Full wwPDB EM Validation Report ⓘ

Oct 8, 2023 – 12:40 AM JST

PDB ID	:	8JD5
EMDB ID	:	EMD-36176
Title	:	Cryo-EM structure of Gi1-bound mGlu2-mGlu4 heterodimer
Authors	:	Wang, X.; Wang, M.; Xu, T.; Feng, Y.; Han, S.; Zhao, Q.; Wu, B.
Deposited on	:	2023-05-12
Resolution	:	3.60 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:

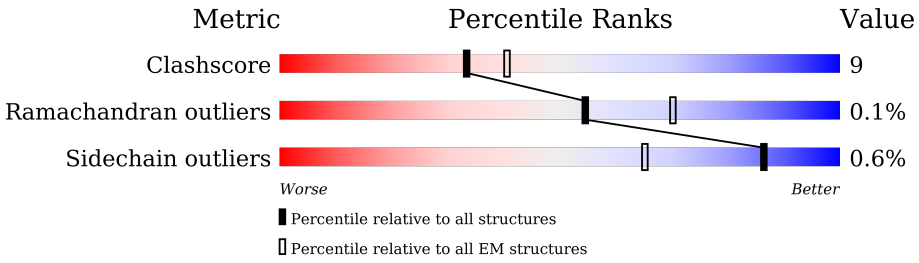
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2	870	75% 15% 10%
2	4	916	67% 16% 16%
3	A	354	49% 13% • 37%
4	B	351	70% 24% • 5%
5	C	71	72% • 27%
6	H	257	73% 16% 11%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18028 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 Metabotropic glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	785	5885	3783	1020	1042	40	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	9	ASP	-	expression tag	UNP Q14416
2	10	TYR	-	expression tag	UNP Q14416
2	11	LYS	-	expression tag	UNP Q14416
2	12	ASP	-	expression tag	UNP Q14416
2	13	ASP	-	expression tag	UNP Q14416
2	14	ASP	-	expression tag	UNP Q14416
2	15	ASP	-	expression tag	UNP Q14416
2	16	GLY	-	expression tag	UNP Q14416
2	17	ALA	-	expression tag	UNP Q14416
2	18	PRO	-	expression tag	UNP Q14416
2	873	LEU	-	expression tag	UNP Q14416
2	874	GLU	-	expression tag	UNP Q14416
2	875	VAL	-	expression tag	UNP Q14416
2	876	LEU	-	expression tag	UNP Q14416
2	877	PHE	-	expression tag	UNP Q14416
2	878	GLN	-	expression tag	UNP Q14416

- Molecule 2 is a protein called Metabotropic glutamate receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	765	5804	3714	1008	1044	38	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	3	ASP	-	expression tag	UNP Q14833

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Chain	Residue	Modelled	Actual	Comment	Reference
4	4	TYR	-	expression tag	UNP Q14833
4	5	LYS	-	expression tag	UNP Q14833
4	6	ASP	-	expression tag	UNP Q14833
4	7	ASP	-	expression tag	UNP Q14833
4	8	ASP	-	expression tag	UNP Q14833
4	9	ASP	-	expression tag	UNP Q14833
4	10	GLY	-	expression tag	UNP Q14833
4	11	ALA	-	expression tag	UNP Q14833
4	12	PRO	-	expression tag	UNP Q14833
4	13	TRP	-	expression tag	UNP Q14833
4	14	SER	-	expression tag	UNP Q14833
4	15	HIS	-	expression tag	UNP Q14833
4	16	PRO	-	expression tag	UNP Q14833
4	17	GLN	-	expression tag	UNP Q14833
4	18	PHE	-	expression tag	UNP Q14833
4	19	GLU	-	expression tag	UNP Q14833
4	20	LYS	-	expression tag	UNP Q14833
4	21	GLY	-	expression tag	UNP Q14833
4	22	SER	-	expression tag	UNP Q14833
4	23	GLY	-	expression tag	UNP Q14833
4	24	SER	-	expression tag	UNP Q14833
4	25	TRP	-	expression tag	UNP Q14833
4	26	SER	-	expression tag	UNP Q14833
4	27	HIS	-	expression tag	UNP Q14833
4	28	PRO	-	expression tag	UNP Q14833
4	29	GLN	-	expression tag	UNP Q14833
4	30	PHE	-	expression tag	UNP Q14833
4	31	GLU	-	expression tag	UNP Q14833
4	32	LYS	-	expression tag	UNP Q14833
4	913	LEU	-	expression tag	UNP Q14833
4	914	GLU	-	expression tag	UNP Q14833
4	915	VAL	-	expression tag	UNP Q14833
4	916	LEU	-	expression tag	UNP Q14833
4	917	PHE	-	expression tag	UNP Q14833
4	918	GLN	-	expression tag	UNP Q14833

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	222	Total	C	N	O	S	0	0
			1644	1053	275	305	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	334	Total	C	N	O	S	0	0
			2380	1487	417	458	18		

There are 12 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

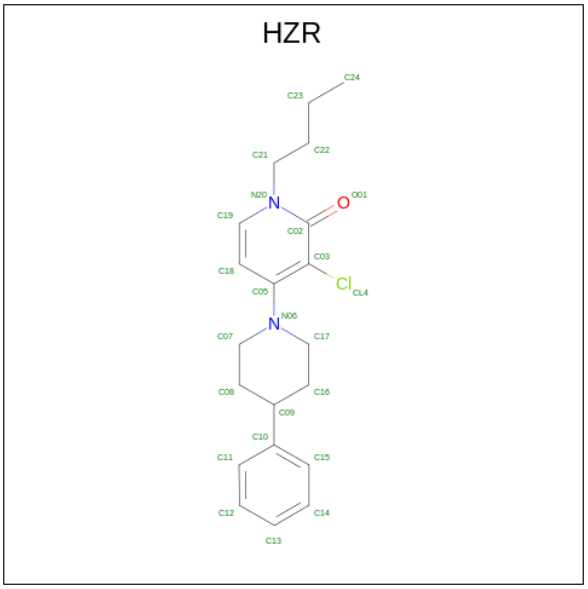
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	52	Total	C	N	O	S	0	0
			334	211	57	64	2		

- Molecule 6 is a protein called scFv.

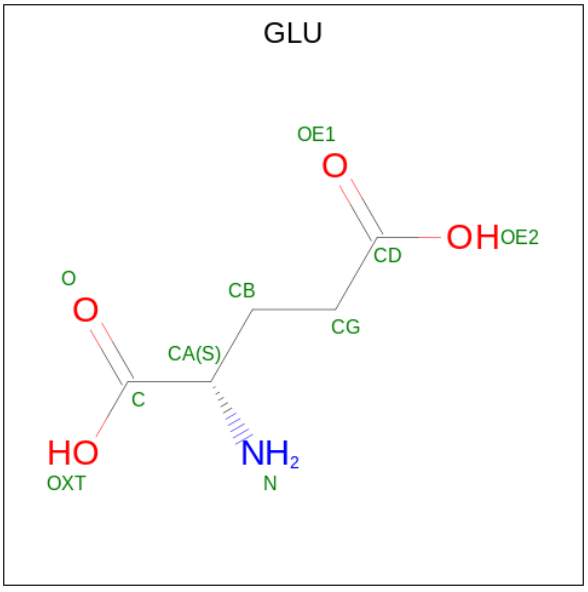
Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	229	Total	C	N	O	S	0	0
			1703	1084	280	329	10		

- Molecule 7 is 1-butyl-3-chloranyl-4-(4-phenylpiperidin-1-yl)pyridin-2-one (three-letter code: HZR) (formula: $C_{20}H_{25}ClN_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total	C	Cl	N	O	0
			24	20	1	2	1	

- Molecule 8 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	2	1	Total	C	N	O	0
			10	5	1	4	

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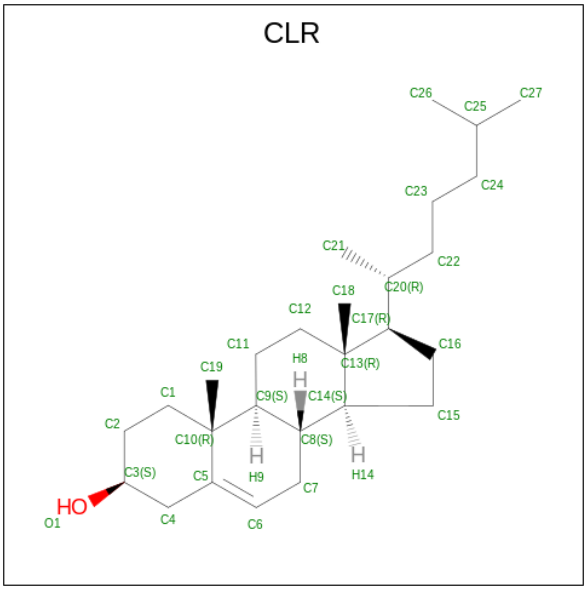
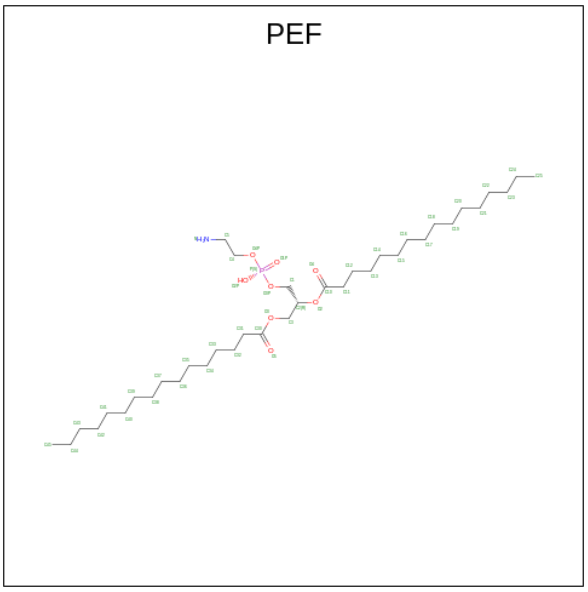
Mol	Chain	Residues	Atoms	AltConf
8	4	1	Total C N O 10 5 1 4	0

