Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2021 – 06:24 AM GMT

PDB ID	:	6RUQ
Title	:	Structure of GluA2cryst in complex the antagonist ZK200775 and the negative allosteric modulator GYKI53655 at 4.65 A resolution
Authors	:	Krintel, C.; Venskutonyte, R.; Mirza, O.A.; Gajhede, M.; Kastrup, J.S.
Deposited on	:	2019-05-28
Resolution	:	4.65 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:

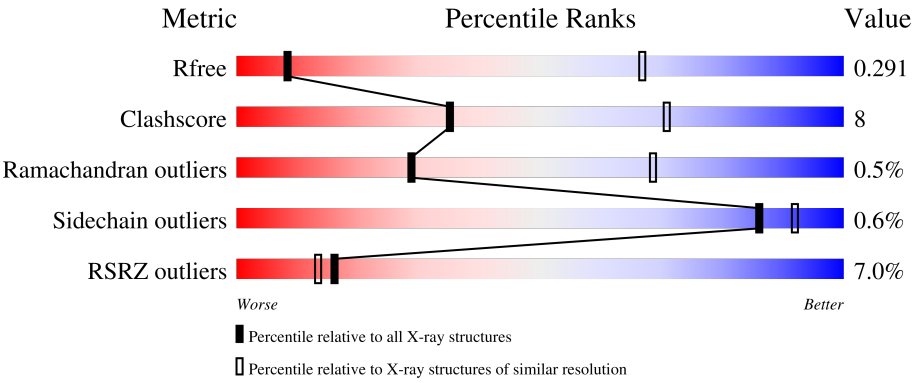
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1.dev1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.65 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	1083 (5.52-3.80)
Clashscore	141614	1156 (5.52-3.80)
Ramachandran outliers	138981	1092 (5.52-3.80)
Sidechain outliers	138945	1072 (5.50-3.80)
RSRZ outliers	127900	1114 (5.54-3.70)

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 <=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	823	4% 76% 19% 5%
1	B	823	4% 76% 18% • 5%
1	C	823	12% 78% 18% • •
1	D	823	7% 78% 17% •
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	G	3	67% 33%
3	F	4	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	F	4	-	-	-	X
4	GYK	A	901	-	-	-	X
4	GYK	B	901	-	-	-	X
4	GYK	C	901	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25050 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	784	Total	C	N	O	S	0	0	0
			6156	3952	1023	1153	28			
1	B	781	Total	C	N	O	S	0	0	0
			6130	3934	1019	1149	28			
1	C	796	Total	C	N	O	S	0	0	0
			6255	4013	1039	1175	28			
1	D	786	Total	C	N	O	S	0	0	0
			6169	3960	1025	1156	28			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	410	ALA	LYS	engineered mutation	UNP P19491
A	413	ALA	GLU	conflict	UNP P19491
A	414	ALA	MET	conflict	UNP P19491
A	416	ALA	GLU	conflict	UNP P19491
A	572	ALA	GLY	conflict	UNP P19491
A	575	GLN	ASN	conflict	UNP P19491
A	577	ALA	LEU	conflict	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	758	LEU	VAL	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
A	832	GLY	-	expression tag	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	410	ALA	LYS	engineered mutation	UNP P19491
B	413	ALA	GLU	conflict	UNP P19491
B	414	ALA	MET	conflict	UNP P19491
B	416	ALA	GLU	conflict	UNP P19491
B	572	ALA	GLY	conflict	UNP P19491
B	575	GLN	ASN	conflict	UNP P19491
B	577	ALA	LEU	conflict	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	758	LEU	VAL	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
B	832	GLY	-	expression tag	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491

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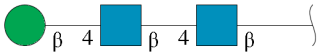
Chain	Residue	Modelled	Actual	Comment	Reference
C	410	ALA	LYS	engineered mutation	UNP P19491
C	413	ALA	GLU	conflict	UNP P19491
C	414	ALA	MET	conflict	UNP P19491
C	416	ALA	GLU	conflict	UNP P19491
C	572	ALA	GLY	conflict	UNP P19491
C	575	GLN	ASN	conflict	UNP P19491
C	577	ALA	LEU	conflict	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	758	LEU	VAL	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
C	832	GLY	-	expression tag	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	410	ALA	LYS	engineered mutation	UNP P19491
D	413	ALA	GLU	conflict	UNP P19491
D	414	ALA	MET	conflict	UNP P19491
D	416	ALA	GLU	conflict	UNP P19491
D	572	ALA	GLY	conflict	UNP P19491
D	575	GLN	ASN	conflict	UNP P19491
D	577	ALA	LEU	conflict	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	758	LEU	VAL	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491
D	832	GLY	-	expression tag	UNP P19491

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

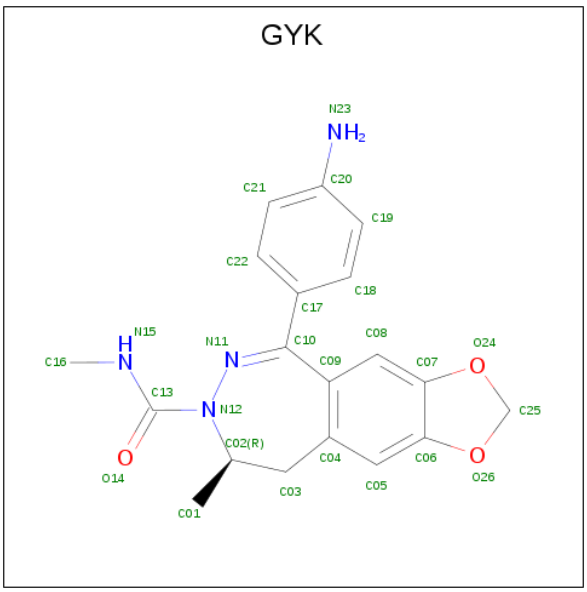


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop yranose.

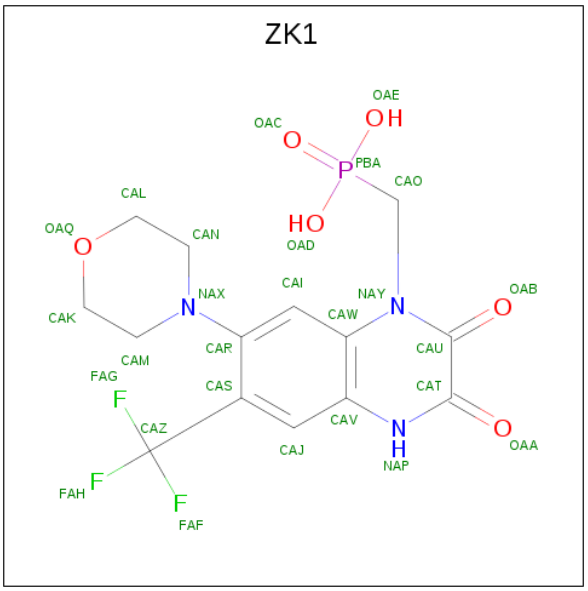
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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: $C_{19}H_{20}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$) (labeled as "Ligand of Interest" by depositor).



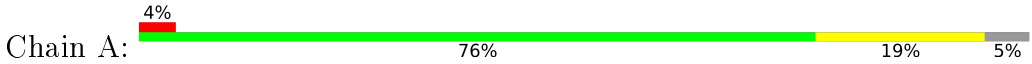
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C F N O P 27 14 3 3 6 1	0	0
5	B	1	Total C F N O P 27 14 3 3 6 1	0	0
5	C	1	Total C F N O P 27 14 3 3 6 1	0	0
5	D	1	Total C F N O P 27 14 3 3 6 1	0	0

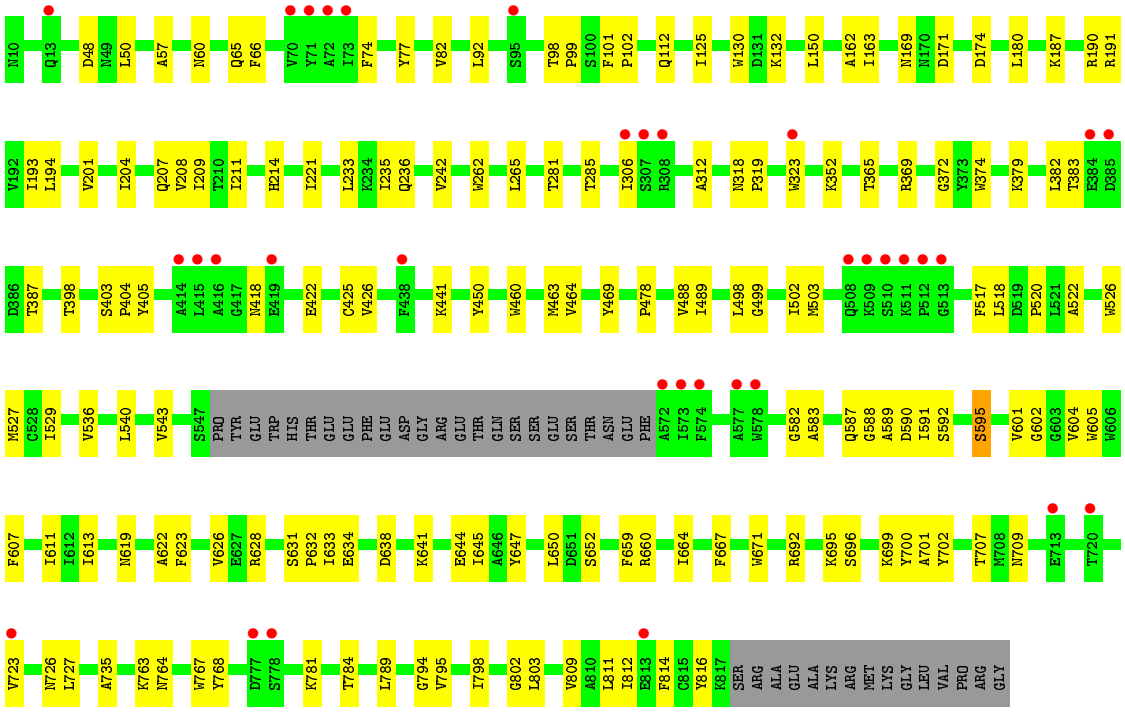
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 2

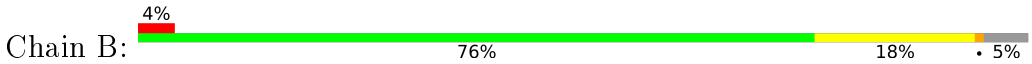
Chain A:

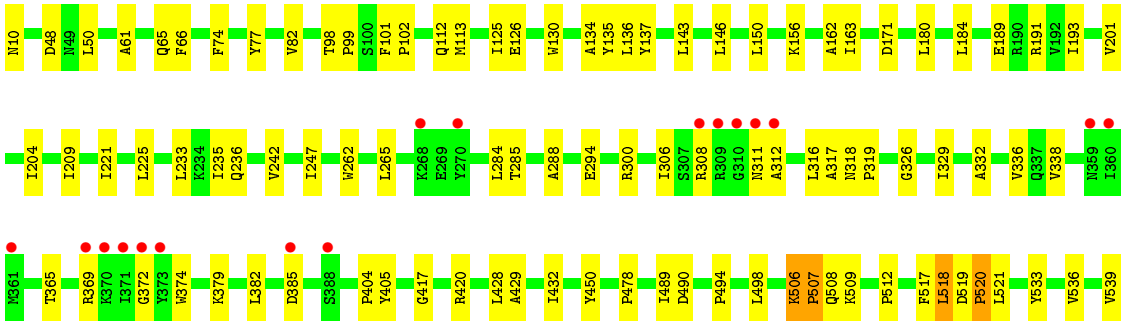


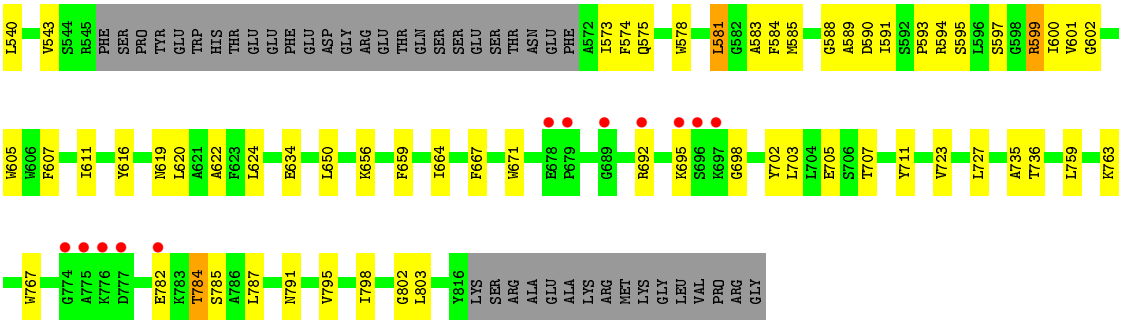


- Molecule 1: Glutamate receptor 2

Chain B:

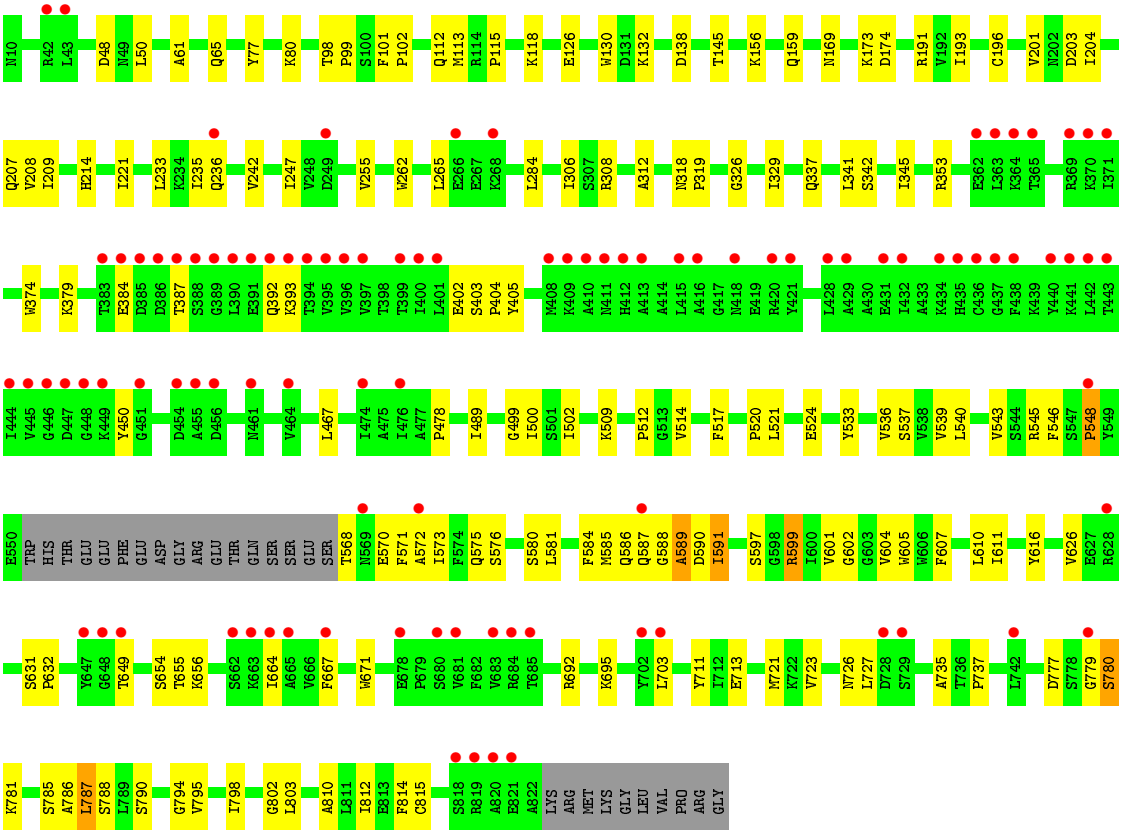






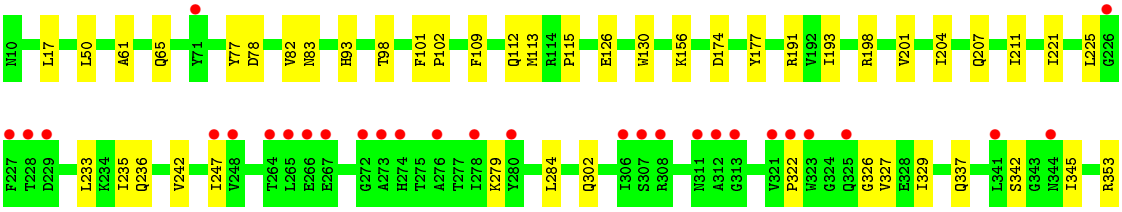
• Molecule 1: Glutamate receptor 2

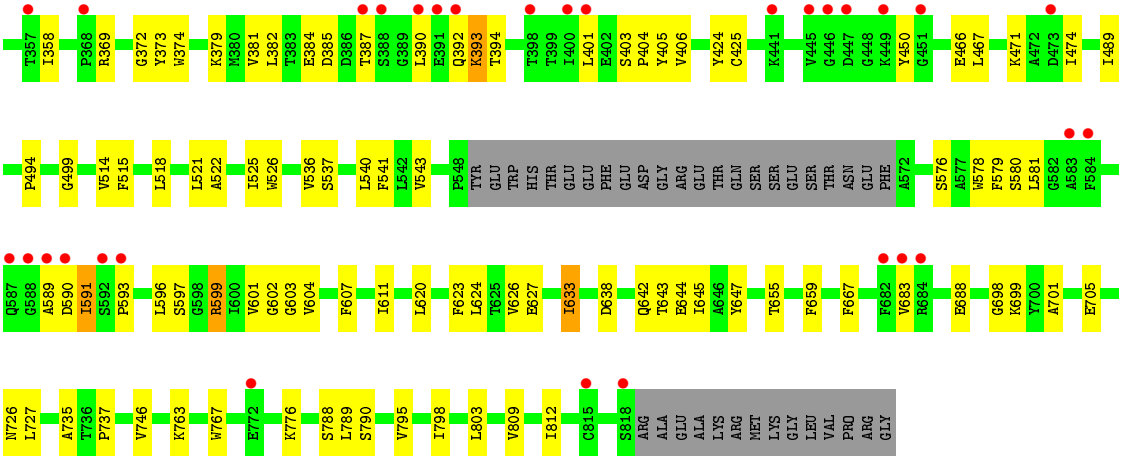
Chain C:



• Molecule 1: Glutamate receptor 2

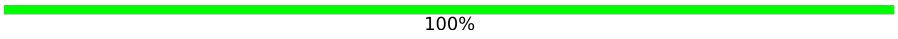
Chain D:





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

Chain E:

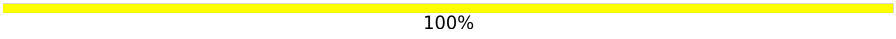


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 3: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.77Å 306.60Å 107.73Å 90.00° 94.26° 90.00°	Depositor
Resolution (Å)	51.10 – 4.65 53.71 – 4.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (51.10-4.65) 99.1 (53.71-4.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 4.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.242 , 0.291 0.243 , 0.291	Depositor DCC
R_{free} test set	1561 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	167.3	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 127.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	25050	wwPDB-VP
Average B, all atoms (Å^2)	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZK1, GYK, NAG, BMA

