



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:36 PM BST

PDB ID : 6MGP
Title : Structure of human 4-1BB / 4-1BBL complex
Authors : Kimberlin, C.R.; Chin, S.M.; Roe-Zurz, Z.; Xu, A.; Yang, Y.
Deposited on : 2018-09-14
Resolution : 2.13 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 : 2.13.1
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

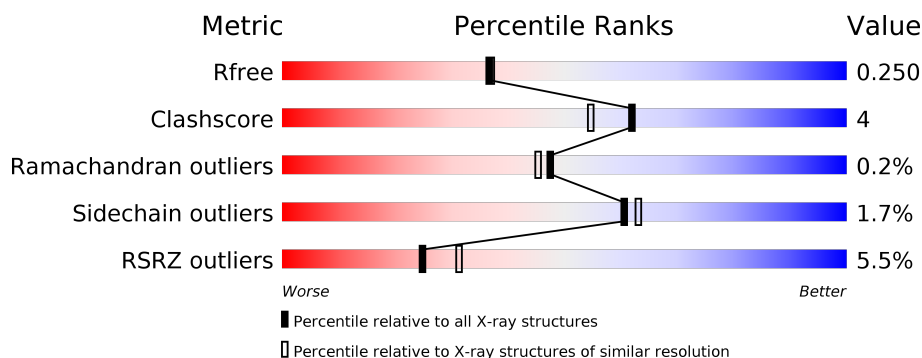
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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.




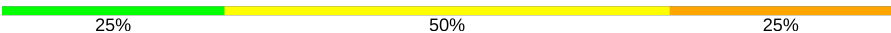

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	207	<div> <div>2%</div> <div>65% 7% 28%</div> </div>
1	B	207	<div> <div>2%</div> <div>64% 9% 27%</div> </div>
1	C	207	<div> <div>8%</div> <div>64% 9% 27%</div> </div>
2	X	144	<div> <div>6%</div> <div>88% 11% .</div> </div>
2	Y	144	<div> <div>6%</div> <div>91% 8% .</div> </div>
2	Z	144	<div> <div>5%</div> <div>89% 10% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	4	 50% 50%
3	E	4	 25% 50% 25%
3	F	4	 25% 25% 50%

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
5	GOL	B	301	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6717 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 Tumor necrosis factor ligand superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1097	705	195	196	1			
1	B	152	Total	C	N	O	S	0	1	0
			1130	723	205	201	1			
1	C	152	Total	C	N	O		0	1	0
			1123	720	200	203				

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLY	-	expression tag	UNP P41273
A	256	SER	-	expression tag	UNP P41273
A	257	HIS	-	expression tag	UNP P41273
A	258	HIS	-	expression tag	UNP P41273
A	259	HIS	-	expression tag	UNP P41273
A	260	HIS	-	expression tag	UNP P41273
A	261	HIS	-	expression tag	UNP P41273
A	262	HIS	-	expression tag	UNP P41273
A	263	HIS	-	expression tag	UNP P41273
A	264	HIS	-	expression tag	UNP P41273
B	255	GLY	-	expression tag	UNP P41273
B	256	SER	-	expression tag	UNP P41273
B	257	HIS	-	expression tag	UNP P41273
B	258	HIS	-	expression tag	UNP P41273
B	259	HIS	-	expression tag	UNP P41273
B	260	HIS	-	expression tag	UNP P41273
B	261	HIS	-	expression tag	UNP P41273
B	262	HIS	-	expression tag	UNP P41273
B	263	HIS	-	expression tag	UNP P41273
B	264	HIS	-	expression tag	UNP P41273
C	255	GLY	-	expression tag	UNP P41273
C	256	SER	-	expression tag	UNP P41273
C	257	HIS	-	expression tag	UNP P41273

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	258	HIS	-	expression tag	UNP P41273
C	259	HIS	-	expression tag	UNP P41273
C	260	HIS	-	expression tag	UNP P41273
C	261	HIS	-	expression tag	UNP P41273
C	262	HIS	-	expression tag	UNP P41273
C	263	HIS	-	expression tag	UNP P41273
C	264	HIS	-	expression tag	UNP P41273

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 9.

