	conflict	UNP Q9GV45
R	373	ALA	GLY	conflict	UNP Q9GV45
R	381	ARG	LYS	conflict	UNP Q9GV45
R	382	ILE	VAL	conflict	UNP Q9GV45
R	384	ARG	LEU	conflict	UNP Q9GV45
R	389	ALA	GLY	conflict	UNP Q9GV45
R	392	ILE	ALA	conflict	UNP Q9GV45
R	405	ALA	GLY	conflict	UNP Q9GV45
R	406	ASP	PHE	conflict	UNP Q9GV45
R	409	ALA	GLY	conflict	UNP Q9GV45
R	410	GLN	LEU	conflict	UNP Q9GV45

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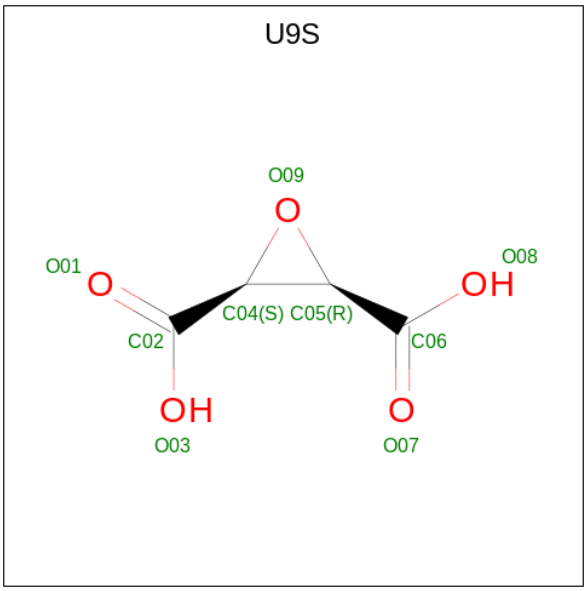
Chain	Residue	Modelled	Actual	Comment	Reference
R	413	GLU	MET	conflict	UNP Q9GV45
R	414	VAL	ILE	conflict	UNP Q9GV45
R	428	VAL	ILE	conflict	UNP Q9GV45
R	431	PRO	HIS	conflict	UNP Q9GV45
R	445	LEU	ILE	conflict	UNP Q9GV45
R	446	ASN	ASP	conflict	UNP Q9GV45
R	453	GLU	PRO	conflict	UNP Q9GV45
R	462	LYS	GLN	conflict	UNP Q9GV45
R	476	ILE	TYR	conflict	UNP Q9GV45
R	482	THR	ASN	conflict	UNP Q9GV45
R	487	MET	LEU	conflict	UNP Q9GV45
R	495	SER	GLY	conflict	UNP Q9GV45

- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	234	Total	C	N	O	S	0	0
			1723	1100	289	324	10		

- Molecule 6 is (2R,3S)-oxirane-2,3-dicarboxylic acid (three-letter code: U9S) (formula: $C_4H_4O_5$) (labeled as "Ligand of Interest" by depositor).



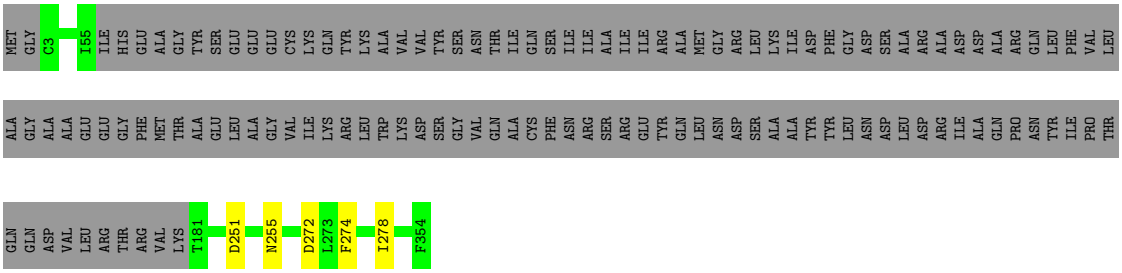
Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	O		0
			9	4	5		

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.

