



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 03:08 PM JST

PDB ID : 8JD3  
EMDB ID : EMD-36174  
Title : Cryo-EM structure of Gi1-bound mGlu2-mGlu3 heterodimer  
Authors : Wang, X.; Wang, M.; Xu, T.; Feng, Y.; Han, S.; Lin, S.; Zhao, Q.; Wu, B.  
Deposited on : 2023-05-12  
Resolution : 3.30 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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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



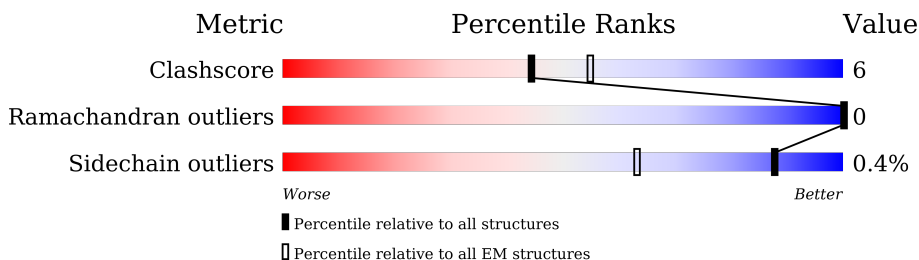
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	2	870	
2	3	894	
3	A	354	
4	B	351	
5	C	71	



## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15770 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
1	2	774	Total	C	N	O	S	0	0
			5793	3730	990	1033	40		

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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	763	Total	C	N	O	S	0	0
			5744	3685	963	1051	45		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-8	ASP	-	expression tag	UNP Q14832

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
3	-7	TYR	-	expression tag	UNP Q14832
3	-6	LYS	-	expression tag	UNP Q14832
3	-5	ASP	-	expression tag	UNP Q14832
3	-4	ASP	-	expression tag	UNP Q14832
3	-3	ASP	-	expression tag	UNP Q14832
3	-2	ASP	-	expression tag	UNP Q14832
3	-1	LYS	-	expression tag	UNP Q14832
3	0	GLY	-	expression tag	UNP Q14832
3	1	ALA	-	expression tag	UNP Q14832
3	2	PRO	-	expression tag	UNP Q14832
3	3	TRP	-	expression tag	UNP Q14832
3	4	SER	-	expression tag	UNP Q14832
3	5	HIS	-	expression tag	UNP Q14832
3	6	PRO	-	expression tag	UNP Q14832
3	7	GLN	-	expression tag	UNP Q14832
3	8	PHE	-	expression tag	UNP Q14832
3	9	GLU	-	expression tag	UNP Q14832
3	10	LYS	-	expression tag	UNP Q14832
3	11	GLY	-	expression tag	UNP Q14832
3	12	SER	-	expression tag	UNP Q14832
3	13	GLY	-	expression tag	UNP Q14832
3	14	SER	-	expression tag	UNP Q14832
3	15	TRP	-	expression tag	UNP Q14832
3	16	SER	-	expression tag	UNP Q14832
3	17	HIS	-	expression tag	UNP Q14832
3	18	PRO	-	expression tag	UNP Q14832
3	19	GLN	-	expression tag	UNP Q14832
3	20	PHE	-	expression tag	UNP Q14832
3	21	GLU	-	expression tag	UNP Q14832
3	22	LYS	-	expression tag	UNP Q14832
3	880	LEU	-	expression tag	UNP Q14832
3	881	GLU	-	expression tag	UNP Q14832
3	882	VAL	-	expression tag	UNP Q14832
3	883	LEU	-	expression tag	UNP Q14832
3	884	PHE	-	expression tag	UNP Q14832
3	885	GLN	-	expression tag	UNP Q14832

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	219	Total	C	N	O	S	0	0
			1491	948	251	282	10		



There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	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	336	Total	C	N	O	S	0	0
			2220	1372	400	431	17		

There are 12 discrepancies between the modelled and reference sequences:

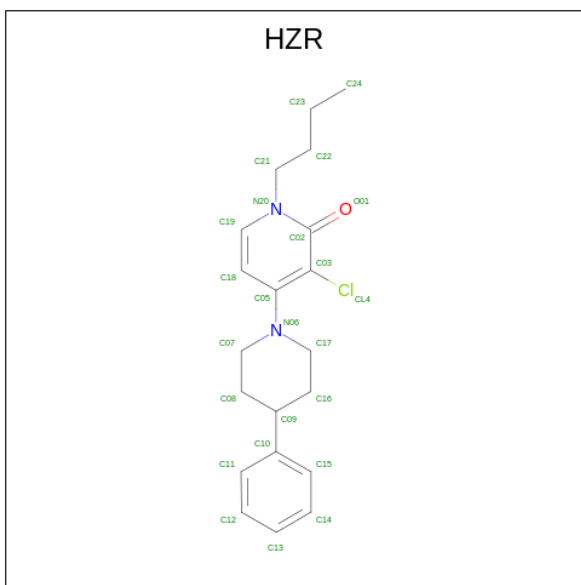
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	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	54	Total	C	N	O	S	0	0
			347	216	63	65	3		

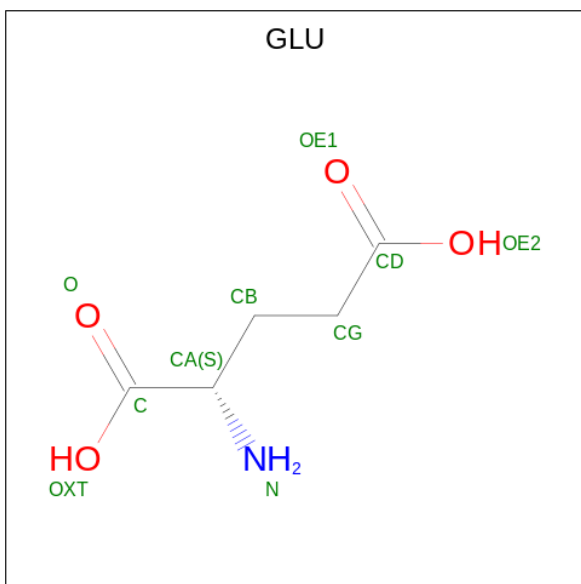
- Molecule 6 is 1-butyl-3-chloranyl-4-(4-phenylpiperidin-1-yl)pyridin-2-one (three-letter code: HZR) (formula: C<sub>20</sub>H<sub>25</sub>ClN<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
6	2	1	Total	C	Cl	N	O	0
			24	20	1	2	1	

