



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:23 PM UTC

PDB ID : 5L1G / pdb_00005l1g
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

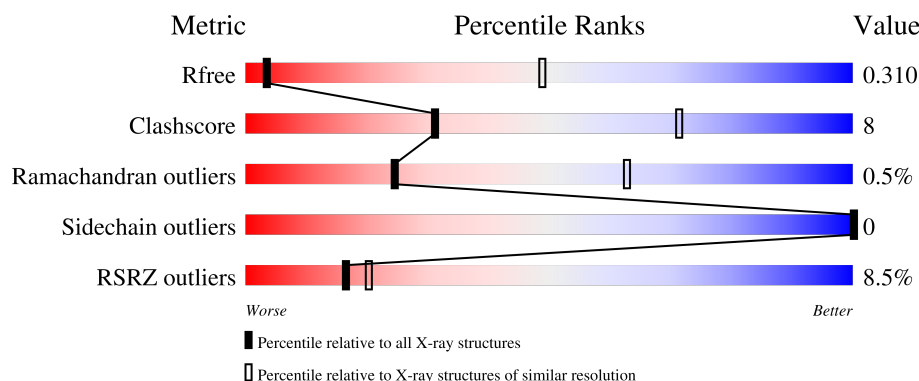
1 Overall quality at a glance

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}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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 of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	803	5% 80% 17% .
1	B	803	11% 76% 20% .
1	C	803	8% 76% 20% ..
1	D	803	8% 79% 18% .

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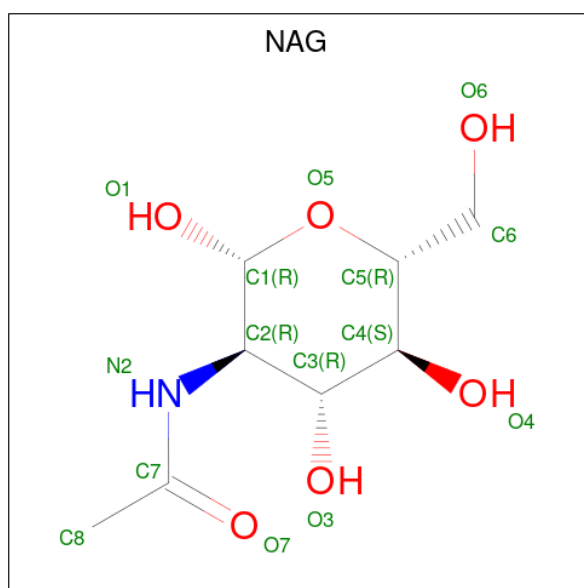
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
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B	564	ASP	-	linker	UNP P19491
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B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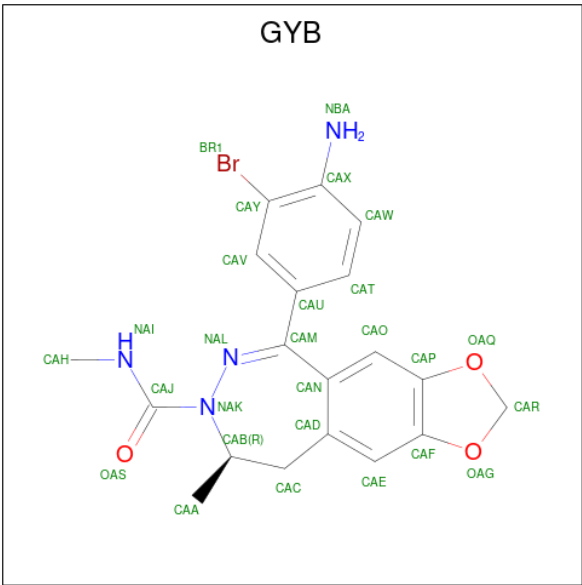
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491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

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: GYB) (formula: $C_{19}H_{19}BrN_4O_3$).

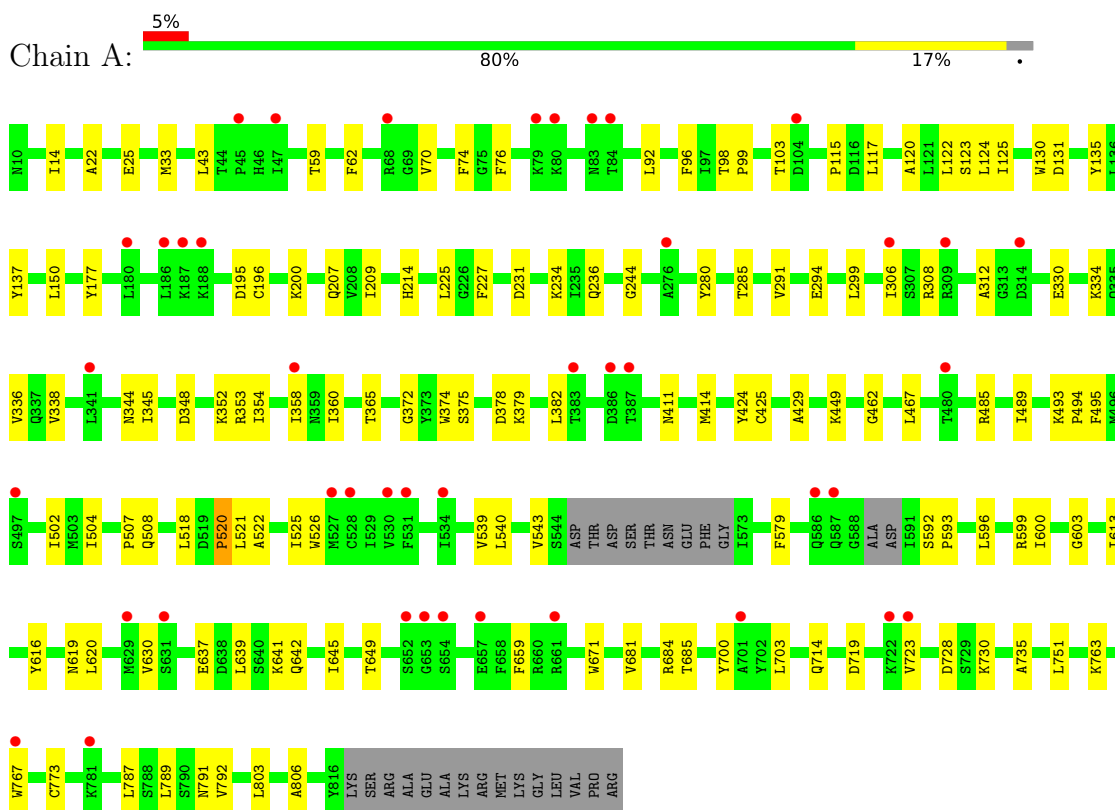


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	A	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	B	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	C	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		
3	D	1	Total	Br	C	N	O	0	0
			27	1	19	4	3		

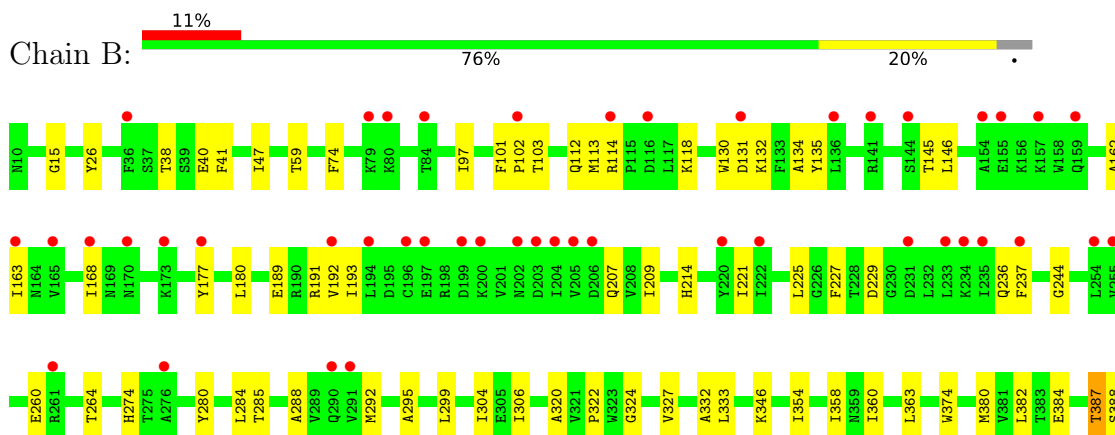
3 Residue-property plots [i](#)

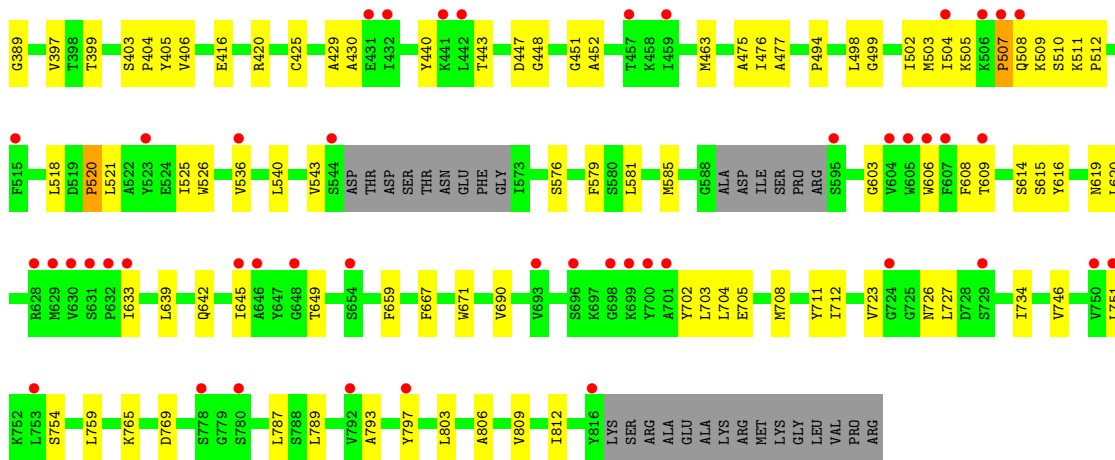
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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

