



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2025 – 12:10 AM JST

PDB ID : 9II3  
EMDB ID : EMD-60589  
Title : Cryo-EM Structure of the 2:1 Complex of mGlu3 and beta-arrestin1  
Authors : Wen, T.L.; Du, M.; Yang, X.; Shen, Y.Q.  
Deposited on : 2024-06-19  
Resolution : 3.90 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) : 2.41.2

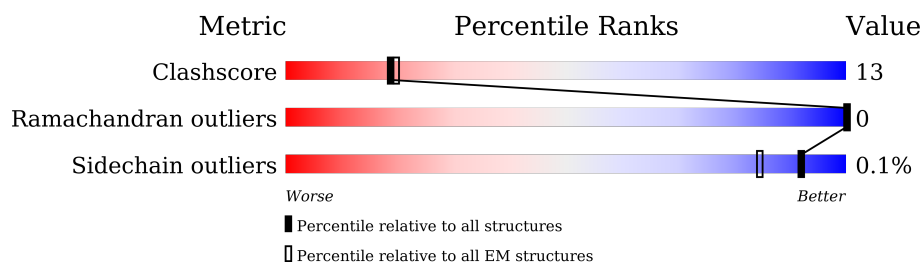
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	B	879	64% 25% 11%
1	R	879	61% 30% 9%
2	A	418	57% 26% 17%
3	S	251	68% 20% 12%
4	C	2	50% 50%
4	D	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	R	859	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16488 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 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	803	Total	C	N	O	P	S	0	0
			6159	3957	1020	1133	3	46		
1	B	782	Total	C	N	O	S		0	0
			5977	3849	991	1091	46			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	347	Total	C	N	O	S	0	0
			2630	1693	453	482	2		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	VAL	CYS	conflict	UNP P49407
A	125	SER	CYS	conflict	UNP P49407
A	140	LEU	CYS	conflict	UNP P49407
A	150	VAL	CYS	conflict	UNP P49407
A	169	GLU	ARG	conflict	UNP P49407
A	242	VAL	CYS	conflict	UNP P49407
A	251	VAL	CYS	conflict	UNP P49407
A	269	SER	CYS	conflict	UNP P49407

- Molecule 3 is a protein called scFv30.

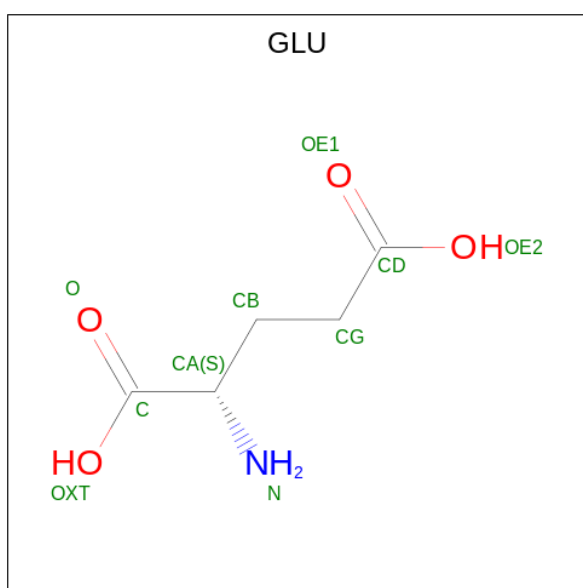
Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	222	Total	C	N	O	S	0	0
			1592	1019	266	301	6		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				AltConf
5	R	1	Total	C	N	O	0
			9	5	1	3	
5	B	1	Total	C	N	O	0
			9	5	1	3	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).

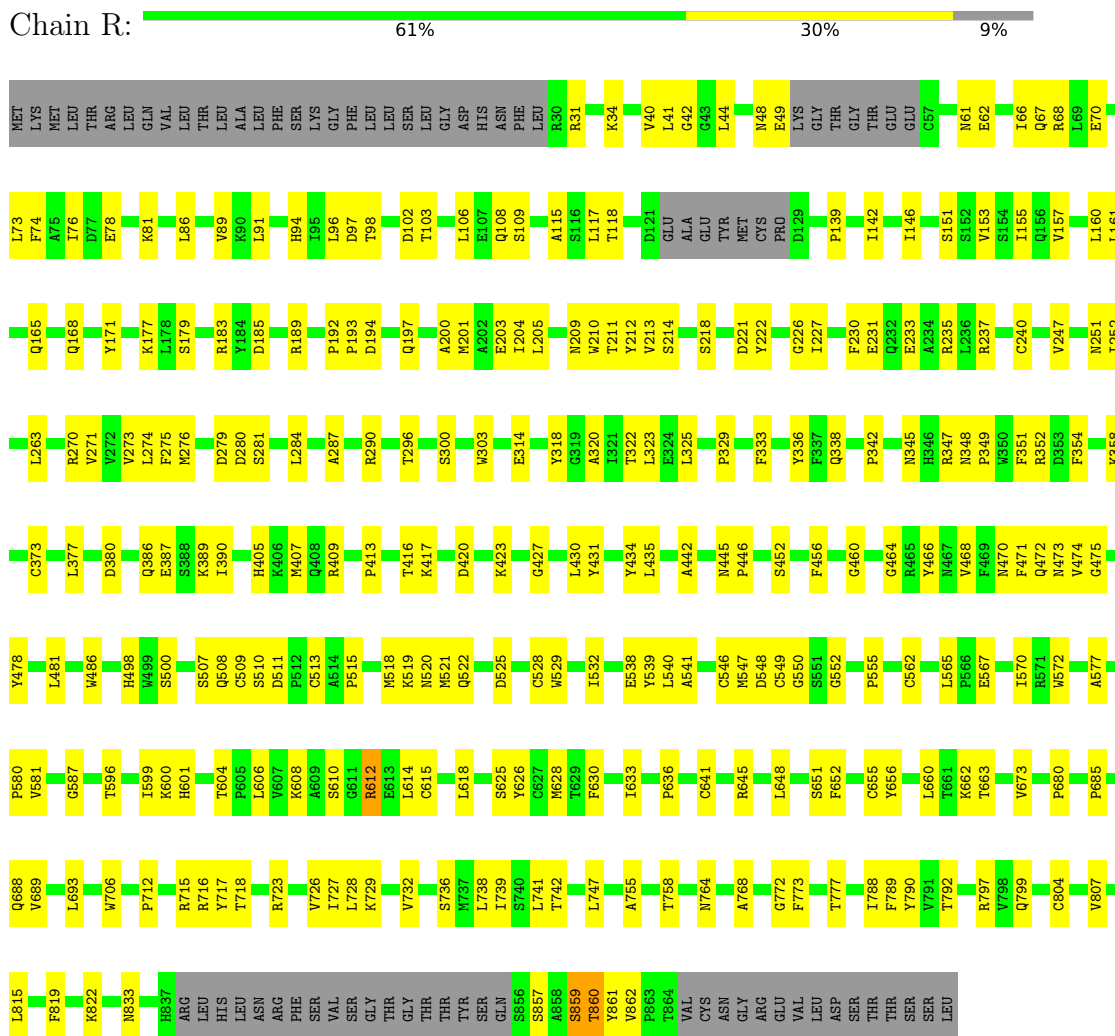


Mol	Chain	Residues	Atoms			AltConf
6	R	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	

