



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:43 AM UTC

PDB ID : 5L1H / pdb_00005l1h
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 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

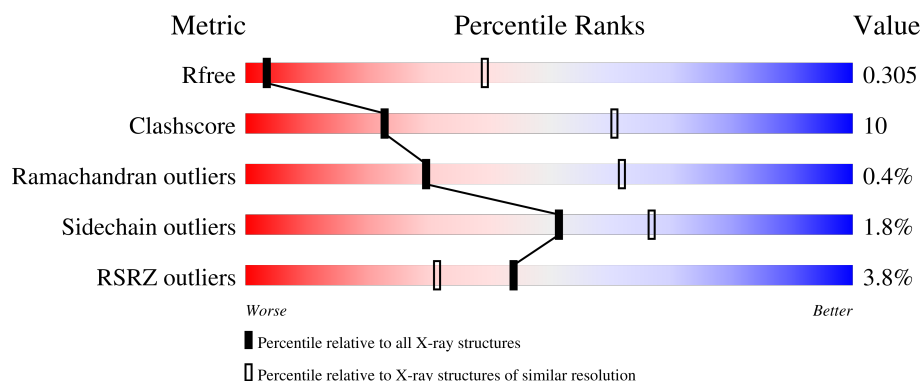
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	
1	B	803	
1	C	803	
1	D	803	

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

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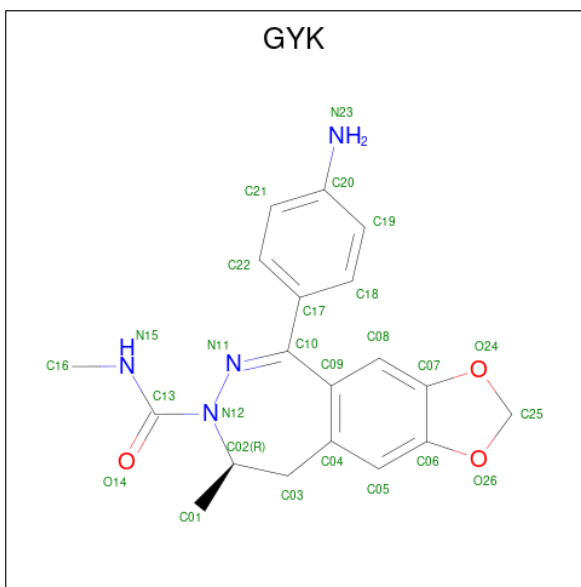
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491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

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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-aminophenyl)-N,8-dimethyl-8,9-dihydro-2H,7H-[1,3]dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide (CCD ID: GYK) (formula: $C_{19}H_{20}N_4O_3$).

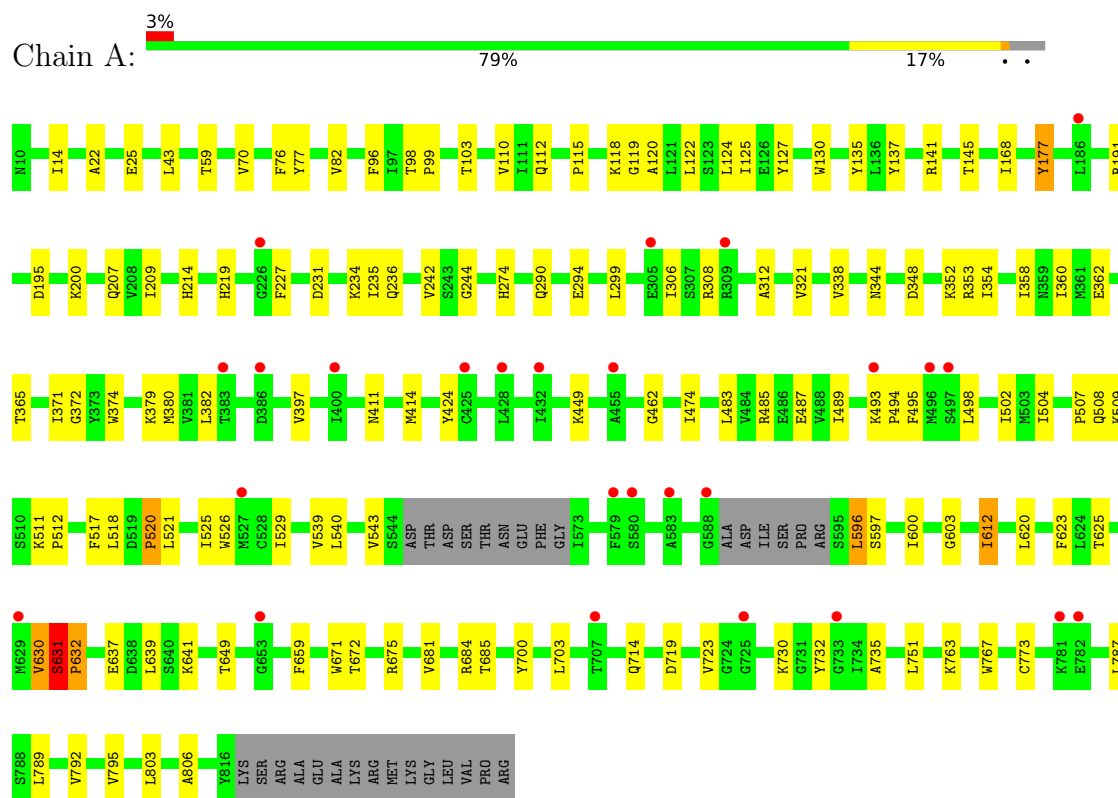


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	4	3		
3	B	1	Total	C	N	O	0	0
			26	19	4	3		
3	C	1	Total	C	N	O	0	0
			26	19	4	3		
3	D	1	Total	C	N	O	0	0
			26	19	4	3		

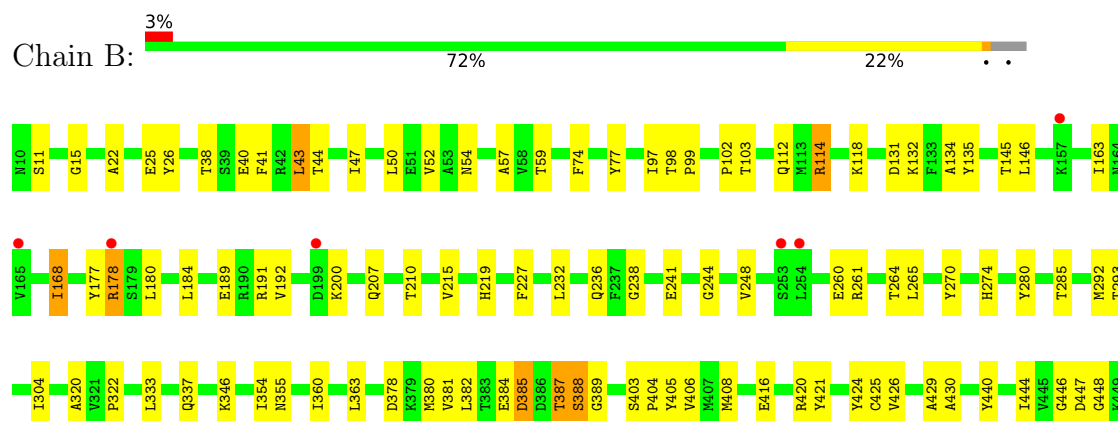
3 Residue-property plots

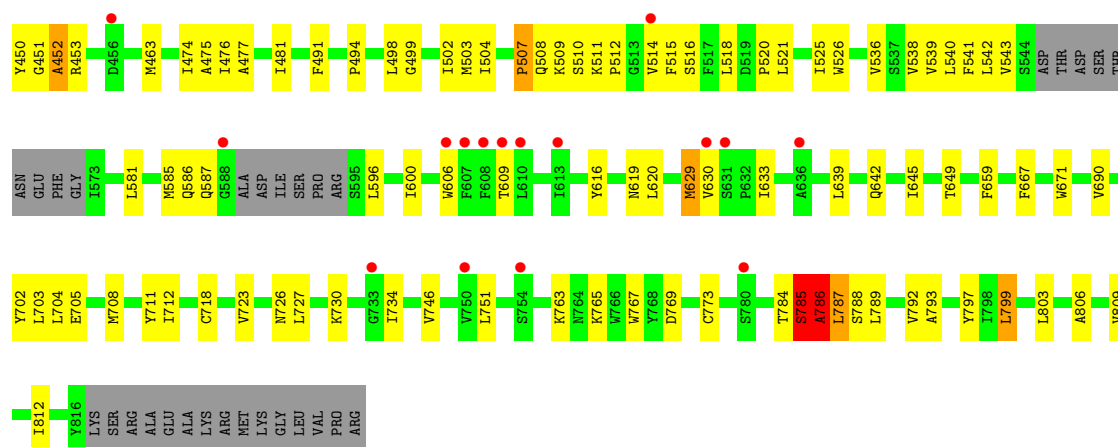
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

