Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2024 – 04:05 PM EDT

PDB ID	:	9AUS
Title	:	Crystal structure of loop-closed dumbbell RNA bridged by glycine
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Deposited on	:	2024-02-29
Resolution	:	2.07 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:

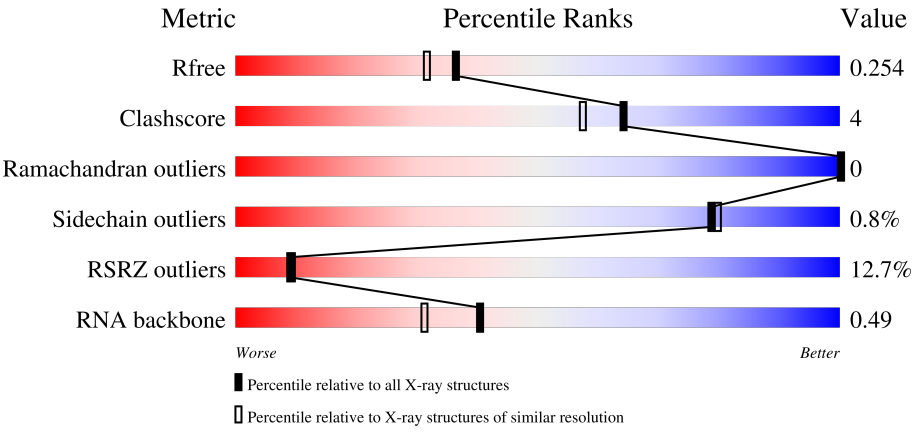
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.07 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}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)
RNA backbone	3690	1038 (2.42-1.70)

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	225	8% 89% 10%
1	H	225	14% 92% 8%
2	B	215	7% 93% 7%
2	L	215	22% 88% 12%

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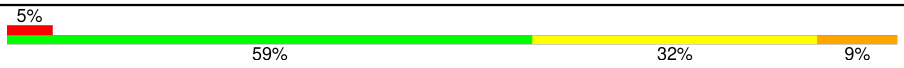
Mol	Chain	Length	Quality of chain
3	C	22	
3	R	22	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8017 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 Fab BL3-6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	225	Total	C	N	O	S	0	0	0
			1678	1055	287	330	6			
1	A	225	Total	C	N	O	S	0	0	0
			1678	1055	287	330	6			

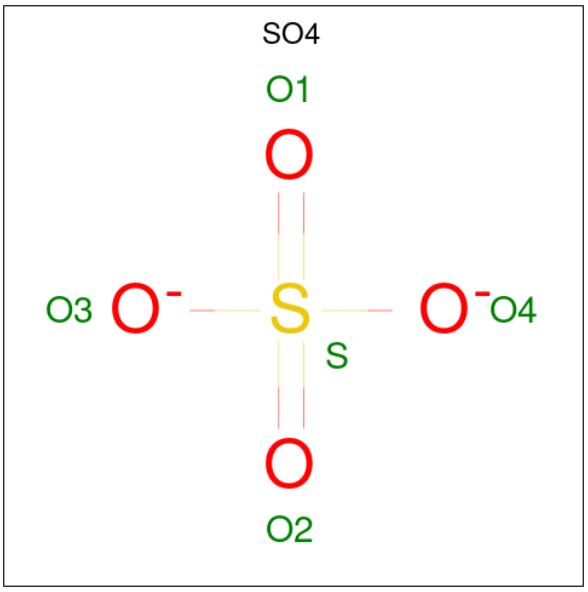
- Molecule 2 is a protein called Fab BL3-6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	2	0	0
			1643	1025	275	337	6			
2	B	215	Total	C	N	O	S	2	0	0
			1643	1025	275	337	6			

- Molecule 3 is a RNA chain called Loop-closed dumbbell RNA bridged by glycine.