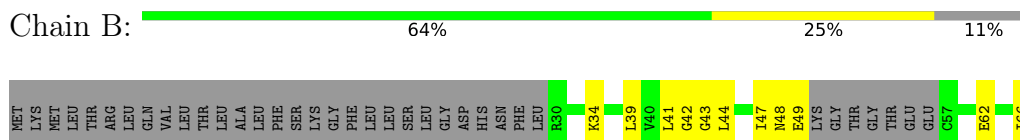
### 3 Residue-property plots

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 3



- Molecule 1: Metabotropic glutamate receptor 3



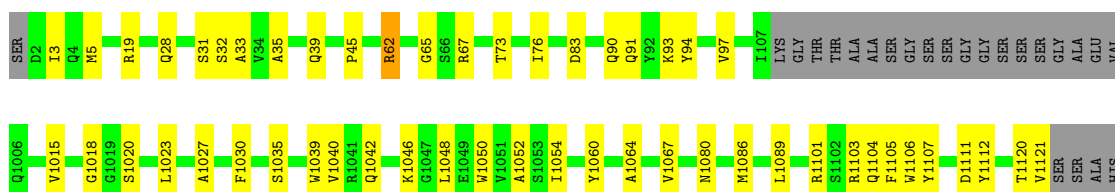
- Molecule 2: Beta-arrestin-1

Chain A:  57% 26% 17%



- Molecule 3: scFv30

Chain S:  68% 20% 12%







- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39446	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CtfFind 4.1.8	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: SEP, NAG, CLR, TPO

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	B	0.26	0/6112	0.48	0/8312
1	R	0.27	0/6263	0.48	0/8516
2	A	0.26	0/2688	0.50	0/3667
3	S	0.27	0/1634	0.51	0/2236
All	All	0.26	0/16697	0.49	0/22731

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	B	5977	0	5772	141	0
1	R	6159	0	5934	168	0
2	A	2630	0	2583	80	0
3	S	1592	0	1406	38	0
4	C	28	0	25	1	0
4	D	28	0	25	0	0
5	B	9	0	5	2	0
5	R	9	0	5	0	0
6	B	28	0	46	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	28	0	46	0	0
All	All	16488	0	15847	411	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 13.

