



## Full wwPDB EM Validation Report ⓘ

Nov 9, 2025 – 12:13 AM JST

PDB ID : 9IJR / pdb\_00009ijr  
EMDB ID : EMD-60642  
Title : Cryo-EM structure of the orphan GPR52 beta-arrestin 1 complex bound to ligand c17  
Authors : Lin, X.; Xu, F.  
Deposited on : 2024-06-25  
Resolution : 3.86 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](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

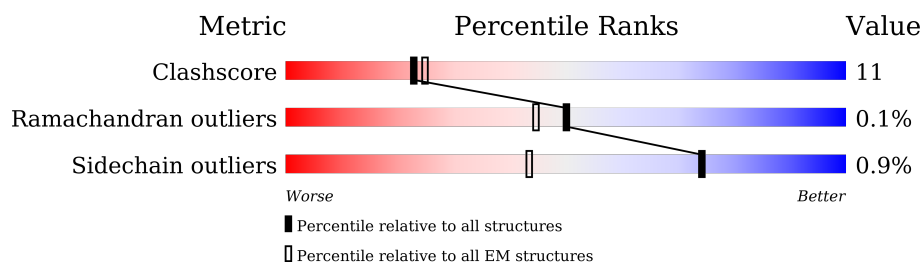
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.86 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  $\geq 3$ , 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	369	
2	C	393	
3	H	266	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6136 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 G-protein coupled receptor 52.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	295	Total	C	N	O	P	S	1	0
			2132	1379	342	394	5	12		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	TRP	ALA	conflict	UNP Q9Y2T5
A	314	PRO	CYS	conflict	UNP Q9Y2T5
A	474	ALA	-	expression tag	UNP Q9Y2T5
A	475	ARG	-	expression tag	UNP Q9Y2T5
A	476	GLY	-	expression tag	UNP Q9Y2T5
A	477	ARG	-	expression tag	UNP Q9Y2T5
A	478	PRO	-	expression tag	UNP Q9Y2T5
A	479	LEU	-	expression tag	UNP Q9Y2T5
A	480	PRO	-	expression tag	UNP Q9Y2T5
A	481	GLU	-	expression tag	UNP Q9Y2T5
A	482	THR	-	expression tag	UNP Q9Y2T5
A	483	GLY	-	expression tag	UNP Q9Y2T5
A	484	GLY	-	expression tag	UNP Q9Y2T5
A	485	GLY	-	expression tag	UNP Q9Y2T5
A	486	ASP	-	expression tag	UNP Q9Y2T5
A	487	GLU	-	expression tag	UNP Q9Y2T5
A	488	SEP	-	expression tag	UNP Q9Y2T5
A	489	ALA	-	expression tag	UNP Q9Y2T5
A	490	TPO	-	expression tag	UNP Q9Y2T5
A	491	TPO	-	expression tag	UNP Q9Y2T5
A	492	ALA	-	expression tag	UNP Q9Y2T5
A	493	SEP	-	expression tag	UNP Q9Y2T5
A	494	SEP	-	expression tag	UNP Q9Y2T5
A	495	SEP	-	expression tag	UNP Q9Y2T5
A	496	LEU	-	expression tag	UNP Q9Y2T5
A	497	ALA	-	expression tag	UNP Q9Y2T5
A	498	LYS	-	expression tag	UNP Q9Y2T5
A	499	ASP	-	expression tag	UNP Q9Y2T5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	500	THR	-	expression tag	UNP Q9Y2T5
A	501	SER	-	expression tag	UNP Q9Y2T5
A	502	SER	-	expression tag	UNP Q9Y2T5

