



wwPDB EM Validation Summary Report ⓘ

Oct 8, 2023 – 12:38 AM 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)

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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

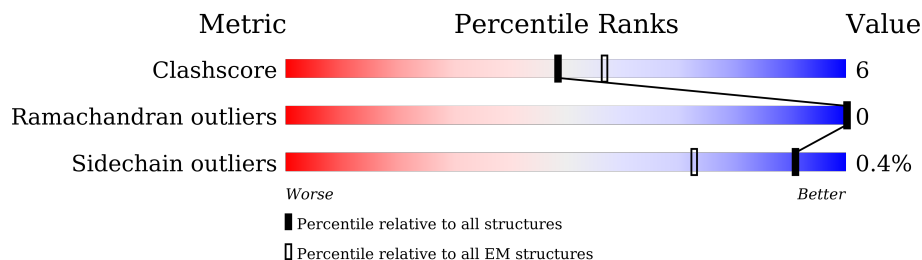
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	870	
2	3	894	
3	A	354	
4	B	351	
5	C	71	

2 Entry composition i

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
			Total	C	N	O	S		
1	2	774	5793	3730	990	1033	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 3.

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

There are 37 discrepancies between the modelled and reference sequences:

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

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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
			Total	C	N	O	S		
3	A	219	1491	948	251	282	10	0	0

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
			Total	C	N	O	S		
4	B	336	2220	1372	400	431	17	0	0

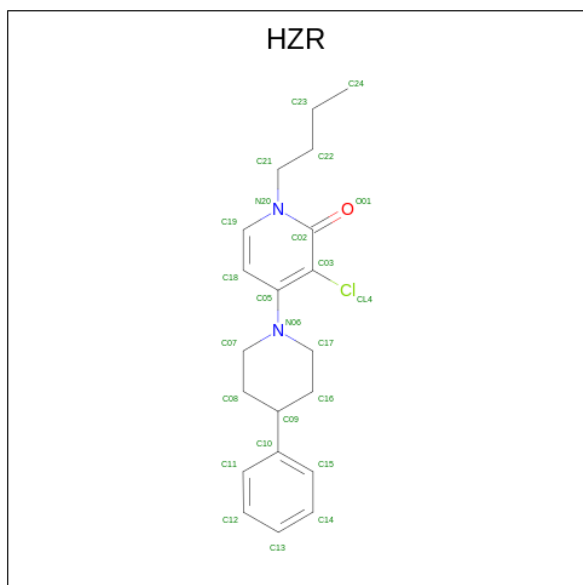
There are 12 discrepancies between the modelled and reference sequences:

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.

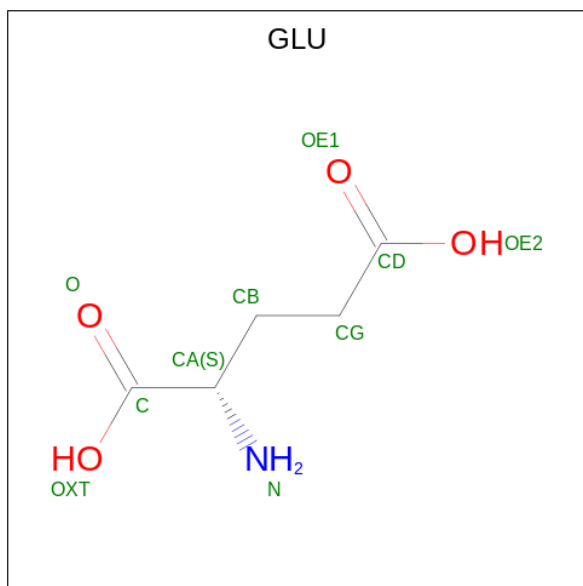
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	54	347	216	63	65	3	0	0

- Molecule 6 is 1-butyl-3-chloranyl-4-(4-phenylpiperidin-1-yl)pyridin-2-one (three-letter code: HZR) (formula: C₂₀H₂₅ClN₂O) (labeled as "Ligand of Interest" by depositor).