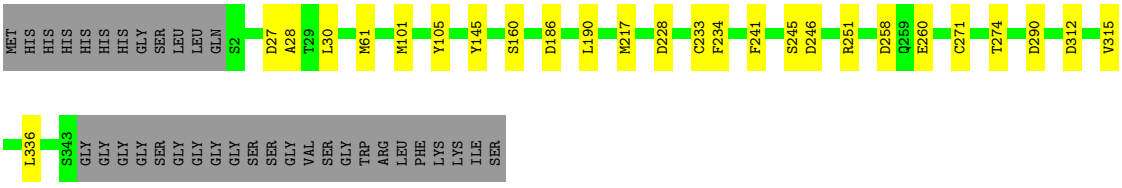
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



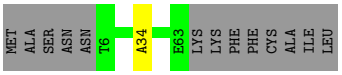
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



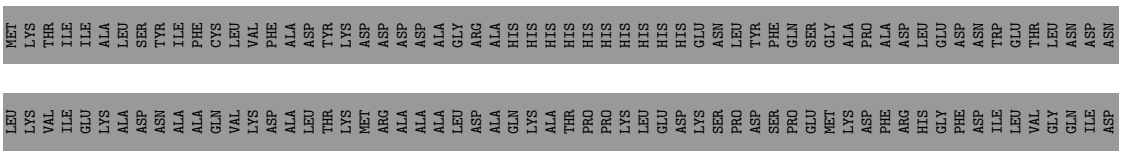
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

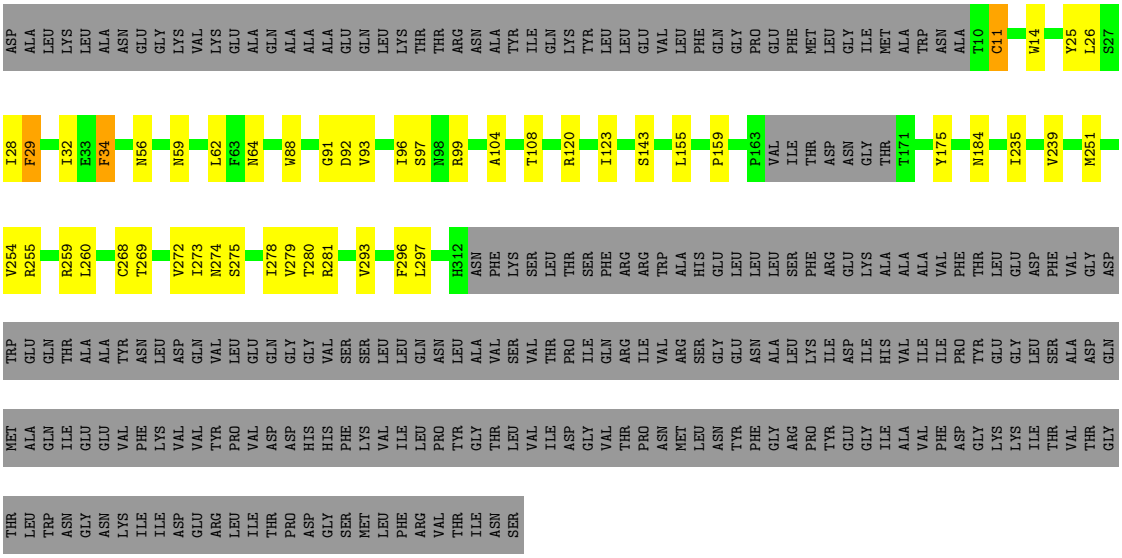
Chain C:



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

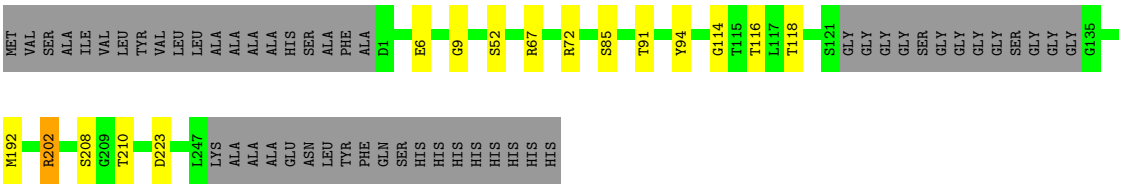
Chain R:





• Molecule 5: scFv16

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	278158	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	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: U9S

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	0.26	0/1743	0.43	0/2350
2	B	0.27	0/2575	0.53	0/3504
3	C	0.24	0/403	0.42	0/554
4	R	0.28	0/2246	0.47	0/3087
5	S	0.30	0/1767	0.54	0/2405
All	All	0.28	0/8734	0.49	0/11900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1713	0	1622	2	0
2	B	2528	0	2353	10	0
3	C	397	0	366	1	0
4	R	2187	0	2019	28	0
5	S	1723	0	1606	9	0
6	R	9	0	0	0	0
All	All	8557	0	7966	49	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 3.