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



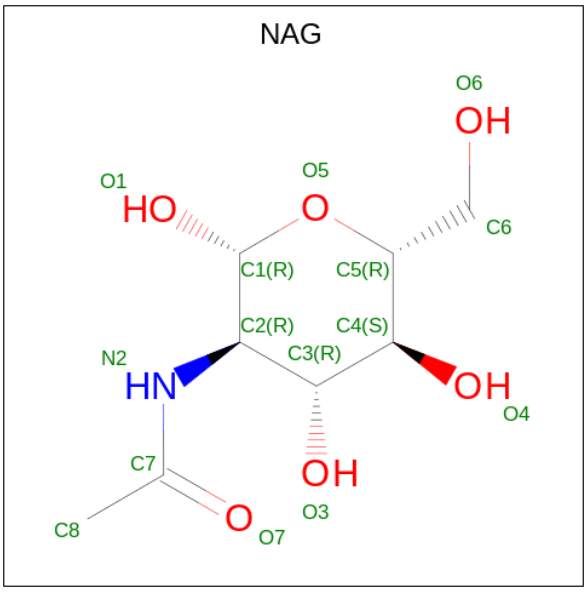
Mol	Chain	Residues	Atoms	AltConf
9	2	1	Total C O 28 27 1	0
9	2	1	Total C O 28 27 1	0
9	2	1	Total C O 28 27 1	0
9	4	1	Total C O 28 27 1	0
9	4	1	Total C O 28 27 1	0

- Molecule 10 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



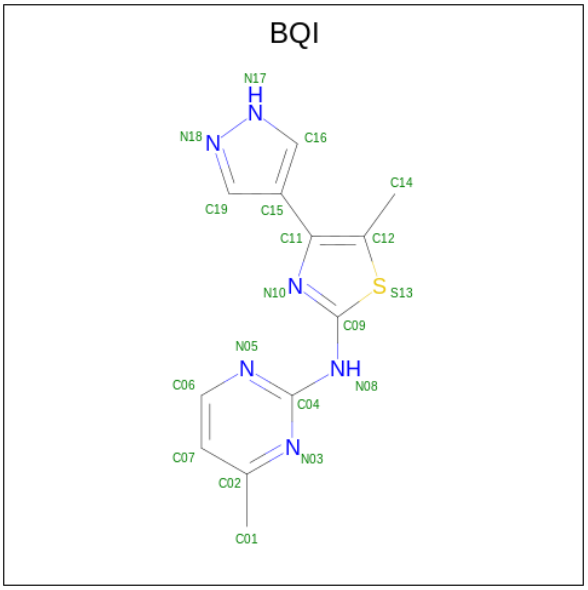
Mol	Chain	Residues	Atoms					AltConf
10	2	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
11	2	1	Total	C	N	O	0
			14	8	1	5	
11	4	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 12 is 5-methyl-N-(4-methylpyrimidin-2-yl)-4-(1H-pyrazol-4-yl)-1,3-thiazol-2-amine (three-letter code: BQI) (formula: $C_{12}H_{12}N_6S$) (labeled as "Ligand of Interest" by depositor).



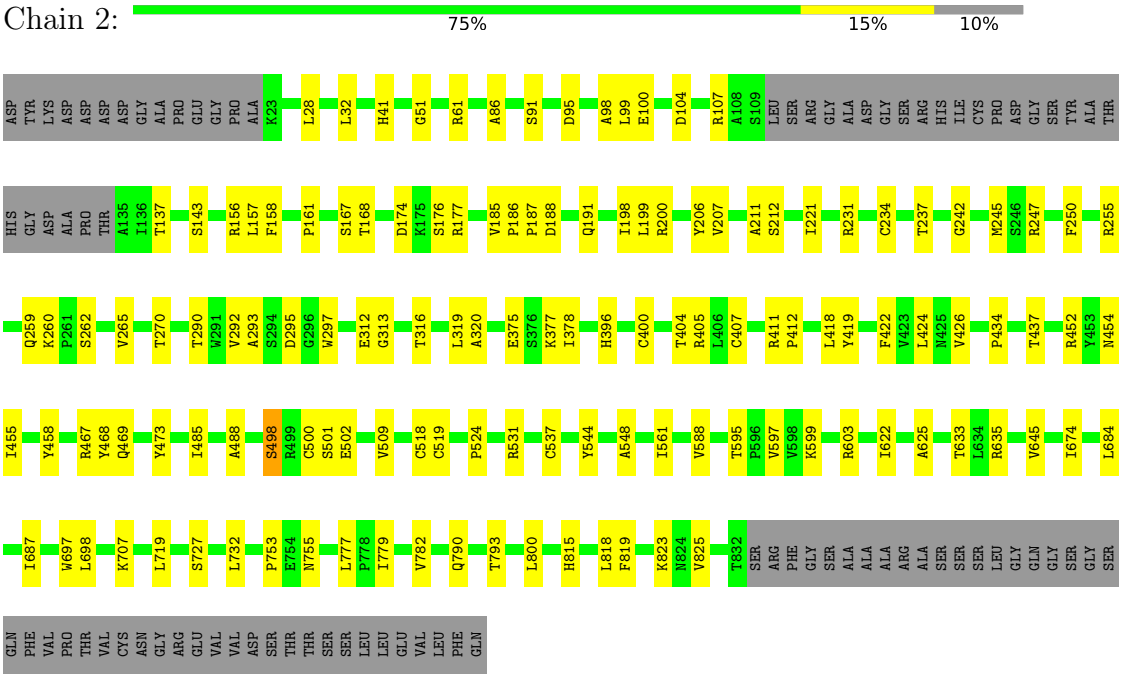
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	S	
12	4	1	19	12	6	1	0

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.

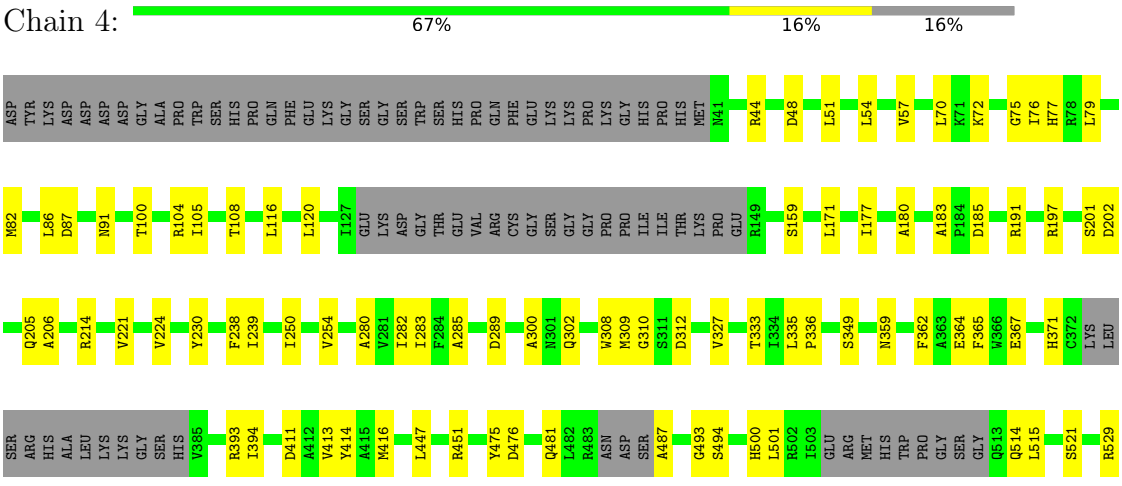
- Molecule 1: Metabotropic glutamate receptor 2

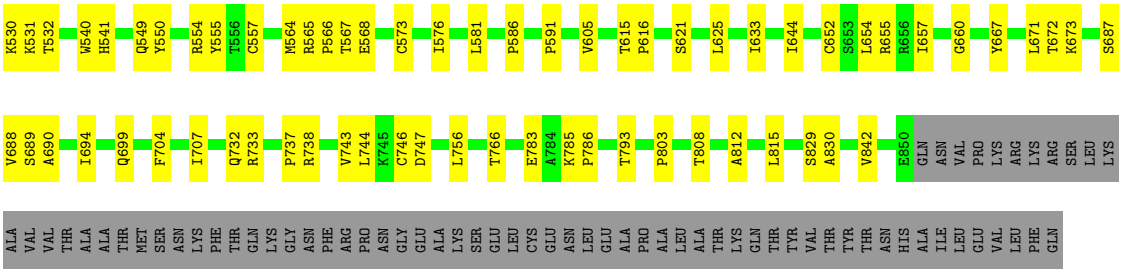
Chain 2:



- Molecule 2: Metabotropic glutamate receptor 4

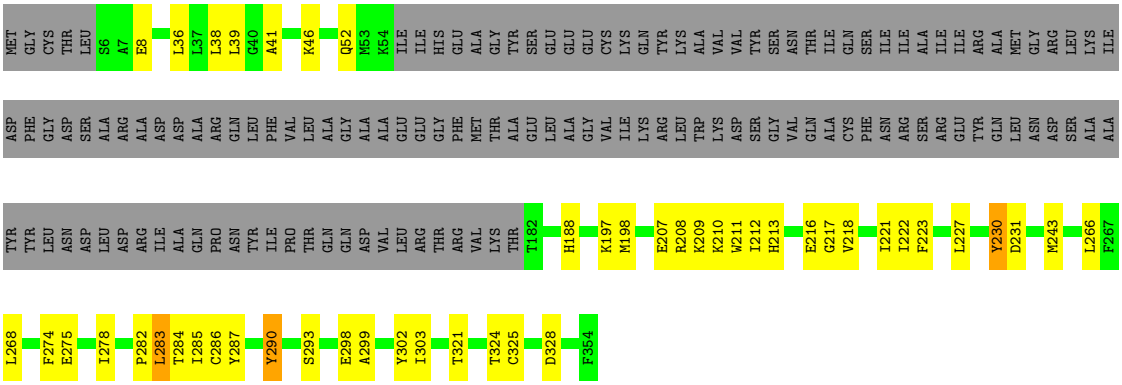
Chain 4:





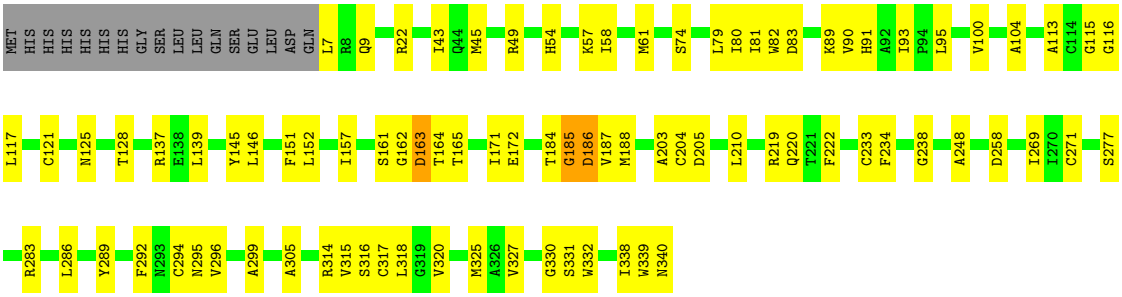
• Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



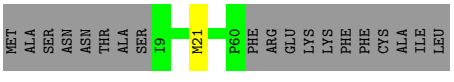
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



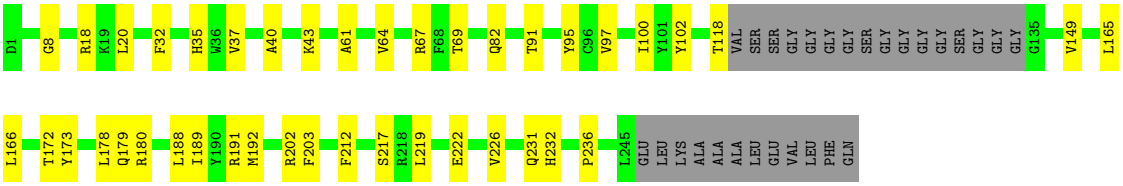
• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:



• Molecule 6: scFv

Chain H:


D1 G8 R18 K19 L20 F32 H35 W36 V37 A40 K43 A61 V64 R67 F68 T69 Q82 T91 Y95 C96 V97 I100 Y101 Y102 T118 VAL SER SER GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY G135 V149 L165
L166 T172 Y173 L178 Q179 R180 L188 I189 Y190 R191 M192 R202 F203 F212 S217 R218 L219 E222 V226 Q231 H232 P236 L245 GLU LEU LYS ALA ALA ALA LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	939819	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 ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	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: PEF, NAG, BQI, CLR, HZR

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	2	0.26	0/6031	0.49	0/8223
2	4	0.24	0/5936	0.48	0/8077
3	A	0.40	0/1674	0.47	0/2271
4	B	0.30	0/2427	0.52	0/3315
5	C	0.23	0/339	0.39	0/469
6	H	0.25	0/1747	0.50	0/2379
All	All	0.27	0/18154	0.49	0/24734