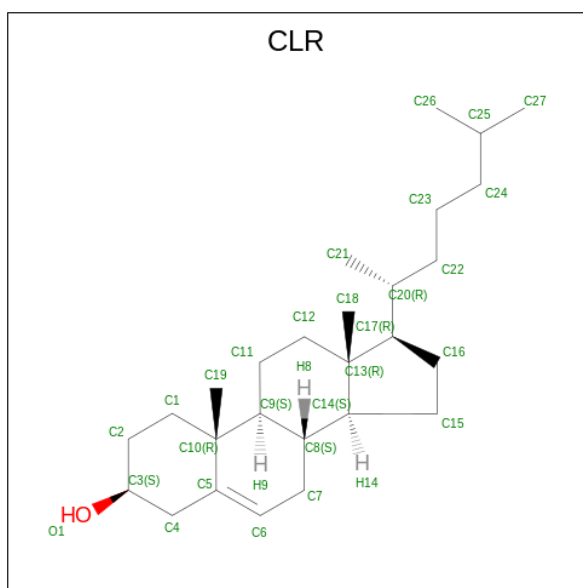
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	N		O
6	2	1	24	20	1	2	1	0

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



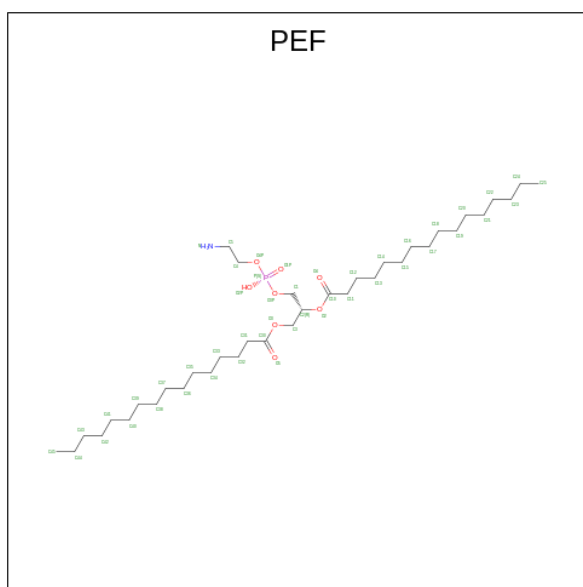
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	2	1	10	5	1	4	0
7	3	1	10	5	1	4	0

- 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

GLY
ARG
GLU
VAL
LEU
ASP
SER
THR
THR
SER
SER
SER
LEU
LEU
GLU
VAL
PHE
LEU
GLN

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

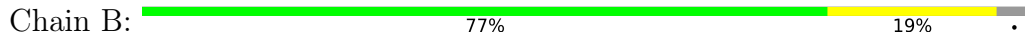


MET
GLY
CYS
THR
LEU
SER
ALA
E9
L37
K53
LYS
ILE
ILE
GLU
GLU
GLY
GLY
ALA
MET
ALA
THR
TYR
SER
SER
GLU
GLU
VAL
VAL
VAL
TYR
SER
SER
GLY
ASN
VAL
THR
THR
ILE
ILE
GLN
SER
ILE
ILE
ILE
ILE
ARG
ARG
MET
MET
GLY
ARG
LEU
LYS
ILE
ILE

ASP
ASP
ALA
ARG
GLN
LEU
PHE
VAL
LEU
LEU
ALA
GLY
GLY
ALA
ALA
GLU
GLU
THR
GLY
HIS
PHE
MET
THR
THR
ALA
GLU
SER
GLY
VAL
VAL
VAL
ILE
LYS
ARG
TRP
LYS
ASP
SER
SER
GLY
VAL
GLN
ALA
ALA
CYS
PHE
ASN
ARG
ILE
ILE
ARG
ARG
GLU
TYR
GLN
LEU
ASN
ASN
ASP
SER
ALA
ALA
TYR
ASP
TYR
PHE
GLY
ASP
SER
ALA
ASP
ARG
ARG

ILE
ALA
GLN
PRO
TYR
ASN
TYR
ILE
PRO
THR
GLN
GLN
ASP
VAL
LEU
ARG
THR
VAL
VAL
LYS
THR
T182
E186
L194
H195
F196
V201
G202
A203
R208
K209
K210
W211
I212
H213
I221
L266
L266
T295
E298
L310
K311
K312
T321
I344
L348
F354

