Full wwPDB EM Validation Report

Jul 8, 2025 – 03:02 PM JST

PDB ID	:	8YKY / pdb_00008yky
EMDB ID	:	EMD-39376
Title	:	Structure of human class T GPCR TAS2R14-Ggustducin complex with agonist 28.1
Authors	:	Hu, X.L.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on	:	2024-03-05
Resolution	:	2.99 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:

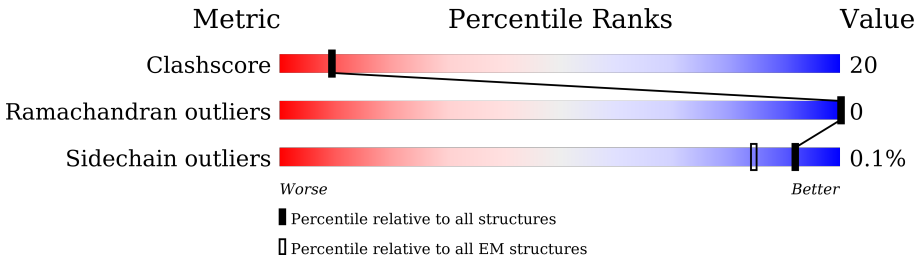
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 2.99 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	369	35% 24% 41%
2	B	366	54% 38% 8%
3	C	71	59% 20% 21%
4	S	286	45% 36% 19%
5	R	990	17% 11% 73%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8800 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 alpha gustducin protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	217	Total	C	N	O	S	0	0
			1749	1113	295	328	13		

- 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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 protein.

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	270	Total	C	N	O	S	0	0
			2188	1481	350	346	11		

There are 50 discrepancies between the modelled and reference sequences:

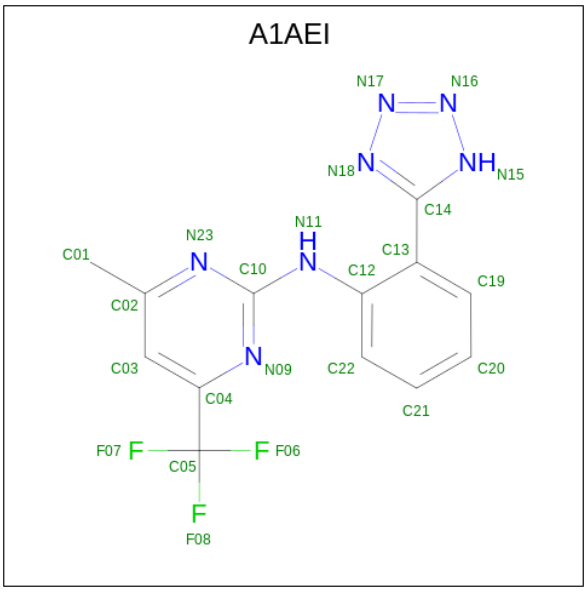
Chain	Residue	Modelled	Actual	Comment	Reference
R	-499	MET	-	initiating methionine	UNP Q59310
R	-498	LYS	-	expression tag	UNP Q59310
R	-497	THR	-	expression tag	UNP Q59310
R	-496	ILE	-	expression tag	UNP Q59310
R	-495	ILE	-	expression tag	UNP Q59310
R	-494	ALA	-	expression tag	UNP Q59310
R	-493	LEU	-	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

Continued on next page...

Continued from previous page...

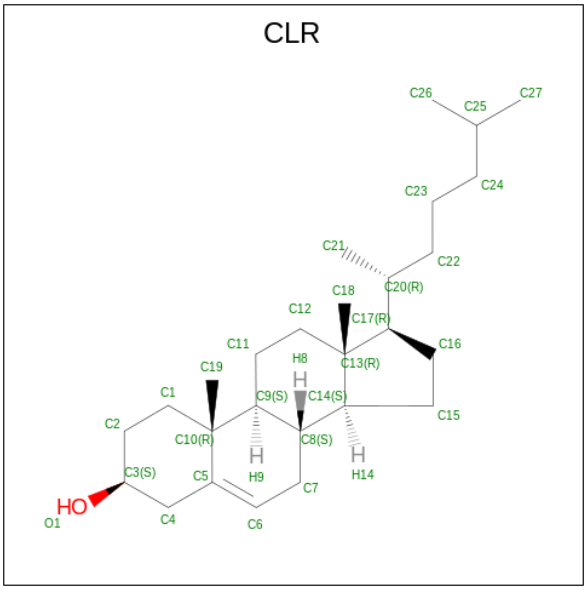
Chain	Residue	Modelled	Actual	Comment	Reference
R	-486	VAL	-	expression tag	UNP Q59310
R	-485	PHE	-	expression tag	UNP Q59310
R	-484	ALA	-	expression tag	UNP Q59310
R	-483	ASP	-	expression tag	UNP Q59310
R	-482	TYR	-	expression tag	UNP Q59310
R	-481	LYS	-	expression tag	UNP Q59310
R	-480	ASP	-	expression 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
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 4-methyl-N-[(2M)-2-(1H-tetrazol-5-yl)phenyl]-6-(trifluoromethyl)pyrimidin-2-amine (CCD ID: A1AEI) (formula: $C_{13}H_{10}F_3N_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	F	N	
6	R	1	23	13	3	7	0

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



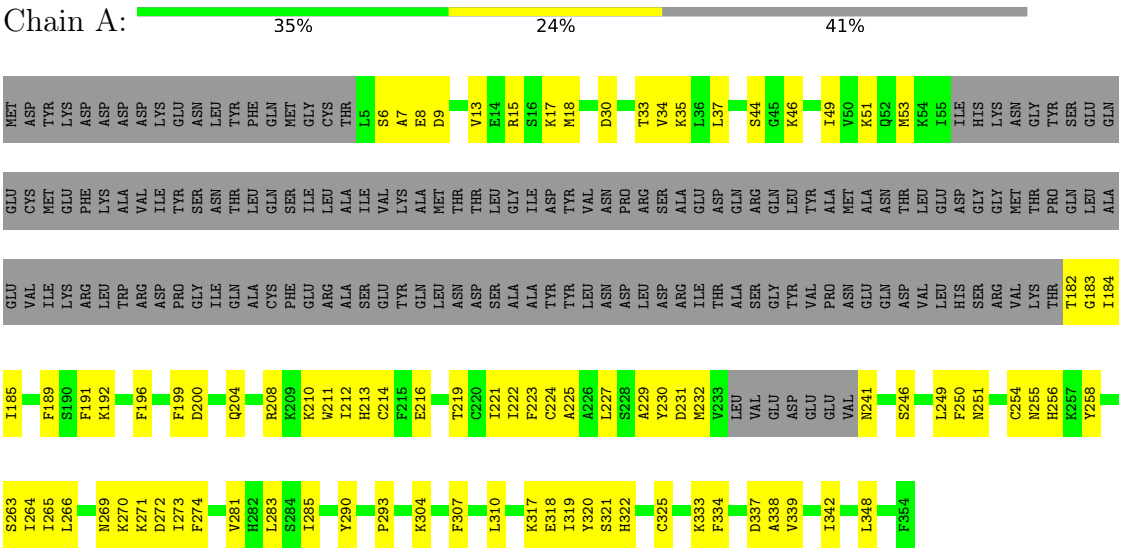
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	R	1	28	27	1	0

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.

