



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:11 PM UTC

PDB ID : 6UMX / pdb_00006umx
Title : Structural basis for specific inhibition of extracellular activation of pro/latent myostatin by SRK-015
Authors : Dagbay, K.B.; Treece, E.; Streich Jr., F.C.; Jackson, J.W.; Faucette, R.R.; Nikiforov, A.; Lin, S.C.; Bostion, C.J.; Nicholls, S.B.; Capili, A.D.; Carven, G.J.
Deposited on : 2019-10-10
Resolution : 2.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

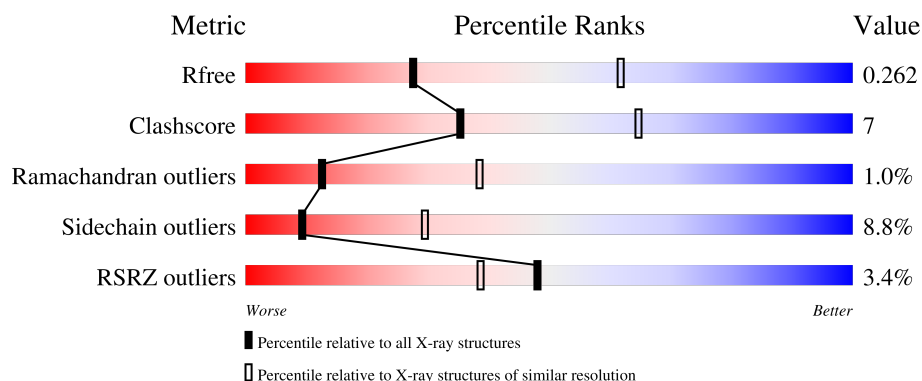
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	5% 57% 18% 24%
1	B	365	4% 54% 17% 25%
2	L	215	2% 78% 20%
2	l	215	69% 25%

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Mol	Chain	Length	Quality of chain
3	H	229	
3	h	229	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10849 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 Growth/differentiation factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2175	1390	364	404	17			
1	B	273	Total	C	N	O	S	0	0	0
			2101	1336	355	393	17			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	HIS	-	expression tag	UNP O14793
A	12	HIS	-	expression tag	UNP O14793
A	13	HIS	-	expression tag	UNP O14793
A	14	HIS	-	expression tag	UNP O14793
A	15	HIS	-	expression tag	UNP O14793
A	16	HIS	-	expression tag	UNP O14793
A	17	GLU	-	expression tag	UNP O14793
A	18	ASN	-	expression tag	UNP O14793
A	19	LEU	-	expression tag	UNP O14793
A	20	TYR	-	expression tag	UNP O14793
A	21	PHE	-	expression tag	UNP O14793
A	22	GLN	-	expression tag	UNP O14793
A	23	SER	-	expression tag	UNP O14793
A	99	ALA	ASP	engineered mutation	UNP O14793
A	263	ALA	ARG	engineered mutation	UNP O14793
A	266	ALA	ARG	engineered mutation	UNP O14793
B	11	HIS	-	expression tag	UNP O14793
B	12	HIS	-	expression tag	UNP O14793
B	13	HIS	-	expression tag	UNP O14793
B	14	HIS	-	expression tag	UNP O14793
B	15	HIS	-	expression tag	UNP O14793
B	16	HIS	-	expression tag	UNP O14793
B	17	GLU	-	expression tag	UNP O14793
B	18	ASN	-	expression tag	UNP O14793
B	19	LEU	-	expression tag	UNP O14793

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	TYR	-	expression tag	UNP O14793
B	21	PHE	-	expression tag	UNP O14793
B	22	GLN	-	expression tag	UNP O14793
B	23	SER	-	expression tag	UNP O14793
B	99	ALA	ASP	engineered mutation	UNP O14793
B	263	ALA	ARG	engineered mutation	UNP O14793
B	266	ALA	ARG	engineered mutation	UNP O14793