- Molecule 2 is a protein called Beta-arrestin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	351	Total	C	N	O	S	0	0
			2427	1569	421	436	1		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-36	PHE	-	expression tag	UNP P49407
C	-35	VAL	-	expression tag	UNP P49407
C	-34	GLN	-	expression tag	UNP P49407
C	-33	PHE	-	expression tag	UNP P49407
C	-32	CYS	-	expression tag	UNP P49407
C	-31	ASN	-	expression tag	UNP P49407
C	-30	LYS	-	expression tag	UNP P49407
C	-29	LYS	-	expression tag	UNP P49407
C	-28	THR	-	expression tag	UNP P49407
C	-27	TYR	-	expression tag	UNP P49407
C	-26	LYS	-	expression tag	UNP P49407
C	-25	TYR	-	expression tag	UNP P49407
C	-24	SER	-	expression tag	UNP P49407
C	-23	GLY	-	expression tag	UNP P49407
C	-22	LEU	-	expression tag	UNP P49407
C	-21	PHE	-	expression tag	UNP P49407
C	-20	ILE	-	expression tag	UNP P49407
C	-19	PRO	-	expression tag	UNP P49407
C	-18	SER	-	expression tag	UNP P49407
C	-17	HIS	-	expression tag	UNP P49407
C	-16	HIS	-	expression tag	UNP P49407
C	-15	ARG	-	expression tag	UNP P49407
C	-14	ALA	-	expression tag	UNP P49407
C	-13	ARG	-	expression tag	UNP P49407
C	-12	ILE	-	expression tag	UNP P49407
C	-11	ARG	-	expression tag	UNP P49407
C	-10	ARG	-	expression tag	UNP P49407
C	-9	ALA	-	expression tag	UNP P49407
C	-8	MET	-	expression tag	UNP P49407

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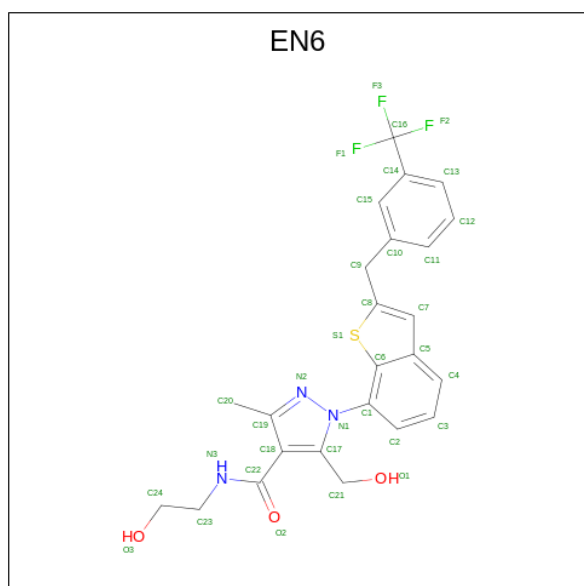
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP P49407
C	-6	SER	-	expression tag	UNP P49407
C	-5	PRO	-	expression tag	UNP P49407
C	-4	GLU	-	expression tag	UNP P49407
C	-3	PHE	-	expression tag	UNP P49407
C	-2	PRO	-	expression tag	UNP P49407
C	-1	GLY	-	expression tag	UNP P49407
C	0	ARG	-	expression tag	UNP P49407
C	1	LEU	-	expression tag	UNP P49407
C	59	VAL	CYS	conflict	UNP P49407
C	125	SER	CYS	conflict	UNP P49407
C	140	LEU	CYS	conflict	UNP P49407
C	150	VAL	CYS	conflict	UNP P49407
C	242	VAL	CYS	conflict	UNP P49407
C	251	VAL	CYS	conflict	UNP P49407
C	269	SER	CYS	conflict	UNP P49407

- Molecule 3 is a protein called scFv30 antibody.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	227	Total	C	N	O	S	0	0
			1543	976	261	302	4		

- Molecule 4 is N-(2-hydroxyethyl)-5-(hydroxymethyl)-3-methyl-1-[2-[[3-(trifluoromethyl)phenyl]methyl]-1-benzothiophen-7-yl]pyrazole-4-carboxamide (CCD ID: EN6) (formula: C<sub>24</sub>H<sub>22</sub>F<sub>3</sub>N<sub>3</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
4	A	1	34	24	3	3	3	1	0



P234				
F237				
K242				
K246				
ALA				
ALA				
ALA				



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218365	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: TPO, SEP, EN6

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	0.23	0/2124	0.47	1/2916 (0.0%)
2	C	0.20	0/2476	0.38	0/3402
3	H	0.15	0/1576	0.34	0/2159
All	All	0.20	0/6176	0.40	1/8477 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	PRO	CA-N-CD	-6.99	102.21	112.00

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	2132	0	1869	54	0
2	C	2427	0	2229	46	0
3	H	1543	0	1305	35	0
4	A	34	0	0	1	0
All	All	6136	0	5403	127	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 11.