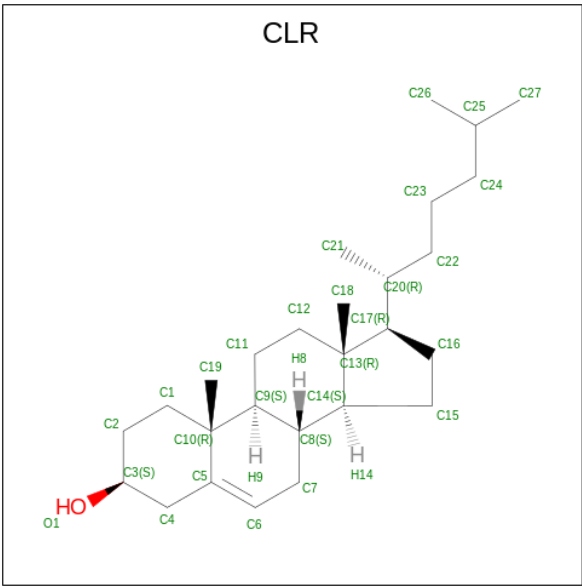
- Molecule 7 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	2	1	Total	C	N	O	0
			10	5	1	4	
7	3	1	Total	C	N	O	0
			10	5	1	4	

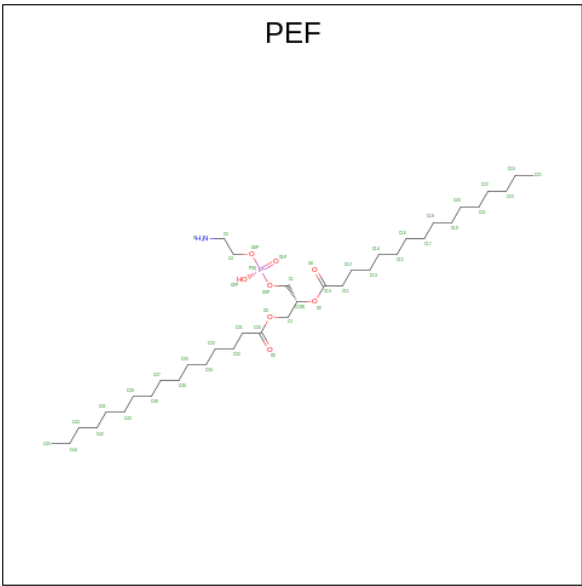


- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			AltConf
8	2	1	Total	C	O	0
			28	27	1	
8	3	1	Total	C	O	0
			28	27	1	
8	3	1	Total	C	O	0
			28	27	1	

- Molecule 9 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula:  $C_{37}H_{74}NO_8P$ ).





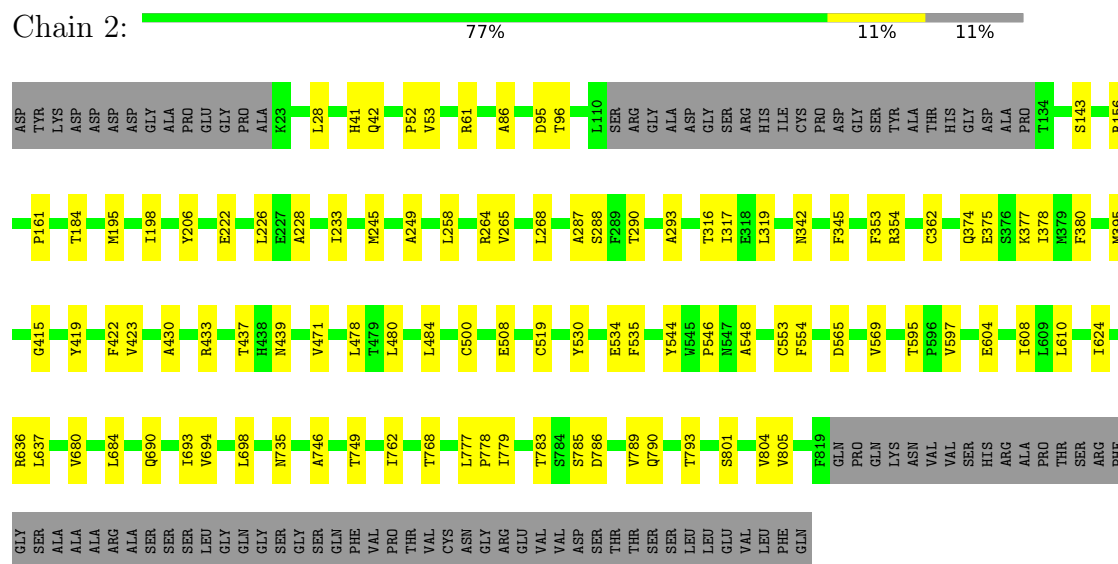
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	3	1	47	37	1	8	1	0



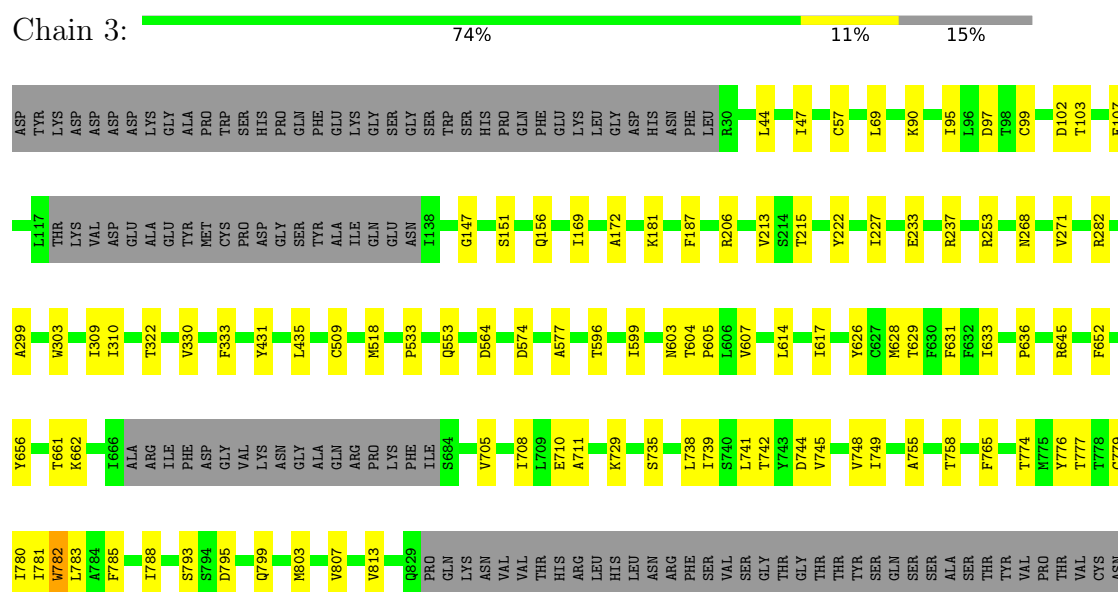
### 3 Residue-property plots

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



#### • Molecule 2: Metabotropic glutamate receptor 3





MET
ALA
SER
ASN
THR
ALA
SER
I9
K46
E47
D48
T52
P53
R62
GLU
LYS
LYS
PHE
PHE
CYS
ALA
ILE
LEU



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	994275	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 ( $e^-/\text{\AA}^2$ )	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, HZR, PEF