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	0.24	0/6285	0.44	0/8493
1	B	0.25	0/6258	0.45	2/8458 (0.0%)
1	C	0.25	0/6387	0.44	0/8632
1	D	0.24	0/6299	0.43	0/8513
All	All	0.25	0/25229	0.44	2/34096 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	518	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	581	LEU	CA-CB-CG	5.42	127.76	115.30

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	6156	0	6156	116	0
1	B	6130	0	6129	116	0
1	C	6255	0	6240	112	0
1	D	6169	0	6169	105	0
2	E	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	39	0	34	0	0
3	F	50	0	43	2	0
4	A	26	0	0	0	0
4	B	26	0	0	2	0
4	C	26	0	0	0	0
4	D	26	0	0	1	0
5	A	27	0	13	1	0
5	B	27	0	13	1	0
5	C	27	0	13	3	0
5	D	27	0	13	2	0
All	All	25050	0	24857	407	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (407) 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:A:498:LEU:HD21	1:A:707:THR:HG23	1.49	0.92
1:B:784:THR:OG1	1:B:785:SER:N	2.07	0.86
1:C:785:SER:O	1:C:787:LEU:N	2.09	0.84
1:C:781:LYS:NZ	1:D:627:GLU:OE2	2.11	0.83
1:D:372:GLY:HA2	1:D:382:LEU:HB3	1.64	0.79
1:A:502:ILE:HG23	1:A:723:VAL:HG23	1.63	0.79
1:A:789:LEU:HD21	1:C:524:GLU:HB2	1.66	0.78
1:D:384:GLU:HG2	1:D:385:ASP:H	1.50	0.77
1:B:599:ARG:HH22	1:D:579:PHE:HA	1.50	0.76
1:C:173:LYS:NZ	1:C:203:ASP:OD2	2.18	0.74
1:C:591:ILE:HD11	1:C:599:ARG:HH21	1.52	0.74
1:C:174:ASP:OD2	1:C:207:GLN:NE2	2.20	0.73
1:C:802:GLY:HA3	1:D:604:VAL:HG21	1.71	0.72
1:B:498:LEU:HD11	1:B:705:GLU:HB2	1.70	0.72
1:B:599:ARG:NH2	1:D:578:TRP:O	2.22	0.72
1:A:520:PRO:O	1:A:619:ASN:ND2	2.23	0.72
1:C:546:PHE:O	1:C:548:PRO:HD3	1.91	0.70
1:C:777:ASP:OD2	1:D:644:GLU:HG3	1.92	0.70
1:B:539:VAL:HG21	1:D:803:LEU:HD22	1.74	0.69
1:C:777:ASP:OD1	1:D:643:THR:N	2.23	0.69
1:B:374:TRP:HE1	1:B:379:LYS:HG3	1.57	0.69
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.57	0.69
1:C:540:LEU:HA	1:C:543:VAL:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:PRO:HA	1:D:112:GLN:HG2	1.75	0.69
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.74	0.68
1:C:585:MET:HB3	1:D:603:GLY:HA2	1.76	0.68
1:A:372:GLY:HA2	1:A:382:LEU:HB3	1.76	0.67
1:A:374:TRP:HE1	1:A:379:LYS:HG2	1.57	0.67
1:D:514:VAL:HG13	1:D:515:PHE:HD2	1.58	0.67
1:B:597:SER:O	1:B:601:VAL:HG23	1.95	0.67
1:B:225:LEU:HD22	1:B:247:ILE:HB	1.78	0.65
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.62	0.64
1:B:308:ARG:HH21	1:B:312:ALA:HB2	1.62	0.64
1:D:644:GLU:HB3	1:D:699:LYS:HE3	1.78	0.64
1:A:77:TYR:OH	1:A:101:PHE:O	2.15	0.64
1:A:587:GLN:NE2	1:C:587:GLN:OE1	2.31	0.63
1:B:584:PHE:HD1	1:B:605:TRP:HZ2	1.46	0.63
1:C:326:GLY:HA2	1:C:329:ILE:HD12	1.81	0.63
1:B:369:ARG:NH2	1:B:385:ASP:OD2	2.33	0.62
1:B:498:LEU:HD13	1:B:707:THR:HG23	1.81	0.62
1:A:811:LEU:HD23	1:A:814:PHE:HE2	1.64	0.62
1:A:628:ARG:NH2	1:A:784:THR:O	2.33	0.62
1:C:102:PRO:HA	1:C:112:GLN:HG2	1.82	0.61
1:B:374:TRP:CD1	1:B:379:LYS:HA	2.34	0.61
1:C:126:GLU:OE2	1:C:156:LYS:NZ	2.33	0.61
1:A:150:LEU:HD22	1:B:162:ALA:HB3	1.81	0.61
1:A:634:GLU:HA	1:A:723:VAL:HB	1.82	0.61
1:D:77:TYR:CD1	1:D:82:VAL:HG22	2.34	0.61
1:D:326:GLY:HA2	1:D:329:ILE:HD12	1.82	0.60
1:C:597:SER:O	1:C:601:VAL:HG23	2.00	0.60
1:B:517:PHE:O	1:B:520:PRO:HD2	2.00	0.60
1:C:589:ALA:HB2	1:C:602:GLY:HA3	1.82	0.60
1:D:77:TYR:HE2	1:D:98:THR:HG21	1.66	0.60
1:D:177:TYR:HB2	1:D:207:GLN:HE21	1.66	0.60
1:C:585:MET:HG3	1:C:586:GLN:H	1.66	0.60
1:B:490:ASP:OD1	1:B:736:THR:OG1	2.19	0.60
1:B:597:SER:O	1:B:600:ILE:HG12	2.01	0.60
1:D:198:ARG:HD3	1:D:279:LYS:HD3	1.83	0.60
1:B:77:TYR:CD1	1:B:82:VAL:HG22	2.37	0.59
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.84	0.59
1:D:374:TRP:CD1	1:D:379:LYS:HA	2.37	0.58
1:A:633:ILE:HD11	1:A:638:ASP:HB2	1.85	0.58
1:C:584:PHE:HB3	1:D:599:ARG:NH1	2.19	0.58
1:D:77:TYR:OH	1:D:101:PHE:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:LEU:HB3	1:D:599:ARG:HD2	1.86	0.57
1:A:489:ILE:HD13	1:A:735:ALA:HB1	1.87	0.57
1:B:705:GLU:OE1	1:B:705:GLU:N	2.35	0.57
1:C:573:ILE:O	1:C:575:GLN:N	2.29	0.57
1:B:10:ASN:HA	1:B:300:ARG:HH22	1.68	0.57
1:C:489:ILE:HD13	1:C:735:ALA:HB1	1.85	0.57
1:A:162:ALA:HB3	1:B:150:LEU:HD22	1.86	0.57
1:A:374:TRP:CD1	1:A:379:LYS:HA	2.40	0.57
1:B:102:PRO:HA	1:B:112:GLN:HG2	1.85	0.57
1:C:812:ILE:HA	1:C:815:CYS:SG	2.45	0.57
1:C:499:GLY:HA3	1:C:726:ASN:HB3	1.85	0.57
1:A:102:PRO:HA	1:A:112:GLN:HG2	1.85	0.57
1:B:417:GLY:O	1:B:420:ARG:NE	2.37	0.57
1:B:536:VAL:HG22	1:D:803:LEU:HD21	1.87	0.57
1:D:499:GLY:HA3	1:D:726:ASN:HB3	1.85	0.57
1:C:785:SER:C	1:C:787:LEU:H	2.07	0.56
1:A:803:LEU:HD21	1:C:536:VAL:HG22	1.87	0.56
1:C:787:LEU:HB3	1:D:521:LEU:O	2.05	0.56
1:D:596:LEU:HD12	1:D:597:SER:N	2.20	0.56
1:D:537:SER:HB2	1:D:580:SER:HB3	1.88	0.56
1:A:803:LEU:HB3	1:C:539:VAL:HG21	1.87	0.56
1:A:814:PHE:HB3	1:C:545:ARG:HD3	1.88	0.56
1:D:521:LEU:O	1:D:525:ILE:HD12	2.05	0.56
1:A:518:LEU:HB2	1:A:526:TRP:CD1	2.41	0.55
1:A:650:LEU:O	1:A:652:SER:N	2.36	0.55
1:D:789:LEU:O	1:D:790:SER:OG	2.23	0.55
1:A:236:GLN:NE2	1:A:365:THR:O	2.37	0.55
1:C:374:TRP:CD1	1:C:379:LYS:HA	2.42	0.55
1:A:582:GLY:HA3	1:C:599:ARG:NH1	2.22	0.55
1:C:512:PRO:HB2	1:C:790:SER:HB2	1.88	0.55
1:B:520:PRO:O	1:B:619:ASN:ND2	2.40	0.55
1:C:584:PHE:HD2	1:D:599:ARG:HH12	1.53	0.55
1:D:50:LEU:HD12	1:D:61:ALA:HB2	1.88	0.55
1:D:193:ILE:HG12	1:D:221:ILE:HB	1.88	0.55
1:D:642:GLN:NE2	1:D:645:ILE:O	2.37	0.55
1:A:502:ILE:HD11	1:A:701:ALA:HB1	1.89	0.55
1:A:696:SER:HB3	1:A:699:LYS:HB2	1.89	0.55
1:D:597:SER:O	1:D:601:VAL:HG23	2.07	0.55
1:B:489:ILE:HD13	1:B:735:ALA:HB1	1.89	0.54
1:A:503:MET:HB2	1:A:709:ASN:HD21	1.71	0.54
1:C:306:ILE:HD12	1:C:306:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:LEU:O	1:D:599:ARG:NE	2.40	0.54
1:D:126:GLU:OE2	1:D:156:LYS:NZ	2.40	0.54
1:B:236:GLN:NE2	1:B:365:THR:O	2.40	0.54
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.73	0.53
1:C:384:GLU:HG2	1:C:387:THR:H	1.73	0.53
3:F:1:NAG:H61	3:F:2:NAG:N2	2.23	0.53
1:B:143:LEU:HD23	1:B:146:LEU:HD23	1.90	0.53
1:B:318:ASN:HB3	1:B:319:PRO:HD3	1.91	0.53
1:D:374:TRP:HD1	1:D:379:LYS:HA	1.72	0.53
1:A:60:ASN:HD21	1:B:317:ALA:H	1.56	0.53
1:A:281:THR:O	1:A:285:THR:HG23	2.09	0.53
1:C:193:ILE:HG12	1:C:221:ILE:HB	1.90	0.53
1:A:422:GLU:HA	1:A:426:VAL:HG21	1.91	0.53
1:C:654:SER:N	5:C:902:ZK1:OAE	2.35	0.53
1:B:193:ILE:HG12	1:B:221:ILE:HB	1.91	0.52
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.90	0.52
1:A:50:LEU:HD21	1:A:57:ALA:HB1	1.91	0.52
1:A:48:ASP:OD2	1:A:65:GLN:NE2	2.42	0.52
1:A:540:LEU:HA	1:A:543:VAL:HG22	1.91	0.52
1:C:537:SER:HB2	1:C:580:SER:HB2	1.90	0.52
1:D:540:LEU:HD21	1:D:580:SER:HA	1.91	0.52
1:B:66:PHE:O	1:B:311:ASN:ND2	2.32	0.52
1:D:795:VAL:O	1:D:798:ILE:HG22	2.09	0.52
1:B:48:ASP:OD2	1:B:65:GLN:NE2	2.43	0.52
1:B:624:LEU:HD21	1:B:787:LEU:HD13	1.92	0.52
1:C:113:MET:HB3	1:C:284:LEU:HD22	1.92	0.52
1:C:392:GLN:HG2	1:C:393:LYS:H	1.75	0.52
1:D:393:LYS:HD2	1:D:394:THR:H	1.75	0.52
1:B:540:LEU:HD22	1:B:590:ASP:HB2	1.92	0.52
1:A:763:LYS:O	1:A:767:TRP:HB2	2.09	0.52
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.75	0.52
1:A:318:ASN:HB3	1:A:319:PRO:HD3	1.93	0.51
1:D:369:ARG:HE	1:D:387:THR:HB	1.75	0.51
1:D:466:GLU:HA	1:D:471:LYS:HE3	1.92	0.51
1:A:306:ILE:HD12	1:A:306:ILE:O	2.10	0.51
1:A:583:ALA:O	1:A:588:GLY:N	2.43	0.51
1:B:235:ILE:HD12	1:B:242:VAL:HG21	1.93	0.51
1:B:507:PRO:HB3	1:B:698:GLY:HA3	1.92	0.51
1:C:50:LEU:HD12	1:C:61:ALA:HB2	1.91	0.51
1:D:809:VAL:O	1:D:812:ILE:HG13	2.11	0.51
1:C:656:LYS:HE2	1:C:671:TRP:HH2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:HG3	1:B:288:ALA:HB2	1.93	0.51
1:A:193:ILE:HG12	1:A:221:ILE:HB	1.93	0.51
1:B:705:GLU:OE2	5:B:902:ZK1:HAM	2.11	0.51
1:B:77:TYR:HD1	1:B:82:VAL:HG22	1.75	0.51
1:C:543:VAL:HG21	1:C:601:VAL:HG21	1.92	0.51
1:D:599:ARG:HD3	1:D:599:ARG:C	2.32	0.51
1:B:622:ALA:HB2	1:D:624:LEU:HB3	1.92	0.50
1:C:521:LEU:HD13	1:C:616:TYR:HD2	1.76	0.50
1:C:405:TYR:CD1	1:C:478:PRO:HG3	2.47	0.50
1:B:134:ALA:HB2	1:B:189:GLU:HG2	1.93	0.50
1:A:125:ILE:HD11	1:A:193:ILE:HD11	1.93	0.50
1:C:533:TYR:CE2	1:C:584:PHE:HB2	2.46	0.50
1:C:781:LYS:O	1:C:781:LYS:HG3	2.11	0.50
1:C:48:ASP:OD2	1:C:65:GLN:NE2	2.44	0.50
1:D:113:MET:HB3	1:D:284:LEU:HD22	1.93	0.50
1:D:518:LEU:H	1:D:518:LEU:HD23	1.77	0.50
1:A:604:VAL:HG11	1:B:802:GLY:HA3	1.93	0.50
1:B:77:TYR:OH	1:B:101:PHE:O	2.21	0.50
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.93	0.50
1:A:233:LEU:HA	1:A:236:GLN:HB2	1.92	0.50
1:D:541:PHE:HA	1:D:576:SER:HB3	1.92	0.50
1:A:536:VAL:HG22	1:B:803:LEU:HD21	1.93	0.50
1:A:809:VAL:O	1:A:812:ILE:HG13	2.11	0.50
1:B:233:LEU:HA	1:B:236:GLN:HB2	1.94	0.50
1:B:583:ALA:HB2	1:B:591:ILE:HG12	1.94	0.50
1:A:613:ILE:HG21	1:C:610:LEU:HD11	1.95	0.49
1:C:337:GLN:HA	1:C:345:ILE:O	2.11	0.49
1:D:390:LEU:HD12	1:D:392:GLN:HB3	1.94	0.49
1:D:607:PHE:O	1:D:611:ILE:HG12	2.12	0.49
1:B:533:TYR:OH	1:B:581:LEU:HB2	2.12	0.49
1:C:201:VAL:HA	1:C:204:ILE:HD12	1.94	0.49
1:C:402:GLU:OE1	5:C:902:ZK1:FAH	2.20	0.49
3:F:1:NAG:H61	3:F:2:NAG:HN2	1.77	0.49
1:B:294:GLU:HG3	1:B:338:VAL:HG11	1.95	0.49
1:A:77:TYR:HE2	1:A:98:THR:HG21	1.78	0.49
1:A:130:TRP:CE2	1:A:191:ARG:HG2	2.48	0.49
1:D:489:ILE:HD13	1:D:735:ALA:HB1	1.95	0.49
1:D:645:ILE:HG12	1:D:698:GLY:O	2.12	0.49
1:B:607:PHE:O	1:B:611:ILE:HG12	2.12	0.49
1:A:405:TYR:CD2	1:A:478:PRO:HG3	2.47	0.48
1:B:519:ASP:O	1:B:521:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:GLU:O	1:C:571:PHE:HB2	2.13	0.48
1:D:384:GLU:CG	1:D:385:ASP:H	2.22	0.48
1:A:811:LEU:HA	1:A:814:PHE:CE2	2.47	0.48
1:A:190:ARG:HG3	1:A:469:TYR:HB3	1.95	0.48
1:B:332:ALA:O	1:B:336:VAL:HG23	2.13	0.48
1:C:77:TYR:OH	1:C:101:PHE:O	2.24	0.48
1:C:467:LEU:HD22	1:C:737:PRO:HG3	1.95	0.48
1:D:705:GLU:OE1	1:D:705:GLU:N	2.34	0.48
1:A:464:VAL:HG13	1:A:489:ILE:HG12	1.95	0.48
1:B:374:TRP:NE1	1:B:379:LYS:HG3	2.28	0.48
1:B:575:GLN:HA	1:B:578:TRP:NE1	2.28	0.48
1:A:590:ASP:OD2	1:A:595:SER:HB3	2.14	0.48
1:B:494:PRO:HG3	1:D:494:PRO:HG3	1.94	0.48
1:D:78:ASP:O	1:D:82:VAL:HG23	2.14	0.48
1:D:390:LEU:HD12	1:D:392:GLN:CB	2.44	0.48
1:A:208:VAL:HG12	1:A:214:HIS:HB3	1.96	0.47
1:B:533:TYR:HD2	1:B:605:TRP:HH2	1.62	0.47
1:C:692:ARG:HA	1:C:695:LYS:HG2	1.96	0.47
1:A:628:ARG:HB3	1:C:626:VAL:HG11	1.96	0.47
1:A:764:ASN:HA	1:A:768:TYR:HD2	1.78	0.47
1:A:811:LEU:HD23	1:A:814:PHE:CE2	2.48	0.47
1:B:656:LYS:HE2	1:B:671:TRP:HH2	1.78	0.47
1:A:802:GLY:HA3	1:C:604:VAL:HG21	1.95	0.47
1:B:306:ILE:HD12	1:B:306:ILE:O	2.14	0.47
1:C:810:ALA:O	1:C:814:PHE:HD1	1.96	0.47
1:A:623:PHE:CE1	1:B:785:SER:HB2	2.49	0.47
1:C:235:ILE:HD12	1:C:242:VAL:HG21	1.96	0.47
1:D:342:SER:HB2	1:D:353:ARG:HH22	1.79	0.47
1:D:384:GLU:HG2	1:D:385:ASP:N	2.24	0.47
1:A:503:MET:HB2	1:A:709:ASN:ND2	2.29	0.47
1:A:607:PHE:O	1:A:611:ILE:HG12	2.13	0.47
1:B:201:VAL:HA	1:B:204:ILE:HD12	1.96	0.47
1:C:318:ASN:HB3	1:C:319:PRO:HD3	1.95	0.47
1:B:518:LEU:HD12	1:B:519:ASP:OD2	2.15	0.47
1:B:536:VAL:HG21	1:B:605:TRP:HE3	1.80	0.47
1:B:634:GLU:HA	1:B:723:VAL:HB	1.95	0.47
1:D:405:TYR:HA	1:D:424:TYR:HB3	1.95	0.47
1:D:590:ASP:OD1	1:D:590:ASP:N	2.48	0.47
1:B:99:PRO:HB3	1:B:284:LEU:HB3	1.96	0.47
1:B:136:LEU:HD21	1:B:184:LEU:HD11	1.96	0.47
1:B:163:ILE:HG21	1:B:180:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:VAL:HG13	1:B:803:LEU:HD23	1.96	0.46
1:A:638:ASP:HA	1:A:641:LYS:HB2	1.95	0.46
1:B:573:ILE:HG13	1:B:574:PHE:H	1.80	0.46
1:C:585:MET:N	1:D:599:ARG:HH11	2.13	0.46
1:D:667:PHE:HE1	1:D:727:LEU:HD13	1.80	0.46
1:A:77:TYR:CD1	1:A:82:VAL:HB	2.50	0.46
1:D:174:ASP:HA	1:D:207:GLN:NE2	2.30	0.46
1:B:50:LEU:HD12	1:B:61:ALA:HB2	1.98	0.46
1:A:132:LYS:HE2	1:A:187:LYS:HD3	1.96	0.46
1:A:590:ASP:N	1:A:590:ASP:OD1	2.49	0.46
1:D:647:TYR:HA	1:D:701:ALA:O	2.15	0.46
1:A:235:ILE:HD12	1:A:242:VAL:HG21	1.97	0.46
1:A:418:ASN:HD21	1:A:441:LYS:HA	1.81	0.46
1:B:583:ALA:HB1	1:B:588:GLY:O	2.15	0.46
1:D:599:ARG:O	1:D:603:GLY:N	2.49	0.46
1:A:517:PHE:CE1	1:A:794:GLY:HA3	2.51	0.46
1:A:194:LEU:HD22	1:A:204:ILE:HG21	1.96	0.46
1:A:312:ALA:HB2	1:A:323:TRP:HZ2	1.80	0.46
1:B:620:LEU:HD11	4:B:901:GYK:C18	2.45	0.46
1:C:607:PHE:O	1:C:611:ILE:HG12	2.15	0.46
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.81	0.46
1:C:589:ALA:O	1:C:591:ILE:N	2.49	0.46
1:D:620:LEU:HD11	4:D:901:GYK:C18	2.46	0.46
1:B:130:TRP:CE2	1:B:191:ARG:HG2	2.51	0.45
1:B:521:LEU:O	1:D:788:SER:OG	2.34	0.45
1:C:588:GLY:HA3	1:C:605:TRP:CD1	2.51	0.45
1:C:654:SER:H	5:C:902:ZK1:PBA	2.40	0.45
1:A:60:ASN:HA	1:B:316:LEU:HD12	1.98	0.45
1:B:262:TRP:HA	1:B:265:LEU:HD12	1.96	0.45
1:C:588:GLY:HA3	1:C:605:TRP:HD1	1.80	0.45
1:D:474:ILE:HD11	1:D:746:VAL:HG21	1.99	0.45
1:D:540:LEU:HA	1:D:543:VAL:HG12	1.98	0.45
1:A:499:GLY:HA3	1:A:726:ASN:HB3	1.99	0.45
1:B:372:GLY:HA2	1:B:382:LEU:HB3	1.99	0.45
1:B:428:LEU:HD13	1:B:759:LEU:HD21	1.99	0.45
1:D:405:TYR:HB3	1:D:425:CYS:SG	2.57	0.45
1:A:667:PHE:HE1	1:A:727:LEU:HD13	1.81	0.45
1:B:584:PHE:CD1	1:B:605:TRP:HZ2	2.32	0.45
1:A:74:PHE:HZ	1:A:285:THR:HG22	1.81	0.45
1:A:150:LEU:HD11	1:B:150:LEU:HD11	1.99	0.45
1:A:163:ILE:HG21	1:A:180:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HA	1:A:204:ILE:HD12	1.99	0.45
1:D:130:TRP:CE2	1:D:191:ARG:HG2	2.52	0.45
1:A:692:ARG:HA	1:A:695:LYS:HE2	1.98	0.45
1:D:93:HIS:ND1	1:D:322:PRO:HB2	2.32	0.45
1:B:126:GLU:OE2	1:B:156:LYS:NZ	2.49	0.44
1:C:209:ILE:HA	1:C:214:HIS:CD2	2.52	0.44
1:C:779:GLY:O	1:C:780:SER:HB3	2.16	0.44
1:D:705:GLU:OE2	5:D:902:ZK1:HAM	2.17	0.44
1:B:209:ILE:HD11	1:B:235:ILE:HG23	1.99	0.44
1:A:403:SER:HA	1:A:404:PRO:HA	1.76	0.44
1:B:575:GLN:HA	1:B:578:TRP:HE1	1.82	0.44
1:C:656:LYS:HE2	1:C:671:TRP:CH2	2.53	0.44
1:D:369:ARG:HD2	1:D:369:ARG:HA	1.74	0.44
1:A:781:LYS:HE3	1:A:781:LYS:HB2	1.75	0.44
1:B:308:ARG:NH2	1:B:312:ALA:HB2	2.31	0.44
1:C:130:TRP:CE2	1:C:191:ARG:HG2	2.52	0.44
1:D:596:LEU:HD12	1:D:597:SER:H	1.82	0.44
1:A:644:GLU:CD	1:B:782:GLU:HG2	2.38	0.44
1:B:429:ALA:O	1:B:432:ILE:HG13	2.18	0.44
1:C:99:PRO:HA	1:C:113:MET:HB2	1.99	0.44
1:A:622:ALA:O	1:A:626:VAL:HG22	2.17	0.44
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.82	0.44
1:A:647:TYR:HA	1:A:701:ALA:O	2.18	0.44
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.52	0.44
1:B:659:PHE:CZ	1:B:703:LEU:HD22	2.53	0.44
1:C:80:LYS:HG2	1:D:83:ASN:OD1	2.18	0.44
1:C:138:ASP:HB2	1:C:196:CYS:SG	2.58	0.43
1:D:589:ALA:HB2	1:D:602:GLY:HA3	1.99	0.43
1:D:233:LEU:HA	1:D:236:GLN:HB2	2.00	0.43
1:B:508:GLN:O	1:B:508:GLN:HG3	2.18	0.43
1:D:17:LEU:HD11	1:D:65:GLN:HG3	2.00	0.43
1:C:132:LYS:HG3	1:C:159:GLN:HB3	2.00	0.43
1:C:502:ILE:HB	1:C:723:VAL:HG23	2.00	0.43
1:C:667:PHE:HE1	1:C:727:LEU:HD13	1.84	0.43
1:C:115:PRO:HG3	1:C:247:ILE:HD13	2.01	0.43
1:C:590:ASP:O	1:C:591:ILE:HG12	2.18	0.43
1:A:659:PHE:HB3	1:A:671:TRP:HB2	2.00	0.43
1:C:233:LEU:HA	1:C:236:GLN:HB2	1.98	0.43
1:C:342:SER:HB2	1:C:353:ARG:HH22	1.83	0.43
1:D:373:TYR:HD1	1:D:382:LEU:HB2	1.83	0.43
1:A:582:GLY:HA3	1:C:599:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:PRO:HG3	1:B:711:TYR:CZ	2.53	0.43
1:B:536:VAL:HG21	1:B:605:TRP:CE3	2.54	0.43
1:B:763:LYS:O	1:B:767:TRP:HB2	2.18	0.43
1:C:795:VAL:O	1:C:798:ILE:HG22	2.19	0.43
1:D:591:ILE:HD12	1:D:593:PRO:HD2	2.01	0.43
1:C:631:SER:N	1:C:632:PRO:HD2	2.33	0.43
1:D:467:LEU:HD22	1:D:737:PRO:HG3	2.00	0.43
1:D:763:LYS:O	1:D:767:TRP:HB2	2.19	0.43
1:B:533:TYR:HD2	1:B:605:TRP:CH2	2.37	0.43
1:B:656:LYS:HE2	1:B:671:TRP:CH2	2.54	0.43
1:D:403:SER:HA	1:D:404:PRO:HA	1.78	0.43
1:A:209:ILE:HD11	1:A:235:ILE:HG23	2.02	0.42
1:B:795:VAL:O	1:B:798:ILE:HG22	2.19	0.42
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.54	0.42
1:C:631:SER:N	1:C:632:PRO:CD	2.82	0.42
1:A:352:LYS:H	1:A:352:LYS:HG2	1.68	0.42
1:A:660:ARG:HG3	1:A:671:TRP:CZ2	2.54	0.42
1:D:373:TYR:CE1	1:D:381:VAL:HB	2.55	0.42
1:A:398:THR:HG23	1:A:463:MET:HG2	2.00	0.42
1:A:619:ASN:ND2	1:B:787:LEU:HB2	2.34	0.42
1:B:125:ILE:HD11	1:B:193:ILE:HD11	2.00	0.42
1:B:650:LEU:HD11	1:B:702:TYR:OH	2.19	0.42
1:D:225:LEU:HD22	1:D:247:ILE:HB	2.02	0.42
1:A:405:TYR:HB3	1:A:425:CYS:SG	2.60	0.42
1:B:692:ARG:HA	1:B:695:LYS:HE2	2.01	0.42
1:C:208:VAL:HG12	1:C:214:HIS:HB3	2.00	0.42
1:A:66:PHE:CE2	1:A:312:ALA:HB1	2.55	0.42
1:A:369:ARG:HH21	1:A:387:THR:HG22	1.84	0.42
1:A:583:ALA:HB1	1:A:588:GLY:HA2	2.01	0.42
1:A:589:ALA:HB2	1:B:585:MET:SD	2.60	0.42
1:B:599:ARG:HG2	1:D:581:LEU:HD12	2.01	0.42
1:C:514:VAL:HG23	1:C:794:GLY:HA3	2.01	0.42
1:C:787:LEU:HD23	1:D:521:LEU:HD23	2.01	0.42
1:D:109:PHE:HZ	1:D:327:VAL:HG22	1.83	0.42
5:A:902:ZK1:HAI	5:A:902:ZK1:HAOA	1.80	0.42
1:C:713:GLU:HG3	1:C:721:MET:HA	2.02	0.42
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.85	0.42
1:A:795:VAL:O	1:A:798:ILE:HG22	2.20	0.42
1:C:500:ILE:HG12	1:C:655:THR:HG23	2.01	0.42
1:C:590:ASP:C	1:C:591:ILE:HG12	2.40	0.42
1:C:509:LYS:HE2	1:C:509:LYS:HB3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:791:ASN:HD21	4:B:901:GYK:C21	2.33	0.42
1:D:207:GLN:O	1:D:211:ILE:HG12	2.20	0.42
1:A:132:LYS:NZ	1:A:187:LYS:HB3	2.35	0.41
1:A:645:ILE:HG12	1:A:699:LYS:HA	2.02	0.41
1:C:572:ALA:HB1	1:C:576:SER:HB2	2.02	0.41
1:A:591:ILE:HG21	1:C:599:ARG:HH12	1.85	0.41
1:B:113:MET:HB3	1:B:284:LEU:HD22	2.02	0.41
1:D:683:VAL:HB	1:D:688:GLU:HG3	2.01	0.41
1:C:392:GLN:HG2	1:C:393:LYS:N	2.35	0.41
1:A:207:GLN:O	1:A:211:ILE:HG12	2.21	0.41
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.56	0.41
1:B:405:TYR:CD2	1:B:478:PRO:HG3	2.56	0.41
1:A:98:THR:HA	1:A:99:PRO:HD3	1.92	0.41
1:A:526:TRP:O	1:A:529:ILE:HG22	2.21	0.41
1:A:631:SER:OG	1:A:632:PRO:HD2	2.21	0.41
1:A:692:ARG:HA	1:A:695:LYS:HG2	2.03	0.41
1:C:308:ARG:HH21	1:C:312:ALA:HB2	1.85	0.41
1:C:404:PRO:HG3	1:C:711:TYR:CD1	2.55	0.41
1:C:803:LEU:HD21	1:D:536:VAL:HG22	2.02	0.41
1:D:518:LEU:HB2	1:D:526:TRP:CD1	2.55	0.41
1:A:169:ASN:ND2	1:A:171:ASP:OD2	2.54	0.41
1:B:308:ARG:HH11	1:B:308:ARG:HA	1.85	0.41
1:D:115:PRO:HG2	1:D:358:ILE:HD11	2.02	0.41
1:A:517:PHE:N	1:A:517:PHE:CD2	2.89	0.41
1:B:98:THR:HA	1:B:99:PRO:HD3	1.92	0.41
1:B:589:ALA:HB2	1:B:602:GLY:HA3	2.02	0.41
1:C:262:TRP:HA	1:C:265:LEU:HD12	2.02	0.41
1:C:568:THR:O	1:C:568:THR:OG1	2.37	0.41
1:D:401:LEU:HD23	1:D:406:VAL:HG12	2.03	0.41
1:A:522:ALA:HB2	1:B:787:LEU:O	2.21	0.41
1:A:650:LEU:HD13	1:A:702:TYR:OH	2.20	0.41
1:A:692:ARG:HD3	1:A:700:TYR:CZ	2.55	0.41
1:B:326:GLY:HA2	1:B:329:ILE:HD12	2.02	0.41
1:B:506:LYS:HA	1:B:507:PRO:HD3	1.90	0.41
1:C:403:SER:HA	1:C:404:PRO:HA	1.86	0.41
1:C:533:TYR:OH	1:C:581:LEU:HA	2.21	0.41
1:D:302:GLN:H	1:D:302:GLN:HG2	1.67	0.41
1:D:623:PHE:HA	1:D:626:VAL:HG12	2.03	0.41
1:A:460:TRP:NE1	1:A:488:VAL:HG11	2.36	0.41
1:B:135:TYR:CE1	1:B:137:TYR:HB3	2.56	0.41
1:C:169:ASN:OD1	1:C:169:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:VAL:HG22	1:C:341:LEU:HA	2.03	0.41
1:A:174:ASP:CG	1:A:207:GLN:HE22	2.22	0.40
1:D:235:ILE:HD12	1:D:242:VAL:HG21	2.03	0.40
1:A:66:PHE:CZ	1:A:92:LEU:HD22	2.56	0.40
1:C:517:PHE:O	1:C:520:PRO:HD2	2.22	0.40
1:D:633:ILE:HG23	1:D:638:ASP:HB2	2.03	0.40
5:D:902:ZK1:HAOA	5:D:902:ZK1:HAI	1.84	0.40
1:A:588:GLY:HA2	1:A:605:TRP:CD1	2.57	0.40
1:D:406:VAL:HG23	1:D:425:CYS:HB2	2.03	0.40
1:D:620:LEU:HD12	1:D:620:LEU:HA	1.87	0.40
1:D:655:THR:O	1:D:659:PHE:HD2	2.05	0.40
1:A:262:TRP:HA	1:A:265:LEU:HD12	2.04	0.40
1:A:589:ALA:HA	1:A:602:GLY:HA3	2.04	0.40
1:B:578:TRP:O	1:B:581:LEU:HD23	2.21	0.40
1:D:337:GLN:HA	1:D:345:ILE:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	780/823 (95%)	729 (94%)	49 (6%)	2 (0%)	41	76
1	B	777/823 (94%)	715 (92%)	57 (7%)	5 (1%)	25	65
1	C	792/823 (96%)	742 (94%)	44 (6%)	6 (1%)	19	60
1	D	782/823 (95%)	730 (93%)	48 (6%)	4 (0%)	29	68
All	All	3131/3292 (95%)	2916 (93%)	198 (6%)	17 (0%)	29	68