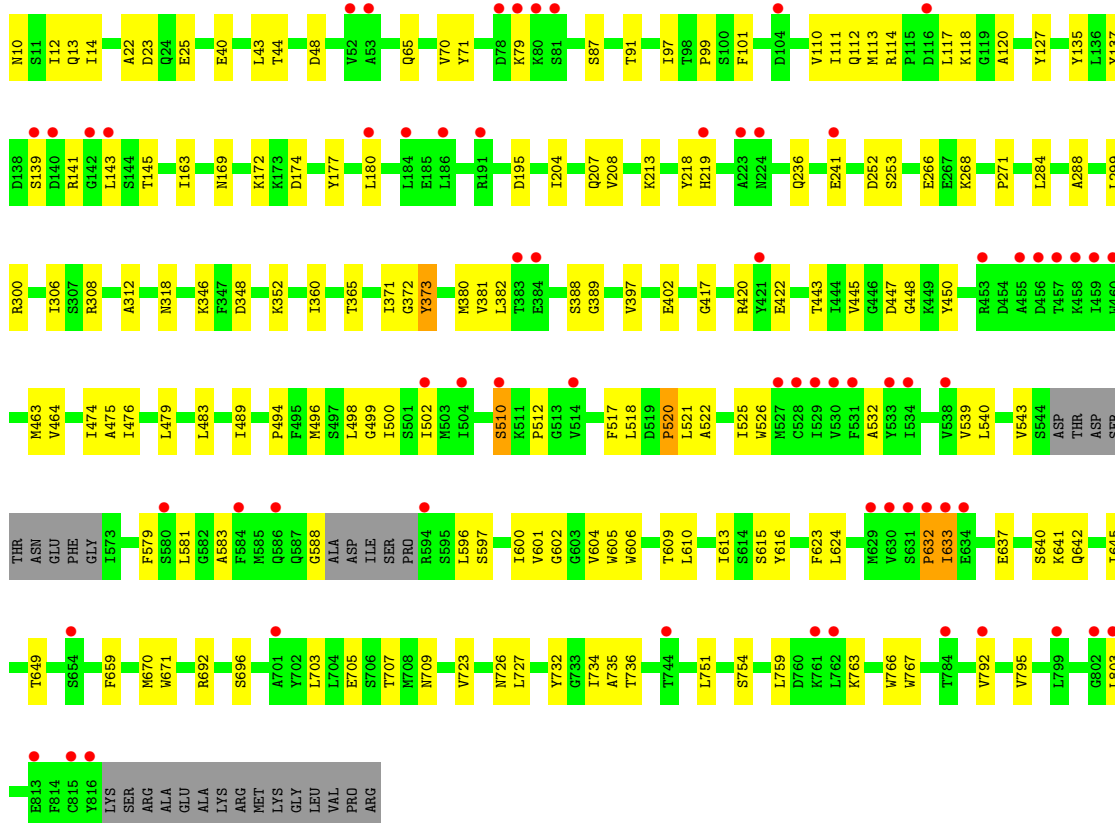
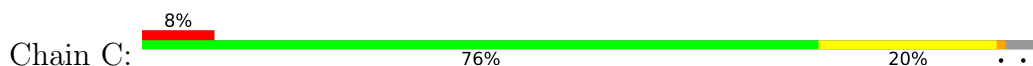


• Molecule 1: Glutamate receptor 2

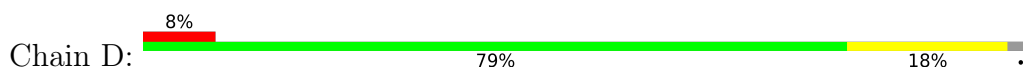


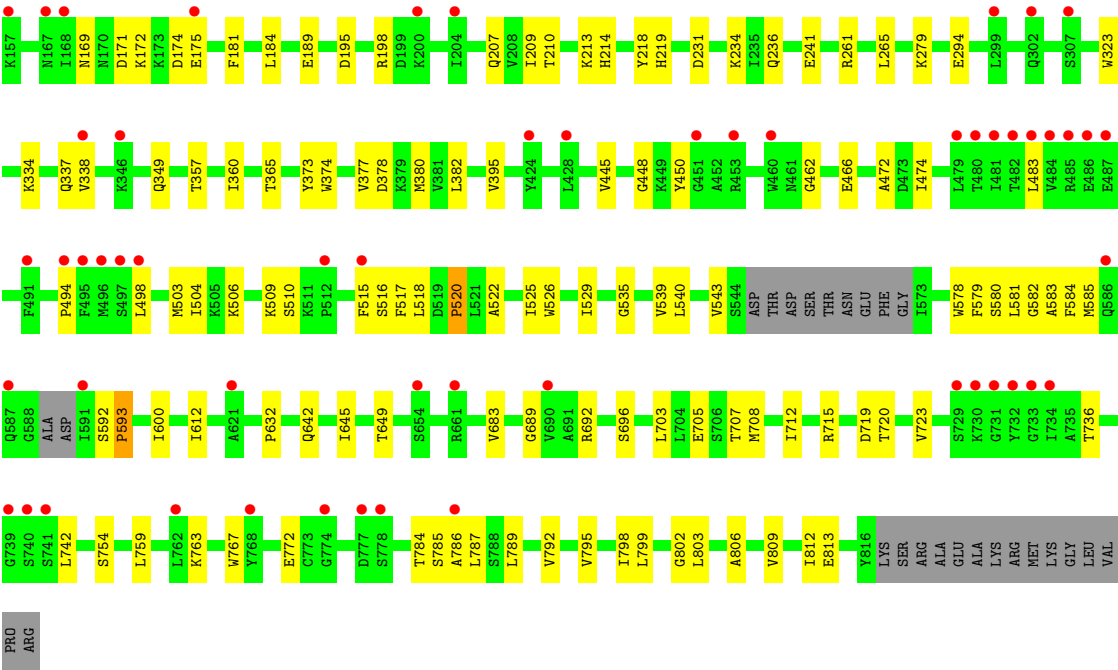


• Molecule 1: Glutamate receptor 2



• 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, α , β , γ	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) 99.1 (48.91-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.257 , 0.295 0.270 , 0.310	Depositor DCC
R_{free} test set	1866 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	206.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 197.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GYB, NAG

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	0.12	0/6110	0.31	0/8271
1	B	0.15	0/6112	0.37	1/8270 (0.0%)
1	C	0.13	0/6074	0.33	4/8225 (0.0%)
1	D	0.12	0/6090	0.32	0/8248
All	All	0.13	0/24386	0.33	5/33014 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	632	PRO	CA-C-N	6.66	133.69	121.70
1	C	632	PRO	C-N-CA	6.66	133.69	121.70
1	B	387	THR	N-CA-C	5.60	121.05	113.21
1	C	510	SER	CA-C-N	5.09	130.86	121.70
1	C	510	SER	C-N-CA	5.09	130.86	121.70