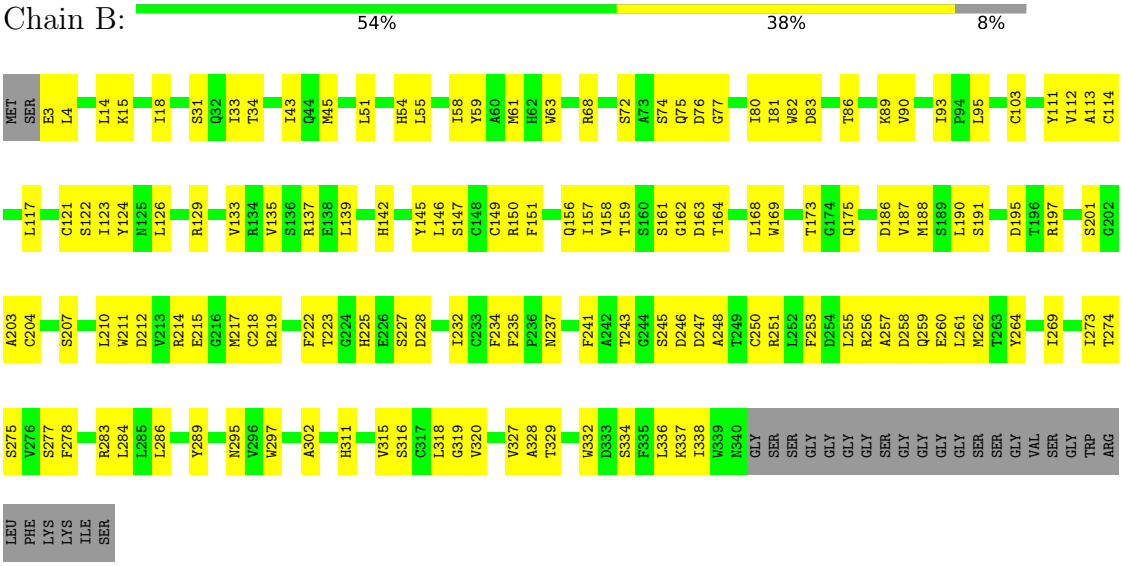
• Molecule 1: G alpha gustducin protein

Chain A:



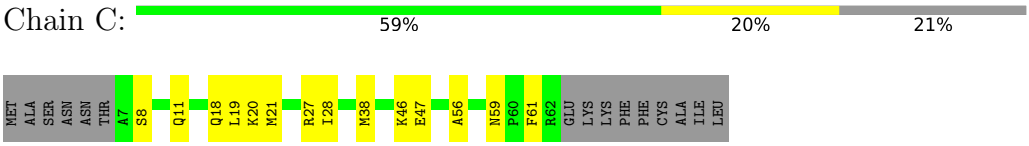
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



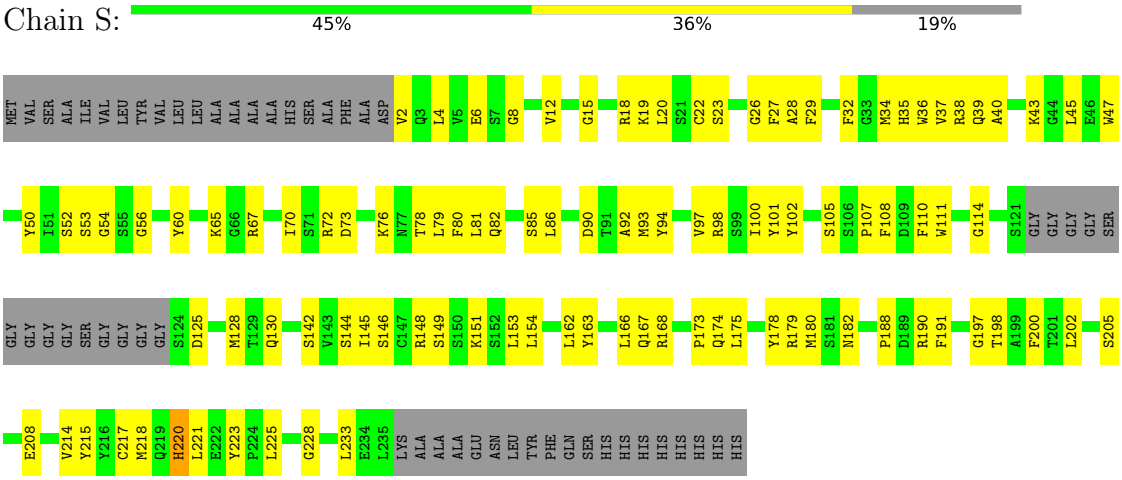
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:



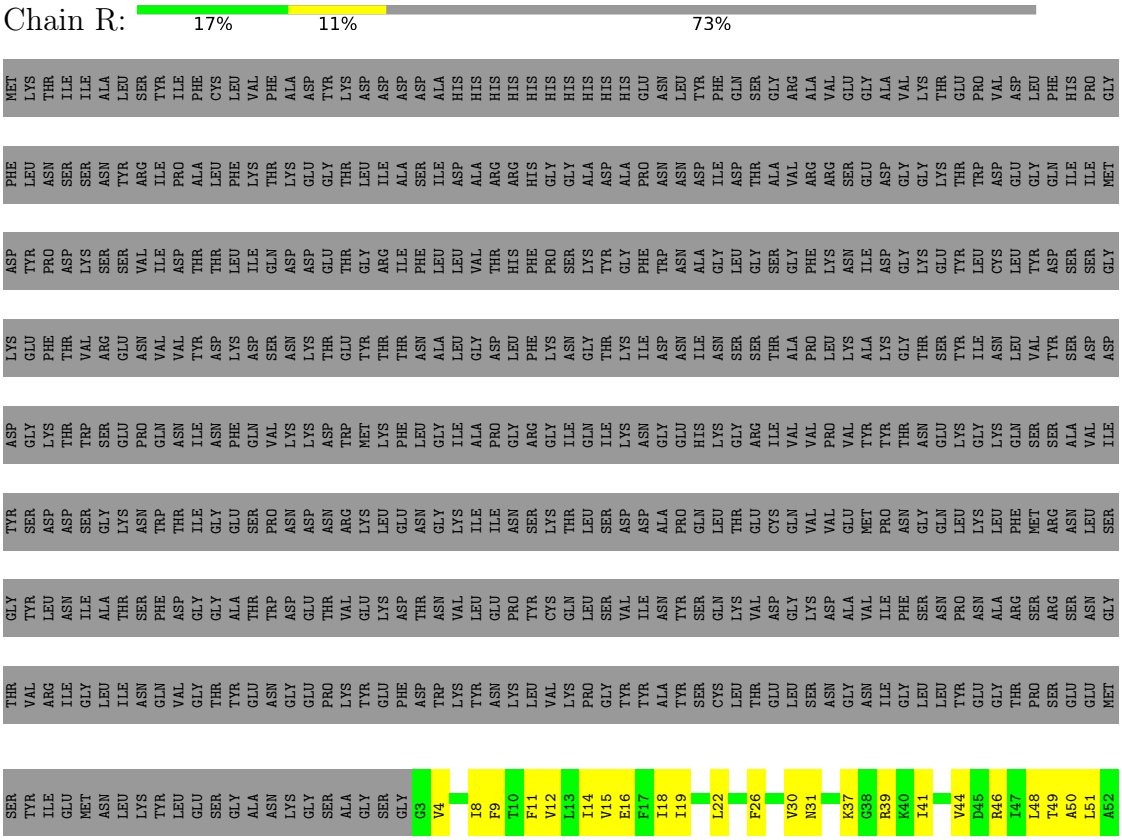
• Molecule 4: ScFv16 protein

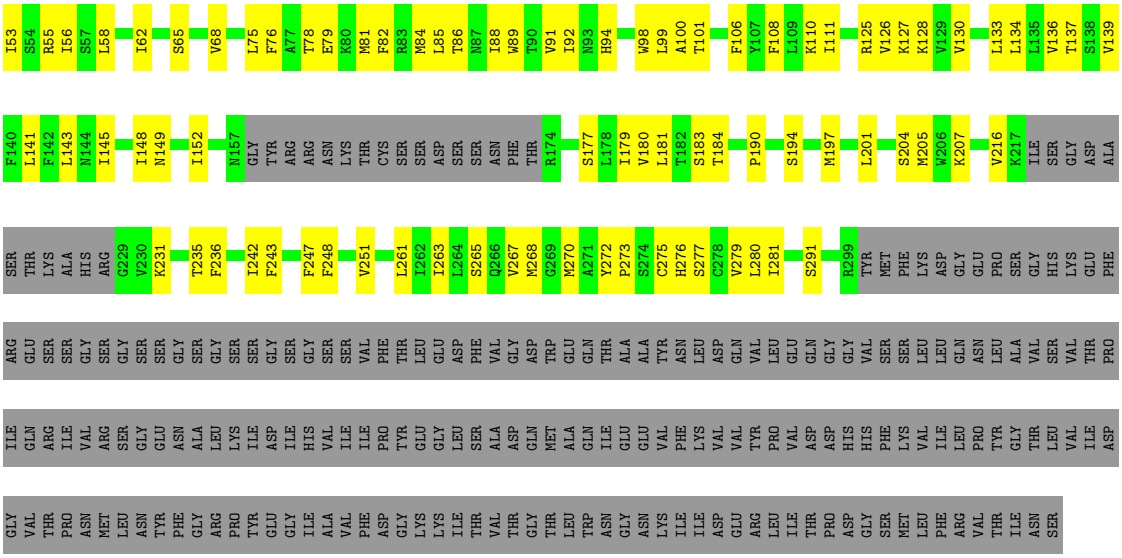
Chain S:



• Molecule 5: exo-alpha-sialidase,Taste receptor type 2 member 14,LgBit

Chain R:




I53 S54 R55 I56 S57 L58 I62 S65 V68 L75 F76 A77 T78 E79 K80 M81 F82 R83 M84 L85 T86 N87 I88 W89 T90 V91 I92 N93 H94 W98 L99 A100 T101 F106 Y107 F108 L109 K110 I111 R125 V126 K127 K128 V129 V130 L133 L134 L135 V136 T137 S138 V139
F140 L141 F142 L143 N144 I145 I148 N149 I152 N157 GLY TYR ARG ARG ASN LYS THR CYS SER SER ASP SER SER ASN PHE THR R174 S177 L178 I179 V180 L181 T182 S183 T184 P190 S194 M197 L201 S204 M205 W206 K207 V216 K217 ILE SER GLY ASP ALA
SER THR LYS ALA HIS ARG G229 V230 K231 T235 F236 I242 F243 F247 F248 V251 L261 I262 I263 L264 S265 Q266 V267 M268 G269 M270 A271 Y272 P273 S274 C275 H276 S277 C278 V279 L280 I281 S291 R299 TYR MET PHE LYS ASP GLY GLU PRO SER GLY HIS LYS GLU PHE
ARG GLU SER SER GLY SER GLY SER SER GLY SER GLY SER SER GLY SER GLY SER SER VAL PHE THR LEU GLU 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 LEU 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 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	174503	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 ($e^-/Å^2$)	57.69	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AEI, 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	0.17	0/1778	0.39	0/2382
2	B	0.20	0/2647	0.33	0/3589
3	C	0.22	0/435	0.26	0/587
4	S	0.17	0/1827	0.36	0/2477
5	R	0.15	0/2242	0.36	0/3038
All	All	0.18	0/8929	0.35	0/12073

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	1749	0	1745	72	0
2	B	2600	0	2505	112	0
3	C	429	0	441	16	0
4	S	1783	0	1717	90	0
5	R	2188	0	2329	84	0
6	R	23	0	0	1	0
7	R	28	0	46	7	0
All	All	8800	0	8783	350	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 20.

