



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:43 AM BST

PDB ID : 5L1G  
Title : AMPA subtype ionotropic glutamate receptor GluA2 in complex with GYKI-Br  
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.  
Deposited on : 2016-07-29  
Resolution : 4.51 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

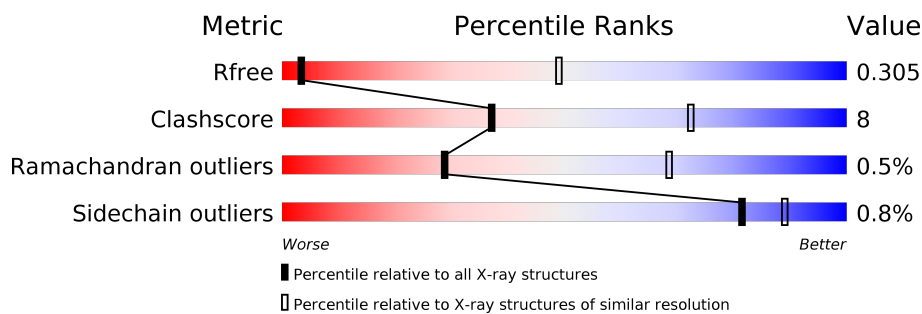
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.51 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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	A	803	<div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	B	803	<div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	C	803	<div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	D	803	<div> <div>78%</div> <div>18%</div> <div>.</div> </div>

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
3	GYB	A	903	X	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24087 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	777	Total	C	N	O	S	0	0	0
			5987	3848	992	1118	29			
1	B	773	Total	C	N	O	S	0	0	0
			5990	3844	989	1128	29			
1	C	774	Total	C	N	O	S	0	0	0
			5952	3824	986	1114	28			
1	D	777	Total	C	N	O	S	0	0	0
			5967	3831	990	1119	27			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	?	-	VAL	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	?	-	GLY	deletion	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	564	ASP	-	linker	UNP P19491
A	565	THR	-	linker	UNP P19491
A	566	ASP	-	linker	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	827	GLY	-	cloning artifact	UNP P19491
A	828	LEU	-	cloning artifact	UNP P19491
A	829	VAL	-	cloning artifact	UNP P19491
A	830	PRO	-	cloning artifact	UNP P19491
A	831	ARG	-	cloning artifact	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	?	-	VAL	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

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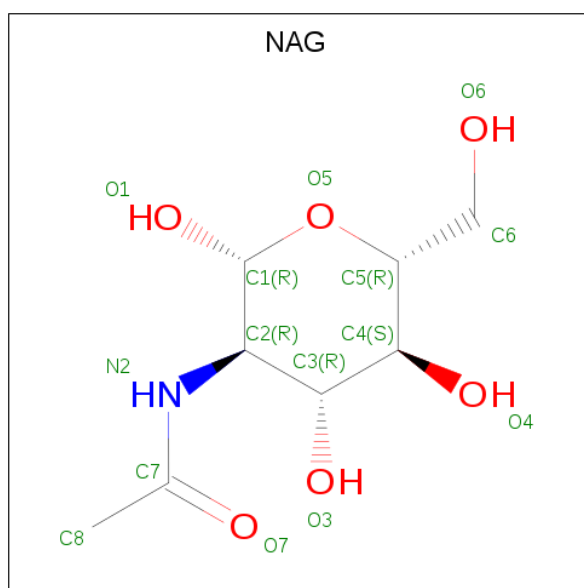
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker	UNP P19491
B	566	ASP	-	linker	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	827	GLY	-	cloning artifact	UNP P19491
B	828	LEU	-	cloning artifact	UNP P19491
B	829	VAL	-	cloning artifact	UNP P19491
B	830	PRO	-	cloning artifact	UNP P19491
B	831	ARG	-	cloning artifact	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	?	-	VAL	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	?	-	GLY	deletion	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	564	ASP	-	linker	UNP P19491
C	565	THR	-	linker	UNP P19491
C	566	ASP	-	linker	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	827	GLY	-	cloning artifact	UNP P19491
C	828	LEU	-	cloning artifact	UNP P19491
C	829	VAL	-	cloning artifact	UNP P19491
C	830	PRO	-	cloning artifact	UNP P19491
C	831	ARG	-	cloning artifact	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	?	-	VAL	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	?	-	GLY	deletion	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491

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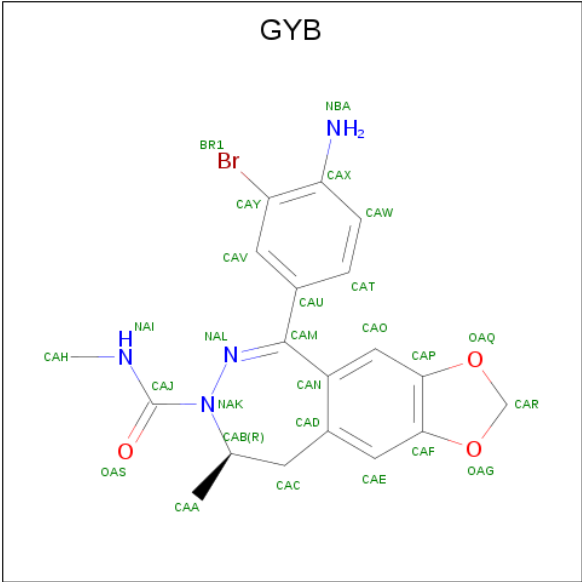
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491
D	830	PRO	-	cloning artifact	UNP P19491
D	831	ARG	-	cloning artifact	UNP P19491

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (8R)-5-(4-amino-3-bromophenyl)-N,8-dimethyl-8,9-dihydro-2H,7H-[1,3]dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide (three-letter code: GYB) (formula:  $C_{19}H_{19}BrN_4O_3$ ).

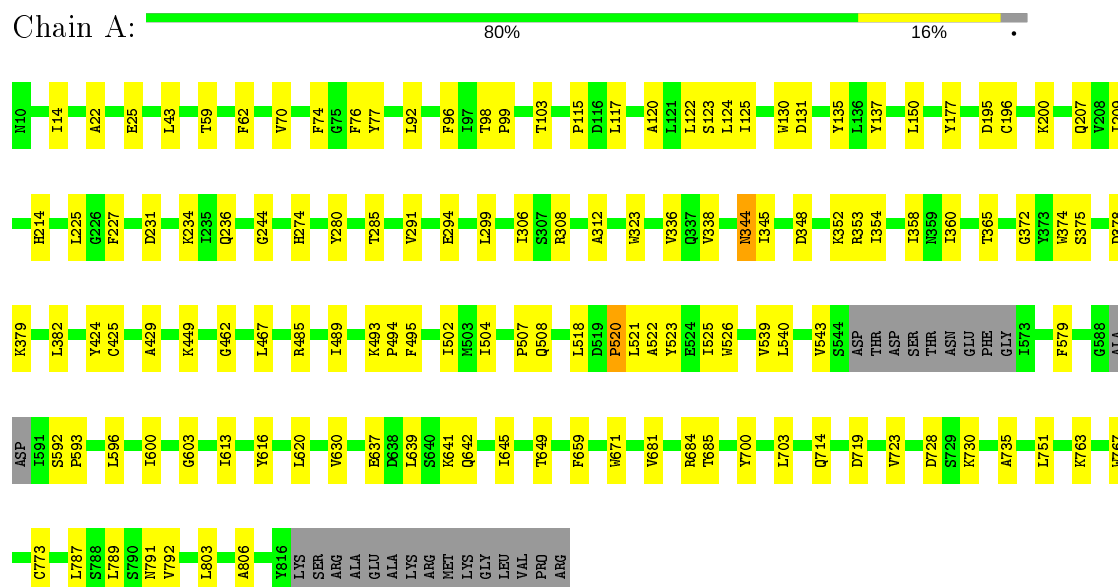


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	A	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	B	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	C	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	D	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		

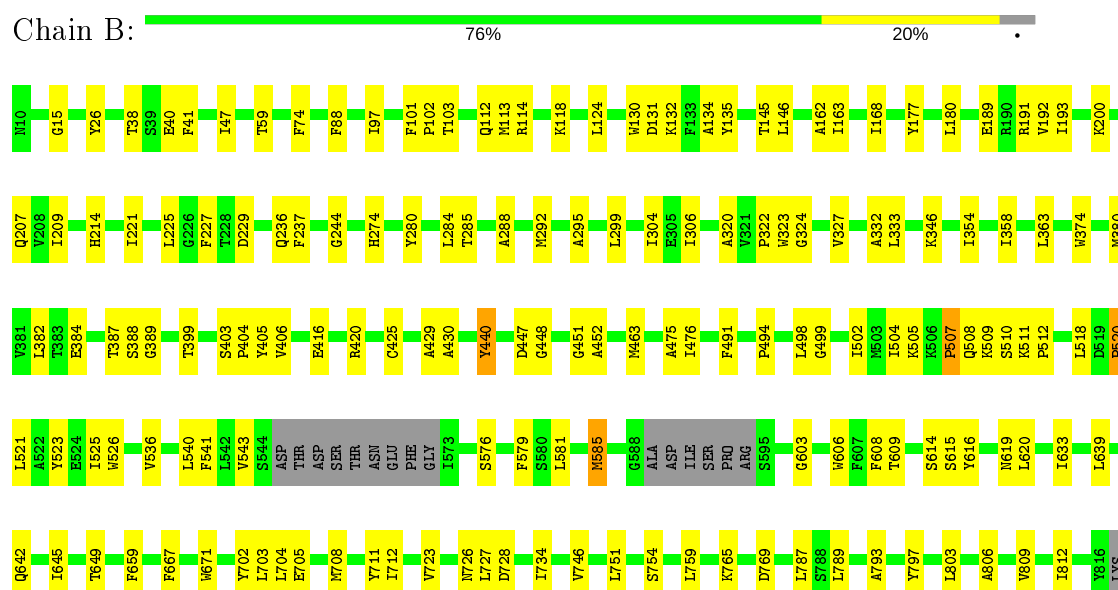
### 3 Residue-property plots

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: Glutamate receptor 2



#### • Molecule 1: Glutamate receptor 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.79Å 110.40Å 600.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 4.51 48.91 – 4.51	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.91-4.51) 99.2 (48.91-4.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, $R_{free}$	0.257 , 0.295 0.265 , 0.305	Depositor DCC
$R_{free}$ test set	1866 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	206.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 181.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	24087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	246.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: NAG, GYB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/6110	0.42	0/8271
1	B	0.26	0/6112	0.45	0/8270
1	C	0.25	0/6074	0.43	0/8225
1	D	0.25	0/6090	0.42	0/8248
All	All	0.25	0/24386	0.43	0/33014

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	A	5987	0	5885	83	0
1	B	5990	0	5902	108	0
1	C	5952	0	5823	124	0
1	D	5967	0	5830	100	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
3	A	54	0	0	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	3	0
3	C	27	0	0	1	0
3	D	27	0	0	3	0
All	All	24087	0	23492	371	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 8.