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	593	PRO
1	B	784	THR
1	C	786	ALA
1	D	522	ALA
1	B	507	PRO
1	B	512	PRO
1	B	520	PRO
1	C	548	PRO
1	C	591	ILE
1	C	787	LEU
1	C	788	SER
1	C	589	ALA
1	A	816	TYR
1	D	633	ILE
1	D	776	LYS
1	A	383	THR
1	D	591	ILE

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	662/696 (95%)	658 (99%)	4 (1%)	86	92
1	B	659/696 (95%)	652 (99%)	7 (1%)	73	85
1	C	672/696 (97%)	669 (100%)	3 (0%)	91	94
1	D	664/696 (95%)	661 (100%)	3 (0%)	88	93
All	All	2657/2784 (95%)	2640 (99%)	17 (1%)	86	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	TYR
1	A	527	MET
1	A	592	SER
1	A	595	SER
1	B	171	ASP

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Mol	Chain	Res	Type
1	B	450	TYR
1	B	506	LYS
1	B	509	LYS
1	B	594	ARG
1	B	595	SER
1	B	599	ARG
1	C	450	TYR
1	C	599	ARG
1	C	780	SER
1	D	393	LYS
1	D	450	TYR
1	D	599	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	112	GLN
1	A	159	GLN
1	A	344	ASN
1	A	586	GLN
1	A	587	GLN
1	A	756	GLN
1	B	83	ASN
1	B	159	GLN
1	B	214	HIS
1	B	302	GLN
1	B	756	GLN
1	B	791	ASN
1	C	112	GLN
1	C	344	ASN
1	C	587	GLN
1	D	207	GLN
1	D	366	ASN
1	D	508	GLN
1	D	756	GLN

5.3.3 RNA

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)

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	E	1	2,1	14,14,15	0.30	0	17,19,21	0.55	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.44	0
2	BMA	E	3	2	11,11,12	0.62	0	15,15,17	0.78	0
3	NAG	F	1	3,1	14,14,15	0.49	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.51	0
3	BMA	F	3	3	11,11,12	1.15	1 (9%)	15,15,17	1.02	1 (6%)
3	BMA	F	4	3	11,11,12	0.98	0	15,15,17	1.42	1 (6%)
2	NAG	G	1	2,1	14,14,15	0.89	1 (7%)	17,19,21	1.40	1 (5%)
2	NAG	G	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	BMA	G	3	2	11,11,12	0.63	0	15,15,17	0.75	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	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	BMA	F	4	3	-	1/2/19/22	1/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	3.24	1.48	1.43
3	F	3	BMA	C4-C3	2.16	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NAG	C1-O5-C5	5.52	119.67	112.19
3	F	4	BMA	C1-O5-C5	4.51	118.30	112.19
3	F	3	BMA	C2-C3-C4	2.13	114.57	110.89

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	4	BMA	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4	BMA	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0