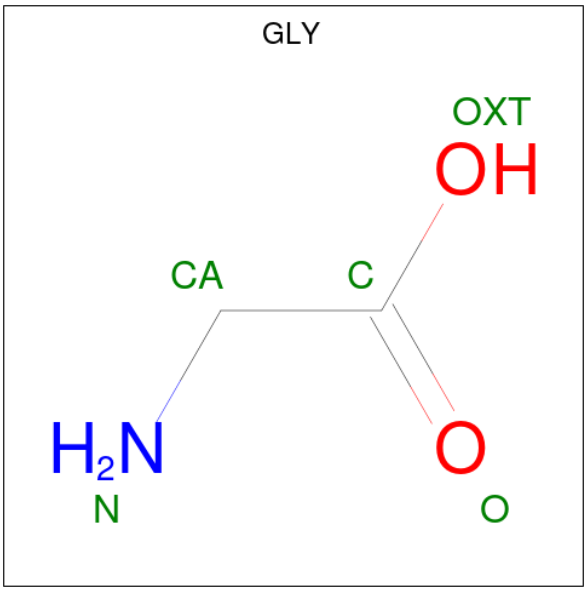
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	22	Total	C	N	O	P	0	0	0
			476	213	93	148	22			
3	C	22	Total	C	N	O	P	0	0	0
			477	213	93	149	22			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	1	Total C N O 4 2 1 1	0	0

- Molecule 6 is water.

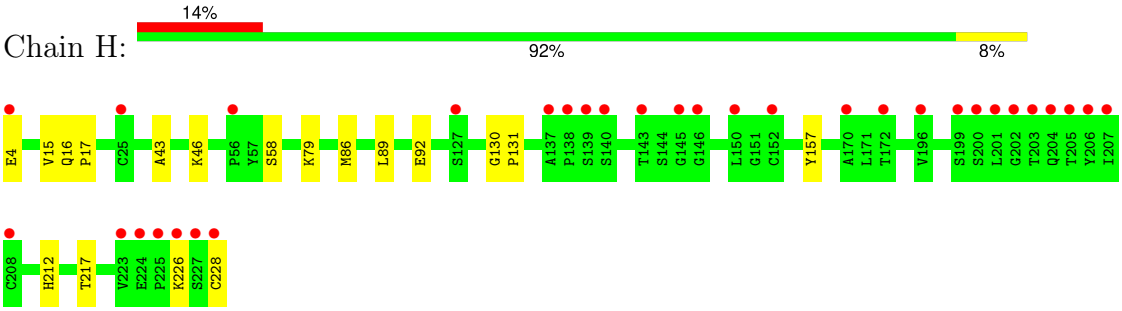
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	108	Total O 108 108	0	0
6	L	53	Total O 53 53	0	0
6	R	30	Total O 30 30	0	0
6	A	102	Total O 102 102	0	0
6	B	76	Total O 76 76	0	0
6	C	19	Total O 19 19	0	0

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.

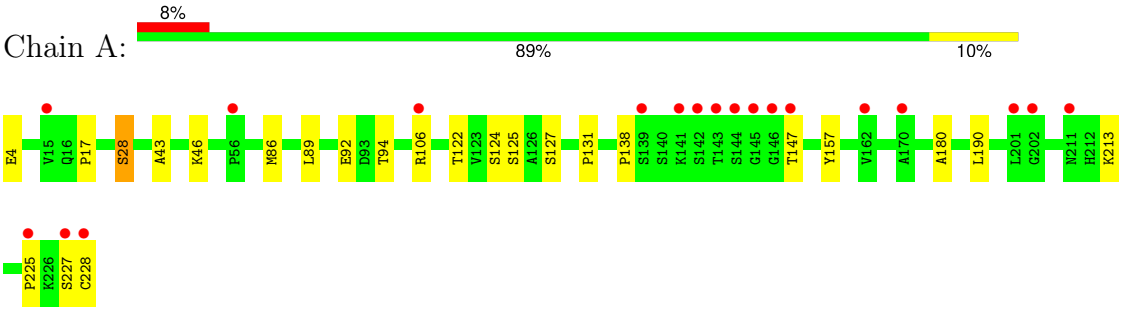
• Molecule 1: Fab BL3-6 heavy chain

Chain H:



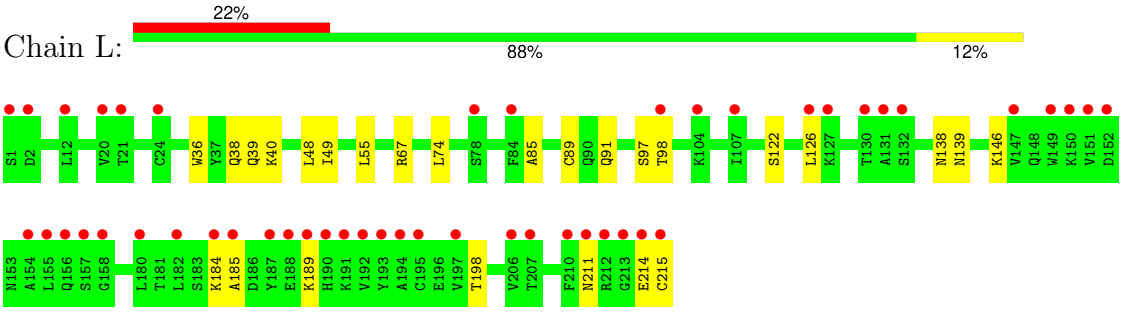
• Molecule 1: Fab BL3-6 heavy chain

Chain A:



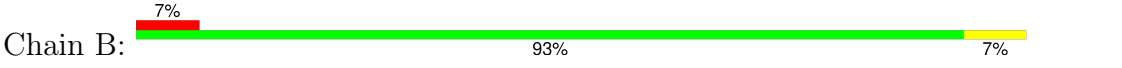
• Molecule 2: Fab BL3-6 light chain

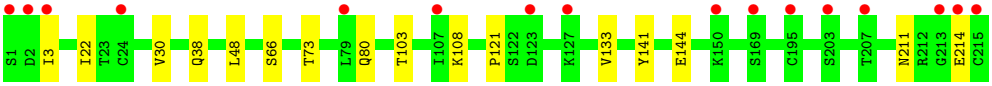
Chain L:



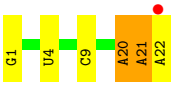
• Molecule 2: Fab BL3-6 light chain

Chain B:

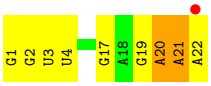




• Molecule 3: Loop-closed dumbbell RNA bridged by glycine



• Molecule 3: Loop-closed dumbbell RNA bridged by glycine



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.51Å 82.08Å 92.67Å 63.95° 88.69° 88.40°	Depositor
Resolution (Å)	46.07 – 2.07 46.07 – 2.07	Depositor EDS
% Data completeness (in resolution range)	91.1 (46.07-2.07) 83.5 (46.07-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.88 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.221 , 0.254 0.221 , 0.254	Depositor DCC
R_{free} test set	54643 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l 0.020 for -h,k,k-l 0.008 for -h,-k,-k+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8017	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/1719	0.50	0/2339
1	H	0.27	0/1719	0.51	0/2339
2	B	0.26	0/1678	0.49	0/2277
2	L	0.25	0/1678	0.48	0/2277
3	C	0.55	1/535 (0.2%)	0.83	0/831
3	R	0.38	1/534 (0.2%)	0.96	3/831 (0.4%)
All	All	0.30	2/7863 (0.0%)	0.57	3/10894 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	G	OP3-P	-10.63	1.48	1.61
3	R	1	G	P-OP1	5.31	1.57	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	1	G	OP1-P-OP2	-12.34	101.09	119.60
3	R	1	G	O5'-P-OP2	-7.33	99.10	105.70
3	R	1	G	O5'-P-OP1	-6.16	100.16	105.70

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	1678	0	1638	14	0
1	H	1678	0	1637	12	0
2	B	1643	0	1595	8	0
2	L	1643	0	1594	17	0
3	C	477	0	240	5	0
3	R	476	0	239	2	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	L	10	0	0	1	0
4	R	5	0	0	0	0
5	R	4	0	2	0	0
6	A	102	0	0	1	0
6	B	76	0	0	1	0
6	C	19	0	0	1	0
6	H	108	0	0	1	0
6	L	53	0	0	2	0
6	R	30	0	0	0	0
All	All	8017	0	6945	55	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 4.