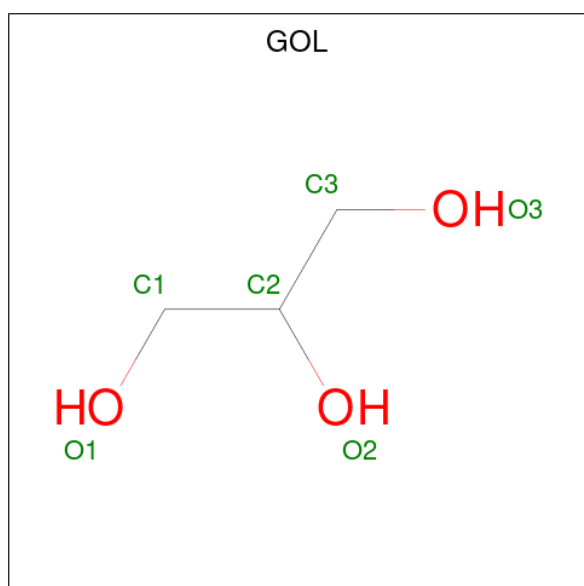
- Molecule 2 is a protein called GL29H4-16 Fab Light Chain, GL29H4-16 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1583	985	266	327	5			
2	l	210	Total	C	N	O	S	0	0	0
			1555	969	261	321	4			

- Molecule 3 is a protein called GL29H4-16 Fab Heavy Chain, GL29H4-16 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	226	Total	C	N	O	S	0	0	0
			1718	1090	293	328	7			
3	h	225	Total	C	N	O	S	0	0	0
			1709	1084	291	327	7			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

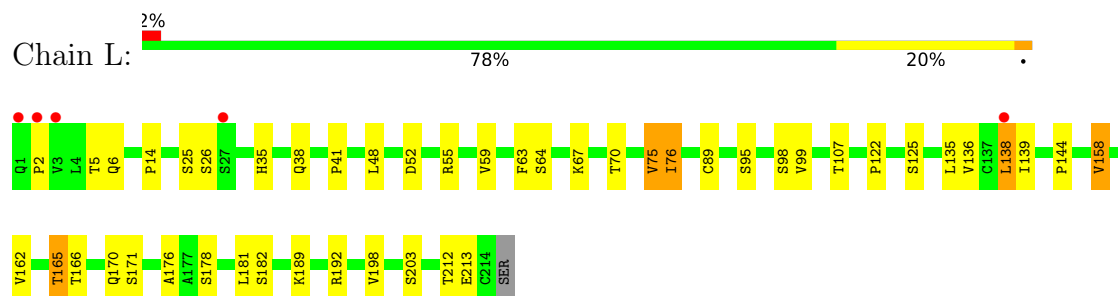


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	h	1	Total	C	O	0	0
			6	3	3		

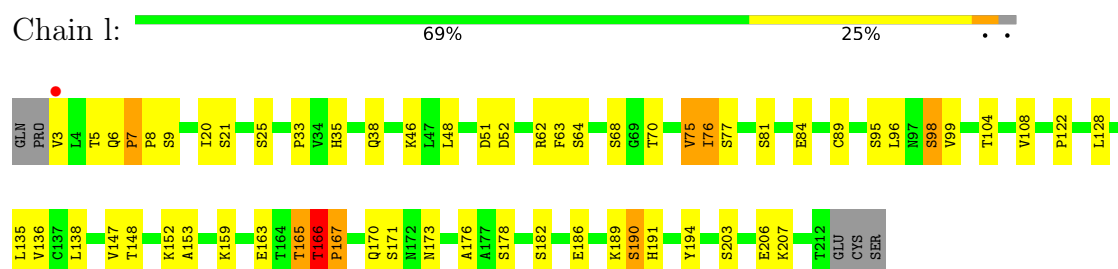
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	O	0	0
			1	1		
5	1	1	Total	O	0	0
			1	1		