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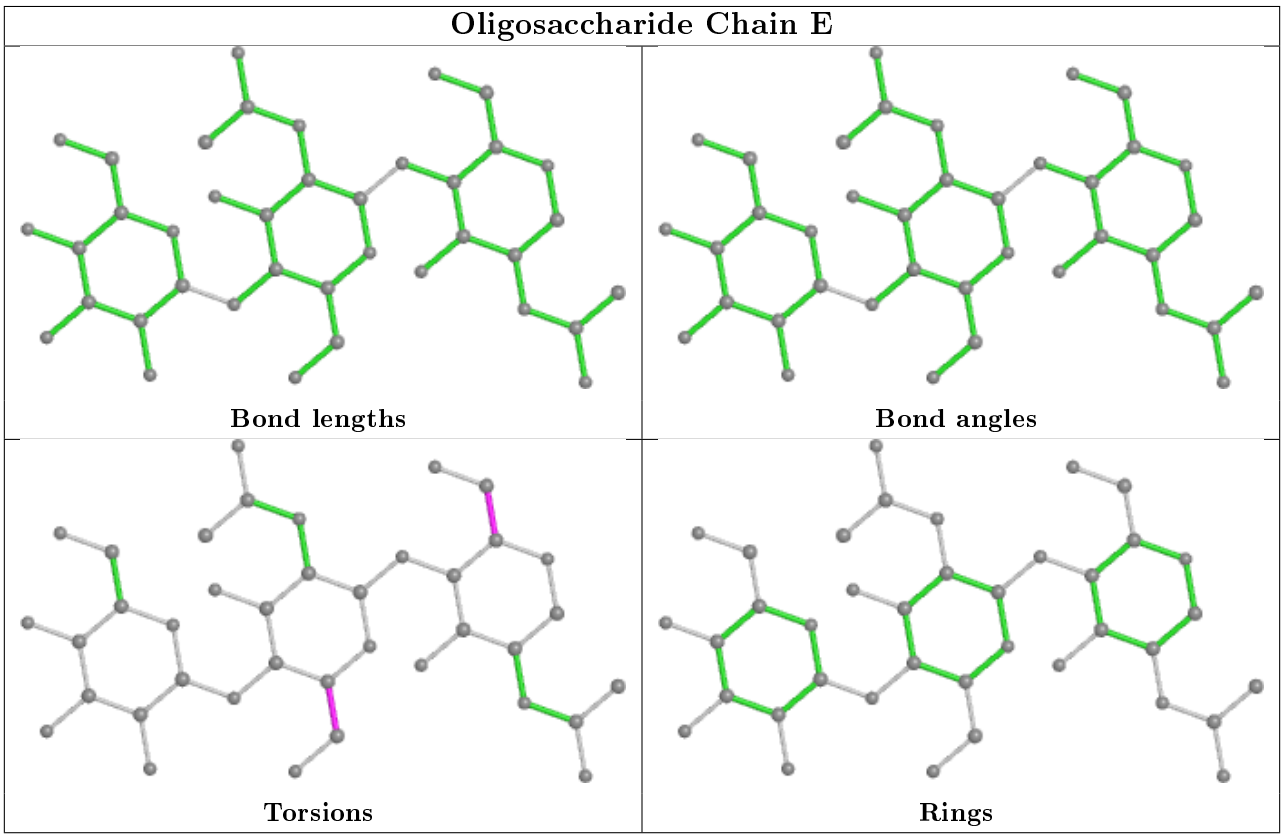
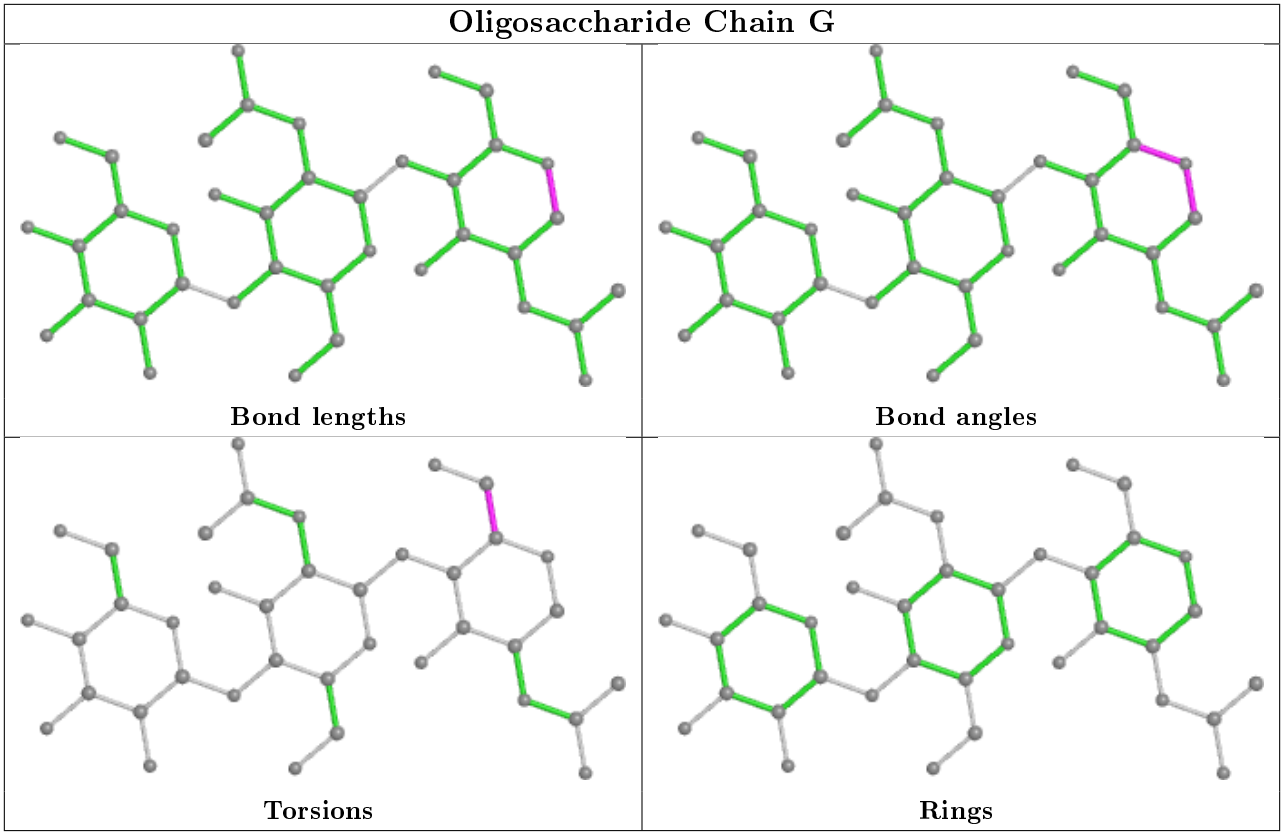
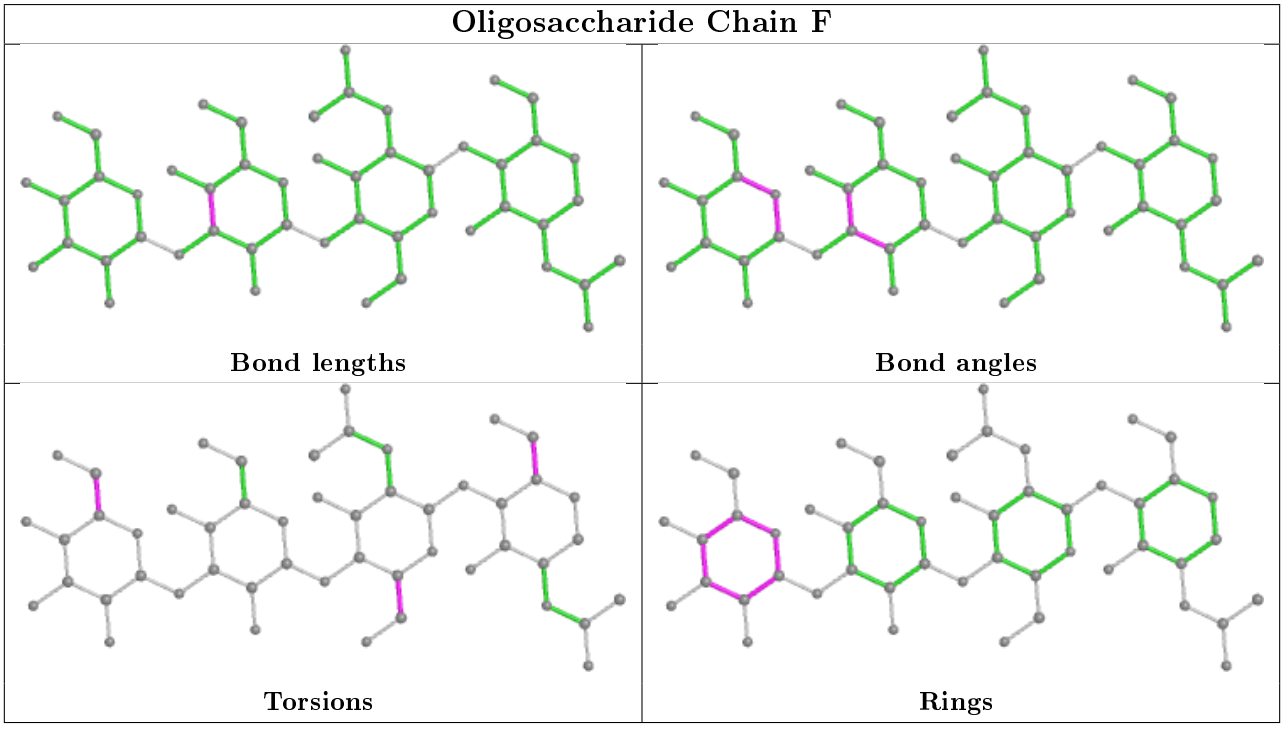
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	2	0

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







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	$\#\|Z\| > 2$
4	GYK	D	901	-	27,29,29	3.79	10 (37%)	30,42,42	2.02	6 (20%)
5	ZK1	C	902	-	28,29,29	3.29	14 (50%)	36,45,45	1.56	6 (16%)
5	ZK1	A	902	-	28,29,29	3.31	14 (50%)	36,45,45	1.57	6 (16%)
4	GYK	C	901	-	27,29,29	3.84	11 (40%)	30,42,42	2.16	11 (36%)
5	ZK1	B	902	-	28,29,29	3.32	14 (50%)	36,45,45	1.52	5 (13%)
4	GYK	A	901	-	27,29,29	3.80	9 (33%)	30,42,42	2.03	6 (20%)
4	GYK	B	901	-	27,29,29	3.85	11 (40%)	30,42,42	2.22	11 (36%)
5	ZK1	D	902	-	28,29,29	3.10	13 (46%)	36,45,45	1.54	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GYK	D	901	-	-	2/6/32/32	0/3/4/4
5	ZK1	C	902	-	-	5/13/23/23	0/3/3/3
5	ZK1	A	902	-	-	4/13/23/23	0/3/3/3
4	GYK	C	901	-	-	2/6/32/32	0/3/4/4
5	ZK1	B	902	-	-	5/13/23/23	0/3/3/3
4	GYK	A	901	-	-	2/6/32/32	0/3/4/4
4	GYK	B	901	-	-	2/6/32/32	0/3/4/4
5	ZK1	D	902	-	-	5/13/23/23	0/3/3/3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	GYK	C10-N11	13.88	1.45	1.30
4	C	901	GYK	C10-N11	13.76	1.45	1.30
4	A	901	GYK	C10-N11	13.72	1.45	1.30
4	D	901	GYK	C10-N11	13.60	1.45	1.30
4	D	901	GYK	C13-N15	8.44	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	GYK	C13-N15	8.44	1.45	1.34
4	C	901	GYK	C13-N15	8.39	1.45	1.34
4	B	901	GYK	C13-N15	8.29	1.45	1.34
5	B	902	ZK1	PBA-OAC	7.39	1.65	1.50
5	C	902	ZK1	PBA-OAC	7.25	1.65	1.50
5	A	902	ZK1	PBA-OAC	7.22	1.65	1.50
5	D	902	ZK1	OAA-CAT	6.64	1.41	1.24
5	A	902	ZK1	OAA-CAT	6.63	1.41	1.24
5	B	902	ZK1	OAA-CAT	6.63	1.41	1.24
5	C	902	ZK1	OAA-CAT	6.59	1.41	1.24
5	B	902	ZK1	OAB-CAU	6.56	1.40	1.24
5	D	902	ZK1	OAB-CAU	6.55	1.40	1.24
5	C	902	ZK1	OAB-CAU	6.55	1.40	1.24
5	A	902	ZK1	OAB-CAU	6.55	1.40	1.24
5	A	902	ZK1	CAT-NAP	6.36	1.44	1.33
5	B	902	ZK1	CAT-NAP	6.33	1.44	1.33
5	D	902	ZK1	CAT-NAP	6.33	1.44	1.33
5	C	902	ZK1	CAT-NAP	6.32	1.44	1.33
4	B	901	GYK	C09-C10	6.11	1.58	1.49
4	C	901	GYK	C09-C10	6.10	1.58	1.49
4	B	901	GYK	O26-C25	-5.71	1.32	1.43
4	D	901	GYK	O26-C25	-5.70	1.32	1.43
4	C	901	GYK	O26-C25	-5.69	1.32	1.43
4	A	901	GYK	O26-C25	-5.68	1.32	1.43
4	D	901	GYK	C09-C10	5.64	1.57	1.49
4	A	901	GYK	C09-C10	5.57	1.57	1.49
4	A	901	GYK	O24-C25	-5.54	1.32	1.43
4	B	901	GYK	O24-C25	-5.53	1.32	1.43
4	D	901	GYK	O24-C25	-5.51	1.32	1.43
4	C	901	GYK	O24-C25	-5.51	1.32	1.43
5	D	902	ZK1	CAW-NAY	5.31	1.47	1.40
5	B	902	ZK1	CAW-NAY	5.22	1.47	1.40
5	A	902	ZK1	CAW-NAY	5.11	1.46	1.40
5	C	902	ZK1	CAW-NAY	4.95	1.46	1.40
5	A	902	ZK1	CAJ-CAS	4.74	1.44	1.37
5	D	902	ZK1	CAJ-CAS	4.71	1.44	1.37
5	B	902	ZK1	CAJ-CAS	4.70	1.44	1.37
5	C	902	ZK1	CAJ-CAS	4.69	1.44	1.37
5	D	902	ZK1	PBA-OAE	4.69	1.65	1.54
5	A	902	ZK1	PBA-OAE	4.68	1.65	1.54
5	C	902	ZK1	PBA-OAE	4.65	1.65	1.54
5	D	902	ZK1	PBA-OAD	4.55	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	ZK1	PBA-OAD	4.54	1.65	1.54
5	B	902	ZK1	PBA-OAE	-3.65	1.46	1.54
5	A	902	ZK1	PBA-OAD	-3.65	1.46	1.54
5	C	902	ZK1	PBA-OAD	-3.64	1.46	1.54
5	D	902	ZK1	CAI-CAR	2.73	1.42	1.38
5	B	902	ZK1	CAI-CAR	2.66	1.42	1.38
5	A	902	ZK1	CAI-CAR	2.60	1.42	1.38
5	C	902	ZK1	CAI-CAR	2.54	1.42	1.38
4	D	901	GYK	C08-C07	2.50	1.43	1.38
4	B	901	GYK	C08-C07	2.44	1.43	1.38
4	C	901	GYK	C05-C04	2.42	1.43	1.39
4	B	901	GYK	C05-C04	2.41	1.43	1.39
4	A	901	GYK	C05-C04	2.41	1.43	1.39
4	B	901	GYK	C17-C10	2.40	1.52	1.49
4	C	901	GYK	C08-C07	2.39	1.43	1.38
4	D	901	GYK	C05-C04	2.35	1.43	1.39
4	B	901	GYK	O14-C13	-2.35	1.18	1.23
4	D	901	GYK	O14-C13	-2.34	1.18	1.23
4	C	901	GYK	O14-C13	-2.34	1.18	1.23
4	C	901	GYK	C17-C10	2.33	1.52	1.49
4	A	901	GYK	O14-C13	-2.33	1.18	1.23
5	D	902	ZK1	CAR-NAX	2.32	1.46	1.41
4	A	901	GYK	C08-C07	2.31	1.43	1.38
5	B	902	ZK1	CAR-NAX	2.30	1.46	1.41
5	C	902	ZK1	CAM-NAX	2.21	1.50	1.46
5	A	902	ZK1	CAR-NAX	2.21	1.46	1.41
5	C	902	ZK1	CAR-NAX	2.21	1.46	1.41
5	D	902	ZK1	PBA-CAO	2.20	1.86	1.81
5	D	902	ZK1	CAM-NAX	2.18	1.50	1.46
5	B	902	ZK1	PBA-CAO	2.16	1.86	1.81
5	A	902	ZK1	PBA-CAO	2.15	1.86	1.81
5	A	902	ZK1	CAM-NAX	2.14	1.50	1.46
5	B	902	ZK1	CAM-NAX	2.14	1.50	1.46
5	D	902	ZK1	CAV-NAP	2.12	1.38	1.35
5	B	902	ZK1	CAV-NAP	2.11	1.38	1.35
5	A	902	ZK1	CAN-NAX	2.11	1.50	1.46
5	A	902	ZK1	CAV-NAP	2.11	1.38	1.35
5	D	902	ZK1	CAN-NAX	2.10	1.50	1.46
4	C	901	GYK	C08-C09	2.09	1.43	1.39
5	C	902	ZK1	CAN-NAX	2.08	1.50	1.46
4	B	901	GYK	C08-C09	2.07	1.43	1.39
5	C	902	ZK1	CAV-NAP	2.07	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	902	ZK1	PBA-CAO	2.05	1.86	1.81
4	A	901	GYK	C20-N23	2.03	1.45	1.38
4	C	901	GYK	C20-N23	2.03	1.45	1.38
4	D	901	GYK	C20-N23	2.03	1.45	1.38
4	B	901	GYK	C20-N23	2.02	1.45	1.38
4	D	901	GYK	C08-C09	2.01	1.43	1.39
5	B	902	ZK1	CAN-NAX	2.01	1.49	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	901	GYK	O24-C07-C08	5.17	134.77	127.85
4	B	901	GYK	O24-C07-C08	5.17	134.76	127.85
4	D	901	GYK	O24-C07-C08	5.14	134.73	127.85
4	A	901	GYK	O24-C07-C08	5.09	134.66	127.85
4	D	901	GYK	O24-C07-C06	-4.58	104.57	109.78
4	B	901	GYK	O24-C07-C06	-4.58	104.57	109.78
4	C	901	GYK	O26-C06-C05	4.51	133.88	127.85
4	A	901	GYK	O26-C06-C05	4.50	133.87	127.85
4	C	901	GYK	O24-C07-C06	-4.47	104.69	109.78
5	C	902	ZK1	CAN-NAX-CAM	4.43	121.29	111.52
4	B	901	GYK	O26-C06-C05	4.42	133.76	127.85
5	A	902	ZK1	CAN-NAX-CAM	4.42	121.27	111.52
4	A	901	GYK	O24-C07-C06	-4.39	104.78	109.78
4	D	901	GYK	O26-C06-C05	4.37	133.69	127.85
5	D	902	ZK1	CAN-NAX-CAM	4.26	120.92	111.52
5	B	902	ZK1	CAN-NAX-CAM	4.01	120.37	111.52
4	D	901	GYK	C25-O24-C07	3.97	110.50	105.34
4	B	901	GYK	C25-O24-C07	3.94	110.46	105.34
4	C	901	GYK	C25-O24-C07	3.90	110.40	105.34
4	A	901	GYK	C25-O24-C07	3.89	110.39	105.34
5	A	902	ZK1	CAV-CAW-NAY	3.39	120.17	117.72
5	C	902	ZK1	CAV-CAW-NAY	3.33	120.13	117.72
5	B	902	ZK1	CAV-CAW-NAY	3.23	120.06	117.72
5	D	902	ZK1	CAV-CAW-NAY	3.10	119.96	117.72
4	A	901	GYK	O26-C06-C07	-2.88	106.50	109.78
4	A	901	GYK	C25-O26-C06	2.88	109.08	105.34
4	D	901	GYK	C25-O26-C06	2.83	109.01	105.34
4	C	901	GYK	C25-O26-C06	2.79	108.96	105.34
4	C	901	GYK	O26-C06-C07	-2.75	106.65	109.78
4	B	901	GYK	C25-O26-C06	2.75	108.91	105.34
4	D	901	GYK	O26-C06-C07	-2.74	106.66	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	GYK	O26-C06-C07	-2.68	106.73	109.78
4	B	901	GYK	C22-C17-C10	2.67	123.99	120.64
4	B	901	GYK	C18-C17-C10	-2.57	117.41	120.64
4	C	901	GYK	C22-C17-C10	2.44	123.70	120.64
4	B	901	GYK	C01-C02-N12	-2.40	108.25	111.14
5	C	902	ZK1	FAG-CAZ-CAS	-2.39	108.54	112.70
5	D	902	ZK1	CAT-NAP-CAV	2.38	120.09	116.83
4	C	901	GYK	C18-C17-C10	-2.36	117.67	120.64
4	B	901	GYK	C09-C10-C17	2.36	120.85	118.11
5	A	902	ZK1	CAT-NAP-CAV	2.32	120.02	116.83
5	B	902	ZK1	CAT-NAP-CAV	2.32	120.02	116.83
5	A	902	ZK1	CAJ-CAS-CAZ	2.27	118.56	116.77
5	C	902	ZK1	CAS-CAR-NAX	2.27	122.52	119.92
5	C	902	ZK1	CAT-NAP-CAV	2.26	119.93	116.83
5	C	902	ZK1	CAO-NAY-CAU	2.24	120.50	117.79
4	B	901	GYK	C08-C09-C10	2.12	121.96	118.88
5	B	902	ZK1	CAS-CAR-NAX	2.11	122.34	119.92
4	C	901	GYK	C09-C10-C17	2.11	120.56	118.11
4	C	901	GYK	C01-C02-N12	-2.10	108.62	111.14
5	A	902	ZK1	CAS-CAR-NAX	2.09	122.31	119.92
5	A	902	ZK1	FAG-CAZ-CAS	-2.07	109.09	112.70
5	D	902	ZK1	CAJ-CAS-CAZ	2.04	118.38	116.77
5	B	902	ZK1	CAJ-CAS-CAZ	2.03	118.37	116.77
4	C	901	GYK	C05-C06-C07	-2.01	119.47	122.02