All (350) 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)
4:S:34:MET:SD	4:S:79:LEU:HD22	1.54	1.45
4:S:34:MET:SD	4:S:79:LEU:CD2	2.38	1.11
4:S:29:PHE:CZ	4:S:34:MET:HE1	1.91	1.05
4:S:29:PHE:CE1	4:S:34:MET:HE1	1.91	1.05
4:S:34:MET:SD	4:S:79:LEU:HD13	2.01	1.01
5:R:268:MET:HE1	7:R:502:CLR:H231	1.61	0.80
5:R:48:LEU:HD22	5:R:280:LEU:HD21	1.62	0.80
1:A:8:GLU:OE2	4:S:163:TYR:OH	2.01	0.79
4:S:34:MET:SD	4:S:79:LEU:CD1	2.71	0.78
4:S:40:ALA:HB3	4:S:43:LYS:HB2	1.66	0.77
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.17	0.77
2:B:253:PHE:CE2	2:B:260:GLU:HG3	2.20	0.75
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.68	0.74
1:A:15:ARG:NH1	2:B:90:VAL:O	2.19	0.74
4:S:29:PHE:CE1	4:S:34:MET:CE	2.73	0.71
1:A:320:TYR:HE1	1:A:342:ILE:HD11	1.58	0.68
5:R:101:THR:HG23	5:R:194:SER:HB2	1.74	0.68
4:S:175:LEU:HD21	4:S:178:TYR:HB3	1.75	0.67
2:B:173:THR:O	2:B:175:GLN:NE2	2.27	0.67
2:B:90:VAL:HG22	4:S:102:TYR:HB2	1.77	0.67
2:B:275:SER:HB2	2:B:318:LEU:HB3	1.75	0.67
4:S:34:MET:SD	4:S:79:LEU:CG	2.83	0.67
4:S:72:ARG:HB3	4:S:79:LEU:HD12	1.77	0.66
1:A:34:VAL:HG13	1:A:219:THR:HG23	1.77	0.65
4:S:130:GLN:NE2	4:S:217:CYS:SG	2.65	0.65
2:B:149:CYS:HB2	2:B:157:ILE:HD11	1.79	0.64
1:A:30:ASP:HA	1:A:33:THR:HB	1.77	0.64
4:S:93:MET:HE2	4:S:114:GLY:HA3	1.79	0.64
5:R:94:HIS:HE2	5:R:137:THR:HG1	1.34	0.64
5:R:79:GLU:HA	5:R:82:PHE:HB3	1.79	0.64
2:B:274:THR:OG1	2:B:315:VAL:O	2.16	0.64
4:S:168:ARG:NH2	4:S:174:GLN:OE1	2.29	0.63
1:A:191:PHE:HE2	1:A:333:LYS:HA	1.63	0.63
4:S:19:LYS:HE2	4:S:80:PHE:HB3	1.79	0.62
5:R:89:TRP:CZ3	7:R:502:CLR:H181	2.34	0.62
2:B:156:GLN:HG2	2:B:168:LEU:HD11	1.81	0.62
1:A:49:ILE:HD13	1:A:269:ASN:HD21	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:261:LEU:O	5:R:265:SER:HB3	1.98	0.62
2:B:112:VAL:HG13	2:B:126:LEU:HD11	1.81	0.62
2:B:150:ARG:HB2	2:B:190:LEU:HD11	1.81	0.62
5:R:247:PHE:HD2	5:R:268:MET:HG3	1.65	0.62
2:B:258:ASP:OD1	3:C:27:ARG:NH1	2.32	0.62
1:A:184:ILE:HD13	2:B:117:LEU:HB2	1.81	0.61
1:A:214:CYS:SG	2:B:75:GLN:NE2	2.73	0.61
2:B:187:VAL:HA	2:B:203:ALA:HA	1.81	0.61
1:A:263:SER:OG	1:A:318:GLU:O	2.18	0.61
2:B:204:CYS:HA	2:B:228:ASP:HB2	1.82	0.60
5:R:94:HIS:NE2	5:R:137:THR:OG1	2.28	0.60
5:R:75:LEU:O	5:R:78:THR:OG1	2.19	0.60
5:R:12:VAL:HA	5:R:15:VAL:HG12	1.84	0.60
2:B:111:TYR:CD2	2:B:123:ILE:HG22	2.37	0.60
4:S:52:SER:HB2	4:S:56:GLY:H	1.66	0.60
2:B:68:ARG:NE	2:B:83:ASP:OD1	2.36	0.59
4:S:130:GLN:HG3	4:S:228:GLY:HA3	1.84	0.59
1:A:270:LYS:HB3	1:A:273:ILE:HD13	1.84	0.59
2:B:114:CYS:HG	2:B:124:TYR:HE1	1.50	0.59
2:B:215:GLU:HB3	2:B:217:MET:HE1	1.84	0.58
3:C:11:GLN:OE1	3:C:11:GLN:N	2.26	0.58
1:A:37:LEU:HB3	1:A:221:ILE:HD13	1.84	0.58
5:R:55:ARG:HB3	5:R:273:PRO:HB3	1.85	0.58
1:A:44:SER:HB2	1:A:225:ALA:HA	1.85	0.58
4:S:35:HIS:NE2	4:S:223:TYR:OH	2.35	0.58
1:A:273:ILE:H	1:A:273:ILE:HD12	1.67	0.58
2:B:58:ILE:HD13	2:B:336:LEU:HG	1.85	0.58
4:S:6:GLU:HA	4:S:22:CYS:HA	1.84	0.58
1:A:216:GLU:OE1	1:A:258:TYR:HB3	2.04	0.58
2:B:251:ARG:HH21	2:B:260:GLU:HG2	1.69	0.57
1:A:13:VAL:HG12	1:A:17:LYS:NZ	2.19	0.57
4:S:163:TYR:N	4:S:218:MET:O	2.35	0.56
2:B:311:HIS:NE2	2:B:329:THR:O	2.39	0.56
4:S:35:HIS:HB2	4:S:97:VAL:HB	1.87	0.56
2:B:114:CYS:SG	2:B:122:SER:HB2	2.46	0.56
4:S:149:SER:OG	4:S:151:LYS:O	2.22	0.56
2:B:77:GLY:HA2	2:B:95:LEU:HD12	1.89	0.55
4:S:188:PRO:HG2	4:S:191:PHE:HE1	1.71	0.55
2:B:212:ASP:OD2	2:B:219:ARG:NH1	2.38	0.55
4:S:67:ARG:NH1	4:S:90:ASP:OD2	2.38	0.55
1:A:222:ILE:HG12	1:A:265:ILE:HB	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:125:ARG:HD3	5:R:128:LYS:HD3	1.87	0.55
1:A:7:ALA:N	4:S:221:LEU:O	2.39	0.55
2:B:74:SER:OG	2:B:76:ASP:OD1	2.24	0.55
5:R:62:ILE:HG13	5:R:270:MET:HB2	1.89	0.55
1:A:338:ALA:O	1:A:342:ILE:HG12	2.07	0.55
5:R:277:SER:O	5:R:281:ILE:HG23	2.07	0.55
4:S:23:SER:HA	4:S:78:THR:HA	1.87	0.55
1:A:232:MET:HE3	1:A:232:MET:H	1.72	0.54
5:R:272:TYR:HB3	5:R:273:PRO:HD3	1.89	0.54
1:A:254:CYS:SG	1:A:255:ASN:N	2.80	0.54
2:B:158:VAL:HG12	2:B:190:LEU:HD22	1.89	0.54