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	2	5885	0	5691	86	0
2	4	5804	0	5634	94	0
3	A	1644	0	1514	64	0
4	B	2380	0	2170	61	0
5	C	334	0	292	1	0
6	H	1703	0	1592	24	0
7	2	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2	10	0	5	0	0
8	4	10	0	5	1	0
9	2	84	0	138	6	0
9	4	56	0	92	5	0
10	2	47	0	73	4	0
11	2	14	0	13	0	0
11	4	14	0	13	0	0
12	4	19	0	0	1	0
All	All	18028	0	17232	320	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 (320) 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)
3:A:230:TYR:HB2	3:A:286:CYS:HB3	1.38	1.03
3:A:210:LYS:HG3	4:B:188:MET:HE1	1.41	1.03
4:B:164:THR:HG22	4:B:185:GLY:O	1.71	0.89
1:2:777:LEU:HD21	9:2:906:CLR:H71	1.69	0.74
4:B:82:TRP:HE1	4:B:89:LYS:HG2	1.53	0.74
2:4:565:ARG:HD2	2:4:566:PRO:HD2	1.70	0.74
3:A:230:TYR:HB2	3:A:286:CYS:CB	2.19	0.72
3:A:227:LEU:HB3	3:A:274:PHE:HB2	1.72	0.71
3:A:287:TYR:HE2	3:A:303:ILE:HA	1.55	0.71
4:B:248:ALA:HB2	4:B:271:CYS:H	1.57	0.70
2:4:633:ILE:HG23	2:4:830:ALA:HB1	1.74	0.69
3:A:208:ARG:HA	3:A:211:TRP:CE2	2.28	0.69
1:2:167:SER:H	1:2:185:VAL:HG21	1.59	0.68
4:B:315:VAL:HA	4:B:331:SER:HA	1.76	0.67
3:A:38:LEU:HG	3:A:222:ILE:HD11	1.77	0.67
4:B:164:THR:CG2	4:B:185:GLY:O	2.42	0.66
3:A:290:TYR:HE1	3:A:299:ALA:HA	1.61	0.65
2:4:76:ILE:HD13	2:4:365:PHE:HB2	1.78	0.64
3:A:39:LEU:HD12	3:A:221:ILE:HD12	1.79	0.64
1:2:777:LEU:HD13	9:4:1001:CLR:H72	1.79	0.64
9:2:906:CLR:H22	9:4:1001:CLR:H191	1.78	0.64
2:4:72:LYS:O	2:4:77:HIS:ND1	2.25	0.64
2:4:239:ILE:HG12	2:4:250:ILE:HG13	1.78	0.64
4:B:233:CYS:SG	4:B:234:PHE:N	2.71	0.64
2:4:185:ASP:OD1	2:4:191:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:283:LEU:HD22	3:A:290:TYR:CE1	2.33	0.63
1:2:206:TYR:O	1:2:498:SER:HB2	1.98	0.63
6:H:69:THR:HB	6:H:82:GLN:HB2	1.81	0.62
1:2:454:ASN:HA	1:2:473:TYR:HA	1.80	0.62
2:4:285:ALA:HB1	2:4:289:ASP:HB3	1.80	0.62
6:H:91:THR:HG23	6:H:118:THR:HA	1.82	0.62
6:H:173:TYR:HB3	6:H:232:HIS:HB3	1.81	0.62
1:2:99:LEU:HG	2:4:171:LEU:HD11	1.82	0.61
1:2:156:ARG:NH1	1:2:177:ARG:O	2.33	0.61
2:4:586:PRO:HB2	9:4:1001:CLR:H21	1.82	0.61
3:A:207:GLU:HG2	3:A:210:LYS:HE2	1.83	0.61
6:H:8:GLY:HA3	6:H:20:LEU:HD13	1.82	0.61
2:4:75:GLY:O	2:4:79:LEU:N	2.34	0.61
2:4:308:TRP:HE1	2:4:327:VAL:HG12	1.66	0.60
3:A:41:ALA:O	3:A:46:LYS:NZ	2.33	0.60
6:H:165:LEU:HD12	6:H:212:PHE:HE2	1.66	0.60
2:4:746:CYS:SG	2:4:747:ASP:N	2.75	0.60
4:B:186:ASP:O	4:B:204:CYS:N	2.24	0.60
1:2:158:PHE:HE1	2:4:120:LEU:HD21	1.67	0.60
2:4:667:TYR:HH	2:4:829:SER:HG	1.50	0.60
1:2:501:SER:CB	1:2:519:CYS:HA	2.32	0.59
3:A:227:LEU:HD13	3:A:274:PHE:CD2	2.36	0.59
2:4:447:LEU:HD11	2:4:451:ARG:HH21	1.68	0.59
1:2:793:THR:HG22	9:2:903:CLR:H183	1.84	0.59
4:B:185:GLY:HA3	4:B:205:ASP:HB3	1.84	0.59
3:A:268:LEU:O	3:A:324:THR:OG1	2.20	0.58
3:A:290:TYR:CE1	3:A:299:ALA:HA	2.38	0.58
2:4:197:ARG:NH1	2:4:201:SER:OG	2.36	0.58
1:2:500:CYS:C	1:2:519:CYS:HB3	2.23	0.58
2:4:565:ARG:NH2	2:4:737:PRO:O	2.37	0.58
1:2:509:VAL:HA	1:2:524:PRO:HA	1.86	0.58
4:B:163:ASP:OD1	4:B:165:THR:HB	2.04	0.57
3:A:208:ARG:HA	3:A:211:TRP:CZ2	2.38	0.57
3:A:284:THR:HA	3:A:287:TYR:O	2.03	0.57
4:B:95:LEU:HD21	4:B:100:VAL:HG11	1.87	0.57
9:2:903:CLR:H71	9:4:1005:CLR:H6	1.85	0.57
2:4:652:CYS:HA	2:4:655:ARG:HD2	1.87	0.56
6:H:189:ILE:HD11	6:H:203:PHE:HB3	1.86	0.56
1:2:790:GLN:O	1:2:793:THR:OG1	2.21	0.56
3:A:227:LEU:HB3	3:A:274:PHE:CG	2.41	0.56
3:A:188:HIS:CD2	3:A:197:LYS:HG2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:70:LEU:HD22	2:4:364:GLU:HG2	1.87	0.56
4:B:145:TYR:H	4:B:162:GLY:H	1.54	0.56
2:4:660:GLY:HA2	2:4:756:LEU:HD21	1.87	0.55
3:A:8:GLU:OE1	6:H:191:ARG:NH2	2.40	0.55
3:A:227:LEU:HB3	3:A:274:PHE:CB	2.35	0.55
3:A:208:ARG:HH22	3:A:209:LYS:HB2	1.70	0.55
4:B:49:ARG:HG3	4:B:338:ILE:HB	1.87	0.55
3:A:208:ARG:HG3	3:A:211:TRP:CH2	2.42	0.55
4:B:292:PHE:HA	4:B:314:ARG:HA	1.88	0.55
1:2:434:PRO:O	1:2:437:THR:OG1	2.23	0.55
3:A:209:LYS:O	3:A:212:ILE:HG22	2.06	0.55
4:B:137:ARG:NE	4:B:171:ILE:O	2.39	0.55
2:4:564:MET:HA	2:4:576:ILE:HG13	1.89	0.55
4:B:283:ARG:O	4:B:299:ALA:N	2.39	0.55
3:A:207:GLU:O	3:A:208:ARG:HB3	2.07	0.55
4:B:79:LEU:HD23	4:B:93:ILE:HD11	1.87	0.55
6:H:37:VAL:HB	6:H:95:TYR:HB2	1.88	0.55
1:2:200:ARG:NH2	1:2:231:ARG:O	2.37	0.55
2:4:180:ALA:O	8:4:1002:GLU:N	2.40	0.54
4:B:152:LEU:H	4:B:157:ILE:HA	1.72	0.54
1:2:237:THR:HG23	1:2:260:LYS:NZ	2.23	0.54
3:A:207:GLU:HB3	3:A:210:LYS:HG2	1.90	0.54
3:A:223:PHE:HB3	3:A:266:LEU:HD23	1.88	0.54
4:B:187:VAL:HA	4:B:203:ALA:HA	1.89	0.54
6:H:35:HIS:HB2	6:H:97:VAL:HB	1.88	0.54
2:4:550:TYR:O	2:4:557:CYS:HA	2.08	0.54
6:H:64:VAL:HG12	6:H:67:ARG:HH21	1.71	0.54
3:A:243:MET:CE	3:A:286:CYS:HB2	2.37	0.54
3:A:287:TYR:CE2	3:A:303:ILE:HA	2.40	0.54
2:4:336:PRO:HA	2:4:475:TYR:HA	1.89	0.54
4:B:219:ARG:HG3	4:B:220:GLN:HG2	1.89	0.54
1:2:168:THR:O	1:2:188:ASP:N	2.41	0.53
4:B:7:LEU:HG	4:B:9:GLN:H	1.73	0.53
3:A:213:HIS:O	3:A:216:GLU:HG2	2.08	0.53
1:2:782:VAL:HG11	2:4:808:THR:HA	1.89	0.53
4:B:61:MET:N	4:B:317:CYS:SG	2.81	0.53
1:2:588:VAL:HG21	1:2:818:LEU:HD11	1.91	0.53
1:2:157:LEU:HD11	2:4:116:LEU:HG	1.89	0.52
1:2:157:LEU:HD13	2:4:120:LEU:HD13	1.90	0.52
6:H:178:LEU:HB2	6:H:188:LEU:HD11	1.91	0.52
1:2:61:ARG:NH1	1:2:143:SER:OG	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:242:GLY:H	1:2:245:MET:HE3	1.75	0.52
1:2:467:ARG:NH1	1:2:469:GLN:OE1	2.43	0.52
3:A:39:LEU:HB2	3:A:223:PHE:HD1	1.74	0.52
4:B:54:HIS:CG	4:B:74:SER:HG	2.28	0.52
6:H:40:ALA:HB3	6:H:43:LYS:HB2	1.92	0.52
6:H:231:GLN:NE2	6:H:236:PRO:O	2.43	0.52
1:2:485:ILE:HB	1:2:488:ALA:HB3	1.92	0.52
3:A:211:TRP:CG	4:B:117:LEU:HD21	2.45	0.52
3:A:325:CYS:HB3	3:A:328:ASP:H	1.75	0.52
2:4:87:ASP:O	2:4:91:ASN:ND2	2.42	0.51
3:A:275:GLU:O	3:A:278:ILE:HG22	2.10	0.51
2:4:531:LYS:HE3	2:4:554:ARG:HD2	1.93	0.51
4:B:234:PHE:CZ	4:B:238:GLY:HA2	2.45	0.51
1:2:211:ALA:HB2	1:2:221:ILE:HG13	1.92	0.51
2:4:202:ASP:OD1	2:4:205:GLN:NE2	2.44	0.51
2:4:221:VAL:HG12	2:4:280:ALA:HB3	1.92	0.51
1:2:290:THR:OG1	1:2:313:GLY:O	2.23	0.51
1:2:297:TRP:NE1	1:2:468:TYR:OH	2.40	0.51
2:4:529:ARG:HD2	2:4:557:CYS:SG	2.51	0.51
2:4:549:GLN:HB3	2:4:557:CYS:HB3	1.91	0.51
2:4:733:ARG:NH2	2:4:812:ALA:O	2.44	0.51
3:A:283:LEU:HD13	3:A:290:TYR:CG	2.46	0.51
1:2:622:ILE:HG22	1:2:635:ARG:HG2	1.93	0.50
1:2:544:TYR:HB2	1:2:548:ALA:HB2	1.93	0.50
4:B:82:TRP:NE1	4:B:89:LYS:HG2	2.24	0.50
1:2:41:HIS:ND1	1:2:51:GLY:O	2.45	0.50
6:H:166:LEU:HA	6:H:172:THR:HG22	1.92	0.50
1:2:158:PHE:CE1	2:4:120:LEU:HD21	2.46	0.50
1:2:674:ILE:HG13	1:2:674:ILE:O	2.11	0.50
1:2:531:ARG:H	1:2:537:CYS:HA	1.75	0.50
3:A:38:LEU:HA	3:A:222:ILE:HG13	1.94	0.50
1:2:32:LEU:HD13	1:2:137:THR:HG21	1.93	0.50
1:2:293:ALA:HB3	1:2:316:THR:HA	1.94	0.50
3:A:52:GLN:O	3:A:52:GLN:HG2	2.12	0.50
3:A:230:TYR:HD1	3:A:230:TYR:H	1.58	0.49
6:H:180:ARG:NH1	6:H:222:GLU:OE2	2.45	0.49
1:2:320:ALA:HB3	1:2:452:ARG:HG3	1.94	0.49
2:4:54:LEU:HD23	2:4:108:THR:HG21	1.94	0.49
2:4:687:SER:OG	2:4:688:VAL:N	2.46	0.49
6:H:61:ALA:HB3	6:H:64:VAL:HG22	1.95	0.49
2:4:282:ILE:HA	2:4:309:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:319:LEU:HD12	1:2:377:LYS:HE2	1.95	0.49
2:4:803:PRO:HG3	9:4:1005:CLR:H152	1.93	0.49
2:4:672:THR:OG1	2:4:699:GLN:OE1	2.22	0.48
3:A:274:PHE:O	3:A:278:ILE:N	2.46	0.48
1:2:732:LEU:HD11	9:2:906:CLR:H152	1.95	0.48
1:2:595:THR:HG22	1:2:597:VAL:HG12	1.96	0.48
1:2:823:LYS:O	1:2:825:VAL:HG23	2.14	0.48
3:A:287:TYR:HD2	3:A:302:TYR:CD2	2.30	0.48
1:2:779:ILE:HG21	9:2:903:CLR:H212	1.95	0.48
2:4:300:ALA:O	2:4:302:GLN:NE2	2.46	0.48
1:2:207:VAL:HG12	1:2:265:VAL:HB	1.95	0.48
1:2:753:PRO:O	1:2:755:ASN:N	2.46	0.48