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	GYK	C09-C10-C17-C18
4	A	901	GYK	C09-C10-C17-C22
4	B	901	GYK	N11-C10-C17-C18
4	B	901	GYK	N11-C10-C17-C22
4	C	901	GYK	N11-C10-C17-C18
4	C	901	GYK	N11-C10-C17-C22
4	D	901	GYK	C09-C10-C17-C18
4	D	901	GYK	C09-C10-C17-C22
5	A	902	ZK1	NAY-CAO-PBA-OAD
5	A	902	ZK1	NAY-CAO-PBA-OAE
5	B	902	ZK1	NAY-CAO-PBA-OAC
5	B	902	ZK1	NAY-CAO-PBA-OAD
5	B	902	ZK1	NAY-CAO-PBA-OAE

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Mol	Chain	Res	Type	Atoms
5	C	902	ZK1	NAY-CAO-PBA-OAE
5	D	902	ZK1	NAY-CAO-PBA-OAE
5	B	902	ZK1	CAI-CAR-NAX-CAN
5	D	902	ZK1	CAI-CAR-NAX-CAN
5	C	902	ZK1	CAI-CAR-NAX-CAN
5	C	902	ZK1	NAY-CAO-PBA-OAD
5	D	902	ZK1	NAY-CAO-PBA-OAD
5	A	902	ZK1	NAY-CAO-PBA-OAC
5	C	902	ZK1	NAY-CAO-PBA-OAC
5	D	902	ZK1	NAY-CAO-PBA-OAC
5	A	902	ZK1	CAI-CAR-NAX-CAN
5	B	902	ZK1	CAS-CAR-NAX-CAN
5	D	902	ZK1	CAS-CAR-NAX-CAN
5	C	902	ZK1	CAS-CAR-NAX-CAN

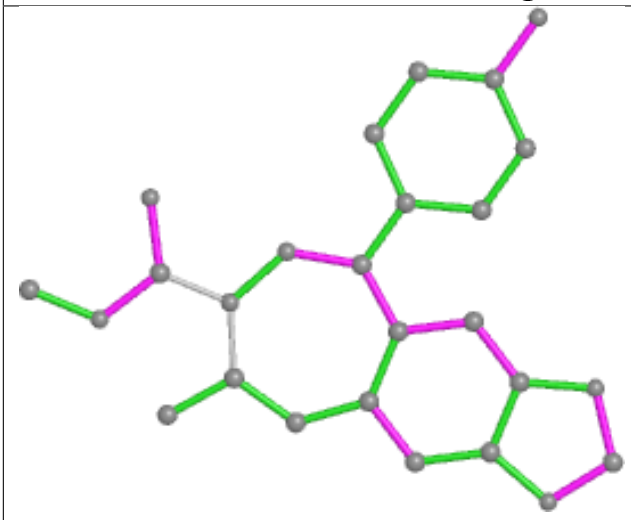
There are no ring outliers.

6 monomers are involved in 10 short contacts:

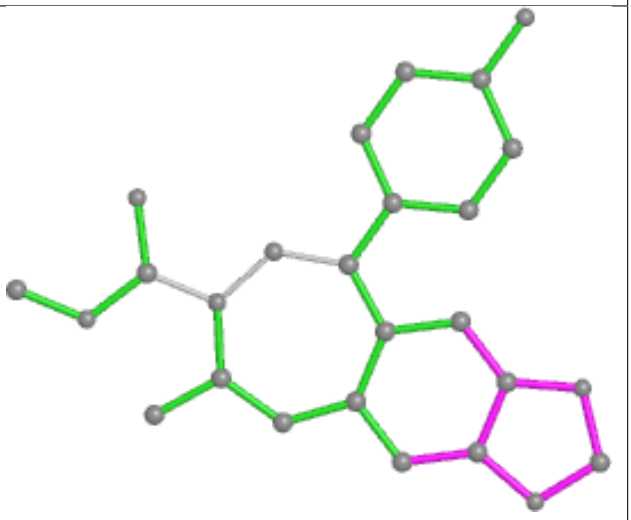
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	GYK	1	0
5	C	902	ZK1	3	0
5	A	902	ZK1	1	0
5	B	902	ZK1	1	0
4	B	901	GYK	2	0
5	D	902	ZK1	2	0