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	0.25	0/5936	0.47	0/8095
2	3	0.25	0/5873	0.47	0/7997
3	A	0.24	0/1515	0.44	0/2069
4	B	0.24	0/2260	0.50	0/3099
5	C	0.24	0/352	0.46	0/483
All	All	0.24	0/15936	0.47	0/21743

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 [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	2	5793	0	5597	63	0
2	3	5744	0	5464	67	0
3	A	1491	0	1253	13	0
4	B	2220	0	1846	41	0
5	C	347	0	298	2	0
6	2	24	0	0	1	0
7	2	10	0	5	0	0
7	3	10	0	5	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2	28	0	46	3	0
8	3	56	0	92	3	0
9	3	47	0	73	7	0
All	All	15770	0	14679	190	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 6.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:745:VAL:HG22	2:3:782:TRP:HD1	1.49	0.77
1:2:265:VAL:HG12	1:2:290:THR:HB	1.73	0.69
2:3:614:LEU:HD23	2:3:662:LYS:HD2	1.74	0.69
1:2:768:THR:HG21	1:2:804:VAL:HG21	1.77	0.66
2:3:735:SER:O	2:3:739:ILE:HD12	1.95	0.66
4:B:9:GLN:O	4:B:13:GLN:NE2	2.28	0.66
4:B:294:CYS:HB3	4:B:308:LEU:O	1.96	0.66
1:2:433:ARG:NH2	1:2:437:THR:O	2.29	0.65
4:B:168:LEU:HB2	4:B:178:THR:HB	1.78	0.65
1:2:471:VAL:HG12	1:2:484:LEU:HB2	1.81	0.63
1:2:430:ALA:HB3	1:2:433:ARG:HG2	1.80	0.63
4:B:230:ASN:HD22	4:B:274:THR:HA	1.64	0.62
1:2:228:ALA:HB1	1:2:233:ILE:HB	1.80	0.62
4:B:104:ALA:HB3	4:B:113:ALA:HB3	1.80	0.62
2:3:645:ARG:HH22	2:3:711:ALA:HA	1.65	0.61
8:3:903:CLR:H3	9:3:904:PEF:H12	1.83	0.61
2:3:577:ALA:HB1	2:3:633:ILE:HD11	1.84	0.60
2:3:813:VAL:HG23	9:3:904:PEF:H401	1.82	0.60
4:B:310:GLY:HA3	4:B:339:TRP:HZ2	1.66	0.60
1:2:28:LEU:HD13	1:2:86:ALA:HB3	1.82	0.59
2:3:215:THR:HB	2:3:227:ILE:HD11	1.84	0.59
2:3:102:ASP:HB2	2:3:156:GLN:HG3	1.84	0.59
2:3:299:ALA:HB3	2:3:322:THR:HG22	1.84	0.59
4:B:212:ASP:OD2	4:B:215:GLU:N	2.34	0.59
2:3:233:GLU:OE1	2:3:237:ARG:NH1	2.33	0.59
2:3:745:VAL:HG22	2:3:782:TRP:CD1	2.36	0.58
3:A:209:LYS:O	3:A:213:HIS:ND1	2.28	0.57
2:3:744:ASP:O	2:3:748:VAL:HG23	2.05	0.57
4:B:313:ASN:OD1	4:B:314:ARG:N	2.36	0.57
1:2:636:ARG:HD3	1:2:698:LEU:HD13	1.85	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:781:ILE:HG22	2:3:782:TRP:CE3	2.40	0.56
2:3:268:ASN:ND2	2:3:509:CYS:O	2.38	0.56
2:3:614:LEU:HD12	2:3:617:ILE:HD11	1.87	0.56
1:2:735:ASN:ND2	6:2:901:HZR:O01	2.38	0.55
3:A:208:ARG:O	3:A:212:ILE:HG12	2.06	0.55
2:3:169:ILE:HD11	2:3:435:LEU:HD11	1.88	0.55
2:3:645:ARG:NH2	2:3:710:GLU:O	2.40	0.55
1:2:793:THR:HG22	8:2:903:CLR:H121	1.87	0.55
1:2:785:SER:H	1:2:790:GLN:HE22	1.55	0.54
2:3:785:PHE:HZ	2:3:803:MET:SD	2.30	0.54
3:A:194:LEU:HD23	3:A:196:PHE:HE1	1.72	0.54
4:B:147:SER:OG	4:B:188:MET:O	2.26	0.54
8:3:903:CLR:H161	9:3:904:PEF:H392	1.89	0.54
1:2:268:LEU:HB2	1:2:293:ALA:HA	1.89	0.54
1:2:779:ILE:HD13	8:2:903:CLR:H122	1.90	0.53
2:3:652:PHE:HZ	2:3:807:VAL:HG22	1.72	0.53
4:B:230:ASN:ND2	4:B:273:ILE:O	2.41	0.53
1:2:195:MET:HG2	1:2:317:ILE:HD12	1.90	0.53
2:3:172:ALA:O	7:3:901:GLU:N	2.42	0.53
2:3:574:ASP:H	2:3:577:ALA:HB3	1.74	0.53
3:A:210:LYS:HA	3:A:213:HIS:HE1	1.73	0.52
1:2:783:THR:HB	1:2:789:VAL:HG11	1.92	0.52
2:3:213:VAL:HG12	2:3:271:VAL:HB	1.92	0.52
4:B:59:TYR:HD2	4:B:101:MET:HG3	1.74	0.52
1:2:95:ASP:OD1	1:2:96:THR:N	2.43	0.52
1:2:61:ARG:NH1	1:2:143:SER:OG	2.43	0.51
1:2:156:ARG:NH1	2:3:107:GLU:OE2	2.37	0.51
2:3:793:SER:HA	2:3:799:GLN:NE2	2.25	0.51
9:3:904:PEF:H442	9:3:904:PEF:H241	1.91	0.51
2:3:181:LYS:NZ	2:3:187:PHE:O	2.44	0.51
4:B:297:TRP:HA	4:B:304:ARG:HA	1.93	0.51
1:2:319:LEU:HD12	1:2:377:LYS:HE3	1.92	0.50
3:A:208:ARG:HD2	3:A:211:TRP:HE1	1.77	0.50
4:B:313:ASN:ND2	4:B:332:TRP:HB2	2.27	0.50
2:3:705:VAL:HA	2:3:708:ILE:HG22	1.92	0.50
1:2:508:GLU:H	1:2:530:TYR:HE1	1.59	0.50
1:2:478:LEU:HD11	1:2:480:LEU:HD23	1.92	0.49
3:A:210:LYS:HA	3:A:213:HIS:CE1	2.47	0.49
1:2:778:PRO:HB2	2:3:788:ILE:HD11	1.92	0.49
2:3:795:ASP:O	2:3:799:GLN:HG2	2.12	0.49
4:B:56:ALA:HB2	4:B:76:ASP:OD2	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:624:ILE:HG13	1:2:624:ILE:O	2.11	0.49
1:2:293:ALA:HB3	1:2:316:THR:HG22	1.93	0.49
8:3:903:CLR:H241	9:3:904:PEF:H421	1.93	0.49
4:B:58:ILE:HD11	4:B:330:GLY:HA3	1.94	0.49
4:B:168:LEU:O	4:B:177:THR:OG1	2.21	0.49
3:A:201:VAL:HG13	3:A:203:ALA:H	1.77	0.49
1:2:375:GLU:HB3	1:2:378:ILE:HG12	1.94	0.49
4:B:169:TRP:CD1	4:B:176:GLN:HA	2.47	0.49
1:2:264:ARG:NH2	1:2:288:SER:O	2.47	0.48
4:B:290:ASP:HA	4:B:314:ARG:HG3	1.94	0.48
1:2:222:GLU:O	1:2:226:LEU:HG	2.14	0.48
2:3:599:ILE:O	2:3:603:ASN:ND2	2.47	0.48
1:2:548:ALA:HB2	1:2:554:PHE:HB3	1.94	0.48
2:3:626:TYR:O	2:3:629:THR:HG22	2.14	0.48
2:3:776:TYR:O	2:3:780:ILE:HG12	2.13	0.48
4:B:67:SER:OG	4:B:68:ARG:N	2.47	0.48
1:2:534:GLU:HG2	1:2:535:PHE:N	2.29	0.48
4:B:57:LYS:HD2	4:B:332:TRP:CD2	2.49	0.47
2:3:741:LEU:O	2:3:745:VAL:HG23	2.14	0.47
1:2:746:ALA:HA	1:2:749:THR:HG22	1.96	0.47
3:A:310:LEU:HB2	3:A:312:LYS:HE2	1.96	0.47
1:2:245:MET:HG3	1:2:249:ALA:HB3	1.96	0.47