All (411) 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:A:59:VAL:HG13	2:A:144:TYR:CE1	1.75	1.21
2:A:222:ASN:O	2:A:265:SER:HA	1.49	1.13
3:S:19:ARG:HA	3:S:76:ILE:O	1.69	0.93
1:R:509:CYS:SG	1:R:510:SER:N	2.49	0.83
2:A:59:VAL:CG1	2:A:144:TYR:CE1	2.63	0.78
1:R:625:SER:HG	1:R:651:SER:HG	1.33	0.76
2:A:148:ALA:O	2:A:163:SER:HA	1.86	0.75
1:R:233:GLU:OE1	1:R:237:ARG:NH1	2.20	0.75
2:A:253:VAL:O	2:A:281:ASN:ND2	2.19	0.74
1:B:303:TRP:HE1	1:B:480:TYR:HH	1.31	0.74
1:R:318:TYR:HD2	1:R:500:SER:HA	1.52	0.74
1:B:174:THR:HG1	5:B:901:GLU:N	1.86	0.73
2:A:361:PRO:HG3	2:A:365:VAL:HG22	1.70	0.73
1:R:161:LEU:HD12	1:R:168:GLN:HB2	1.70	0.72
3:S:1035:SER:O	3:S:1104:GLN:NE2	2.23	0.71
2:A:365:VAL:HG11	3:S:1107:TYR:HB3	1.73	0.71
1:R:706:TRP:HZ2	1:R:736:SER:HB3	1.57	0.69
2:A:187:THR:HG1	2:A:198:HIS:HD1	1.38	0.69
1:R:456:PHE:HB3	1:R:460:GLY:HA2	1.75	0.68
1:B:151:SER:HB2	1:B:222:TYR:HB2	1.74	0.68
2:A:56:THR:OG1	2:A:83:ASN:OD1	2.11	0.67
1:R:44:LEU:O	1:R:171:TYR:OH	2.11	0.67
2:A:327:LEU:O	2:A:342:ASP:HA	1.95	0.66
2:A:18:LEU:HD22	2:A:43:VAL:HG12	1.75	0.66
1:B:320:ALA:O	1:B:470:ASN:ND2	2.29	0.66
1:R:540:LEU:HA	1:R:546:CYS:HA	1.78	0.65
1:R:552:GLY:HA2	1:R:718:THR:HG21	1.76	0.65
1:R:68:ARG:NH2	1:R:387:GLU:OE2	2.29	0.65
1:R:685:PRO:HB2	1:B:685:PRO:HB2	1.78	0.65
1:B:68:ARG:NH2	1:B:387:GLU:OE2	2.29	0.65
1:B:96:LEU:HD13	1:B:108:GLN:HB3	1.79	0.65
1:B:430:LEU:HA	1:B:434:TYR:HD2	1.61	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:VAL:H	1:B:478:TYR:HB3	1.61	0.64
1:R:641:CYS:SG	1:R:645:ARG:NH2	2.69	0.64
1:B:373:CYS:HB3	1:B:377:LEU:HD22	1.79	0.64
1:B:718:THR:HG22	1:B:726:VAL:HG22	1.78	0.64
1:R:862:VAL:O	2:A:5:GLY:N	2.31	0.64
1:B:285:ILE:HD13	1:B:310:ILE:HG22	1.80	0.64
1:R:62:GLU:OE2	1:R:358:LYS:NZ	2.31	0.63
1:R:859:SEP:O2P	3:S:67:ARG:NH2	2.31	0.63
1:R:109:SER:HB3	1:R:160:LEU:HD23	1.80	0.63
1:R:513:CYS:HB2	1:R:529:TRP:CD1	2.33	0.63
1:B:636:PRO:HG2	1:B:728:LEU:HB2	1.80	0.63
3:S:32:SER:HB3	3:S:67:ARG:HD2	1.81	0.62
1:R:41:LEU:HD12	1:R:76:ILE:HD11	1.80	0.62
1:R:693:LEU:HD21	1:B:693:LEU:HD21	1.79	0.62
2:A:299:ASN:HB3	3:S:1105:PHE:HE1	1.64	0.62
2:A:187:THR:OG1	2:A:198:HIS:ND1	2.28	0.62
2:A:219:HIS:NE2	2:A:267:THR:OG1	2.33	0.62
1:R:221:ASP:OD1	1:R:222:TYR:N	2.33	0.62
1:B:233:GLU:OE1	1:B:237:ARG:NH1	2.32	0.62
1:R:96:LEU:HB3	1:R:108:GLN:HG2	1.82	0.61
2:A:222:ASN:O	2:A:265:SER:CA	2.37	0.61
1:R:275:PHE:HA	1:R:300:SER:HB3	1.80	0.61
1:B:568:ASP:N	1:B:726:VAL:O	2.33	0.61
1:R:860:TPO:OG1	2:A:107:LYS:NZ	2.34	0.61
1:B:716:ARG:HE	1:B:726:VAL:HG11	1.64	0.61
1:B:449:ASP:O	1:B:452:SER:OG	2.19	0.61
1:B:615:CYS:SG	1:B:822:LYS:NZ	2.75	0.60
1:B:513:CYS:HB2	1:B:529:TRP:CD1	2.37	0.60
1:B:472:GLN:OE1	1:B:498:HIS:ND1	2.34	0.60
2:A:147:LYS:HA	2:A:164:VAL:O	2.01	0.60
3:S:62:ARG:NH2	3:S:83:ASP:OD2	2.35	0.60
1:B:540:LEU:HA	1:B:546:CYS:HA	1.84	0.59
2:A:213:PRO:HA	2:A:275:THR:HG22	1.85	0.59
1:R:115:ALA:HB2	1:R:139:PRO:HB2	1.83	0.59
1:R:539:TYR:O	1:R:547:MET:N	2.35	0.59
1:B:353:ASP:HA	1:B:356:GLU:HG2	1.85	0.59
1:R:342:PRO:O	1:R:352:ARG:NE	2.36	0.59
3:S:39:GLN:NE2	3:S:45:PRO:HG3	2.18	0.59
1:B:826:ILE:HA	1:B:833:ASN:HD22	1.68	0.59
1:B:214:SER:HB2	1:B:272:VAL:HG22	1.85	0.59
1:R:97:ASP:OD1	1:R:98:THR:N	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:212:TYR:HB3	1:R:508:GLN:HA	1.85	0.59
1:R:281:SER:HG	1:R:303:TRP:HE3	1.51	0.58
1:R:192:PRO:HG3	1:R:464:GLY:HA2	1.85	0.58
1:R:203:GLU:OE1	1:R:486:TRP:NE1	2.29	0.58
1:R:511:ASP:O	1:R:529:TRP:NE1	2.36	0.58
1:B:423:LYS:HG3	1:B:424:ILE:HD12	1.85	0.58
2:A:299:ASN:HB3	3:S:1105:PHE:CE1	2.39	0.58
1:B:206:ARG:NH1	1:B:237:ARG:O	2.36	0.58
1:R:320:ALA:O	1:R:470:ASN:ND2	2.36	0.58
1:R:329:PRO:HB3	1:R:386:GLN:NE2	2.19	0.58
1:R:226:GLY:HA3	1:R:275:PHE:CE2	2.39	0.58
1:R:625:SER:OG	1:R:651:SER:OG	2.12	0.58
1:R:521:MET:O	1:R:529:TRP:HA	2.04	0.57
2:A:341:SER:OG	2:A:342:ASP:N	2.37	0.57
1:B:567:GLU:HA	1:B:726:VAL:HB	1.85	0.57
1:B:773:PHE:O	1:B:777:THR:HG22	2.04	0.57
1:R:581:VAL:HG13	1:R:630:PHE:HE2	1.69	0.56
1:R:656:TYR:HB2	1:R:747:LEU:HD23	1.86	0.56
2:A:303:SER:HA	2:A:319:VAL:HG13	1.86	0.56
2:A:252:PRO:O	2:A:284:LYS:NZ	2.36	0.56
1:B:719:LEU:O	1:B:723:ARG:N	2.23	0.56
1:R:715:ARG:HG3	1:R:729:LYS:HB2	1.87	0.56
1:R:189:ARG:HH21	1:R:193:PRO:HB3	1.71	0.56
1:B:251:ASN:OD1	1:B:252:ILE:N	2.39	0.56
1:R:373:CYS:HB3	1:R:377:LEU:HD22	1.88	0.56
1:R:431:TYR:HD1	1:R:435:LEU:HD23	1.71	0.56
1:R:738:LEU:HD11	1:R:790:TYR:HB2	1.88	0.56
1:R:279:ASP:OD1	1:R:280:ASP:N	2.40	0.56
1:R:520:ASN:ND2	1:R:522:GLN:OE1	2.39	0.55
1:R:442:ALA:H	1:R:452:SER:HB3	1.72	0.55
1:R:550:GLY:O	1:R:723:ARG:NH2	2.39	0.55
1:R:567:GLU:HA	1:R:726:VAL:HB	1.88	0.55
1:R:614:LEU:HD21	1:R:688:GLN:HB3	1.87	0.55
3:S:1042:GLN:NE2	3:S:1046:LYS:O	2.38	0.55
3:S:1111:ASP:OD1	3:S:1112:TYR:N	2.40	0.55
1:B:594:VAL:HG22	1:B:823:VAL:HG21	1.89	0.55
1:B:795:ASP:HB2	1:B:798:VAL:HG22	1.87	0.55
1:R:303:TRP:HE1	1:R:322:THR:HG21	1.72	0.55
1:R:209:ASN:OD1	4:C:1:NAG:N2	2.40	0.54
