



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:44 PM BST

PDB ID : 6UMX
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

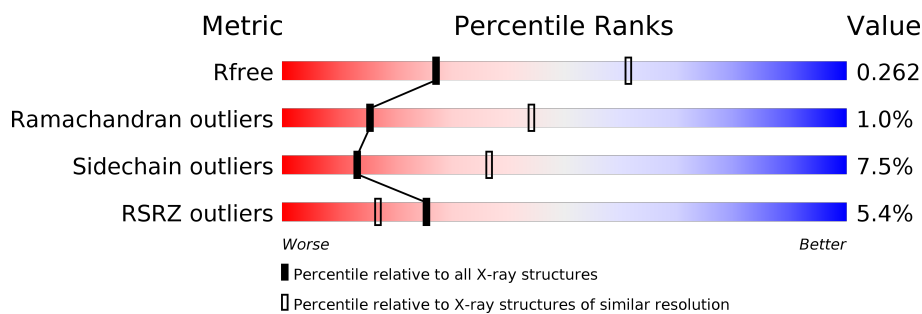
1 Overall quality at a glance ⓘ

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}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	<div> <div>7%</div> <div>69%</div> <div>7%</div> <div>24%</div> </div>
1	B	365	<div> <div>8%</div> <div>67%</div> <div>7%</div> <div>25%</div> </div>
2	L	215	<div> <div>0%</div> <div>91%</div> <div>9%</div> </div>
2	l	215	<div> <div>4%</div> <div>85%</div> <div>13%</div> </div>
3	H	229	<div> <div>0%</div> <div>89%</div> <div>9%</div> </div>
3	h	229	<div> <div>4%</div> <div>90%</div> <div>8%</div> </div>

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

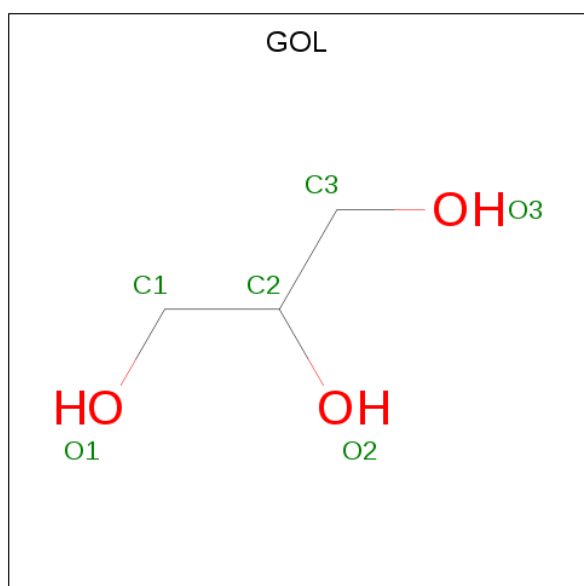
- Molecule 2 is a protein called GL29H4-16 Fab Light Chain, GL29H4-16 Fab Light Chain.

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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

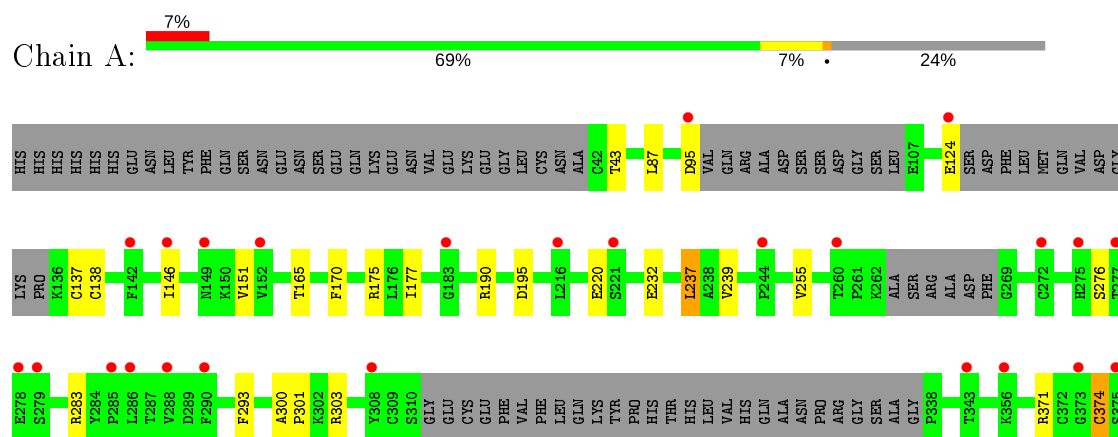
- Molecule 5 is water.