All (371) 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:903:GYB:CAR	1:C:610:LEU:HA	1.68	1.22
3:A:903:GYB:OAQ	1:C:613:ILE:CD1	1.89	1.20
3:A:903:GYB:CAP	1:C:613:ILE:HD11	1.72	1.19
3:A:903:GYB:CAR	1:C:613:ILE:HD11	1.76	1.15
3:A:903:GYB:OAQ	1:C:613:ILE:HD11	0.92	1.09
3:A:903:GYB:OAQ	1:C:610:LEU:HD12	1.52	1.07
1:C:498:LEU:HD11	1:C:705:GLU:HB2	1.47	0.97
3:A:903:GYB:CAR	1:C:613:ILE:CD1	2.40	0.97
1:A:449:LYS:HB3	1:A:462:GLY:HA2	1.44	0.96
1:A:613:ILE:HG21	3:A:903:GYB:CAH	2.03	0.89
3:A:903:GYB:CAR	1:C:610:LEU:CA	2.54	0.83
3:A:903:GYB:CAP	1:C:613:ILE:CD1	2.50	0.83
1:D:198:ARG:HH21	1:D:279:LYS:HD3	1.45	0.80
1:C:360:ILE:HB	1:C:372:GLY:HA3	1.66	0.78
1:B:346:LYS:HG3	1:B:354:ILE:HG13	1.67	0.77
1:B:451:GLY:HA2	1:B:452:ALA:HB3	1.67	0.76
1:C:596:LEU:HD13	1:D:578:TRP:HA	1.68	0.75
1:C:521:LEU:HG	1:C:616:TYR:HD2	1.52	0.75
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.68	0.75
3:A:903:GYB:OAQ	1:C:610:LEU:CD1	2.33	0.74
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.72	0.72
1:B:504:ILE:HD13	1:B:633:ILE:HD12	1.72	0.69
1:C:143:LEU:HG	1:D:143:LEU:HD11	1.75	0.69
1:B:102:PRO:HA	1:B:112:GLN:HG2	1.75	0.68
1:C:177:TYR:HB3	1:C:207:GLN:HG2	1.75	0.68
1:C:12:ILE:HG23	1:C:71:TYR:HD2	1.59	0.68
1:D:377:VAL:HG13	1:D:378:ASP:H	1.57	0.68
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.76	0.67
1:C:522:ALA:H	1:D:787:LEU:HD22	1.58	0.67
1:A:70:VAL:O	1:A:308:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.75	0.67
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.77	0.67
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.77	0.67
1:B:494:PRO:HG3	1:C:494:PRO:HG3	1.77	0.66
1:C:346:LYS:NZ	2:C:901:NAG:O7	2.29	0.66
3:A:903:GYB:BR1	1:B:614:SER:OG	2.66	0.66
3:A:903:GYB:CAP	1:C:610:LEU:HD12	2.25	0.66
1:C:498:LEU:HD13	1:C:707:THR:HG23	1.78	0.65
3:A:903:GYB:CAP	1:C:610:LEU:CD1	2.75	0.65
1:B:510:SER:OG	3:B:902:GYB:OAS	2.13	0.65
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.78	0.64
1:A:603:GLY:HA2	1:B:585:MET:HB3	1.79	0.63
1:B:416:GLU:HA	1:B:420:ARG:HD3	1.80	0.63
1:D:71:TYR:HA	1:D:323:TRP:HH2	1.63	0.63
1:C:596:LEU:HG	1:D:809:VAL:HG11	1.81	0.62
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.65	0.61
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.81	0.61
1:D:172:LYS:NZ	1:D:175:GLU:OE1	2.33	0.61
1:C:588:GLY:HA2	1:C:605:TRP:HD1	1.65	0.61
1:B:608:PHE:HD1	1:C:795:VAL:HG12	1.66	0.61
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.83	0.61
1:C:518:LEU:O	1:C:526:TRP:NE1	2.34	0.61
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.82	0.61
1:D:337:GLN:NE2	2:D:901:NAG:O7	2.34	0.60
1:C:517:PHE:CE1	1:C:795:VAL:HG22	2.38	0.59
1:A:135:TYR:CE1	1:A:137:TYR:HB3	2.38	0.59
1:B:508:GLN:N	1:B:509:LYS:HA	2.18	0.59
1:A:525:ILE:HG13	1:B:789:LEU:HD12	1.85	0.59
1:A:522:ALA:H	1:B:787:LEU:HD22	1.67	0.59
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.85	0.59
1:C:540:LEU:HA	1:C:543:VAL:HG22	1.85	0.59
1:B:498:LEU:HD12	1:B:705:GLU:HB2	1.84	0.58
1:B:447:ASP:N	1:B:448:GLY:HA2	2.18	0.58
1:C:445:VAL:HG22	1:C:448:GLY:H	1.68	0.58
1:C:640:SER:HB3	1:C:670:MET:HG2	1.84	0.58
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.86	0.58
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.86	0.58
1:C:522:ALA:HB3	1:C:525:ILE:HD13	1.85	0.58
1:C:597:SER:N	1:D:813:GLU:OE2	2.37	0.58
1:B:425:CYS:O	1:B:429:ALA:N	2.37	0.57
1:B:103:THR:HG23	1:B:112:GLN:HE21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ILE:HG22	1:B:734:ILE:HG23	1.87	0.57
1:D:498:LEU:HD12	1:D:705:GLU:HB2	1.86	0.57
1:A:124:LEU:HD13	1:A:360:ILE:HD13	1.86	0.57
1:B:168:ILE:HD11	1:B:200:LYS:HZ1	1.70	0.57
1:C:299:LEU:HD13	1:C:306:ILE:HD13	1.87	0.57
3:A:903:GYB:CAR	1:C:613:ILE:HD13	2.33	0.57
1:A:344:ASN:HD22	1:A:345:ILE:H	1.51	0.57
1:A:344:ASN:O	1:A:353:ARG:NH2	2.38	0.56
1:D:22:ALA:HB1	1:D:25:GLU:HB2	1.87	0.56
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.22	0.56
1:A:806:ALA:HA	1:D:600:ILE:HD11	1.85	0.56
1:B:168:ILE:O	1:B:168:ILE:HD12	2.05	0.56
1:B:382:LEU:HD13	1:B:384:GLU:HG3	1.88	0.56
1:D:231:ASP:HB3	1:D:234:LYS:HE2	1.86	0.56
1:D:134:ALA:HB2	1:D:189:GLU:HG2	1.87	0.56
1:A:714:GLN:HA	1:A:773:CYS:HB2	1.88	0.56
1:C:13:GLN:HA	1:C:44:THR:HB	1.87	0.56
1:C:447:ASP:OD1	1:C:447:ASP:N	2.40	0.55
1:B:606:TRP:HA	1:B:609:THR:HG22	1.88	0.55
1:C:623:PHE:HZ	1:D:786:ALA:HA	1.71	0.55
1:B:615:SER:HB3	3:C:902:GYB:BR1	2.61	0.55
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.87	0.55
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.87	0.55
1:A:792:VAL:HG21	1:D:525:ILE:HG12	1.89	0.55
1:C:604:VAL:HG12	1:D:799:LEU:HD12	1.88	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.88	0.55
1:C:48:ASP:OD1	1:C:65:GLN:NE2	2.40	0.54
1:B:603:GLY:HA3	1:C:581:LEU:HD21	1.87	0.54
1:C:10:ASN:HB3	1:C:300:ARG:HH22	1.70	0.54
1:A:177:TYR:HD2	1:A:207:GLN:HG3	1.72	0.54
1:A:521:LEU:HD13	1:A:616:TYR:HD2	1.73	0.54
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.88	0.54
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.42	0.54
1:B:15:GLY:O	1:B:74:PHE:N	2.38	0.54
3:A:903:GYB:CAR	1:C:610:LEU:HD12	2.36	0.54
1:A:59:THR:HG21	1:B:59:THR:HG21	1.91	0.53
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.73	0.53
1:B:751:LEU:HB2	1:C:483:LEU:HD13	1.90	0.53
1:A:684:ARG:HG2	1:A:685:THR:HG23	1.89	0.53
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.43	0.53
1:B:633:ILE:HD13	1:B:639:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:PHE:HE1	1:A:592:SER:H	1.56	0.53
1:B:131:ASP:OD1	1:B:132:LYS:N	2.42	0.53
1:B:510:SER:HB3	1:B:512:PRO:HD3	1.90	0.53
1:B:754:SER:HB2	1:B:759:LEU:HD12	1.91	0.52
1:B:274:HIS:ND1	1:B:274:HIS:O	2.42	0.52
1:D:540:LEU:HA	1:D:543:VAL:HG22	1.91	0.52
1:D:213:LYS:NZ	1:D:218:TYR:OH	2.34	0.52
1:A:231:ASP:HB3	1:A:234:LYS:HE2	1.92	0.52
1:A:294:GLU:HG3	1:A:338:VAL:HG11	1.91	0.52
1:B:510:SER:HB3	1:B:511:LYS:HA	1.92	0.52
1:A:751:LEU:HB2	1:D:483:LEU:HD13	1.90	0.52
1:C:600:ILE:HA	1:D:581:LEU:HD21	1.91	0.52
1:A:344:ASN:HD22	1:A:345:ILE:N	2.07	0.52
1:A:803:LEU:HD22	1:D:539:VAL:HG21	1.92	0.52
1:D:498:LEU:HB3	1:D:707:THR:HG23	1.91	0.52
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.43	0.51
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.42	0.51
1:A:137:TYR:HA	1:A:195:ASP:HB3	1.92	0.51
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.91	0.51
1:B:620:LEU:HD21	3:B:902:GYB:BR1	2.65	0.51
1:C:521:LEU:HD23	1:D:787:LEU:HD13	1.92	0.51
1:B:708:MET:O	1:B:712:ILE:HG12	2.10	0.51
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.75	0.51
1:D:12:ILE:HG23	1:D:71:TYR:HD2	1.76	0.51
1:D:715:ARG:HD3	1:D:772:GLU:HG2	1.92	0.51
1:B:388:SER:HB3	1:B:389:GLY:HA3	1.92	0.51
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.93	0.51
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.93	0.50
1:D:517:PHE:CE1	1:D:795:VAL:HG22	2.46	0.50
1:A:681:VAL:O	1:A:700:TYR:OH	2.24	0.50
1:B:163:ILE:HG21	1:B:180:LEU:HD13	1.93	0.50
1:D:174:ASP:OD1	1:D:207:GLN:NE2	2.44	0.50
1:D:509:LYS:HA	1:D:510:SER:C	2.31	0.50
1:A:520:PRO:HG3	1:A:620:LEU:HD13	1.94	0.50
3:A:903:GYB:CAR	1:C:610:LEU:CD1	2.89	0.50
1:C:97:ILE:HA	1:C:111:ILE:HB	1.94	0.50
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.93	0.50
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.48	0.49
1:B:97:ILE:HD11	1:B:333:LEU:HD22	1.95	0.49
1:D:450:TYR:HA	1:D:462:GLY:HA3	1.94	0.49
1:A:502:ILE:HD13	1:A:639:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:ASN:HA	1:C:624:LEU:HD13	1.94	0.49
1:D:236:GLN:NE2	1:D:365:THR:O	2.44	0.49
1:A:117:LEU:HD13	1:A:225:LEU:HD21	1.93	0.49
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.95	0.49
1:A:308:ARG:NE	1:A:312:ALA:HB2	2.27	0.49
1:B:135:TYR:CD2	1:B:146:LEU:HD13	2.48	0.49
1:B:502:ILE:HD13	1:B:639:LEU:HD13	1.94	0.49
1:B:702:TYR:CE2	1:B:704:LEU:HB3	2.47	0.49
1:C:252:ASP:OD1	1:C:253:SER:N	2.45	0.49
1:D:784:THR:HA	1:D:785:SER:HB3	1.93	0.49
1:B:508:GLN:H	1:B:509:LYS:HA	1.78	0.48
1:A:425:CYS:O	1:A:429:ALA:N	2.43	0.48
1:C:13:GLN:HG2	1:C:70:VAL:HG12	1.95	0.48
1:D:516:SER:HB2	3:D:902:GYB:CAA	2.43	0.48
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.96	0.48
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.54	0.48
1:D:382:LEU:H	1:D:382:LEU:HD23	1.77	0.48
1:C:579:PHE:O	1:C:583:ALA:N	2.47	0.48
1:A:493:LYS:HG3	1:A:751:LEU:HD21	1.94	0.48
1:B:38:THR:HG23	1:B:40:GLU:H	1.78	0.48
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.95	0.48
1:B:225:LEU:HB2	1:B:280:TYR:CD2	2.49	0.48
1:B:499:GLY:HA3	1:B:726:ASN:HB3	1.95	0.47
1:C:213:LYS:NZ	1:C:218:TYR:OH	2.39	0.47
1:A:485:ARG:O	1:A:489:ILE:HG13	2.14	0.47
1:C:373:TYR:HB3	1:C:381:VAL:O	2.14	0.47
1:D:708:MET:O	1:D:712:ILE:HG12	2.14	0.47
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.48	0.47
1:A:150:LEU:HD22	1:B:162:ALA:HB3	1.96	0.47
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.49	0.47