4:S:163:TYR:HB2	4:S:218:MET:HB3	1.90	0.54
5:R:263:ILE:O	5:R:267:VAL:HG12	2.08	0.54
5:R:51:LEU:HD13	5:R:99:LEU:HB3	1.88	0.54
2:B:15:LYS:O	2:B:18:ILE:HG13	2.07	0.54
2:B:311:HIS:CE1	2:B:337:LYS:HD3	2.42	0.54
4:S:108:PHE:HB3	4:S:111:TRP:HE1	1.73	0.53
4:S:215:TYR:CE1	4:S:233:LEU:HD22	2.43	0.53
5:R:106:PHE:HE1	5:R:127:LYS:HG3	1.72	0.53
1:A:13:VAL:HG12	1:A:17:LYS:HZ2	1.72	0.53
5:R:133:LEU:HA	5:R:136:VAL:HG12	1.90	0.53
2:B:61:MET:HE1	2:B:319:GLY:N	2.23	0.53
2:B:227:SER:HB3	2:B:245:SER:HB3	1.91	0.53
4:S:2:VAL:HG21	4:S:98:ARG:HH11	1.74	0.53
4:S:73:ASP:HB3	4:S:76:LYS:HB2	1.90	0.53
1:A:191:PHE:CE1	1:A:192:LYS:HD3	2.44	0.53
2:B:277:SER:HB3	2:B:320:VAL:HG23	1.90	0.53
5:R:184:THR:HA	7:R:502:CLR:H242	1.91	0.53
2:B:54:HIS:CE1	2:B:80:ILE:HD12	2.43	0.53
5:R:94:HIS:CE1	5:R:141:LEU:HB2	2.44	0.52
1:A:272:ASP:OD1	1:A:272:ASP:N	2.42	0.52
2:B:334:SER:O	2:B:334:SER:OG	2.24	0.52
4:S:145:ILE:HG22	4:S:202:LEU:HB3	1.91	0.52
1:A:213:HIS:HB3	1:A:258:TYR:CE2	2.44	0.52
4:S:29:PHE:CZ	4:S:34:MET:CE	2.79	0.52
4:S:38:ARG:HB2	4:S:92:ALA:HB3	1.92	0.52
5:R:180:VAL:HG23	7:R:502:CLR:H212	1.89	0.52
5:R:15:VAL:O	5:R:18:ILE:HG13	2.08	0.52
3:C:8:SER:HA	3:C:11:GLN:NE2	2.24	0.52
5:R:65:SER:HB2	5:R:85:LEU:HD11	1.92	0.52
1:A:348:LEU:HG	5:R:111:ILE:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ARG:O	4:S:98:ARG:NH1	2.43	0.52
2:B:207:SER:HB2	2:B:223:THR:HG22	1.90	0.52
4:S:125:ASP:OD1	4:S:125:ASP:N	2.40	0.52
4:S:128:MET:HE1	4:S:153:LEU:HD11	1.92	0.52
2:B:18:ILE:HG22	3:C:27:ARG:HH22	1.75	0.52
1:A:13:VAL:O	1:A:17:LYS:HG3	2.10	0.51
1:A:229:ALA:HA	1:A:232:MET:SD	2.49	0.51
5:R:62:ILE:HD11	5:R:89:TRP:CD1	2.45	0.51
2:B:90:VAL:HG13	4:S:102:TYR:CD2	2.45	0.51
2:B:111:TYR:HD2	2:B:123:ILE:HG22	1.73	0.51
2:B:262:MET:HE3	2:B:302:ALA:HB2	1.91	0.51
5:R:148:ILE:HD11	5:R:179:ILE:HG23	1.92	0.51
5:R:270:MET:O	5:R:273:PRO:HD2	2.09	0.51
4:S:146:SER:HA	4:S:200:PHE:O	2.10	0.51
2:B:159:THR:OG1	2:B:169:TRP:NE1	2.39	0.51
5:R:76:PHE:HA	5:R:81:MET:HE2	1.92	0.50
6:R:501:A1AEI:N11	6:R:501:A1AEI:N15	2.58	0.50
4:S:36:TRP:CZ3	4:S:94:TYR:HB3	2.46	0.50
4:S:60:TYR:HB2	4:S:65:LYS:HD2	1.94	0.50
5:R:18:ILE:O	5:R:22:LEU:HG	2.11	0.50
5:R:98:TRP:CE2	5:R:190:PRO:HB3	2.46	0.50
5:R:108:PHE:HA	5:R:201:LEU:HD21	1.93	0.50
5:R:242:ILE:HG13	5:R:243:PHE:HD1	1.75	0.50
5:R:50:ALA:O	5:R:53:ILE:HG13	2.11	0.50
4:S:70:ILE:HG12	4:S:81:LEU:HD12	1.93	0.50
5:R:26:PHE:O	5:R:30:VAL:HG13	2.11	0.50
4:S:52:SER:O	4:S:72:ARG:NH1	2.44	0.50
5:R:4:VAL:O	5:R:8:ILE:HG13	2.11	0.50
1:A:246:SER:O	1:A:249:LEU:HD23	2.11	0.49
5:R:51:LEU:O	5:R:55:ARG:HG3	2.12	0.49
5:R:180:VAL:HG11	5:R:251:VAL:HG11	1.94	0.49
1:A:230:TYR:CE1	1:A:283:LEU:HA	2.46	0.49
4:S:4:LEU:HD11	4:S:98:ARG:HG3	1.94	0.49
5:R:106:PHE:CD1	5:R:126:VAL:HG22	2.47	0.49
2:B:121:CYS:HB3	2:B:139:LEU:HD12	1.95	0.49
4:S:102:TYR:CG	4:S:105:SER:HB3	2.48	0.49
2:B:31:SER:HA	2:B:34:THR:HG22	1.95	0.49
5:R:58:LEU:HD23	5:R:273:PRO:HG2	1.95	0.49
1:A:185:ILE:HD13	1:A:200:ASP:HB3	1.94	0.48
3:C:21:MET:HE3	3:C:21:MET:HB2	1.79	0.48
5:R:91:VAL:HA	5:R:141:LEU:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:LEU:HD11	3:C:20:LYS:HG3	1.95	0.48
2:B:286:LEU:HB2	2:B:318:LEU:HD21	1.95	0.48
1:A:264:ILE:HB	1:A:319:ILE:HG12	1.95	0.48
2:B:195:ASP:OD1	2:B:195:ASP:N	2.42	0.48
1:A:196:PHE:HE1	1:A:339:VAL:HG11	1.78	0.48
2:B:162:GLY:HA2	2:B:186:ASP:HB2	1.93	0.48
2:B:218:CYS:O	3:C:18:GLN:NE2	2.36	0.48
1:A:204:GLN:O	1:A:204:GLN:NE2	2.46	0.48
1:A:204:GLN:NE2	1:A:211:TRP:HE1	2.11	0.48
1:A:320:TYR:CE1	1:A:342:ILE:HD11	2.44	0.48
2:B:33:ILE:HG22	3:C:38:MET:HE2	1.96	0.48
2:B:173:THR:HG22	2:B:175:GLN:HE21	1.79	0.48
4:S:19:LYS:HE3	4:S:82:GLN:HB2	1.95	0.48
4:S:142:SER:HA	4:S:205:SER:HA	1.96	0.48
1:A:337:ASP:OD1	1:A:338:ALA:N	2.46	0.48
2:B:146:LEU:HD22	2:B:159:THR:HB	1.96	0.48
4:S:32:PHE:CE1	4:S:98:ARG:HG2	2.49	0.48
4:S:39:GLN:H	4:S:92:ALA:HB1	1.79	0.48
4:S:168:ARG:HH12	4:S:174:GLN:HG2	1.79	0.48
5:R:62:ILE:HD11	5:R:89:TRP:NE1	2.28	0.48