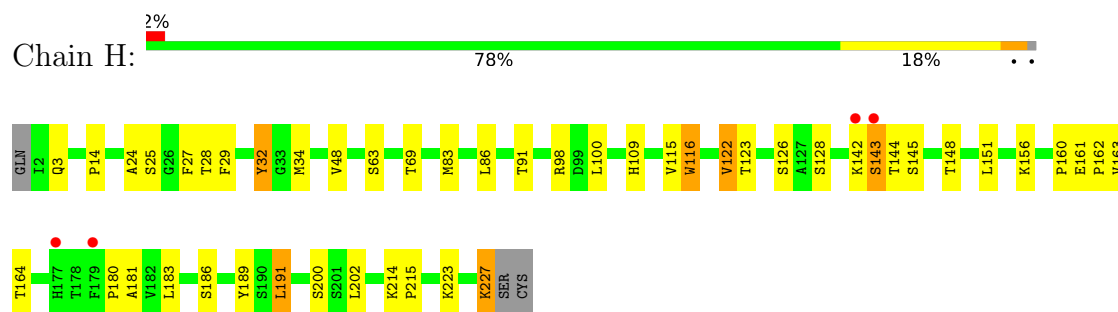
• Molecule 2: GL29H4-16 Fab Light Chain, GL29H4-16 Fab Light Chain



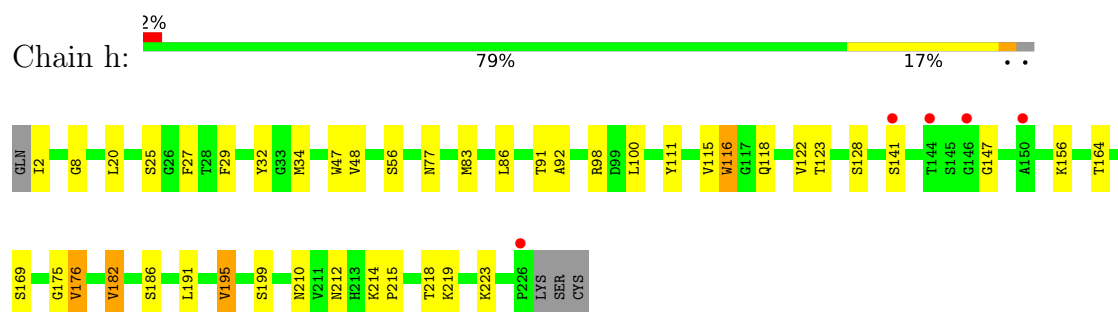
• Molecule 2: GL29H4-16 Fab Light Chain, GL29H4-16 Fab Light Chain



• Molecule 3: GL29H4-16 Fab Heavy Chain, GL29H4-16 Fab Heavy Chain



• Molecule 3: GL29H4-16 Fab Heavy Chain, GL29H4-16 Fab Heavy Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.62Å 110.01Å 293.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.43 – 2.79 40.43 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.43-2.79) 99.8 (40.43-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.217 , 0.264 0.220 , 0.262	Depositor DCC
R_{free} test set	2372 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	81.1	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10849	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	1.13	2/2222 (0.1%)	1.21	6/3016 (0.2%)
1	B	1.13	1/2142 (0.0%)	1.37	10/2910 (0.3%)
2	L	1.32	6/1623 (0.4%)	1.24	7/2221 (0.3%)
2	l	1.23	5/1594 (0.3%)	1.25	5/2181 (0.2%)
3	H	1.38	11/1762 (0.6%)	1.34	6/2398 (0.3%)
3	h	1.43	7/1753 (0.4%)	1.30	3/2387 (0.1%)
All	All	1.26	32/11096 (0.3%)	1.29	37/15113 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	116	TRP	N-CA	10.91	1.60	1.46
3	H	116	TRP	N-CA	9.06	1.57	1.46
3	H	180	PRO	CA-C	-7.65	1.43	1.52
2	l	182	SER	CA-C	-7.50	1.43	1.52
2	L	162	VAL	C-O	-7.33	1.15	1.24

