



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:11 PM BST

PDB ID : 5L1H
Title : AMPA subtype ionotropic glutamate receptor GluA2 in complex with non-competitive inhibitor GYKI53655
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.
Deposited on : 2016-07-29
Resolution : 3.80 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 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

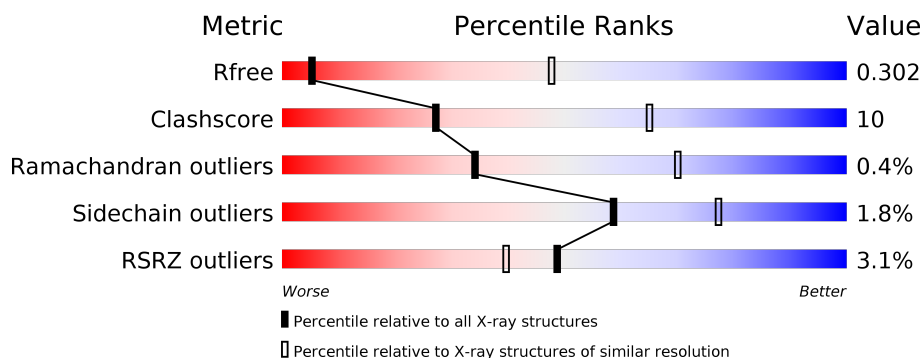
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 ≥ 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	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>
1	B	803	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>••</div> </div> </div>
1	C	803	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>••</div> </div> </div>
1	D	803	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	901	-	-	-	X
2	NAG	C	901	-	-	-	X
3	GYK	C	902	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24066 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	773	Total	C	N	O	S	0	0	0
			5970	3835	990	1116	29			
1	B	773	Total	C	N	O	S	0	0	0
			6001	3850	991	1131	29			
1	C	773	Total	C	N	O	S	0	0	0
			5960	3829	987	1116	28			
1	D	776	Total	C	N	O	S	0	0	0
			5975	3835	991	1121	28			

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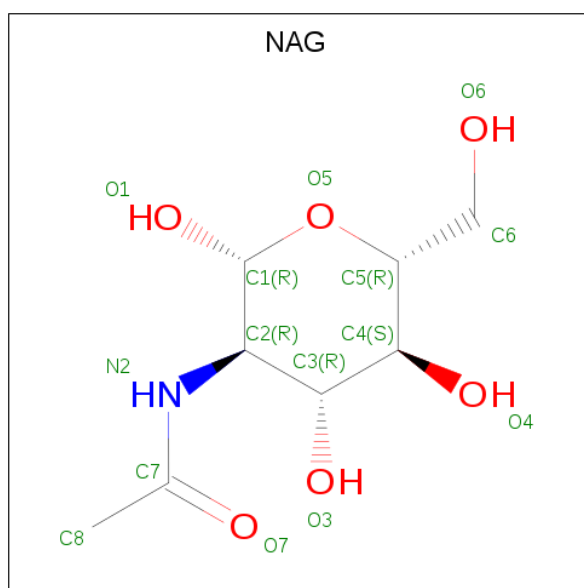
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker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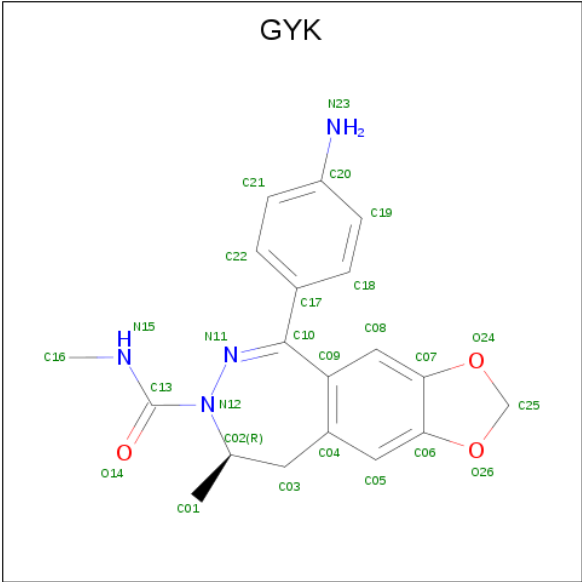
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491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

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



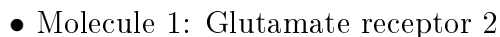
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

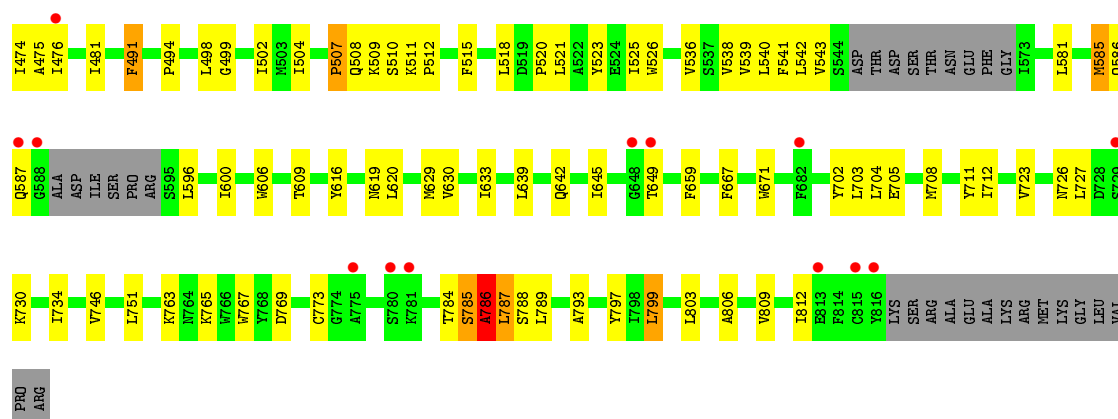
- Molecule 3 is (8R)-5-(4-aminophenyl)-N,8-dimethyl-8,9-dihydro-2H,7H-[1,3]dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide (three-letter code: GYK) (formula: $C_{19}H_{20}N_4O_3$).



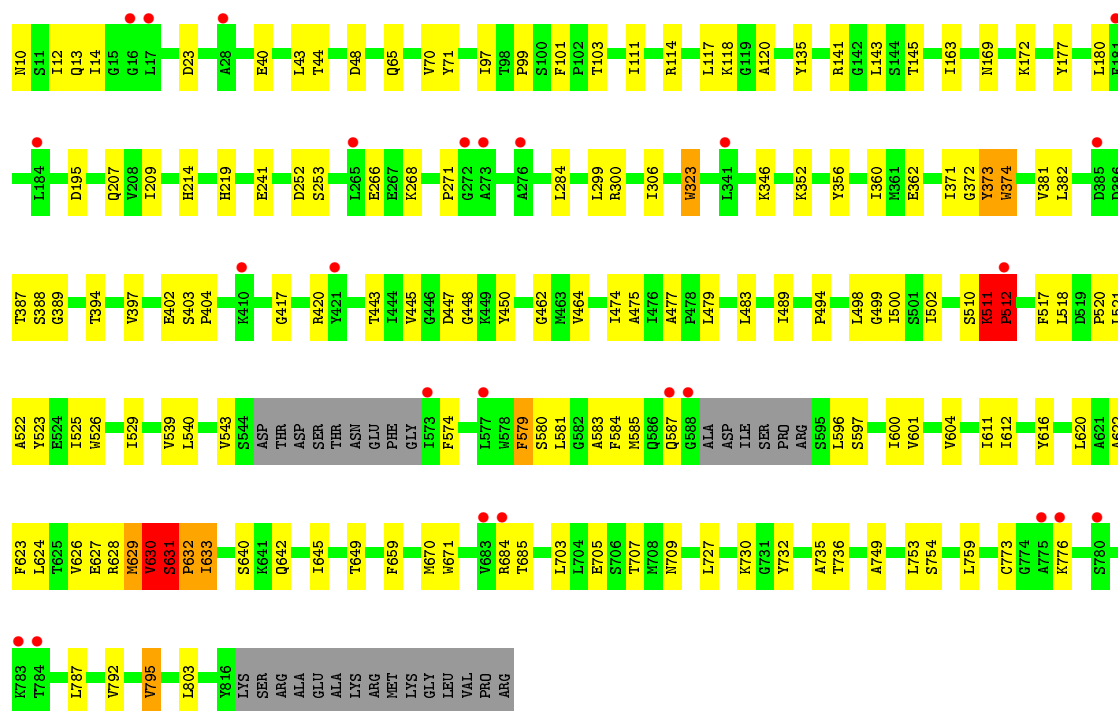
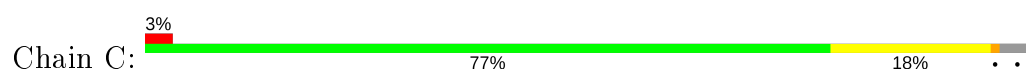
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	4	3		
3	B	1	Total	C	N	O	0	0
			26	19	4	3		
3	C	1	Total	C	N	O	0	0
			26	19	4	3		
3	D	1	Total	C	N	O	0	0
			26	19	4	3		

- Molecule 1: Glutamate receptor 2

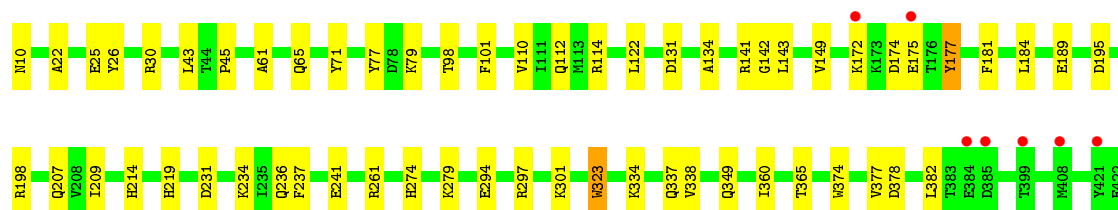
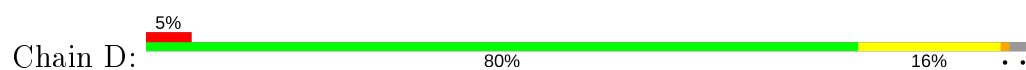