1:2:28:LEU:HB2	1:2:86:ALA:HB3	1.96	0.47
1:2:501:SER:O	1:2:502:GLU:C	2.51	0.47
2:4:359:ASN:HB3	2:4:362:PHE:HB2	1.96	0.47
6:H:8:GLY:C	6:H:18:ARG:HH12	2.16	0.47
1:2:599:LYS:HE3	1:2:603:ARG:HH21	1.79	0.47
4:B:83:ASP:OD1	4:B:83:ASP:N	2.46	0.47
3:A:38:LEU:HG	3:A:222:ILE:CD1	2.44	0.47
3:A:243:MET:HE2	3:A:286:CYS:HB2	1.96	0.47
1:2:212:SER:HB2	1:2:270:THR:HG22	1.97	0.47
1:2:633:THR:HG23	1:2:698:LEU:HD11	1.97	0.47
2:4:224:VAL:HB	2:4:283:ILE:HG22	1.95	0.47
3:A:290:TYR:OH	3:A:298:GLU:HG2	2.14	0.47
4:B:121:CYS:HB2	4:B:146:LEU:CD1	2.45	0.47
4:B:220:GLN:HA	5:C:21:MET:HG3	1.96	0.47
3:A:282:PRO:O	3:A:285:ILE:HG22	2.15	0.47
10:2:904:PEF:H362	2:4:793:THR:HG21	1.97	0.47
6:H:202:ARG:HD3	6:H:217:SER:H	1.80	0.47
10:2:904:PEF:H141	10:2:904:PEF:H171	1.77	0.46
4:B:125:ASN:ND2	4:B:128:THR:OG1	2.48	0.46
1:2:411:ARG:HB3	1:2:412:PRO:HD3	1.97	0.46
1:2:426:VAL:HG12	1:2:426:VAL:O	2.15	0.46
4:B:316:SER:OG	4:B:330:GLY:O	2.34	0.46
1:2:104:ASP:HA	1:2:107:ARG:HG2	1.97	0.46
1:2:645:VAL:HG22	1:2:687:ILE:HD13	1.98	0.46
1:2:199:LEU:HD11	1:2:292:VAL:HG21	1.98	0.46
4:B:22:ARG:NH1	4:B:258:ASP:O	2.49	0.46
1:2:500:CYS:HB3	1:2:519:CYS:HB3	1.22	0.45
1:2:255:ARG:O	1:2:259:GLN:HG2	2.16	0.45
4:B:320:VAL:HG22	4:B:327:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:312:GLU:HA	1:2:458:TYR:HD2	1.81	0.45
2:4:690:ALA:HB1	2:4:694:ILE:HD13	1.97	0.45
1:2:91:SER:HB2	1:2:98:ALA:HB2	1.99	0.45
1:2:375:GLU:HB3	1:2:378:ILE:HG12	1.99	0.45
4:B:269:ILE:HG12	4:B:289:TYR:CD2	2.52	0.45
1:2:95:ASP:OD1	1:2:95:ASP:N	2.49	0.45
1:2:234:CYS:HB2	1:2:518:CYS:HB3	1.46	0.45
2:4:481:GLN:O	2:4:487:ALA:N	2.49	0.45
2:4:615:THR:N	2:4:616:PRO:HD3	2.31	0.45
4:B:137:ARG:NH2	4:B:172:GLU:O	2.50	0.45
2:4:159:SER:HB3	2:4:230:TYR:HB2	1.98	0.45
2:4:310:GLY:HA3	2:4:333:THR:HG22	1.98	0.45
1:2:707:LYS:HB2	1:2:719:LEU:HA	1.98	0.45
2:4:335:LEU:O	2:4:476:ASP:N	2.39	0.45
3:A:207:GLU:CG	3:A:210:LYS:HG2	2.47	0.45
4:B:294:CYS:SG	4:B:295:ASN:N	2.90	0.45
4:B:90:VAL:HG23	6:H:102:TYR:HB2	1.98	0.45
2:4:177:ILE:HD12	2:4:416:MET:HB2	1.98	0.44
2:4:349:SER:HA	2:4:394:ILE:HB	1.98	0.44
2:4:733:ARG:HG3	2:4:743:VAL:HG13	1.99	0.44
4:B:325:MET:O	4:B:340:ASN:ND2	2.49	0.44
2:4:230:TYR:OH	2:4:312:ASP:OD1	2.27	0.44
2:4:565:ARG:HB2	2:4:576:ILE:HG12	1.99	0.44
2:4:689:SER:OG	2:4:690:ALA:N	2.51	0.44
2:4:159:SER:OG	2:4:183:ALA:HB2	2.17	0.44
3:A:8:GLU:HG3	6:H:232:HIS:CD2	2.52	0.44
4:B:43:ILE:HD11	4:B:296:VAL:HG11	1.99	0.44
1:2:174:ASP:OD2	1:2:176:SER:OG	2.30	0.44
3:A:290:TYR:HB2	3:A:302:TYR:CE2	2.53	0.44
1:2:404:THR:O	1:2:405:ARG:HD2	2.17	0.44
3:A:216:GLU:C	3:A:218:VAL:H	2.21	0.44
2:4:550:TYR:OH	2:4:573:CYS:HA	2.18	0.44
3:A:293:SER:N	3:A:298:GLU:OE1	2.50	0.44
4:B:188:MET:HE3	4:B:204:CYS:HB2	2.00	0.44
4:B:286:LEU:HB3	4:B:318:LEU:HD21	1.99	0.44
4:B:210:LEU:HD22	4:B:219:ARG:HG2	2.00	0.44
4:B:316:SER:HB3	4:B:332:TRP:CD1	2.53	0.44
10:2:904:PEF:H352	10:2:904:PEF:H161	1.99	0.43
3:A:286:CYS:SG	3:A:287:TYR:N	2.91	0.43
6:H:149:VAL:HB	6:H:219:LEU:HD13	2.00	0.43
1:2:419:TYR:HA	1:2:422:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:697:TRP:HE1	1:2:727:SER:HG	1.66	0.43
1:2:622:ILE:HA	1:2:625:ALA:HB2	2.01	0.43
2:4:349:SER:O	2:4:393:ARG:NH2	2.51	0.43
3:A:290:TYR:CD1	3:A:302:TYR:HD2	2.36	0.43
1:2:684:LEU:HD23	1:2:687:ILE:HD12	1.99	0.43
2:4:79:LEU:HD11	2:4:105:ILE:HD12	1.99	0.43
2:4:744:LEU:H	2:4:815:LEU:HD13	1.83	0.43
4:B:115:GLY:HA3	4:B:146:LEU:HD12	2.00	0.43
1:2:375:GLU:HG3	1:2:377:LYS:H	1.83	0.43
2:4:411:ASP:HA	2:4:414:TYR:HB2	1.99	0.43
4:B:100:VAL:HA	4:B:116:GLY:HA3	2.00	0.43
4:B:222:PHE:HE1	4:B:258:ASP:HA	1.83	0.43
1:2:191:GLN:HE22	1:2:295:ASP:HB2	1.83	0.43
1:2:198:ILE:HD11	1:2:455:ILE:HD12	2.00	0.43
2:4:529:ARG:HD3	2:4:530:LYS:N	2.34	0.43
2:4:605:VAL:HG12	2:4:842:VAL:HG21	2.01	0.43
3:A:207:GLU:HG2	3:A:210:LYS:HG2	2.01	0.43
2:4:82:MET:HG3	2:4:413:VAL:HG11	2.00	0.43
3:A:208:ARG:NH2	3:A:209:LYS:HB2	2.32	0.43
3:A:38:LEU:O	3:A:39:LEU:HD23	2.18	0.42
1:2:237:THR:HG23	1:2:260:LYS:HZ2	1.83	0.42
4:B:81:ILE:HD12	4:B:91:HIS:HB2	2.01	0.42
1:2:815:HIS:HA	1:2:819:PHE:HD2	1.85	0.42
2:4:704:PHE:HA	2:4:707:ILE:HD12	2.01	0.42
3:A:216:GLU:O	3:A:218:VAL:N	2.52	0.42
10:2:904:PEF:H191	10:2:904:PEF:H162	1.75	0.42
1:2:396:HIS:NE2	1:2:404:THR:HA	2.35	0.42
2:4:625:LEU:HD23	2:4:673:LYS:HG3	2.01	0.42
1:2:782:VAL:HG22	2:4:812:ALA:HB2	2.01	0.42
2:4:521:SER:OG	2:4:540:TRP:O	2.29	0.42
4:B:54:HIS:CE1	4:B:80:ILE:HD12	2.54	0.42
4:B:58:ILE:O	4:B:316:SER:OG	2.29	0.42
4:B:184:THR:O	4:B:185:GLY:O	2.38	0.42
2:4:44:ARG:HG2	2:4:104:ARG:HD3	2.02	0.42
2:4:367:GLU:O	2:4:371:HIS:ND1	2.46	0.42
4:B:113:ALA:HB2	4:B:151:PHE:HE1	1.83	0.42
4:B:296:VAL:HG13	4:B:305:ALA:HB3	2.01	0.42
1:2:265:VAL:HG23	1:2:498:SER:OG	2.19	0.41
1:2:424:LEU:HD12	1:2:424:LEU:HA	1.90	0.41
3:A:207:GLU:CB	3:A:210:LYS:HG2	2.50	0.41
4:B:146:LEU:HD23	4:B:146:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:247:ARG:HH21	1:2:250:PHE:HE2	1.67	0.41
3:A:38:LEU:HD12	3:A:38:LEU:H	1.85	0.41
6:H:32:PHE:HE1	6:H:100:ILE:HD12	1.85	0.41
1:2:186:PRO:HA	1:2:187:PRO:HD3	1.94	0.41
2:4:51:LEU:HD12	2:4:86:LEU:HD21	2.03	0.41
2:4:591:PRO:HD3	12:4:1004:BQI:C16	2.50	0.41
6:H:179:GLN:HB3	6:H:226:VAL:HB	2.02	0.41
2:4:654:LEU:HD23	2:4:657:ILE:HD11	2.03	0.41
2:4:785:LYS:N	2:4:786:PRO:HD2	2.36	0.41
3:A:274:PHE:CZ	3:A:278:ILE:HD13	2.55	0.41
4:B:121:CYS:HB2	4:B:146:LEU:HD11	2.02	0.41
1:2:800:LEU:HD23	1:2:800:LEU:HA	1.93	0.41
2:4:206:ALA:HB1	2:4:238:PHE:HA	2.02	0.41
2:4:621:SER:HB3	2:4:783:GLU:OE2	2.21	0.41
3:A:266:LEU:HB2	3:A:321:THR:HA	2.02	0.41
2:4:532:THR:HB	2:4:541:HIS:CE1	2.55	0.41
2:4:550:TYR:OH	2:4:566:PRO:HA	2.21	0.41
4:B:104:ALA:HB3	4:B:113:ALA:HB3	2.01	0.41
3:A:36:LEU:HB2	3:A:198:MET:HG2	2.01	0.41
4:B:45:MET:HG3	4:B:339:TRP:HB3	2.03	0.41
1:2:161:PRO:HG2	1:2:418:LEU:HD23	2.03	0.41
1:2:400:CYS:HB3	1:2:407:CYS:HB3	1.85	0.41
1:2:561:ILE:HG13	1:2:561:ILE:O	2.21	0.41
2:4:57:VAL:HG11	2:4:79:LEU:HD22	2.03	0.41
2:4:57:VAL:HA	2:4:75:GLY:HA3	2.03	0.41
2:4:494:SER:O	2:4:500:HIS:N	2.54	0.41
2:4:514:GLN:HG3	2:4:515:LEU:N	2.36	0.41
2:4:581:LEU:HG	2:4:644:ILE:HG22	2.01	0.41
3:A:211:TRP:CD2	4:B:117:LEU:HD21	2.55	0.41
4:B:121:CYS:O	4:B:139:LEU:HD13	2.21	0.41
2:4:224:VAL:HG22	2:4:254:VAL:HB	2.02	0.41
2:4:493:GLY:HA3	2:4:501:LEU:HA	2.01	0.41
2:4:529:ARG:HE	2:4:555:TYR:C	2.24	0.41
3:A:283:LEU:H	3:A:283:LEU:HG	1.53	0.41
6:H:172:THR:OG1	6:H:192:MET:SD	2.72	0.41
2:4:671:LEU:HD13	2:4:766:THR:HG23	2.03	0.40
4:B:233:CYS:SG	4:B:277:SER:HA	2.60	0.40
2:4:48:ASP:H	2:4:100:THR:HG23	1.85	0.40
2:4:214:ARG:HD2	2:4:214:ARG:HA	1.96	0.40
3:A:207:GLU:HG3	3:A:209:LYS:HB3	2.03	0.40
1:2:100:GLU:HA	2:4:171:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:567:THR:OG1	2:4:568:GLU:N	2.54	0.40
2:4:732:GLN:HG3	2:4:733:ARG:N	2.37	0.40
1:2:259:GLN:NE2	1:2:259:GLN:HA	2.36	0.40
1:2:265:VAL:CG2	1:2:498:SER:OG	2.70	0.40
4:B:269:ILE:HG12	4:B:289:TYR:CE2	2.56	0.40
2:4:531:LYS:HD2	2:4:540:TRP:CD1	2.57	0.40
3:A:266:LEU:HD23	3:A:266:LEU:HA	1.95	0.40
4:B:57:LYS:HD3	4:B:332:TRP:CE2	2.57	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	2	781/870 (90%)	723 (93%)	58 (7%)	0	100	100
2	4	755/916 (82%)	704 (93%)	51 (7%)	0	100	100
3	A	218/354 (62%)	204 (94%)	13 (6%)	1 (0%)	29	68
4	B	332/351 (95%)	303 (91%)	28 (8%)	1 (0%)	41	75
5	C	50/71 (70%)	50 (100%)	0	0	100	100
6	H	225/257 (88%)	216 (96%)	9 (4%)	0	100	100
All	All	2361/2819 (84%)	2200 (93%)	159 (7%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	217	GLY
4	B	185	GLY