1:2:530:TYR:HB3	1:2:546:PRO:HB2	1.95	0.47
4:B:77:GLY:O	4:B:95:LEU:N	2.35	0.47
3:A:295:THR:OG1	3:A:298:GLU:OE1	2.33	0.47
1:2:419:TYR:HA	1:2:423:VAL:HB	1.96	0.47
2:3:656:TYR:CE2	2:3:748:VAL:HG22	2.50	0.47
4:B:75:GLN:N	4:B:75:GLN:OE1	2.48	0.47
2:3:102:ASP:OD1	2:3:103:THR:N	2.47	0.47
2:3:742:THR:HA	2:3:745:VAL:HB	1.95	0.47
1:2:637:LEU:HA	1:2:694:VAL:HG21	1.97	0.47
4:B:296:VAL:O	4:B:305:ALA:N	2.48	0.46
2:3:745:VAL:O	2:3:749:ILE:HG12	2.14	0.46
2:3:69:LEU:HD13	2:3:95:ILE:HG21	1.96	0.46
1:2:433:ARG:NH2	1:2:439:ASN:H	2.14	0.46
2:3:330:VAL:HG12	2:3:333:PHE:H	1.81	0.46
4:B:231:ALA:HB3	4:B:275:SER:HA	1.98	0.46
4:B:16:ASN:O	4:B:19:ARG:HG3	2.16	0.45
1:2:801:SER:O	1:2:805:VAL:HG23	2.16	0.45
4:B:145:TYR:O	4:B:162:GLY:N	2.49	0.45
2:3:553:GLN:HG2	2:3:564:ASP:HA	1.97	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3:904:PEF:H31	9:3:904:PEF:H312	1.64	0.45
4:B:75:GLN:HG2	4:B:99:TRP:HD1	1.80	0.45
8:2:903:CLR:H183	8:2:903:CLR:H212	1.99	0.45
2:3:253:ARG:HD3	2:3:253:ARG:HA	1.75	0.45
4:B:148:CYS:SG	4:B:149:CYS:N	2.90	0.45
1:2:785:SER:N	1:2:790:GLN:HE22	2.15	0.44
2:3:518:MET:HA	2:3:533:PRO:HA	1.97	0.44
2:3:604:THR:OG1	2:3:605:PRO:HD3	2.16	0.44
9:3:904:PEF:H352	9:3:904:PEF:H381	1.57	0.44
1:2:161:PRO:HD3	1:2:415:GLY:HA3	1.99	0.44
1:2:374:GLN:HE21	1:2:378:ILE:HG21	1.82	0.44
2:3:774:THR:HA	2:3:777:THR:HG22	1.99	0.44
2:3:738:LEU:O	2:3:742:THR:HG23	2.17	0.44
1:2:41:HIS:HA	1:2:53:VAL:HA	2.00	0.44
1:2:534:GLU:HG2	1:2:535:PHE:H	1.82	0.44
2:3:282:ARG:HA	2:3:309:ILE:HG23	1.99	0.44
2:3:774:THR:O	2:3:777:THR:HG22	2.18	0.44
1:2:342:ASN:HB3	1:2:345:PHE:HB2	2.00	0.43
2:3:151:SER:HB2	2:3:222:TYR:HB2	1.99	0.43
4:B:235:PHE:HA	4:B:278:PHE:HD2	1.82	0.43
1:2:42:GLN:N	1:2:52:PRO:O	2.40	0.43
2:3:636:PRO:HG3	2:3:729:LYS:HA	2.01	0.43
1:2:258:LEU:HD11	1:2:287:ALA:HB2	2.00	0.43
4:B:254:ASP:HB3	4:B:257:ALA:HB3	1.99	0.43
1:2:500:CYS:HB3	1:2:519:CYS:HB3	1.53	0.43
1:2:544:TYR:HB3	1:2:553:CYS:HB3	2.01	0.43
1:2:353:PHE:HB2	1:2:362:CYS:SG	2.59	0.42
1:2:680:VAL:O	1:2:684:LEU:HD23	2.19	0.42
2:3:781:ILE:HG22	2:3:782:TRP:CZ3	2.54	0.42
1:2:777:LEU:HB3	1:2:778:PRO:HD3	2.01	0.42
2:3:303:TRP:HZ2	2:3:310:ILE:HD11	1.85	0.42
2:3:607:VAL:HG13	2:3:765:PHE:HZ	1.85	0.42
3:A:186:GLU:OE1	3:A:186:GLU:N	2.52	0.42
2:3:781:ILE:HG22	2:3:782:TRP:HE3	1.81	0.42
4:B:52:ARG:NE	4:B:52:ARG:HA	2.34	0.42
1:2:637:LEU:HD23	1:2:637:LEU:H	1.85	0.42
2:3:431:TYR:HA	2:3:435:LEU:HB3	2.01	0.42
1:2:604:GLU:O	1:2:608:ILE:HG12	2.19	0.42
3:A:344:ILE:O	3:A:348:LEU:HG	2.18	0.42
1:2:786:ASP:HA	1:2:790:GLN:OE1	2.20	0.42
4:B:7:LEU:O	4:B:10:GLU:HG3	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:746:ALA:HB2	1:2:762:ILE:HD11	2.02	0.42
1:2:779:ILE:HG13	2:3:788:ILE:HG13	2.01	0.42
2:3:607:VAL:HG13	2:3:765:PHE:CZ	2.55	0.42
1:2:610:LEU:HD23	1:2:610:LEU:HA	1.85	0.42
4:B:241:PHE:HE2	4:B:255:LEU:HA	1.85	0.42
2:3:44:LEU:H	2:3:147:GLY:HA3	1.85	0.41
1:2:595:THR:HG22	1:2:597:VAL:HG22	2.02	0.41
1:2:690:GLN:HA	1:2:693:ILE:HG22	2.01	0.41
2:3:628:MET:HA	2:3:631:PHE:HD2	1.85	0.41
4:B:101:MET:N	4:B:101:MET:SD	2.92	0.41
2:3:57:CYS:HB3	2:3:99:CYS:HB3	1.25	0.41
4:B:59:TYR:CD2	4:B:101:MET:HG3	2.52	0.41
2:3:596:THR:HA	2:3:599:ILE:HG22	2.03	0.41
4:B:331:SER:OG	4:B:332:TRP:N	2.53	0.41
1:2:184:THR:HG22	1:2:380:PHE:HD1	1.84	0.41
2:3:47:ILE:HD12	2:3:97:ASP:HB2	2.02	0.41
2:3:206:ARG:HA	2:3:206:ARG:HD3	1.84	0.41
2:3:656:TYR:CD2	2:3:748:VAL:HG22	2.56	0.41
2:3:779:CYS:O	2:3:783:LEU:HD23	2.21	0.41
4:B:164:THR:HG21	4:B:183:HIS:O	2.21	0.41
4:B:333:ASP:OD1	4:B:333:ASP:N	2.54	0.41
1:2:206:TYR:CD1	1:2:500:CYS:HB2	2.55	0.41
3:A:266:LEU:HD23	3:A:321:THR:HG23	2.02	0.41
5:C:52:THR:OG1	5:C:53:PRO:HD3	2.21	0.41
1:2:395:MET:HG3	1:2:422:PHE:CE2	2.55	0.41
1:2:785:SER:O	1:2:789:VAL:HG12	2.21	0.40
2:3:614:LEU:HD21	2:3:661:THR:HB	2.03	0.40
3:A:37:LEU:HB3	3:A:221:ILE:HG22	2.03	0.40
4:B:110:ASN:O	4:B:126:LEU:N	2.53	0.40
4:B:229:ILE:HA	4:B:245:SER:HA	2.03	0.40
1:2:198:ILE:HD12	1:2:317:ILE:HD11	2.03	0.40
1:2:565:ASP:HA	1:2:569:VAL:HG23	2.03	0.40
2:3:90:LYS:HB3	2:3:90:LYS:HE3	1.87	0.40
2:3:755:ALA:HA	2:3:758:THR:HG22	2.02	0.40
2:3:793:SER:HA	2:3:799:GLN:HE22	1.86	0.40
4:B:164:THR:HG22	4:B:182:GLY:HA3	2.02	0.40
5:C:48:ASP:O	5:C:52:THR:HG23	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	770/870 (88%)	737 (96%)	33 (4%)	0	100	100
2	3	757/894 (85%)	732 (97%)	25 (3%)	0	100	100
3	A	215/354 (61%)	207 (96%)	8 (4%)	0	100	100
4	B	334/351 (95%)	317 (95%)	17 (5%)	0	100	100
5	C	52/71 (73%)	49 (94%)	3 (6%)	0	100	100
All	All	2128/2540 (84%)	2042 (96%)	86 (4%)	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	2	581/712 (82%)	580 (100%)	1 (0%)	92	95
2	3	588/781 (75%)	587 (100%)	1 (0%)	92	95
3	A	123/305 (40%)	122 (99%)	1 (1%)	79	87
4	B	180/293 (61%)	179 (99%)	1 (1%)	84	90
5	C	26/58 (45%)	25 (96%)	1 (4%)	28	56
All	All	1498/2149 (70%)	1493 (100%)	5 (0%)	88	94