2:A:217:ASN:ND2	2:A:270:LYS:O	2.40	0.54
1:R:472:GLN:NE2	1:R:481:LEU:HD21	2.23	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ASN:HB2	1:B:351:PHE:HB2	1.88	0.54
2:A:86:SER:OG	2:A:114:PRO:O	2.26	0.54
1:R:70:GLU:OE2	1:R:348:ASN:ND2	2.40	0.54
1:R:211:THR:O	1:R:240:CYS:N	2.35	0.54
1:B:39:LEU:HD22	1:B:143:ALA:HB2	1.89	0.54
1:B:66:ILE:HG13	1:B:354:PHE:CD1	2.43	0.54
1:R:48:ASN:OD1	1:R:49:GLU:N	2.38	0.53
1:R:859:SEP:O1P	2:A:7:ARG:NH1	2.40	0.53
2:A:59:VAL:HG13	2:A:144:TYR:HE1	1.62	0.53
1:R:604:THR:OG1	1:R:833:ASN:ND2	2.41	0.53
1:R:636:PRO:HG2	1:R:728:LEU:HB3	1.90	0.53
2:A:130:GLN:NE2	2:A:282:ARG:O	2.38	0.53
1:B:389:LYS:NZ	5:B:901:GLU:OE2	2.31	0.53
1:B:684:SER:O	1:B:688:GLN:HB2	2.09	0.53
2:A:59:VAL:HG13	2:A:144:TYR:CD1	2.39	0.53
2:A:56:THR:HA	2:A:82:ALA:O	2.08	0.53
1:B:242:ALA:O	1:B:266:LYS:NZ	2.42	0.53
2:A:25:ARG:NH2	2:A:167:VAL:O	2.38	0.53
1:B:314:GLU:HG2	1:B:471:PHE:CZ	2.43	0.53
1:B:471:PHE:HE1	1:B:479:SER:HA	1.74	0.53
1:R:271:VAL:N	1:R:507:SER:OG	2.40	0.53
1:R:329:PRO:HB3	1:R:386:GLN:HE22	1.74	0.52
2:A:105:ILE:HD11	2:A:114:PRO:HG3	1.90	0.52
1:B:44:LEU:HD13	1:B:157:VAL:HG21	1.92	0.52
2:A:201:ALA:HB3	2:A:347:LEU:HD11	1.92	0.52
1:B:319:GLY:HA3	1:B:500:SER:HB2	1.90	0.52
1:R:515:PRO:HA	1:R:518:MET:O	2.08	0.52
1:R:151:SER:HB2	1:R:222:TYR:HB2	1.90	0.52
2:A:301:ALA:HB3	2:A:319:VAL:HG21	1.91	0.52
1:B:420:ASP:HA	1:B:423:LYS:HG2	1.91	0.52
1:B:602:ASN:OD1	1:B:616:TYR:OH	2.25	0.52
1:B:554:TRP:HB2	1:B:723:ARG:HH22	1.75	0.52
1:R:230:PHE:CZ	1:R:273:VAL:HG21	2.45	0.52
1:B:330:VAL:HG12	1:B:333:PHE:H	1.75	0.52
3:S:1030:PHE:O	3:S:1080:ASN:ND2	2.29	0.52
1:R:270:ARG:O	1:R:296:THR:OG1	2.20	0.51
1:B:62:GLU:HA	1:B:354:PHE:HE1	1.75	0.51
1:R:67:GLN:HB3	1:R:390:ILE:HD11	1.93	0.51
3:S:1064:ALA:HB3	3:S:1067:VAL:HG22	1.92	0.51
1:B:359:PHE:CD2	1:B:377:LEU:HD23	2.45	0.51
1:B:553:GLN:O	1:B:723:ARG:NH2	2.44	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:78:GLU:HA	1:R:81:LYS:HG2	1.92	0.51
1:R:773:PHE:O	1:R:777:THR:HG22	2.10	0.51
1:B:226:GLY:HA3	1:B:275:PHE:CZ	2.46	0.51
1:B:210:TRP:HH2	1:B:499:TRP:CH2	2.27	0.51
1:B:473:ASN:HA	1:B:478:TYR:CG	2.45	0.51
2:A:20:VAL:HG22	2:A:41:VAL:HG12	1.93	0.51
1:B:595:VAL:HG22	1:B:619:LEU:HD13	1.92	0.51
1:R:565:LEU:O	1:R:716:ARG:NH2	2.44	0.51
2:A:361:PRO:HD2	3:S:1106:TRP:CE3	2.45	0.51
3:S:1018:GLY:HA2	3:S:1089:LEU:HA	1.93	0.51
1:B:181:LYS:NZ	1:B:187:PHE:O	2.44	0.51
1:B:226:GLY:HA3	1:B:275:PHE:CE2	2.46	0.51
1:B:739:ILE:O	1:B:742:THR:HG22	2.11	0.50
2:A:42:LEU:HD21	2:A:108:LEU:HB3	1.93	0.50
1:R:31:ARG:HD2	1:R:349:PRO:HB2	1.94	0.50
1:R:179:SER:OG	1:R:189:ARG:NH2	2.43	0.50
2:A:29:ASP:OD2	2:A:170:LYS:NZ	2.45	0.50
1:B:41:LEU:HG	1:B:91:LEU:HD11	1.93	0.50
1:B:263:LEU:HD13	1:B:272:VAL:HG21	1.93	0.50
1:R:42:GLY:O	1:R:146:ILE:N	2.44	0.50
1:R:472:GLN:HB2	1:R:498:HIS:HB2	1.94	0.50
1:R:416:THR:OG1	1:R:417:LYS:NZ	2.45	0.50
1:B:710:GLU:HB3	1:B:732:VAL:HG21	1.94	0.50
1:B:809:LEU:O	1:B:813:VAL:HG23	2.11	0.50
1:R:859:SEP:O3P	3:S:67:ARG:NH1	2.45	0.49
1:R:34:LYS:HG2	1:R:94:HIS:ND1	2.27	0.49
1:R:205:LEU:HD13	1:R:213:VAL:HG11	1.94	0.49
2:A:63:TYR:CE2	2:A:246:THR:HG21	2.46	0.49
2:A:79:LEU:HD21	2:A:243:LEU:HD11	1.94	0.49
1:B:323:LEU:HD22	1:B:468:VAL:HG22	1.92	0.49
1:R:66:ILE:HG13	1:R:354:PHE:CD1	2.48	0.49
1:R:606:LEU:HD21	1:R:822:LYS:HG2	1.95	0.49
1:R:815:LEU:HD23	1:R:819:PHE:HD2	1.78	0.49
3:S:1042:GLN:HB2	3:S:1048:LEU:HD23	1.94	0.49
1:B:169:ILE:HD12	1:B:400:MET:HB2	1.94	0.49
1:B:210:TRP:NE1	1:B:505:PRO:O	2.43	0.49
1:B:521:MET:SD	1:B:523:PRO:HD3	2.53	0.49
1:R:348:ASN:HB2	1:R:351:PHE:HB2	1.94	0.49
1:R:86:LEU:HG	1:R:405:HIS:HB2	1.95	0.49
2:A:128:THR:HA	2:A:141:GLY:HA3	1.95	0.48
1:B:213:VAL:HG23	1:B:241:ILE:HD12	1.94	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:645:ARG:HH22	1:R:712:PRO:HA	1.79	0.48
3:S:1040:VAL:HG22	3:S:1050:TRP:HA	1.94	0.48
1:R:333:PHE:CD2	1:R:390:ILE:HG21	2.49	0.48
1:R:555:PRO:HA	1:R:562:CYS:HA	1.96	0.48
3:S:97:VAL:HG12	3:S:97:VAL:O	2.14	0.48
3:S:1020:SER:HA	3:S:1086:MET:O	2.13	0.48
1:R:155:ILE:HD12	1:R:221:ASP:OD2	2.14	0.48
2:A:197:LEU:HG	2:A:222:ASN:HA	1.96	0.48
3:S:1027:ALA:HB1	3:S:1030:PHE:CE1	2.49	0.48
1:R:231:GLU:OE2	1:R:235:ARG:NE	2.44	0.47
1:R:271:VAL:HG23	1:R:507:SER:HB2	1.96	0.47
1:R:157:VAL:HB	1:R:168:GLN:HE22	1.77	0.47
1:R:717:TYR:HB3	1:R:727:ILE:HB	1.96	0.47
2:A:19:THR:OG1	2:A:42:LEU:HB2	2.14	0.47
1:R:183:ARG:NH1	1:B:184:TYR:OH	2.47	0.47
1:R:185:ASP:OD1	1:R:185:ASP:N	2.47	0.47
1:B:43:GLY:HA3	1:B:95:ILE:HG12	1.96	0.47
1:B:187:PHE:HE2	1:B:189:ARG:HH11	1.62	0.47
1:R:407:MET:SD	1:R:430:LEU:HB2	2.55	0.47
1:R:608:LYS:HB3	2:A:71:LEU:HD11	1.96	0.47
1:B:97:ASP:OD1	1:B:98:THR:N	2.47	0.47
1:B:788:ILE:HA	1:B:791:VAL:HG12	1.95	0.47
1:R:610:SER:HA	1:R:764:ASN:ND2	2.28	0.47
1:B:42:GLY:HA3	1:B:145:VAL:HG22	1.96	0.47
1:B:648:LEU:HD21	1:B:741:LEU:HD21	1.96	0.47
1:R:194:ASP:OD1	1:R:197:GLN:NE2	2.47	0.47
1:R:197:GLN:HA	1:R:466:TYR:HE2	1.79	0.47