All (127) 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)
1:A:322:SER:HA	1:A:325:ARG:HB2	1.73	0.70
1:A:36:VAL:HA	1:A:41:ILE:HD11	1.76	0.67
2:C:307:ARG:HG3	2:C:310:ALA:HB2	1.76	0.66
1:A:139:ARG:NH2	1:A:260:ASP:O	2.22	0.64
1:A:130:TRP:HD1	1:A:165:ILE:HG13	1.61	0.64
3:H:228:GLN:OE1	3:H:229:GLN:N	2.30	0.63
3:H:5:VAL:N	3:H:28:SER:O	2.31	0.63
2:C:25:ARG:HH21	2:C:293:LEU:HD22	1.66	0.60
1:A:491:TPO:O2P	2:C:11:LYS:NZ	2.35	0.59
2:C:315:LEU:HD22	2:C:318:ILE:HD11	1.84	0.59
3:H:50:TRP:NE1	3:H:53:SER:OG	2.28	0.59
2:C:179:GLY:N	2:C:206:GLU:OE2	2.22	0.59
2:C:186:THR:HB	2:C:345:VAL:HG22	1.83	0.59
1:A:280:PRO:HB2	1:A:302:THR:HG22	1.84	0.58
1:A:129:MET:HE1	1:A:275:TYR:HE1	1.67	0.57
1:A:257:HIS:HA	1:A:261:ARG:HD3	1.86	0.57
3:H:50:TRP:HE1	3:H:53:SER:HG	1.47	0.57
1:A:72:HIS:HA	2:C:247:ALA:HB2	1.86	0.56
2:C:29:ASP:OD2	2:C:170:LYS:NZ	2.33	0.56
1:A:496:LEU:O	2:C:6:THR:N	2.38	0.56
3:H:139:SER:OG	3:H:140:ASP:N	2.36	0.56
2:C:205:LYS:HG3	2:C:208:TYR:CE1	2.41	0.56
2:C:235:VAL:HG13	2:C:274:LEU:HD23	1.88	0.55
2:C:77:LYS:HD3	2:C:243:LEU:HD11	1.89	0.55
1:A:139:ARG:O	1:A:139:ARG:HD3	2.06	0.55
1:A:139:ARG:HH22	1:A:264:ALA:N	2.05	0.55
1:A:134:CYS:HA	1:A:137:VAL:HG12	1.89	0.54
1:A:494:SEP:OG	1:A:495:SEP:N	2.39	0.54
1:A:309:ASN:OD1	1:A:310:SER:N	2.41	0.53
3:H:216:SER:OG	3:H:218:GLN:OE1	2.26	0.53
1:A:129:MET:HE3	1:A:215:ALA:HB1	1.92	0.52
2:C:294:LYS:O	2:C:295:HIS:ND1	2.43	0.52
1:A:491:TPO:O1P	2:C:25:ARG:NH1	2.42	0.52
1:A:284:TYR:HE2	1:A:299:SER:HB3	1.75	0.52
2:C:214:ILE:N	2:C:274:LEU:O	2.43	0.51
2:C:182:PRO:HG2	2:C:203:LEU:HD12	1.92	0.51
2:C:282:ARG:NH2	3:H:60:TYR:OH	2.45	0.50
1:A:258:SER:H	1:A:261:ARG:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:ASN:OD1	2:C:299:ASN:N	2.37	0.50
1:A:300:PHE:HB2	4:A:601:EN6:C4	2.42	0.50
2:C:53:VAL:O	2:C:86:SER:OG	2.27	0.49
1:A:87:ASP:O	1:A:90:VAL:HG12	2.12	0.49
3:H:177:GLN:O	3:H:224:THR:OG1	2.30	0.49
2:C:6:THR:OG1	2:C:7:ARG:N	2.40	0.49
3:H:22:ARG:HA	3:H:85:GLN:HA	1.94	0.49
1:A:269:ARG:O	1:A:273:VAL:HG22	2.13	0.49
3:H:144:THR:O	3:H:163:ARG:N	2.42	0.48
2:C:214:ILE:HB	2:C:274:LEU:HB3	1.95	0.48
2:C:301:ALA:HB1	2:C:319:VAL:HG21	1.95	0.48
2:C:197:LEU:HB2	2:C:222:ASN:HA	1.95	0.47
1:A:201:ALA:HA	1:A:204:THR:HG22	1.96	0.47
2:C:210:HIS:HA	2:C:351:LEU:HD11	1.95	0.47
3:H:42:GLN:HA	3:H:48:LEU:HA	1.97	0.47
1:A:75:THR:HG21	1:A:149:TYR:HE1	1.80	0.47
2:C:78:ASP:OD1	2:C:78:ASP:N	2.40	0.47
2:C:215:SER:O	2:C:215:SER:OG	2.28	0.47
1:A:223:TYR:HE2	1:A:268:PHE:HA	1.80	0.47
3:H:157:ARG:HA	3:H:215:SER:HA	1.97	0.47
1:A:125:LYS:NZ	1:A:306:ALA:O	2.46	0.47
1:A:139:ARG:HH12	1:A:264:ALA:HA	1.80	0.46
2:C:22:LEU:HD13	2:C:166:LEU:HD11	1.96	0.46
1:A:117:PHE:O	1:A:121:ILE:HG22	2.16	0.46
1:A:303:THR:O	1:A:307:ILE:HG22	2.16	0.46
2:C:21:TYR:HE2	2:C:108:LEU:HD11	1.80	0.46
2:C:12:ALA:HA	2:C:19:THR:HA	1.97	0.46
1:A:162:ILE:O	1:A:165:ILE:HG22	2.15	0.46
1:A:495:SEP:O	2:C:107:LYS:NZ	2.40	0.46