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



Mol	Chain	Res	Type
1	2	354	ARG
2	3	782	TRP
3	A	209	LYS
4	B	19	ARG
5	C	46	LYS

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

Mol	Chain	Res	Type
4	B	13	GLN
4	B	230	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](#)

7 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	GLU	2	902	-	8,9,9	1.02	0	10,11,11	1.18	0
8	CLR	3	903	-	31,31,31	0.27	0	48,48,48	0.40	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	HZR	2	901	-	25,26,26	3.13	12 (48%)	31,35,35	1.80	8 (25%)
8	CLR	2	903	-	31,31,31	0.29	0	48,48,48	0.64	1 (2%)
9	PEF	3	904	-	46,46,46	1.30	4 (8%)	49,51,51	0.81	2 (4%)
8	CLR	3	902	-	31,31,31	0.27	0	48,48,48	0.40	0
7	GLU	3	901	-	8,9,9	1.02	0	10,11,11	1.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLU	2	902	-	-	4/9/9/9	-
8	CLR	3	903	-	-	4/10/68/68	0/4/4/4
6	HZR	2	901	-	-	7/12/22/22	0/3/3/3
8	CLR	2	903	-	-	5/10/68/68	0/4/4/4
9	PEF	3	904	-	-	34/50/50/50	-
8	CLR	3	902	-	-	4/10/68/68	0/4/4/4
7	GLU	3	901	-	-	6/9/9/9	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	901	HZR	C19-N20	7.93	1.48	1.37
6	2	901	HZR	C19-C18	7.70	1.53	1.35
6	2	901	HZR	C02-N20	5.57	1.48	1.39
6	2	901	HZR	C03-C02	4.62	1.53	1.44
6	2	901	HZR	C18-C05	4.30	1.49	1.41
9	3	904	PEF	O2-C10	4.06	1.45	1.34
6	2	901	HZR	C17-N06	3.21	1.52	1.47
6	2	901	HZR	C07-N06	3.16	1.52	1.47
9	3	904	PEF	O3-C30	3.06	1.42	1.33
6	2	901	HZR	C03-CL4	2.82	1.79	1.72
9	3	904	PEF	C11-C10	2.62	1.58	1.50
6	2	901	HZR	C08-C09	-2.61	1.46	1.53
6	2	901	HZR	C16-C09	-2.56	1.46	1.53
9	3	904	PEF	P-O4P	2.09	1.67	1.59
6	2	901	HZR	C05-N06	2.05	1.45	1.38
6	2	901	HZR	O01-C02	-2.02	1.18	1.23



All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	901	HZR	C05-C03-C02	-4.15	119.76	123.11
6	2	901	HZR	C19-N20-C02	-3.83	120.05	122.89
9	3	904	PEF	O2-C10-C11	3.55	119.14	111.50
6	2	901	HZR	O01-C02-C03	-3.22	119.84	125.19
6	2	901	HZR	C07-C08-C09	2.91	114.48	111.04
6	2	901	HZR	C16-C09-C08	2.86	115.52	109.56
6	2	901	HZR	C17-C16-C09	2.72	114.26	111.04
9	3	904	PEF	O3-C30-C31	2.59	120.05	111.91
6	2	901	HZR	C16-C09-C10	-2.54	106.84	112.79
6	2	901	HZR	C18-C19-N20	-2.44	120.15	122.44
8	2	903	CLR	C13-C17-C20	2.38	123.22	119.49