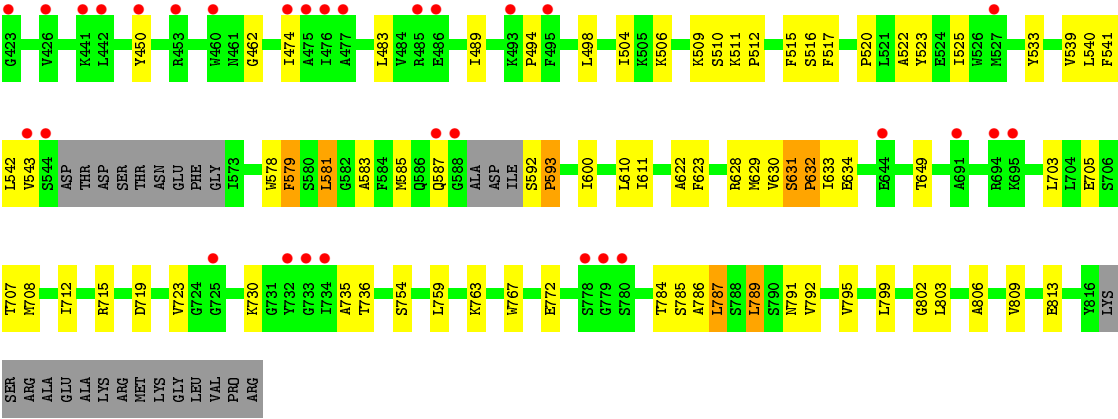


• Molecule 1: Glutamate receptor 2



• 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	92.59Å 110.64Å 599.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 3.80 47.49 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.49-3.80) 98.9 (47.49-3.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.276 , 0.292 0.283 , 0.302	Depositor DCC
R_{free} test set	3071 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	141.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 101.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24066	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: GYK, 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	0.27	2/6092 (0.0%)	0.44	1/8244 (0.0%)
1	B	0.27	1/6123 (0.0%)	0.55	8/8284 (0.1%)
1	C	0.27	2/6082 (0.0%)	0.50	6/8235 (0.1%)
1	D	0.29	2/6098 (0.0%)	0.45	4/8257 (0.0%)
All	All	0.28	7/24395 (0.0%)	0.49	19/33020 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	632	PRO	N-CD	9.86	1.61	1.47
1	B	388	SER	N-CA	6.05	1.58	1.46
1	D	512	PRO	N-CD	5.47	1.55	1.47
1	C	632	PRO	N-CD	5.45	1.55	1.47
1	A	632	PRO	N-CD	5.38	1.55	1.47
1	A	512	PRO	N-CD	5.27	1.55	1.47
1	C	512	PRO	N-CD	5.11	1.55	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	ALA	CB-CA-C	-14.64	88.14	110.10
1	C	629	MET	CB-CA-C	-12.59	85.22	110.40
1	B	452	ALA	N-CA-C	12.33	144.30	111.00
1	B	785	SER	CB-CA-C	10.37	129.81	110.10
1	B	453	ARG	N-CA-CB	-10.05	92.51	110.60
1	B	786	ALA	N-CA-CB	9.57	123.50	110.10
1	D	632	PRO	CA-N-CD	-8.14	100.10	111.50
1	B	388	SER	N-CA-C	-6.97	92.19	111.00
1	B	388	SER	CB-CA-C	6.92	123.24	110.10
1	D	631	SER	C-N-CD	6.91	142.92	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	512	PRO	CA-N-CD	-6.66	102.17	111.50
1	B	388	SER	N-CA-CB	6.12	119.67	110.50
1	C	373	TYR	CB-CA-C	5.86	122.12	110.40
1	D	631	SER	CB-CA-C	5.76	121.05	110.10
1	A	511	LYS	C-N-CD	5.57	140.10	128.40
1	D	511	LYS	C-N-CD	5.46	139.86	128.40
1	C	630	VAL	N-CA-C	-5.27	96.76	111.00
1	C	511	LYS	C-N-CD	5.10	139.10	128.40
1	C	374	TRP	N-CA-CB	5.05	119.69	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5970	0	5874	124	0
1	B	6001	0	5924	139	1
1	C	5960	0	5850	154	0
1	D	5975	0	5855	109	1
2	A	14	0	13	1	0
2	B	14	0	13	1	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
3	A	26	0	0	1	0
3	B	26	0	0	3	0
3	C	26	0	0	3	0
3	D	26	0	0	2	0
All	All	24066	0	23555	482	1

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 10.