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	TYR	N-CA-C	-21.02	77.00	110.20
1	B	149	ASN	N-CA-CB	19.10	142.76	110.49
1	B	65	ARG	N-CA-CB	18.33	141.47	110.49
1	A	237	LEU	N-CA-C	-11.67	84.91	107.44
1	B	64	LEU	CB-CA-C	11.05	127.97	110.96

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	ALA	Peptide,Mainchain
1	A	43	THR	Peptide
1	B	137	CYS	Peptide
1	B	300	ALA	Peptide

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	2175	0	2135	39	0
1	B	2101	0	2048	44	0
2	L	1583	0	1517	13	0
2	l	1555	0	1498	30	0
3	H	1718	0	1687	20	0
3	h	1709	0	1674	25	0
4	h	6	0	8	0	0
5	H	1	0	0	0	0
5	l	1	0	0	0	0
All	All	10849	0	10567	158	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 7.

The worst 5 of 158 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:91:THR:HG23	3:H:123:THR:HA	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:91:THR:HG23	3:h:123:THR:HA	1.58	0.85
1:A:272:CYS:HG	1:A:282:CYS:HG	0.82	0.81
1:B:280:ARG:NH2	1:B:374:CYS:SG	2.56	0.77
3:H:183:LEU:HD13	3:H:189:TYR:CE1	2.23	0.74

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	269/365 (74%)	255 (95%)	9 (3%)	5 (2%)	6	22
1	B	263/365 (72%)	246 (94%)	12 (5%)	5 (2%)	6	22
2	L	212/215 (99%)	200 (94%)	10 (5%)	2 (1%)	14	41
2	l	208/215 (97%)	194 (93%)	14 (7%)	0	100	100
3	H	224/229 (98%)	211 (94%)	12 (5%)	1 (0%)	30	60
3	h	223/229 (97%)	210 (94%)	12 (5%)	1 (0%)	30	60
All	All	1399/1618 (86%)	1316 (94%)	69 (5%)	14 (1%)	12	38

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	CYS
2	L	165	THR
1	B	65	ARG
1	B	149	ASN
2	L	95	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/328 (72%)	220 (93%)	17 (7%)	13	39
1	B	227/328 (69%)	210 (92%)	17 (8%)	12	37
2	L	179/182 (98%)	158 (88%)	21 (12%)	5	18
2	l	177/182 (97%)	156 (88%)	21 (12%)	5	17
3	H	191/194 (98%)	175 (92%)	16 (8%)	10	32
3	h	190/194 (98%)	176 (93%)	14 (7%)	13	37
All	All	1201/1408 (85%)	1095 (91%)	106 (9%)	9	29

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	l	9	SER
2	l	171	SER
1	B	276	SER
2	l	25	SER
2	l	76	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	h	210	ASN
3	h	212	ASN
1	B	358	GLN
1	B	307	ASN
1	B	349	ASN

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	h	301	-	5,5,5	0.93	0	5,5,5	1.02	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
4	GOL	h	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	h	301	GOL	O1-C1-C2-O2
4	h	301	GOL	O1-C1-C2-C3
4	h	301	GOL	C1-C2-C3-O3
4	h	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/365 (76%)	0.37	19 (6%) 23 17	69, 110, 160, 196	0
1	B	273/365 (74%)	0.50	15 (5%) 30 23	77, 118, 187, 220	0
2	L	214/215 (99%)	-0.06	5 (2%) 61 51	54, 81, 113, 151	0
2	l	210/215 (97%)	-0.01	1 (0%) 87 82	62, 101, 132, 149	0
3	H	226/229 (98%)	-0.10	4 (1%) 67 58	53, 74, 100, 136	0
3	h	225/229 (98%)	-0.06	5 (2%) 62 52	52, 71, 142, 227	0
All	All	1427/1618 (88%)	0.13	49 (3%) 48 39	52, 91, 154, 227	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	h	146	GLY	4.7
2	l	3	VAL	4.0
1	A	47	ASN	3.8
1	B	118	ILE	3.4
1	A	343	THR	3.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	h	301	6/6	0.82	0.16	76,87,88,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.