3:S:1103:ARG:HH11	3:S:1106:TRP:H	1.62	0.47
1:R:587:GLY:HA3	1:R:626:TYR:CE1	2.50	0.47
3:S:1103:ARG:NH1	3:S:1106:TRP:H	2.12	0.47
1:R:165:GLN:O	1:R:427:GLY:HA3	2.14	0.47
1:R:652:PHE:HZ	1:R:807:VAL:HG12	1.80	0.47
1:B:146:ILE:HG13	1:B:397:VAL:HG22	1.97	0.47
1:R:660:LEU:HA	1:R:663:THR:HG22	1.97	0.46
2:A:342:ASP:N	2:A:342:ASP:OD1	2.48	0.46
3:S:35:ALA:O	3:S:90:GLN:N	2.45	0.46
1:B:398:TYR:HD2	1:B:443:PRO:HG3	1.80	0.46
1:R:201:MET:HG3	1:R:323:LEU:HD12	1.96	0.46
2:A:322:LYS:HG2	2:A:348:PRO:HA	1.97	0.46
1:B:171:TYR:CG	1:B:393:VAL:HG22	2.50	0.46
1:B:212:TYR:OH	1:B:266:LYS:HD3	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:LYS:HE2	1:B:735:SER:HB3	1.98	0.46
1:B:767:GLU:HA	1:B:770:PHE:CD2	2.50	0.46
1:R:287:ALA:HA	1:R:290:ARG:HD2	1.97	0.46
2:A:124:PRO:HG3	2:A:316:GLY:HA3	1.97	0.46
2:A:43:VAL:HG11	2:A:53:VAL:HG11	1.97	0.46
1:B:774:THR:HG23	1:B:817:CYS:HB3	1.98	0.46
1:R:115:ALA:O	1:R:118:THR:OG1	2.26	0.46
1:R:73:LEU:HB3	1:R:347:ARG:HH22	1.81	0.45
1:R:539:TYR:CE2	1:R:541:ALA:HA	2.52	0.45
1:R:61:ASN:OD1	1:R:62:GLU:N	2.49	0.45
2:A:190:PHE:CD2	2:A:224:THR:HG21	2.51	0.45
1:R:153:VAL:O	1:R:157:VAL:HG23	2.16	0.45
1:R:739:ILE:O	1:R:742:THR:HG22	2.17	0.45
3:S:1030:PHE:CE1	3:S:1101:ARG:HG3	2.52	0.45
1:R:86:LEU:HB3	1:R:89:VAL:HB	1.99	0.45
2:A:277:PHE:CE2	2:A:280:ASN:HB2	2.51	0.45
1:R:102:ASP:OD1	1:R:103:THR:N	2.48	0.45
1:B:788:ILE:O	1:B:792:THR:OG1	2.27	0.45
1:R:612:ARG:HA	1:R:615:CYS:SG	2.57	0.45
3:S:39:GLN:HE21	3:S:45:PRO:HG3	1.82	0.45
1:B:44:LEU:HB2	1:B:147:GLY:HA2	1.99	0.45
1:B:598:PHE:HD2	1:B:619:LEU:HD11	1.81	0.45
1:R:325:LEU:HD23	1:R:466:TYR:CE1	2.52	0.45
1:R:473:ASN:HA	1:R:478:TYR:CG	2.51	0.45
1:R:628:MET:SD	1:R:648:LEU:HA	2.57	0.45
3:S:1023:LEU:HB3	3:S:1039:TRP:CH2	2.51	0.45
1:B:511:ASP:O	1:B:529:TRP:NE1	2.34	0.45
1:R:420:ASP:O	1:R:423:LYS:HG2	2.17	0.45
1:B:213:VAL:O	1:B:242:ALA:N	2.49	0.45
1:B:43:GLY:N	1:B:94:HIS:O	2.49	0.44
1:R:572:TRP:NE1	1:R:633:ILE:O	2.49	0.44
1:B:430:LEU:HA	1:B:434:TYR:CD2	2.46	0.44
2:A:55:VAL:HG11	2:A:115:PHE:CD2	2.53	0.44
2:A:130:GLN:HB2	2:A:289:LEU:HD13	1.98	0.44
2:A:201:ALA:HA	2:A:217:ASN:O	2.17	0.44
1:B:321:ILE:HD13	1:B:470:ASN:HD22	1.83	0.44
1:R:445:ASN:N	1:R:446:PRO:HD2	2.32	0.44
1:B:152:SER:O	1:B:156:GLN:HG2	2.17	0.44
1:R:409:ARG:O	1:R:413:PRO:HB3	2.18	0.44
2:A:26:ASP:HB3	2:A:362:HIS:CE1	2.52	0.44
1:B:453:ILE:HG22	1:B:455:LYS:HB2	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:600:LYS:HE3	1:R:601:HIS:NE2	2.32	0.44
1:R:612:ARG:H	1:R:612:ARG:HD3	1.83	0.44
2:A:29:ASP:HB3	2:A:172:GLN:HG2	2.00	0.44
1:B:274:LEU:HD12	1:B:274:LEU:HA	1.83	0.44
1:R:323:LEU:HD23	1:R:468:VAL:HG22	2.00	0.43
2:A:104:LEU:O	2:A:108:LEU:HD13	2.18	0.43
2:A:205:LYS:HG2	2:A:208:TYR:HE1	1.83	0.43
1:B:102:ASP:OD1	1:B:103:THR:N	2.50	0.43
1:B:409:ARG:O	1:B:413:PRO:HB3	2.18	0.43
1:R:276:MET:HE3	1:R:284:LEU:HD22	2.00	0.43
2:A:59:VAL:HG12	2:A:59:VAL:O	2.18	0.43
1:B:539:TYR:N	1:B:547:MET:O	2.45	0.43
1:B:816:GLY:HA2	1:B:820:ALA:HB2	2.00	0.43
1:R:518:MET:HA	1:R:532:ILE:O	2.19	0.43
1:R:570:ILE:HD13	1:R:797:ARG:HG2	2.00	0.43
1:B:277:ARG:NH2	1:B:279:ASP:OD2	2.51	0.43
1:B:642:ALA:HA	1:B:645:ARG:HD3	1.99	0.43
1:B:715:ARG:HH21	1:B:729:LYS:HD3	1.82	0.43
1:R:287:ALA:O	1:R:290:ARG:HB2	2.19	0.43
2:A:216:VAL:HG21	2:A:323:VAL:HG11	2.00	0.43
1:R:673:VAL:HG22	1:R:680:PRO:HD3	1.99	0.43
1:B:194:ASP:OD1	1:B:197:GLN:NE2	2.51	0.43
1:B:587:GLY:HA3	1:B:626:TYR:CZ	2.53	0.43
1:R:430:LEU:HA	1:R:434:TYR:HD2	1.84	0.43
2:A:143:ASP:OD1	2:A:143:ASP:N	2.52	0.43
1:B:48:ASN:OD1	1:B:49:GLU:N	2.52	0.43
1:B:345:ASN:ND2	1:B:348:ASN:OD1	2.47	0.43
1:B:438:ILE:HG13	1:B:440:PHE:HD1	1.83	0.43
1:R:214:SER:HB3	1:R:263:LEU:HD22	2.00	0.43
1:R:325:LEU:HD12	1:R:389:LYS:CE	2.48	0.43
1:R:596:THR:HA	1:R:599:ILE:HG12	2.01	0.43
2:A:32:ASP:OD1	2:A:33:LEU:N	2.51	0.43
1:B:416:THR:O	1:B:417:LYS:HE2	2.18	0.43
1:B:614:LEU:HD11	1:B:688:GLN:OE1	2.18	0.43
1:R:251:ASN:OD1	1:R:252:ILE:N	2.51	0.43
2:A:199:LEU:HD13	2:A:220:VAL:HG22	2.01	0.43
1:B:221:ASP:OD1	1:B:221:ASP:N	2.51	0.43
1:B:614:LEU:HA	1:B:617:ILE:HG22	2.00	0.43
2:A:80:PHE:CZ	2:A:82:ALA:HB2	2.53	0.43
1:B:279:ASP:OD1	1:B:280:ASP:N	2.51	0.43
1:B:285:ILE:HD12	1:B:309:ILE:HG22	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:THR:HB	1:B:798:VAL:HG23	2.01	0.42
1:R:102:ASP:O	1:R:106:LEU:HB2	2.20	0.42
2:A:87:PHE:O	2:A:89:PRO:HD3	2.18	0.42
1:B:185:ASP:N	1:B:185:ASP:OD1	2.53	0.42
1:B:390:ILE:O	1:B:393:VAL:HB	2.19	0.42
2:A:199:LEU:HD22	2:A:327:LEU:HD13	2.02	0.42
2:A:203:LEU:HB3	2:A:208:TYR:OH	2.19	0.42
1:B:47:ILE:HG21	1:B:350:TRP:CD2	2.54	0.42
1:B:274:LEU:N	1:B:298:VAL:O	2.35	0.42
1:B:642:ALA:O	1:B:645:ARG:HG2	2.18	0.42
1:R:789:PHE:HE1	1:R:799:GLN:HG3	1.84	0.42
2:A:33:LEU:HA	2:A:121:PRO:HG3	2.01	0.42
3:S:1054:ILE:HD12	3:S:1060:TYR:O	2.19	0.42
1:B:34:LYS:HG2	1:B:94:HIS:ND1	2.34	0.42
3:S:3:ILE:HG23	3:S:28:GLN:H	1.84	0.42
3:S:5:MET:SD	3:S:91:GLN:HG2	2.59	0.42
3:S:33:ALA:HB3	3:S:93:LYS:HB2	2.02	0.42