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	902	GLU	N-CA-CB-CG
7	2	902	GLU	C-CA-CB-CG
8	2	903	CLR	C13-C17-C20-C21
9	3	904	PEF	O4-C10-O2-C2
9	3	904	PEF	C31-C30-O3-C3
9	3	904	PEF	O5-C30-O3-C3
9	3	904	PEF	C1-O3P-P-O1P
9	3	904	PEF	C1-O3P-P-O2P
9	3	904	PEF	C1-O3P-P-O4P
9	3	904	PEF	C11-C10-O2-C2
8	2	903	CLR	C16-C17-C20-C22
9	3	904	PEF	C40-C41-C42-C43
9	3	904	PEF	C17-C18-C19-C20
9	3	904	PEF	C35-C36-C37-C38
9	3	904	PEF	C13-C14-C15-C16
8	3	902	CLR	C13-C17-C20-C22
6	2	901	HZR	N20-C21-C22-C23
8	2	903	CLR	C16-C17-C20-C21
6	2	901	HZR	C22-C21-N20-C19
9	3	904	PEF	C30-C31-C32-C33
8	3	902	CLR	C16-C17-C20-C21
8	3	902	CLR	C13-C17-C20-C21
9	3	904	PEF	C37-C38-C39-C40
8	2	903	CLR	C13-C17-C20-C22
9	3	904	PEF	C34-C35-C36-C37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	3	904	PEF	C1-C2-O2-C10
9	3	904	PEF	C19-C20-C21-C22
9	3	904	PEF	C33-C34-C35-C36
9	3	904	PEF	C38-C39-C40-C41
9	3	904	PEF	C36-C37-C38-C39
9	3	904	PEF	C42-C43-C44-C45
9	3	904	PEF	C32-C33-C34-C35
9	3	904	PEF	C31-C32-C33-C34
9	3	904	PEF	O3P-C1-C2-C3
9	3	904	PEF	C14-C15-C16-C17
9	3	904	PEF	C16-C17-C18-C19
8	3	902	CLR	C16-C17-C20-C22
9	3	904	PEF	C1-C2-C3-O3
7	3	901	GLU	OXT-C-CA-N
9	3	904	PEF	O2-C2-C3-O3
7	3	901	GLU	O-C-CA-N
9	3	904	PEF	O3P-C1-C2-O2
6	2	901	HZR	C22-C21-N20-C02
8	2	903	CLR	C21-C20-C22-C23
8	3	903	CLR	C16-C17-C20-C22
8	3	903	CLR	C13-C17-C20-C22
8	3	903	CLR	C13-C17-C20-C21
9	3	904	PEF	C18-C19-C20-C21
8	3	903	CLR	C16-C17-C20-C21
9	3	904	PEF	O4P-C4-C5-N
6	2	901	HZR	C16-C09-C10-C11
7	3	901	GLU	O-C-CA-CB
6	2	901	HZR	C16-C09-C10-C15
7	2	902	GLU	OE1-CD-CG-CB
7	2	902	GLU	OE2-CD-CG-CB
9	3	904	PEF	C39-C40-C41-C42
9	3	904	PEF	C2-C1-O3P-P
6	2	901	HZR	C18-C05-N06-C07
6	2	901	HZR	C18-C05-N06-C17
7	3	901	GLU	OE1-CD-CG-CB
7	3	901	GLU	OE2-CD-CG-CB
7	3	901	GLU	OXT-C-CA-CB
9	3	904	PEF	O3-C30-C31-C32
9	3	904	PEF	O5-C30-C31-C32

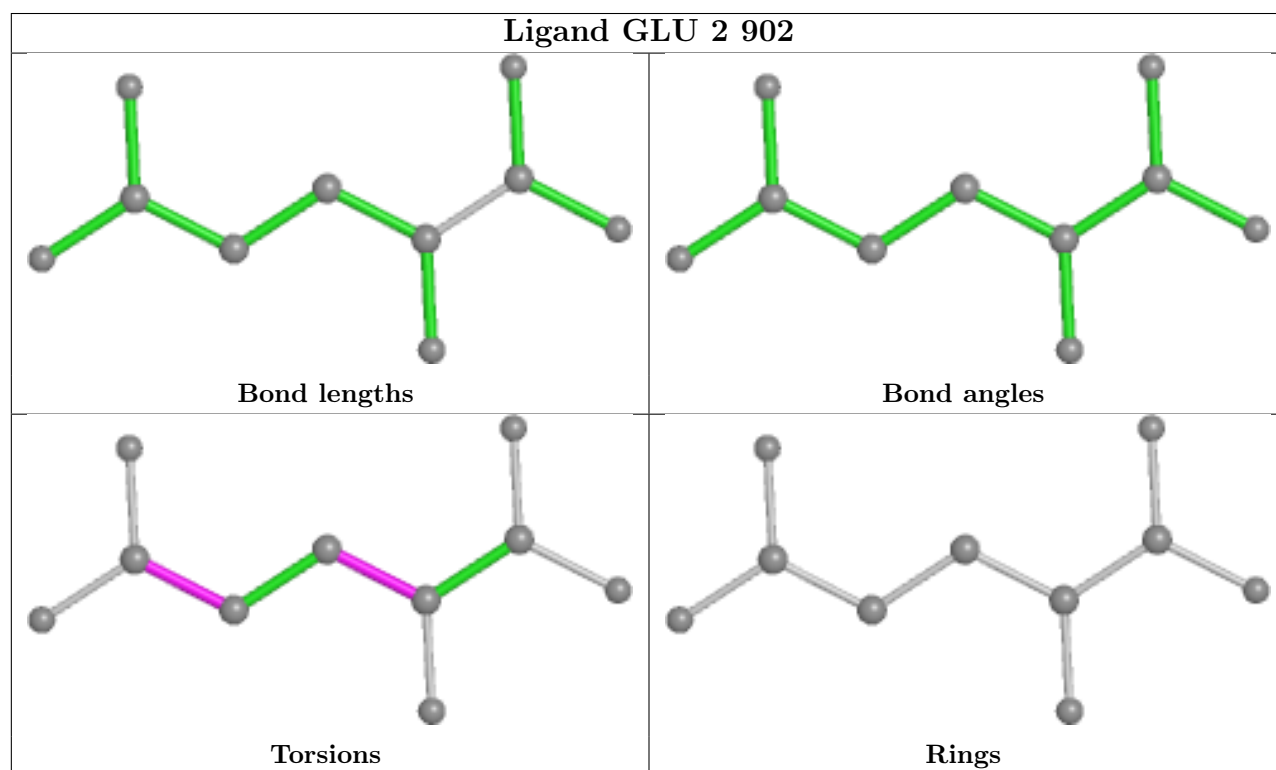
There are no ring outliers.