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	89	0
1	B	5990	0	5902	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5952	0	5823	131	0
1	D	5967	0	5830	103	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
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	390	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 (390) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:97:ILE:HD12	1:B:292:MET:HE3	1.79	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:450:TYR:HA	1:C:463:MET:HE2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:503:MET:HE1	1:B:690:VAL:HG22	1.85	0.57
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
3:A:903:GYB:CAR	1:C:613:ILE:HD13	2.33	0.57
1:C:299:LEU:HD13	1:C:306:ILE:HD13	1.87	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:C:402:GLU:OE1	1:C:450:TYR:OH	2.22	0.56
1:D:22:ALA:HB1	1:D:25:GLU:HB2	1.87	0.56
1:A:806:ALA:HA	1:D:600:ILE:HD11	1.85	0.56
1:B:168:ILE:HD12	1:B:168:ILE:O	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:C:127:TYR:HB2	1:C:380:MET:HE3	1.87	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:D:509:LYS:HA	1:D:510:SER:C	2.31	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:582:GLY:O	1:D:585:MET:HE3	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LYS:NZ	1:D:349:GLN:O	2.34	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:A:681:VAL:O	1:A:700:TYR:OH	2.24	0.54
1:B:15:GLY:O	1:B:74:PHE:N	2.38	0.54
1:A:33:MET:HE1	1:A:43:LEU:HB2	1.90	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
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:O	1:B:274:HIS:ND1	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:B:360:ILE:HD13	1:B:380:MET:HE2	1.91	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:620:LEU:HD21	3:B:902:GYB:BR1	2.65	0.51
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.91	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:D:360:ILE:HD13	1:D:380:MET:HE1	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:ARG:HD3	1:D:772:GLU:HG2	1.92	0.51
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.93	0.51
1:B:388:SER:HB3	1:B:389:GLY:HA3	1.92	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: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: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:B:463:MET:HE1	1:B:477:ALA:HB3	1.94	0.49
1:D:450:TYR:HA	1:D:462:GLY:HA3	1.94	0.49
1:B:260:GLU:O	1:B:264:THR:OG1	2.22	0.49
1:A:502:ILE:HD13	1:A:639:LEU:HD13	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:150:LEU:HD22	1:B:162:ALA:HB3	1.96	0.47
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.48	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:C:113:MET:HE3	1:C:288:ALA:HA	1.96	0.47
1:D:592:SER:N	1:D:593:PRO:HD3	2.29	0.47
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:692:ARG:O	1:C:696:SER:OG	2.26	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:C:588:GLY:C	1:C:602:GLY:HA2	2.41	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: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:330:GLU:OE2	1:A:334:LYS:NZ	2.42	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:LEU:O	1:D:522:ALA:HB2	2.16	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:236:GLN:NE2	1:A:365:THR:O	2.49	0.45
1:A:719:ASP:OD1	1:A:719:ASP:N	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
1:C:236:GLN:NE2	1:C:365:THR:O	2.45	0.45
1:D:131:ASP:OD1	1:D:131:ASP:N	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:498:LEU:HD22	1:C:732:TYR:CZ	2.53	0.44
1:C:499:GLY:HA3	1:C:726:ASN:HB3	1.98	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:A:599:ARG:C	1:B:581:LEU:CD2	2.91	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:C:521:LEU:HA	1:D:787:LEU:HD13	1.99	0.44
1:D:143:LEU:H	1:D:143:LEU:HD23	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:HE2	1:A:92:LEU:HD12	1.82	0.44
1:A:507:PRO:HA	1:A:508:GLN:CB	2.48	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:411:ASN:HB2	1:A:414:MET:HE2	2.00	0.43
1:C:397:VAL:O	1:C:443:THR:OG1	2.27	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:C:496:MET:HE2	1:C:763:LYS:HD3	2.00	0.43
1:D:518:LEU:O	1:D:526:TRP:NE1	2.51	0.43
1:C:22:ALA:HB1	1:C:25:GLU:HB2	2.00	0.43
1:C:163:ILE:HG21	1:C:180:LEU:HD13	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:A:619:ASN:CG	1:B:787:LEU:HD12	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:692:ARG:O	1:D:696:SER:OG	2.33	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:D:219:HIS:HA	1:D:241:GLU:O	2.20	0.41
1:A:600:ILE:HA	1:B:581:LEU:HD21	2.01	0.41
1:A:728:ASP:OD2	1:A:730:LYS:HE3	2.20	0.41
1:B:397:VAL:O	1:B:443:THR:OG1	2.36	0.41
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: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:C:380:MET:HE2	1:C:380:MET:HB2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:637:GLU:H	1:A:637:GLU:CD	2.28	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:C:600:ILE:HG22	1:D:581:LEU:HD13	2.03	0.41
1:D:515:PHE:HD2	1:D:515:PHE:HA	1.77	0.41
1:D:535:GLY:O	1:D:539:VAL:HG23	2.21	0.41
1:D:715:ARG:HD3	1:D:715:ARG:HA	1.91	0.41
1:A:348:ASP:HB3	1:A:354:ILE:HG21	2.03	0.41
1:B:236:GLN:HG3	1:B:363:LEU:HD11	2.03	0.41
1:C:502:ILE:O	1:C:709:ASN:ND2	2.52	0.41
1:C:583:ALA:HB1	1:C:588:GLY:C	2.46	0.41
1:C:751:LEU:HD23	1:C:751:LEU:HA	1.86	0.41
1:D:96:PHE:CE2	1:D:98:THR:HB	2.56	0.41
1:D:377:VAL:HG13	1:D:378:ASP:N	2.32	0.41
1:A:76:PHE:CE2	1:A:99:PRO:HG2	2.56	0.41
1:B:463:MET:HE3	1:B:475:ALA:HB1	2.02	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:C:422:GLU:HB2	1:C:766:TRP:HH2	1.87	0.40
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.03	0.40
1:A:122:LEU:HD23	1:A:122:LEU:HA	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

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 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%)	24	63
1	B	767/803 (96%)	708 (92%)	57 (7%)	2 (0%)	36	71
1	C	768/803 (96%)	715 (93%)	48 (6%)	5 (1%)	18	55
1	D	771/803 (96%)	720 (93%)	48 (6%)	3 (0%)	30	67
All	All	3077/3212 (96%)	2858 (93%)	205 (7%)	14 (0%)	24	63

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	510	SER
1	A	596	LEU
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%)	627 (100%)	0	100	100
1	B	634/683 (93%)	634 (100%)	0	100	100
1	C	619/683 (91%)	619 (100%)	0	100	100
1	D	620/683 (91%)	620 (100%)	0	100	100
All	All	2500/2732 (92%)	2500 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	83	ASN
1	A	290	GLN
1	A	714	GLN
1	A	726	ASN
1	B	619	ASN
1	B	726	ASN
1	B	791	ASN
1	C	24	GLN
1	C	49	ASN
1	C	93	HIS
1	C	207	GLN
1	C	274	HIS
1	C	337	GLN
1	C	344	ASN
1	D	764	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	902	-	28,30,30	4.40	12 (42%)	32,44,44	2.14	8 (25%)
2	NAG	D	901	1	14,14,15	0.54	0	17,19,21	0.62	0
3	GYB	A	902	-	28,30,30	4.42	13 (46%)	32,44,44	2.32	12 (37%)
3	GYB	C	902	-	28,30,30	4.29	13 (46%)	32,44,44	2.69	13 (40%)
2	NAG	A	901	1	14,14,15	0.80	1 (7%)	17,19,21	0.67	0
2	NAG	B	901	1	14,14,15	0.37	0	17,19,21	0.62	1 (5%)
2	NAG	C	901	1	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
3	GYB	A	903	-	28,30,30	2.47	9 (32%)	32,44,44	2.29	9 (28%)
3	GYB	D	902	-	28,30,30	4.34	12 (42%)	32,44,44	2.46	12 (37%)

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

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GYB	CAM-NAL	14.89	1.46	1.30
3	D	902	GYB	CAM-NAL	14.52	1.46	1.30
3	C	902	GYB	CAM-NAL	14.51	1.46	1.30
3	B	902	GYB	CAM-NAL	14.27	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
3	C	902	GYB	CAJ-NAI	9.98	1.47	1.34
3	A	903	GYB	CAU-CAM	-6.18	1.40	1.49
3	B	902	GYB	CAN-CAM	5.64	1.57	1.49
3	A	903	GYB	CAN-CAM	-5.53	1.41	1.49
3	A	902	GYB	CAN-CAM	5.37	1.56	1.49
3	A	903	GYB	CAM-NAL	5.34	1.36	1.30
3	C	902	GYB	CAN-CAM	5.32	1.56	1.49
3	D	902	GYB	CAN-CAM	5.31	1.56	1.49
3	D	902	GYB	OAG-CAR	-5.13	1.33	1.43
3	C	902	GYB	OAG-CAR	-5.12	1.33	1.43
3	A	902	GYB	OAG-CAR	-5.12	1.33	1.43
3	C	902	GYB	OAQ-CAR	-5.11	1.33	1.43
3	D	902	GYB	OAQ-CAR	-5.08	1.33	1.43
3	A	902	GYB	OAQ-CAR	-5.04	1.33	1.43
3	B	902	GYB	OAG-CAR	-5.03	1.33	1.43
3	B	902	GYB	OAQ-CAR	-5.01	1.33	1.43
3	B	902	GYB	CAE-CAD	4.71	1.46	1.39
3	D	902	GYB	OAS-CAJ	-4.64	1.14	1.23
3	B	902	GYB	OAS-CAJ	-4.61	1.14	1.23
3	A	902	GYB	OAS-CAJ	-4.58	1.14	1.23
3	C	902	GYB	OAS-CAJ	-4.55	1.15	1.23
3	A	903	GYB	CAA-CAB	4.37	1.66	1.52
3	A	902	GYB	CAE-CAD	4.32	1.46	1.39
3	C	902	GYB	CAE-CAD	4.26	1.46	1.39
3	D	902	GYB	CAE-CAD	4.24	1.46	1.39
3	A	902	GYB	CAU-CAM	4.13	1.55	1.49
3	D	902	GYB	CAO-CAN	3.96	1.46	1.39
3	B	902	GYB	CAO-CAN	3.92	1.46	1.39
3	C	902	GYB	CAU-CAM	3.92	1.55	1.49
3	D	902	GYB	CAU-CAM	3.84	1.55	1.49
3	A	902	GYB	CAO-CAP	3.80	1.45	1.38
3	B	902	GYB	CAU-CAM	3.80	1.54	1.49
3	B	902	GYB	CAO-CAP	3.79	1.45	1.38
3	A	902	GYB	CAO-CAN	3.78	1.45	1.39
3	B	902	GYB	CAE-CAF	3.72	1.45	1.38
3	C	902	GYB	CAO-CAP	3.70	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	GYB	CAO-CAN	3.62	1.45	1.39
3	D	902	GYB	CAO-CAP	3.61	1.45	1.38
3	C	902	GYB	CAX-NBA	3.54	1.49	1.38
3	A	902	GYB	CAX-NBA	3.54	1.49	1.38
3	D	902	GYB	CAX-NBA	3.53	1.49	1.38
3	D	902	GYB	CAE-CAF	3.50	1.44	1.38
3	B	902	GYB	CAX-NBA	3.43	1.49	1.38
3	A	903	GYB	NAK-NAL	-3.33	1.28	1.38
3	A	902	GYB	CAE-CAF	3.31	1.44	1.38
3	C	902	GYB	CAE-CAF	3.18	1.44	1.38
3	A	903	GYB	CAC-CAD	-3.02	1.44	1.51
3	A	903	GYB	CAO-CAP	-2.96	1.33	1.38
3	A	903	GYB	CAE-CAF	-2.84	1.34	1.38
2	A	901	NAG	C1-C2	2.79	1.56	1.52
3	A	902	GYB	CAT-CAW	2.09	1.42	1.38
3	C	902	GYB	CAT-CAW	2.08	1.42	1.38
3	A	903	GYB	CAP-CAF	-2.05	1.34	1.39