3:S:1023:LEU:HD23	3:S:1023:LEU:HA	1.94	0.42
1:B:74:PHE:HB2	1:B:336:TYR:CD2	2.55	0.42
1:B:97:ASP:OD1	1:B:99:CYS:N	2.52	0.42
1:R:755:ALA:HB1	1:R:772:GLY:HA2	2.01	0.42
1:R:859:SEP:O2P	3:S:31:SER:OG	2.27	0.42
2:A:119:ILE:HG23	2:A:123:LEU:HD12	2.01	0.42
1:R:338:GLN:HB3	1:R:380:ASP:OD1	2.20	0.42
2:A:8:VAL:HG21	2:A:104:LEU:HD21	2.01	0.42
2:A:233:ILE:HG12	2:A:274:LEU:HD11	2.01	0.42
1:B:216:VAL:HG22	1:B:245:GLU:HB2	2.02	0.42
1:R:538:GLU:HA	1:R:548:ASP:HA	2.01	0.42
1:R:577:ALA:O	1:R:581:VAL:HG23	2.19	0.42
1:R:758:THR:O	1:R:768:ALA:HB1	2.20	0.42
3:S:1015:VAL:HB	3:S:1121:VAL:HA	2.01	0.42
1:B:203:GLU:HB3	1:B:490:LEU:HD11	2.00	0.42
1:B:314:GLU:HG2	1:B:471:PHE:CE2	2.55	0.42
1:B:756:PHE:O	1:B:759:ARG:NE	2.42	0.42
1:R:117:LEU:HD12	1:B:117:LEU:HD12	2.02	0.42
2:A:65:ARG:H	2:A:68:LEU:HD12	1.85	0.42
1:R:345:ASN:HD21	1:R:348:ASN:HD22	1.68	0.41
1:R:689:VAL:HG12	1:R:693:LEU:HD13	2.00	0.41
1:R:788:ILE:O	1:R:792:THR:OG1	2.31	0.41
1:R:860:TPO:OG1	1:R:861:TYR:N	2.52	0.41
3:S:1015:VAL:N	3:S:1120:THR:O	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:732:VAL:HG13	1:R:736:SER:HB2	2.02	0.41
1:B:512:PRO:HA	1:B:529:TRP:HZ2	1.85	0.41
1:B:659:LEU:HD13	1:B:775:MET:SD	2.60	0.41
2:A:22:LEU:HD23	2:A:22:LEU:HA	1.83	0.41
2:A:124:PRO:HG2	2:A:142:VAL:HG11	2.01	0.41
2:A:208:TYR:HE2	2:A:214:ILE:HG23	1.86	0.41
2:A:227:THR:HG23	2:A:262:VAL:O	2.20	0.41
1:R:40:VAL:HG23	1:R:142:ILE:HA	2.02	0.41
1:R:41:LEU:HD11	1:R:91:LEU:HD21	2.02	0.41
1:R:200:ALA:O	1:R:204:ILE:HG12	2.21	0.41
1:B:287:ALA:O	1:B:290:ARG:HB2	2.20	0.41
1:B:299:ALA:HB3	1:B:322:THR:HG22	2.02	0.41
1:B:431:TYR:CD2	1:B:435:LEU:HD23	2.55	0.41
1:R:474:VAL:HG13	1:R:475:GLY:N	2.36	0.41
1:R:662:LYS:HE3	1:R:662:LYS:HB2	1.81	0.41
3:S:1050:TRP:HE1	3:S:1052:ALA:C	2.23	0.41
1:B:255:SER:O	1:B:259:VAL:HG23	2.20	0.41
1:R:386:GLN:HG3	1:R:387:GLU:O	2.21	0.41
1:R:741:LEU:HD23	1:R:741:LEU:HA	1.88	0.41
1:B:770:PHE:O	1:B:774:THR:OG1	2.31	0.41
1:R:227:ILE:HD12	1:R:227:ILE:HA	1.89	0.41
1:R:274:LEU:HD12	1:R:274:LEU:HA	1.79	0.41
2:A:62:ARG:HG2	2:A:76:ARG:HB2	2.02	0.41
2:A:65:ARG:H	2:A:68:LEU:HB2	1.86	0.41
1:R:618:LEU:HD12	1:R:655:CYS:HA	2.02	0.41
1:R:210:TRP:CE3	1:R:271:VAL:HG21	2.56	0.41
1:R:314:GLU:HG2	1:R:471:PHE:CZ	2.56	0.41
1:R:587:GLY:HA3	1:R:626:TYR:CZ	2.56	0.41
2:A:47:TYR:CZ	2:A:51:ARG:HA	2.56	0.41
1:B:174:THR:HG21	1:B:325:LEU:HD11	2.03	0.41
1:B:625:SER:O	1:B:628:MET:HG2	2.21	0.41
1:B:684:SER:HB2	1:B:688:GLN:HE21	1.85	0.41
1:R:160:LEU:HD13	1:B:163:LEU:HD13	2.03	0.41
1:R:177:LYS:HE2	1:R:177:LYS:HB3	1.97	0.40
1:R:519:LYS:HB3	1:R:546:CYS:SG	2.62	0.40
1:R:549:CYS:HB3	1:R:562:CYS:HB3	1.89	0.40
3:S:65:GLY:HA2	3:S:73:THR:O	2.20	0.40
1:B:79:ILE:HA	1:B:82:ASP:OD2	2.21	0.40
1:R:580:PRO:HB3	1:R:804:CYS:SG	2.62	0.40
1:B:605:PRO:HA	1:B:608:LYS:HD3	2.03	0.40
1:R:525:ASP:HB2	1:R:528:CYS:HB2	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:93:LYS:HG3	3:S:94:TYR:CD1	2.57	0.40
1:B:109:SER:OG	1:B:157:VAL:HG22	2.20	0.40
2:A:59:VAL:CG1	2:A:144:TYR:CZ	3.05	0.40
1:B:142:ILE:HG21	1:B:145:VAL:HG23	2.04	0.40
1:B:273:VAL:HA	1:B:298:VAL:HB	2.02	0.40
1:B:660:LEU:HD11	1:B:747:LEU:CD1	2.51	0.40
1:R:74:PHE:HB2	1:R:336:TYR:CE2	2.56	0.40
1:R:218:SER:HA	1:R:247:VAL:HG22	2.03	0.40
2:A:160:LYS:HA	2:A:160:LYS:HD2	1.77	0.40
1:B:256:TYR:O	1:B:260:ILE:HG12	2.21	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	B	774/879 (88%)	721 (93%)	53 (7%)	0	100	100
1	R	792/879 (90%)	742 (94%)	50 (6%)	0	100	100
2	A	339/418 (81%)	316 (93%)	23 (7%)	0	100	100
3	S	218/251 (87%)	208 (95%)	10 (5%)	0	100	100
All	All	2123/2427 (88%)	1987 (94%)	136 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	624/764 (82%)	624 (100%)	0	100	100
1	R	640/764 (84%)	639 (100%)	1 (0%)	92	94
2	A	274/372 (74%)	274 (100%)	0	100	100
3	S	145/205 (71%)	144 (99%)	1 (1%)	81	86
All	All	1683/2105 (80%)	1681 (100%)	2 (0%)	92	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	612	ARG
3	S	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	348	ASN
1	R	472	GLN
1	R	498	HIS
1	R	520	ASN
1	R	833	ASN
1	B	386	GLN
1	B	470	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SEP	R	859	1	8,9,10	1.54	1 (12%)	8,12,14	1.39	1 (12%)
1	TPO	R	860	1	8,10,11	1.09	0	10,14,16	1.97	1 (10%)
1	SEP	R	857	1	8,9,10	1.54	1 (12%)	8,12,14	1.53	2 (25%)
1	SEP	R	856	1	3,4,10	0.64	0	2,4,14	0.82	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
1	SEP	R	859	1	-	0/5/8/10	-
1	TPO	R	860	1	-	1/9/11/13	-
1	SEP	R	857	1	-	1/5/8/10	-
1	SEP	R	856	1	-	0/0/2/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	857	SEP	P-O1P	3.38	1.61	1.50
1	R	859	SEP	P-O1P	3.33	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	860	TPO	P-OG1-CB	-5.72	105.94	123.21
1	R	859	SEP	P-OG-CB	-2.99	110.06	118.30
1	R	857	SEP	P-OG-CB	-2.81	110.56	118.30
1	R	857	SEP	OG-CB-CA	2.68	110.76	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	R	860	TPO	N-CA-CB-OG1
1	R	857	SEP	CA-CB-OG-P