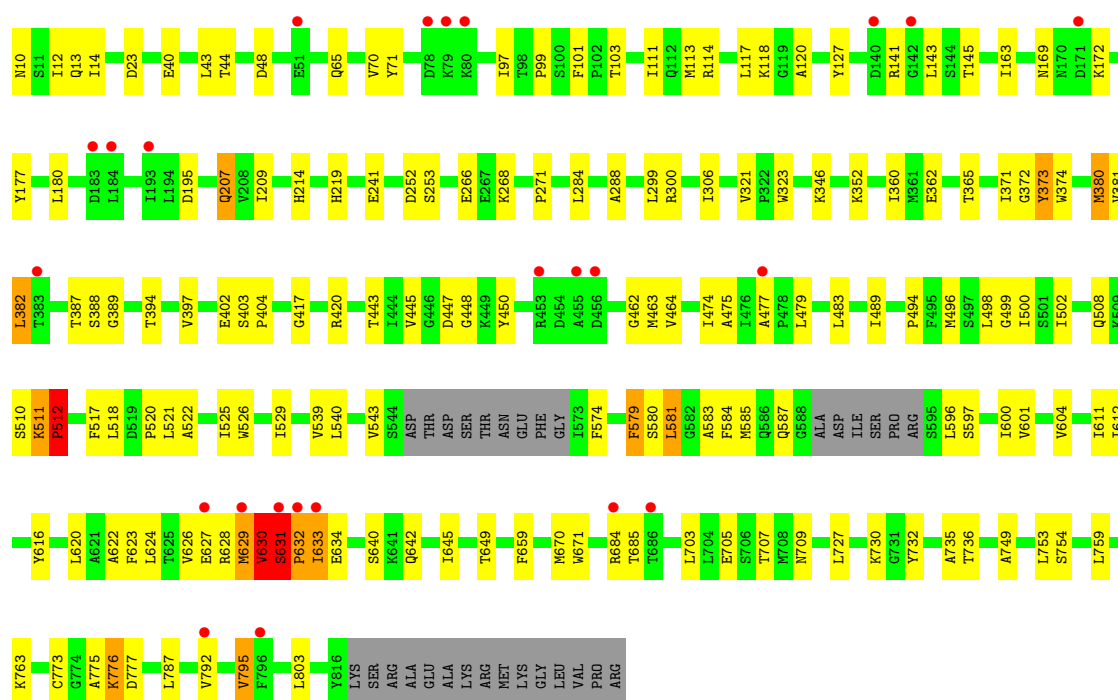
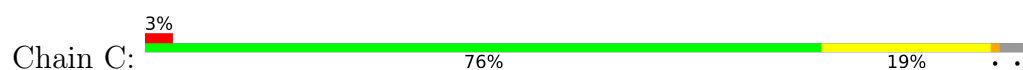


• Molecule 1: Glutamate receptor 2

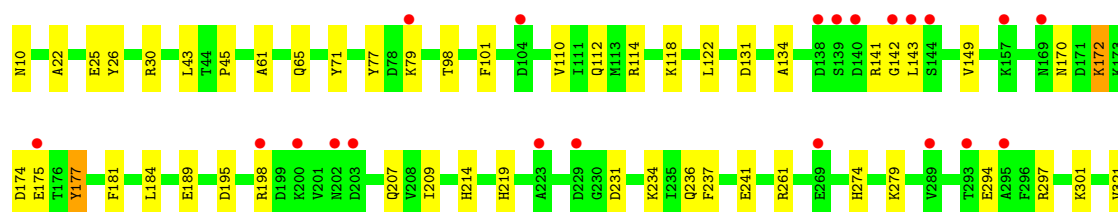
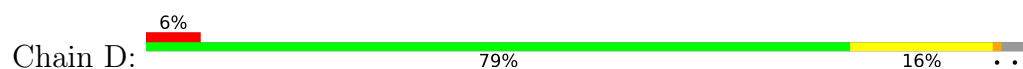


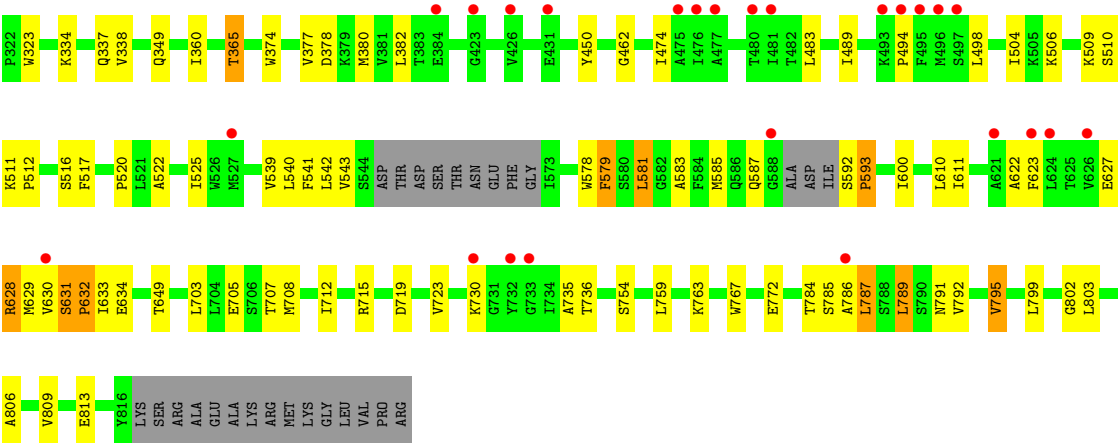


• Molecule 1: Glutamate receptor 2



• 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	92.59Å 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 0.285 , 0.305	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)	0.26 , 105.8	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	0.87	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: NAG, GYK

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	0.18	3/6092 (0.0%)	0.39	5/8244 (0.1%)
1	B	0.19	1/6123 (0.0%)	0.51	12/8284 (0.1%)
1	C	0.18	2/6082 (0.0%)	0.50	15/8235 (0.2%)
1	D	0.21	3/6098 (0.0%)	0.40	8/8257 (0.1%)
All	All	0.19	9/24395 (0.0%)	0.46	40/33020 (0.1%)

All (9) 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	6.42	1.58	1.46
1	D	511	LYS	C-N	6.10	1.40	1.33
1	A	511	LYS	C-N	5.73	1.41	1.33
1	D	512	PRO	N-CD	5.54	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	5.34	1.55	1.47
1	C	512	PRO	N-CD	5.18	1.55	1.47