All (55) 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)
2:L:122:SER:O	6:L:401:HOH:O	2.09	0.70
2:L:38:GLN:HB2	2:L:48:LEU:HD11	1.78	0.66
2:B:22:ILE:HD12	2:B:103:THR:HG21	1.78	0.65
1:H:4:GLU:N	6:H:304:HOH:O	2.29	0.64
2:B:3:ILE:HD13	2:B:30:VAL:HG12	1.79	0.64
1:A:4:GLU:N	6:A:302:HOH:O	2.31	0.62
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.81	0.62
1:H:217:THR:HG22	1:A:127:SER:HB2	1.82	0.61
2:L:91:GLN:HE21	2:L:98:THR:HG22	1.66	0.59
2:L:40:LYS:HD3	2:L:85:ALA:HB2	1.85	0.58
1:A:43:ALA:HB3	1:A:46:LYS:HD2	1.86	0.58
2:B:121:PRO:HD3	2:B:133:VAL:HG22	1.87	0.57
1:H:79:LYS:HZ1	1:A:28:SER:HB3	1.71	0.56
2:L:138:ASN:ND2	2:L:139:ASN:OD1	2.40	0.55
1:A:92:GLU:OE1	1:A:92:GLU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:PRO:HB3	1:H:157:TYR:HB3	1.91	0.53
2:B:80:GLN:NE2	6:B:407:HOH:O	2.42	0.52
1:H:43:ALA:HB3	1:H:46:LYS:HD3	1.92	0.52
2:L:185:ALA:O	2:L:189:LYS:HG2	2.10	0.52
1:H:92:GLU:OE1	1:H:92:GLU:N	2.38	0.51
2:L:97:SER:OG	6:L:402:HOH:O	2.20	0.51
2:L:146:LYS:HB3	2:L:198:THR:HB	1.93	0.51
3:C:17:G:H1'	3:C:21:A:H61	1.76	0.50
2:B:66:SER:OG	2:B:73:THR:OG1	2.30	0.49
2:L:49:ILE:HD13	2:L:55:LEU:HA	1.94	0.49
3:C:20:A:H1'	3:C:21:A:H5"	1.95	0.49
1:H:16:GLN:HG3	1:H:17:PRO:HD2	1.95	0.48
3:R:20:A:H4'	3:R:21:A:OP1	2.11	0.48
3:C:19:G:C6	3:C:21:A:C6	3.03	0.46
1:A:227:SER:OG	1:A:228:CYS:N	2.47	0.46
1:A:131:PRO:HB3	1:A:157:TYR:HB3	1.98	0.45
1:H:58:SER:OG	3:R:9:C:N3	2.36	0.45
1:H:212:HIS:HB3	1:H:217:THR:OG1	2.17	0.45
2:L:211:ASN:HB2	2:L:214:GLU:HB3	1.99	0.45
2:L:36:TRP:CZ3	2:L:89:CYS:HB3	2.53	0.44
1:H:130:GLY:HA3	1:H:217:THR:HG21	1.99	0.44
2:L:67:ARG:NH2	4:L:301:SO4:O3	2.41	0.43
2:B:211:ASN:O	2:B:214:GLU:HG2	2.19	0.43
1:A:86:MET:HB3	1:A:89:LEU:HD21	2.01	0.43
2:B:108:LYS:HA	2:B:141:TYR:OH	2.19	0.43
1:H:86:MET:HB3	1:H:89:LEU:HD21	2.01	0.42
1:A:106:ARG:HB2	6:C:202:HOH:O	2.19	0.42
2:L:39:GLN:O	2:L:85:ALA:HB1	2.19	0.42
1:A:138:PRO:HG2	1:A:225:PRO:HG3	2.01	0.42
2:L:126:LEU:HD12	2:L:184:LYS:HG3	2.01	0.42
3:C:20:A:N3	3:C:21:A:H2'	2.34	0.42
2:L:189:LYS:HA	2:L:189:LYS:HD3	1.90	0.41
2:L:214:GLU:O	2:L:215:CYS:HB2	2.21	0.41
1:H:15:VAL:HG11	1:H:89:LEU:HD13	2.02	0.41
1:A:213:LYS:HE2	1:A:213:LYS:HB3	1.83	0.41
3:C:17:G:H1'	3:C:21:A:N6	2.36	0.41
1:A:180:ALA:HA	1:A:190:LEU:HB3	2.03	0.40
2:L:36:TRP:CD2	2:L:74:LEU:HB2	2.56	0.40
1:A:17:PRO:HD3	1:A:124:SER:C	2.42	0.40
1:A:94:THR:HG23	1:A:122:THR:HA	2.02	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	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
1	H	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
2	B	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
2	L	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
All	All	872/880 (99%)	848 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	186/186 (100%)	183 (98%)	3 (2%)	58	57
1	H	186/186 (100%)	184 (99%)	2 (1%)	70	70
2	B	190/190 (100%)	189 (100%)	1 (0%)	86	88
2	L	190/190 (100%)	190 (100%)	0	100	100
All	All	752/752 (100%)	746 (99%)	6 (1%)	79	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	226	LYS
1	H	228	CYS