There are no ring outliers.



2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	859	SEP	4	0
1	R	860	TPO	2	0

## 5.5 Carbohydrates

4 monosaccharides 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
4	NAG	C	1	1,4	14,14,15	2.10	6 (42%)	17,19,21	1.60	4 (23%)
4	NAG	C	2	4	14,14,15	1.99	6 (42%)	17,19,21	1.16	2 (11%)
4	NAG	D	1	1,4	14,14,15	1.95	6 (42%)	17,19,21	1.19	2 (11%)
4	NAG	D	2	4	14,14,15	1.98	5 (35%)	17,19,21	1.23	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	C7-N2	4.03	1.48	1.34
4	C	2	NAG	C7-N2	4.02	1.48	1.34
4	C	1	NAG	C7-N2	3.94	1.47	1.34
4	D	1	NAG	C7-N2	3.93	1.47	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	3.77	1.49	1.43
4	C	2	NAG	O5-C1	3.49	1.49	1.43
4	D	2	NAG	O5-C1	3.46	1.49	1.43
4	D	1	NAG	O5-C1	3.36	1.49	1.43
4	C	1	NAG	O5-C5	2.72	1.48	1.43
4	C	1	NAG	C3-C2	-2.66	1.46	1.52
4	C	2	NAG	C2-N2	2.47	1.50	1.46
4	D	2	NAG	C2-N2	2.43	1.50	1.46
4	D	1	NAG	O7-C7	-2.37	1.17	1.23
4	C	1	NAG	C2-N2	2.37	1.50	1.46
4	C	1	NAG	O7-C7	-2.32	1.18	1.23
4	D	1	NAG	C3-C2	-2.30	1.47	1.52
4	D	1	NAG	O5-C5	2.30	1.48	1.43
4	D	2	NAG	O7-C7	-2.29	1.18	1.23
4	D	1	NAG	C2-N2	2.28	1.50	1.46
4	C	2	NAG	O7-C7	-2.27	1.18	1.23
4	C	2	NAG	O5-C5	2.18	1.47	1.43
4	D	2	NAG	O5-C5	2.14	1.47	1.43
4	C	2	NAG	C3-C2	-2.10	1.48	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C1-O5-C5	4.54	118.34	112.19
4	D	2	NAG	C4-C3-C2	3.11	115.57	111.02
4	D	1	NAG	C2-N2-C7	-2.73	119.02	122.90
4	C	2	NAG	C4-C3-C2	2.68	114.94	111.02
4	C	1	NAG	C2-N2-C7	-2.57	119.25	122.90
4	D	1	NAG	C8-C7-N2	2.47	120.29	116.10
4	C	1	NAG	C8-C7-N2	2.15	119.74	116.10
4	C	2	NAG	C8-C7-N2	2.07	119.61	116.10
4	C	1	NAG	O5-C5-C4	2.01	115.73	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

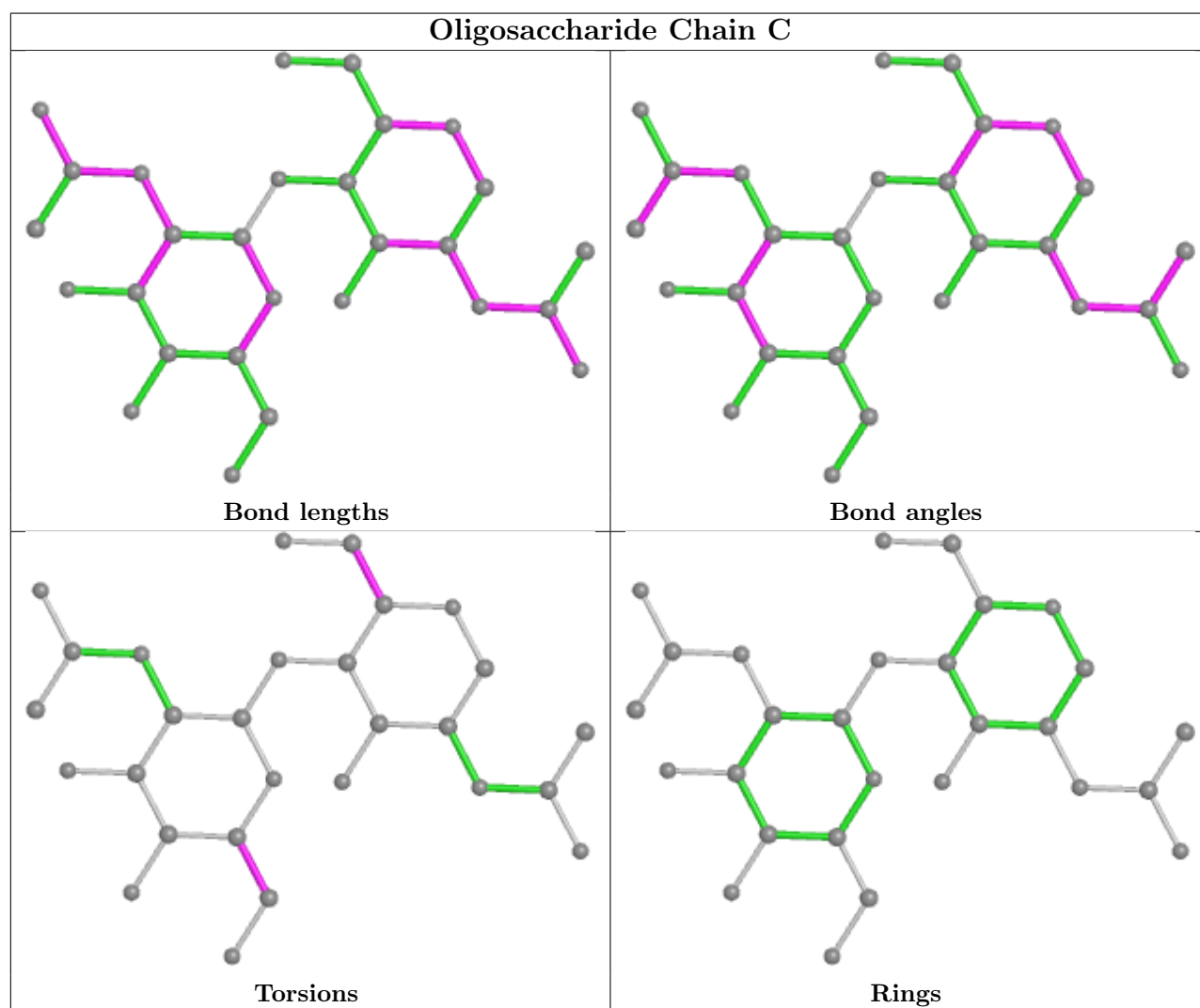
Mol	Chain	Res	Type	Atoms
4	C	1	NAG	O5-C5-C6-O6