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	629	MET	CB-CA-C	-18.14	85.22	112.07
1	B	452	ALA	CB-CA-C	-14.90	88.14	110.50
1	B	452	ALA	N-CA-C	11.89	144.30	111.00
1	B	453	ARG	N-CA-CB	-11.80	92.51	110.45
1	C	380	MET	N-CA-C	10.98	123.76	110.91
1	D	631	SER	C-N-CD	10.14	142.92	120.60
1	B	453	ARG	N-CA-C	8.75	122.36	110.55
1	C	382	LEU	N-CA-C	8.71	123.79	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	632	PRO	CA-N-CD	-8.14	100.10	111.50
1	A	631	SER	C-N-CD	8.12	138.47	120.60
1	C	631	SER	C-N-CD	7.92	138.01	120.60
1	A	597	SER	N-CA-C	7.77	120.73	111.33
1	B	786	ALA	N-CA-CB	7.70	123.50	110.49
1	B	785	SER	CB-CA-C	7.50	129.81	111.95
1	D	511	LYS	CA-C-N	-7.07	113.38	120.31
1	D	511	LYS	C-N-CA	-7.07	113.38	120.31
1	D	628	ARG	N-CA-C	7.06	118.77	111.14
1	C	512	PRO	CA-N-CD	-7.02	102.17	112.00
1	B	388	SER	CB-CA-C	6.92	123.24	110.10
1	C	777	ASP	N-CA-C	6.90	121.74	113.12
1	B	388	SER	N-CA-C	-6.72	92.19	111.00
1	A	511	LYS	CA-C-N	-6.58	113.20	119.85
1	A	511	LYS	C-N-CA	-6.58	113.20	119.85
1	C	373	TYR	N-CA-C	-6.15	97.69	110.80
1	B	387	THR	N-CA-C	6.14	120.08	112.03
1	D	365	THR	N-CA-C	6.06	117.97	111.36
1	C	630	VAL	N-CA-C	-6.05	96.76	109.34
1	D	172	LYS	N-CA-CB	-5.88	102.36	110.42
1	C	373	TYR	CB-CA-C	5.88	122.12	110.42
1	C	508	GLN	N-CA-C	5.79	119.56	111.74
1	B	516	SER	N-CA-C	-5.76	106.25	113.28
1	C	365	THR	N-CA-C	5.64	118.19	111.71
1	C	374	TRP	N-CA-CB	5.51	119.69	110.59
1	C	512	PRO	N-CA-C	5.41	123.61	112.47
1	B	388	SER	N-CA-CB	5.40	119.67	110.50
1	B	514	VAL	N-CA-C	5.18	117.56	111.09
1	C	775	ALA	N-CA-C	-5.18	106.64	113.17
1	C	776	LYS	N-CA-C	5.10	119.50	113.28
1	D	170	ASN	N-CA-C	-5.08	106.59	112.89
1	A	596	LEU	N-CA-C	-5.00	100.32	108.67

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	126	0
1	B	6001	0	5924	144	1
1	C	5960	0	5850	158	0
1	D	5975	0	5855	110	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	3	0
All	All	24066	0	23555	494	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 (494) 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:623:PHE:CD2	1:D:629:MET:HE3	1.77	1.18
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:D:623:PHE:HD2	1:D:629:MET:HE3	0.94	1.07
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:A:630:VAL:HG22	1:A:631:SER:C	1.92	0.95
1:C:629:MET:CG	1:C:629:MET:O	2.03	0.95
1:B:232:LEU:HD23	1:B:232:LEU:O	1.66	0.95
1:C:632:PRO:CD	1:C:633:ILE:HB	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:77:TYR:HD1	1:A:82:VAL:HB	1.30	0.93
1:C:629:MET:O	1:C:629:MET:HG2	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: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
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: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:D:509:LYS:HA	1:D:510:SER:C	2.13	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:629:MET:HE1	3:D:902:GYK:C03	2.21	0.71
1:D:377:VAL:CG1	1:D:378:ASP:H	2.01	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:77:TYR:CZ	1:A:82:VAL:HG23	2.28	0.68
1:B:118:LYS:HB3	1:B:145:THR:HG22	1.76	0.68
1:A:603:GLY:HA2	1:B:585:MET:HB3	1.76	0.67
1:B:382:LEU:HD13	1:B:384:GLU:HG3	1.75	0.67
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.59	0.67
1:C:631:SER:OG	1:C:632:PRO:O	2.10	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:C:12:ILE:HG23	1:C:71:TYR:HD2	1.61	0.66
1:C:450:TYR:HA	1:C:463:MET:HE2	1.78	0.65
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
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:HG12	1:D:630:VAL:O	1.97	0.64
1:C:177:TYR:HB3	1:C:207:GLN:HG2	1.80	0.64
1:D:334:LYS:NZ	1:D:349:GLN:O	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:623:PHE:CD2	1:D:629:MET:CE	2.69	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:50:LEU:C	1:B:50:LEU:HD12	2.26	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:B:97:ILE:HD12	1:B:292:MET:HE3	1.83	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:B:503:MET:HE1	1:B:690:VAL:HG22	1.84	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
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.86	0.58
1:C:632:PRO:CG	1:C:633:ILE:HB	2.33	0.58
1:A:792:VAL:HG21	1:D:525:ILE:HG12	1.85	0.58
1:B:508:GLN:N	1:B:509:LYS:HA	2.19	0.58
1:A:498:LEU:CD1	1:A:730:LYS:HG3	2.33	0.58
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.86	0.58
1:C:518:LEU:O	1:C:526:TRP:NE1	2.36	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:498:LEU:HD12	1:A:730:LYS:HG3	1.87	0.57
1:A:520:PRO:HG3	1:A:620:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:784:THR:C	1:B:785:SER:OG	2.49	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: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:C	1:C:382:LEU:HD22	2.32	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
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: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:A:751:LEU:HB2	1:D:483:LEU:HD13	1.89	0.54
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.41	0.54
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.88	0.54
1:A:517:PHE:HE1	1:D:611:ILE:HG21	1.73	0.54
1:A:77:TYR:CD1	1:A:82:VAL:CG2	2.83	0.53
1:B:360:ILE:HD13	1:B:380:MET:HE2	1.88	0.53
1:C:498:LEU:CD1	1:C:730:LYS:HD2	2.38	0.53
1:C:631:SER:HG	1:C:632:PRO:C	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:LEU:HD12	1:D:705:GLU:HB2	1.89	0.53
1:D:540:LEU:HA	1:D:543:VAL:HG22	1.90	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:463:MET:HE1	1:B:477:ALA:HB3	1.90	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:C:113:MET:HE3	1:C:288:ALA:HA	1.92	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:A:168:ILE:HD11	1:A:200:LYS:HZ1	1.74	0.52
1:B:606:TRP:HA	1:B:609:THR:HG22	1.91	0.52
1:B:510:SER:OG	3:B:902:GYK:O14	2.27	0.51
1:A:411:ASN:HB2	1:A:414:MET:HE2	1.91	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
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:97:ILE:HA	1:C:111:ILE:HB	1.93	0.51
1:C:127:TYR:HB2	1:C:380:MET:HE3	1.92	0.51
1:C:604:VAL:HG12	1:D:799:LEU:HD12	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:10:ASN:ND2	1:C:40:GLU:O	2.45	0.49
1:C:252:ASP:OD1	1:C:253:SER:N	2.45	0.49
1:C:631:SER:CB	1:C:632:PRO:C	2.85	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:A:96:PHE:CE2	1:A:98:THR:HB	2.48	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:C:525:ILE:HD11	1:D:789:LEU:HA	1.94	0.49
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.94	0.49
1:B:508:GLN:CB	1:B:629:MET:HE3	2.41	0.49
1:C:10:ASN:HB3	1:C:300:ARG:HH22	1.76	0.49
1:A:623:PHE:CZ	1:B:786:ALA:N	2.81	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: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
1:A:631:SER:HA	1:A:632:PRO:C	2.37	0.49
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:D:632:PRO:O	1:D:633:ILE:C	2.56	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:A:520:PRO:C	1:B:787:LEU:HD12	2.38	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:387:THR:OG1	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:787:LEU:C	1:B:787:LEU:CD2	2.86	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: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:97:ILE:HD11	1:B:333:LEU:HD22	1.96	0.47
1:B:227:PHE:CZ	1:B:232:LEU:CD1	2.95	0.47
1:C:388:SER:H	1:C:389:GLY:HA2	1.80	0.47
1:D:360:ILE:HD13	1:D:380:MET:HE1	1.94	0.47
1:B:734:ILE:HG21	1:B:746:VAL:HG11	1.97	0.47
1:D:377:VAL:CG1	1:D:378:ASP:N	2.65	0.47
1:A:498:LEU:HD12	1:A:498:LEU:C	2.40	0.47
1:D:630:VAL:O	1:D:630:VAL:CG1	2.62	0.47
1:A:596:LEU:HD12	1:A:596:LEU:HA	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: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:381:VAL:HG13	1:B:381:VAL:O	2.14	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
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:499:GLY:HA3	1:B:726:ASN:HB3	1.97	0.46
1:B:708:MET:O	1:B:712:ILE:HG12	2.15	0.46
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.98	0.46
1:D:131:ASP:OD1	1:D:131:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ALA:HB1	1:B:25:GLU:HB2	1.97	0.46
1:B:630:VAL:HG23	1:B:630:VAL:O	2.15	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:C:631:SER:HB2	1:C:632:PRO:C	2.41	0.45
1:B:809:VAL:O	1:B:812:ILE:HG12	2.16	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:O	1:B:515:PHE:CG	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:38:THR:HG23	1:B:41:PHE:H	1.81	0.45
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.99	0.45
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.81	0.45
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.99	0.45
1:C:521:LEU:HA	1:D:787:LEU:HG	1.98	0.45
1:D:143:LEU:H	1:D:143:LEU:HD23	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:A:127:TYR:CG	1:A:380:MET:HE2	2.52	0.45
1:B:751:LEU:HB2	1:C:483:LEU:HD13	1.97	0.45
1:D:541:PHE:CD2	1:D:542:LEU:HD23	2.51	0.45
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:A:787:LEU:O	1:D:522:ALA:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASN:HD21	1:C:172:LYS:HD3	1.81	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: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: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: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:C:611:ILE:HB	1:D:795:VAL:HG11	1.98	0.44
1:D:297:ARG:HG2	1:D:301:LYS:HE3	2.00	0.44
1:D:627:GLU:C	1:D:629:MET:HB2	2.43	0.44
1:D:754:SER:HB2	1:D:759:LEU:HD12	2.00	0.44
1:B:54:ASN:OD1	1:B:57:ALA:N	2.48	0.44
1:B:430:ALA:HA	1:B:440:TYR:HE1	1.83	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:59:THR:HG21	1:B:59:THR:HG21	2.00	0.44
1:A:236:GLN:NE2	1:A:365:THR:O	2.49	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
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:178:ARG:HD3	1:B:178:ARG:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:PHE:CZ	1:B:285:THR:HG23	2.53	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: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:O	1:C:629:MET:SD	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:B:619:ASN:HA	1:C:624:LEU:HD13	2.01	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:D:261:ARG:HD2	1:D:261:ARG:HA	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: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:43:LEU:O	1:D:45:PRO:HD3	2.20	0.42
1:D:274:HIS:O	1:D:274:HIS:CG	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:496:MET:HE2	1:C:763:LYS:HD3	2.02	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:C:627:GLU:C	1:C:629:MET:N	2.75	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:H	1:D:234:LYS:HG2	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:A:168:ILE:HD11	1:A:200:LYS:NZ	2.34	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:C:498:LEU:HD12	1:C:498:LEU:C	2.45	0.41
1:A:110:VAL:HG12	1:A:112:GLN:CD	2.46	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
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:B:215:VAL:HA	1:B:238:GLY:O	2.21	0.41
1:C:177:TYR:HD1	1:C:177:TYR:HA	1.78	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: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:377:VAL:CG1	1:D:378:ASP:OD1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:623:PHE:CE2	1:D:629:MET:HE3	2.46	0.40
1:B:219:HIS:HD2	1:B:241:GLU:O	2.05	0.40
1:B:260:GLU:O	1:B:264:THR:OG1	2.27	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: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:HD23	1:A:122:LEU:HA	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:B:705:GLU:H	1:B:705:GLU:CD	2.28	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 ⓘ