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



MET
HIS
HIS
HIS
HIS
HIS
HIS
GLY
SER
LEU
LEU
LEU
GLN
SER
SER
GLU
L4
L7
R8
Q9
E10
Q13
M16
R19
R52
A56
K57
I58
Y59
S67
R68
Q75
D76
G77
L95
W99
Y100
M101
A104
M110
A113
L126
Y145
L146
S147
C148
C149

G162
D163
T164
L168
W169
Q176
T177
T178
G182
H183
M188
D212
E215
I229
N230
A231
F235
F241
S245
D254
L255
R256
A257
I273
T274
S275
F278
D290
C294
M295
Y296
W297
R304
A305
L308
G310
R313
R314
G330

S331
W332
D333
W339
ASN

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



MET
ALA
SER
ASN
ASN
THR
ALA
SER
I9
K46
E47
D48
T52
P53
R62
GLU
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: PEF, 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	0.25	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

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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.

The worst 5 of 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

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	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 [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	581/712 (82%)	580 (100%)	1 (0%)	93	97
2	3	588/781 (75%)	587 (100%)	1 (0%)	93	97
3	A	123/305 (40%)	122 (99%)	1 (1%)	81	89
4	B	180/293 (61%)	179 (99%)	1 (1%)	86	91
5	C	26/58 (45%)	25 (96%)	1 (4%)	33	62
All	All	1498/2149 (70%)	1493 (100%)	5 (0%)	91	96

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 monosaccharides 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	902	-	31,31,31	0.27	0	48,48,48	0.40	0
8	CLR	3	903	-	31,31,31	0.27	0	48,48,48	0.40	0
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%)
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	902	-	-	4/10/68/68	0/4/4/4
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	-
7	GLU	3	901	-	-	6/9/9/9	-

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

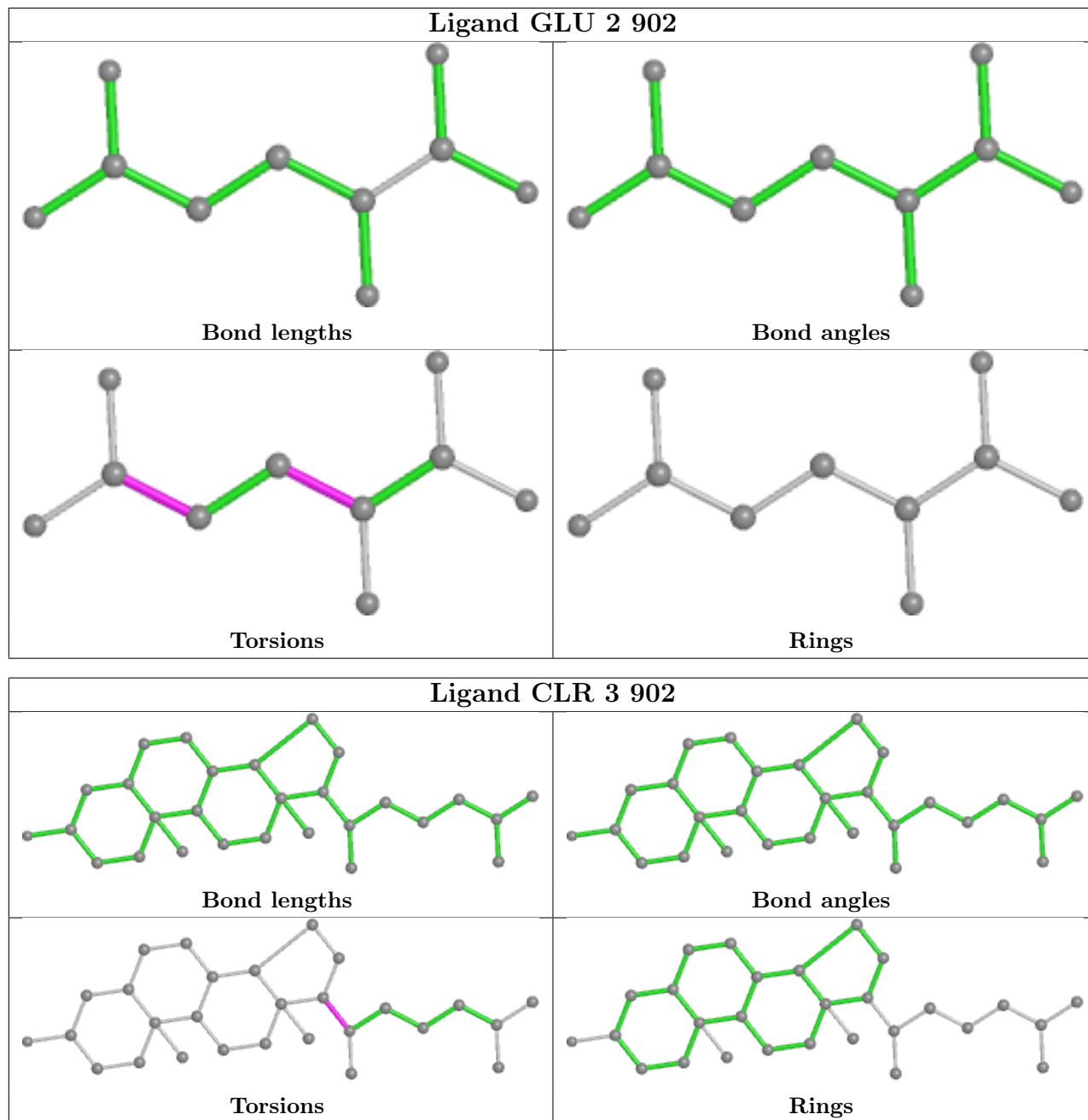
There are no ring outliers.