1:A:522:ALA:N	1:B:787:LEU:HD22	2.29	0.47
1:C:169:ASN:HD21	1:C:172:LYS:HD3	1.79	0.47
1:D:763:LYS:O	1:D:767:TRP:HB2	2.14	0.47
1:B:430:ALA:HA	1:B:440:TYR:HE1	1.79	0.47
1:B:505:LYS:HE2	1:B:507:PRO:HB3	1.96	0.47
1:C:632:PRO:HB2	1:C:633:ILE:HB	1.96	0.47
1:D:787:LEU:HD21	1:D:792:VAL:HG21	1.95	0.47
1:A:196:CYS:HB3	1:A:200:LYS:HB2	1.96	0.47
1:C:502:ILE:HB	1:C:723:VAL:HG23	1.96	0.47
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.96	0.47
1:D:592:SER:N	1:D:593:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ILE:HA	1:C:382:LEU:HD22	1.97	0.47
1:C:600:ILE:HD11	1:D:806:ALA:HA	1.97	0.47
1:C:177:TYR:CB	1:C:207:GLN:HG2	2.45	0.46
1:A:291:VAL:HA	1:A:336:VAL:HG11	1.97	0.46
1:A:489:ILE:HD13	1:A:735:ALA:HB1	1.98	0.46
1:B:124:LEU:HA	1:B:380:MET:HE1	1.95	0.46
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.97	0.46
1:D:504:ILE:HD11	1:D:723:VAL:HG11	1.96	0.46
1:D:754:SER:HB2	1:D:759:LEU:HD12	1.98	0.46
1:A:375:SER:N	1:A:378:ASP:O	2.46	0.46
1:C:79:LYS:HD2	1:C:139:SER:O	2.16	0.46
1:D:789:LEU:HA	1:D:792:VAL:HB	1.98	0.46
1:A:789:LEU:HA	1:D:525:ILE:HD11	1.96	0.46
1:B:463:MET:HE3	1:B:475:ALA:HB1	1.98	0.46
1:A:620:LEU:HD21	3:A:902:GYB:BR1	2.71	0.46
1:A:637:GLU:O	1:A:641:LYS:N	2.49	0.46
1:A:358:ILE:HD12	1:A:374:TRP:HE1	1.79	0.46
1:B:387:THR:N	1:B:388:SER:HA	2.31	0.46
1:B:404:PRO:HG3	1:B:711:TYR:CD1	2.51	0.46
1:A:540:LEU:HA	1:A:543:VAL:HG22	1.98	0.45
1:D:181:PHE:HA	1:D:184:LEU:HB2	1.97	0.45
1:B:734:ILE:HG21	1:B:746:VAL:HG11	1.98	0.45
1:B:132:LYS:NZ	1:B:189:GLU:OE2	2.49	0.45
1:B:399:THR:HG21	1:B:406:VAL:HG21	1.97	0.45
1:A:787:LEU:O	1:D:522:ALA:HB2	2.16	0.45
1:A:236:GLN:NE2	1:A:365:THR:O	2.49	0.45
1:A:719:ASP:N	1:A:719:ASP:OD1	2.47	0.45
1:B:26:TYR:HE1	1:B:47:ILE:HG12	1.81	0.45
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.51	0.45
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.97	0.45
1:C:604:VAL:HG21	1:D:802:GLY:HA3	1.99	0.45
1:A:131:ASP:N	1:A:131:ASP:OD1	2.49	0.45
1:D:357:THR:HG23	1:D:373:TYR:HB2	1.99	0.45
1:B:118:LYS:HB3	1:B:145:THR:HG22	1.98	0.45
1:B:177:TYR:HB3	1:B:207:GLN:HG2	1.98	0.45
1:B:406:VAL:HG23	1:B:425:CYS:HB2	1.99	0.45
1:B:502:ILE:HB	1:B:723:VAL:HG23	1.97	0.45
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.99	0.45
1:C:600:ILE:HG22	1:D:581:LEU:CD1	2.46	0.45
1:A:372:GLY:HA2	1:A:382:LEU:HB3	1.99	0.45
1:B:520:PRO:HG3	1:B:620:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLN:NE2	1:C:365:THR:O	2.45	0.45
1:D:131:ASP:N	1:D:131:ASP:OD1	2.47	0.45
1:D:198:ARG:NH2	1:D:279:LYS:HD3	2.22	0.45
1:C:464:VAL:HG22	1:C:479:LEU:HD21	1.98	0.45
1:D:683:VAL:HG11	1:D:689:GLY:HA2	1.98	0.45
1:A:103:THR:O	1:A:352:LYS:NZ	2.43	0.44
1:A:125:ILE:HG23	1:A:130:TRP:HB2	1.99	0.44
1:A:518:LEU:O	1:A:526:TRP:NE1	2.50	0.44
1:B:387:THR:O	1:B:387:THR:OG1	2.24	0.44
1:C:499:GLY:HA3	1:C:726:ASN:HB3	1.98	0.44
1:C:498:LEU:HD22	1:C:732:TYR:CZ	2.53	0.44
1:D:360:ILE:HD11	1:D:374:TRP:HB2	1.98	0.44
1:A:504:ILE:HD11	1:A:723:VAL:HG11	1.99	0.44
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.99	0.44
1:C:135:TYR:CE2	1:C:137:TYR:HB3	2.53	0.44
1:C:476:ILE:HG12	1:C:734:ILE:HG23	1.99	0.44
1:D:143:LEU:HD23	1:D:143:LEU:H	1.82	0.44
1:C:521:LEU:HA	1:D:787:LEU:HD13	1.99	0.44
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.83	0.44
1:B:358:ILE:O	1:B:374:TRP:N	2.49	0.44
1:C:539:VAL:HG21	1:D:803:LEU:HD22	1.99	0.44
1:A:507:PRO:HA	1:A:508:GLN:CB	2.48	0.44
1:A:62:PHE:HE2	1:A:92:LEU:HD12	1.82	0.44
1:B:130:TRP:CE2	1:B:191:ARG:HD3	2.52	0.44
1:D:79:LYS:HD2	1:D:142:GLY:HA2	1.98	0.44
1:B:576:SER:HA	1:B:579:PHE:HB3	1.99	0.44
1:B:74:PHE:HA	1:B:97:ILE:O	2.18	0.44
1:A:791:ASN:OD1	3:A:902:GYB:NAI	2.50	0.43
3:A:903:GYB:OAG	1:C:606:TRP:NE1	2.51	0.43
1:B:299:LEU:HD21	1:B:332:ALA:HB2	2.00	0.43
1:C:388:SER:H	1:C:389:GLY:HA2	1.82	0.43
1:C:417:GLY:O	1:C:420:ARG:NE	2.51	0.43
1:D:122:LEU:HD21	1:D:149:VAL:HA	2.01	0.43
1:A:467:LEU:HD23	1:A:467:LEU:HA	1.88	0.43
1:A:600:ILE:HD11	1:B:806:ALA:HA	1.99	0.43
1:B:304:ILE:HD12	1:B:304:ILE:O	2.19	0.43
1:B:793:ALA:HB1	1:B:797:TYR:CE2	2.54	0.43
1:B:809:VAL:O	1:B:812:ILE:HG12	2.19	0.43
1:D:101:PHE:HA	1:D:114:ARG:HD2	2.00	0.43
1:D:169:ASN:ND2	1:D:171:ASP:OD1	2.51	0.43
1:D:518:LEU:O	1:D:526:TRP:NE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ILE:HG21	1:C:180:LEU:HD13	2.00	0.43
1:C:22:ALA:HB1	1:C:25:GLU:HB2	2.00	0.43
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.99	0.43
1:C:500:ILE:O	1:C:727:LEU:N	2.51	0.43
1:D:171:ASP:OD1	1:D:172:LYS:N	2.51	0.43
1:D:506:LYS:N	1:D:719:ASP:O	2.43	0.43
1:C:763:LYS:HD2	1:C:767:TRP:CE3	2.54	0.43
1:D:26:TYR:CE2	1:D:30:ARG:HD2	2.53	0.43
1:C:520:PRO:HB2	1:C:616:TYR:CE2	2.54	0.43
1:A:115:PRO:HA	1:A:353:ARG:HB2	2.01	0.43
1:C:615:SER:OG	3:D:902:GYB:NBA	2.52	0.43
1:D:517:PHE:O	1:D:520:PRO:HD2	2.18	0.43
1:B:608:PHE:CD1	1:C:795:VAL:HG12	2.49	0.42
1:C:87:SER:OG	1:D:54:ASN:OD1	2.36	0.42
1:D:529:ILE:HD13	1:D:612:ILE:HD12	2.01	0.42
1:B:295:ALA:HB2	1:B:333:LEU:HD23	2.02	0.42
1:C:219:HIS:HA	1:C:241:GLU:O	2.19	0.42
1:C:464:VAL:HG13	1:C:489:ILE:HG12	2.00	0.42
1:D:503:MET:HG3	1:D:720:THR:HB	2.02	0.42
1:B:320:ALA:O	1:B:322:PRO:HD3	2.19	0.42
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.84	0.42
1:D:61:ALA:O	1:D:65:GLN:HG2	2.18	0.42
1:A:120:ALA:HB2	1:A:374:TRP:NE1	2.34	0.42
1:D:466:GLU:O	1:D:472:ALA:N	2.52	0.42
1:D:580:SER:O	1:D:584:PHE:N	2.53	0.42
1:D:809:VAL:HA	1:D:812:ILE:HG12	2.02	0.42
1:A:613:ILE:CG2	3:A:903:GYB:CAH	2.87	0.42
1:B:518:LEU:HB2	1:B:526:TRP:CE2	2.54	0.42
1:C:266:GLU:HG2	1:C:268:LYS:H	1.85	0.42
1:D:261:ARG:HA	1:D:261:ARG:HD2	1.81	0.42
1:D:43:LEU:O	1:D:45:PRO:HD3	2.20	0.42
1:B:237:PHE:HB2	1:D:210:THR:HG22	2.02	0.42
1:B:403:SER:HA	1:B:404:PRO:HA	1.87	0.42
1:D:13:GLN:HG3	1:D:70:VAL:HG12	2.02	0.42
1:A:225:LEU:HB2	1:A:280:TYR:CD2	2.55	0.42
1:B:209:ILE:HG23	1:B:214:HIS:NE2	2.33	0.42
1:A:123:SER:OG	1:A:379:LYS:HD3	2.20	0.41
1:C:588:GLY:C	1:C:602:GLY:HA2	2.41	0.41
1:D:219:HIS:HA	1:D:241:GLU:O	2.20	0.41
1:A:728:ASP:OD2	1:A:730:LYS:HE3	2.20	0.41
1:A:600:ILE:HA	1:B:581:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:HG23	1:B:41:PHE:H	1.84	0.41
1:C:110:VAL:HG12	1:C:112:GLN:HG3	2.02	0.41
1:C:308:ARG:HE	1:C:312:ALA:HB2	1.85	0.41
1:C:597:SER:O	1:C:601:VAL:HG23	2.20	0.41
1:D:334:LYS:NZ	1:D:349:GLN:O	2.34	0.41
1:A:424:TYR:HE2	1:A:495:PHE:HE2	1.68	0.41
1:C:637:GLU:HG2	1:C:641:LYS:HE3	2.01	0.41
1:C:659:PHE:HB3	1:C:671:TRP:HB2	2.02	0.41
1:D:395:VAL:HG21	1:D:742:LEU:HD21	2.02	0.41
3:D:902:GYB:CAT	3:D:902:GYB:CAO	2.97	0.41
1:D:795:VAL:O	1:D:798:ILE:HG22	2.20	0.41
1:B:518:LEU:O	1:B:526:TRP:NE1	2.53	0.41
1:B:525:ILE:HG12	1:C:792:VAL:HG11	2.02	0.41
1:D:579:PHE:O	1:D:583:ALA:N	2.54	0.41
1:A:763:LYS:O	1:A:767:TRP:HB2	2.20	0.41
1:B:324:GLY:O	1:B:327:VAL:HG12	2.21	0.41
1:C:204:ILE:O	1:C:208:VAL:HG23	2.20	0.41
1:C:525:ILE:HD11	1:D:789:LEU:HB3	2.03	0.41
1:C:604:VAL:HG11	1:D:802:GLY:HA3	2.02	0.41
1:B:288:ALA:O	1:B:292:MET:HG3	2.20	0.41
1:B:507:PRO:HD2	1:B:508:GLN:HA	2.02	0.41
1:D:515:PHE:HA	1:D:515:PHE:HD2	1.77	0.41
1:D:535:GLY:O	1:D:539:VAL:HG23	2.21	0.41
1:C:600:ILE:HG22	1:D:581:LEU:HD13	2.03	0.41
1:D:715:ARG:HA	1:D:715:ARG:HD3	1.91	0.41
1:B:236:GLN:HG3	1:B:363:LEU:HD11	2.03	0.41
1:C:751:LEU:HD23	1:C:751:LEU:HA	1.86	0.41
1:D:377:VAL:HG13	1:D:378:ASP:N	2.32	0.41
1:A:348:ASP:HB3	1:A:354:ILE:HG21	2.03	0.41
1:C:135:TYR:HH	1:C:145:THR:HG1	1.64	0.41
1:C:502:ILE:O	1:C:709:ASN:ND2	2.52	0.41
1:D:96:PHE:CE2	1:D:98:THR:HB	2.56	0.41
1:A:76:PHE:CE2	1:A:99:PRO:HG2	2.56	0.41
1:C:532:ALA:HB1	1:C:605:TRP:HZ3	1.86	0.41
1:D:642:GLN:HE22	1:D:645:ILE:HB	1.86	0.41
1:B:113:MET:HB3	1:B:284:LEU:HD22	2.03	0.40
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.54	0.40
1:C:318:ASN:HB2	1:D:60:ASN:HD21	1.86	0.40
3:A:903:GYB:CAP	1:C:610:LEU:HD13	2.51	0.40
1:B:728:ASP:OD1	1:B:728:ASP:N	2.54	0.40
1:C:422:GLU:HB2	1:C:766:TRP:HH2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.03	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.93	0.40
1:A:308:ARG:HE	1:A:312:ALA:HB2	1.85	0.40
1:B:229:ASP:OD2	1:B:280:TYR:N	2.54	0.40
1:C:91:THR:HG21	1:D:56:PHE:CE1	2.56	0.40
1:A:96:PHE:CE2	1:A:98:THR:HB	2.57	0.40
1:C:10:ASN:ND2	1:C:40:GLU:O	2.51	0.40
1:C:606:TRP:HA	1:C:609:THR:HG22	2.03	0.40
1:D:261:ARG:O	1:D:265:LEU:HG	2.22	0.40
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.56	0.40
1:B:620:LEU:HD11	3:B:902:GYB:CAY	2.52	0.40
1:C:348:ASP:OD1	1:C:352:LYS:N	2.54	0.40
1:C:388:SER:N	1:C:389:GLY:HA2	2.37	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	771/803 (96%)	715 (93%)	52 (7%)	4 (0%)	29	68
1	B	767/803 (96%)	708 (92%)	57 (7%)	2 (0%)	41	76
1	C	768/803 (96%)	715 (93%)	48 (6%)	5 (1%)	22	62
1	D	771/803 (96%)	720 (93%)	48 (6%)	3 (0%)	34	72
All	All	3077/3212 (96%)	2858 (93%)	205 (7%)	14 (0%)	29	68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	510	SER
1	A	596	LEU