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	767/803 (96%)	720 (94%)	45 (6%)	2 (0%)	36	67
1	B	767/803 (96%)	713 (93%)	51 (7%)	3 (0%)	30	62
1	C	767/803 (96%)	716 (93%)	45 (6%)	6 (1%)	16	48
1	D	770/803 (96%)	718 (93%)	50 (6%)	2 (0%)	36	67
All	All	3071/3212 (96%)	2867 (93%)	191 (6%)	13 (0%)	30	62

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 ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/683 (92%)	622 (99%)	5 (1%)	73	76
1	B	638/683 (93%)	618 (97%)	20 (3%)	35	57
1	C	624/683 (91%)	615 (99%)	9 (1%)	59	70
1	D	625/683 (92%)	614 (98%)	11 (2%)	51	67
All	All	2514/2732 (92%)	2469 (98%)	45 (2%)	51	67

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

Mol	Chain	Res	Type
1	A	177	TYR
1	A	321	VAL
1	A	612	ILE
1	A	630	VAL
1	A	795	VAL
1	B	43	LEU
1	B	114	ARG
1	B	168	ILE
1	B	178	ARG
1	B	191	ARG
1	B	248	VAL
1	B	274	HIS
1	B	304	ILE
1	B	385	ASP
1	B	450	TYR
1	B	581	LEU
1	B	586	GLN
1	B	629	MET
1	B	639	LEU
1	B	718	CYS
1	B	773	CYS
1	B	785	SER
1	B	787	LEU
1	B	792	VAL
1	B	799	LEU
1	C	207	GLN
1	C	321	VAL
1	C	579	PHE
1	C	581	LEU
1	C	585	MET
1	C	631	SER
1	C	634	GLU
1	C	787	LEU
1	C	795	VAL
1	D	118	LYS
1	D	177	TYR
1	D	321	VAL
1	D	579	PHE
1	D	581	LEU
1	D	585	MET
1	D	610	LEU
1	D	787	LEU
1	D	789	LEU

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Mol	Chain	Res	Type
1	D	791	ASN
1	D	795	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	A	418	ASN
1	A	714	GLN
1	A	726	ASN
1	B	83	ASN
1	B	112	GLN
1	B	219	HIS
1	B	586	GLN
1	B	619	ASN
1	C	46	HIS
1	C	93	HIS
1	C	337	GLN
1	C	344	ASN
1	C	587	GLN
1	D	619	ASN
1	D	714	GLN
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 ⓘ