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

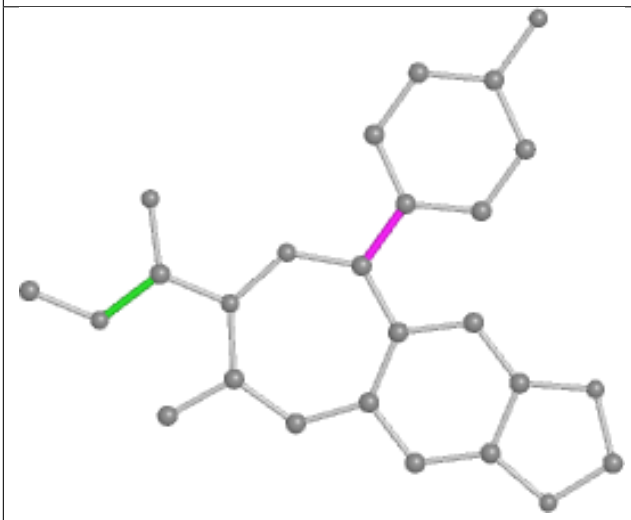
Ligand GYK D 901



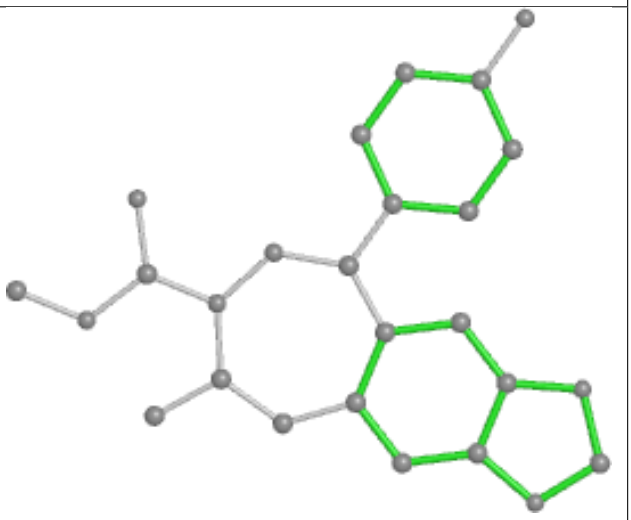
Bond lengths



Bond angles

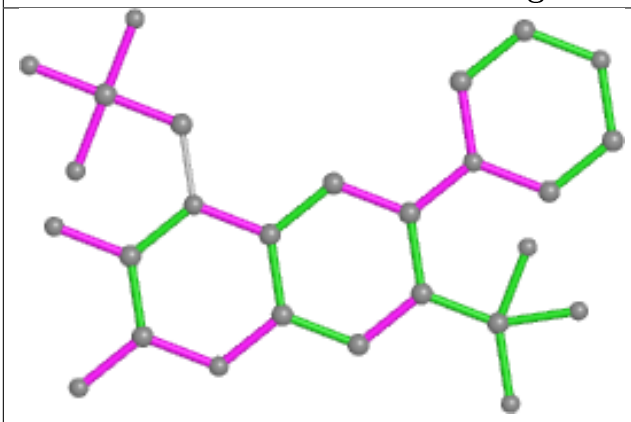


Torsions

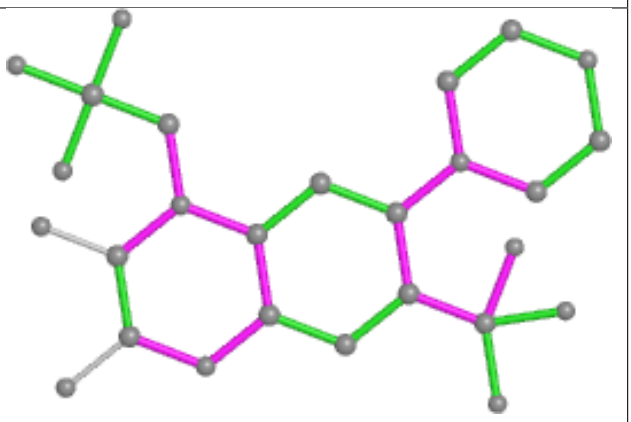


Rings

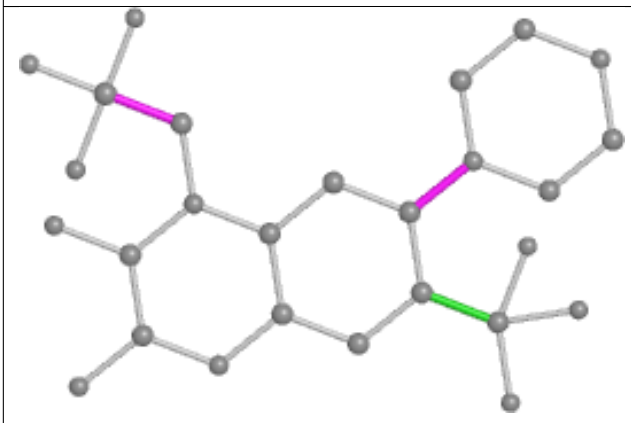
Ligand ZK1 C 902



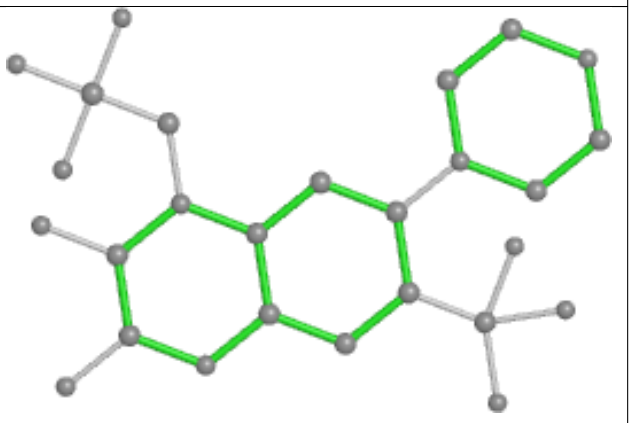
Bond lengths



Bond angles

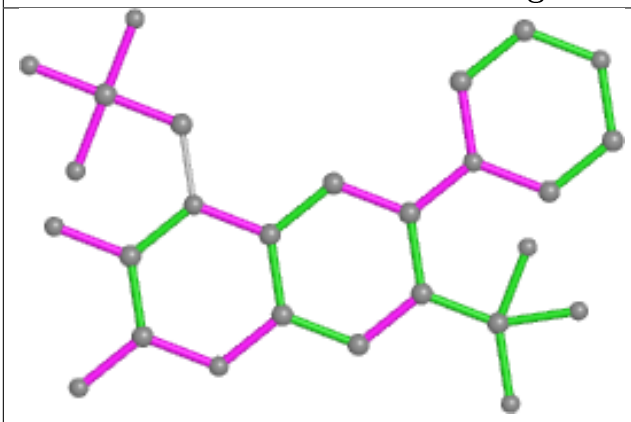


Torsions

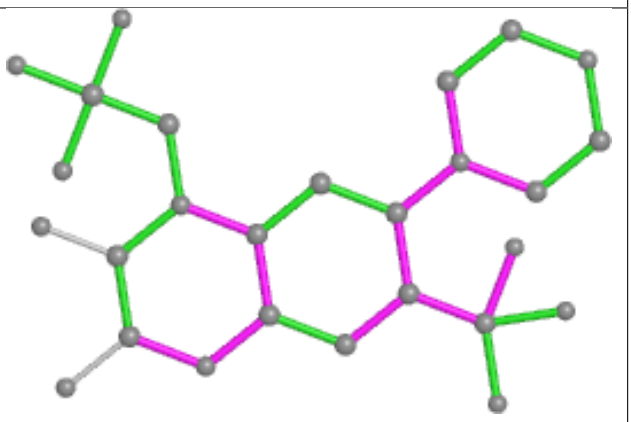


Rings

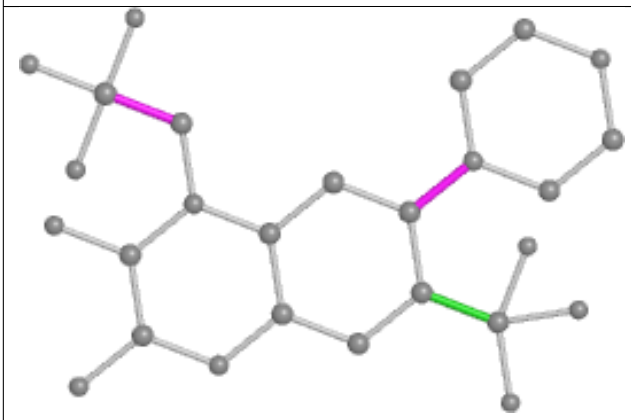
Ligand ZK1 A 902



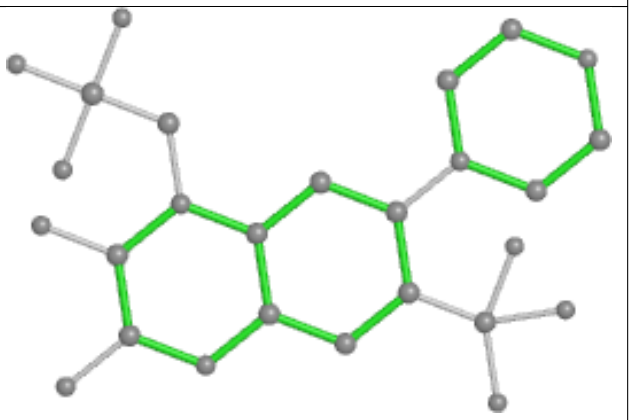
Bond lengths



Bond angles

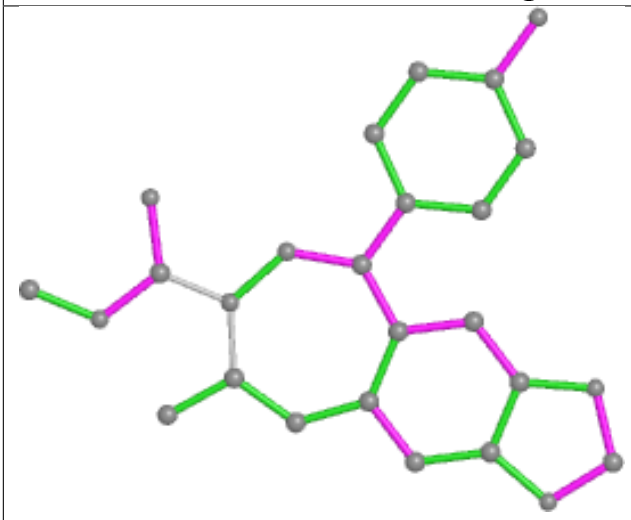


Torsions

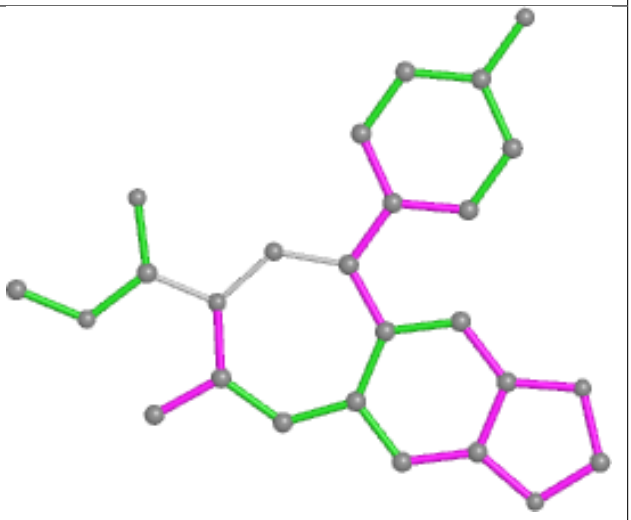


Rings

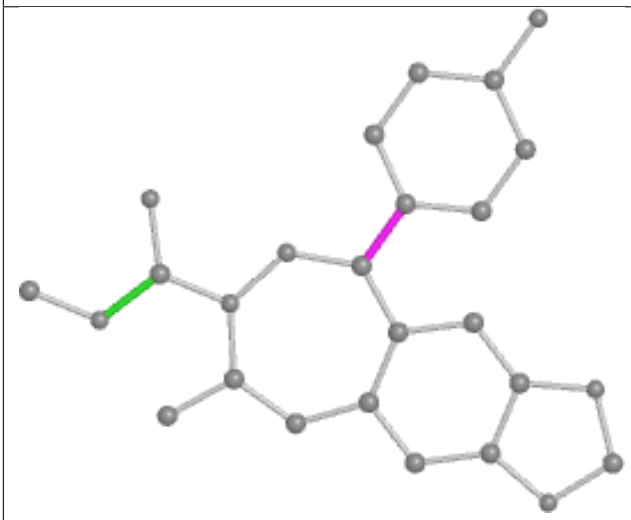
Ligand GYK C 901



Bond lengths



Bond angles



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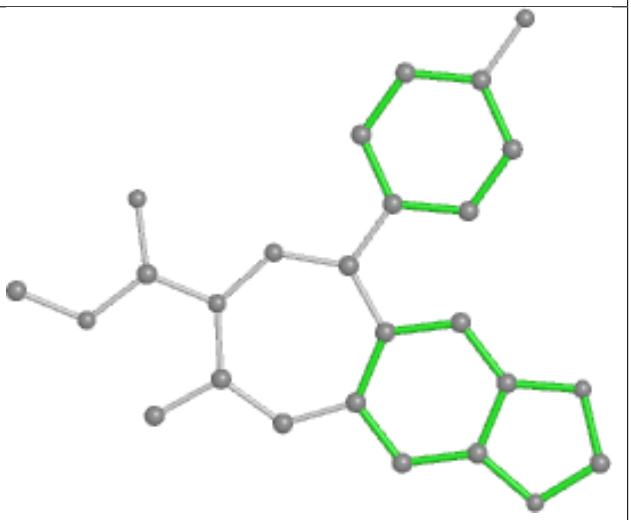
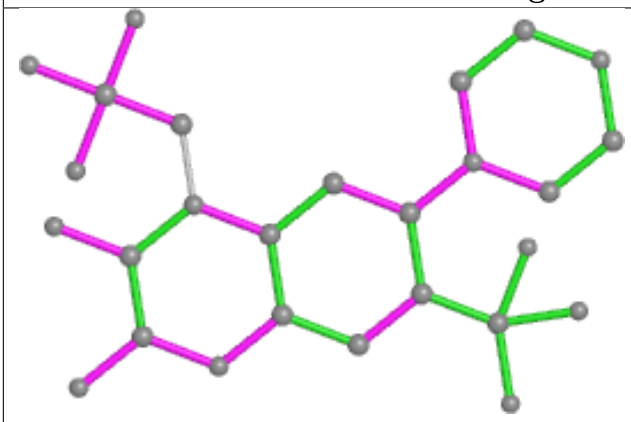
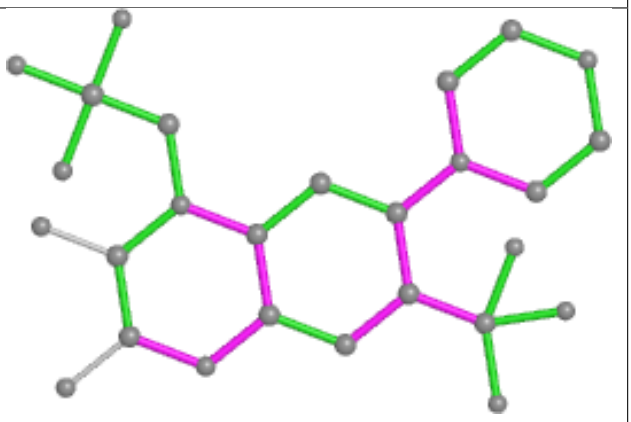