1:A:70:LEU:HD22	1:A:72:HIS:HB3	1.99	0.45
1:A:130:TRP:HH2	1:A:214:PRO:HB2	1.81	0.45
1:A:182:LYS:HB3	1:A:197:TRP:CD2	2.52	0.45
3:H:35:SER:HB3	3:H:101:ARG:HG3	1.99	0.45
3:H:171:ALA:HB1	3:H:230:TYR:CE2	2.51	0.45
3:H:177:GLN:HB2	3:H:183:PRO:HB3	1.97	0.45
1:A:225:HIS:O	1:A:229:ILE:HG13	2.16	0.45
2:C:37:VAL:HG22	2:C:117:PHE:HB2	1.99	0.45
3:H:147:PRO:HD2	3:H:160:ILE:HG23	1.99	0.45
1:A:58:ASN:HD22	1:A:58:ASN:HA	1.56	0.44
3:H:64:ALA:HB3	3:H:67:VAL:HG23	2.00	0.44
3:H:91:ALA:HA	3:H:121:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:200:ARG:NH2	3:H:214:ILE:HA	2.32	0.44
2:C:13:SER:N	2:C:18:LEU:O	2.50	0.44
2:C:198:HIS:ND1	2:C:198:HIS:C	2.74	0.44
3:H:48:LEU:H	3:H:48:LEU:HD12	1.83	0.44
1:A:320:SER:OG	1:A:321:ASN:N	2.51	0.43
2:C:173:TYR:C	2:C:352:MET:HE1	2.43	0.43
3:H:48:LEU:HB2	3:H:237:PHE:CD2	2.53	0.43
1:A:190:PHE:HB2	1:A:193:CYS:SG	2.58	0.43
1:A:211:LEU:HD22	1:A:212:TYR:CE1	2.53	0.43
3:H:139:SER:OG	3:H:140:ASP:OD1	2.36	0.43
2:C:321:TYR:CE2	2:C:351:LEU:HD23	2.54	0.43
3:H:221:ASP:N	3:H:221:ASP:OD1	2.52	0.43
1:A:58:ASN:HB3	1:A:88:LEU:HB2	2.00	0.43
2:C:235:VAL:HG23	2:C:253:VAL:HB	2.01	0.43
1:A:47:ILE:O	1:A:51:THR:HG23	2.19	0.43
3:H:200:ARG:HH21	3:H:201:PHE:HD1	1.67	0.43
2:C:342:ASP:OD1	2:C:342:ASP:N	2.52	0.42
3:H:144:THR:OG1	3:H:163:ARG:O	2.35	0.42
1:A:261:ARG:HH21	1:A:262:ARG:HA	1.85	0.42
1:A:261:ARG:NH2	1:A:262:ARG:HA	2.34	0.42
1:A:100:SER:O	1:A:100:SER:OG	2.32	0.42
2:C:128:THR:HG21	2:C:292:LYS:HB2	2.02	0.42
2:C:303:SER:H	2:C:352:MET:HB3	1.85	0.42
2:C:237:GLN:NE2	2:C:321:TYR:OH	2.52	0.42
3:H:73:ILE:HB	3:H:84:LEU:HD13	2.01	0.42
2:C:34:VAL:HG11	2:C:119:ILE:HB	2.02	0.42
1:A:44:THR:HA	1:A:47:ILE:HG13	2.01	0.41
1:A:70:LEU:HD11	2:C:243:LEU:HD22	2.02	0.41
1:A:129:MET:HE1	1:A:275:TYR:CE1	2.51	0.41
2:C:208:TYR:CE2	2:C:214:ILE:HD13	2.55	0.41
1:A:257:HIS:HD1	1:A:261:ARG:HD3	1.84	0.41
2:C:210:HIS:HB3	3:H:105:PHE:HE2	1.85	0.41
3:H:102:SER:HB3	3:H:110:LEU:HD13	2.02	0.41
3:H:176:GLN:HB2	3:H:186:LEU:HD11	2.02	0.41
3:H:67:VAL:HG13	3:H:71:PHE:HD2	1.84	0.41
3:H:231:LYS:HA	3:H:231:LYS:HD2	1.71	0.41
1:A:124:LEU:O	1:A:127:VAL:HG12	2.21	0.41
1:A:126:SER:HB2	1:A:211:LEU:HD11	2.03	0.41
2:C:321:TYR:HE2	2:C:351:LEU:HD23	1.85	0.41
3:H:200:ARG:NH1	3:H:215:SER:H	2.18	0.41
1:A:127:VAL:HG21	1:A:166:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:CYS:HB3	1:A:197:TRP:HE3	1.85	0.41
1:A:94:CYS:C	1:A:97:PRO:HD2	2.47	0.40
3:H:36:SER:O	3:H:36:SER:OG	2.39	0.40
3:H:101:ARG:HD3	3:H:112:TYR:HD2	1.86	0.40
1:A:189:ILE:HD12	1:A:189:ILE:HA	1.89	0.40
2:C:79:LEU:H	2:C:79:LEU:HD12	1.85	0.40
3:H:224:THR:HG22	3:H:242:LYS:HA	2.04	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	283/369 (77%)	256 (90%)	27 (10%)	0	100	100
2	C	349/393 (89%)	319 (91%)	30 (9%)	0	100	100
3	H	223/266 (84%)	217 (97%)	5 (2%)	1 (0%)	30	65
All	All	855/1028 (83%)	792 (93%)	62 (7%)	1 (0%)	50	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	234	PRO