1:A:212:ILE:HG21	1:A:256:HIS:NE2	2.29	0.47
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.68	0.47
5:R:91:VAL:HG22	5:R:145:ILE:HD11	1.96	0.47
5:R:100:ALA:HB1	5:R:276:HIS:HE1	1.79	0.47
1:A:8:GLU:HG3	4:S:220:HIS:HB3	1.95	0.47
4:S:36:TRP:CE3	4:S:94:TYR:HB3	2.49	0.47
5:R:110:LYS:HG3	5:R:126:VAL:HG21	1.97	0.47
2:B:157:ILE:HG23	2:B:169:TRP:HB2	1.97	0.47
4:S:167:GLN:HB3	4:S:214:VAL:HG22	1.97	0.47
5:R:183:SER:OG	7:R:502:CLR:H20	2.14	0.47
1:A:6:SER:OG	1:A:9:ASP:HB2	2.14	0.47
1:A:334:PHE:HA	1:A:337:ASP:OD2	2.14	0.47
4:S:29:PHE:CZ	4:S:79:LEU:HB2	2.49	0.47
1:A:322:HIS:HB2	1:A:334:PHE:CE1	2.49	0.47
4:S:86:LEU:HD12	4:S:86:LEU:H	1.78	0.47
4:S:107:PRO:HB2	4:S:108:PHE:HD1	1.80	0.47
1:A:231:ASP:HB3	1:A:285:ILE:HD11	1.96	0.47
4:S:28:ALA:O	4:S:32:PHE:HB3	2.15	0.47
4:S:29:PHE:HZ	4:S:79:LEU:HB2	1.81	0.46
5:R:84:MET:HE1	5:R:88:ILE:HD11	1.97	0.46
2:B:80:ILE:HD13	2:B:89:LYS:HZ2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:TYR:CE1	2:B:295:ASN:HB2	2.50	0.46
1:A:272:ASP:OD1	1:A:273:ILE:HD12	2.16	0.46
2:B:234:PHE:CD1	2:B:241:PHE:HB3	2.51	0.46
2:B:275:SER:OG	2:B:316:SER:O	2.33	0.46
5:R:204:SER:HA	5:R:207:LYS:HG2	1.98	0.46
3:C:56:ALA:HA	3:C:59:ASN:HB3	1.97	0.46
2:B:234:PHE:HD1	2:B:241:PHE:HB3	1.80	0.46
4:S:8:GLY:HA3	4:S:20:LEU:HG	1.98	0.46
5:R:44:VAL:O	5:R:48:LEU:HG	2.15	0.46
2:B:250:CYS:SG	2:B:273:ILE:HD13	2.56	0.46
4:S:162:LEU:HB3	4:S:180:MET:HB2	1.98	0.46
1:A:49:ILE:HG21	1:A:224:CYS:SG	2.56	0.46
5:R:16:GLU:HB3	5:R:270:MET:HE2	1.98	0.46
5:R:16:GLU:HA	5:R:19:ILE:HG22	1.98	0.46
2:B:51:LEU:HD12	2:B:336:LEU:HB2	1.98	0.46
4:S:37:VAL:HG11	4:S:45:LEU:HD13	1.98	0.46
2:B:164:THR:HA	2:B:186:ASP:HA	1.96	0.45
1:A:53:MET:HE1	1:A:189:PHE:HZ	1.81	0.45
1:A:271:LYS:HB3	1:A:325:CYS:HA	1.98	0.45
2:B:142:HIS:CD2	2:B:146:LEU:HD21	2.51	0.45
1:A:290:TYR:OH	1:A:293:PRO:O	2.33	0.45
2:B:188:MET:HE3	2:B:188:MET:HB3	1.64	0.45
2:B:223:THR:O	2:B:223:THR:OG1	2.31	0.45
1:A:210:LYS:HB3	2:B:188:MET:HE1	1.98	0.45
4:S:223:TYR:O	4:S:225:LEU:HG	2.16	0.45
2:B:161:SER:OG	2:B:162:GLY:N	2.49	0.45
3:C:47:GLU:OE2	3:C:47:GLU:N	2.49	0.45
1:A:263:SER:HA	1:A:317:LYS:HB2	1.99	0.45
2:B:235:PHE:HD2	2:B:237:ASN:H	1.63	0.45
1:A:250:PHE:HD2	1:A:310:LEU:HD12	1.82	0.45
2:B:54:HIS:NE2	2:B:72:SER:OG	2.35	0.45
4:S:166:LEU:O	4:S:173:PRO:HA	2.17	0.45
5:R:106:PHE:HB2	5:R:130:VAL:HG21	1.99	0.45
2:B:257:ALA:HB1	2:B:259:GLN:HE21	1.82	0.44
5:R:82:PHE:O	5:R:86:THR:OG1	2.25	0.44
2:B:54:HIS:O	2:B:334:SER:OG	2.30	0.44
2:B:146:LEU:HD23	2:B:161:SER:HB2	1.98	0.44
4:S:20:LEU:HB2	4:S:81:LEU:HB3	1.98	0.44
4:S:182:ASN:OD1	4:S:182:ASN:N	2.49	0.44
2:B:187:VAL:HG11	2:B:201:SER:HB2	2.00	0.44
3:C:8:SER:HA	3:C:11:GLN:HE22	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:16:GLU:OE1	5:R:267:VAL:HG23	2.17	0.44
5:R:99:LEU:HG	5:R:134:LEU:HD11	1.99	0.44
2:B:83:ASP:OD2	2:B:86:THR:OG1	2.34	0.44
2:B:113:ALA:HB2	2:B:151:PHE:HE1	1.83	0.44
4:S:50:TYR:CD2	4:S:223:TYR:HE2	2.35	0.44
4:S:162:LEU:HD11	4:S:217:CYS:HB2	2.00	0.44
5:R:125:ARG:HB3	5:R:128:LYS:HB3	1.99	0.44
1:A:8:GLU:OE1	4:S:179:ARG:NH1	2.51	0.44
1:A:227:LEU:HB3	1:A:274:PHE:CG	2.53	0.44
5:R:26:PHE:HZ	5:R:291:SER:HA	1.81	0.44
5:R:53:ILE:O	5:R:56:ILE:HG22	2.16	0.44
5:R:231:LYS:O	5:R:235:THR:OG1	2.23	0.44
1:A:46:LYS:HD2	1:A:200:ASP:OD2	2.17	0.44
1:A:304:LYS:HD3	1:A:304:LYS:HA	1.81	0.44
5:R:82:PHE:CD1	7:R:502:CLR:H22	2.53	0.44
1:A:210:LYS:NZ	2:B:246:ASP:OD2	2.51	0.43
5:R:31:ASN:ND2	5:R:49:THR:OG1	2.37	0.43
5:R:58:LEU:O	5:R:62:ILE:HG12	2.18	0.43
2:B:43:ILE:HG21	2:B:45:MET:HE2	2.00	0.43
2:B:145:TYR:HE1	2:B:147:SER:HB3	1.82	0.43
4:S:144:SER:HA	4:S:202:LEU:O	2.18	0.43
2:B:142:HIS:CE1	2:B:161:SER:HB3	2.54	0.43
2:B:284:LEU:HD12	2:B:297:TRP:O	2.18	0.43
4:S:54:GLY:N	4:S:72:ARG:HD3	2.33	0.43
2:B:234:PHE:HA	2:B:241:PHE:HB3	2.00	0.43
5:R:177:SER:O	5:R:181:LEU:HD23	2.18	0.43
2:B:146:LEU:HD23	2:B:146:LEU:HA	1.79	0.43
7:R:502:CLR:H221	7:R:502:CLR:H162	1.45	0.43
2:B:81:ILE:O	2:B:90:VAL:N	2.48	0.43
2:B:283:ARG:HA	2:B:283:ARG:HD2	1.82	0.43