Rings

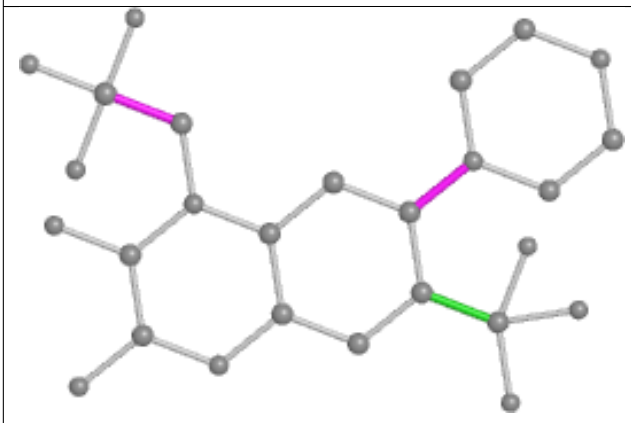
Ligand ZK1 B 902



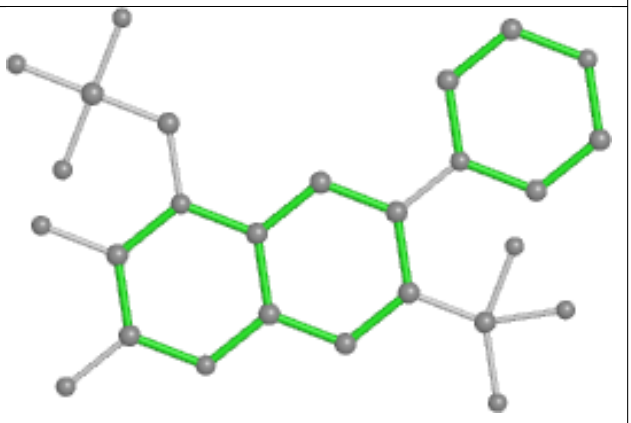
Bond lengths



Bond angles

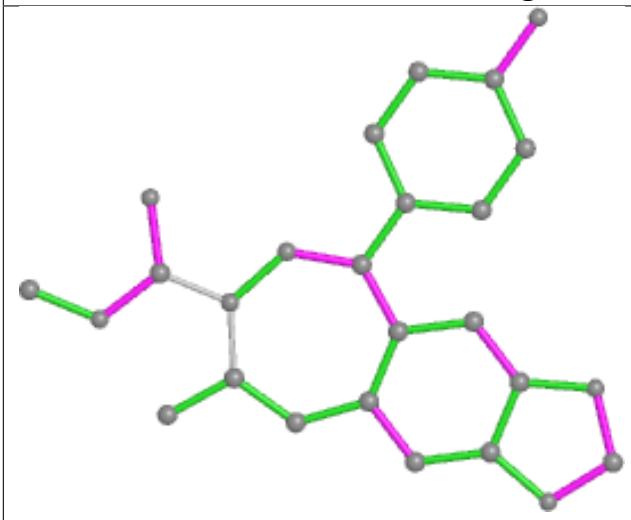


Torsions

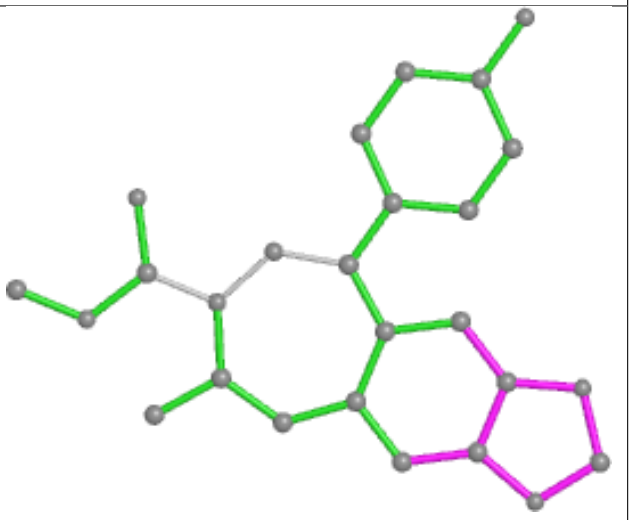


Rings

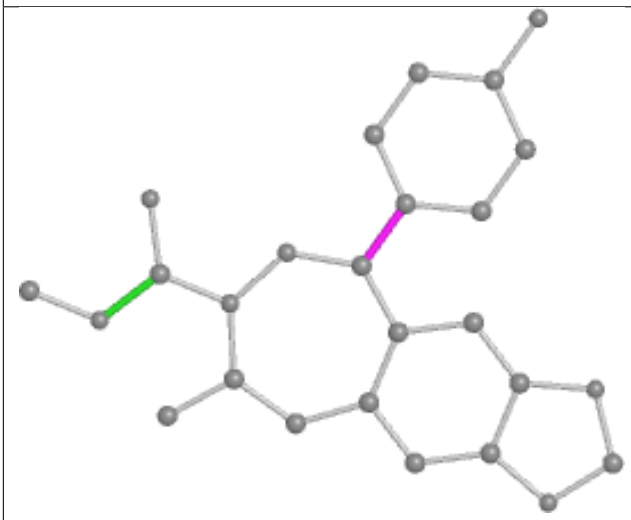
Ligand GYK A 901



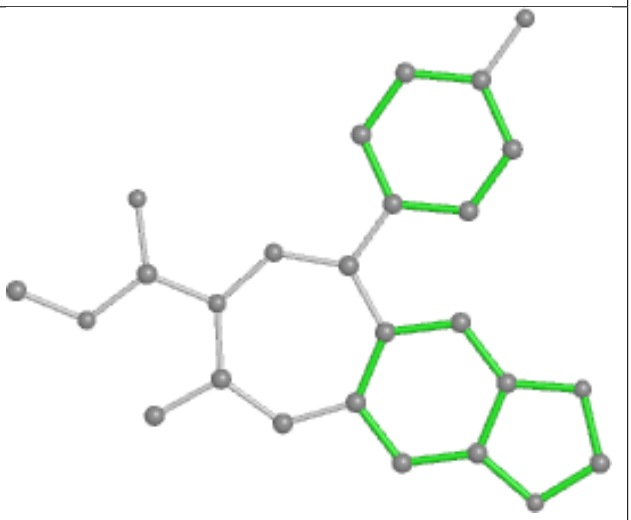
Bond lengths



Bond angles

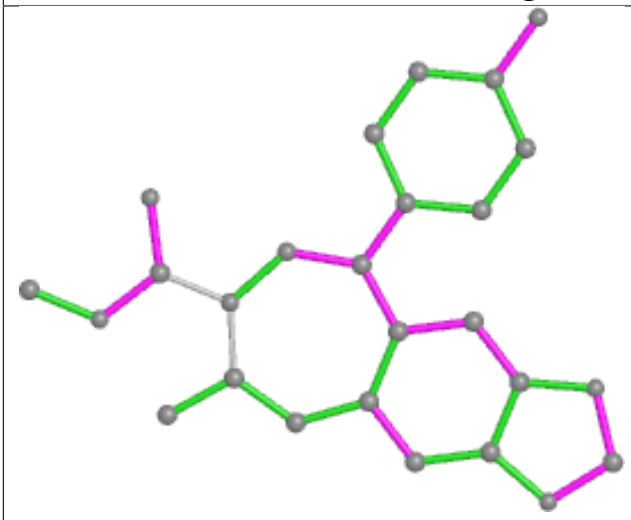


Torsions

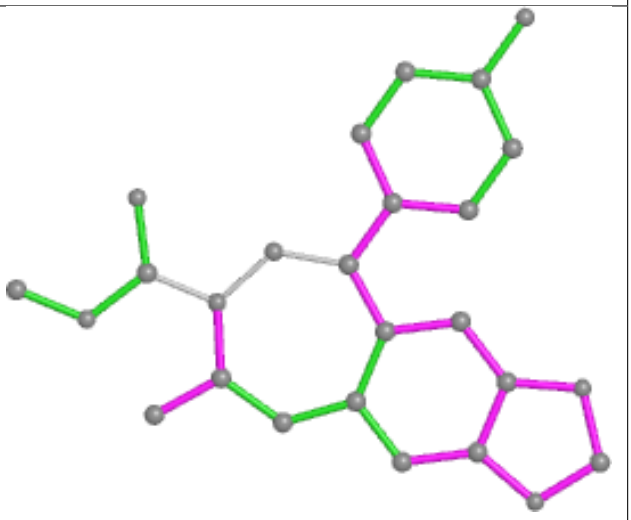


Rings

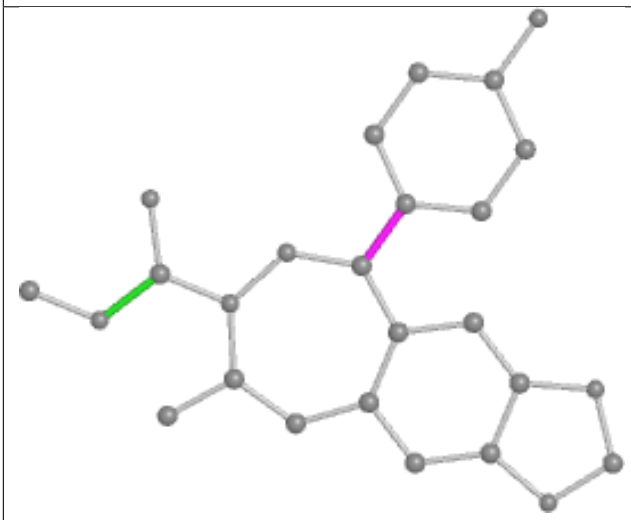
Ligand GYK B 901



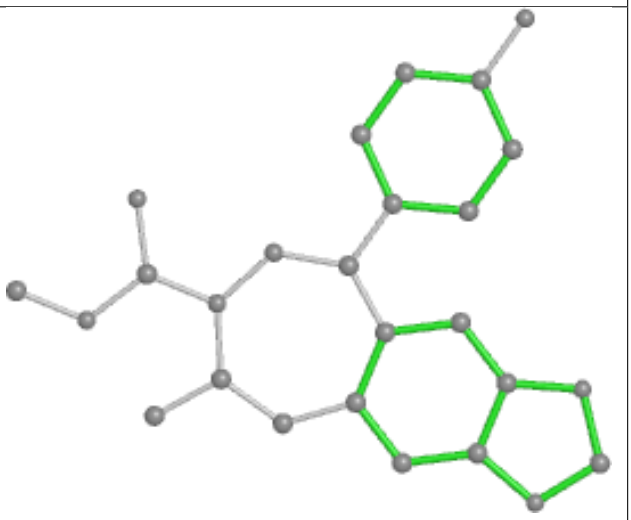
Bond lengths



Bond angles

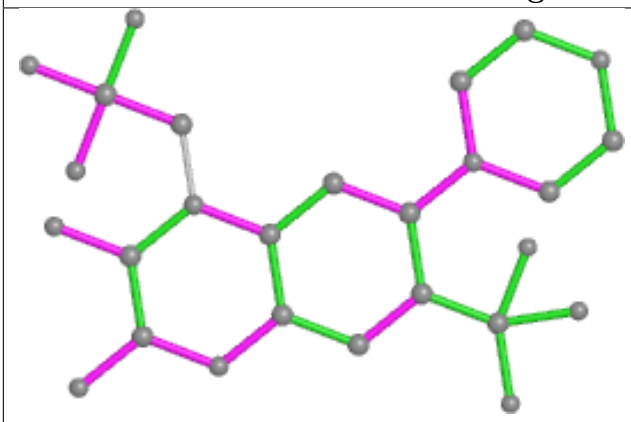


Torsions

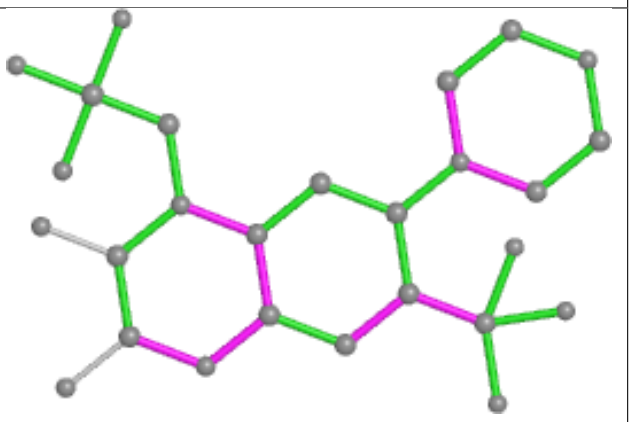


Rings

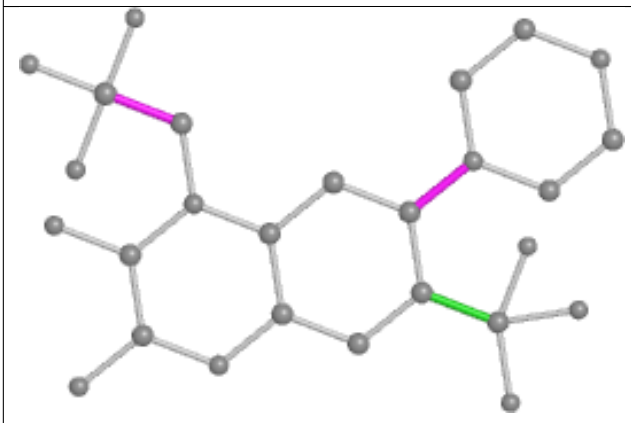
Ligand ZK1 D 902



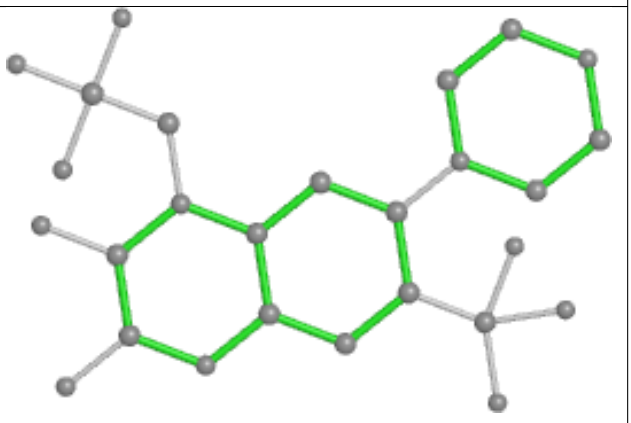
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	784/823 (95%)	0.03	34 (4%) 35 29	126, 201, 264, 306	0
1	B	781/823 (94%)	0.04	29 (3%) 41 33	113, 187, 267, 319	0
1	C	796/823 (96%)	0.39	98 (12%) 4 5	106, 224, 293, 351	0
1	D	786/823 (95%)	0.34	60 (7%) 13 12	142, 219, 290, 354	0
All	All	3147/3292 (95%)	0.20	221 (7%) 16 13	106, 208, 282, 354	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	ALA	7.0
1	D	313	GLY	6.3
1	D	588	GLY	6.2
1	A	512	PRO	6.2
1	C	447	ASP	6.0
1	C	684	ARG	5.8
1	C	649	THR	5.6
1	C	456	ASP	5.6
1	D	589	ALA	5.5
1	A	71	TYR	5.4
1	A	572	ALA	5.4
1	C	421	TYR	5.2
1	D	272	GLY	5.0
1	C	648	GLY	4.8
1	C	369	ARG	4.8
1	B	782	GLU	4.8
1	C	400	ILE	4.7
1	C	386	ASP	4.7
1	A	573	ILE	4.7
1	C	665	ALA	4.6
1	A	308	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	364	LYS	4.6
1	C	454	ASP	4.6
1	C	663	LYS	4.5
1	A	510	SER	4.5
1	C	362	GLU	4.4
1	A	508	GLN	4.4
1	C	412	HIS	4.4
1	C	438	PHE	4.4
1	C	416	ALA	4.2
1	C	401	LEU	4.2
1	A	720	THR	4.2
1	C	819	ARG	4.2
1	C	370	LYS	4.1
1	A	509	LYS	4.1
1	C	440	TYR	4.1
1	D	401	LEU	4.1
1	D	584	PHE	4.1
1	C	435	HIS	4.0
1	C	444	ILE	4.0
1	C	371	ILE	4.0
1	C	664	ILE	3.9
1	A	306	ILE	3.9
1	C	441	LYS	3.9
1	C	448	GLY	3.8
1	C	415	LEU	3.8
1	D	266	GLU	3.8
1	C	437	GLY	3.8
1	C	455	ALA	3.7
1	A	307	SER	3.7
1	A	70	VAL	3.7
1	C	385	ASP	3.6
1	B	775	ALA	3.6
1	B	697	LYS	3.6
1	C	392	GLN	3.6
1	C	394	THR	3.6
1	D	587	GLN	3.5
1	A	72	ALA	3.5
1	C	436	CYS	3.5
1	C	418	ASN	3.5
1	B	310	GLY	3.5
1	D	71	TYR	3.4
1	C	395	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	13	GLN	3.4
1	B	695	LYS	3.4
1	A	578	TRP	3.4
1	A	384	GLU	3.3
1	C	678	GLU	3.3
1	D	392	GLN	3.3
1	A	511	LYS	3.3
1	B	370	LYS	3.3
1	C	442	LEU	3.3
1	C	388	SER	3.3
1	D	278	ILE	3.3
1	C	703	LEU	3.2
1	B	359	ASN	3.2
1	C	399	THR	3.2
1	B	312	ALA	3.2
1	D	341	LEU	3.2
1	B	309	ARG	3.2
1	A	385	ASP	3.2
1	D	344	ASN	3.1
1	C	393	LYS	3.1
1	A	414	ALA	3.1
1	B	373	TYR	3.0
1	B	371	ILE	3.0
1	C	396	VAL	3.0
1	B	372	GLY	3.0
1	C	667	PHE	3.0
1	C	431	GLU	3.0
1	D	267	GLU	2.9
1	C	411	ASN	2.9
1	D	447	ASP	2.9
1	A	778	SER	2.9
1	C	363	LEU	2.9
1	D	590	ASP	2.9
1	C	266	GLU	2.9
1	D	306	ILE	2.9
1	C	569	ASN	2.9
1	C	383	THR	2.9
1	C	449	LYS	2.9
1	C	681	VAL	2.9
1	C	391	GLU	2.9
1	D	323	TRP	2.8
1	B	776	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	95	SER	2.8
1	A	415	LEU	2.8
1	C	572	ALA	2.8
1	D	307	SER	2.8
1	B	268	LYS	2.8
1	D	772	GLU	2.8
1	B	777	ASP	2.8
1	C	820	ALA	2.8
1	C	389	GLY	2.7
1	C	680	SER	2.7
1	C	42	ARG	2.7
1	D	308	ARG	2.7
1	D	274	HIS	2.7
1	C	476	ILE	2.7
1	C	647	TYR	2.7
1	D	387	THR	2.7
1	B	689	GLY	2.7
1	A	713	GLU	2.7
1	D	311	ASN	2.7
1	C	742	LEU	2.6
1	C	365	THR	2.6
1	C	268	LYS	2.6
1	D	593	PRO	2.6
1	A	577	ALA	2.6
1	B	360	ILE	2.6
1	C	390	LEU	2.6
1	D	451	GLY	2.6
1	C	451	GLY	2.6
1	D	445	VAL	2.6
1	B	774	GLY	2.6
1	A	777	ASP	2.6
1	D	248	VAL	2.6
1	D	449	LYS	2.6
1	D	441	LYS	2.5
1	D	265	LEU	2.5
1	A	438	PHE	2.5
1	C	429	ALA	2.5
1	D	684	ARG	2.5
1	C	397	VAL	2.5
1	C	43	LEU	2.5
1	D	273	ALA	2.5
1	D	398	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	249	ASP	2.5
1	C	409	LYS	2.5
1	C	443	THR	2.5
1	D	400	ILE	2.5
1	C	434	LYS	2.4
1	C	779	GLY	2.4
1	C	446	GLY	2.4
1	C	821	GLU	2.4
1	C	387	THR	2.4
1	B	311	ASN	2.4
1	C	420	ARG	2.4
1	C	474	ILE	2.4
1	C	413	ALA	2.4
1	C	432	ILE	2.4
1	C	702	TYR	2.4
1	C	685	THR	2.4
1	C	410	ALA	2.4
1	B	388	SER	2.4
1	D	280	TYR	2.4
1	B	369	ARG	2.3
1	C	548	PRO	2.3
1	C	461	ASN	2.3
1	D	473	ASP	2.3
1	B	696	SER	2.3
1	A	513	GLY	2.3
1	C	587	GLN	2.3
1	D	446	GLY	2.3
1	C	818	SER	2.3
1	D	683	VAL	2.3
1	A	323	TRP	2.3
1	B	361	MET	2.3
1	D	357	THR	2.3
1	D	227	PHE	2.3
1	D	322	PRO	2.3
1	A	574	PHE	2.3
1	C	464	VAL	2.3
1	D	321	VAL	2.3
1	D	815	CYS	2.3
1	D	228	THR	2.3
1	D	264	THR	2.2
1	B	692	ARG	2.2
1	D	388	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	229	ASP	2.2
1	C	662	SER	2.2
1	D	325	GLN	2.2
1	B	678	GLU	2.2
1	C	445	VAL	2.2
1	D	368	PRO	2.2
1	C	408	MET	2.2
1	D	583	ALA	2.2
1	D	818	SER	2.2
1	D	390	LEU	2.2
1	A	813	GLU	2.1
1	B	308	ARG	2.1
1	D	226	GLY	2.1
1	C	729	SER	2.1
1	D	391	GLU	2.1
1	A	416	ALA	2.1
1	C	728	ASP	2.1
1	A	419	GLU	2.1
1	A	723	VAL	2.1
1	C	428	LEU	2.1
1	D	276	ALA	2.1
1	D	682	PHE	2.1
1	C	628	ARG	2.0
1	B	270	TYR	2.0
1	B	679	PRO	2.0
1	B	385	ASP	2.0
1	D	592	SER	2.0
1	A	73	ILE	2.0
1	D	247	ILE	2.0
1	C	236	GLN	2.0
1	C	384	GLU	2.0
1	C	683	VAL	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)

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,

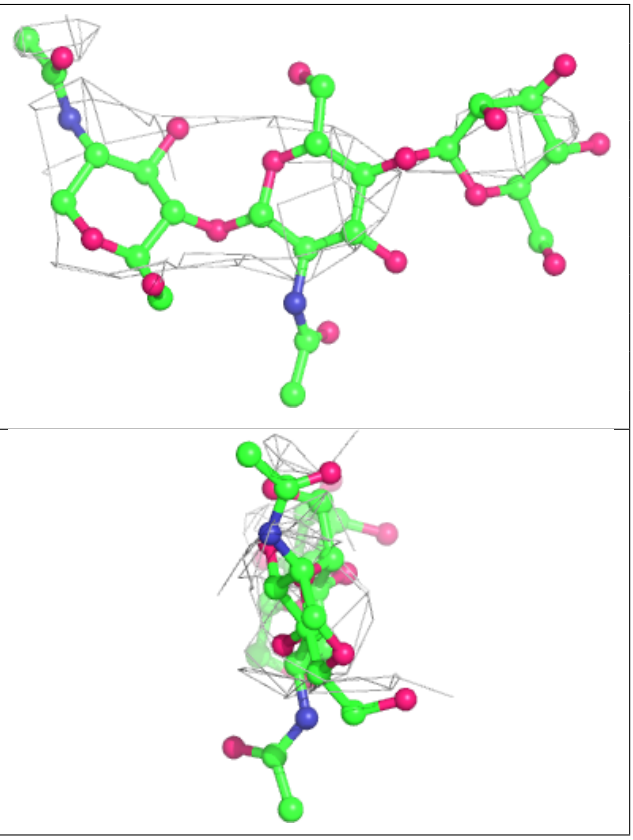
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

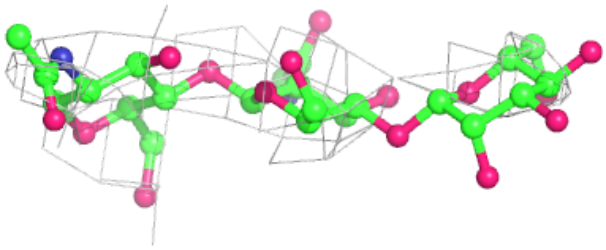
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	F	4	11/12	0.75	0.54	270,299,314,326	0
3	BMA	F	3	11/12	0.81	0.54	280,298,312,316	0
2	NAG	E	1	14/15	0.81	0.35	223,243,260,263	0
2	BMA	E	3	11/12	0.82	0.51	261,282,295,304	0
3	NAG	F	1	14/15	0.82	0.42	225,253,262,279	0
3	NAG	F	2	14/15	0.84	0.37	206,268,284,292	0
2	NAG	E	2	14/15	0.85	0.48	259,283,301,303	0
2	NAG	G	2	14/15	0.85	0.48	229,268,279,281	0
2	NAG	G	1	14/15	0.86	0.34	211,245,258,268	0
2	BMA	G	3	11/12	0.86	0.41	268,290,297,297	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

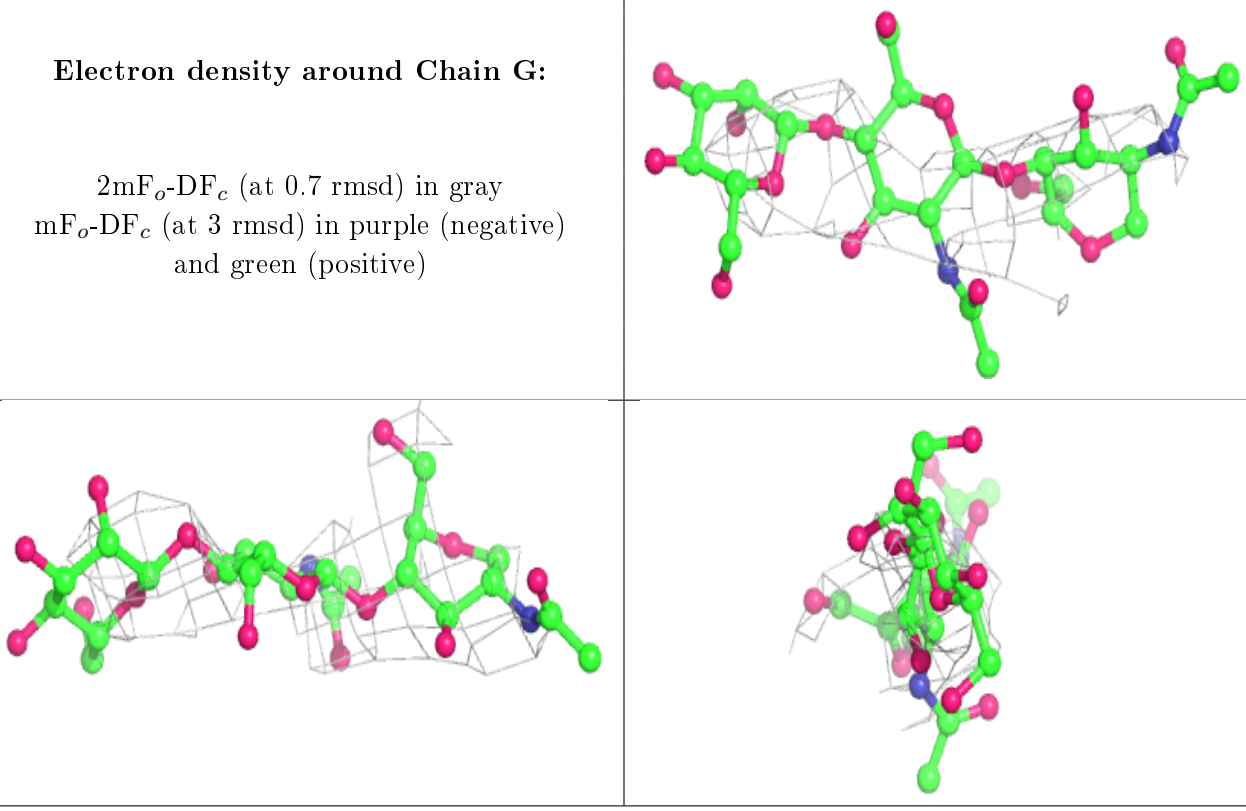
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





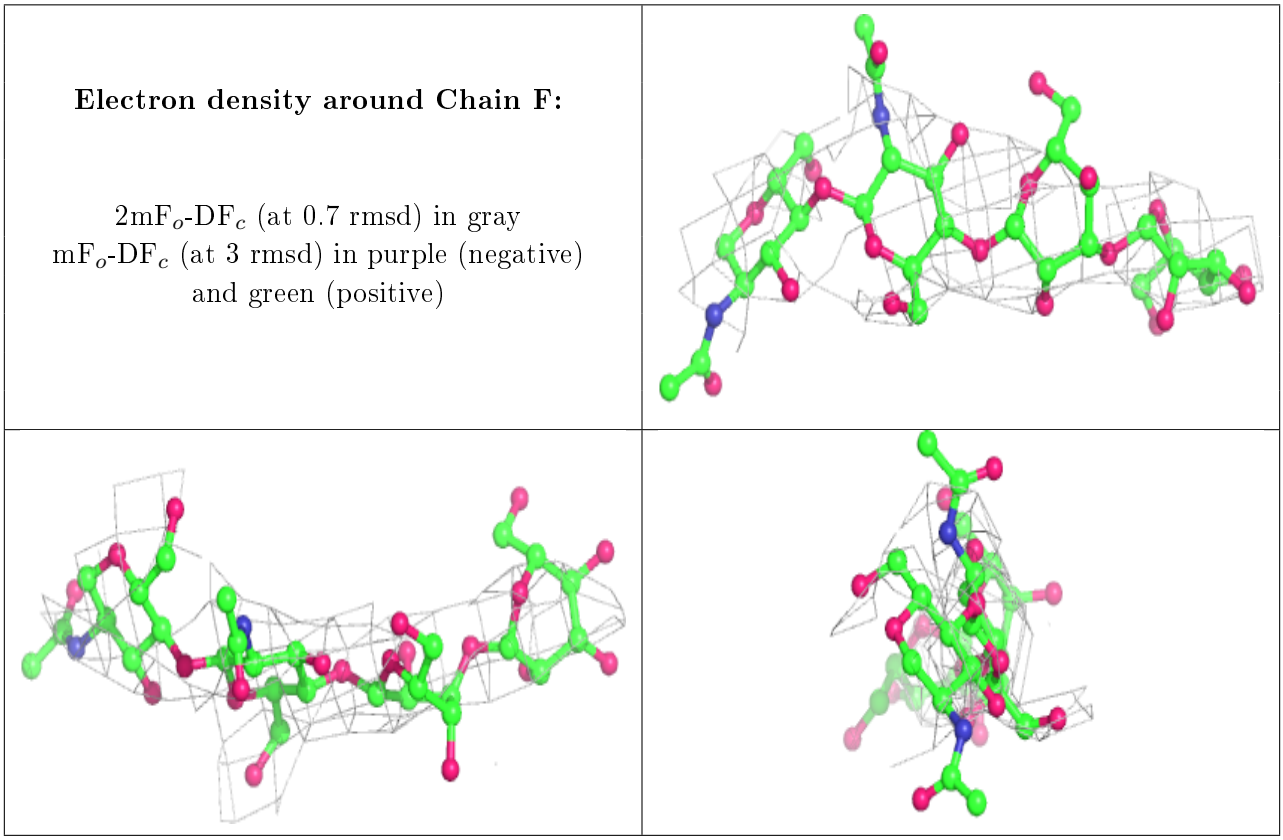
Electron density around Chain G:

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



Electron density around Chain F:

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



6.4 Ligands (i)

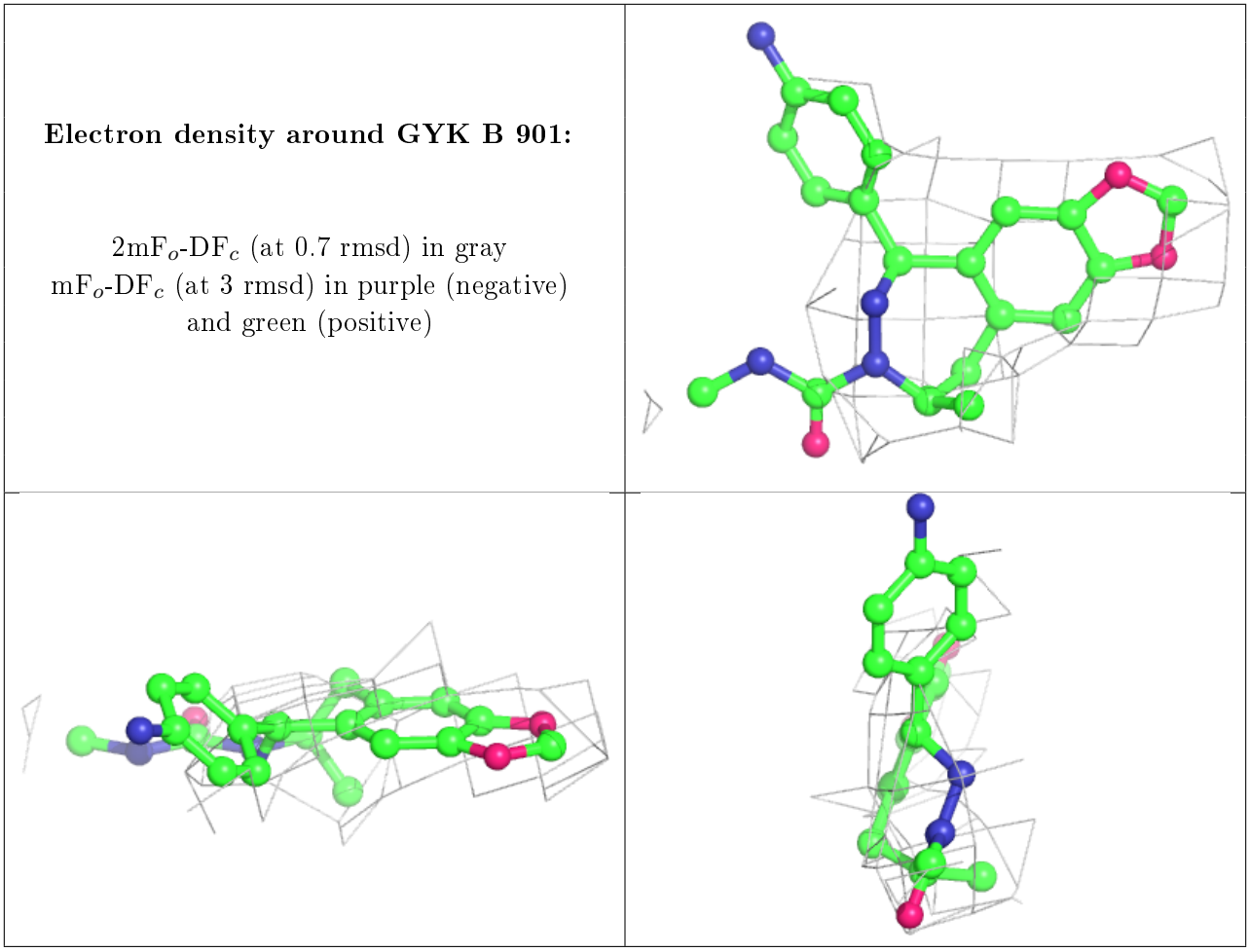
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GYK	B	901	26/26	0.72	0.46	208,225,234,240	0
4	GYK	C	901	26/26	0.74	0.47	205,219,233,237	0
4	GYK	A	901	26/26	0.76	0.60	214,240,251,254	0
5	ZK1	B	902	27/27	0.85	0.33	172,184,201,204	0
5	ZK1	D	902	27/27	0.86	0.35	171,201,216,218	0
5	ZK1	A	902	27/27	0.87	0.26	180,196,223,232	0
5	ZK1	C	902	27/27	0.89	0.41	230,249,268,278	0
4	GYK	D	901	26/26	0.89	0.32	223,244,265,275	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.