All (49) 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)
5:S:94:TYR:O	5:S:114:GLY:HA2	1.88	0.73
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.33	0.61
4:R:56:ASN:OD1	4:R:59:ASN:ND2	2.34	0.60
4:R:88:TRP:NE1	4:R:91:GLY:O	2.34	0.59
5:S:52:SER:O	5:S:72:ARG:NH1	2.38	0.56
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.87	0.56
5:S:202:ARG:NH2	5:S:223:ASP:OD2	2.40	0.55
4:R:99:ARG:HH11	4:R:99:ARG:HG3	1.70	0.55
4:R:251:MET:HG3	4:R:280:THR:HG21	1.89	0.54
2:B:245:SER:OG	2:B:246:ASP:N	2.43	0.52
4:R:25:TYR:CE2	4:R:29:PHE:HD2	2.29	0.50
4:R:235:ILE:O	4:R:239:VAL:HG23	2.12	0.50
5:S:67:ARG:NH1	5:S:85:SER:O	2.45	0.49
5:S:208:SER:O	5:S:210:THR:N	2.43	0.49
4:R:56:ASN:OD1	4:R:56:ASN:N	2.45	0.49
5:S:6:GLU:OE1	5:S:114:GLY:N	2.33	0.48
4:R:104:ALA:O	4:R:108:THR:OG1	2.27	0.48
4:R:274:ASN:O	4:R:278:ILE:HG13	2.14	0.48
4:R:92:ASP:O	4:R:96:ILE:HD12	2.13	0.47
4:R:26:LEU:HD21	4:R:278:ILE:HG22	1.95	0.47
2:B:27:ASP:OD1	2:B:28:ALA:N	2.44	0.47
4:R:28:ILE:O	4:R:32:ILE:HG13	2.15	0.46
5:S:91:THR:HG23	5:S:118:THR:HA	1.98	0.46
4:R:25:TYR:HE1	4:R:279:VAL:HA	1.79	0.46
2:B:30:LEU:HD13	3:C:34:ALA:HB1	1.96	0.46
4:R:293:VAL:HA	4:R:297:LEU:HB2	1.98	0.46
4:R:260:LEU:HD23	4:R:260:LEU:HA	1.80	0.45
4:R:184:ASN:HD22	4:R:259:ARG:HH21	1.64	0.44
4:R:269:THR:O	4:R:273:ILE:HG22	2.16	0.44
4:R:14:TRP:CD2	4:R:272:VAL:HG12	2.53	0.44
4:R:120:ARG:O	4:R:123:ILE:HG22	2.17	0.44
2:B:160:SER:HB3	2:B:190:LEU:HD23	2.00	0.43
4:R:64:ASN:ND2	4:R:143:SER:HB3	2.33	0.43
4:R:272:VAL:O	4:R:275:SER:OG	2.28	0.43
4:R:184:ASN:HD22	4:R:259:ARG:NH2	2.16	0.43
2:B:233:CYS:O	2:B:241:PHE:HB2	2.18	0.43
4:R:254:VAL:HG12	4:R:273:ILE:HD11	2.01	0.43
4:R:11:CYS:HB3	4:R:268:CYS:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:HE1	2:B:145:TYR:CD1	2.54	0.42
2:B:274:THR:OG1	2:B:315:VAL:O	2.30	0.42
5:S:9:GLY:HA3	5:S:116:THR:O	2.18	0.42
4:R:155:LEU:HD23	4:R:155:LEU:HA	1.91	0.42
2:B:186:ASP:N	2:B:186:ASP:OD1	2.53	0.42
1:A:274:PHE:CE2	1:A:278:ILE:HD11	2.56	0.41
4:R:93:VAL:HA	4:R:96:ILE:HD12	2.02	0.41
2:B:251:ARG:HD3	2:B:260:GLU:OE1	2.21	0.41
4:R:34:PHE:CD2	4:R:34:PHE:C	2.94	0.41
5:S:192:MET:O	5:S:192:MET:HG2	2.21	0.40
4:R:62:LEU:HB3	4:R:296:PHE:CE1	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	223/354 (63%)	220 (99%)	3 (1%)	0	100	100
2	B	340/377 (90%)	328 (96%)	12 (4%)	0	100	100
3	C	56/71 (79%)	56 (100%)	0	0	100	100
4	R	292/658 (44%)	281 (96%)	11 (4%)	0	100	100
5	S	230/286 (80%)	218 (95%)	12 (5%)	0	100	100
All	All	1141/1746 (65%)	1103 (97%)	38 (3%)	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	168/305 (55%)	167 (99%)	1 (1%)	84 95
2	B	261/308 (85%)	253 (97%)	8 (3%)	35 70
3	C	35/58 (60%)	35 (100%)	0	100 100
4	R	203/576 (35%)	195 (96%)	8 (4%)	27 62
5	S	175/229 (76%)	174 (99%)	1 (1%)	84 95
All	All	842/1476 (57%)	824 (98%)	18 (2%)	49 78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	ASP
2	B	61	MET
2	B	105	TYR
2	B	217	MET
2	B	228	ASP
2	B	234	PHE
2	B	258	ASP
2	B	312	ASP
2	B	336	LEU
4	R	11	CYS
4	R	29	PHE
4	R	34	PHE
4	R	97	SER
4	R	159	PRO
4	R	175	TYR
4	R	255	ARG
4	R	281	ARG
5	S	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	R	59	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	$\#\|Z\| > 2$
6	U9S	R	501	-	9,9,9	1.36	0	11,13,13	1.65	3 (27%)