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Mol	Chain	Res	Type
1	D	593	PRO
1	C	373	TYR
1	A	520	PRO
1	A	630	VAL
1	D	520	PRO
1	C	512	PRO
1	C	520	PRO
1	B	520	PRO
1	C	633	ILE
1	D	632	PRO
1	A	593	PRO
1	B	507	PRO

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/683 (92%)	622 (99%)	5 (1%)	81	89
1	B	634/683 (93%)	627 (99%)	7 (1%)	73	85
1	C	619/683 (91%)	617 (100%)	2 (0%)	92	95
1	D	620/683 (91%)	613 (99%)	7 (1%)	73	85
All	All	2500/2732 (92%)	2479 (99%)	21 (1%)	81	89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	TYR
1	A	274	HIS
1	A	323	TRP
1	A	344	ASN
1	A	523	TYR
1	B	88	PHE
1	B	323	TRP
1	B	440	TYR
1	B	491	PHE

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Mol	Chain	Res	Type
1	B	523	TYR
1	B	541	PHE
1	B	585	MET
1	C	323	TRP
1	C	523	TYR
1	D	177	TYR
1	D	323	TRP
1	D	523	TYR
1	D	533	TYR
1	D	541	PHE
1	D	585	MET
1	D	791	ASN

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

Mol	Chain	Res	Type
1	B	791	ASN
1	C	207	GLN

### 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](#)

9 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	$\# Z  > 2$
3	GYB	A	902	-	28,30,30	4.35	12 (42%)	31,44,44	2.33	10 (32%)
3	GYB	B	902	-	28,30,30	4.34	12 (42%)	31,44,44	2.15	8 (25%)
2	NAG	C	901	1	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
2	NAG	B	901	1	14,14,15	0.36	0	17,19,21	0.60	1 (5%)
2	NAG	D	901	1	14,14,15	0.50	0	17,19,21	0.60	0
3	GYB	A	903	-	28,30,30	2.43	9 (32%)	31,44,44	2.19	8 (25%)
2	NAG	A	901	1	14,14,15	0.74	1 (7%)	17,19,21	0.66	0
3	GYB	C	902	-	28,30,30	4.23	12 (42%)	31,44,44	2.70	12 (38%)
3	GYB	D	902	-	28,30,30	4.28	12 (42%)	31,44,44	2.47	10 (32%)