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	2	590/712 (83%)	588 (100%)	2 (0%)	92 97
2	4	602/787 (76%)	601 (100%)	1 (0%)	93 98
3	A	158/305 (52%)	154 (98%)	4 (2%)	47 75
4	B	230/293 (78%)	227 (99%)	3 (1%)	69 86
5	C	26/58 (45%)	26 (100%)	0	100 100
6	H	179/207 (86%)	179 (100%)	0	100 100
All	All	1785/2362 (76%)	1775 (99%)	10 (1%)	86 94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	262	SER
1	2	498	SER
2	4	738	ARG
3	A	230	TYR
3	A	231	ASP
3	A	283	LEU
3	A	290	TYR
4	B	161	SER
4	B	163	ASP
4	B	186	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	259	GLN
2	4	91	ASN
4	B	119	ASN
4	B	142	HIS
6	H	183	GLN
6	H	231	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

12 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	$\#\|Z\| > 2$
8	GLU	2	902	-	8,9,9	1.03	0	10,11,11	1.19	0
9	CLR	4	1001	-	31,31,31	0.30	0	48,48,48	0.59	1 (2%)
9	CLR	2	903	-	31,31,31	0.29	0	48,48,48	0.38	0
9	CLR	2	907	-	31,31,31	0.28	0	48,48,48	0.37	0
9	CLR	2	906	-	31,31,31	0.31	0	48,48,48	0.55	1 (2%)
11	NAG	2	905	1	14,14,15	0.45	0	17,19,21	0.38	0
12	BQI	4	1004	-	14,21,21	2.21	4 (28%)	13,29,29	2.30	3 (23%)
11	NAG	4	1003	2	14,14,15	0.41	0	17,19,21	0.33	0
9	CLR	4	1005	-	31,31,31	0.30	0	48,48,48	0.41	0
8	GLU	4	1002	-	8,9,9	1.03	0	10,11,11	1.18	0
7	HZR	2	901	-	25,26,26	3.18	12 (48%)	31,35,35	1.70	6 (19%)
10	PEF	2	904	-	46,46,46	1.30	4 (8%)	49,51,51	0.93	2 (4%)

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
8	GLU	2	902	-	-	5/9/9/9	-
9	CLR	4	1001	-	-	4/10/68/68	0/4/4/4
9	CLR	2	903	-	-	1/10/68/68	0/4/4/4
9	CLR	2	907	-	-	0/10/68/68	0/4/4/4
9	CLR	2	906	-	-	4/10/68/68	0/4/4/4
11	NAG	2	905	1	-	0/6/23/26	0/1/1/1
12	BQI	4	1004	-	-	2/2/8/8	0/3/3/3
11	NAG	4	1003	2	-	1/6/23/26	0/1/1/1
9	CLR	4	1005	-	-	4/10/68/68	0/4/4/4
8	GLU	4	1002	-	-	2/9/9/9	-
7	HZR	2	901	-	-	3/12/22/22	0/3/3/3
10	PEF	2	904	-	-	23/50/50/50	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	901	HZR	C19-N20	8.13	1.49	1.37
7	2	901	HZR	C19-C18	7.66	1.52	1.35
7	2	901	HZR	C02-N20	5.72	1.49	1.39
12	4	1004	BQI	C09-N08	4.89	1.45	1.36
7	2	901	HZR	C03-C02	4.52	1.53	1.44
12	4	1004	BQI	C04-N08	4.41	1.45	1.36
7	2	901	HZR	C18-C05	4.40	1.49	1.41
10	2	904	PEF	O2-C10	4.02	1.45	1.34
12	4	1004	BQI	C15-C11	3.45	1.53	1.49
7	2	901	HZR	C07-N06	3.35	1.53	1.47
7	2	901	HZR	C17-N06	3.31	1.52	1.47
10	2	904	PEF	O3-C30	3.03	1.42	1.33
7	2	901	HZR	C16-C09	-2.79	1.45	1.53
7	2	901	HZR	C03-CL4	2.77	1.79	1.72
7	2	901	HZR	C08-C09	-2.74	1.45	1.53
10	2	904	PEF	C11-C10	2.60	1.58	1.50
12	4	1004	BQI	N18-N17	-2.26	1.33	1.37
10	2	904	PEF	P-O4P	2.13	1.67	1.59
7	2	901	HZR	C05-N06	2.04	1.45	1.38
7	2	901	HZR	O01-C02	-2.02	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	4	1004	BQI	C06-N05-C04	5.37	120.21	115.45
12	4	1004	BQI	N05-C04-N03	-4.39	122.39	126.55
10	2	904	PEF	O2-C10-C11	4.27	120.70	111.50
7	2	901	HZR	C05-C03-C02	-4.10	119.81	123.11
7	2	901	HZR	C19-N20-C02	-3.71	120.14	122.89
7	2	901	HZR	C08-C09-C10	-3.66	104.21	112.79
12	4	1004	BQI	C07-C06-N05	-3.35	119.79	123.96
7	2	901	HZR	O01-C02-C03	-3.17	119.92	125.19
9	4	1001	CLR	C13-C17-C20	2.74	123.78	119.49
10	2	904	PEF	O3-C30-C31	2.66	120.24	111.91
7	2	901	HZR	C18-C19-N20	-2.63	119.98	122.44
7	2	901	HZR	C02-C03-CL4	2.45	119.77	116.00
9	2	906	CLR	C13-C17-C20	2.44	123.30	119.49

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	901	HZR	C22-C21-N20-C02
7	2	901	HZR	C22-C21-N20-C19
9	2	906	CLR	C13-C17-C20-C22
10	2	904	PEF	C11-C10-O2-C2
10	2	904	PEF	O4-C10-O2-C2
12	4	1004	BQI	N03-C04-N08-C09
12	4	1004	BQI	N05-C04-N08-C09
9	2	906	CLR	C16-C17-C20-C22
10	2	904	PEF	C33-C34-C35-C36
10	2	904	PEF	C35-C36-C37-C38
9	4	1001	CLR	C13-C17-C20-C22
10	2	904	PEF	C14-C15-C16-C17
9	2	906	CLR	C16-C17-C20-C21
9	4	1001	CLR	C16-C17-C20-C22
9	4	1001	CLR	C16-C17-C20-C21
10	2	904	PEF	C16-C17-C18-C19
9	2	903	CLR	C22-C23-C24-C25
10	2	904	PEF	C42-C43-C44-C45
10	2	904	PEF	C15-C16-C17-C18
9	2	906	CLR	C13-C17-C20-C21
10	2	904	PEF	C34-C35-C36-C37
11	4	1003	NAG	O5-C5-C6-O6
10	2	904	PEF	C22-C23-C24-C25
10	2	904	PEF	O3P-C1-C2-O2
10	2	904	PEF	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	4	1005	CLR	C16-C17-C20-C22
10	2	904	PEF	C18-C19-C20-C21
10	2	904	PEF	C12-C13-C14-C15
10	2	904	PEF	C4-O4P-P-O1P
9	4	1005	CLR	C13-C17-C20-C22
8	2	902	GLU	N-CA-CB-CG
10	2	904	PEF	O3P-C1-C2-C3
10	2	904	PEF	C10-C11-C12-C13
9	4	1005	CLR	C16-C17-C20-C21
10	2	904	PEF	C4-O4P-P-O3P
10	2	904	PEF	C1-C2-C3-O3
8	2	902	GLU	OE2-CD-CG-CB
9	4	1005	CLR	C13-C17-C20-C21
8	2	902	GLU	OE1-CD-CG-CB
9	4	1001	CLR	C13-C17-C20-C21
7	2	901	HZR	C18-C05-N06-C17
8	4	1002	GLU	OE2-CD-CG-CB
10	2	904	PEF	C11-C12-C13-C14
8	4	1002	GLU	OE1-CD-CG-CB
8	2	902	GLU	C-CA-CB-CG
10	2	904	PEF	C19-C20-C21-C22
10	2	904	PEF	O3-C30-C31-C32
8	2	902	GLU	OXT-C-CA-CB
10	2	904	PEF	O5-C30-C31-C32

There are no ring outliers.