All (482) 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)
1:D:628:ARG:CB	1:D:630:VAL:HG22	1.12	1.55
1:C:512:PRO:HG3	3:C:902:GYK:C16	1.51	1.40
1:D:628:ARG:CB	1:D:630:VAL:CG2	2.02	1.35
1:A:77:TYR:CD1	1:A:82:VAL:HB	1.65	1.28
1:C:622:ALA:O	1:C:626:VAL:HG23	1.39	1.20
1:D:631:SER:HB3	1:D:632:PRO:HA	1.23	1.14
1:A:77:TYR:CE1	1:A:82:VAL:CG2	2.32	1.12
1:C:630:VAL:HG22	1:C:632:PRO:HA	1.30	1.10
1:A:630:VAL:HA	1:A:631:SER:HB2	1.21	1.06
1:A:77:TYR:CD1	1:A:82:VAL:CB	2.41	1.02
1:C:632:PRO:HD2	1:C:633:ILE:HB	1.38	1.01
1:A:77:TYR:CE1	1:A:82:VAL:HB	1.96	0.99
1:D:377:VAL:HG13	1:D:378:ASP:H	1.26	0.98
1:C:630:VAL:HG22	1:C:631:SER:H	1.29	0.98
1:C:631:SER:H	1:C:632:PRO:HA	1.30	0.97
1:C:521:LEU:HG	1:C:616:TYR:HD2	1.29	0.96
1:C:629:MET:CG	1:C:629:MET:O	2.03	0.95
1:B:232:LEU:O	1:B:232:LEU:HD23	1.66	0.95
1:C:632:PRO:CD	1:C:633:ILE:HB	1.95	0.95
1:C:622:ALA:O	1:C:626:VAL:CG2	2.14	0.95
1:A:449:LYS:HB3	1:A:462:GLY:HA2	1.49	0.94
1:D:623:PHE:HD2	1:D:629:MET:HE3	1.31	0.93
1:A:77:TYR:HD1	1:A:82:VAL:HB	1.30	0.93
1:C:629:MET:HG2	1:C:629:MET:O	1.66	0.92
1:D:631:SER:CB	1:D:632:PRO:HA	2.00	0.91
1:A:77:TYR:CE1	1:A:82:VAL:CB	2.53	0.90
1:A:77:TYR:CE1	1:A:82:VAL:HG23	2.06	0.90
1:A:630:VAL:HG22	1:A:631:SER:C	1.92	0.90
1:A:631:SER:HB3	1:A:632:PRO:HA	1.54	0.90
1:B:541:PHE:HD2	1:B:542:LEU:CD2	1.84	0.90
1:A:630:VAL:HA	1:A:631:SER:CB	2.02	0.88
1:D:623:PHE:HD2	1:D:629:MET:CE	1.86	0.87
1:C:512:PRO:CG	3:C:902:GYK:C16	2.48	0.86
1:B:232:LEU:HD21	1:B:363:LEU:HD22	1.56	0.86
1:B:541:PHE:CD2	1:B:542:LEU:HD23	2.11	0.85
1:B:541:PHE:CD2	1:B:542:LEU:CD2	2.62	0.83
1:C:632:PRO:CB	1:C:633:ILE:HB	2.09	0.82
1:B:382:LEU:HD13	1:B:384:GLU:CG	2.10	0.81
1:C:632:PRO:HB2	1:C:633:ILE:HB	1.60	0.81
1:C:631:SER:N	1:C:632:PRO:HA	1.96	0.80
1:C:632:PRO:HB2	1:C:633:ILE:CG1	2.12	0.80
1:D:377:VAL:HG13	1:D:378:ASP:N	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:PRO:HD2	1:C:633:ILE:CB	2.13	0.79
1:A:77:TYR:CE1	1:A:82:VAL:HG21	2.20	0.76
1:D:623:PHE:CD2	1:D:629:MET:CE	2.69	0.76
1:B:114:ARG:HD2	1:B:280:TYR:HE2	1.51	0.76
1:C:521:LEU:HG	1:C:616:TYR:CD2	2.18	0.76
1:C:632:PRO:HB2	1:C:633:ILE:CB	2.15	0.75
1:B:451:GLY:HA2	1:B:452:ALA:HB3	1.67	0.75
1:B:541:PHE:HD2	1:B:542:LEU:HD21	1.51	0.74
1:D:715:ARG:HD3	1:D:772:GLU:HG2	1.68	0.74
1:B:227:PHE:CZ	1:B:232:LEU:HD11	2.23	0.74
1:C:630:VAL:HG22	1:C:631:SER:N	2.02	0.74
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.68	0.73
1:B:346:LYS:HG3	1:B:354:ILE:HG13	1.71	0.72
1:C:360:ILE:HB	1:C:372:GLY:HA3	1.70	0.72
1:A:520:PRO:O	1:B:787:LEU:HD12	1.89	0.72
1:C:630:VAL:HG22	1:C:632:PRO:CA	2.16	0.72
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.72	0.72
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.72	0.71
1:D:377:VAL:CG1	1:D:378:ASP:H	2.01	0.71
1:B:382:LEU:HD13	1:B:384:GLU:HG2	1.73	0.70
1:C:632:PRO:HB2	1:C:633:ILE:HG13	1.73	0.70
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.74	0.69
1:D:198:ARG:HH21	1:D:279:LYS:HD3	1.58	0.68
1:D:509:LYS:HA	1:D:510:SER:C	2.13	0.68
1:A:77:TYR:CZ	1:A:82:VAL:HG23	2.28	0.68
1:C:631:SER:OG	1:C:632:PRO:O	2.10	0.68
1:B:118:LYS:HB3	1:B:145:THR:HG22	1.76	0.68
1:B:382:LEU:HD13	1:B:384:GLU:HG3	1.75	0.67
1:A:603:GLY:HA2	1:B:585:MET:HB3	1.76	0.67
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.59	0.67
1:C:640:SER:HB3	1:C:670:MET:HG2	1.77	0.67
1:C:522:ALA:HB3	1:C:525:ILE:HD13	1.76	0.67
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.77	0.66
1:A:70:VAL:O	1:A:308:ARG:NH1	2.29	0.66
1:C:371:ILE:O	1:C:382:LEU:HD22	1.95	0.66
1:D:623:PHE:CD2	1:D:629:MET:HE2	2.30	0.66
1:C:12:ILE:HG23	1:C:71:TYR:HD2	1.61	0.66
1:D:631:SER:HB3	1:D:632:PRO:CA	2.15	0.65
1:C:596:LEU:HD13	1:D:578:TRP:HA	1.79	0.65
1:B:388:SER:HB3	1:B:389:GLY:HA3	1.77	0.64
1:B:494:PRO:HG3	1:C:494:PRO:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:HIS:O	1:A:274:HIS:ND1	2.30	0.64
1:A:630:VAL:HG13	1:A:631:SER:O	1.97	0.64
1:D:630:VAL:O	1:D:630:VAL:HG12	1.97	0.64
1:C:177:TYR:HB3	1:C:207:GLN:HG2	1.80	0.64
1:A:344:ASN:ND2	2:A:901:NAG:O6	2.31	0.64
1:B:385:ASP:OD2	1:B:385:ASP:N	2.29	0.64
1:B:541:PHE:CD2	1:B:542:LEU:HD21	2.31	0.64
1:D:172:LYS:NZ	1:D:175:GLU:OE1	2.31	0.64
1:D:377:VAL:HG13	1:D:378:ASP:OD1	1.98	0.63
1:C:498:LEU:HD21	1:C:732:TYR:CZ	2.33	0.63
1:A:630:VAL:HG22	1:A:631:SER:O	1.98	0.63
1:D:71:TYR:HA	1:D:323:TRP:HH2	1.64	0.63
1:A:110:VAL:CG1	1:A:112:GLN:NE2	2.61	0.63
1:B:103:THR:HG23	1:B:112:GLN:HE21	1.64	0.62
1:C:587:GLN:HE22	1:D:587:GLN:HG3	1.64	0.62
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.81	0.62
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.80	0.62
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.81	0.62
1:A:529:ILE:HD13	1:A:612:ILE:HD12	1.81	0.62
1:C:511:LYS:H	1:C:512:PRO:HD2	1.64	0.61
1:C:626:VAL:O	1:C:629:MET:HB3	2.00	0.61
1:C:630:VAL:CG2	1:C:631:SER:H	2.11	0.61
1:C:346:LYS:NZ	2:C:901:NAG:O7	2.34	0.60
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.84	0.60
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.67	0.60
1:C:540:LEU:HA	1:C:543:VAL:HG22	1.84	0.60
1:D:628:ARG:CB	1:D:629:MET:HA	2.32	0.60
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.82	0.59
1:A:623:PHE:HZ	1:B:786:ALA:O	1.85	0.59
1:A:124:LEU:HD13	1:A:360:ILE:HD13	1.84	0.59
1:C:623:PHE:HZ	1:D:786:ALA:HA	1.67	0.59
1:A:806:ALA:HA	1:D:600:ILE:HD11	1.85	0.59
1:D:337:GLN:NE2	2:D:901:NAG:O7	2.35	0.59
1:B:498:LEU:HD12	1:B:705:GLU:HB2	1.83	0.59
1:D:516:SER:HB2	3:D:902:GYK:C01	2.33	0.59
1:C:521:LEU:HB2	1:C:526:TRP:CE2	2.38	0.58
1:A:493:LYS:HG3	1:A:751:LEU:HD21	1.86	0.58
1:A:681:VAL:O	1:A:700:TYR:OH	2.20	0.58
1:B:447:ASP:N	1:B:448:GLY:HA2	2.18	0.58
1:C:143:LEU:HG	1:D:143:LEU:HD11	1.85	0.58
1:C:773:CYS:HB3	1:C:776:LYS:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:PRO:CG	1:C:633:ILE:HB	2.33	0.58
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.86	0.58
1:B:508:GLN:N	1:B:509:LYS:HA	2.19	0.58
1:A:792:VAL:HG21	1:D:525:ILE:HG12	1.85	0.58
1:A:498:LEU:CD1	1:A:730:LYS:HG3	2.33	0.58
1:C:518:LEU:O	1:C:526:TRP:NE1	2.36	0.58
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.86	0.58
1:A:630:VAL:CA	1:A:631:SER:HB2	2.14	0.57
1:C:498:LEU:HD12	1:C:730:LYS:HG3	1.85	0.57
1:B:416:GLU:HA	1:B:420:ARG:HD3	1.84	0.57
1:A:374:TRP:CE3	1:A:379:LYS:NZ	2.70	0.57
1:A:520:PRO:HG3	1:A:620:LEU:HD13	1.87	0.57
1:A:498:LEU:HD12	1:A:730:LYS:HG3	1.87	0.57
1:A:684:ARG:HG2	1:A:685:THR:HG23	1.87	0.56
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.23	0.56
1:A:344:ASN:O	1:A:353:ARG:NH2	2.38	0.56
1:A:631:SER:CB	1:A:632:PRO:HA	2.33	0.56
1:B:102:PRO:HA	1:B:112:GLN:HG2	1.87	0.56
1:C:597:SER:N	1:D:813:GLU:OE2	2.39	0.56
1:B:620:LEU:HD11	3:B:902:GYK:C18	2.35	0.56
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.88	0.56
1:D:219:HIS:HA	1:D:241:GLU:O	2.06	0.56
1:C:450:TYR:O	1:C:462:GLY:HA3	2.06	0.56
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.88	0.56
1:B:50:LEU:C	1:B:50:LEU:HD12	2.26	0.56
1:C:522:ALA:H	1:D:787:LEU:HD12	1.71	0.56
1:B:784:THR:O	1:B:785:SER:OG	2.22	0.56
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.87	0.56
1:D:134:ALA:HB2	1:D:189:GLU:HG2	1.87	0.55
1:C:445:VAL:HG22	1:C:448:GLY:H	1.72	0.55
1:C:13:GLN:HA	1:C:44:THR:HB	1.89	0.55
1:C:48:ASP:OD1	1:C:65:GLN:NE2	2.40	0.55
1:B:232:LEU:CD2	1:B:363:LEU:HD22	2.33	0.55
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.88	0.55
1:A:135:TYR:CE1	1:A:137:TYR:HB3	2.41	0.55
1:A:358:ILE:HD12	1:A:374:TRP:HE1	1.70	0.55
1:B:538:VAL:O	1:B:541:PHE:HB3	2.07	0.54
1:C:371:ILE:HA	1:C:382:LEU:HD22	1.89	0.54
1:C:510:SER:CB	1:C:511:LYS:CB	2.85	0.54
1:C:510:SER:CB	1:C:511:LYS:CA	2.85	0.54
1:B:38:THR:HG23	1:B:40:GLU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD13	1:C:306:ILE:HD13	1.90	0.54
1:D:498:LEU:HB3	1:D:707:THR:HG23	1.90	0.54
1:D:623:PHE:CD2	1:D:629:MET:HE3	2.24	0.54
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.73	0.54
1:B:799:LEU:O	1:B:803:LEU:N	2.39	0.54
1:D:334:LYS:NZ	1:D:349:GLN:O	2.27	0.54
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.41	0.54
1:A:751:LEU:HB2	1:D:483:LEU:HD13	1.89	0.54
1:A:517:PHE:HE1	1:D:611:ILE:HG21	1.73	0.54
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.88	0.54
1:A:77:TYR:CD1	1:A:82:VAL:CG2	2.83	0.53
1:C:498:LEU:CD1	1:C:730:LYS:HD2	2.38	0.53
1:A:714:GLN:HA	1:A:773:CYS:HB2	1.91	0.53
1:D:450:TYR:HA	1:D:462:GLY:HA3	1.91	0.53
1:D:540:LEU:HA	1:D:543:VAL:HG22	1.90	0.53
1:D:498:LEU:HD12	1:D:705:GLU:HB2	1.89	0.53
1:C:539:VAL:HG21	1:D:803:LEU:HD22	1.91	0.53
1:A:77:TYR:CZ	1:A:82:VAL:CG2	2.88	0.53
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.44	0.53
1:A:141:ARG:NH2	1:A:195:ASP:O	2.33	0.53
1:B:236:GLN:HG3	1:B:363:LEU:HD11	1.90	0.53
1:B:600:ILE:HG22	1:C:581:LEU:HD13	1.91	0.53
1:B:114:ARG:HD2	1:B:280:TYR:CE2	2.38	0.52
1:D:509:LYS:N	1:D:510:SER:CB	2.72	0.52
1:B:596:LEU:HB2	1:C:574:PHE:O	2.09	0.52
1:C:596:LEU:HG	1:D:809:VAL:HG11	1.91	0.52
1:B:620:LEU:HD11	3:B:902:GYK:C19	2.39	0.52
1:B:504:ILE:HD13	1:B:633:ILE:HD12	1.91	0.52
1:D:231:ASP:HB3	1:D:234:LYS:HE2	1.91	0.52
1:A:119:GLY:O	1:A:379:LYS:NZ	2.41	0.52
1:B:163:ILE:HG21	1:B:180:LEU:HD13	1.92	0.52
1:D:22:ALA:HB1	1:D:25:GLU:HB2	1.90	0.52
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.91	0.52
1:B:606:TRP:HA	1:B:609:THR:HG22	1.91	0.52
1:B:784:THR:C	1:B:785:SER:OG	2.49	0.51
1:B:510:SER:OG	3:B:902:GYK:O14	2.27	0.51
1:B:510:SER:HB3	1:B:512:PRO:HD3	1.92	0.51
1:C:394:THR:HG23	1:C:394:THR:O	2.10	0.51
1:D:784:THR:HA	1:D:785:SER:HB3	1.92	0.51
1:B:787:LEU:HD23	1:B:788:SER:N	2.24	0.51
1:D:541:PHE:HD2	1:D:542:LEU:HD23	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:HD21	1:B:293:THR:HG22	1.93	0.51
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.93	0.51
1:C:511:LYS:H	1:C:512:PRO:CD	2.24	0.51
1:B:26:TYR:HE1	1:B:47:ILE:HG12	1.75	0.51
1:C:604:VAL:HG12	1:D:799:LEU:HD12	1.92	0.51
1:C:97:ILE:HA	1:C:111:ILE:HB	1.93	0.51
1:C:477:ALA:O	1:C:479:LEU:N	2.42	0.51
1:D:517:PHE:CE1	1:D:795:VAL:HG22	2.46	0.51
1:A:803:LEU:HD22	1:D:539:VAL:HG21	1.93	0.51
1:B:177:TYR:HB3	1:B:207:GLN:HG2	1.92	0.50
1:C:498:LEU:CD1	1:C:730:LYS:CD	2.88	0.50
1:A:631:SER:HB3	1:A:632:PRO:CA	2.34	0.50
1:C:498:LEU:HD12	1:C:499:GLY:N	2.26	0.50
1:A:502:ILE:HD13	1:A:639:LEU:HD13	1.92	0.50
1:A:525:ILE:HG13	1:B:789:LEU:HD12	1.92	0.50
1:B:15:GLY:O	1:B:74:PHE:N	2.40	0.50
1:C:500:ILE:O	1:C:727:LEU:N	2.44	0.50
1:A:103:THR:O	1:A:352:LYS:NZ	2.43	0.50
1:B:232:LEU:O	1:B:232:LEU:CD2	2.50	0.50
1:B:508:GLN:H	1:B:509:LYS:HA	1.77	0.50
1:A:77:TYR:CD1	1:A:82:VAL:CA	2.94	0.50
1:B:131:ASP:OD1	1:B:132:LYS:N	2.45	0.50
1:C:252:ASP:OD1	1:C:253:SER:N	2.45	0.49
1:C:10:ASN:ND2	1:C:40:GLU:O	2.45	0.49
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.46	0.49
1:D:382:LEU:H	1:D:382:LEU:HD23	1.76	0.49
1:B:168:ILE:HD11	1:B:200:LYS:HZ3	1.77	0.49
1:A:96:PHE:CE2	1:A:98:THR:HB	2.48	0.49
1:B:124:LEU:HA	1:B:380:MET:HE1	1.93	0.49
1:C:579:PHE:O	1:C:583:ALA:N	2.46	0.49
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.47	0.49
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.94	0.49