### 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	193/327 (59%)	192 (100%)	1 (0%)	86	90
2	C	214/346 (62%)	211 (99%)	3 (1%)	62	75
3	H	132/207 (64%)	131 (99%)	1 (1%)	79	84
All	All	539/880 (61%)	534 (99%)	5 (1%)	74	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
2	C	26	ASP
2	C	150	VAL
2	C	198	HIS
3	H	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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$
1	SEP	A	494	1	8,9,10	1.52	1 (12%)	8,12,14	1.53	2 (25%)
1	SEP	A	493	1	8,9,10	1.52	1 (12%)	8,12,14	1.70	2 (25%)
1	TPO	A	491	1	8,10,11	1.03	0	10,14,16	1.79	2 (20%)
1	SEP	A	488	1	8,9,10	1.53	1 (12%)	8,12,14	1.87	2 (25%)
1	TPO	A	490	1	3,4,11	0.69	0	2,4,16	0.88	0
1	SEP	A	495	1	8,9,10	1.54	1 (12%)	8,12,14	1.59	2 (25%)

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
1	SEP	A	494	1	-	2/5/8/10	-
1	SEP	A	493	1	-	2/5/8/10	-
1	TPO	A	491	1	-	1/9/11/13	-
1	SEP	A	488	1	-	0/5/8/10	-
1	TPO	A	490	1	-	0/0/2/13	-
1	SEP	A	495	1	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	495	SEP	P-O1P	3.35	1.61	1.50
1	A	488	SEP	P-O1P	3.34	1.61	1.50
1	A	493	SEP	P-O1P	3.32	1.61	1.50
1	A	494	SEP	P-O1P	3.30	1.61	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	TPO	P-OG1-CB	-4.74	108.90	123.21
1	A	488	SEP	P-OG-CB	-3.49	108.68	118.30
1	A	488	SEP	OG-CB-CA	3.47	111.53	108.14
1	A	493	SEP	P-OG-CB	-3.29	109.24	118.30
1	A	494	SEP	P-OG-CB	-3.10	109.76	118.30
1	A	493	SEP	OG-CB-CA	2.97	111.03	108.14
1	A	495	SEP	P-OG-CB	-2.95	110.18	118.30
1	A	495	SEP	OG-CB-CA	2.80	110.87	108.14
1	A	494	SEP	OG-CB-CA	2.35	110.43	108.14
1	A	491	TPO	CG2-CB-CA	-2.33	108.56	113.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	493	SEP	CB-OG-P-O2P
1	A	494	SEP	N-CA-CB-OG
1	A	493	SEP	CB-OG-P-O3P
1	A	494	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
1	A	491	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	494	SEP	1	0
1	A	491	TPO	2	0
1	A	495	SEP	2	0