5 monomers are involved in 12 short contacts:



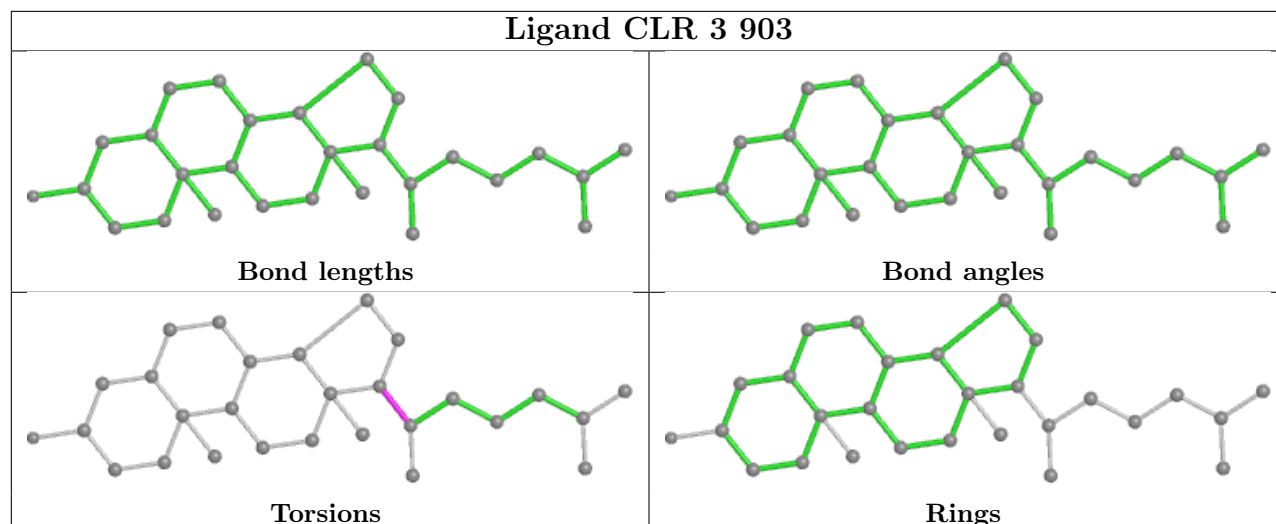
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	3	903	CLR	3	0
6	2	901	HZR	1	0
8	2	903	CLR	3	0
9	3	904	PEF	7	0
7	3	901	GLU	1	0

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.