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

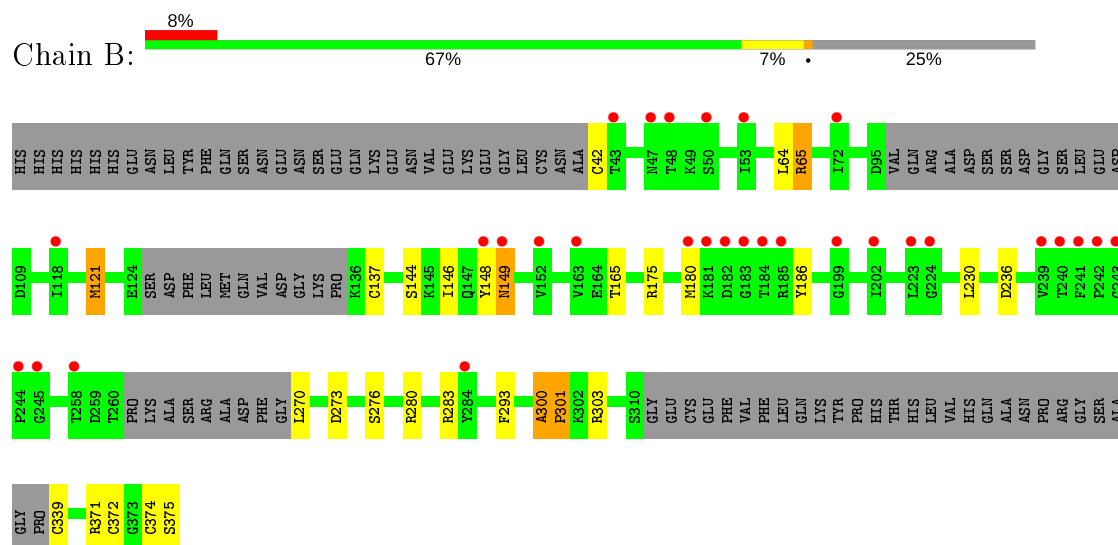
3 Residue-property plots

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

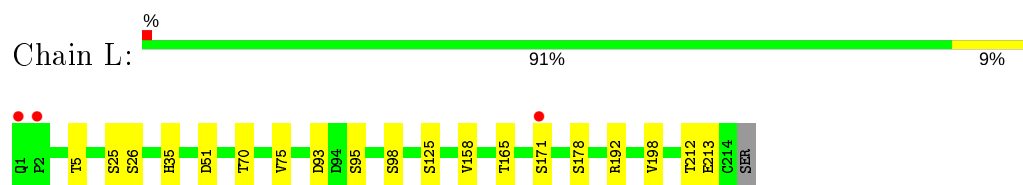
- Molecule 1: Growth/differentiation factor 8



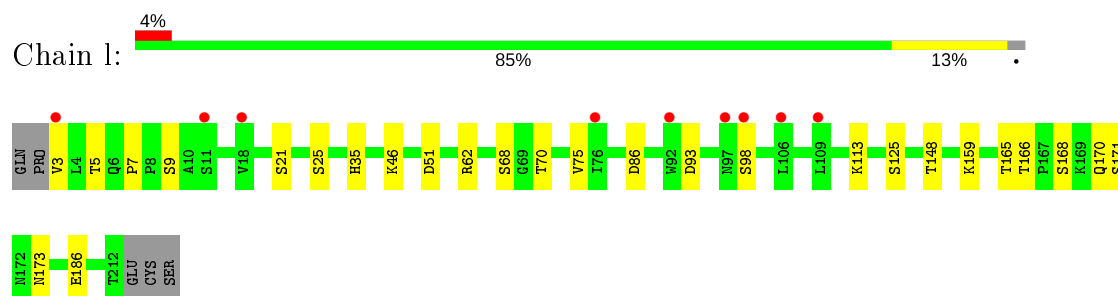
- Molecule 1: Growth/differentiation factor 8