## 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	$\# Z  > 2$
4	EN6	A	601	-	32,37,37	1.29	2 (6%)	35,54,54	1.49	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EN6	A	601	-	-	3/16/24/24	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	EN6	C22-N3	5.43	1.45	1.33
4	A	601	EN6	O2-C22	-2.19	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	EN6	C1-C6-S1	4.64	133.64	124.94
4	A	601	EN6	C20-C19-N2	3.09	126.44	119.78
4	A	601	EN6	C17-C18-C19	2.74	107.22	103.88
4	A	601	EN6	C4-C5-C7	-2.53	124.39	133.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

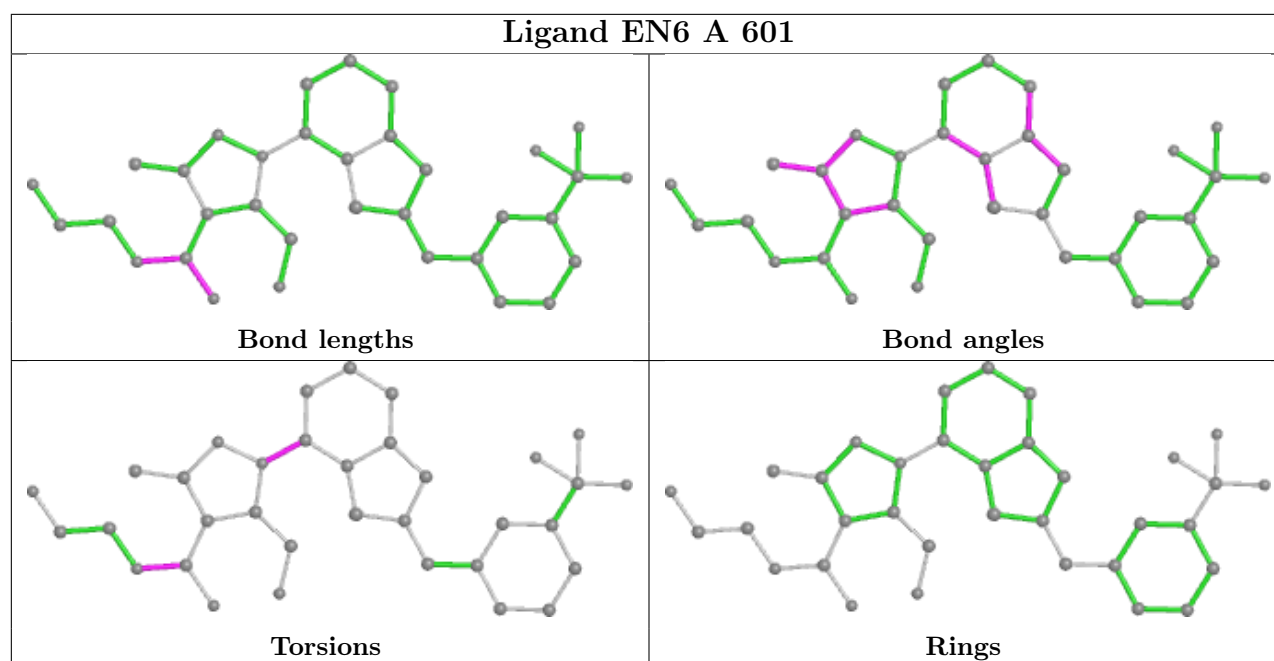
Mol	Chain	Res	Type	Atoms
4	A	601	EN6	O2-C22-N3-C23
4	A	601	EN6	C18-C22-N3-C23
4	A	601	EN6	C2-C1-N1-N2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	EN6	1	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.