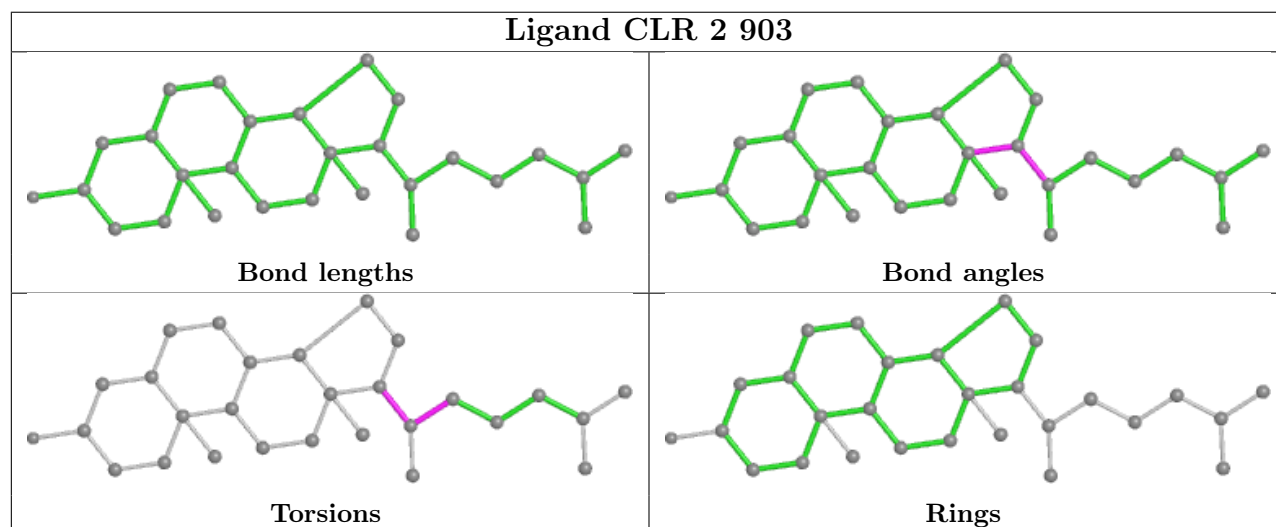
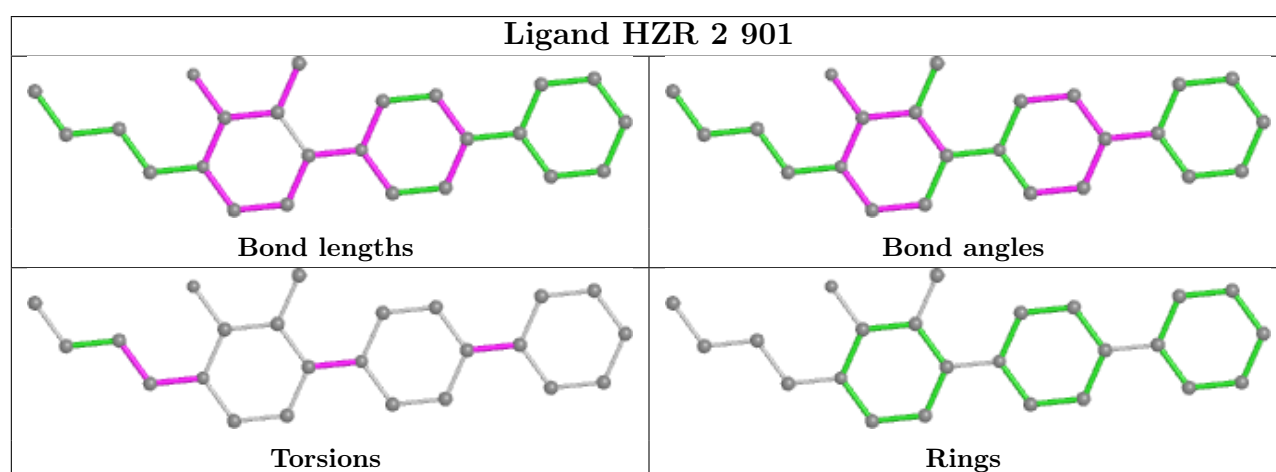