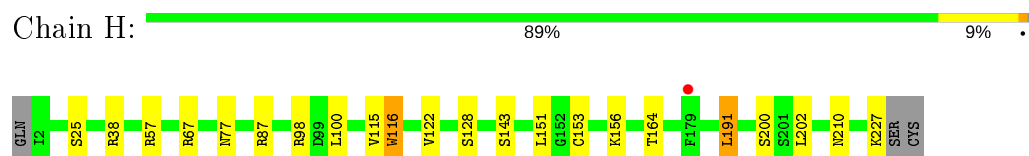
- Molecule 2: GL29H4-16 Fab Light Chain, GL29H4-16 Fab Light Chain



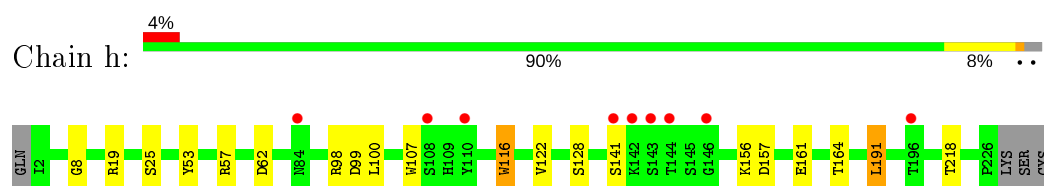
- Molecule 2: GL29H4-16 Fab Light Chain, GL29H4-16 Fab Light Chain



- 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) 99.9 (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 (4.83%)	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)	0.29 , 57.9	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	0.82	1/2222 (0.0%)	1.01	5/3016 (0.2%)
1	B	0.82	0/2142	1.16	13/2910 (0.4%)
2	L	1.01	0/1623	0.99	2/2221 (0.1%)
2	l	0.94	2/1594 (0.1%)	0.99	5/2181 (0.2%)
3	H	1.06	3/1762 (0.2%)	1.14	9/2398 (0.4%)
3	h	1.10	4/1753 (0.2%)	1.14	8/2387 (0.3%)
All	All	0.95	10/11096 (0.1%)	1.08	42/15113 (0.3%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h	116	TRP	N-CA	6.96	1.60	1.46
3	h	161	GLU	CD-OE2	6.89	1.33	1.25
3	H	116	TRP	N-CA	5.77	1.57	1.46
3	h	53	TYR	CE1-CZ	5.65	1.45	1.38
2	l	125	SER	CB-OG	-5.50	1.35	1.42
3	H	153	CYS	CB-SG	-5.42	1.73	1.81
3	H	98	ARG	CZ-NH1	-5.34	1.26	1.33
1	A	170	PHE	CG-CD1	-5.04	1.31	1.38
3	h	8	GLY	C-O	5.03	1.31	1.23
2	l	168	SER	CB-OG	5.01	1.48	1.42