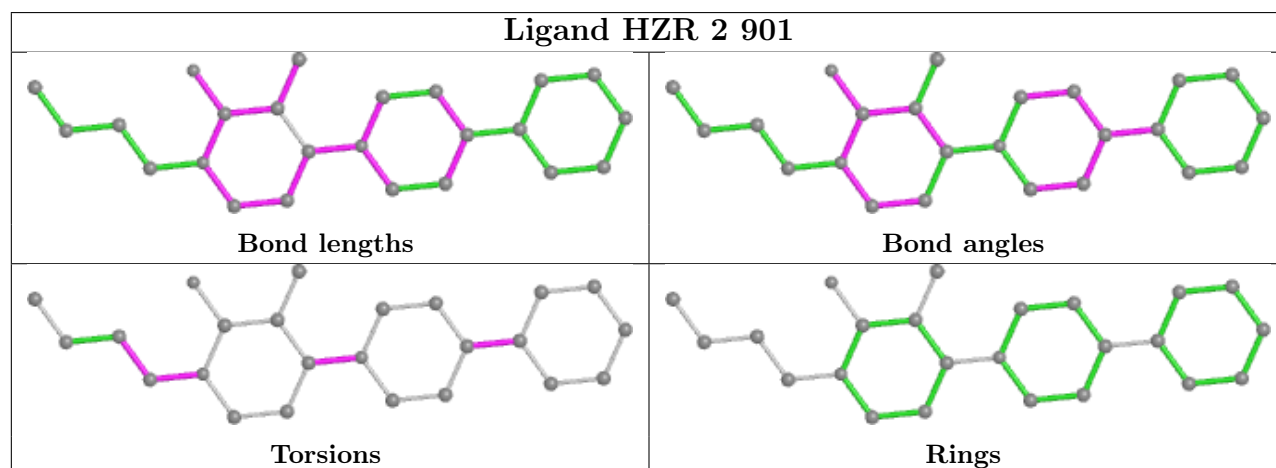




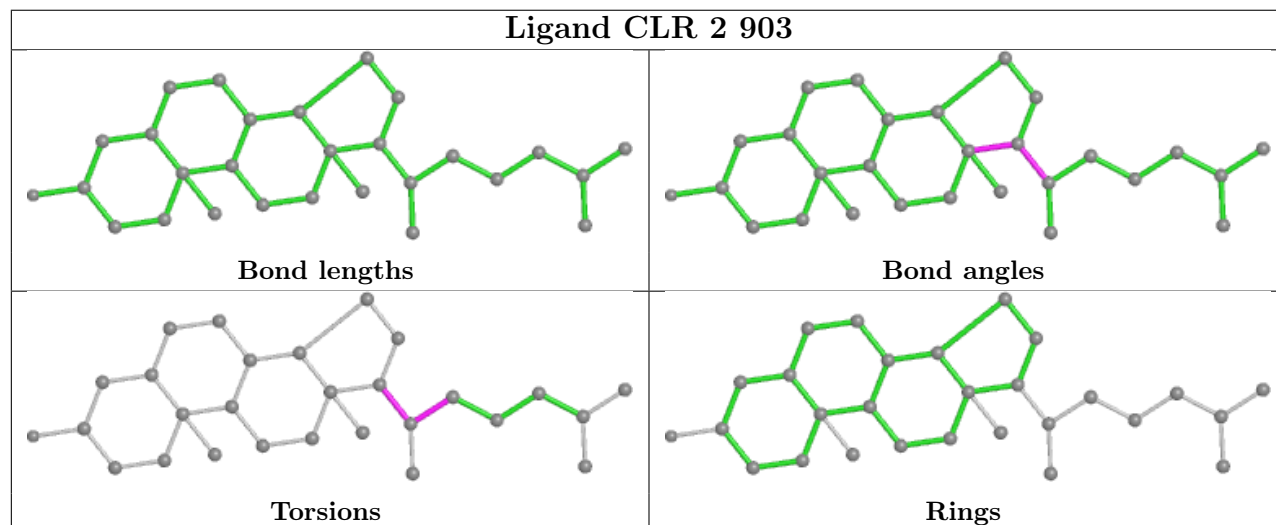
## Ligand CLR 3 903



## Ligand HZR 2 901

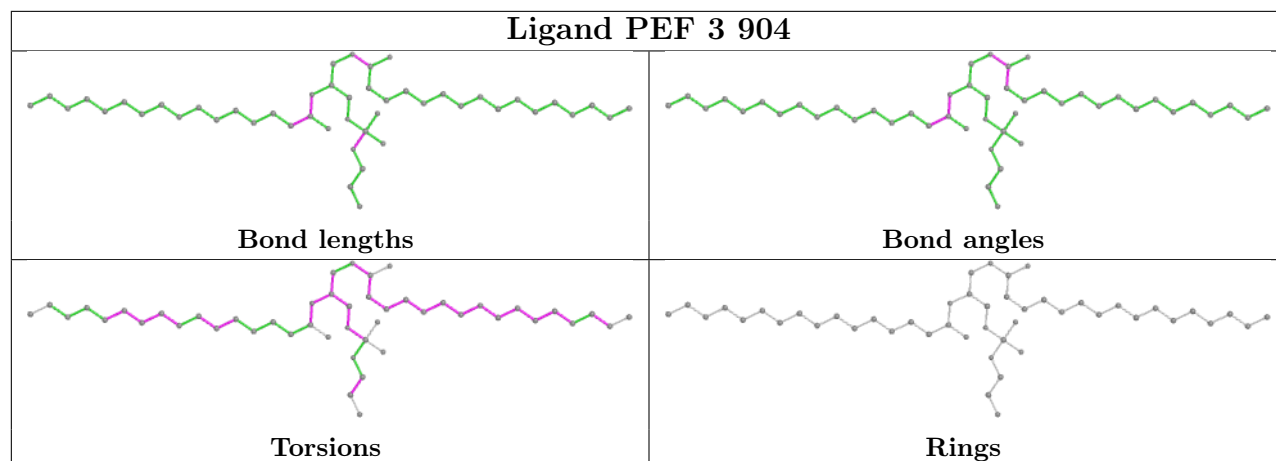


## Ligand CLR 2 903

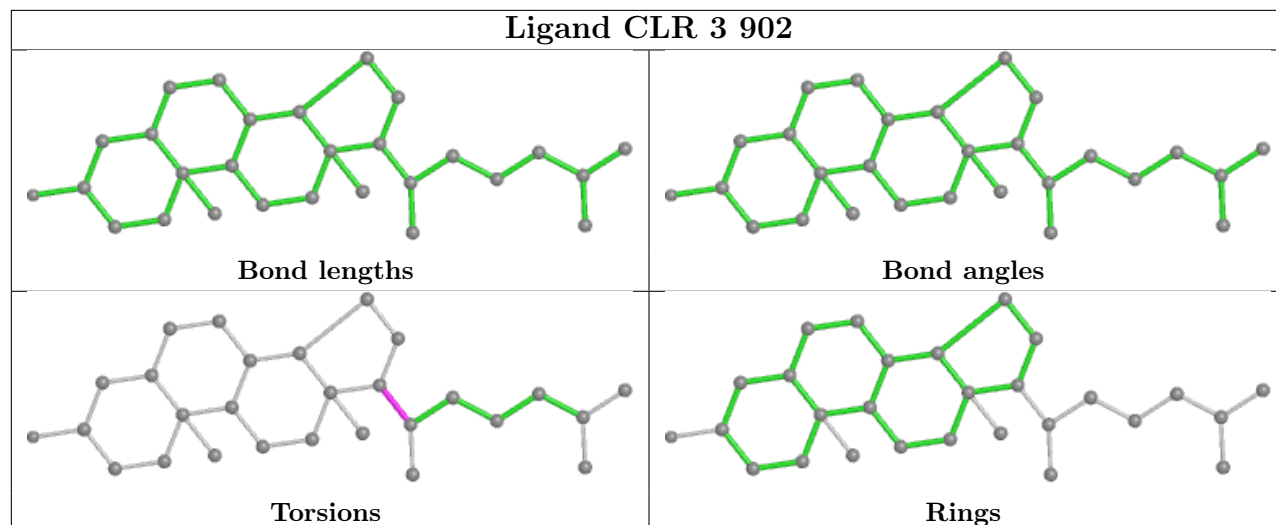




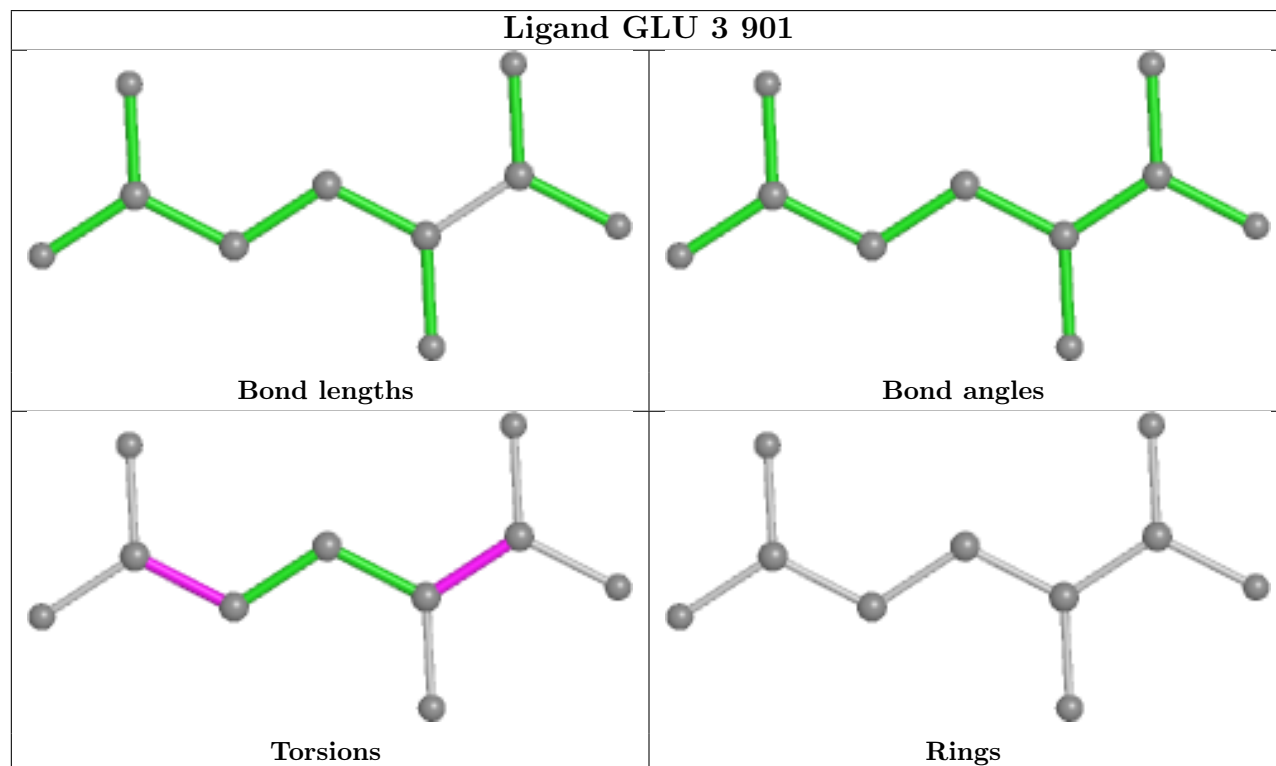
## Ligand PEF 3 904



## Ligand CLR 3 902



## Ligand GLU 3 901





## 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.