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
3	GYB	A	902	-	-	3/6/32/32	0/3/4/4
3	GYB	B	902	-	-	4/6/32/32	0/3/4/4
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1
3	GYB	A	903	-	1/1/4/5	4/6/32/32	0/3/4/4
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
3	GYB	C	902	-	-	2/6/32/32	0/3/4/4
3	GYB	D	902	-	-	3/6/32/32	0/3/4/4

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GYB	CAM-NAL	14.52	1.46	1.30
3	D	902	GYB	CAM-NAL	14.16	1.46	1.30
3	C	902	GYB	CAM-NAL	14.15	1.46	1.30
3	B	902	GYB	CAM-NAL	13.91	1.45	1.30
3	B	902	GYB	CAJ-NAI	11.00	1.48	1.34
3	A	902	GYB	CAJ-NAI	10.66	1.48	1.34
3	D	902	GYB	CAJ-NAI	10.35	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	GYB	CAJ-NAI	9.98	1.47	1.34
3	A	903	GYB	CAU-CAM	-6.15	1.40	1.49
3	B	902	GYB	CAN-CAM	5.55	1.57	1.49
3	A	903	GYB	CAN-CAM	-5.43	1.41	1.49
3	D	902	GYB	OAG-CAR	-5.36	1.33	1.43
3	C	902	GYB	OAG-CAR	-5.36	1.33	1.43
3	A	902	GYB	OAG-CAR	-5.35	1.33	1.43
3	C	902	GYB	OAQ-CAR	-5.35	1.33	1.43
3	D	902	GYB	OAQ-CAR	-5.32	1.33	1.43
3	A	902	GYB	OAQ-CAR	-5.27	1.33	1.43
3	A	902	GYB	CAN-CAM	5.27	1.56	1.49
3	B	902	GYB	OAG-CAR	-5.26	1.33	1.43
3	B	902	GYB	OAQ-CAR	-5.24	1.33	1.43
3	C	902	GYB	CAN-CAM	5.22	1.56	1.49
3	D	902	GYB	CAN-CAM	5.22	1.56	1.49
3	A	903	GYB	CAM-NAL	5.20	1.36	1.30
3	D	902	GYB	OAS-CAJ	-4.49	1.14	1.23
3	B	902	GYB	OAS-CAJ	-4.46	1.14	1.23
3	A	902	GYB	OAS-CAJ	-4.43	1.14	1.23
3	C	902	GYB	OAS-CAJ	-4.40	1.15	1.23
3	B	902	GYB	CAE-CAD	4.33	1.46	1.39
3	A	903	GYB	CAA-CAB	4.27	1.66	1.52
3	A	902	GYB	CAU-CAM	4.11	1.55	1.49
3	A	902	GYB	CAE-CAD	3.97	1.46	1.39
3	D	902	GYB	CAO-CAN	3.95	1.46	1.39
3	C	902	GYB	CAE-CAD	3.91	1.46	1.39
3	B	902	GYB	CAO-CAN	3.91	1.46	1.39
3	C	902	GYB	CAU-CAM	3.90	1.55	1.49
3	D	902	GYB	CAE-CAD	3.90	1.46	1.39
3	D	902	GYB	CAU-CAM	3.82	1.55	1.49
3	B	902	GYB	CAU-CAM	3.78	1.54	1.49
3	A	902	GYB	CAO-CAN	3.77	1.45	1.39
3	C	902	GYB	CAO-CAN	3.60	1.45	1.39
3	A	902	GYB	CAO-CAP	3.58	1.45	1.38
3	B	902	GYB	CAO-CAP	3.57	1.45	1.38
3	C	902	GYB	CAX-NBA	3.53	1.49	1.37
3	A	902	GYB	CAX-NBA	3.53	1.49	1.37
3	D	902	GYB	CAX-NBA	3.52	1.49	1.37
3	B	902	GYB	CAE-CAF	3.50	1.45	1.38
3	C	902	GYB	CAO-CAP	3.49	1.45	1.38
3	B	902	GYB	CAX-NBA	3.42	1.49	1.37
3	D	902	GYB	CAO-CAP	3.40	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	GYB	CAC-CAD	-3.31	1.44	1.51
3	D	902	GYB	CAE-CAF	3.30	1.44	1.38
3	A	903	GYB	NAK-NAL	-3.21	1.28	1.38
3	A	902	GYB	CAE-CAF	3.12	1.44	1.38
3	C	902	GYB	CAE-CAF	3.00	1.44	1.38
3	A	903	GYB	CAO-CAP	-2.71	1.33	1.38
3	A	903	GYB	CAE-CAF	-2.59	1.34	1.38
2	A	901	NAG	C1-C2	2.55	1.56	1.52
3	A	903	GYB	CAP-CAF	-2.02	1.34	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	GYB	CAH-NAI-CAJ	-8.88	111.55	120.69
3	A	903	GYB	CAT-CAU-CAM	-5.93	113.19	120.64
3	A	903	GYB	CAD-CAC-CAB	-5.86	100.17	115.55
3	D	902	GYB	CAH-NAI-CAJ	-5.83	114.69	120.69
3	D	902	GYB	CAN-CAM-CAU	-5.82	111.35	118.11
3	B	902	GYB	OAG-CAF-CAE	5.60	135.35	127.85
3	D	902	GYB	OAG-CAF-CAE	5.55	135.28	127.85
3	A	902	GYB	OAG-CAF-CAE	5.12	134.70	127.85
3	C	902	GYB	OAG-CAF-CAE	5.05	134.61	127.85
3	C	902	GYB	CAN-CAM-CAU	-5.01	112.28	118.11
3	A	902	GYB	CAN-CAM-CAU	-4.85	112.47	118.11
3	A	903	GYB	CAV-CAU-CAM	4.68	128.20	120.38
3	A	902	GYB	CAH-NAI-CAJ	-4.34	116.23	120.69
3	B	902	GYB	OAG-CAF-CAP	-4.18	105.02	109.78
3	D	902	GYB	OAQ-CAP-CAO	4.10	133.34	127.85
3	B	902	GYB	OAQ-CAP-CAO	4.05	133.26	127.85
3	A	902	GYB	OAQ-CAP-CAO	4.00	133.20	127.85
3	D	902	GYB	OAG-CAF-CAP	-3.98	105.25	109.78
3	C	902	GYB	OAG-CAF-CAP	-3.73	105.53	109.78
3	A	902	GYB	OAG-CAF-CAP	-3.65	105.63	109.78
3	C	902	GYB	OAQ-CAP-CAO	3.65	132.73	127.85
3	B	902	GYB	CAN-CAM-CAU	-3.64	113.87	118.11
3	B	902	GYB	CAR-OAG-CAF	3.20	109.50	105.34
3	A	903	GYB	CAO-CAN-CAM	-3.18	114.27	118.88
3	B	902	GYB	CAV-CAY-CAX	-3.14	119.13	122.15
3	D	902	GYB	CAR-OAG-CAF	3.08	109.34	105.34
3	A	902	GYB	OAQ-CAP-CAF	-2.99	106.38	109.78
3	A	903	GYB	CAY-CAX-NBA	-2.96	119.16	122.36
3	A	902	GYB	CAR-OAG-CAF	2.89	109.09	105.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	GYB	OAQ-CAP-CAF	-2.82	106.57	109.78
3	A	903	GYB	CAC-CAD-CAE	-2.76	111.52	118.44
3	C	902	GYB	CAR-OAG-CAF	2.76	108.92	105.34
3	C	902	GYB	OAS-CAJ-NAI	-2.72	117.42	122.79
3	A	902	GYB	OAS-CAJ-NAI	-2.62	117.62	122.79
3	D	902	GYB	OAQ-CAP-CAF	-2.58	106.84	109.78
3	A	902	GYB	CAR-OAQ-CAP	2.55	108.66	105.34
3	A	903	GYB	CAT-CAW-CAX	-2.51	118.75	121.42
3	B	902	GYB	OAQ-CAP-CAF	-2.45	107.00	109.78
3	A	902	GYB	CAV-CAY-CAX	-2.43	119.81	122.15
3	C	902	GYB	CAR-OAQ-CAP	2.38	108.43	105.34
3	D	902	GYB	CAR-OAQ-CAP	2.34	108.38	105.34
2	C	901	NAG	C1-O5-C5	2.23	115.21	112.19
3	B	902	GYB	CAR-OAQ-CAP	2.19	108.19	105.34
3	A	903	GYB	CAH-NAI-CAJ	-2.19	118.43	120.69
3	C	902	GYB	CAV-CAY-CAX	-2.18	120.06	122.15
3	C	902	GYB	CAO-CAN-CAM	-2.17	115.74	118.88
3	D	902	GYB	OAS-CAJ-NAI	-2.13	118.58	122.79
2	B	901	NAG	C1-O5-C5	2.09	115.02	112.19
3	C	902	GYB	CAY-CAX-NBA	-2.04	120.15	122.36
3	D	902	GYB	CAE-CAF-CAP	-2.01	119.47	122.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	903	GYB	CAB

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	902	GYB	NAL-CAM-CAU-CAV
3	A	903	GYB	NAL-CAM-CAU-CAV
3	A	903	GYB	NAL-CAM-CAU-CAT
3	A	903	GYB	CAN-CAM-CAU-CAV
3	A	903	GYB	CAN-CAM-CAU-CAT
3	A	902	GYB	CAN-CAM-CAU-CAT
3	C	902	GYB	CAN-CAM-CAU-CAV
3	C	902	GYB	CAN-CAM-CAU-CAT
3	A	902	GYB	CAN-CAM-CAU-CAV
3	B	902	GYB	CAN-CAM-CAU-CAT
3	D	902	GYB	CAN-CAM-CAU-CAV
3	D	902	GYB	CAN-CAM-CAU-CAT