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ASN	N-CA-CB	17.87	142.76	110.60
1	B	65	ARG	N-CA-CB	17.15	141.47	110.60
1	B	148	TYR	N-CA-C	-12.59	77.00	111.00
1	A	237	LEU	N-CA-C	-9.66	84.91	111.00
1	B	64	LEU	CB-CA-C	9.35	127.97	110.20
1	B	273	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	B	149	ASN	N-CA-C	-8.51	88.01	111.00
3	H	38	ARG	NE-CZ-NH2	-7.29	116.66	120.30
3	h	57	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	h	98	ARG	NE-CZ-NH1	7.20	123.90	120.30
3	H	57	ARG	NE-CZ-NH1	7.20	123.90	120.30
3	h	191	LEU	CB-CG-CD1	-6.49	99.98	111.00
3	h	157	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	A	283	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	371	ARG	NE-CZ-NH1	6.01	123.30	120.30
2	l	62	ARG	NE-CZ-NH1	5.91	123.25	120.30
3	H	191	LEU	CB-CG-CD1	-5.88	101.00	111.00
1	A	175	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	l	86	ASP	CB-CG-OD2	5.85	123.57	118.30
3	H	67	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	121	MET	CA-CB-CG	5.77	123.11	113.30
3	h	19	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	283	ARG	NE-CZ-NH1	5.65	123.12	120.30
3	H	87	ARG	NE-CZ-NH2	-5.61	117.50	120.30
3	H	191	LEU	CB-CG-CD2	5.53	120.40	111.00
1	B	300	ALA	C-N-CD	-5.48	108.54	120.60
3	h	57	ARG	NE-CZ-NH2	-5.48	117.56	120.30
3	H	151	LEU	CB-CG-CD2	5.43	120.23	111.00
2	L	93	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	B	303	ARG	NE-CZ-NH2	-5.38	117.61	120.30
3	H	38	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	h	99	ASP	CB-CG-OD1	5.32	123.09	118.30
2	l	93	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	B	273	ASP	CB-CG-OD2	5.20	122.98	118.30
2	l	113	LYS	CD-CE-NZ	5.19	123.64	111.70
1	B	175	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	l	51	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	236	ASP	CB-CG-OD1	5.11	122.90	118.30
2	L	51	ASP	CB-CG-OD2	-5.10	113.71	118.30
3	h	62	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	195	ASP	CB-CG-OD1	5.08	122.87	118.30
3	H	115	VAL	CG1-CB-CG2	-5.06	102.81	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	8	26
1	B	263/365 (72%)	246 (94%)	12 (5%)	5 (2%)	8	26
2	L	212/215 (99%)	200 (94%)	10 (5%)	2 (1%)	17	46
2	l	208/215 (97%)	194 (93%)	14 (7%)	0	100	100
3	H	224/229 (98%)	211 (94%)	12 (5%)	1 (0%)	34	66
3	h	223/229 (97%)	210 (94%)	12 (5%)	1 (0%)	34	66
All	All	1399/1618 (86%)	1316 (94%)	69 (5%)	14 (1%)	15	44

All (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

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Mol	Chain	Res	Type
1	A	146	ILE
1	B	146	ILE
1	A	374	CYS
3	H	116	TRP
1	A	301	PRO
3	h	116	TRP
1	B	144	SER
1	B	301	PRO
1	A	151	VAL

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%)	221 (93%)	16 (7%)	16	42
1	B	227/328 (69%)	211 (93%)	16 (7%)	15	40
2	L	179/182 (98%)	164 (92%)	15 (8%)	11	31
2	l	177/182 (97%)	157 (89%)	20 (11%)	6	18
3	H	191/194 (98%)	178 (93%)	13 (7%)	16	42
3	h	190/194 (98%)	180 (95%)	10 (5%)	22	54
All	All	1201/1408 (85%)	1111 (92%)	90 (8%)	13	37

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LEU
1	A	95	ASP
1	A	124	GLU
1	A	137	CYS
1	A	165	THR
1	A	177	ILE
1	A	190	ARG
1	A	220	GLU
1	A	232	GLU

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Mol	Chain	Res	Type
1	A	237	LEU
1	A	239	VAL
1	A	255	VAL
1	A	276	SER
1	A	293	PHE
1	A	303	ARG
1	A	374	CYS
2	L	5	THR
2	L	25	SER
2	L	26	SER
2	L	35	HIS
2	L	70	THR
2	L	75	VAL
2	L	98	SER
2	L	125	SER
2	L	158	VAL
2	L	171	SER
2	L	178	SER
2	L	192	ARG
2	L	198	VAL
2	L	212	THR
2	L	213	GLU
3	H	25	SER
3	H	77	ASN
3	H	100	LEU
3	H	122	VAL
3	H	128	SER
3	H	143	SER
3	H	156	LYS
3	H	164	THR
3	H	191	LEU
3	H	200	SER
3	H	202	LEU
3	H	210	ASN
3	H	227	LYS
2	1	3	VAL
2	1	5	THR
2	1	7	PRO
2	1	9	SER
2	1	21	SER
2	1	25	SER
2	1	35	HIS