All (56) 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	CAD-CAC-CAB	-6.21	100.17	115.48
3	A	903	GYB	CAT-CAU-CAM	-6.02	113.19	120.64
3	D	902	GYB	CAN-CAM-CAU	-5.89	111.35	118.12
3	D	902	GYB	CAH-NAI-CAJ	-5.83	114.69	120.69
3	B	902	GYB	OAG-CAF-CAE	5.63	135.35	127.86
3	D	902	GYB	OAG-CAF-CAE	5.58	135.28	127.86
3	A	902	GYB	OAG-CAF-CAE	5.15	134.70	127.86
3	C	902	GYB	OAG-CAF-CAE	5.08	134.61	127.86
3	C	902	GYB	CAN-CAM-CAU	-5.07	112.28	118.12
3	A	903	GYB	CAV-CAU-CAM	4.96	128.20	120.34
3	A	902	GYB	CAN-CAM-CAU	-4.91	112.47	118.12
3	A	902	GYB	CAH-NAI-CAJ	-4.34	116.23	120.69
3	D	902	GYB	OAQ-CAP-CAO	4.12	133.34	127.86
3	B	902	GYB	OAQ-CAP-CAO	4.06	133.26	127.86
3	A	902	GYB	OAQ-CAP-CAO	4.02	133.20	127.86
3	B	902	GYB	OAG-CAF-CAP	-3.93	105.02	109.79
3	D	902	GYB	OAG-CAF-CAP	-3.75	105.25	109.79
3	B	902	GYB	CAN-CAM-CAU	-3.69	113.87	118.12
3	C	902	GYB	OAQ-CAP-CAO	3.66	132.73	127.86
3	C	902	GYB	OAG-CAF-CAP	-3.52	105.53	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	GYB	OAG-CAF-CAP	-3.44	105.63	109.79
3	B	902	GYB	CAV-CAY-CAX	-3.40	119.13	122.56
3	A	903	GYB	CAD-CAN-CAM	3.21	126.82	121.45
3	A	903	GYB	CAO-CAN-CAM	-3.15	114.27	118.87
3	B	902	GYB	CAR-OAG-CAF	3.12	109.50	105.32
3	D	902	GYB	CAR-OAG-CAF	3.00	109.34	105.32
3	A	903	GYB	CAY-CAX-NBA	-2.89	119.16	122.38
3	A	902	GYB	CAR-OAG-CAF	2.82	109.09	105.32
3	A	902	GYB	OAQ-CAP-CAF	-2.81	106.38	109.79
3	A	902	GYB	CAV-CAY-CAX	-2.72	119.81	122.56
3	C	902	GYB	OAS-CAJ-NAI	-2.72	117.42	122.79
3	C	902	GYB	CAR-OAG-CAF	2.69	108.92	105.32
3	C	902	GYB	OAQ-CAP-CAF	-2.66	106.57	109.79
3	A	903	GYB	CAT-CAW-CAX	-2.66	118.75	121.42
3	A	902	GYB	OAS-CAJ-NAI	-2.62	117.62	122.79
3	A	903	GYB	CAC-CAD-CAE	-2.61	111.52	118.52
3	A	902	GYB	CAR-OAQ-CAP	2.50	108.66	105.32
3	C	902	GYB	CAV-CAY-CAX	-2.48	120.06	122.56
3	D	902	GYB	OAQ-CAP-CAF	-2.43	106.84	109.79
3	C	902	GYB	CAR-OAQ-CAP	2.33	108.43	105.32
3	B	902	GYB	OAQ-CAP-CAF	-2.31	107.00	109.79
3	D	902	GYB	CAR-OAQ-CAP	2.28	108.38	105.32
2	C	901	NAG	C1-O5-C5	2.25	115.21	112.19
3	A	903	GYB	CAH-NAI-CAJ	-2.19	118.43	120.69
3	D	902	GYB	CAV-CAY-CAX	-2.18	120.36	122.56
3	C	902	GYB	CAO-CAN-CAM	-2.15	115.74	118.87
3	B	902	GYB	CAR-OAQ-CAP	2.14	108.19	105.32
3	D	902	GYB	OAS-CAJ-NAI	-2.13	118.58	122.79
2	B	901	NAG	C1-O5-C5	2.12	115.02	112.19
3	A	902	GYB	BR1-CAY-CAX	2.10	120.85	118.75
3	C	902	GYB	CAD-CAN-CAM	2.06	124.91	121.45
3	D	902	GYB	CAD-CAN-CAM	2.05	124.89	121.45
3	D	902	GYB	CAE-CAF-CAP	-2.04	119.47	122.03
3	A	902	GYB	CAD-CAN-CAM	2.04	124.86	121.45
3	C	902	GYB	CAT-CAU-CAM	2.02	123.14	120.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	903	GYB	CAB

All (16) torsion outliers are listed below:

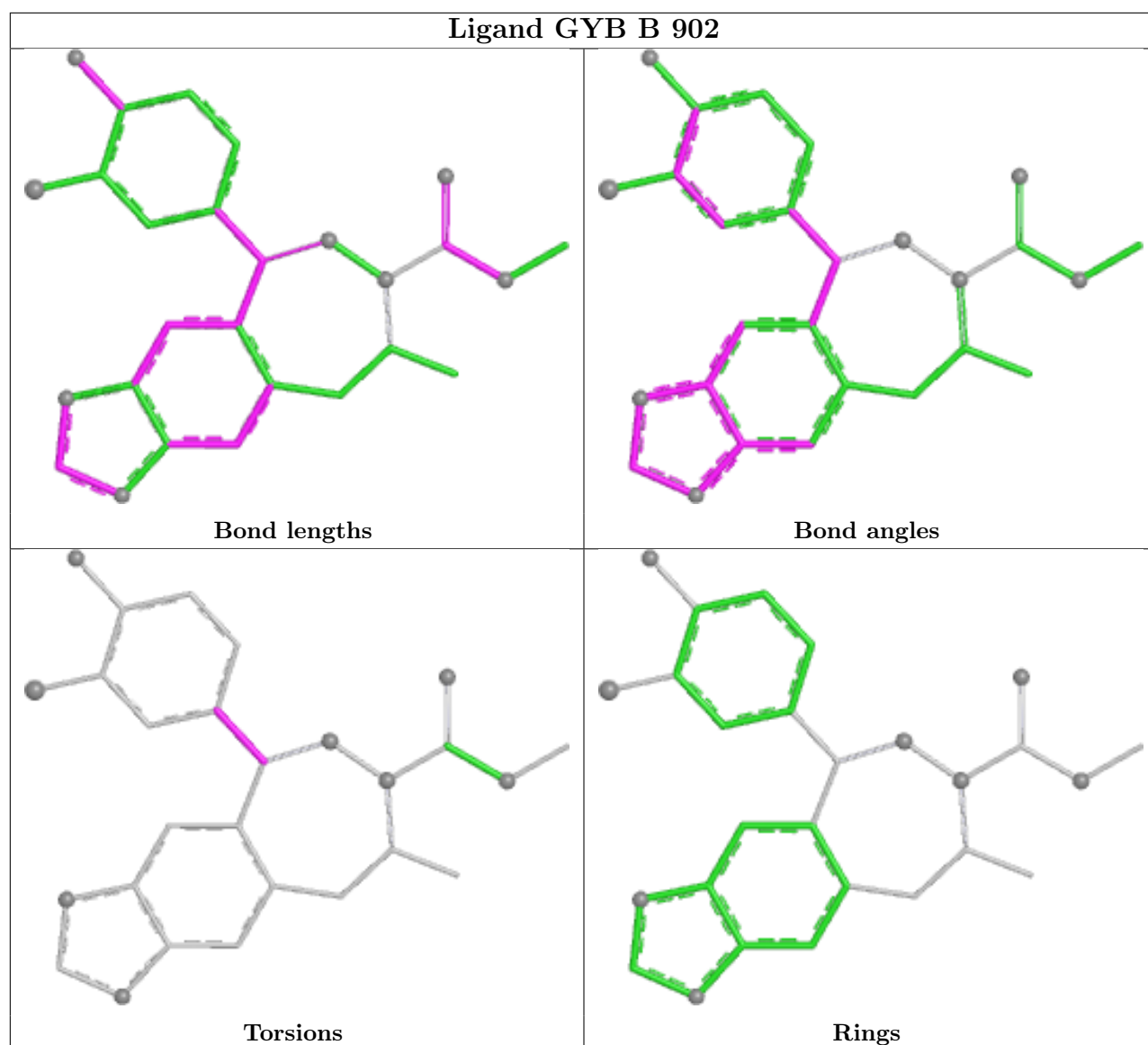
Mol	Chain	Res	Type	Atoms
3	A	903	GYB	NAL-CAM-CAU-CAV
3	A	903	GYB	NAL-CAM-CAU-CAT
3	A	903	GYB	CAN-CAM-CAU-CAV
3	A	903	GYB	CAN-CAM-CAU-CAT
3	B	902	GYB	NAL-CAM-CAU-CAV
3	A	902	GYB	CAN-CAM-CAU-CAT
3	C	902	GYB	CAN-CAM-CAU-CAV
3	C	902	GYB	CAN-CAM-CAU-CAT
3	A	902	GYB	CAN-CAM-CAU-CAV
3	B	902	GYB	CAN-CAM-CAU-CAT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