1:C:525:ILE:HD11	1:D:789:LEU:HA	1.94	0.49
1:C:10:ASN:HB3	1:C:300:ARG:HH22	1.76	0.49
1:B:11:SER:OG	1:B:44:THR:OG1	2.27	0.49
1:B:510:SER:HB3	1:B:511:LYS:HA	1.94	0.49
1:A:623:PHE:CZ	1:B:786:ALA:N	2.81	0.49
1:C:371:ILE:C	1:C:382:LEU:HD22	2.32	0.49
1:D:628:ARG:N	1:D:629:MET:HB2	2.28	0.49
1:A:177:TYR:HD2	1:A:207:GLN:HG3	1.77	0.49
1:A:294:GLU:HG3	1:A:338:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:LYS:N	1:D:719:ASP:O	2.40	0.49
1:C:498:LEU:HB3	1:C:707:THR:HG23	1.94	0.49
1:A:308:ARG:NE	1:A:312:ALA:HB2	2.28	0.49
1:C:373:TYR:HB3	1:C:381:VAL:O	2.13	0.49
1:C:604:VAL:HG11	1:D:802:GLY:HA3	1.95	0.49
1:B:50:LEU:CD1	1:B:52:VAL:HA	2.43	0.48
1:D:708:MET:O	1:D:712:ILE:HG12	2.14	0.48
1:B:525:ILE:HG12	1:C:792:VAL:HG11	1.94	0.48
1:D:26:TYR:CE2	1:D:30:ARG:HD2	2.48	0.48
1:A:125:ILE:HG23	1:A:130:TRP:HB2	1.95	0.48
1:B:387:THR:OG1	1:B:387:THR:O	2.31	0.48
1:B:184:LEU:O	1:B:189:GLU:HB2	2.13	0.48
3:D:902:GYK:C08	3:D:902:GYK:C22	2.92	0.48
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.94	0.48
1:B:381:VAL:O	1:B:381:VAL:HG13	2.14	0.48
1:C:219:HIS:HA	1:C:241:GLU:O	2.14	0.48
1:A:498:LEU:HD21	1:A:732:TYR:CZ	2.49	0.48
1:A:637:GLU:O	1:A:641:LYS:N	2.47	0.47
1:B:210:THR:HG22	1:D:237:PHE:HB2	1.96	0.47
1:A:789:LEU:HA	1:D:525:ILE:HD11	1.96	0.47
1:C:135:TYR:HH	1:C:145:THR:HG1	1.57	0.47
1:C:498:LEU:HD12	1:C:730:LYS:CG	2.43	0.47
1:D:236:GLN:NE2	1:D:365:THR:O	2.39	0.47
1:B:227:PHE:CZ	1:B:232:LEU:CD1	2.95	0.47
1:B:97:ILE:HD11	1:B:333:LEU:HD22	1.96	0.47
1:C:388:SER:H	1:C:389:GLY:HA2	1.80	0.47
1:D:377:VAL:CG1	1:D:378:ASP:N	2.65	0.47
1:B:734:ILE:HG21	1:B:746:VAL:HG11	1.97	0.47
1:D:630:VAL:CG1	1:D:630:VAL:O	2.62	0.47
1:A:596:LEU:HA	1:A:596:LEU:HD12	1.84	0.47
1:A:623:PHE:CZ	1:B:786:ALA:O	2.67	0.47
1:D:174:ASP:OD1	1:D:207:GLN:NE2	2.48	0.47
1:D:763:LYS:O	1:D:767:TRP:HB2	2.15	0.47
1:B:630:VAL:HG23	1:B:630:VAL:O	2.15	0.47
1:C:632:PRO:HD2	1:C:633:ILE:CG2	2.44	0.47
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.55	0.46
1:A:110:VAL:HG12	1:A:112:GLN:NE2	2.30	0.46
1:B:99:PRO:O	1:B:114:ARG:HB2	2.15	0.46
1:B:425:CYS:O	1:B:429:ALA:N	2.49	0.46
1:C:510:SER:CB	1:C:511:LYS:HA	2.46	0.46
1:B:444:ILE:HG22	1:B:446:GLY:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LEU:HD12	1:C:730:LYS:HD2	1.98	0.46
1:A:120:ALA:HB2	1:A:374:TRP:NE1	2.31	0.46
1:C:498:LEU:CD2	1:C:732:TYR:CZ	2.98	0.46
1:B:708:MET:O	1:B:712:ILE:HG12	2.15	0.46
1:B:499:GLY:HA3	1:B:726:ASN:HB3	1.97	0.46
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.98	0.46
1:D:131:ASP:N	1:D:131:ASP:OD1	2.47	0.46
1:B:22:ALA:HB1	1:B:25:GLU:HB2	1.97	0.46
1:C:387:THR:HA	1:C:388:SER:HA	1.62	0.46
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.97	0.46
1:A:274:HIS:O	1:A:274:HIS:CG	2.69	0.46
1:C:371:ILE:HA	1:C:382:LEU:CD2	2.44	0.46
1:C:447:ASP:OD1	1:C:447:ASP:N	2.44	0.46
1:D:715:ARG:HA	1:D:772:GLU:CG	2.46	0.46
1:C:371:ILE:CA	1:C:382:LEU:HD22	2.44	0.46
1:C:600:ILE:HD11	1:D:806:ALA:HA	1.98	0.46
1:D:787:LEU:HD11	1:D:792:VAL:HG21	1.97	0.46
1:D:632:PRO:O	1:D:632:PRO:HD2	2.16	0.45
1:A:521:LEU:HB2	1:A:526:TRP:NE1	2.31	0.45
1:C:520:PRO:HG3	1:C:620:LEU:HD13	1.98	0.45
1:B:809:VAL:O	1:B:812:ILE:HG12	2.16	0.45
1:D:623:PHE:CE2	1:D:629:MET:HE2	2.52	0.45
1:A:507:PRO:HA	1:A:508:GLN:CB	2.47	0.45
1:A:507:PRO:HB2	1:A:509:LYS:CB	2.45	0.45
1:B:515:PHE:CG	1:B:515:PHE:O	2.69	0.45
1:B:587:GLN:HB3	1:B:606:TRP:CD1	2.51	0.45
1:C:177:TYR:CB	1:C:207:GLN:HG2	2.45	0.45
1:C:464:VAL:HG22	1:C:479:LEU:HD21	1.99	0.45
1:D:181:PHE:HA	1:D:184:LEU:HB2	1.98	0.45
1:A:424:TYR:HE2	1:A:495:PHE:HE2	1.65	0.45
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.99	0.45
1:B:38:THR:HG23	1:B:41:PHE:H	1.81	0.45
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.81	0.45
1:C:521:LEU:HA	1:D:787:LEU:HG	1.98	0.45
1:C:631:SER:CB	1:C:632:PRO:C	2.85	0.45
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.99	0.45
1:D:143:LEU:HD23	1:D:143:LEU:H	1.80	0.45
1:B:406:VAL:HG23	1:B:425:CYS:HB2	1.99	0.45
1:B:498:LEU:HG	1:B:730:LYS:HG3	1.99	0.45
1:A:231:ASP:HB3	1:A:234:LYS:HE2	1.98	0.45
1:B:751:LEU:HB2	1:C:483:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:LYS:CA	1:D:510:SER:C	2.85	0.45
1:D:541:PHE:CD2	1:D:542:LEU:HD23	2.51	0.45
1:A:630:VAL:CA	1:A:631:SER:CB	2.85	0.44
1:B:232:LEU:HD21	1:B:363:LEU:CD2	2.37	0.44
1:C:464:VAL:HG13	1:C:489:ILE:HG12	1.98	0.44
1:D:592:SER:N	1:D:593:PRO:HD3	2.31	0.44
1:A:397:VAL:HG13	1:A:474:ILE:HG23	1.99	0.44
1:C:169:ASN:HD21	1:C:172:LYS:HD3	1.81	0.44
1:A:787:LEU:O	1:D:522:ALA:HB2	2.16	0.44
1:A:235:ILE:HD12	1:A:242:VAL:HG21	1.99	0.44
1:A:485:ARG:O	1:A:489:ILE:HG13	2.17	0.44
1:A:631:SER:HA	1:A:632:PRO:C	2.37	0.44
1:B:406:VAL:HG22	1:B:426:VAL:HG23	1.99	0.44
1:A:115:PRO:HA	1:A:353:ARG:HB2	1.99	0.44
1:B:260:GLU:O	1:B:264:THR:OG1	2.27	0.44
1:B:404:PRO:HG3	1:B:711:TYR:CD1	2.52	0.44
1:A:498:LEU:HD12	1:A:730:LYS:CG	2.47	0.44
1:C:498:LEU:HD11	1:C:730:LYS:CD	2.48	0.44
3:C:902:GYK:C22	3:C:902:GYK:C08	2.95	0.44
1:D:632:PRO:O	1:D:633:ILE:C	2.56	0.44
1:A:449:LYS:CB	1:A:462:GLY:HA2	2.35	0.44
1:A:620:LEU:HD11	3:A:902:GYK:C18	2.48	0.44
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.99	0.44
1:D:297:ARG:HG2	1:D:301:LYS:HE3	2.00	0.44
1:D:754:SER:HB2	1:D:759:LEU:HD12	2.00	0.44
1:C:611:ILE:HB	1:D:795:VAL:HG11	1.98	0.44
1:B:430:ALA:HA	1:B:440:TYR:HE1	1.83	0.44
1:B:54:ASN:OD1	1:B:57:ALA:N	2.48	0.44
1:A:520:PRO:C	1:B:787:LEU:HD12	2.38	0.44
1:B:787:LEU:CD2	1:B:788:SER:N	2.80	0.44
1:A:540:LEU:HA	1:A:543:VAL:HG22	1.99	0.44
1:C:521:LEU:HB2	1:C:526:TRP:NE1	2.33	0.44
1:A:236:GLN:NE2	1:A:365:THR:O	2.49	0.44
1:A:59:THR:HG21	1:B:59:THR:HG21	2.00	0.44
1:B:11:SER:HG	1:B:44:THR:HG1	1.64	0.44
1:B:539:VAL:HG21	1:C:803:LEU:HD22	1.99	0.44
1:A:489:ILE:HD13	1:A:735:ALA:HB1	2.00	0.43
1:D:579:PHE:O	1:D:583:ALA:N	2.50	0.43
1:A:14:ILE:HD13	1:A:43:LEU:HD23	2.00	0.43
1:A:623:PHE:HZ	1:B:786:ALA:N	2.15	0.43
1:A:130:TRP:HZ2	1:A:219:HIS:CD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:TYR:CE1	1:B:47:ILE:HG12	2.54	0.43
1:A:504:ILE:HD11	1:A:723:VAL:HG11	2.00	0.43
1:C:163:ILE:HG21	1:C:180:LEU:HD13	1.98	0.43
1:C:517:PHE:CE1	1:C:795:VAL:HG22	2.54	0.43
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.50	0.43
1:A:76:PHE:CE2	1:A:99:PRO:HG2	2.54	0.43
1:B:787:LEU:CD2	1:B:787:LEU:C	2.86	0.43
1:C:209:ILE:HG23	1:C:214:HIS:CE1	2.54	0.43
1:D:504:ILE:HD11	1:D:723:VAL:HG11	2.00	0.43
1:B:481:ILE:HG23	1:B:491:PHE:CD2	2.54	0.43
1:C:627:GLU:O	1:C:629:MET:N	2.52	0.43
1:A:372:GLY:HA2	1:A:382:LEU:HB3	2.00	0.43
1:B:763:LYS:O	1:B:767:TRP:HB2	2.18	0.43
1:B:168:ILE:HD11	1:B:200:LYS:NZ	2.34	0.43
1:B:476:ILE:HG22	1:B:734:ILE:HG23	2.00	0.43
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.53	0.43
1:D:177:TYR:HD1	1:D:177:TYR:HA	1.73	0.43
1:D:634:GLU:HA	1:D:723:VAL:HB	2.00	0.43
1:A:521:LEU:HA	1:B:787:LEU:HD11	1.16	0.43
1:C:397:VAL:O	1:C:443:THR:OG1	2.30	0.43
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.53	0.43
1:B:702:TYR:CE2	1:B:704:LEU:HB3	2.54	0.43
1:C:502:ILE:O	1:C:709:ASN:ND2	2.48	0.43
1:A:118:LYS:HG2	1:A:145:THR:HG22	2.00	0.42
1:C:403:SER:HA	1:C:404:PRO:HA	1.83	0.42
1:C:629:MET:SD	1:C:629:MET:O	2.75	0.42
1:C:498:LEU:HD12	1:C:730:LYS:CD	2.48	0.42
1:C:600:ILE:HG22	1:D:581:LEU:HD13	1.99	0.42
1:A:290:GLN:HG2	1:A:338:VAL:HG21	2.00	0.42
1:B:507:PRO:HD2	1:B:508:GLN:HA	2.01	0.42
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.55	0.42
1:B:408:MET:HG2	1:B:421:TYR:CE1	2.53	0.42
1:C:103:THR:O	1:C:352:LYS:NZ	2.52	0.42
1:C:580:SER:O	1:C:584:PHE:N	2.51	0.42
1:B:619:ASN:HA	1:C:624:LEU:HD13	2.01	0.42
1:D:261:ARG:HA	1:D:261:ARG:HD2	1.83	0.42
1:A:763:LYS:O	1:A:767:TRP:HB2	2.20	0.42
1:C:597:SER:O	1:C:601:VAL:HG23	2.18	0.42
1:C:749:ALA:O	1:C:753:LEU:HG	2.19	0.42
1:A:110:VAL:HG11	1:A:112:GLN:NE2	2.32	0.42
1:A:498:LEU:C	1:A:498:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HA	1:A:195:ASP:HB3	2.02	0.42
1:A:362:GLU:HG3	1:A:371:ILE:HG21	2.02	0.42
1:C:498:LEU:CD1	1:C:730:LYS:HG3	2.50	0.42
1:D:474:ILE:HG13	1:D:736:THR:HG22	2.00	0.42
1:A:518:LEU:O	1:A:526:TRP:NE1	2.53	0.42
1:A:719:ASP:OD1	1:A:719:ASP:N	2.52	0.42
1:C:13:GLN:HG2	1:C:70:VAL:HG12	2.01	0.42
1:D:274:HIS:O	1:D:274:HIS:CG	2.72	0.42
1:D:43:LEU:O	1:D:45:PRO:HD3	2.20	0.42
1:B:507:PRO:N	1:B:508:GLN:HA	2.34	0.42
1:C:520:PRO:HB2	1:C:616:TYR:CE2	2.54	0.42
1:A:358:ILE:HB	1:A:374:TRP:CD1	2.54	0.42
1:A:483:LEU:O	1:A:487:GLU:HG3	2.20	0.42
1:C:611:ILE:HG21	1:D:517:PHE:HE1	1.84	0.42
1:D:122:LEU:HD21	1:D:149:VAL:HA	2.00	0.42
1:C:362:GLU:HG3	1:C:371:ILE:HG21	2.01	0.41
1:C:498:LEU:CD2	1:C:732:TYR:CE2	3.03	0.41
1:A:130:TRP:CZ3	1:A:191:ARG:HB3	2.55	0.41
1:D:79:LYS:HD2	1:D:142:GLY:HA2	2.02	0.41
1:A:625:THR:HG22	1:D:622:ALA:HA	2.02	0.41
1:C:356:TYR:HH	1:C:374:TRP:HZ3	1.68	0.41
1:C:388:SER:N	1:C:389:GLY:HA2	2.35	0.41
1:C:659:PHE:HB3	1:C:671:TRP:HB2	2.02	0.41
1:A:168:ILE:HD11	1:A:200:LYS:NZ	2.34	0.41
1:B:265:LEU:HD13	1:B:270:TYR:CD2	2.56	0.41
1:C:266:GLU:HG2	1:C:268:LYS:H	1.85	0.41
1:D:61:ALA:O	1:D:65:GLN:HG2	2.20	0.41
1:D:489:ILE:HD13	1:D:735:ALA:HB1	2.03	0.41
1:B:337:GLN:NE2	2:B:901:NAG:O7	2.53	0.41
1:C:623:PHE:HA	1:C:626:VAL:HG23	2.02	0.41
1:B:793:ALA:HB1	1:B:797:TYR:CE2	2.55	0.41
1:C:71:TYR:HA	1:C:323:TRP:HH2	1.85	0.41
1:C:529:ILE:HD13	1:C:612:ILE:HD12	2.02	0.41
1:D:234:LYS:HG2	1:D:234:LYS:H	1.66	0.41
1:A:77:TYR:CD1	1:A:82:VAL:HA	2.55	0.41
1:A:77:TYR:CD1	1:A:82:VAL:HG23	2.50	0.41
1:B:518:LEU:O	1:B:526:TRP:NE1	2.52	0.41
1:C:475:ALA:HB3	1:C:735:ALA:HB3	2.02	0.41
1:B:320:ALA:O	1:B:322:PRO:HD3	2.20	0.41
1:B:521:LEU:HB2	1:B:526:TRP:CE2	2.56	0.41
1:A:517:PHE:O	1:A:520:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ILE:HD11	1:B:806:ALA:HA	2.03	0.41
1:B:135:TYR:CD2	1:B:146:LEU:HD13	2.56	0.41
1:C:417:GLY:O	1:C:420:ARG:NE	2.53	0.41
1:C:631:SER:N	1:C:632:PRO:CA	2.77	0.41
1:D:377:VAL:CG1	1:D:378:ASP:OD1	2.68	0.41
1:B:215:VAL:HA	1:B:238:GLY:O	2.21	0.41
1:C:177:TYR:HA	1:C:177:TYR:HD1	1.78	0.41
1:C:684:ARG:HG2	1:C:685:THR:HG23	2.02	0.41
1:D:110:VAL:HG12	1:D:112:GLN:HG3	2.02	0.41
1:D:498:LEU:HG	1:D:730:LYS:HG3	2.03	0.41
1:B:74:PHE:HA	1:B:97:ILE:O	2.21	0.41
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.56	0.41
1:C:631:SER:HB2	1:C:632:PRO:C	2.41	0.41
1:A:348:ASP:HB3	1:A:354:ILE:HG21	2.02	0.40
1:B:261:ARG:O	1:B:265:LEU:HG	2.21	0.40
1:B:346:LYS:HE3	1:B:355:ASN:HD22	1.87	0.40
1:B:474:ILE:HG12	1:B:475:ALA:H	1.85	0.40
1:B:219:HIS:HD2	1:B:241:GLU:O	2.05	0.40
1:B:507:PRO:CD	1:B:508:GLN:HA	2.51	0.40
1:C:447:ASP:OD2	1:C:462:GLY:N	2.53	0.40
1:C:627:GLU:C	1:C:629:MET:N	2.75	0.40
1:A:131:ASP:N	1:A:131:ASP:OD1	2.55	0.40
1:B:502:ILE:HB	1:B:723:VAL:HG23	2.04	0.40
1:C:705:GLU:OE1	1:C:705:GLU:N	2.52	0.40
1:D:715:ARG:HA	1:D:772:GLU:HG2	2.02	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.94	0.40
1:A:672:THR:HG22	1:A:675:ARG:NH2	2.37	0.40
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.57	0.40
1:B:403:SER:HA	1:B:404:PRO:HA	1.86	0.40
1:D:360:ILE:HD11	1:D:374:TRP:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ASP:O	1:D:10:ASN:N[1_455]	2.18	0.02