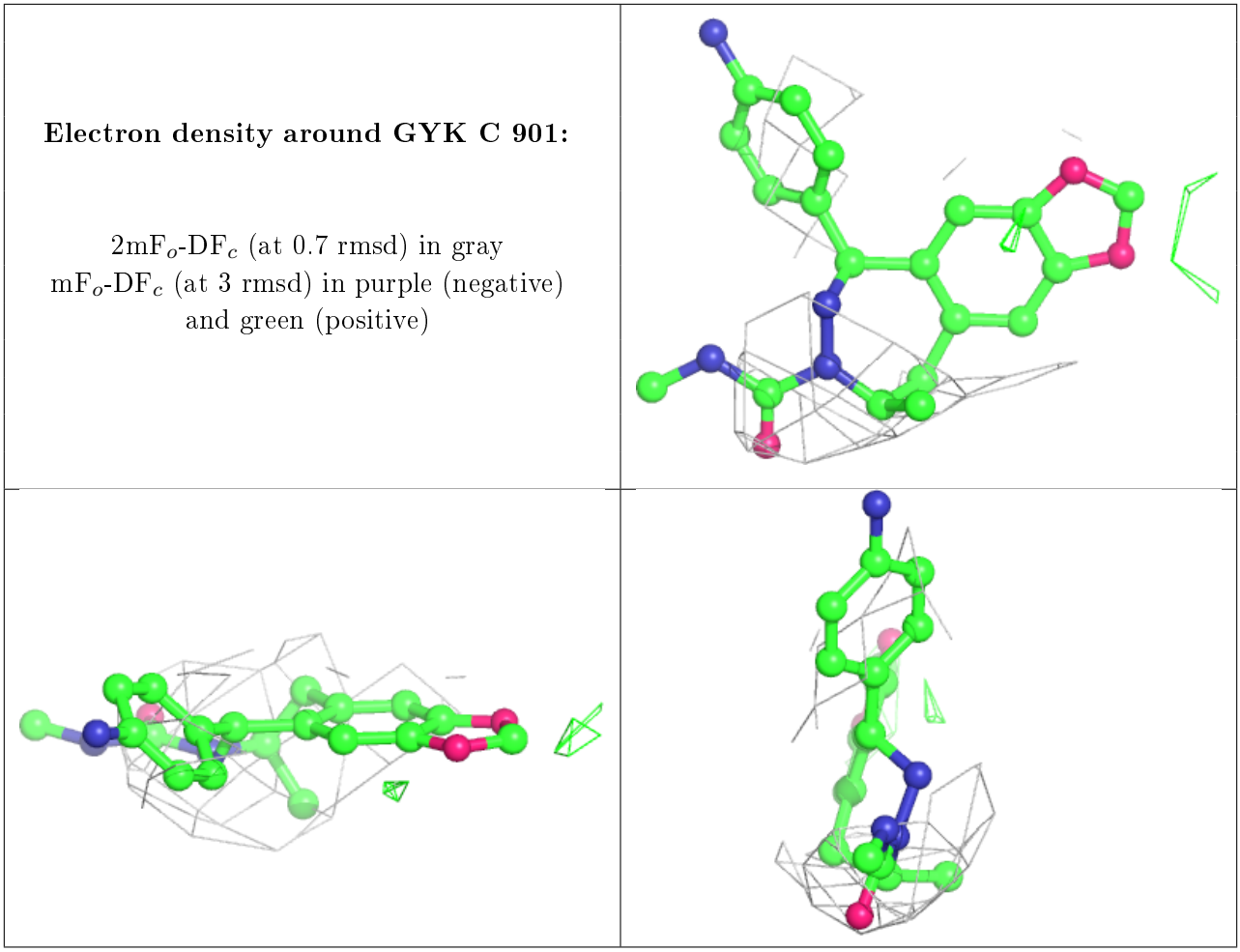
Electron density around GYK B 901:

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



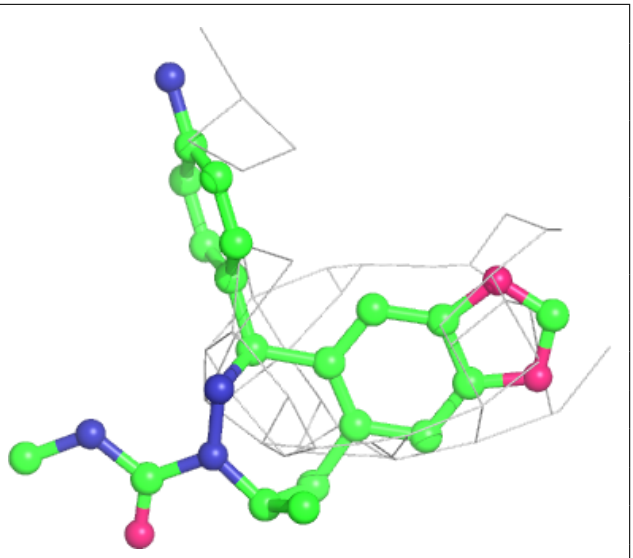
Electron density around GYK C 901:

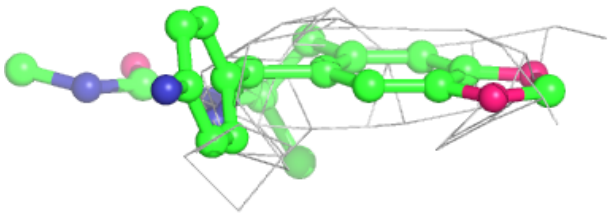
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

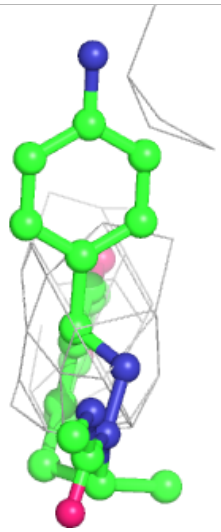


Electron density around GYK A 901:

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

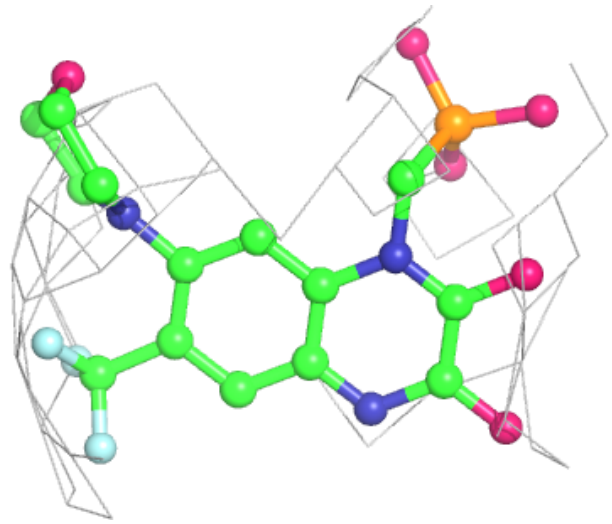


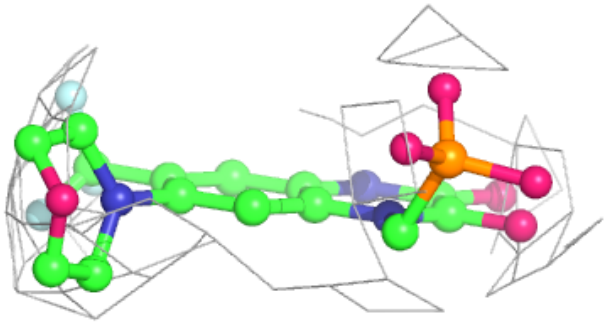


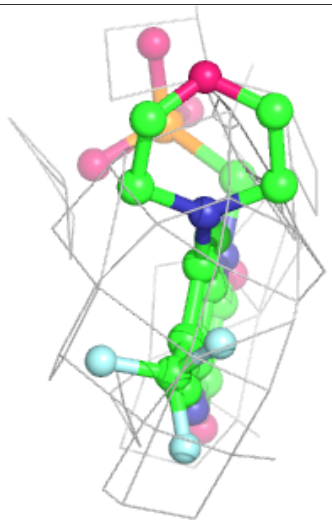


Electron density around ZK1 B 902:

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

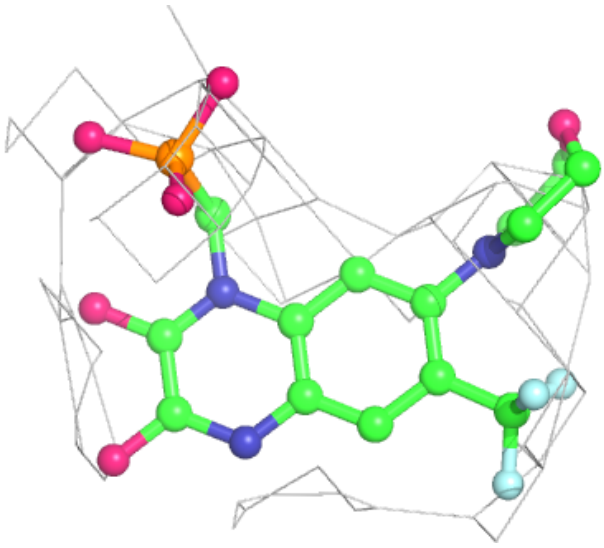


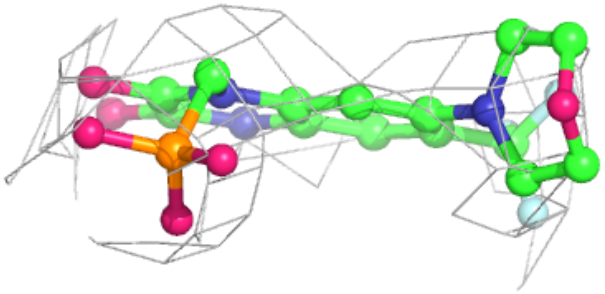


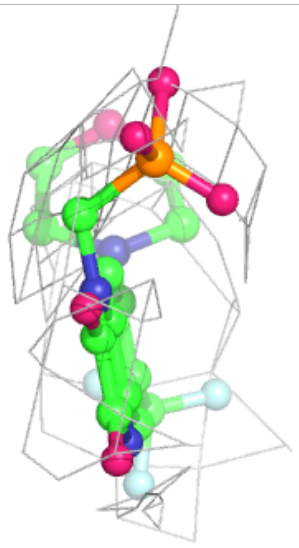


Electron density around ZK1 D 902:

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

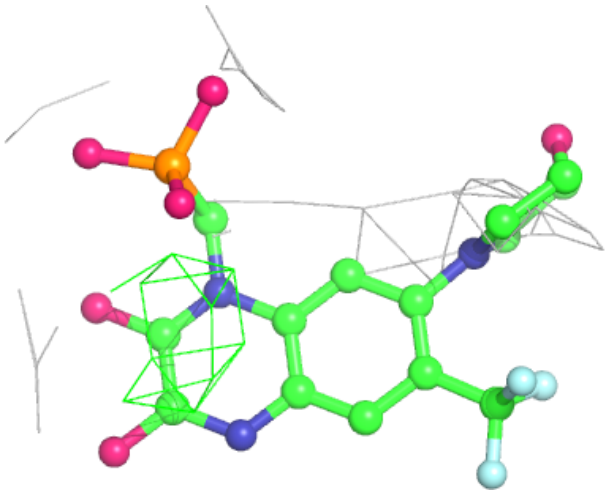


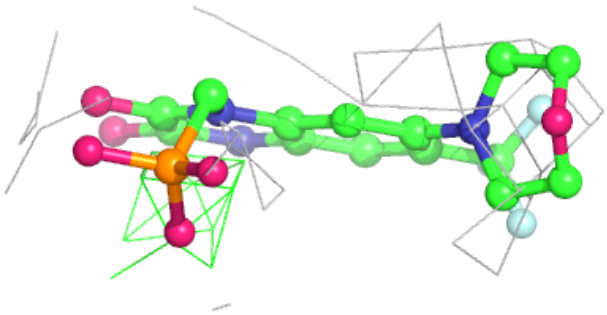


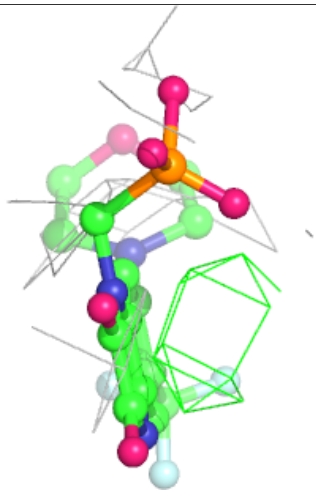


Electron density around ZK1 A 902:

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

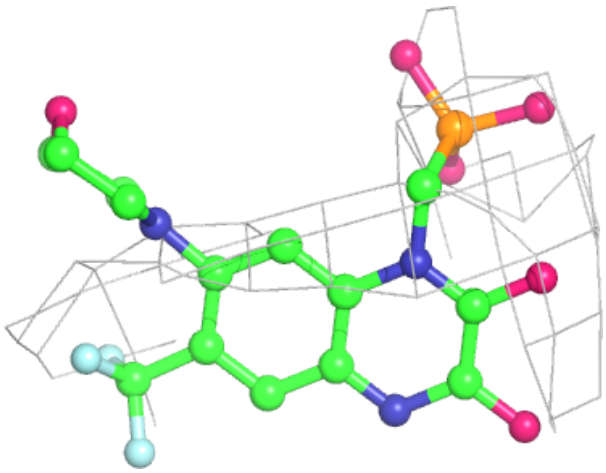


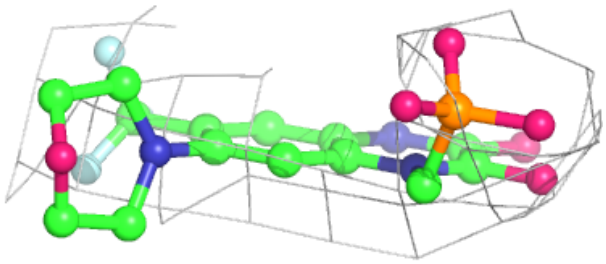


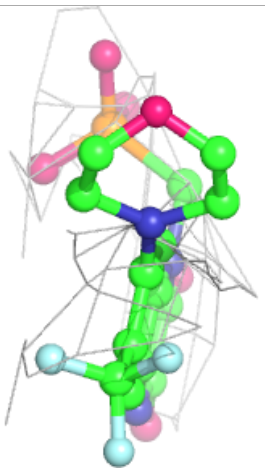


Electron density around ZK1 C 902:

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

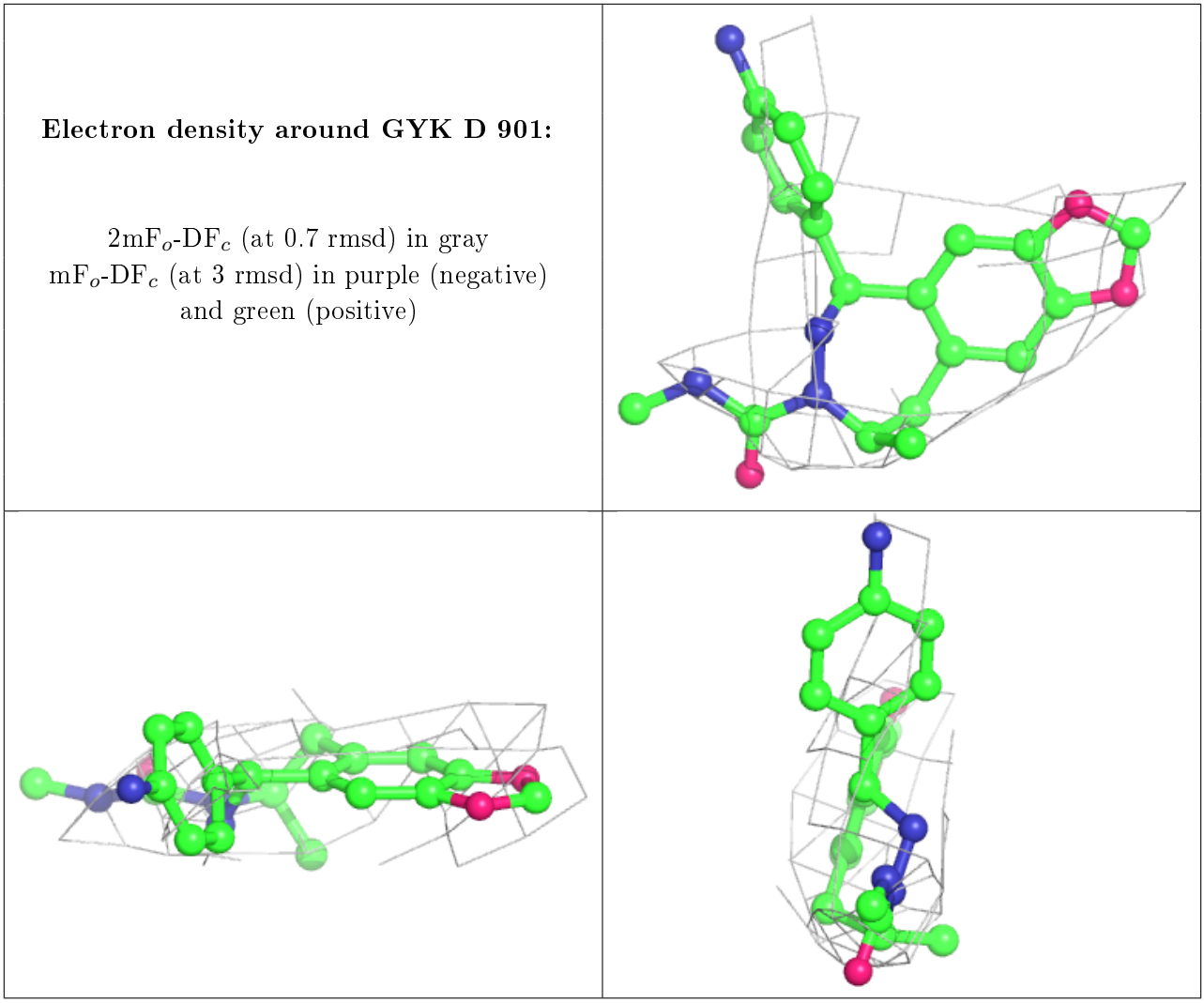






Electron density around GYK D 901:

$2mF_o$-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

There are no such residues in this entry.