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	U9S	R	501	-	-	3/6/13/13	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	501	U9S	C05-O09-C04	2.39	64.18	61.94
6	R	501	U9S	O09-C04-C02	2.10	119.62	116.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	501	U9S	O09-C05-C04	-2.07	57.86	59.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

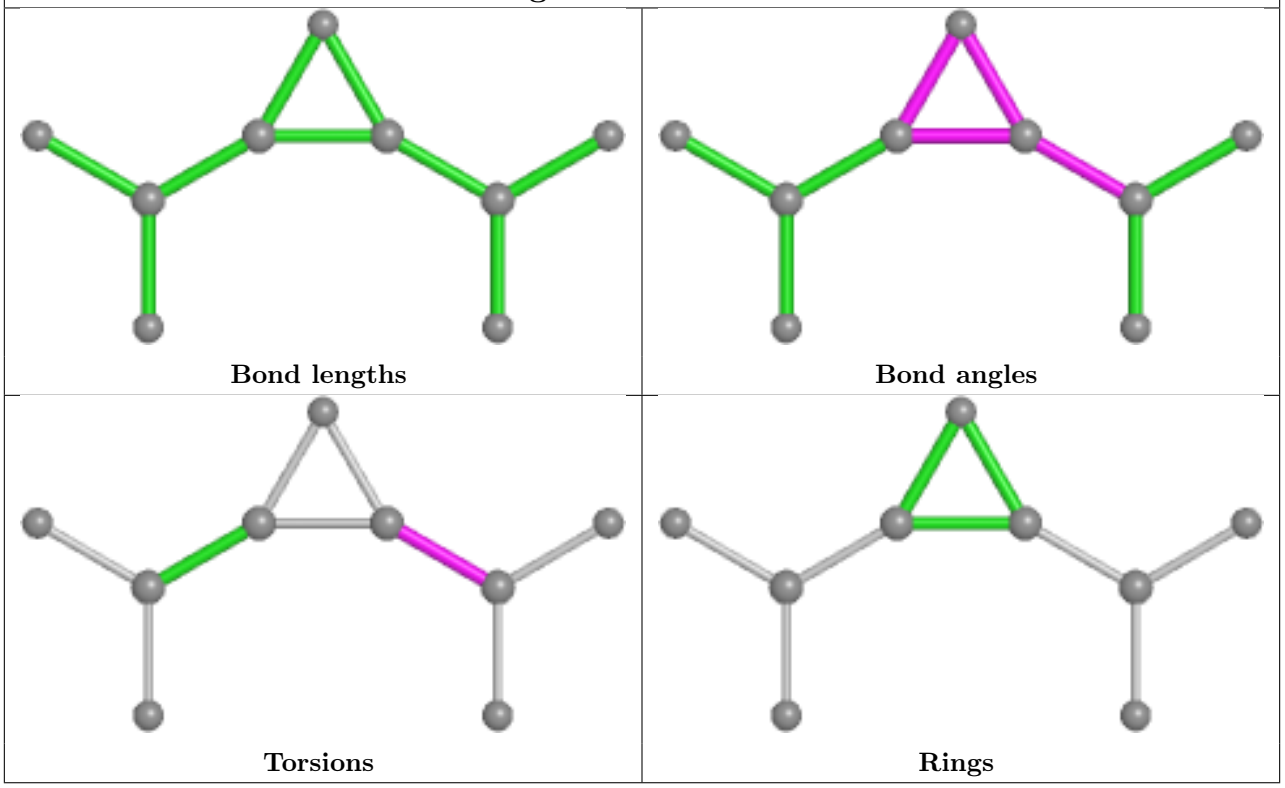
Mol	Chain	Res	Type	Atoms
6	R	501	U9S	O01-C02-C04-C05
6	R	501	U9S	O01-C02-C04-O09
6	R	501	U9S	O03-C02-C04-C05

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 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 U9S R 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.