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	767/803 (96%)	720 (94%)	45 (6%)	2 (0%)	41	74
1	B	767/803 (96%)	713 (93%)	51 (7%)	3 (0%)	34	70
1	C	767/803 (96%)	716 (93%)	45 (6%)	6 (1%)	19	57
1	D	770/803 (96%)	718 (93%)	50 (6%)	2 (0%)	41	74
All	All	3071/3212 (96%)	2867 (93%)	191 (6%)	13 (0%)	34	70

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	786	ALA
1	C	511	LYS
1	C	512	PRO
1	C	628	ARG
1	D	593	PRO
1	D	520	PRO
1	A	520	PRO
1	B	520	PRO
1	A	631	SER
1	C	633	ILE
1	C	631	SER
1	C	630	VAL
1	B	507	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	621 (99%)	6 (1%)	76	86
1	B	638/683 (93%)	618 (97%)	20 (3%)	40	65
1	C	624/683 (91%)	617 (99%)	7 (1%)	73	85
1	D	625/683 (92%)	613 (98%)	12 (2%)	57	76
All	All	2514/2732 (92%)	2469 (98%)	45 (2%)	59	77

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	TYR
1	A	323	TRP
1	A	515	PHE
1	A	523	TYR
1	A	585	MET
1	A	630	VAL
1	B	88	PHE
1	B	114	ARG
1	B	143	LEU
1	B	178	ARG
1	B	191	ARG
1	B	274	HIS
1	B	323	TRP
1	B	385	ASP
1	B	440	TYR
1	B	450	TYR
1	B	491	PHE
1	B	523	TYR
1	B	581	LEU
1	B	585	MET
1	B	586	GLN
1	B	629	MET
1	B	639	LEU
1	B	773	CYS
1	B	787	LEU
1	B	799	LEU
1	C	323	TRP
1	C	523	TYR
1	C	579	PHE
1	C	585	MET
1	C	631	SER
1	C	787	LEU
1	C	795	VAL