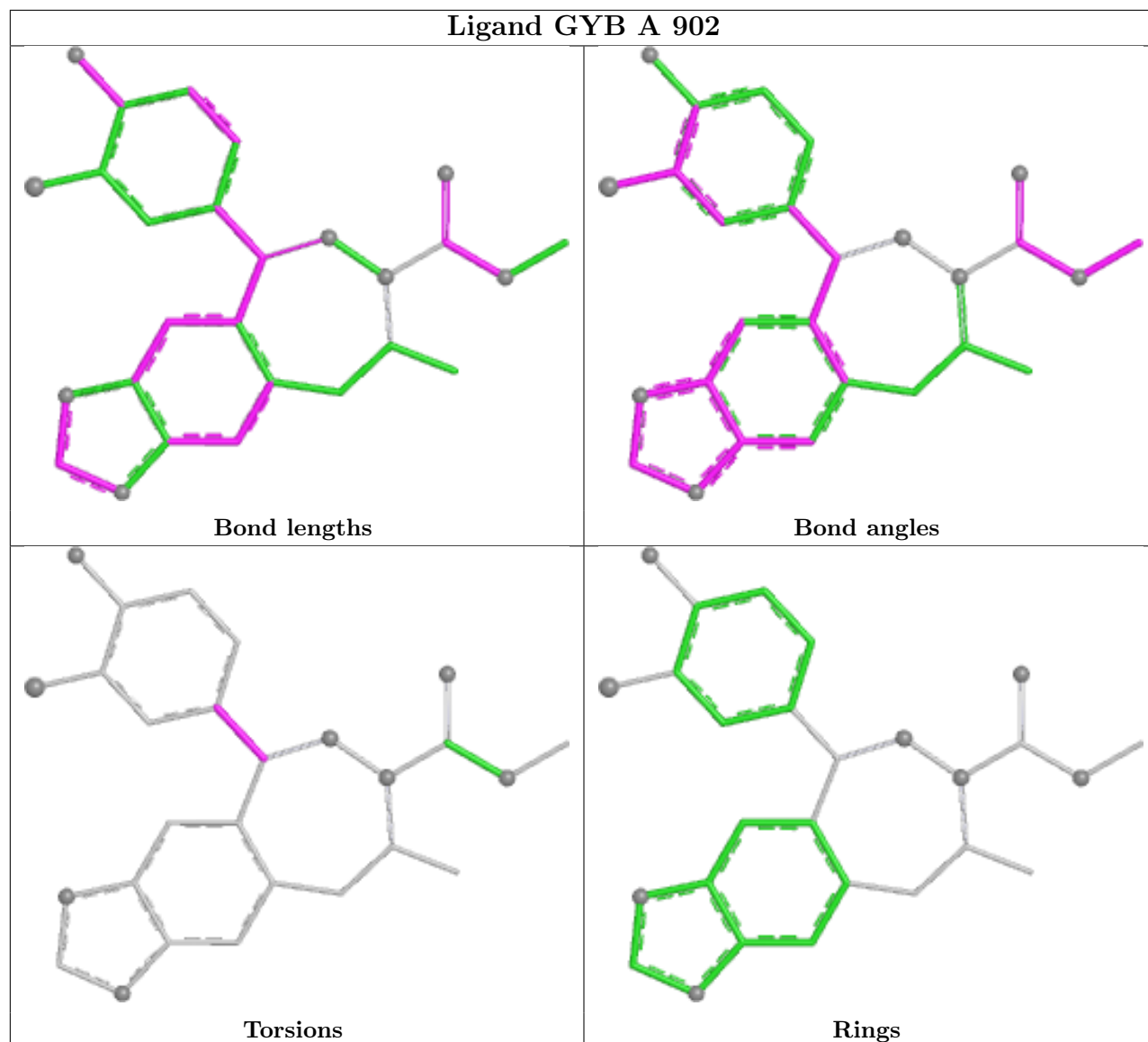
There are no ring outliers.

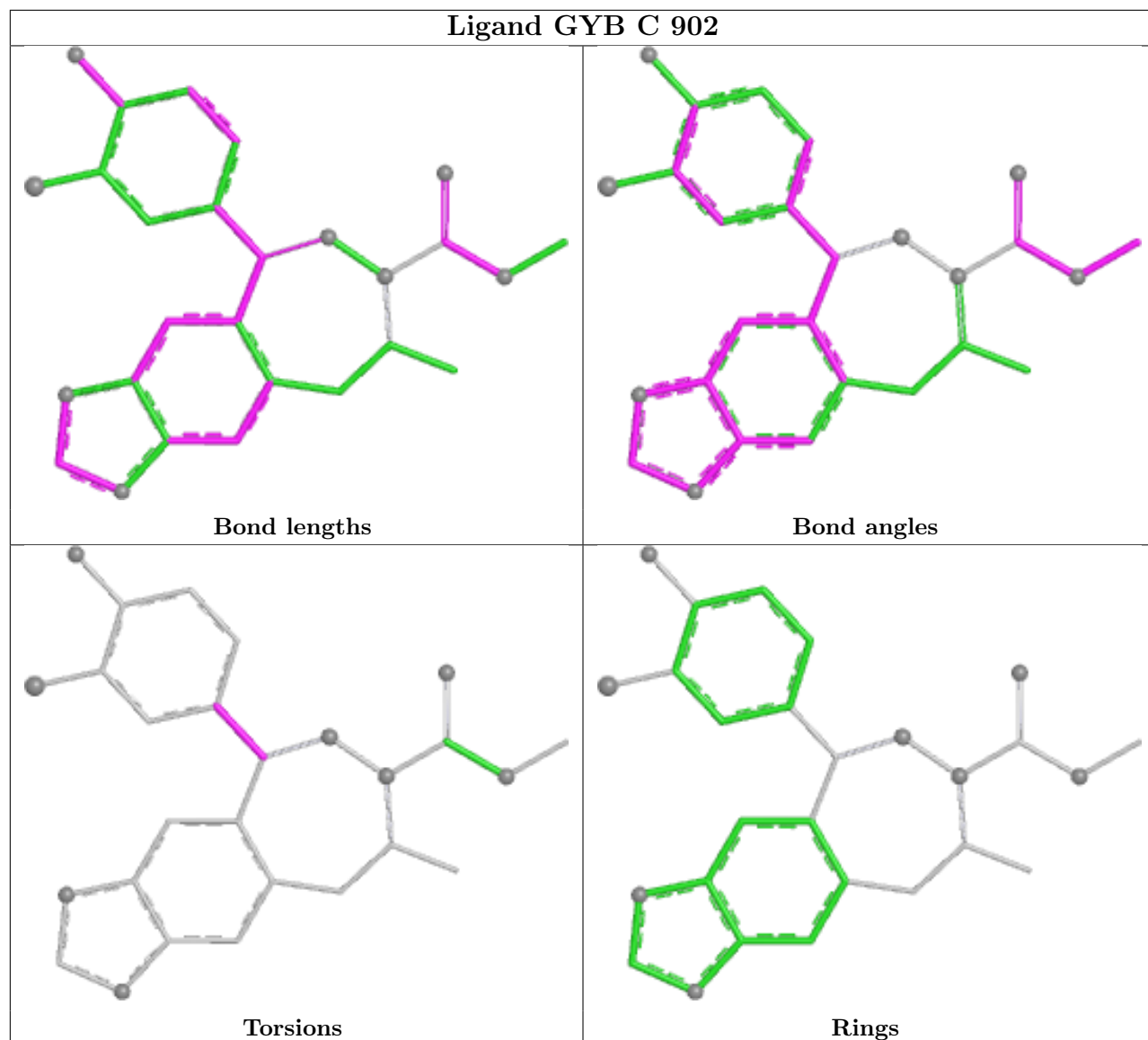
7 monomers are involved in 31 short contacts:

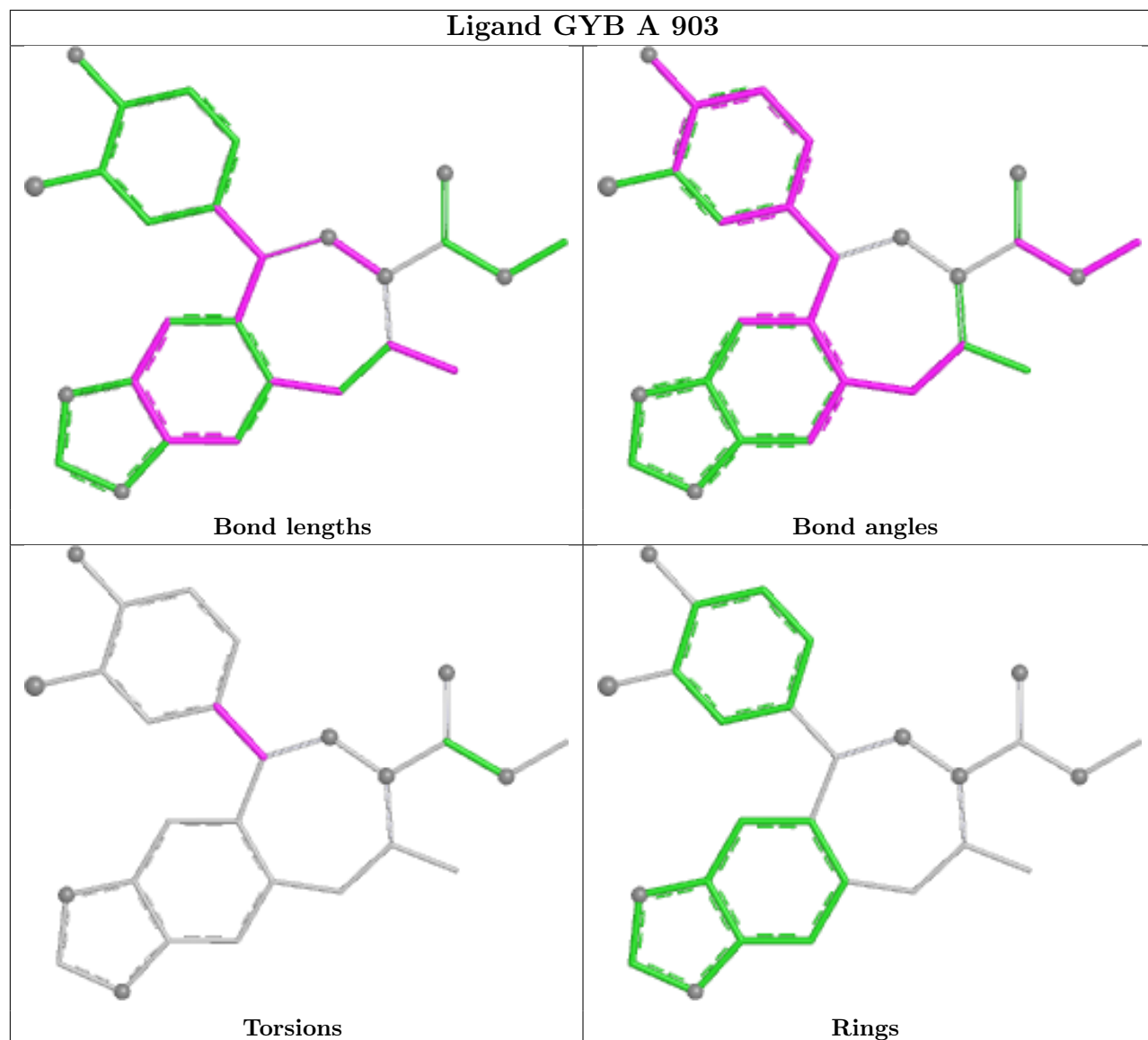
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	GYB	3	0
2	D	901	NAG	1	0
3	A	902	GYB	2	0
3	C	902	GYB	1	0
2	C	901	NAG	1	0
3	A	903	GYB	20	0
3	D	902	GYB	3	0

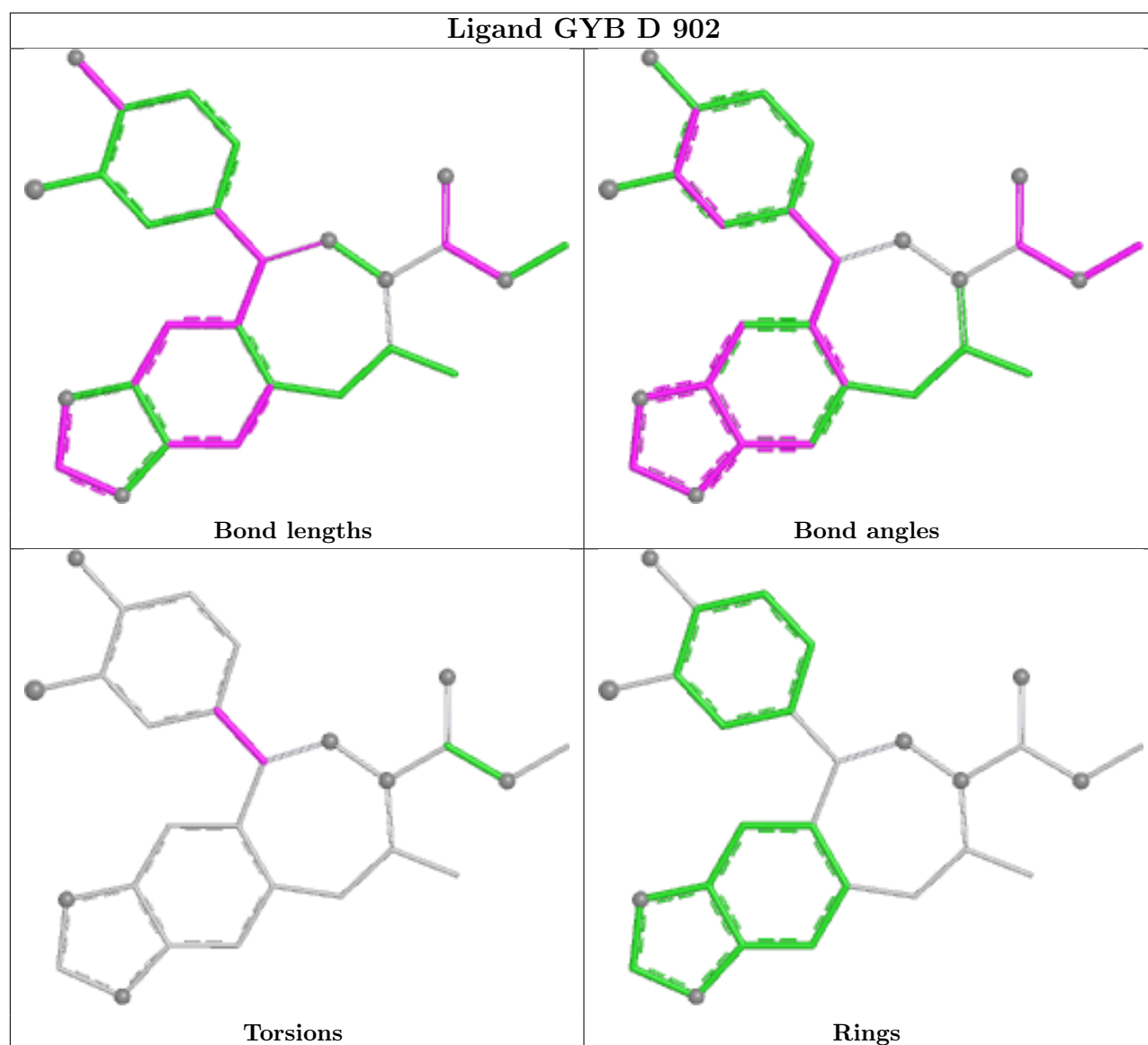
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	777/803 (96%)	0.36	42 (5%)	31 30	153, 228, 329, 363	0
1	B	773/803 (96%)	0.59	91 (11%)	9 13	172, 212, 312, 365	0
1	C	774/803 (96%)	0.50	65 (8%)	17 21	146, 255, 314, 341	0
1	D	777/803 (96%)	0.54	66 (8%)	16 20	202, 266, 336, 372	0
All	All	3101/3212 (96%)	0.50	264 (8%)	16 20	146, 242, 325, 372	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	732	TYR	9.5
1	C	534	ILE	8.8
1	D	731	GLY	8.2
1	D	481	ILE	8.0
1	D	157	LYS	7.8
1	A	186	LEU	7.4
1	D	494	PRO	7.3
1	B	698	GLY	7.0
1	B	165	VAL	6.9
1	B	157	LYS	6.9
1	C	530	VAL	6.8
1	C	632	PRO	6.8
1	D	484	VAL	6.7
1	C	531	PHE	6.4
1	D	480	THR	6.4
1	C	633	ILE	6.3
1	B	604	VAL	6.3
1	B	631	SER	6.2
1	B	630	VAL	6.2
1	D	79	LYS	6.1
1	C	457	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	79	LYS	6.0
1	A	527	MET	5.9
1	C	458	LYS	5.8
1	B	196	CYS	5.8
1	C	186	LEU	5.7
1	D	175	GLU	5.6
1	D	485	ARG	5.6
1	B	203	ASP	5.6
1	C	527	MET	5.6
1	B	200	LYS	5.6
1	D	139	SER	5.4
1	D	495	PHE	5.3
1	D	453	ARG	5.2
1	D	733	GLY	5.2
1	A	309	ARG	5.2
1	C	459	ILE	5.2
1	D	496	MET	5.1
1	D	497	SER	4.9
1	A	387	THR	4.9
1	B	254	LEU	4.9
1	D	479	LEU	4.9
1	C	78	ASP	4.8
1	D	424	TYR	4.7
1	A	383	THR	4.7
1	B	629	MET	4.7
1	B	234	LYS	4.6
1	D	482	THR	4.6
1	B	170	ASN	4.6
1	C	538	VAL	4.6
1	B	204	ILE	4.6
1	C	586	GLN	4.5
1	D	302	GLN	4.5
1	D	428	LEU	4.4
1	B	699	LYS	4.4
1	B	197	GLU	4.3
1	C	761	LYS	4.3
1	C	143	LEU	4.3
1	B	544	SER	4.3
1	D	483	LEU	4.3
1	D	167	ASN	4.2
1	D	586	GLN	4.2
1	B	780	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	140	ASP	4.2
1	A	654	SER	4.1
1	B	194	LEU	4.0
1	C	80	LYS	4.0
1	D	143	LEU	4.0
1	B	750	VAL	4.0
1	B	141	ARG	3.9
1	D	140	ASP	3.9
1	D	587	GLN	3.8
1	A	47	ILE	3.8
1	B	607	PHE	3.7
1	A	306	ILE	3.7
1	D	168	ILE	3.7
1	B	205	VAL	3.6
1	D	729	SER	3.6
1	B	507	PRO	3.6
1	C	510	SER	3.5
1	B	235	ILE	3.5
1	B	199	ASP	3.5
1	D	154	ALA	3.5
1	A	386	ASP	3.5
1	B	192	VAL	3.5
1	B	700	TYR	3.5
1	A	531	PHE	3.5
1	D	730	LYS	3.4
1	C	456	ASP	3.4
1	B	696	SER	3.4
1	B	595	SER	3.4
1	A	276	ALA	3.3
1	D	487	GLU	3.3
1	A	68	ARG	3.3
1	D	486	GLU	3.3
1	B	646	ALA	3.3
1	D	491	PHE	3.3
1	D	451	GLY	3.3
1	A	84	THR	3.3
1	A	701	ALA	3.3
1	A	586	GLN	3.2
1	A	534	ILE	3.2
1	B	632	PRO	3.2
1	C	241	GLU	3.2
1	B	609	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	606	TRP	3.2
1	B	206	ASP	3.2
1	B	155	GLU	3.2
1	B	233	LEU	3.2
1	A	631	SER	3.1
1	A	722	LYS	3.1
1	C	533	TYR	3.1
1	C	529	ILE	3.1
1	C	453	ARG	3.1
1	A	497	SER	3.1
1	B	116	ASP	3.1
1	A	723	VAL	3.1
1	B	816	TYR	3.0
1	B	605	TRP	3.0
1	D	739	GLY	3.0
1	C	514	VAL	3.0
1	D	740	SER	3.0
1	B	729	SER	2.9
1	B	523	TYR	2.9
1	B	441	LYS	2.9
1	B	173	LYS	2.9
1	C	631	SER	2.9
1	D	621	ALA	2.9
1	C	142	GLY	2.9
1	D	762	LEU	2.9
1	B	457	THR	2.9
1	C	784	THR	2.9
1	A	629	MET	2.8
1	C	629	MET	2.8
1	C	799	LEU	2.8
1	B	792	VAL	2.8
1	B	751	LEU	2.8
1	B	255	VAL	2.8
1	A	83	ASN	2.8
1	A	187	LYS	2.8
1	C	584	PHE	2.8
1	C	594	ARG	2.8
1	C	224	ASN	2.7
1	C	802	GLY	2.7
1	B	131	ASP	2.7
1	B	231	ASP	2.7
1	A	653	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	177	TYR	2.7
1	B	515	PHE	2.7
1	C	384	GLU	2.7
1	C	53	ALA	2.6
1	C	762	LEU	2.6
1	C	139	SER	2.6
1	B	136	LEU	2.6
1	C	816	TYR	2.6
1	B	431	GLU	2.6
1	C	52	VAL	2.6
1	B	168	ILE	2.6
1	D	104	ASP	2.6
1	A	104	ASP	2.5
1	D	498	LEU	2.5
1	D	661	ARG	2.5
1	C	104	ASP	2.5
1	C	184	LEU	2.5
1	D	786	ALA	2.5
1	D	101	PHE	2.5
1	D	591	ILE	2.5
1	B	291	VAL	2.5
1	D	460	TRP	2.5
1	B	508	GLN	2.5
1	B	154	ALA	2.5
1	A	188	LYS	2.5
1	D	200	LYS	2.5
1	C	803	LEU	2.5
1	B	459	ILE	2.4
1	B	778	SER	2.4
1	C	421	TYR	2.4
1	B	159	GLN	2.4
1	C	813	GLU	2.4
1	D	307	SER	2.4
1	D	690	VAL	2.4
1	B	276	ALA	2.4
1	C	455	ALA	2.4
1	B	202	ASN	2.4
1	D	778	SER	2.4
1	D	515	PHE	2.4
1	B	504	ILE	2.4
1	B	633	ILE	2.4
1	B	220	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	744	THR	2.4
1	B	753	LEU	2.4
1	D	11	SER	2.4
1	C	383	THR	2.4
1	C	701	ALA	2.4
1	D	346	LYS	2.4
1	B	163	ILE	2.3
1	C	630	VAL	2.3
1	A	480	THR	2.3
1	C	180	LEU	2.3
1	A	45	PRO	2.3
1	A	530	VAL	2.3
1	B	102	PRO	2.3
1	A	781	LYS	2.3
1	B	80	LYS	2.3
1	A	652	SER	2.3
1	C	81	SER	2.3
1	B	432	ILE	2.3
1	B	506	LYS	2.3
1	C	223	ALA	2.3
1	A	314	ASP	2.3
1	D	777	ASP	2.3
1	D	107	HIS	2.2
1	A	767	TRP	2.2
1	B	797	TYR	2.2
1	D	654	SER	2.2
1	B	645	ILE	2.2
1	C	502	ILE	2.2
1	B	724	GLY	2.2
1	D	512	PRO	2.2
1	B	654	SER	2.2
1	A	661	ARG	2.2
1	B	701	ALA	2.2
1	C	191	ARG	2.2
1	C	580	SER	2.2
1	C	815	CYS	2.2
1	B	222	ILE	2.2
1	C	460	TRP	2.2
1	D	338	VAL	2.2
1	D	741	SER	2.2
1	A	528	CYS	2.2
1	C	116	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	774	GLY	2.2
1	B	79	LYS	2.2
1	B	144	SER	2.2
1	D	147	GLN	2.2
1	B	648	GLY	2.1
1	B	36	PHE	2.1
1	A	80	LYS	2.1
1	C	792	VAL	2.1
1	B	628	ARG	2.1
1	D	768	TYR	2.1
1	C	528	CYS	2.1
1	B	84	THR	2.1
1	A	657	GLU	2.1
1	A	358	ILE	2.1
1	D	131	ASP	2.1
1	D	204	ILE	2.1
1	D	734	ILE	2.1
1	A	180	LEU	2.1
1	B	442	LEU	2.1
1	A	341	LEU	2.1
1	B	237	PHE	2.1
1	C	634	GLU	2.1
1	C	219	HIS	2.0
1	B	261	ARG	2.0
1	D	299	LEU	2.0
1	C	504	ILE	2.0
1	A	587	GLN	2.0
1	B	290	GLN	2.0
1	B	536	VAL	2.0
1	B	114	ARG	2.0
1	C	654	SER	2.0
1	B	693	VAL	2.0
1	A	79	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