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	B	901	1	14,14,15	0.35	0	17,19,21	0.54	0
3	GYK	A	902	-	27,29,29	3.85	9 (33%)	31,42,42	2.11	10 (32%)
3	GYK	C	902	-	27,29,29	3.79	10 (37%)	31,42,42	2.14	10 (32%)
3	GYK	D	902	-	27,29,29	3.81	8 (29%)	31,42,42	2.45	8 (25%)
3	GYK	B	902	-	27,29,29	3.80	9 (33%)	31,42,42	1.98	7 (22%)
2	NAG	D	901	1	14,14,15	0.39	0	17,19,21	0.53	0
2	NAG	C	901	1	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
2	NAG	A	901	1	14,14,15	0.51	0	17,19,21	0.52	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	B	901	1	-	0/6/23/26	0/1/1/1
3	GYK	A	902	-	-	2/6/32/32	0/3/4/4
3	GYK	C	902	-	-	2/6/32/32	0/3/4/4
3	GYK	D	902	-	-	2/6/32/32	0/3/4/4
3	GYK	B	902	-	-	4/6/32/32	0/3/4/4
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1
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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GYK	C10-N11	14.53	1.46	1.30
3	D	902	GYK	C10-N11	14.40	1.46	1.30
3	C	902	GYK	C10-N11	14.29	1.45	1.30
3	B	902	GYK	C10-N11	13.94	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	-5.57	1.32	1.43
3	B	902	GYK	O26-C25	-5.45	1.32	1.43
3	D	902	GYK	O26-C25	-5.44	1.32	1.43
3	C	902	GYK	O26-C25	-5.39	1.32	1.43
3	A	902	GYK	C09-C10	5.37	1.56	1.49
3	A	902	GYK	O24-C25	-5.34	1.32	1.43
3	D	902	GYK	C09-C10	5.33	1.56	1.49
3	B	902	GYK	C09-C10	5.33	1.56	1.49
3	C	902	GYK	O24-C25	-5.29	1.32	1.43
3	D	902	GYK	O24-C25	-5.29	1.32	1.43
3	B	902	GYK	O24-C25	-5.28	1.32	1.43
3	C	902	GYK	C09-C10	4.91	1.56	1.49
3	A	902	GYK	C08-C07	2.63	1.43	1.38
3	B	902	GYK	C08-C07	2.62	1.43	1.38
3	B	902	GYK	C05-C04	2.57	1.43	1.39
3	B	902	GYK	O14-C13	-2.44	1.18	1.23
3	D	902	GYK	O14-C13	-2.43	1.18	1.23
3	C	902	GYK	C05-C04	2.36	1.43	1.39
3	C	902	GYK	O14-C13	-2.36	1.18	1.23
3	A	902	GYK	O14-C13	-2.35	1.18	1.23
3	D	902	GYK	C05-C04	2.27	1.43	1.39
3	A	902	GYK	C05-C04	2.24	1.43	1.39
3	D	902	GYK	C08-C07	2.13	1.42	1.38
3	C	902	GYK	C17-C10	2.12	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	C	902	GYK	C08-C07	2.02	1.42	1.38
3	B	902	GYK	C20-N23	2.02	1.45	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	GYK	C09-C10-C17	-7.76	109.19	118.12
3	C	902	GYK	C09-C10-C17	-5.69	111.58	118.12
3	D	902	GYK	O24-C07-C08	5.15	134.70	127.86
3	B	902	GYK	O24-C07-C08	5.12	134.66	127.86
3	A	902	GYK	O24-C07-C08	5.06	134.58	127.86
3	C	902	GYK	O24-C07-C08	4.61	133.99	127.86
3	A	902	GYK	O24-C07-C06	-4.59	104.23	109.79
3	D	902	GYK	O26-C06-C05	4.49	133.83	127.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	GYK	O26-C06-C05	4.41	133.72	127.86
3	B	902	GYK	O26-C06-C05	4.37	133.67	127.86
3	B	902	GYK	O24-C07-C06	-4.24	104.66	109.79
3	A	902	GYK	O26-C06-C05	4.11	133.32	127.86
3	A	902	GYK	C25-O24-C07	4.08	110.78	105.32
3	D	902	GYK	O24-C07-C06	-3.83	105.15	109.79
3	B	902	GYK	C25-O24-C07	3.82	110.44	105.32
3	D	902	GYK	C16-N15-C13	-3.80	116.78	120.69
3	D	902	GYK	C25-O24-C07	3.36	109.81	105.32
3	C	902	GYK	O24-C07-C06	-3.29	105.81	109.79
3	C	902	GYK	O26-C06-C07	-3.25	105.85	109.79
3	A	902	GYK	C09-C10-C17	-3.22	114.42	118.12
3	C	902	GYK	C25-O24-C07	2.98	109.30	105.32
3	C	902	GYK	C25-O26-C06	2.89	109.18	105.32
3	A	902	GYK	C04-C03-C02	-2.83	108.50	115.48
3	B	902	GYK	C25-O26-C06	2.79	109.06	105.32
3	A	902	GYK	C01-C02-N12	-2.73	107.91	111.15
3	D	902	GYK	O26-C06-C07	-2.73	106.48	109.79
3	B	902	GYK	O26-C06-C07	-2.69	106.53	109.79
3	A	902	GYK	C25-O26-C06	2.62	108.83	105.32
3	D	902	GYK	C25-O26-C06	2.56	108.74	105.32
3	A	902	GYK	O26-C06-C07	-2.37	106.91	109.79
3	A	902	GYK	C05-C04-C09	2.32	122.24	119.11
3	B	902	GYK	C01-C02-N12	-2.27	108.46	111.15
3	C	902	GYK	C16-N15-C13	-2.11	118.52	120.69
3	C	902	GYK	C01-C02-N12	-2.10	108.66	111.15
2	C	901	NAG	C1-O5-C5	2.03	114.90	112.19
3	C	902	GYK	C04-C03-C02	-2.01	110.52	115.48

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

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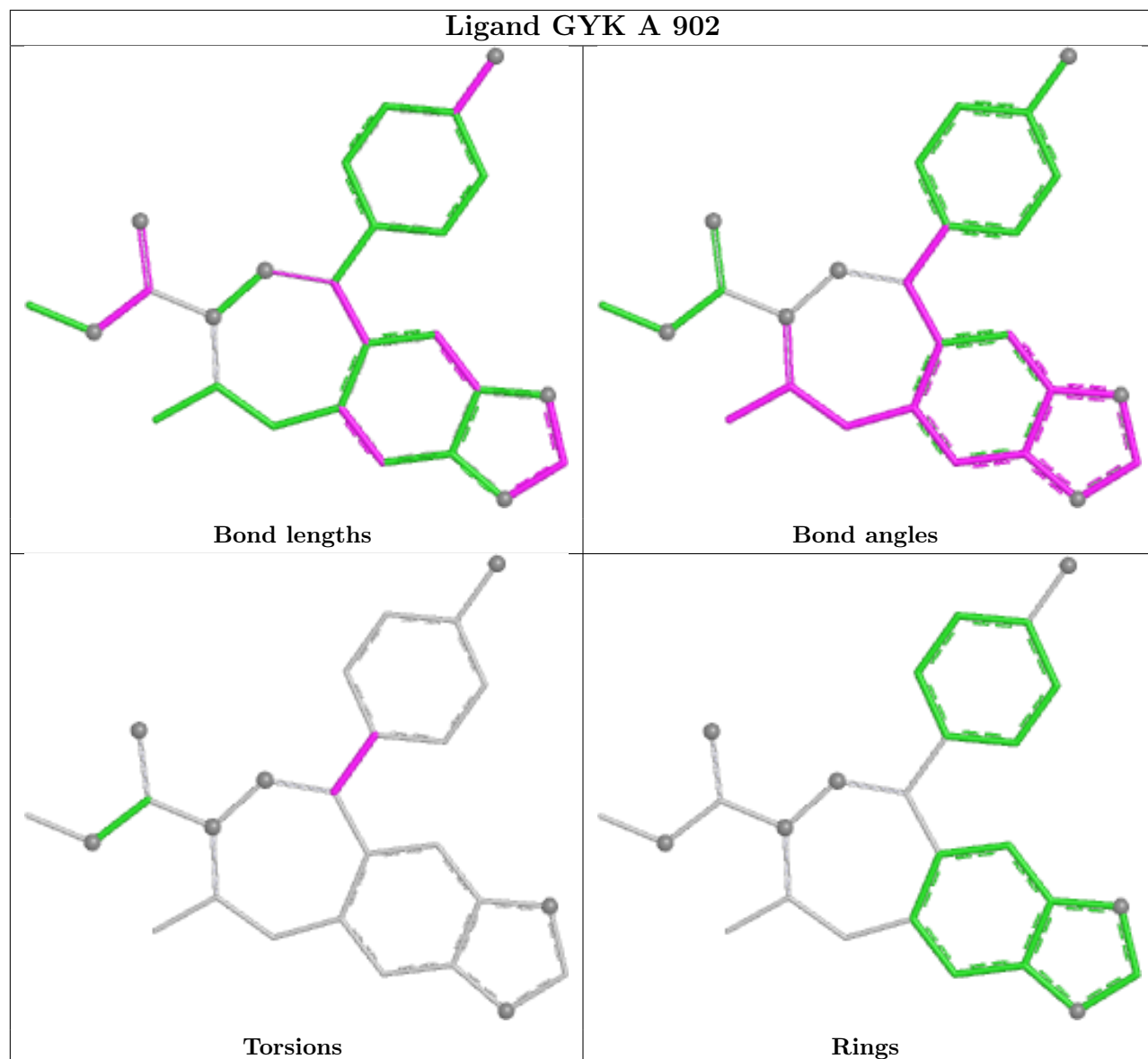
Mol	Chain	Res	Type	Atoms
3	B	902	GYK	N11-C10-C17-C22