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Mol	Chain	Res	Type
1	D	177	TYR
1	D	323	TRP
1	D	515	PHE
1	D	523	TYR
1	D	533	TYR
1	D	579	PHE
1	D	581	LEU
1	D	585	MET
1	D	610	LEU
1	D	787	LEU
1	D	789	LEU
1	D	791	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	B	112	GLN
1	B	219	HIS
1	C	219	HIS
1	C	587	GLN
1	D	791	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
2	NAG	C	901	1	14,14,15	0.29	0	17,19,21	0.58	0
2	NAG	A	901	1	14,14,15	0.48	0	17,19,21	0.51	0
3	GYK	C	902	-	27,29,29	3.75	9 (33%)	30,42,42	2.18	9 (30%)
3	GYK	A	902	-	27,29,29	3.81	9 (33%)	30,42,42	2.16	10 (33%)
3	GYK	B	902	-	27,29,29	3.76	9 (33%)	30,42,42	2.03	7 (23%)
3	GYK	D	902	-	27,29,29	3.77	8 (29%)	30,42,42	2.48	8 (26%)
2	NAG	D	901	1	14,14,15	0.37	0	17,19,21	0.51	0
2	NAG	B	901	1	14,14,15	0.33	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
3	GYK	C	902	-	-	2/6/32/32	0/3/4/4
3	GYK	A	902	-	-	2/6/32/32	0/3/4/4
3	GYK	B	902	-	-	4/6/32/32	0/3/4/4
3	GYK	D	902	-	-	2/6/32/32	0/3/4/4
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GYK	C10-N11	14.17	1.46	1.30
3	D	902	GYK	C10-N11	14.04	1.46	1.30
3	C	902	GYK	C10-N11	13.93	1.45	1.30
3	B	902	GYK	C10-N11	13.59	1.45	1.30
3	B	902	GYK	C13-N15	8.42	1.45	1.34
3	C	902	GYK	C13-N15	8.25	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GYK	C13-N15	8.07	1.45	1.34
3	D	902	GYK	C13-N15	7.93	1.44	1.34
3	A	902	GYK	O26-C25	-5.82	1.32	1.43
3	B	902	GYK	O26-C25	-5.70	1.32	1.43
3	D	902	GYK	O26-C25	-5.68	1.32	1.43
3	C	902	GYK	O26-C25	-5.64	1.32	1.43
3	A	902	GYK	O24-C25	-5.59	1.32	1.43
3	C	902	GYK	O24-C25	-5.53	1.32	1.43
3	D	902	GYK	O24-C25	-5.53	1.32	1.43
3	B	902	GYK	O24-C25	-5.52	1.32	1.43
3	A	902	GYK	C09-C10	5.28	1.56	1.49
3	D	902	GYK	C09-C10	5.24	1.56	1.49
3	B	902	GYK	C09-C10	5.23	1.56	1.49
3	C	902	GYK	C09-C10	4.82	1.56	1.49
3	A	902	GYK	C08-C07	2.49	1.43	1.38
3	B	902	GYK	C08-C07	2.48	1.43	1.38
3	B	902	GYK	O14-C13	-2.35	1.18	1.23
3	B	902	GYK	C05-C04	2.35	1.43	1.39
3	D	902	GYK	O14-C13	-2.34	1.18	1.23
3	C	902	GYK	O14-C13	-2.28	1.18	1.23
3	A	902	GYK	O14-C13	-2.27	1.18	1.23
3	C	902	GYK	C05-C04	2.17	1.43	1.39
3	C	902	GYK	C17-C10	2.11	1.52	1.49
3	A	902	GYK	C20-N23	2.10	1.45	1.38
3	C	902	GYK	C20-N23	2.09	1.45	1.38
3	D	902	GYK	C05-C04	2.08	1.43	1.39
3	A	902	GYK	C05-C04	2.06	1.43	1.39
3	D	902	GYK	C08-C07	2.03	1.42	1.38
3	B	902	GYK	C20-N23	2.02	1.45	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	GYK	C09-C10-C17	-7.67	109.19	118.11
3	C	902	GYK	C09-C10-C17	-5.62	111.58	118.11
3	D	902	GYK	O24-C07-C08	5.12	134.70	127.85
3	B	902	GYK	O24-C07-C08	5.09	134.66	127.85
3	A	902	GYK	O24-C07-C08	5.03	134.58	127.85
3	A	902	GYK	O24-C07-C06	-4.88	104.23	109.78
3	C	902	GYK	O24-C07-C08	4.59	133.99	127.85
3	B	902	GYK	O24-C07-C06	-4.50	104.66	109.78
3	D	902	GYK	O26-C06-C05	4.47	133.83	127.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	GYK	O26-C06-C05	4.39	133.72	127.85
3	B	902	GYK	O26-C06-C05	4.35	133.67	127.85
3	A	902	GYK	C25-O24-C07	4.18	110.78	105.34
3	A	902	GYK	O26-C06-C05	4.09	133.32	127.85
3	D	902	GYK	O24-C07-C06	-4.07	105.15	109.78
3	B	902	GYK	C25-O24-C07	3.92	110.44	105.34
3	D	902	GYK	C16-N15-C13	-3.80	116.78	120.69
3	C	902	GYK	O24-C07-C06	-3.49	105.81	109.78
3	C	902	GYK	O26-C06-C07	-3.45	105.85	109.78
3	D	902	GYK	C25-O24-C07	3.44	109.81	105.34
3	A	902	GYK	C09-C10-C17	-3.17	114.42	118.11
3	C	902	GYK	C25-O24-C07	3.05	109.30	105.34
3	C	902	GYK	C25-O26-C06	2.96	109.18	105.34
3	D	902	GYK	O26-C06-C07	-2.90	106.48	109.78
3	B	902	GYK	C25-O26-C06	2.86	109.06	105.34
3	B	902	GYK	O26-C06-C07	-2.85	106.53	109.78
3	A	902	GYK	C01-C02-N12	-2.69	107.91	111.14
3	A	902	GYK	C04-C03-C02	-2.69	108.50	115.55
3	A	902	GYK	C25-O26-C06	2.69	108.83	105.34
3	D	902	GYK	C25-O26-C06	2.62	108.74	105.34
3	A	902	GYK	O26-C06-C07	-2.52	106.91	109.78
3	A	902	GYK	C05-C04-C09	2.24	122.24	119.24
3	B	902	GYK	C01-C02-N12	-2.23	108.46	111.14
3	C	902	GYK	C16-N15-C13	-2.11	118.52	120.69
3	C	902	GYK	C01-C02-N12	-2.06	108.66	111.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

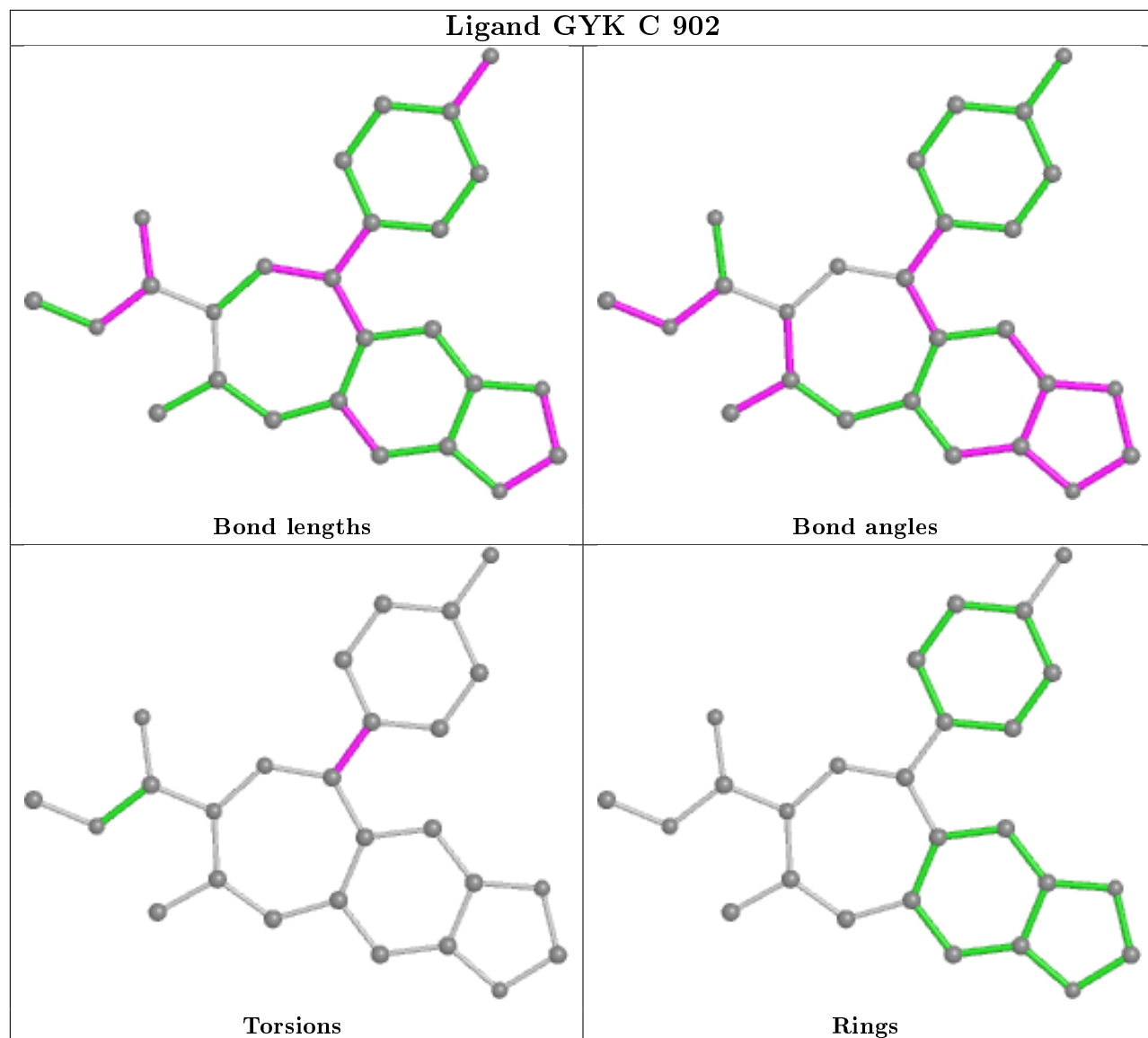
Mol	Chain	Res	Type	Atoms
3	A	902	GYK	C09-C10-C17-C18
3	A	902	GYK	C09-C10-C17-C22
3	B	902	GYK	N11-C10-C17-C18
3	C	902	GYK	C09-C10-C17-C18
3	C	902	GYK	C09-C10-C17-C22
3	D	902	GYK	C09-C10-C17-C22
3	D	902	GYK	C09-C10-C17-C18
3	B	902	GYK	C09-C10-C17-C18
3	B	902	GYK	C09-C10-C17-C22
3	B	902	GYK	N11-C10-C17-C22

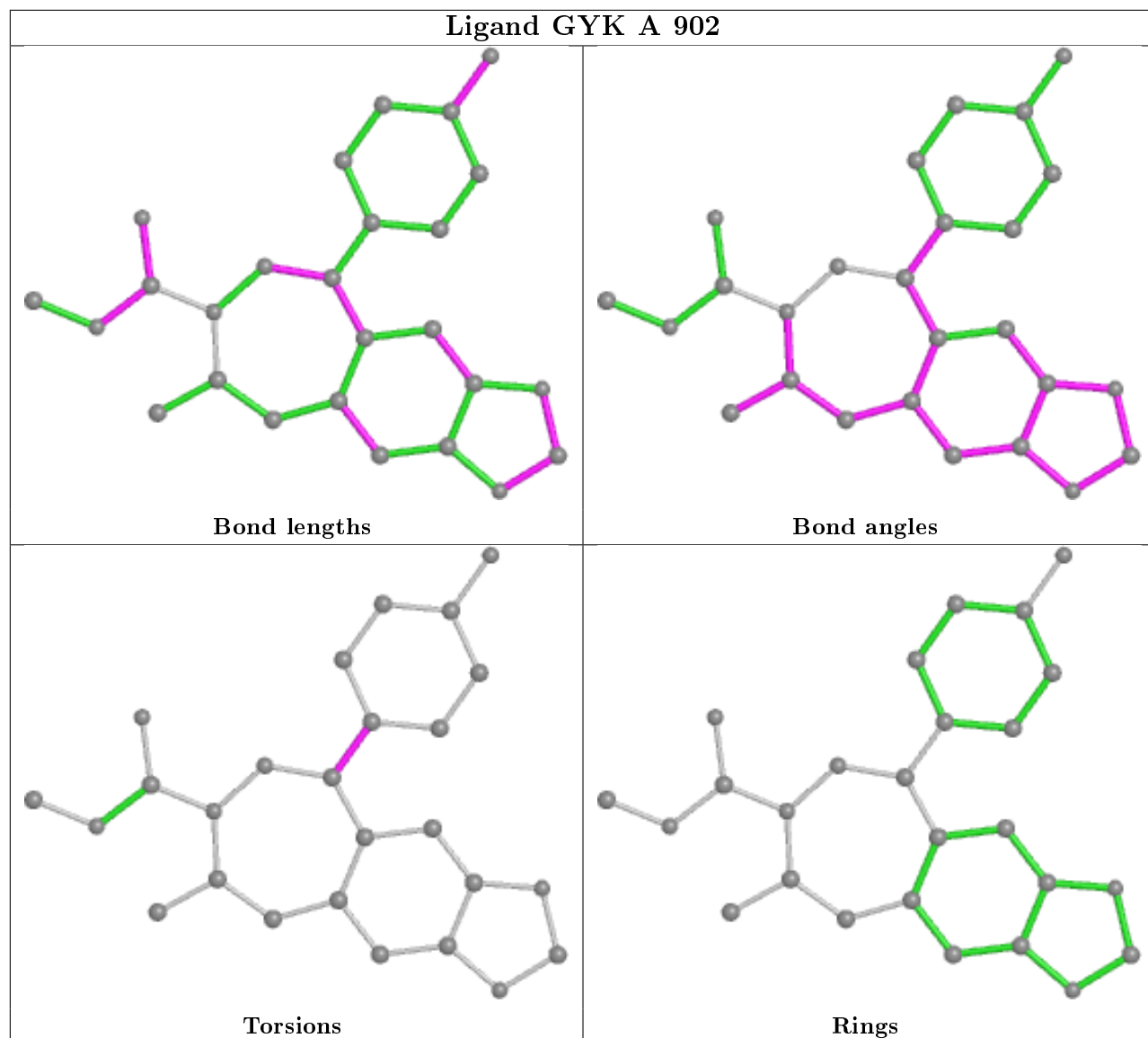
There are no ring outliers.