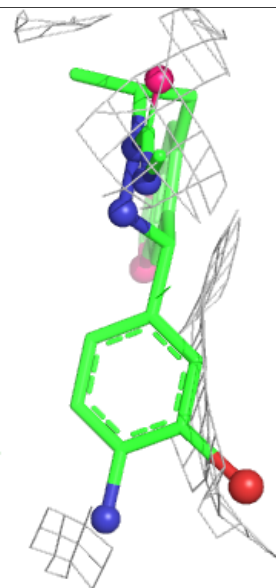
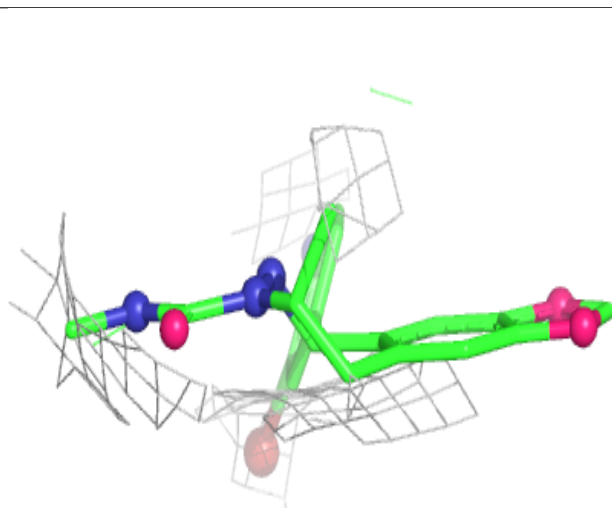
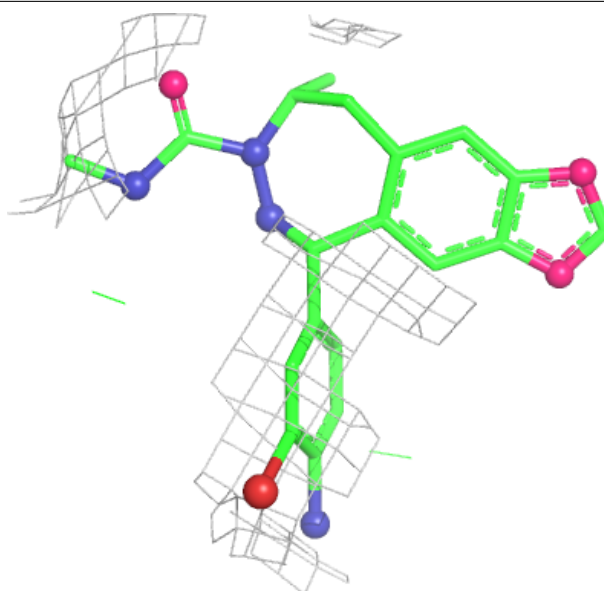
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	901	14/15	0.51	0.20	344,344,346,352	0
2	NAG	D	901	14/15	0.55	0.19	358,358,359,362	0
3	GYB	D	902	27/27	0.61	0.11	253,264,269,292	0
3	GYB	C	902	27/27	0.62	0.16	252,261,270,281	0
3	GYB	A	902	27/27	0.64	0.12	259,264,270,279	0
2	NAG	C	901	14/15	0.65	0.27	505,505,507,515	0
2	NAG	B	901	14/15	0.78	0.14	285,285,287,290	0
3	GYB	B	902	27/27	0.78	0.11	253,263,269,275	0
3	GYB	A	903	27/27	0.89	0.64	58,205,248,257	27

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.