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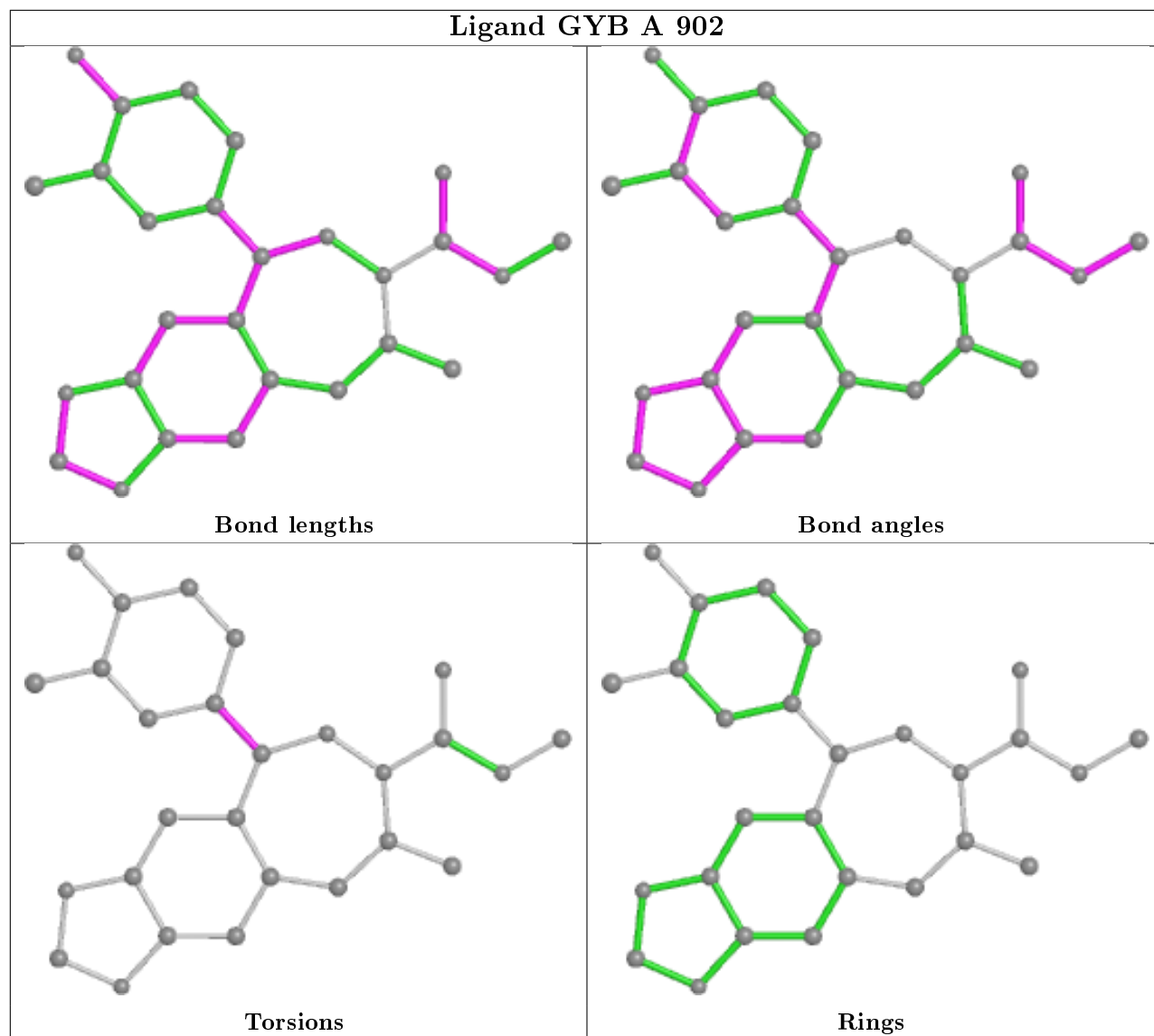
Mol	Chain	Res	Type	Atoms
3	B	902	GYB	NAL-CAM-CAU-CAT
3	B	902	GYB	CAN-CAM-CAU-CAV
3	A	902	GYB	NAL-CAM-CAU-CAV
3	D	902	GYB	NAL-CAM-CAU-CAV

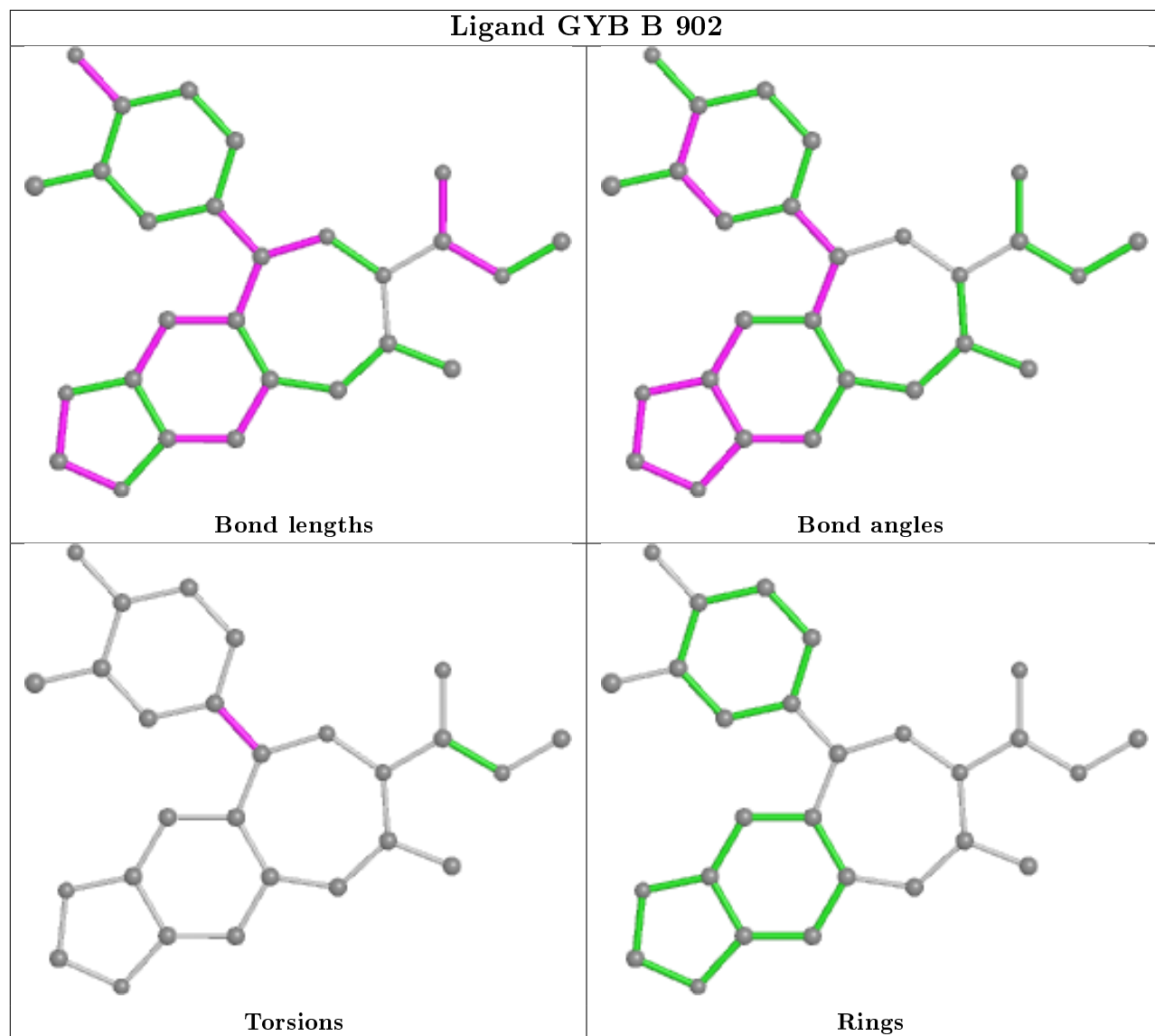
There are no ring outliers.

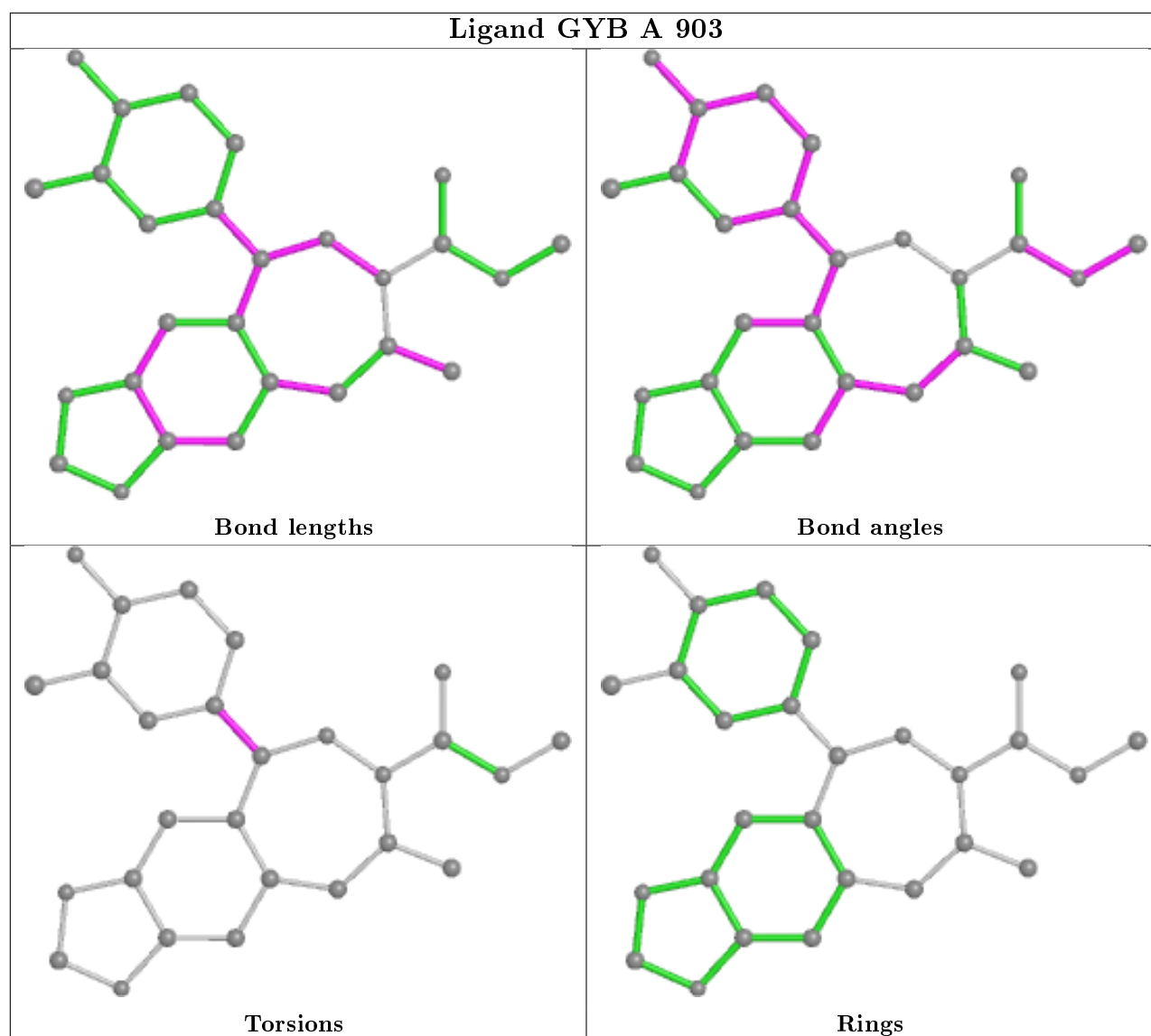
7 monomers are involved in 31 short contacts:

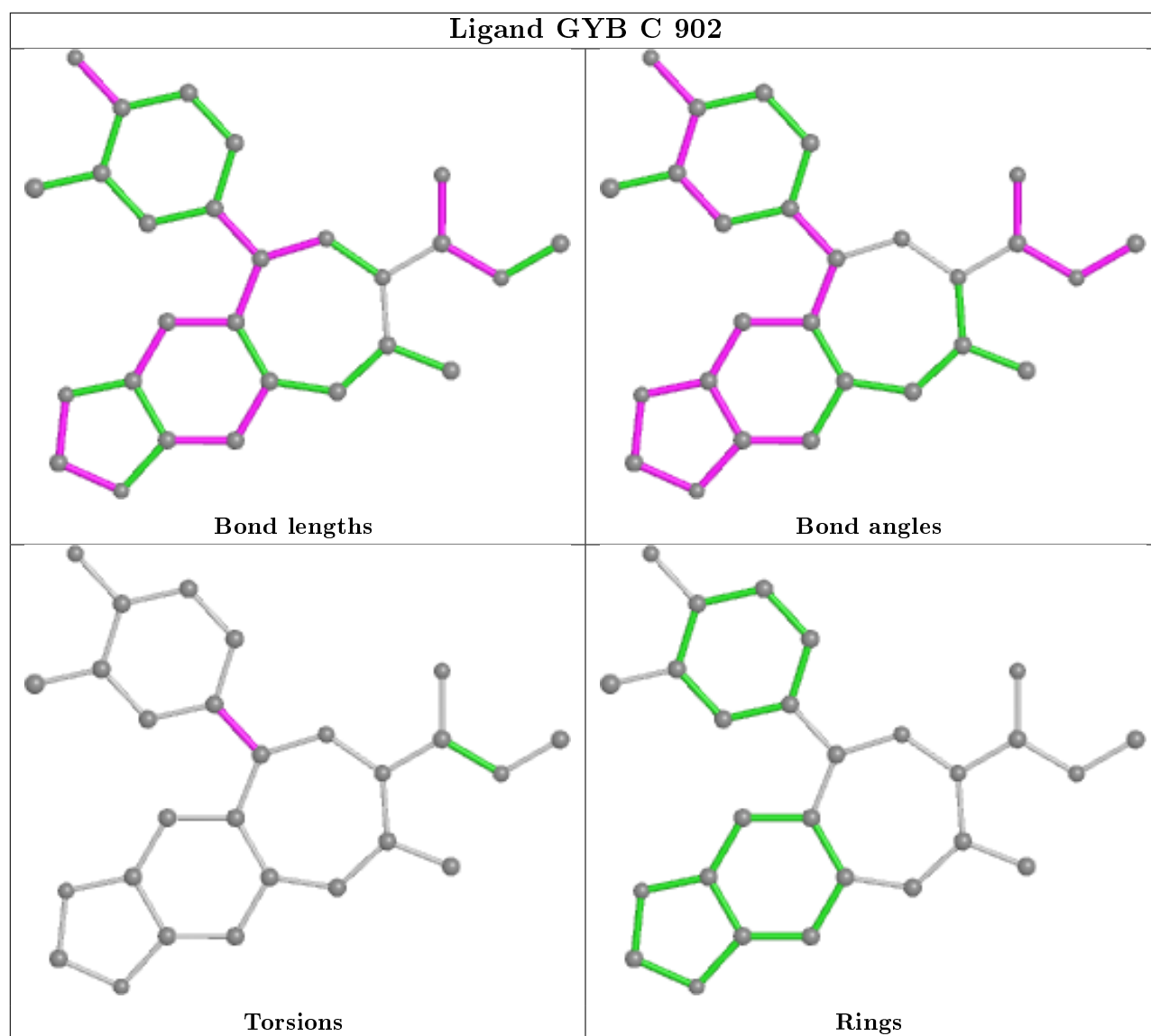
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GYB	2	0
3	B	902	GYB	3	0
2	C	901	NAG	1	0
2	D	901	NAG	1	0
3	A	903	GYB	20	0
3	C	902	GYB	1	0
3	D	902	GYB	3	0

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.

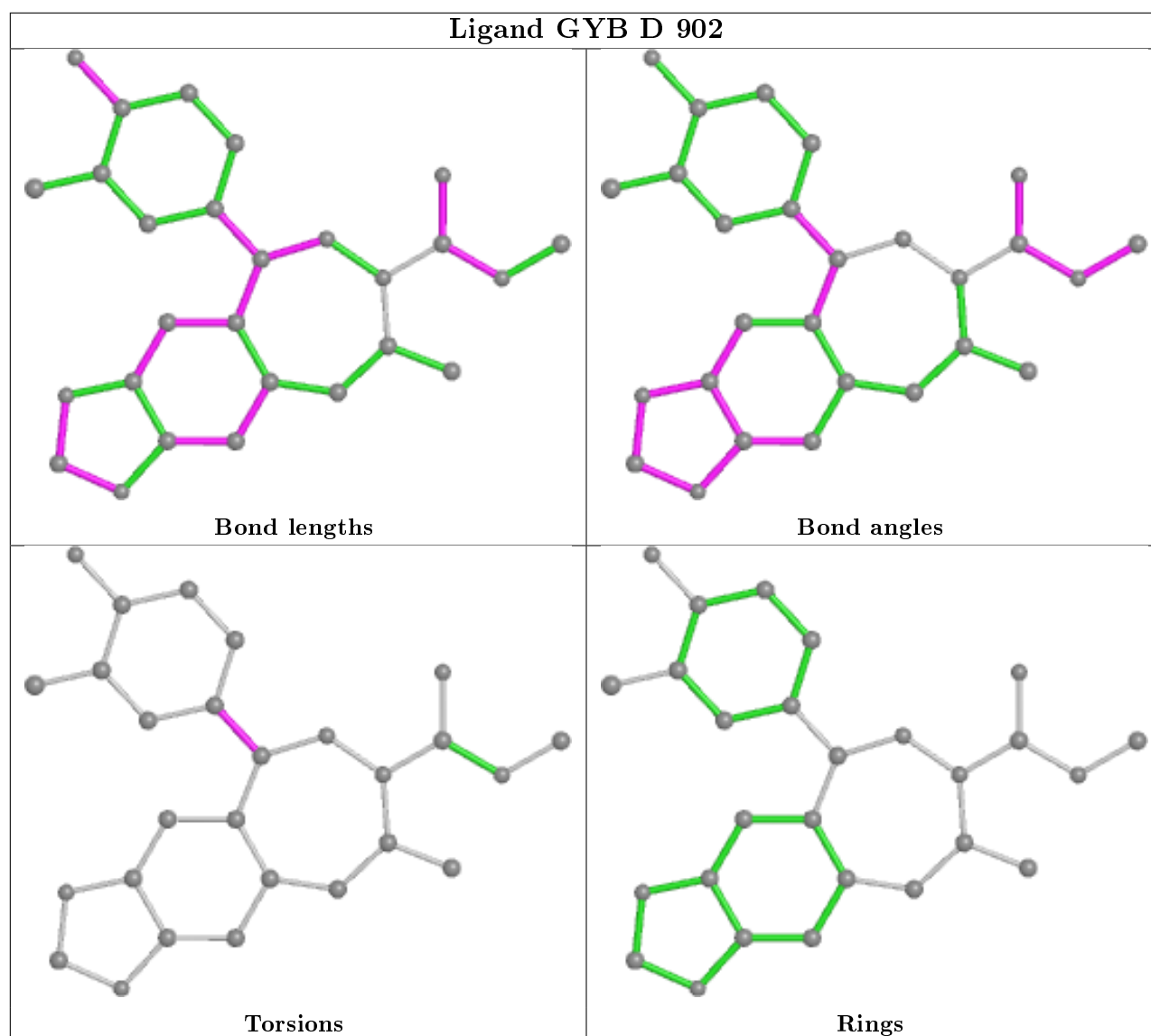












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

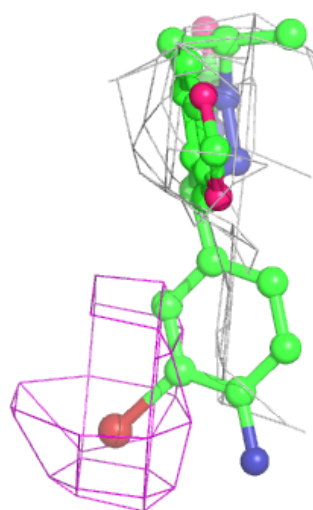
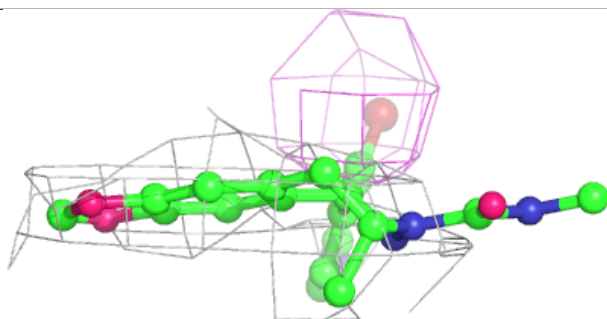
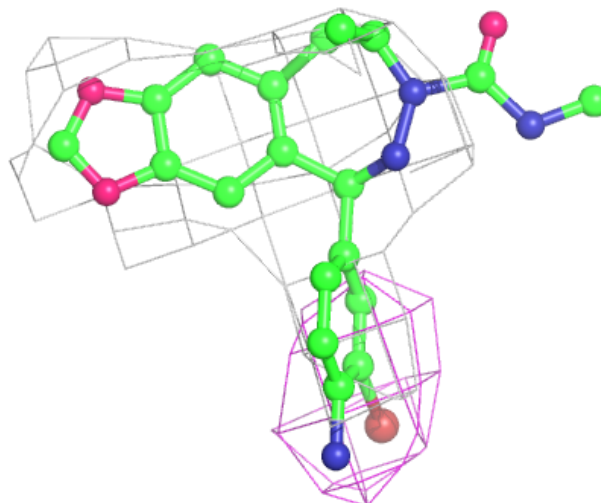
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