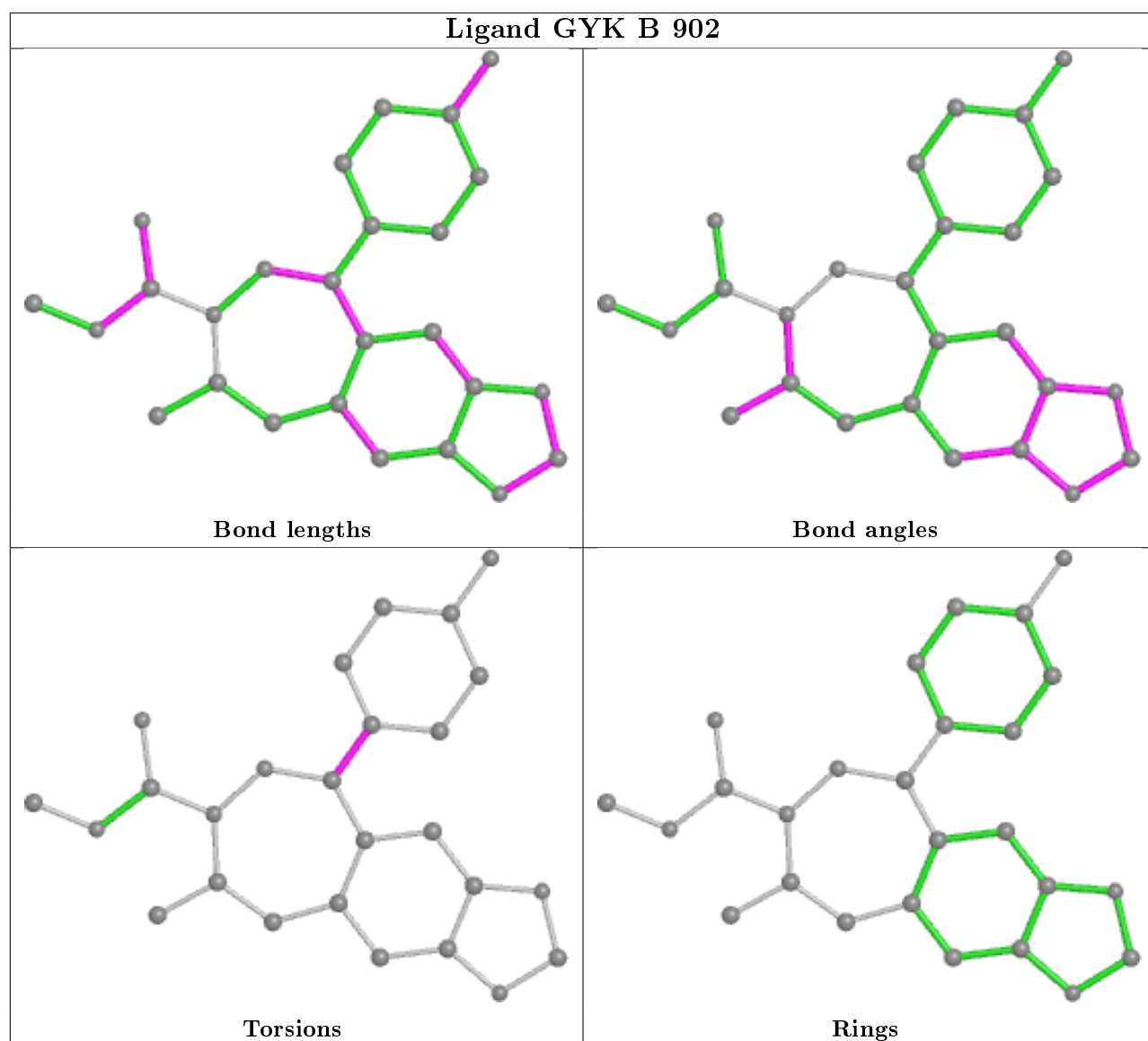
8 monomers are involved in 13 short contacts:

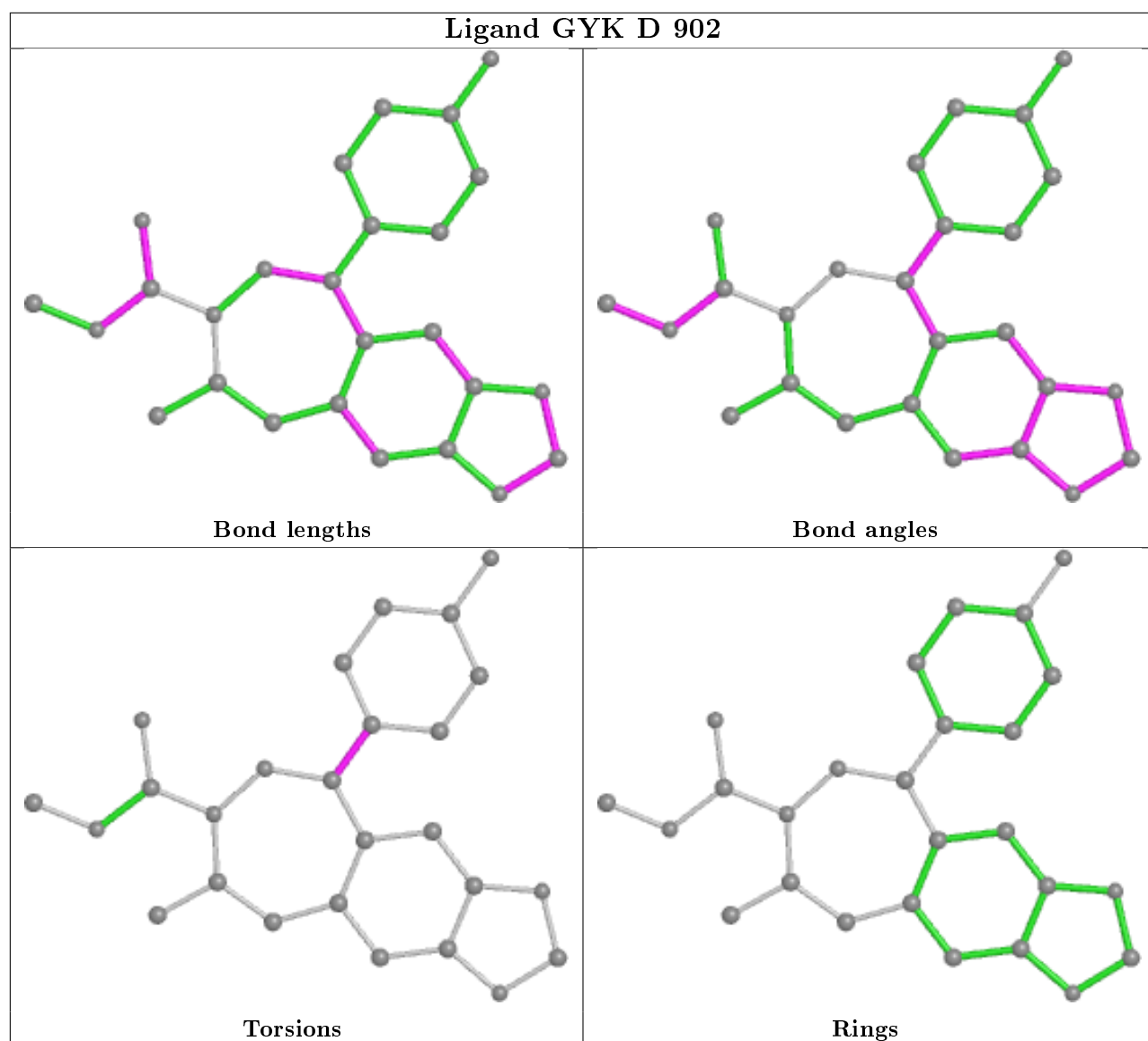
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	NAG	1	0
2	A	901	NAG	1	0
3	C	902	GYK	3	0
3	A	902	GYK	1	0
3	B	902	GYK	3	0
3	D	902	GYK	2	0
2	D	901	NAG	1	0
2	B	901	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 ⓘ