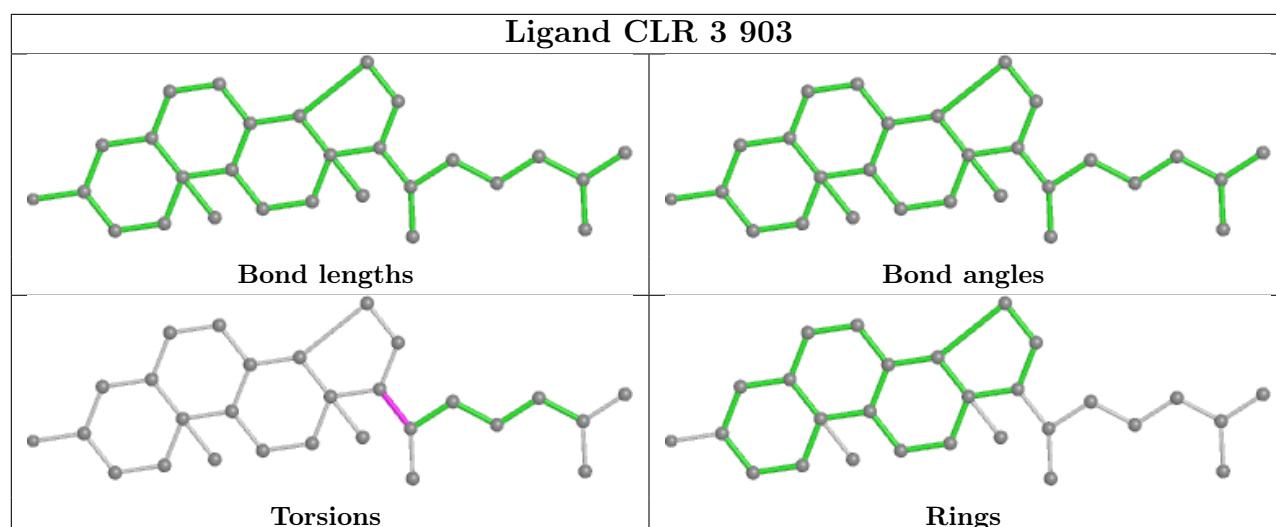
5 monomers are involved in 12 short contacts:

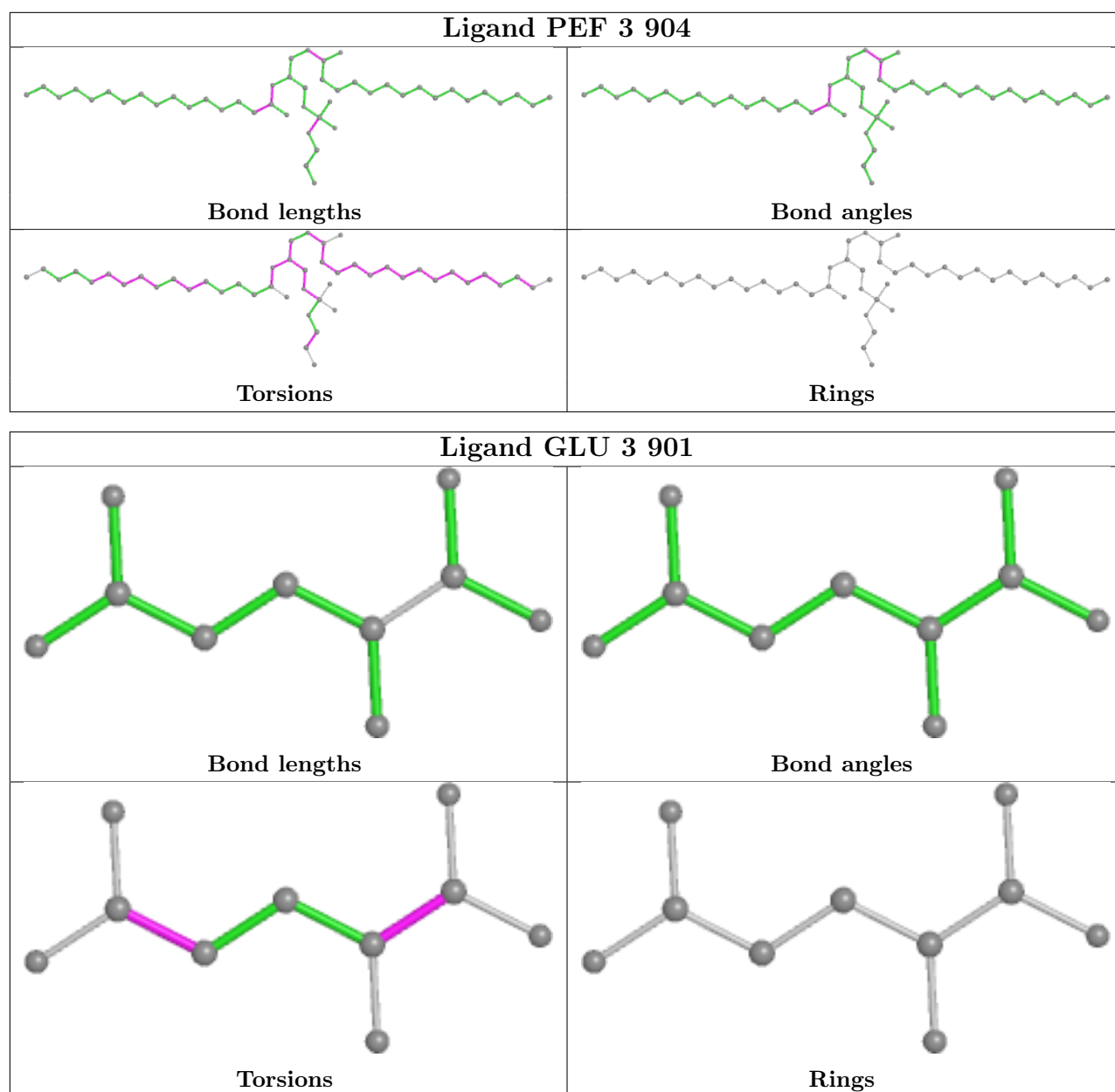
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	3	903	CLR	3	0
6	2	901	HZR	1	0
8	2	903	CLR	3	0
9	3	904	PEF	7	0
7	3	901	GLU	1	0

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.







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.