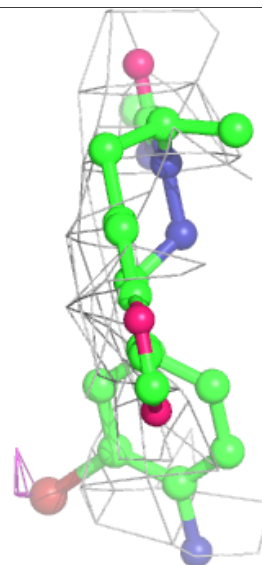
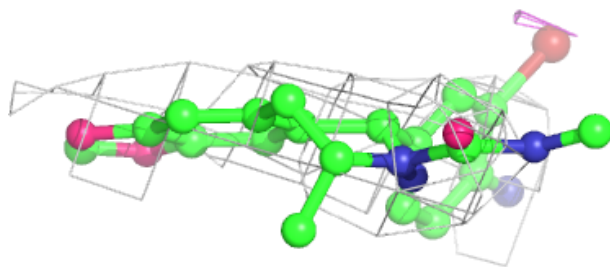
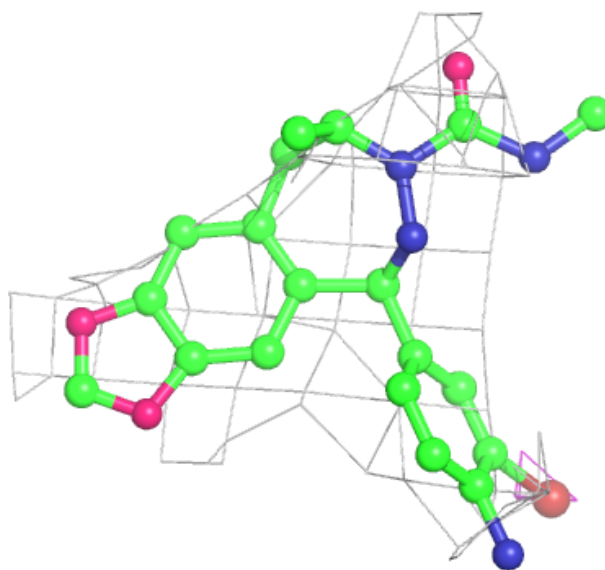
**Electron density around GYB A 902:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



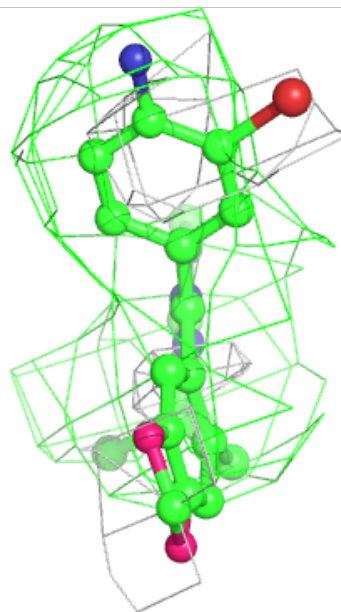
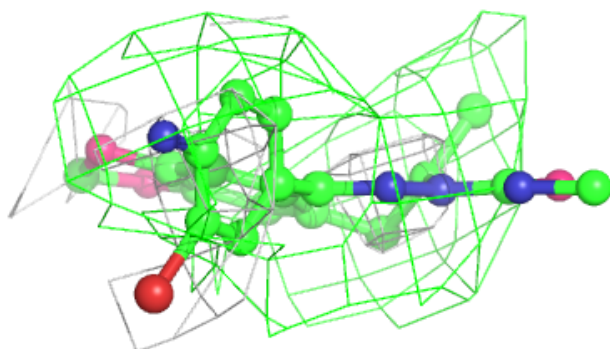
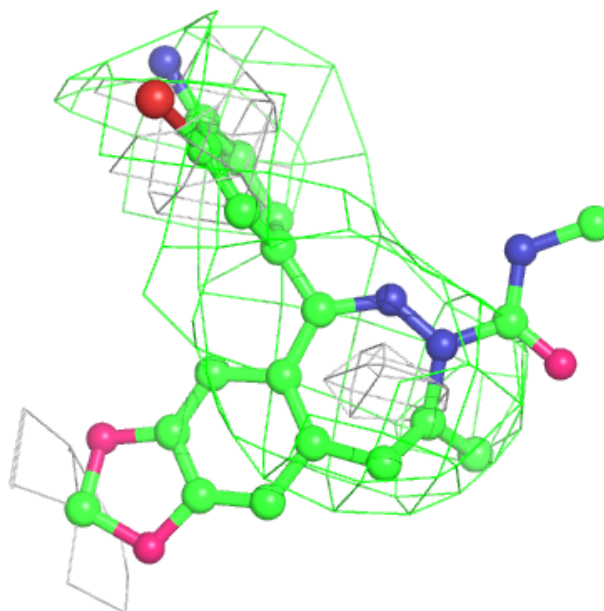
**Electron density around GYB B 902:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



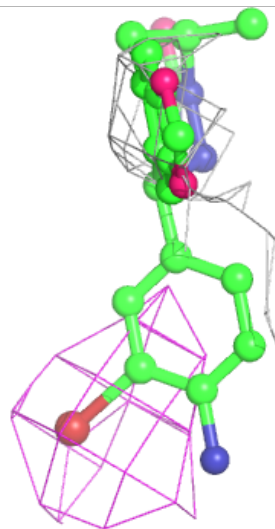
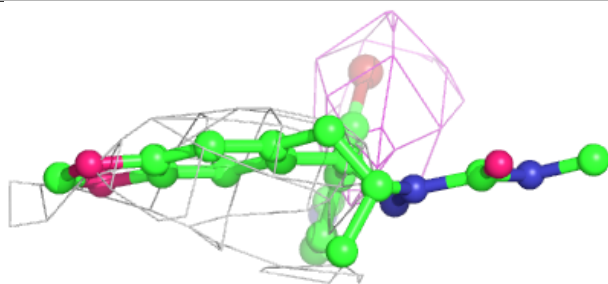
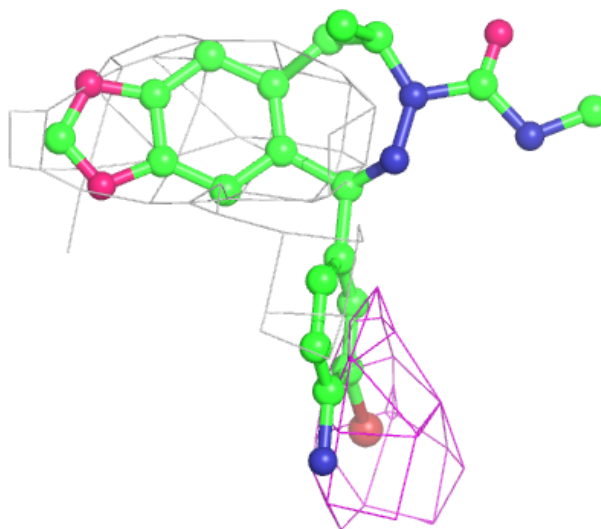
**Electron density around GYB A 903:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



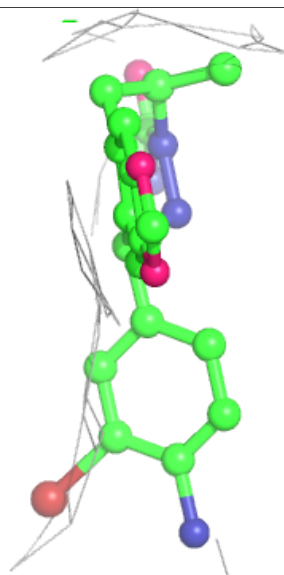
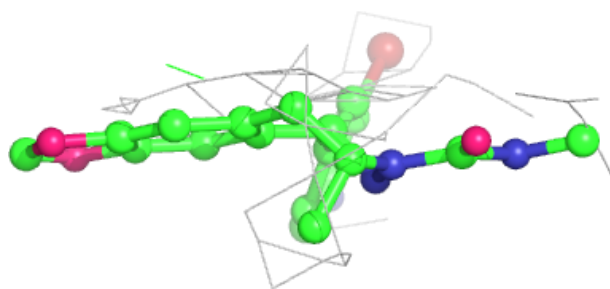
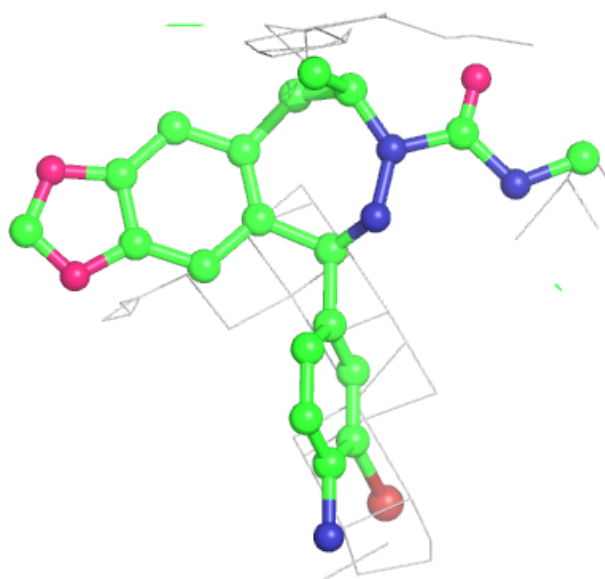
**Electron density around GYB C 902:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GYB D 902:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.