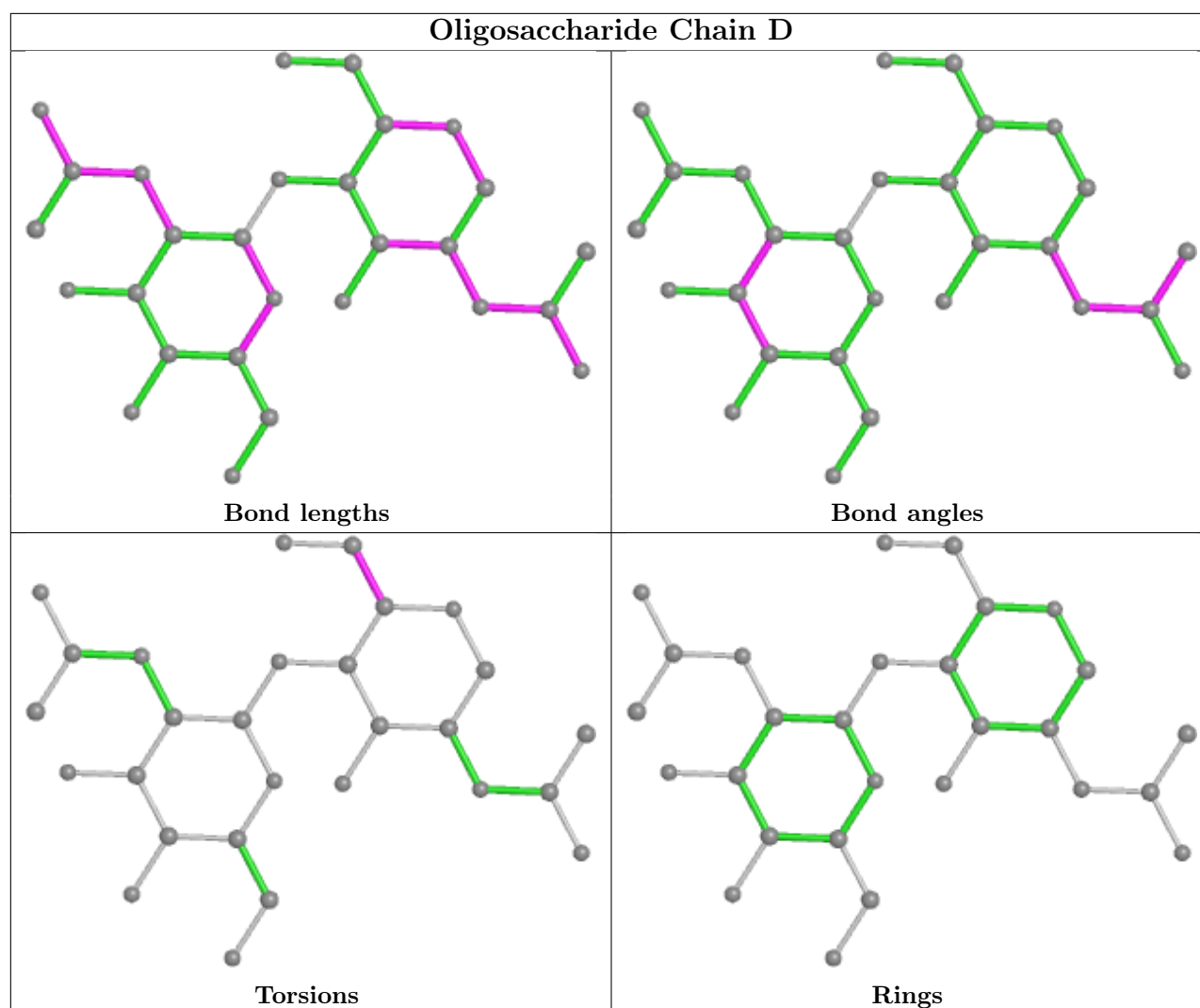
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	NAG	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 oligosaccharide.





## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
6	CLR	R	902	-	31,31,31	0.30	0	48,48,48	0.64	0
5	GLU	B	901	-	7,8,9	0.86	0	4,9,11	1.04	0
5	GLU	R	901	-	7,8,9	0.85	0	4,9,11	1.00	0
6	CLR	B	902	-	31,31,31	0.29	0	48,48,48	0.53	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
6	CLR	R	902	-	-	1/10/68/68	0/4/4/4
5	GLU	B	901	-	-	0/6/7/9	-
5	GLU	R	901	-	-	1/6/7/9	-
6	CLR	B	902	-	-	4/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

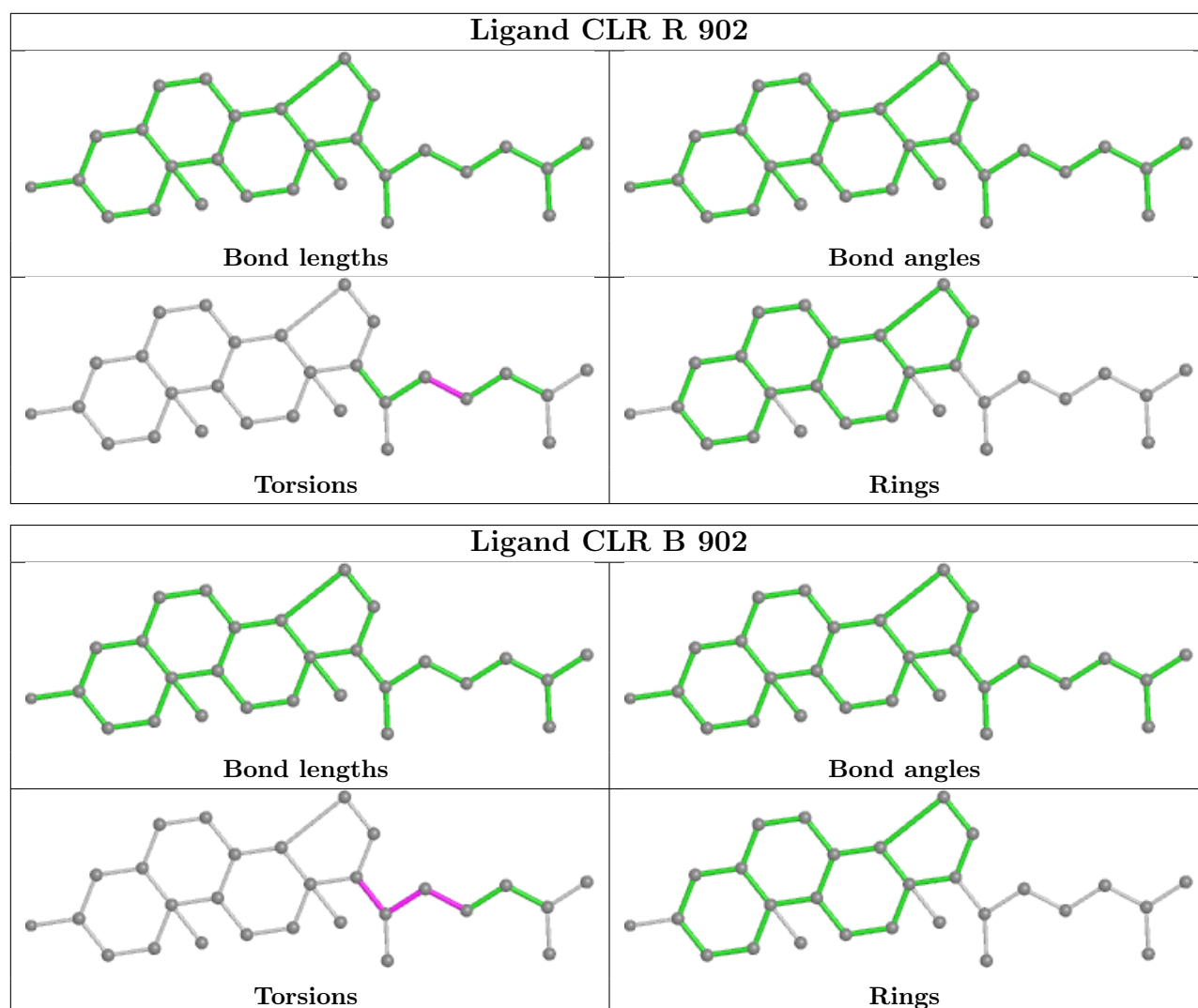
Mol	Chain	Res	Type	Atoms
5	R	901	GLU	O-C-CA-CB
6	B	902	CLR	C21-C20-C22-C23
6	B	902	CLR	C17-C20-C22-C23
6	R	902	CLR	C20-C22-C23-C24
6	B	902	CLR	C20-C22-C23-C24
6	B	902	CLR	C16-C17-C20-C22

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	GLU	2	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.