4:S:54:GLY:H	4:S:72:ARG:HD3	1.82	0.43
4:S:100:ILE:HD12	4:S:100:ILE:HA	1.89	0.43
5:R:149:ASN:HA	5:R:152:ILE:HG22	2.01	0.43
2:B:80:ILE:HD13	2:B:89:LYS:NZ	2.32	0.43
2:B:3:GLU:OE2	2:B:4:LEU:N	2.52	0.43
5:R:9:PHE:HA	5:R:12:VAL:HG22	2.00	0.43
1:A:18:MET:SD	4:S:53:SER:OG	2.76	0.43
5:R:106:PHE:CE1	5:R:127:LYS:HG3	2.51	0.43
5:R:136:VAL:O	5:R:139:VAL:HG12	2.19	0.43
4:S:98:ARG:HD3	4:S:110:PHE:HB3	2.00	0.42
1:A:211:TRP:HB2	2:B:117:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD13	2:B:82:TRP:CG	2.55	0.42
2:B:264:TYR:HB3	2:B:297:TRP:CD2	2.54	0.42
4:S:32:PHE:HA	4:S:100:ILE:HD13	2.01	0.42
1:A:51:LYS:HA	1:A:51:LYS:HD3	1.67	0.42
1:A:208:ARG:O	1:A:212:ILE:HB	2.20	0.42
2:B:103:CYS:HA	2:B:113:ALA:O	2.19	0.42
2:B:124:TYR:CE2	2:B:135:VAL:HG12	2.55	0.42
5:R:98:TRP:CZ2	5:R:190:PRO:HB3	2.53	0.42
1:A:46:LYS:HA	1:A:49:ILE:HG22	2.01	0.42
5:R:37:LYS:HE2	5:R:39:ARG:HG3	2.01	0.42
5:R:11:PHE:O	5:R:14:ILE:HG22	2.20	0.42
4:S:12:VAL:HG11	4:S:18:ARG:HB2	2.00	0.42
4:S:37:VAL:HG13	4:S:47:TRP:HA	2.02	0.42
1:A:35:LYS:HD3	1:A:199:PHE:CE2	2.55	0.42
5:R:149:ASN:O	5:R:152:ILE:HG22	2.19	0.42
1:A:213:HIS:ND1	2:B:59:TYR:HE2	2.18	0.42
4:S:35:HIS:HE1	4:S:101:TYR:HE2	1.67	0.42
1:A:182:THR:OG1	1:A:183:GLY:N	2.52	0.41
2:B:191:SER:HB2	2:B:232:ILE:HG23	2.02	0.41
2:B:338:ILE:HG21	3:C:61:PHE:CE2	2.55	0.41
4:S:190:ARG:H	4:S:190:ARG:HG2	1.70	0.41
5:R:275:CYS:O	5:R:279:VAL:HG13	2.20	0.41
2:B:14:LEU:HD13	3:C:19:LEU:HB3	2.02	0.41
2:B:163:ASP:O	2:B:164:THR:OG1	2.32	0.41
2:B:227:SER:HB2	2:B:247:ASP:HB3	2.01	0.41
4:S:154:LEU:HD21	4:S:197:GLY:HA2	2.01	0.41
5:R:55:ARG:HH22	5:R:100:ALA:HB2	1.85	0.41
5:R:184:THR:HG21	5:R:248:PHE:HB2	2.02	0.41
2:B:121:CYS:SG	2:B:123:ILE:HD11	2.60	0.41
2:B:316:SER:HB3	2:B:332:TRP:NE1	2.35	0.41
2:B:258:ASP:OD1	3:C:27:ARG:HD3	2.20	0.41
5:R:134:LEU:HD23	5:R:134:LEU:HA	1.83	0.41
2:B:137:ARG:HE	2:B:137:ARG:HB2	1.56	0.41
2:B:197:ARG:HA	2:B:214:ARG:HH12	1.86	0.41
4:S:223:TYR:HE1	4:S:225:LEU:HD11	1.85	0.41
5:R:205:MET:HE3	5:R:205:MET:HB3	1.93	0.41
1:A:230:TYR:O	1:A:241:ASN:ND2	2.39	0.41
2:B:235:PHE:HA	2:B:278:PHE:CD2	2.56	0.41
4:S:15:GLY:HA2	4:S:85:SER:HA	2.02	0.41
4:S:98:ARG:HB2	4:S:110:PHE:O	2.20	0.41
4:S:148:ARG:HA	4:S:198:THR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:108:PHE:CD2	5:R:197:MET:HE2	2.56	0.41
2:B:210:LEU:HD22	2:B:255:LEU:HD22	2.02	0.41
2:B:222:PHE:HE1	2:B:258:ASP:HA	1.86	0.41
2:B:248:ALA:HB1	2:B:269:ILE:HG22	2.02	0.41
3:C:46:LYS:HE2	3:C:46:LYS:HB2	1.88	0.41
4:S:2:VAL:HA	4:S:26:GLY:HA3	2.03	0.41
5:R:236:PHE:HZ	5:R:272:TYR:CE1	2.39	0.41
1:A:321:SER:O	5:R:216:VAL:HG11	2.21	0.40
2:B:256:ARG:NH1	3:C:28:ILE:HD12	2.35	0.40
5:R:58:LEU:HD13	5:R:92:ILE:HG22	2.03	0.40
1:A:192:LYS:HB2	1:A:192:LYS:HE2	1.76	0.40
1:A:230:TYR:OH	1:A:281:VAL:HG23	2.20	0.40
2:B:55:LEU:HD13	2:B:55:LEU:HA	1.95	0.40
2:B:201:SER:OG	2:B:211:TRP:NE1	2.30	0.40
4:S:102:TYR:CD2	4:S:105:SER:HB3	2.56	0.40
1:A:223:PHE:CD2	1:A:307:PHE:HZ	2.39	0.40
1:A:232:MET:HE3	1:A:232:MET:N	2.37	0.40
2:B:261:LEU:HA	2:B:261:LEU:HD23	1.87	0.40
4:S:2:VAL:HG23	4:S:27:PHE:CD1	2.56	0.40
5:R:41:ILE:HD12	5:R:46:ARG:HE	1.86	0.40
1:A:251:ASN:HD22	1:A:310:LEU:HD22	1.86	0.40
2:B:63:TRP:CZ2	2:B:328:ALA:HB2	2.57	0.40
4:S:190:ARG:NH1	4:S:208:GLU:OE1	2.55	0.40
2:B:93:ILE:HG12	2:B:133:VAL:HG11	2.03	0.40
5:R:68:VAL:HG12	5:R:76:PHE:HD1	1.87	0.40
5:R:139:VAL:O	5:R:143:LEU:HD23	2.21	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	211/369 (57%)	200 (95%)	11 (5%)	0	100	100
2	B	336/366 (92%)	317 (94%)	19 (6%)	0	100	100
3	C	54/71 (76%)	50 (93%)	4 (7%)	0	100	100
4	S	228/286 (80%)	207 (91%)	21 (9%)	0	100	100
5	R	264/990 (27%)	259 (98%)	5 (2%)	0	100	100
All	All	1093/2082 (52%)	1033 (94%)	60 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/328 (60%)	195 (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%)	196 (100%)	1 (0%)	86	94
5	R	247/864 (29%)	247 (100%)	0	100	100
All	All	965/1777 (54%)	964 (100%)	1 (0%)	92	98