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	773/803 (96%)	-0.13	16 (2%) 63 55	72, 144, 238, 285	0
1	B	773/803 (96%)	-0.14	17 (2%) 62 54	69, 131, 228, 272	0
1	C	773/803 (96%)	0.07	25 (3%) 47 38	101, 167, 232, 261	0
1	D	776/803 (96%)	0.09	38 (4%) 29 25	109, 180, 249, 281	0
All	All	3095/3212 (96%)	-0.03	96 (3%) 49 40	69, 155, 240, 285	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	476	ILE	9.3
1	D	475	ALA	7.8
1	D	477	ALA	5.5
1	D	544	SER	5.3
1	A	782	GLU	5.2
1	D	733	GLY	5.1
1	A	580	SER	4.8
1	C	588	GLY	4.8
1	C	780	SER	4.6
1	A	400	ILE	4.5
1	B	816	TYR	4.1
1	D	543	VAL	4.1
1	D	779	GLY	4.1
1	D	780	SER	3.9
1	B	815	CYS	3.8
1	B	781	LYS	3.7
1	C	272	GLY	3.7
1	B	649	THR	3.6
1	C	784	THR	3.6
1	D	175	GLU	3.5
1	B	588	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	442	LEU	3.5
1	C	684	ARG	3.5
1	A	512	PRO	3.4
1	D	527	MET	3.4
1	B	813	GLU	3.3
1	D	453	ARG	3.3
1	C	775	ALA	3.2
1	B	104	ASP	3.2
1	D	426	VAL	3.1
1	D	384	GLU	3.1
1	B	780	SER	3.1
1	B	456	ASP	3.0
1	C	276	ALA	3.0
1	A	401	LEU	3.0
1	D	172	LYS	3.0
1	A	579	PHE	2.9
1	D	485	ARG	2.9
1	D	486	GLU	2.9
1	D	460	TRP	2.8
1	B	144	SER	2.8
1	C	16	GLY	2.8
1	C	573	ILE	2.8
1	D	732	TYR	2.7
1	A	574	PHE	2.7
1	D	474	ILE	2.7
1	A	587	GLN	2.7
1	C	410	LYS	2.7
1	B	476	ILE	2.7
1	B	775	ALA	2.7
1	D	734	ILE	2.7
1	C	587	GLN	2.7
1	D	493	LYS	2.6
1	C	181	PHE	2.5
1	D	423	GLY	2.5
1	D	644	GLU	2.5
1	C	783	LYS	2.5
1	C	184	LEU	2.5
1	D	441	LYS	2.4
1	C	776	LYS	2.4
1	D	399	THR	2.4
1	D	421	TYR	2.4
1	D	588	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	587	GLN	2.3
1	D	408	MET	2.3
1	D	694	ARG	2.3
1	A	386	ASP	2.3
1	D	495	PHE	2.3
1	D	385	ASP	2.3
1	A	511	LYS	2.2
1	B	440	TYR	2.2
1	C	17	LEU	2.2
1	A	543	VAL	2.2
1	C	577	LEU	2.2
1	C	28	ALA	2.2
1	A	523	TYR	2.2
1	A	399	THR	2.2
1	C	265	LEU	2.2
1	D	587	GLN	2.2
1	A	588	GLY	2.1
1	C	273	ALA	2.1
1	C	421	TYR	2.1
1	B	729	SER	2.1
1	C	683	VAL	2.1
1	C	385	ASP	2.1
1	D	691	ALA	2.1
1	D	695	LYS	2.1
1	C	341	LEU	2.1
1	D	725	GLY	2.1
1	D	778	SER	2.1
1	D	450	TYR	2.1
1	C	512	PRO	2.0
1	B	682	PHE	2.0
1	A	43	LEU	2.0
1	A	388	SER	2.0
1	B	648	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

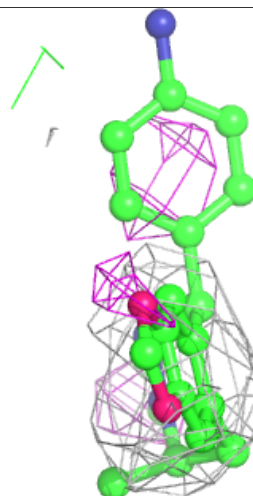
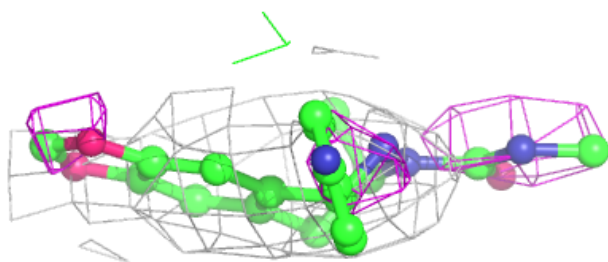
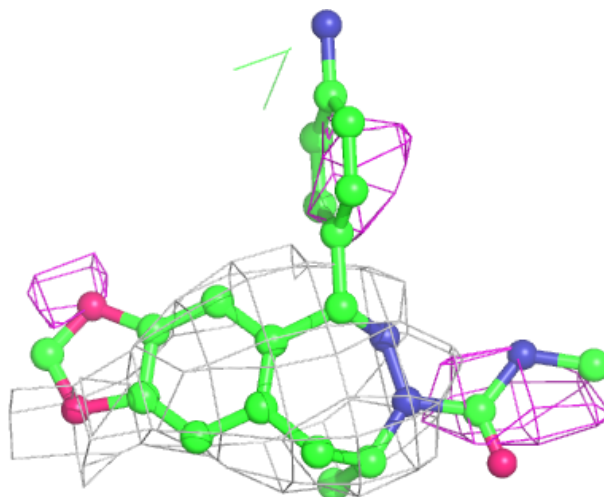
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	901	14/15	0.27	0.67	416,416,418,424	0
2	NAG	A	901	14/15	0.62	1.02	255,255,257,262	0
2	NAG	D	901	14/15	0.66	0.36	269,269,270,272	0
2	NAG	B	901	14/15	0.71	0.28	196,196,199,200	0
3	GYK	C	902	26/26	0.74	0.68	128,169,210,219	0
3	GYK	A	902	26/26	0.82	0.41	128,169,210,219	0
3	GYK	D	902	26/26	0.90	0.18	128,169,210,219	0
3	GYK	B	902	26/26	0.91	0.21	128,169,210,219	0

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.

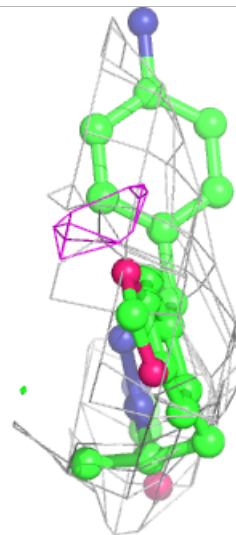
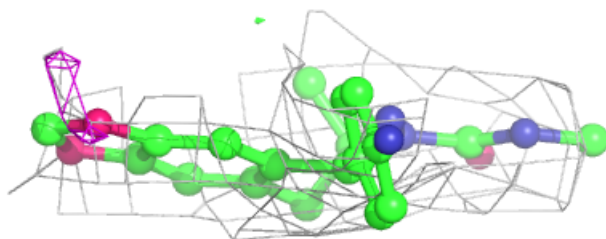
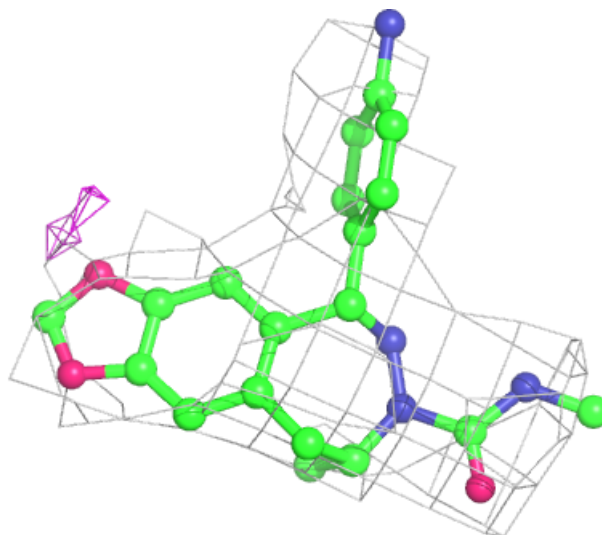
Electron density around GYK C 902:

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



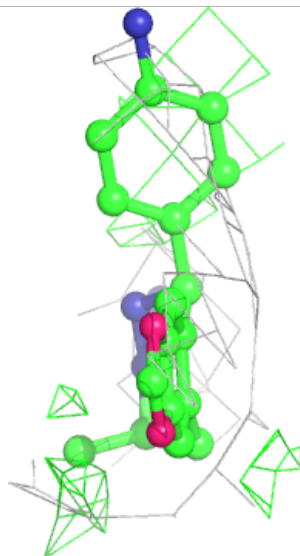
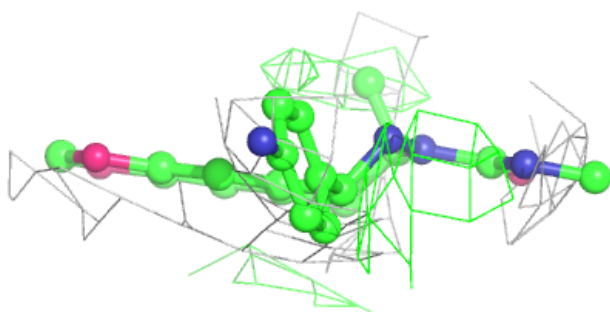
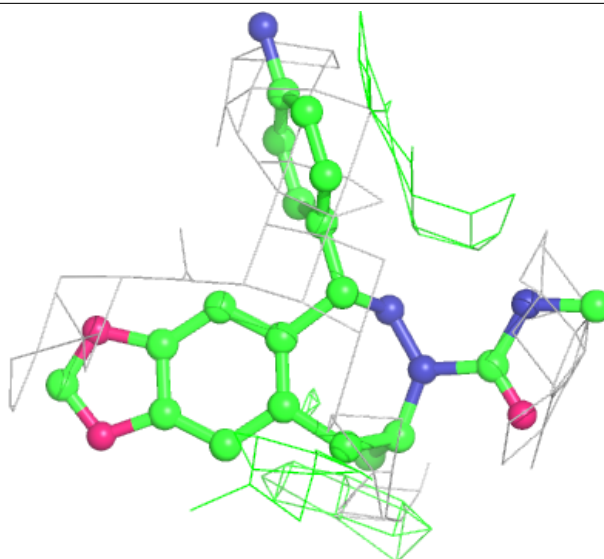
Electron density around GYK A 902:

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



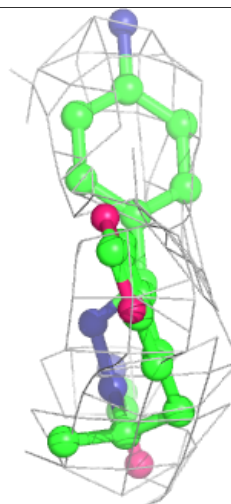
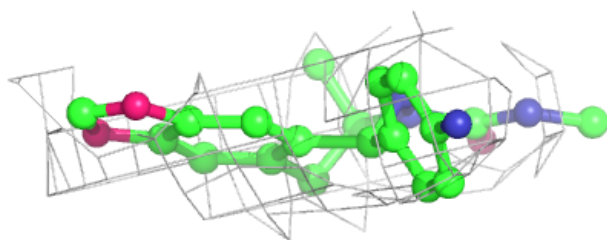
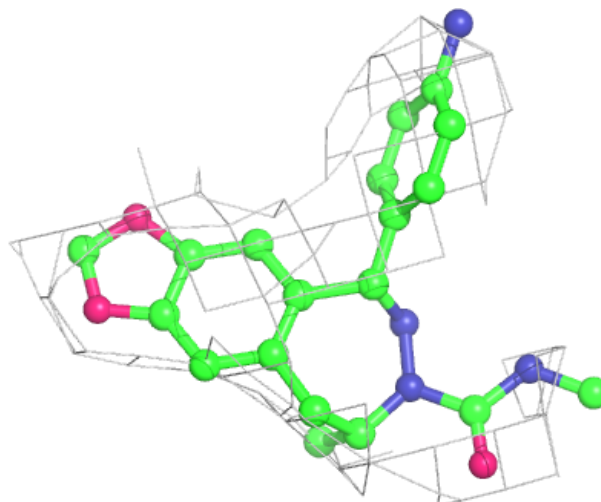
Electron density around GYK D 902:

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



Electron density around GYK 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.