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Mol	Chain	Res	Type
1	A	28	SER
1	A	125	SER
1	A	147	THR
2	B	144	GLU

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

Mol	Chain	Res	Type
1	H	176	HIS
2	L	138	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	21/22 (95%)	6 (28%)	1 (4%)
3	R	21/22 (95%)	4 (19%)	1 (4%)
All	All	42/44 (95%)	10 (23%)	2 (4%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	4	U
3	R	20	A
3	R	21	A
3	R	22	A
3	C	2	G
3	C	3	U
3	C	4	U
3	C	20	A
3	C	21	A
3	C	22	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	R	20	A
3	C	20	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	R	101	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	C	101	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	L	302	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.08	0
5	GLY	R	102	3	3,3,4	0.61	0	1,2,4	0.24	0
4	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.08	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
5	GLY	R	102	3	-	0/0/1/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

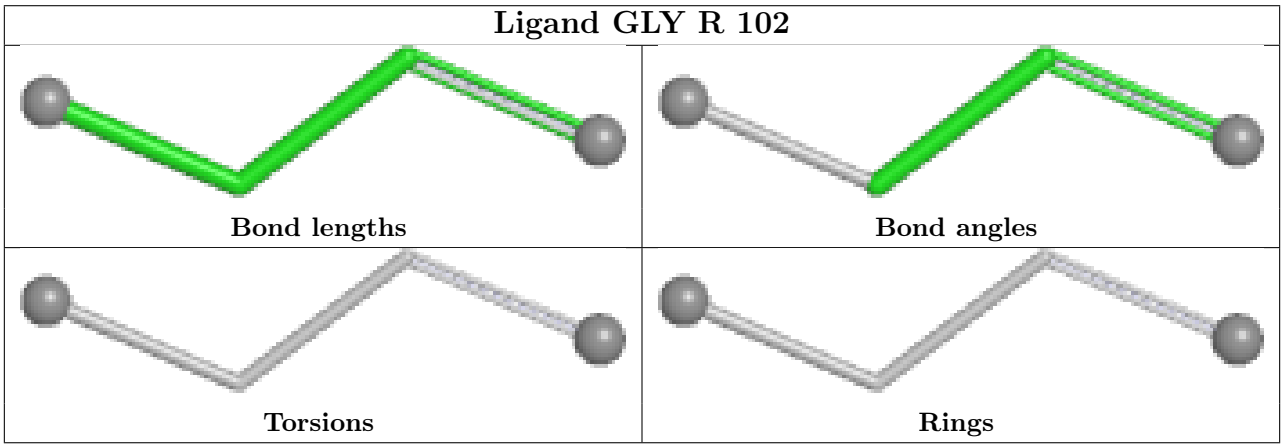
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	SO4	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 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.