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

Mol	Chain	Res	Type
4	S	220	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	HIS
1	A	347	ASN
2	B	75	GLN
2	B	175	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	220	GLN
3	C	44	HIS
5	R	31	ASN
5	R	260	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)

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	$\#\|Z\| > 2$
7	CLR	R	502	-	31,31,31	0.46	0	48,48,48	0.91	2 (4%)
6	A1AEI	R	501	-	25,25,25	0.55	0	35,36,36	1.32	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
7	CLR	R	502	-	-	7/10/68/68	0/4/4/4
6	A1AEI	R	501	-	-	2/14/14/14	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	501	A1AEI	N15-N16-N17	4.33	112.37	109.53
6	R	501	A1AEI	N18-N17-N16	-4.09	106.86	109.53
6	R	501	A1AEI	C03-C04-C05	2.71	123.53	120.10
7	R	502	CLR	C14-C8-C9	-2.53	105.70	109.09
6	R	501	A1AEI	C13-C12-N11	-2.37	116.96	119.64
7	R	502	CLR	C7-C8-C9	2.01	112.14	109.71

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	502	CLR	C13-C17-C20-C21
7	R	502	CLR	C13-C17-C20-C22
7	R	502	CLR	C16-C17-C20-C21
7	R	502	CLR	C16-C17-C20-C22
7	R	502	CLR	C21-C20-C22-C23
7	R	502	CLR	C17-C20-C22-C23
7	R	502	CLR	C20-C22-C23-C24
6	R	501	A1AEI	C19-C13-C14-N15
6	R	501	A1AEI	C19-C13-C14-N18

There are no ring outliers.

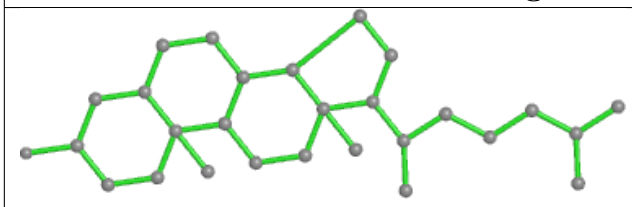
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	502	CLR	7	0
6	R	501	A1AEI	1	0

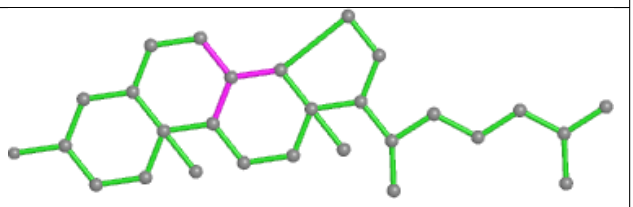
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

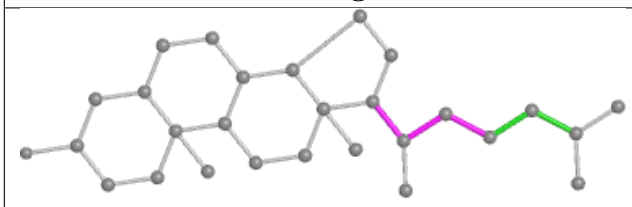
Ligand CLR R 502



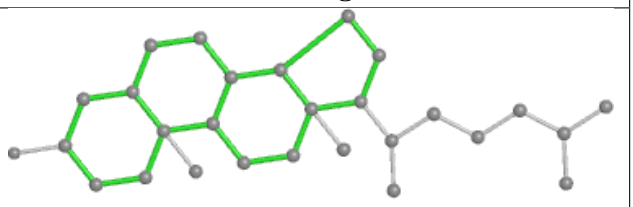
Bond lengths



Bond angles

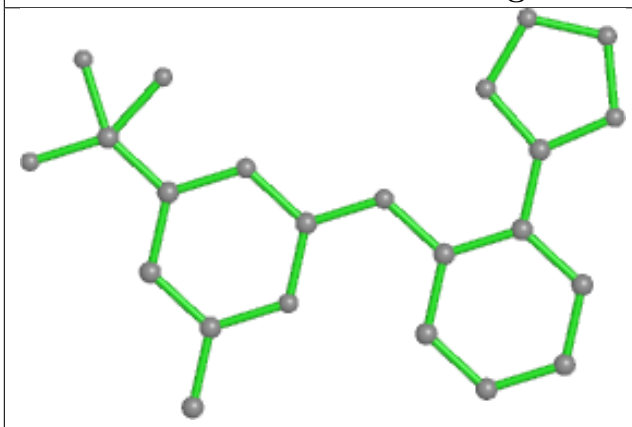


Torsions

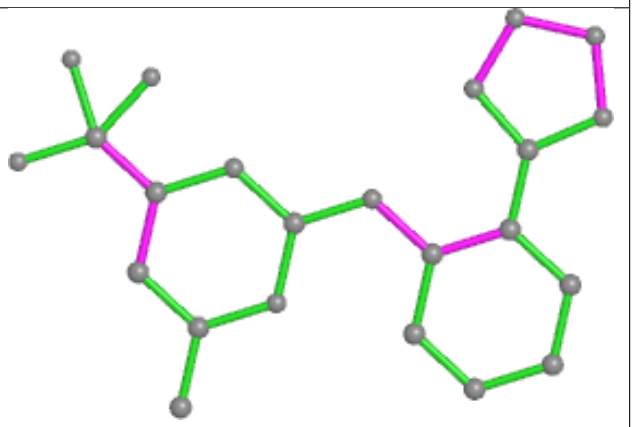


Rings

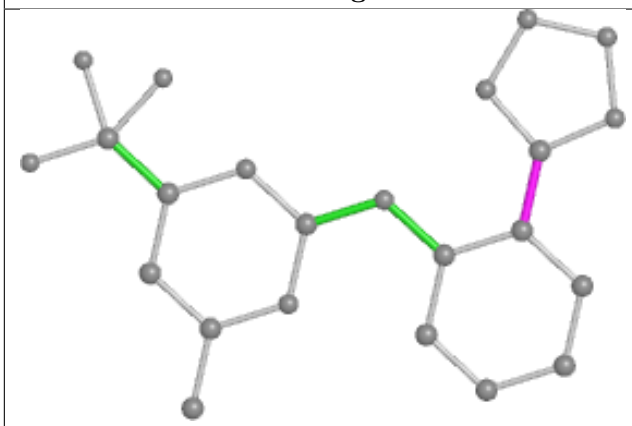
Ligand A1AEI R 501



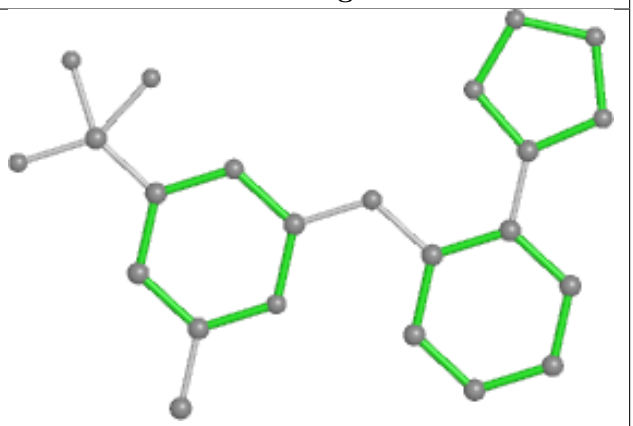
Bond lengths



Bond angles



Torsions



Rings

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.