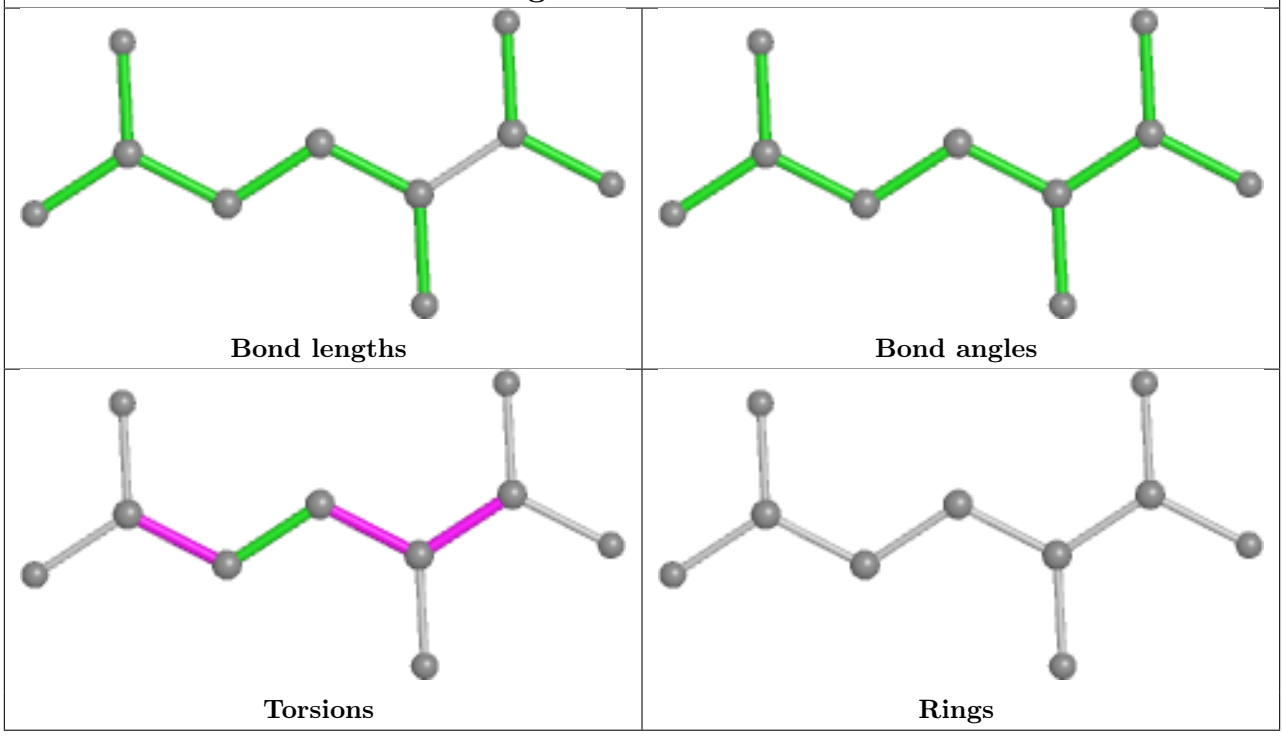
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	4	1001	CLR	3	0
9	2	903	CLR	3	0
9	2	906	CLR	3	0
12	4	1004	BQI	1	0
9	4	1005	CLR	2	0
8	4	1002	GLU	1	0
10	2	904	PEF	4	0

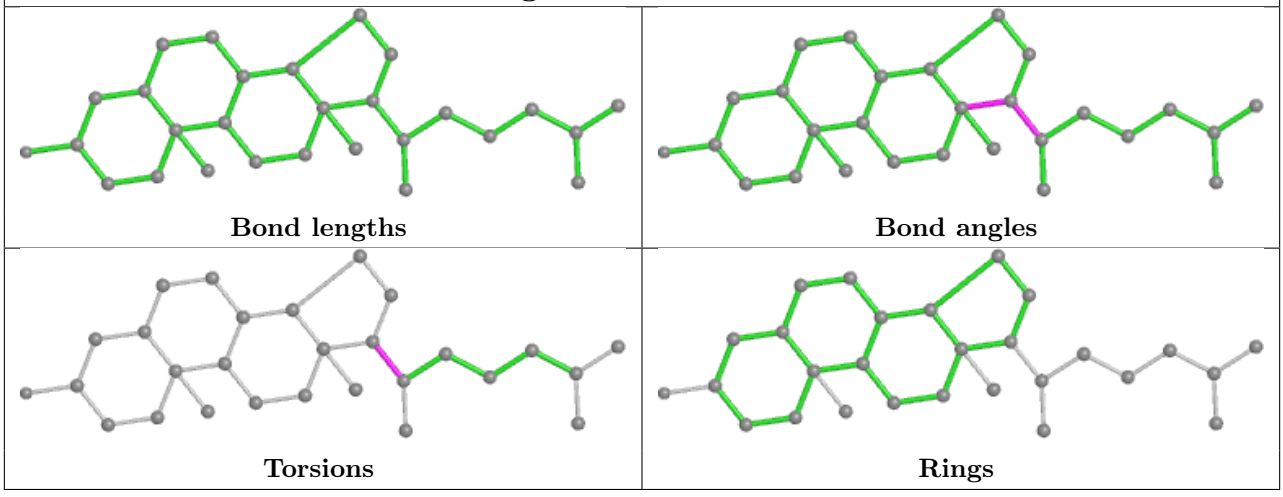
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