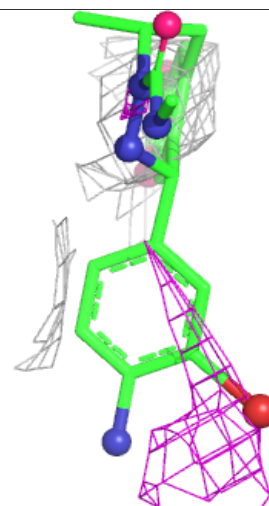
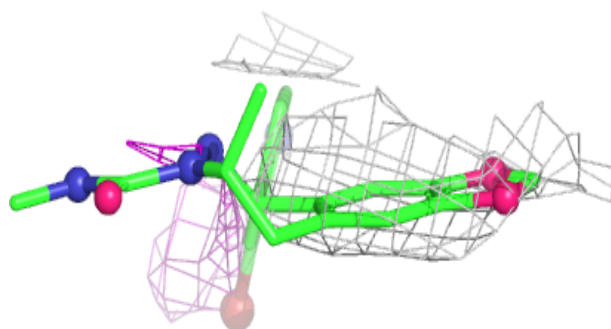
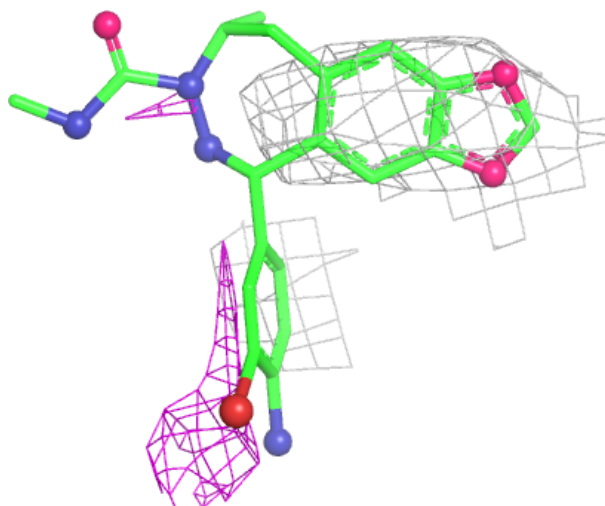
Electron density around GYB D 902:

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



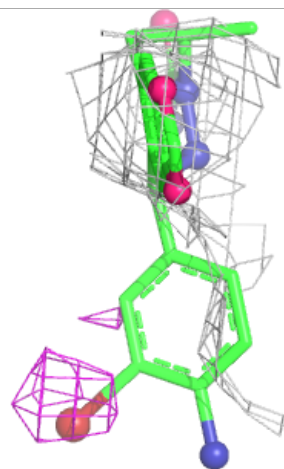
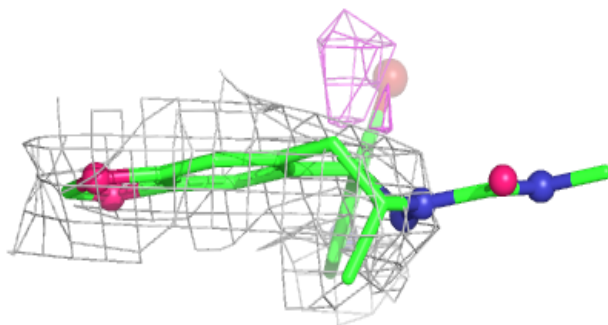
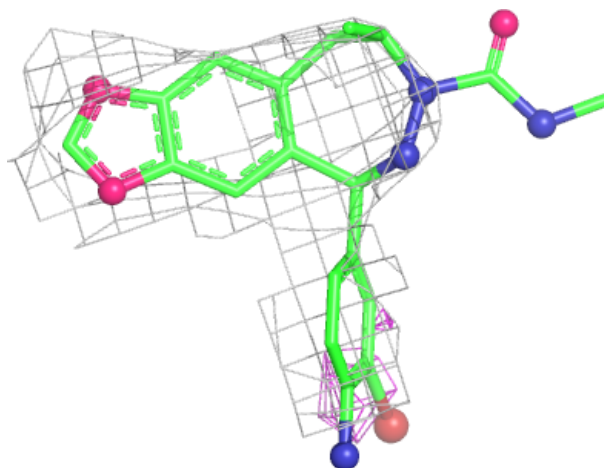
Electron density around GYB C 902:

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



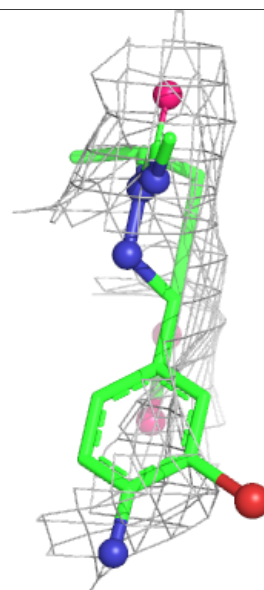
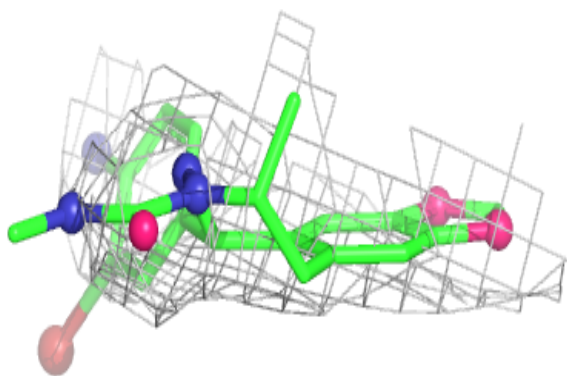
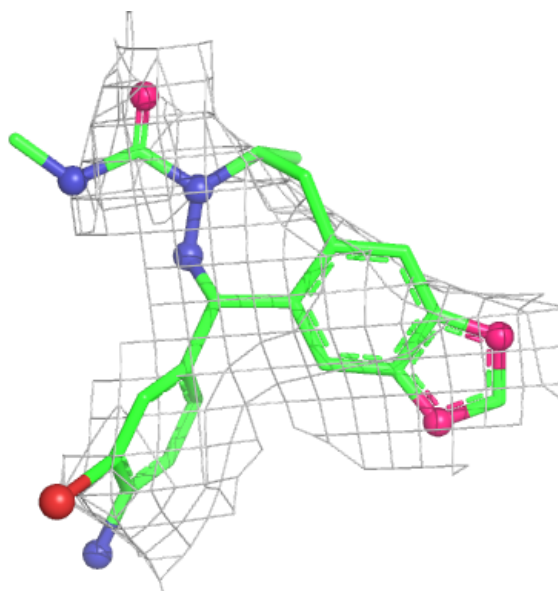
Electron density around GYB A 902:

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



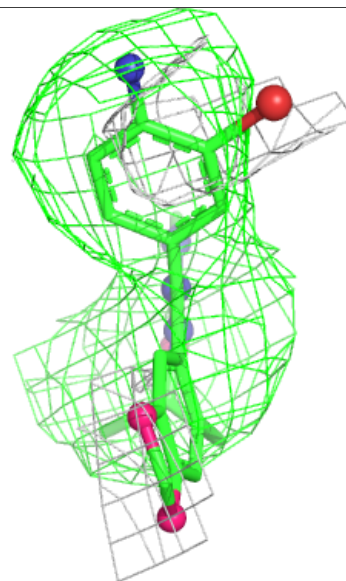
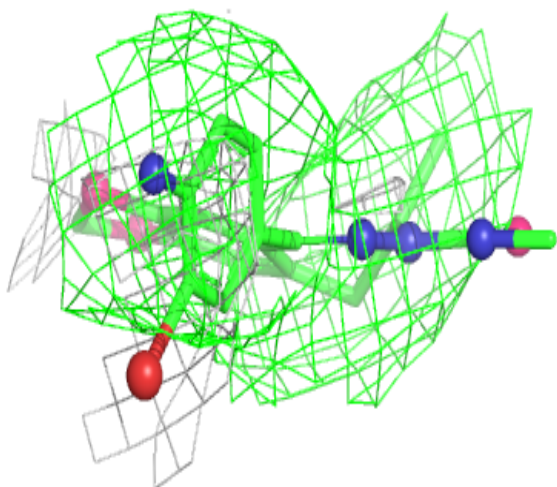
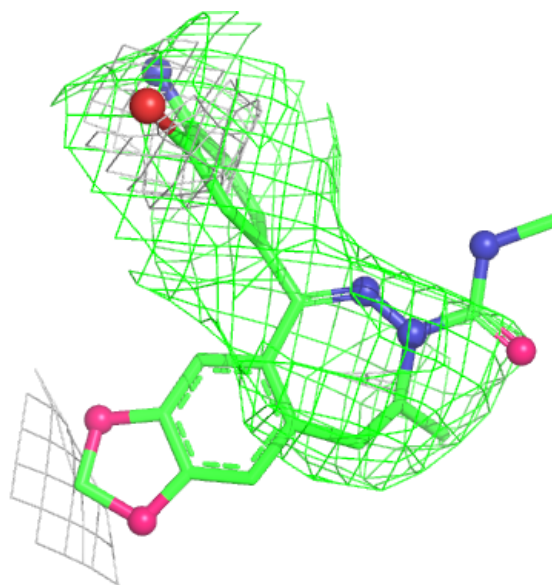
Electron density around GYB B 902:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.