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, 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	225/225 (100%)	0.77	19 (8%) 18 20	27, 40, 73, 116	1 (0%)
1	H	225/225 (100%)	0.92	32 (14%) 7 8	28, 40, 90, 132	1 (0%)
2	B	215/215 (100%)	0.91	16 (7%) 22 24	31, 46, 64, 114	2 (0%)
2	L	215/215 (100%)	1.22	48 (22%) 3 2	31, 52, 97, 128	2 (0%)
3	C	22/22 (100%)	0.88	1 (4%) 39 40	41, 91, 127, 135	0
3	R	22/22 (100%)	0.45	1 (4%) 39 40	35, 47, 58, 67	0
All	All	924/924 (100%)	0.94	117 (12%) 9 9	27, 45, 92, 135	6 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	185	ALA	4.7
1	H	206	TYR	4.7
1	H	202	GLY	4.6
2	B	1	SER	4.6
2	L	192	VAL	4.5
1	H	143	THR	4.4
1	H	200	SER	4.3
1	H	201	LEU	4.2
2	L	212	ARG	4.1
2	L	190	HIS	4.0
1	H	140	SER	4.0
2	L	154	ALA	3.9
1	A	145	GLY	3.9
2	B	24	CYS	3.8
1	H	150	LEU	3.7
2	L	210	PHE	3.7
1	H	203	THR	3.5
1	H	205	THR	3.3
2	L	188	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	137	ALA	3.2
1	H	223	VAL	3.2
2	B	3	ILE	3.1
1	H	227	SER	3.1
2	L	193	TYR	3.1
2	L	215	CYS	3.1
2	L	151	VAL	3.1
2	B	195	CYS	3.1
1	H	228	CYS	3.0
2	L	126	LEU	3.0
2	L	152	ASP	2.9
1	H	207	ILE	2.9
1	H	152	CYS	2.9
2	L	2	ASP	2.9
2	B	2	ASP	2.9
1	A	143	THR	2.9
1	A	202	GLY	2.9
1	A	146	GLY	2.8
1	H	56	PRO	2.8
2	L	184	LYS	2.8
2	L	189	LYS	2.8
2	L	131	ALA	2.8
3	C	22	A	2.8
2	L	191	LYS	2.7
1	H	225	PRO	2.7
2	B	214	GLU	2.7
2	L	104	LYS	2.7
2	L	107	ILE	2.7
1	A	201	LEU	2.7
1	A	15	VAL	2.7
2	B	215	CYS	2.6
1	A	170	ALA	2.6
1	H	224	GLU	2.6
2	L	194	ALA	2.6
2	L	211	ASN	2.6
2	L	213	GLY	2.6
2	L	187	TYR	2.6
2	L	84	PHE	2.6
2	L	98	THR	2.5
1	A	106	ARG	2.5
1	A	144	SER	2.5
2	L	12	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	4	GLU	2.5
2	B	79	LEU	2.5
2	L	21	THR	2.5
1	A	142	SER	2.4
2	L	207	THR	2.4
1	H	196	VAL	2.4
1	A	228	CYS	2.4
2	L	149	TRP	2.4
2	L	206	VAL	2.4
2	L	150	LYS	2.3
2	L	1	SER	2.3
2	B	203	SER	2.3
2	B	123	ASP	2.3
2	L	214	GLU	2.3
2	L	182	LEU	2.3
2	L	24	CYS	2.3
1	H	199	SER	2.3
2	L	78	SER	2.3
2	B	127	LYS	2.3
2	L	180	LEU	2.3
1	H	138	PRO	2.3
1	H	139	SER	2.3
2	L	156	GLN	2.3
2	L	155	LEU	2.2
2	L	130	THR	2.2
1	H	145	GLY	2.2
1	A	147	THR	2.2
2	L	132	SER	2.2
1	H	226	LYS	2.2
2	L	158	GLY	2.2
1	H	170	ALA	2.2
1	A	141	LYS	2.2
1	A	162	VAL	2.2
2	L	20	VAL	2.2
1	H	127	SER	2.1
2	L	157	SER	2.1
2	B	213	GLY	2.1
2	L	147	VAL	2.1
2	L	197	VAL	2.1
2	L	127	LYS	2.1
1	A	139	SER	2.1
1	A	227	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	107	ILE	2.1
1	A	56	PRO	2.1
2	B	169	SER	2.1
1	H	172	THR	2.1
2	B	207	THR	2.1
1	H	146	GLY	2.0
1	H	204	GLN	2.1
1	A	225	PRO	2.0
3	R	22	A	2.0
1	H	25	CYS	2.0
2	L	195	CYS	2.0
1	A	211	ASN	2.0
2	B	150	LYS	2.0
1	H	208	CYS	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 monosaccharides 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, 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.