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Mol	Chain	Res	Type
2	l	46	LYS
2	l	68	SER
2	l	70	THR
2	l	75	VAL
2	l	98	SER
2	l	148	THR
2	l	159	LYS
2	l	165	THR
2	l	166	THR
2	l	170	GLN
2	l	171	SER
2	l	173	ASN
2	l	186	GLU
3	h	25	SER
3	h	100	LEU
3	h	107	TRP
3	h	122	VAL
3	h	128	SER
3	h	141	SER
3	h	156	LYS
3	h	164	THR
3	h	191	LEU
3	h	218	THR
1	B	42	CYS
1	B	121	MET
1	B	165	THR
1	B	180	MET
1	B	186	TYR
1	B	230	LEU
1	B	270	LEU
1	B	276	SER
1	B	280	ARG
1	B	293	PHE
1	B	301	PRO
1	B	339	CYS
1	B	371	ARG
1	B	372	CYS
1	B	374	CYS
1	B	375	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	77	ASN
3	H	210	ASN
3	h	210	ASN
3	h	212	ASN
1	B	307	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.89	0	5,5,5	0.98	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/365 (76%)	0.49	25 (8%) 9 5	69, 110, 160, 196	0
1	B	273/365 (74%)	0.67	30 (10%) 5 3	77, 118, 187, 220	0
2	L	214/215 (99%)	0.06	3 (1%) 75 70	54, 81, 113, 151	0
2	l	210/215 (97%)	0.13	9 (4%) 35 25	62, 101, 132, 149	0
3	H	226/229 (98%)	-0.12	1 (0%) 92 91	53, 74, 100, 136	0
3	h	225/229 (98%)	0.12	9 (4%) 38 28	52, 71, 142, 227	0
All	All	1427/1618 (88%)	0.25	77 (5%) 25 17	52, 91, 154, 227	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	h	143	SER	7.1
2	L	1	GLN	7.1
2	l	3	VAL	6.6
1	B	239	VAL	6.5
1	B	244	PRO	6.3
1	A	275	HIS	5.5
1	B	242	PRO	5.3
3	h	144	THR	5.2
1	B	245	GLY	5.0
1	B	149	ASN	4.7
1	B	243	GLY	4.5
1	B	181	LYS	4.4
1	A	152	VAL	4.2
1	A	146	ILE	4.2
1	A	373	GLY	4.0
1	B	118	ILE	4.0
3	h	146	GLY	4.0
1	A	286	LEU	3.9
1	B	240	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	180	MET	3.8
1	B	185	ARG	3.7
1	B	53	ILE	3.7
1	B	241	PHE	3.7
1	B	43	THR	3.7
1	B	223	LEU	3.5
1	A	343	THR	3.5
1	A	277	THR	3.4
1	B	182	ASP	3.4
1	B	50	SER	3.3
1	B	47	ASN	3.3
1	B	48	THR	3.3
1	B	199	GLY	3.3
1	B	258	THR	3.2
1	A	308	TYR	3.2
2	l	76	ILE	3.2
2	l	98	SER	3.1
2	l	109	LEU	3.1
1	A	183	GLY	3.1
1	A	285	PRO	3.0
3	h	141	SER	2.8
1	B	183	GLY	2.8
1	A	260	THR	2.7
2	l	97	ASN	2.6
2	L	171	SER	2.6
1	A	244	PRO	2.6
1	A	216	LEU	2.6
1	B	184	THR	2.5
1	A	290	PHE	2.5
1	B	72	ILE	2.4
2	l	18	VAL	2.4
2	l	106	LEU	2.4
1	A	288	VAL	2.4
3	h	196	THR	2.3
1	B	163	VAL	2.3
1	B	284	TYR	2.2
3	h	142	LYS	2.2
2	l	92	TRP	2.2
1	B	148	TYR	2.2
1	B	152	VAL	2.2
1	B	224	GLY	2.2
1	A	149	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	SER	2.1
3	H	179	PHE	2.1
1	A	95	ASP	2.1
2	l	11	SER	2.1
3	h	110	TYR	2.1
1	A	221	SER	2.1
1	A	375	SER	2.1
1	A	272	CYS	2.1
3	h	108	SER	2.1
1	B	202	ILE	2.0
2	L	2	PRO	2.0
1	A	142	PHE	2.0
3	h	84	ASN	2.0
1	A	356	LYS	2.0
1	A	124	GLU	2.0
1	A	278	GLU	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, 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(\AA^2)	Q<0.9
4	GOL	h	301	6/6	0.68	0.22	76,87,88,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.