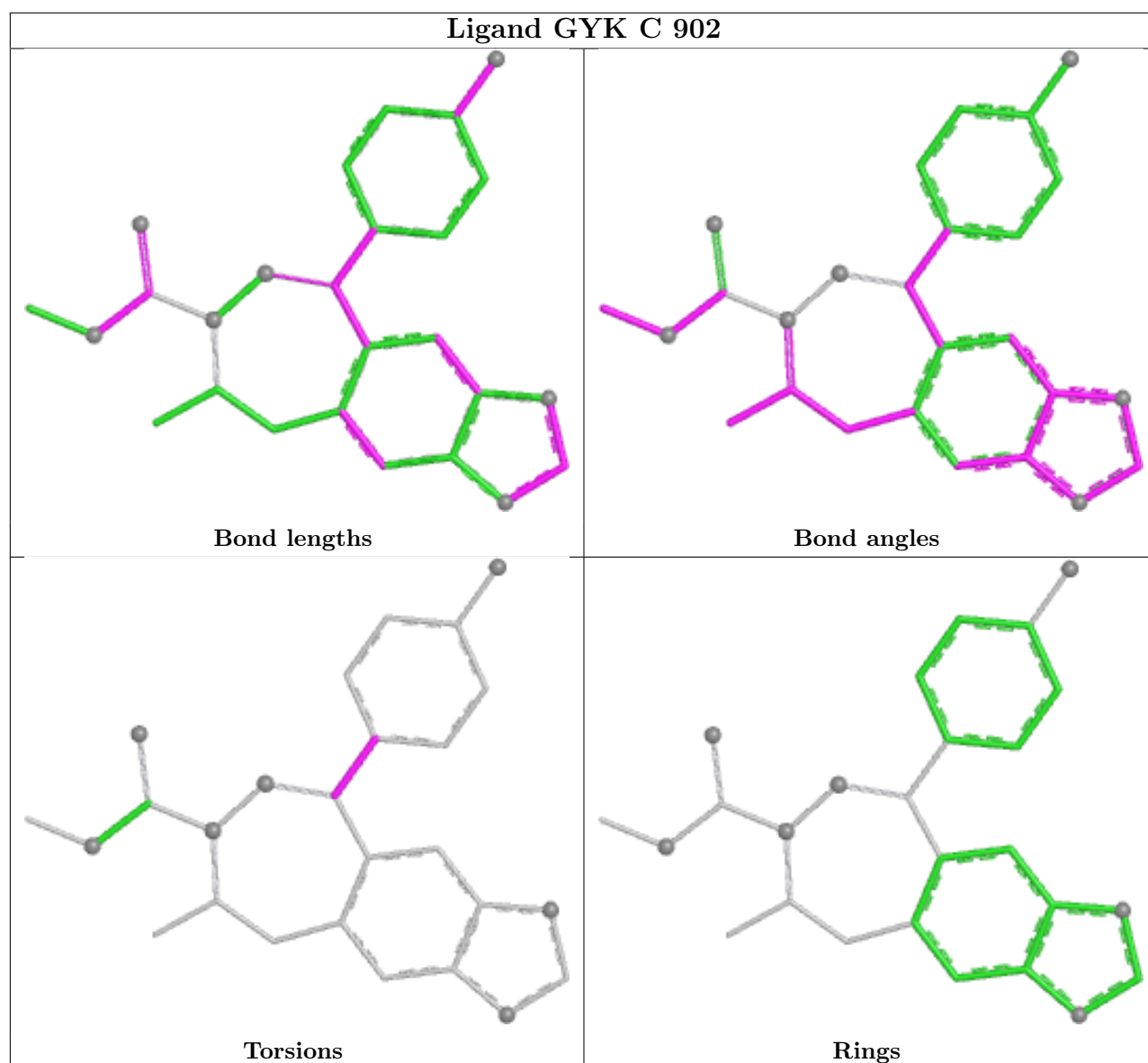
There are no ring outliers.

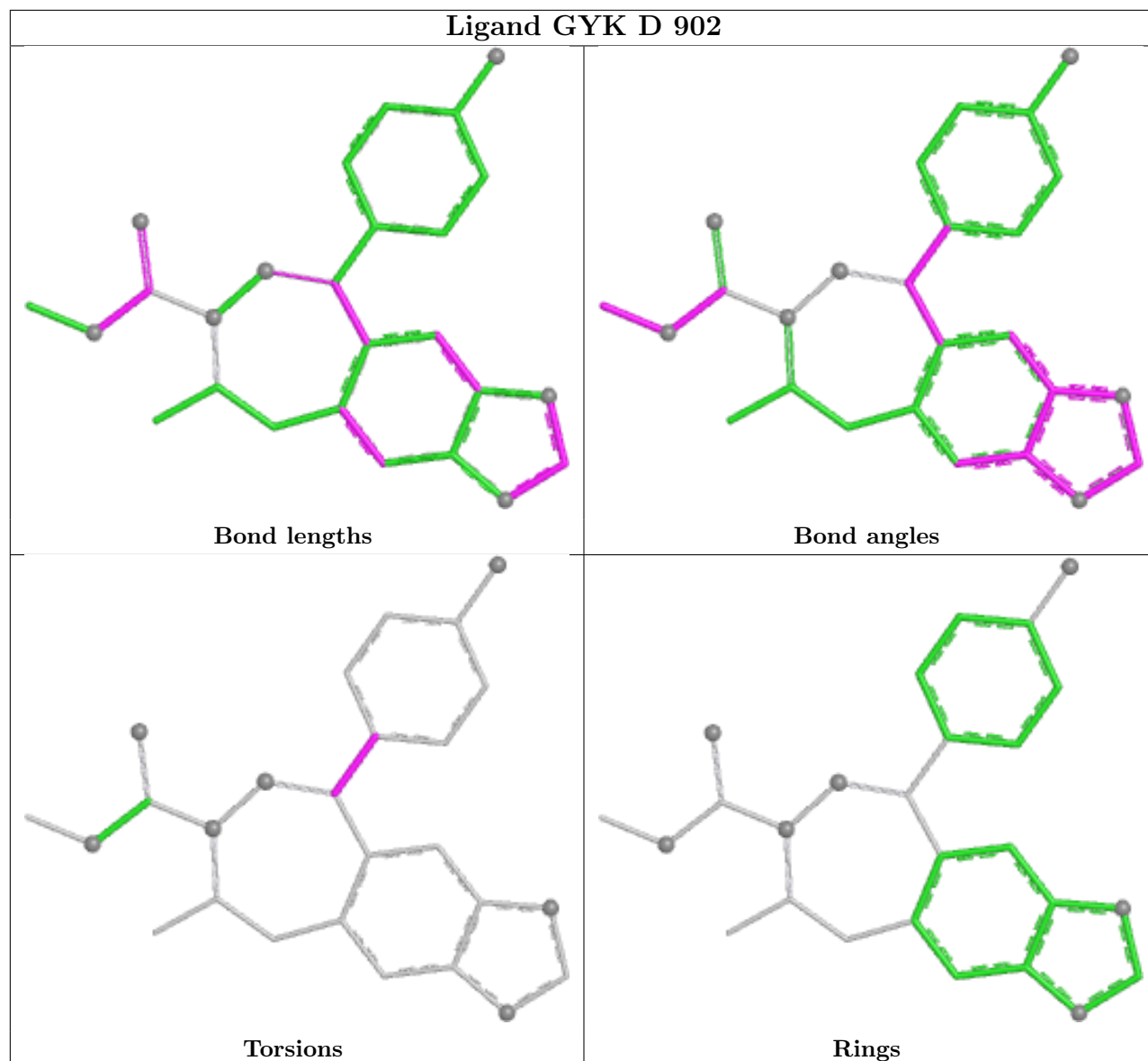
8 monomers are involved in 14 short contacts:

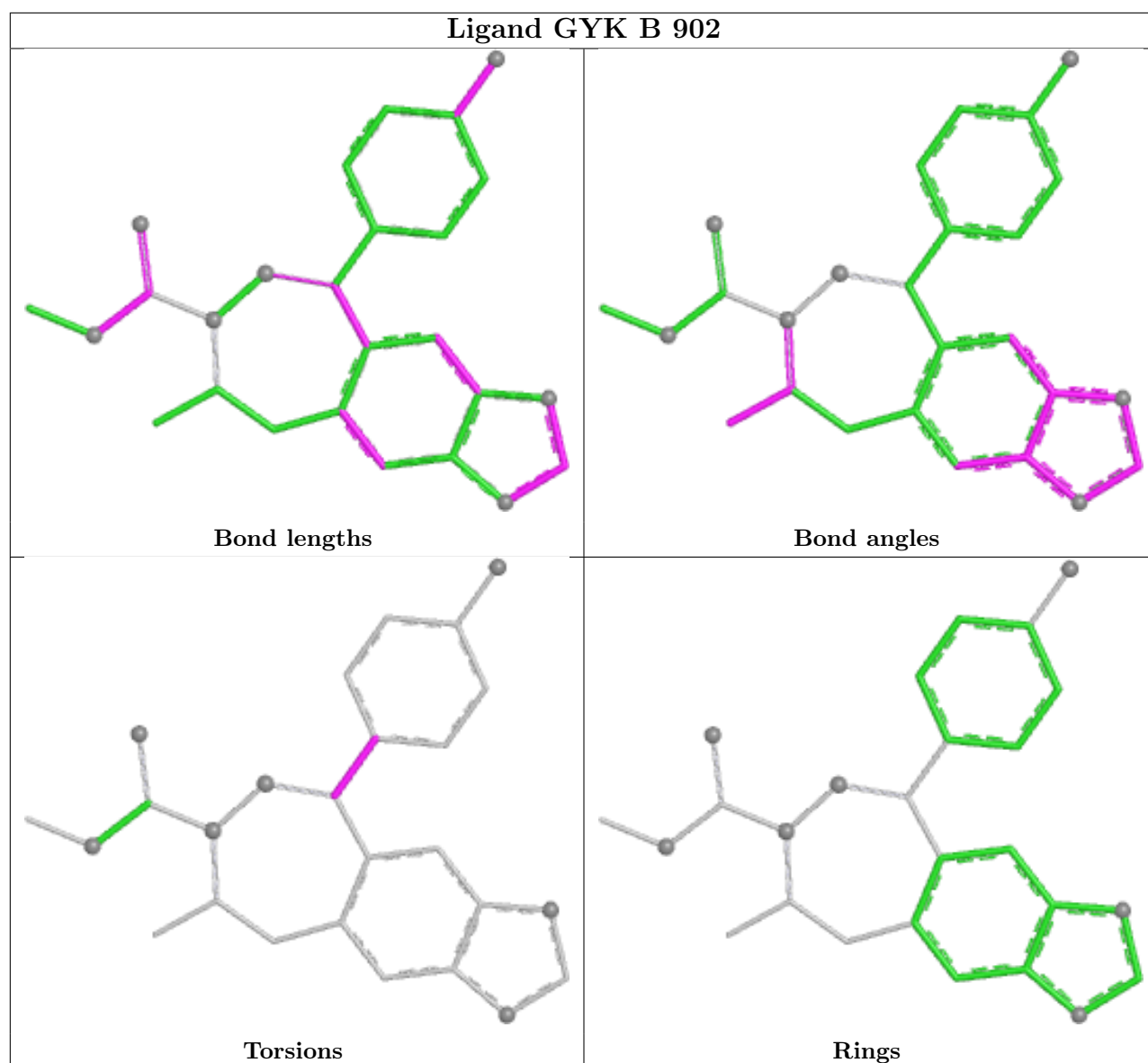
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	NAG	1	0
3	A	902	GYK	1	0
3	C	902	GYK	3	0
3	D	902	GYK	3	0
3	B	902	GYK	3	0
2	D	901	NAG	1	0
2	C	901	NAG	1	0
2	A	901	NAG	1	0

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%)	0.11	26 (3%)	48	33	72, 144, 238, 285	0
1	B	773/803 (96%)	0.03	22 (2%)	55	38	69, 131, 228, 272	0
1	C	773/803 (96%)	0.08	24 (3%)	51	35	101, 167, 232, 261	0
1	D	776/803 (96%)	0.22	46 (5%)	28	23	109, 180, 249, 281	0
All	All	3095/3212 (96%)	0.11	118 (3%)	44	31	69, 155, 240, 285	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	ARG	6.5
1	B	780	SER	6.1
1	D	477	ALA	6.0
1	B	609	THR	5.8
1	D	203	ASP	5.2
1	D	200	LYS	5.1
1	D	527	MET	5.0
1	D	476	ILE	4.9
1	A	400	ILE	4.7
1	A	186	LEU	4.6
1	B	607	PHE	4.5
1	B	254	LEU	4.2
1	A	496	MET	4.1
1	B	157	LYS	4.1
1	A	497	SER	4.0
1	D	139	SER	4.0
1	A	733	GLY	4.0
1	D	104	ASP	3.9
1	D	732	TYR	3.6
1	D	493	LYS	3.5
1	A	588	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	202	ASN	3.4
1	B	253	SER	3.4
1	D	79	LYS	3.4
1	C	632	PRO	3.4
1	C	455	ALA	3.3
1	D	175	GLU	3.2
1	D	495	PHE	3.2
1	A	432	ILE	3.2
1	D	140	ASP	3.1
1	B	613	ILE	3.1
1	C	142	GLY	3.1
1	A	425	CYS	3.1
1	B	456	ASP	3.1
1	C	80	LYS	3.1
1	D	138	ASP	3.1
1	C	383	THR	3.0
1	C	78	ASP	3.0
1	A	629	MET	2.9
1	D	497	SER	2.9
1	D	630	VAL	2.9
1	A	580	SER	2.9
1	B	631	SER	2.9
1	C	140	ASP	2.9
1	B	750	VAL	2.8
1	A	493	LYS	2.8
1	B	754	SER	2.8
1	C	796	PHE	2.8
1	D	621	ALA	2.8
1	D	426	VAL	2.8
1	D	496	MET	2.7
1	B	608	PHE	2.7
1	D	588	GLY	2.7
1	A	386	ASP	2.7
1	B	199	ASP	2.7
1	C	633	ILE	2.6
1	A	583	ALA	2.6
1	C	79	LYS	2.6
1	D	480	THR	2.6
1	D	144	SER	2.6
1	A	782	GLU	2.6
1	C	184	LEU	2.6
1	B	165	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	630	VAL	2.5
1	D	229	ASP	2.5
1	A	527	MET	2.5
1	D	481	ILE	2.5
1	D	494	PRO	2.5
1	B	606	TRP	2.5
1	C	453	ARG	2.4
1	A	653	GLY	2.4
1	C	684	ARG	2.4
1	A	383	THR	2.4
1	D	143	LEU	2.4
1	D	475	ALA	2.4
1	D	623	PHE	2.4
1	C	477	ALA	2.4
1	D	295	ALA	2.4
1	A	579	PHE	2.4
1	C	631	SER	2.4
1	D	293	THR	2.4
1	D	384	GLU	2.4
1	D	142	GLY	2.3
1	B	636	ALA	2.3
1	C	627	GLU	2.3
1	D	423	GLY	2.3
1	C	183	ASP	2.3
1	D	289	VAL	2.3
1	B	610	LEU	2.3
1	D	786	ALA	2.3
1	A	305	GLU	2.3
1	C	629	MET	2.3
1	D	730	LYS	2.2
1	C	792	VAL	2.2
1	D	626	VAL	2.2
1	D	733	GLY	2.2
1	D	169	ASN	2.2
1	A	781	LYS	2.2
1	C	686	THR	2.2
1	A	226	GLY	2.2
1	A	455	ALA	2.2
1	B	588	GLY	2.2
1	C	51	GLU	2.2
1	B	514	VAL	2.1
1	B	178	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	456	ASP	2.1
1	D	269	GLU	2.1
1	A	428	LEU	2.1
1	A	707	THR	2.1
1	D	624	LEU	2.1
1	D	198	ARG	2.0
1	D	223	ALA	2.0
1	A	725	GLY	2.0
1	C	193	ILE	2.0
1	D	157	LYS	2.0
1	C	171	ASP	2.0
1	D	431	GLU	2.0
1	B	733	GLY	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 [i](#)

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.