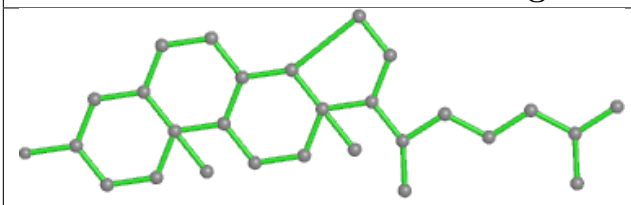
Ligand GLU 2 902

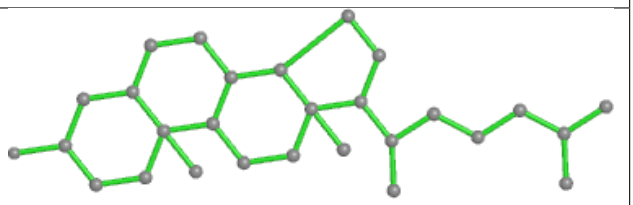


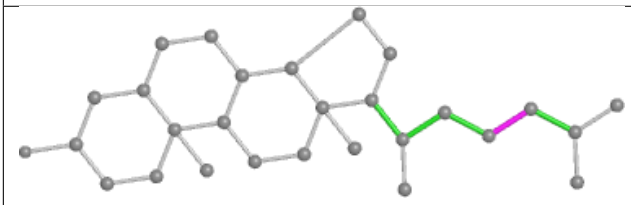
Ligand CLR 4 1001

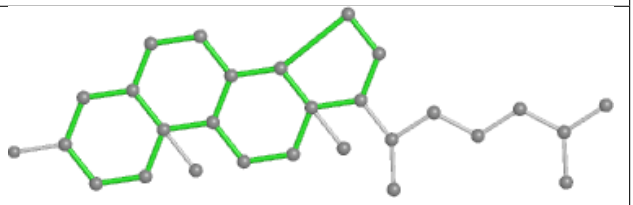


Ligand CLR 2 903

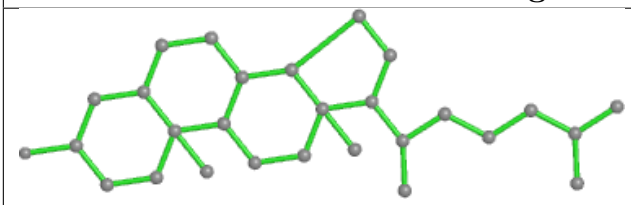

Bond lengths

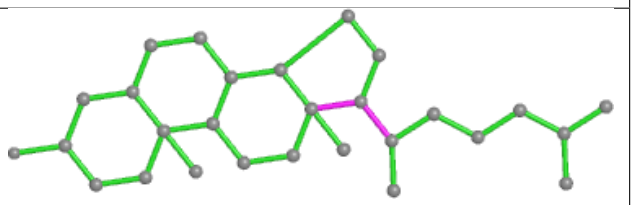

Bond angles

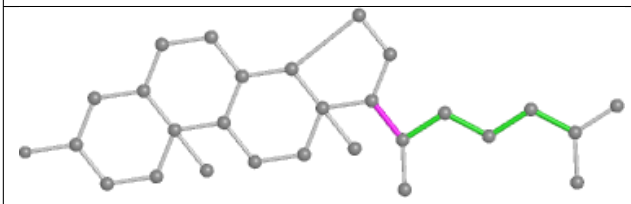

Torsions

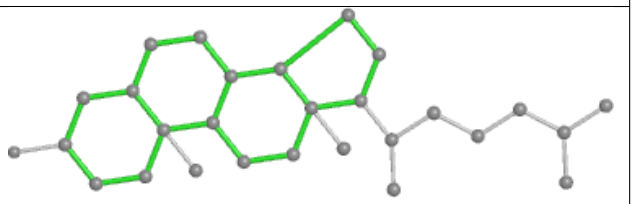

Rings

Ligand CLR 2 906

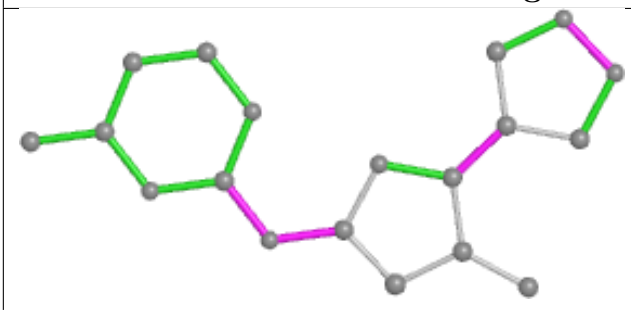

Bond lengths

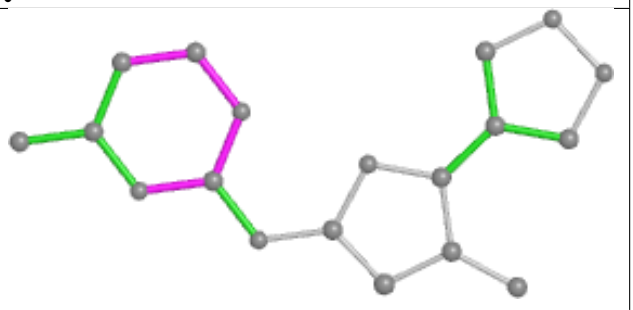

Bond angles

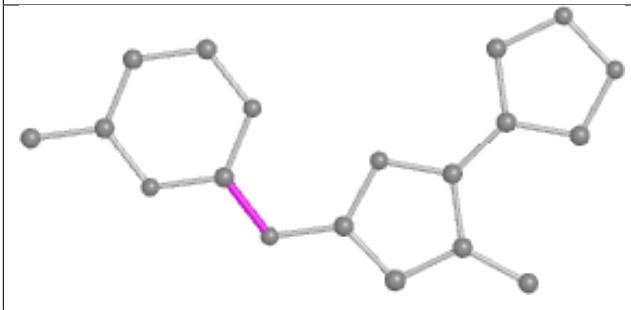

Torsions

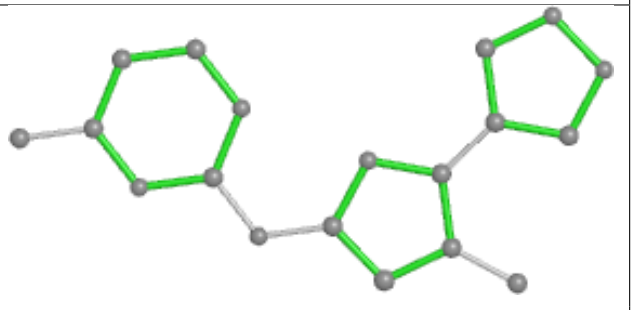

Rings

Ligand BQI 4 1004

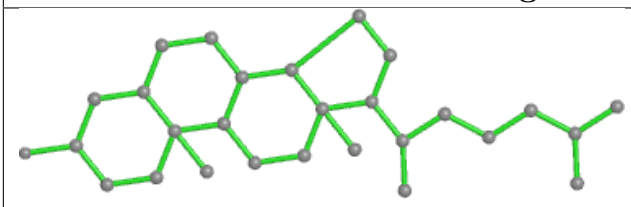

Bond lengths


Bond angles

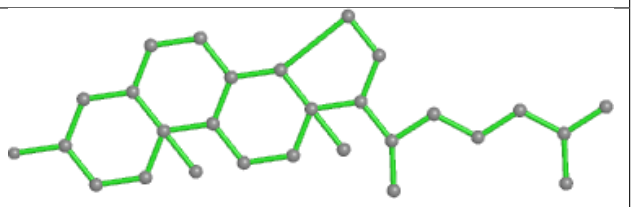

Torsions


Rings

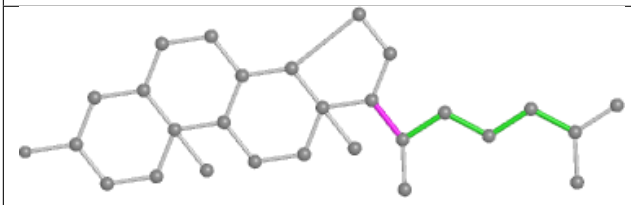
Ligand CLR 4 1005



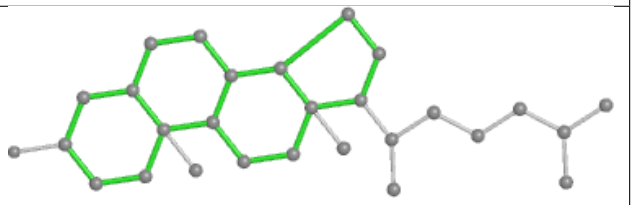
Bond lengths



Bond angles

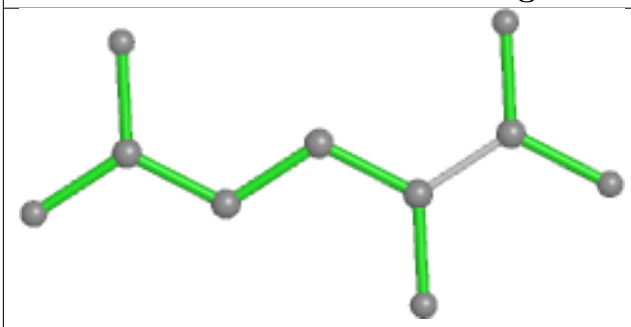


Torsions

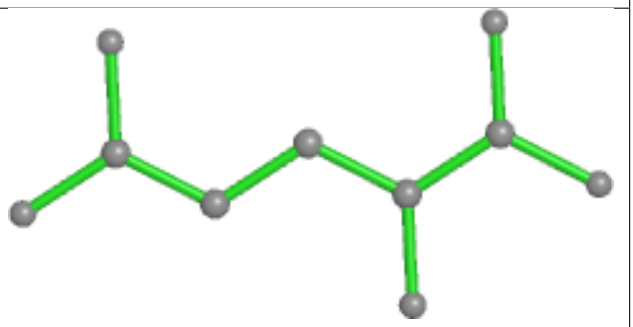


Rings

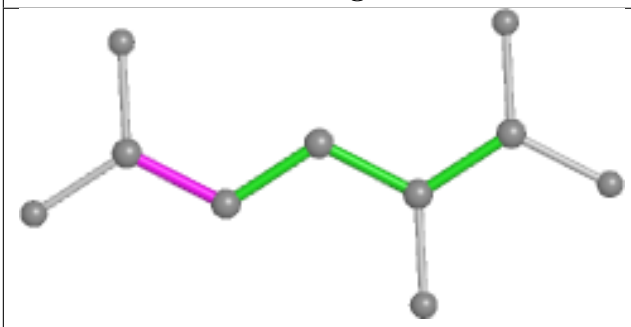
Ligand GLU 4 1002



Bond lengths



Bond angles



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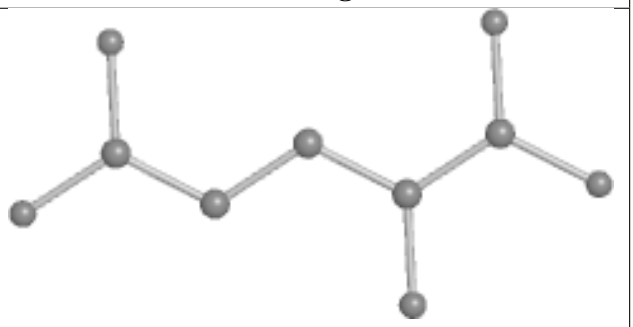
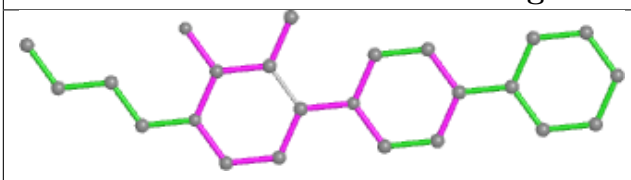
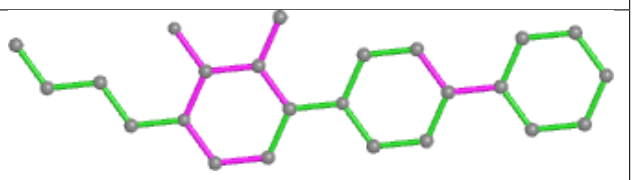


Rings

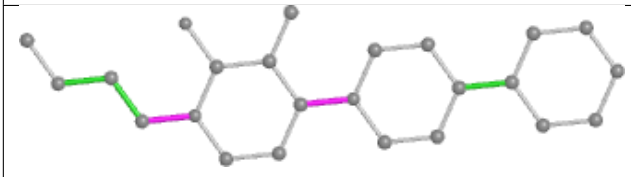
Ligand HZR 2 901



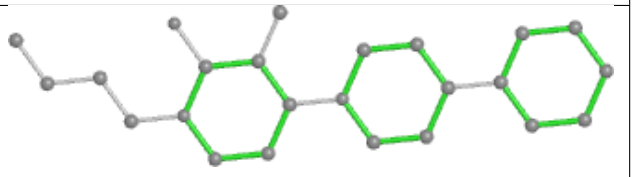
Bond lengths



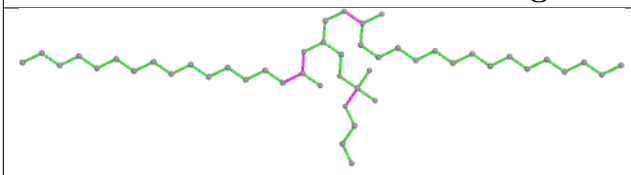
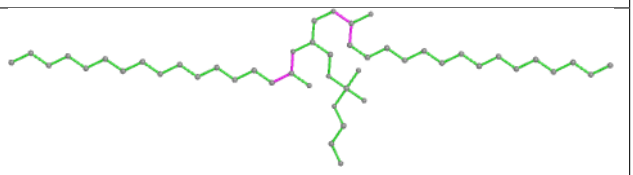
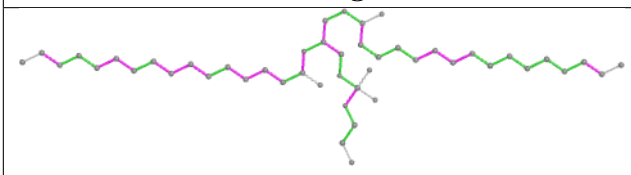
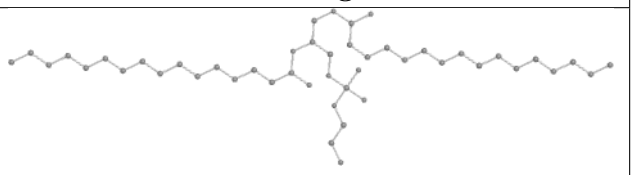
Bond angles



Torsions



Rings

Ligand PEF 2 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.