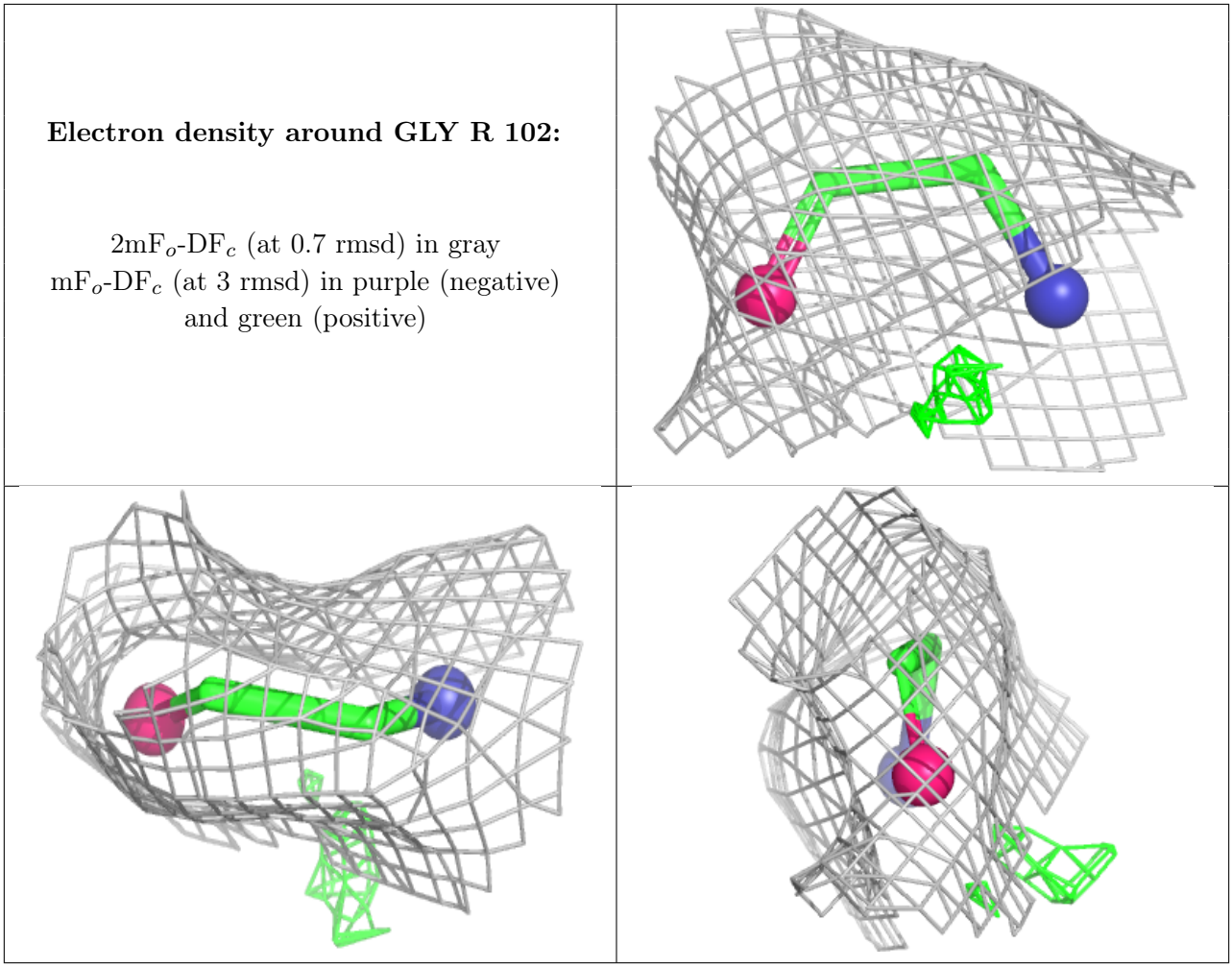
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	101	5/5	0.58	0.12	130,131,136,137	0
4	SO4	L	302	5/5	0.64	0.12	94,95,101,125	0
4	SO4	B	301	5/5	0.73	0.10	83,84,100,116	0
4	SO4	R	101	5/5	0.73	0.13	60,64,72,75	0
5	GLY	R	102	4/5	0.77	0.12	63,64,65,66	0
4	SO4	B	302	5/5	0.78	0.09	67,71,88,88	0
4	SO4	L	301	5/5	0.84	0.08	66,67,69,71	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 GLY R 102:

$2mF_o$-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.