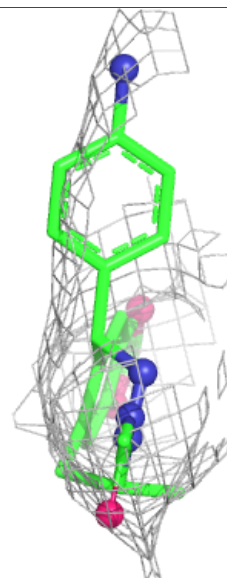
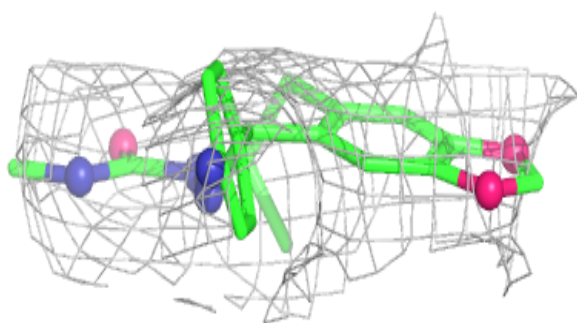
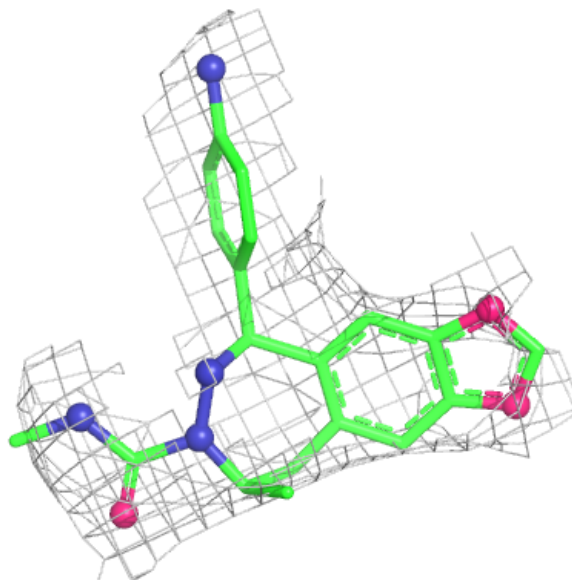
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	901	14/15	0.24	0.20	255,255,257,262	0
2	NAG	B	901	14/15	0.36	0.17	196,196,199,200	0
2	NAG	C	901	14/15	0.38	0.21	416,416,418,424	0
2	NAG	D	901	14/15	0.52	0.15	269,269,270,272	0
3	GYK	A	902	26/26	0.81	0.12	128,169,210,219	0
3	GYK	C	902	26/26	0.82	0.14	128,169,210,219	0
3	GYK	D	902	26/26	0.83	0.14	128,169,210,219	0
3	GYK	B	902	26/26	0.88	0.10	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.

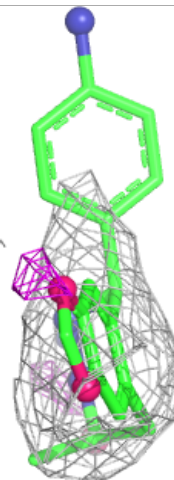
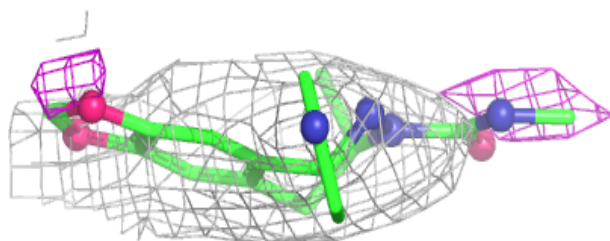
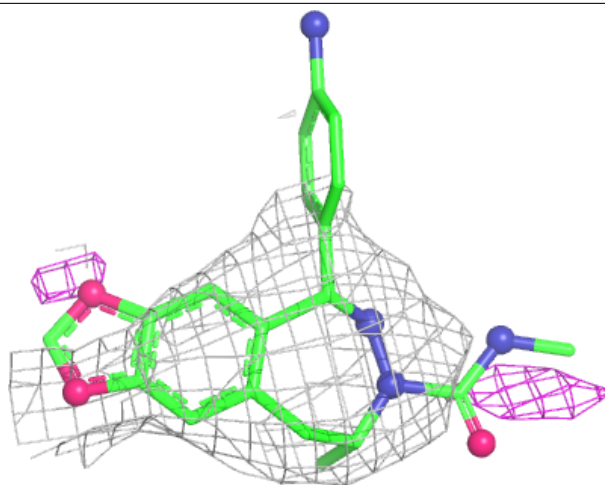
Electron density around GYK A 902:

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



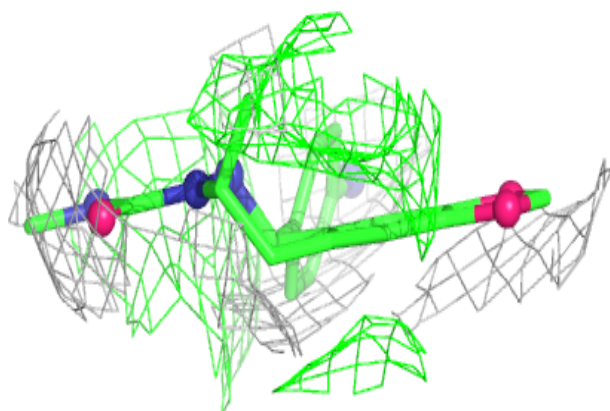
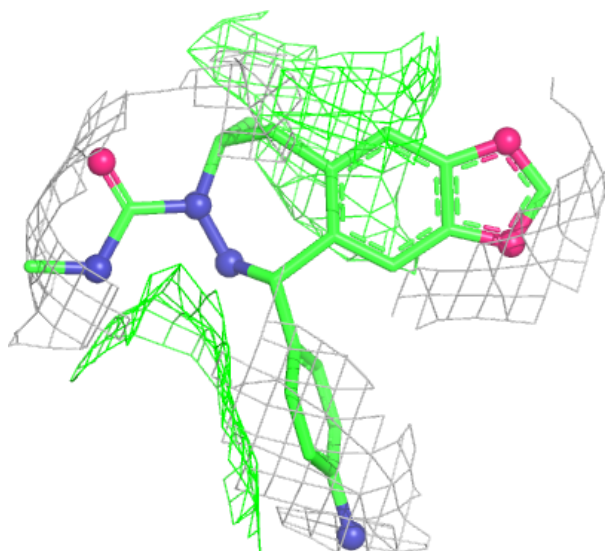
Electron density around GYK C 902:

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



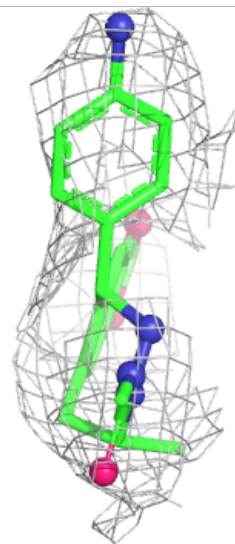
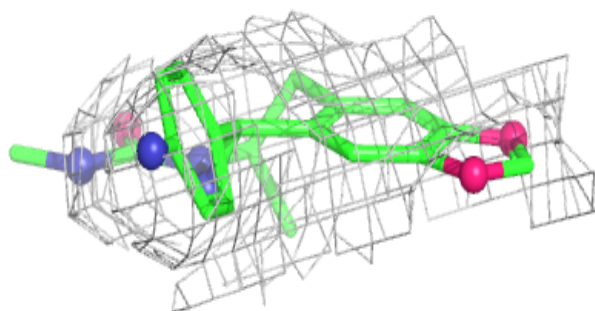
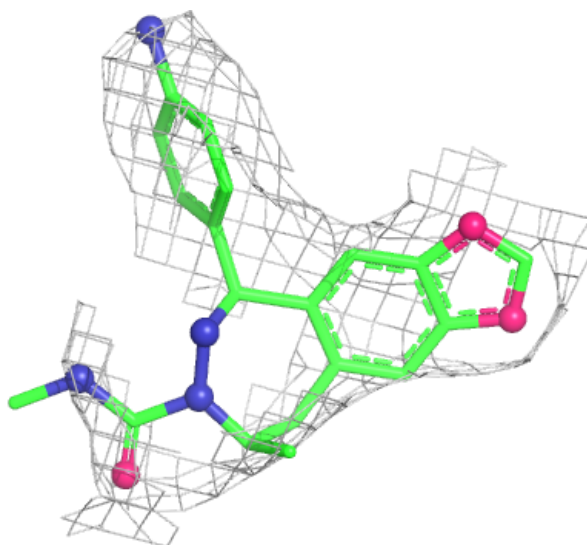
Electron density around GYK D 902:

$2mF_o-DF_c$ (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.