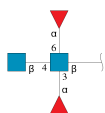
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	144	Total	C	N	O	S	0	0	0
			1040	612	193	213	22			
2	Y	143	Total	C	N	O	S	0	0	0
			1024	607	185	210	22			
2	Z	144	Total	C	N	O	S	0	0	0
			1027	610	186	209	22			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	163	GLU	-	expression tag	UNP Q07011
X	164	ASN	-	expression tag	UNP Q07011
X	165	LEU	-	expression tag	UNP Q07011
X	166	TYR	-	expression tag	UNP Q07011
X	167	PHE	-	expression tag	UNP Q07011
X	168	GLN	-	expression tag	UNP Q07011
Y	163	GLU	-	expression tag	UNP Q07011
Y	164	ASN	-	expression tag	UNP Q07011
Y	165	LEU	-	expression tag	UNP Q07011
Y	166	TYR	-	expression tag	UNP Q07011
Y	167	PHE	-	expression tag	UNP Q07011
Y	168	GLN	-	expression tag	UNP Q07011
Z	163	GLU	-	expression tag	UNP Q07011
Z	164	ASN	-	expression tag	UNP Q07011
Z	165	LEU	-	expression tag	UNP Q07011
Z	166	TYR	-	expression tag	UNP Q07011
Z	167	PHE	-	expression tag	UNP Q07011
Z	168	GLN	-	expression tag	UNP Q07011

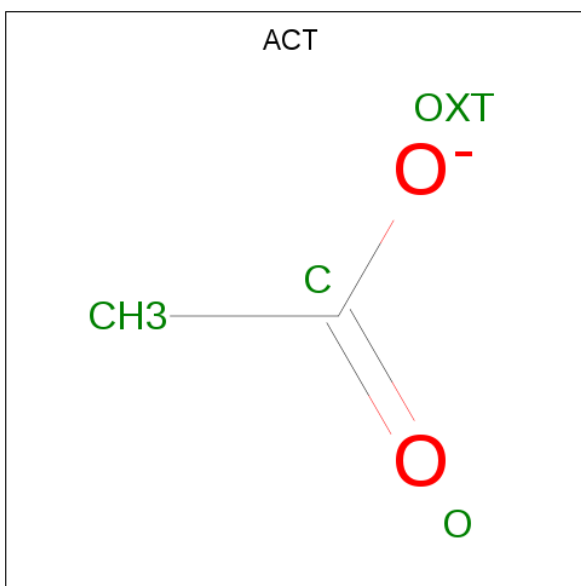
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyr

anose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total 48	C 28	N 2	O 18	0	0	0
3	E	4	Total 48	C 28	N 2	O 18	0	0	0
3	F	4	Total 48	C 28	N 2	O 18	0	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	X	1	Total	C	O	0	0
			4	2	2		
4	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	Z	1	Total	C	O	0	0
			6	3	3		
5	Z	1	Total	C	O	0	0
			6	3	3		

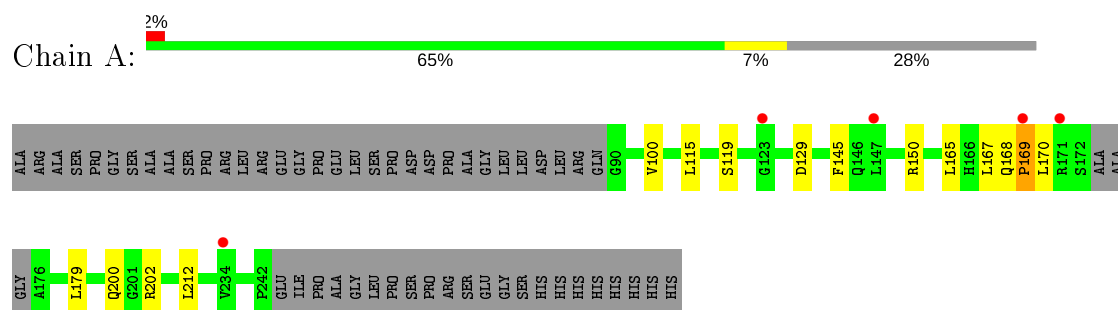
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	20	Total	O	0	0
			20	20		
6	C	14	Total	O	0	0
			14	14		
6	X	10	Total	O	0	0
			10	10		
6	Y	16	Total	O	0	0
			16	16		
6	Z	14	Total	O	0	0
			14	14		

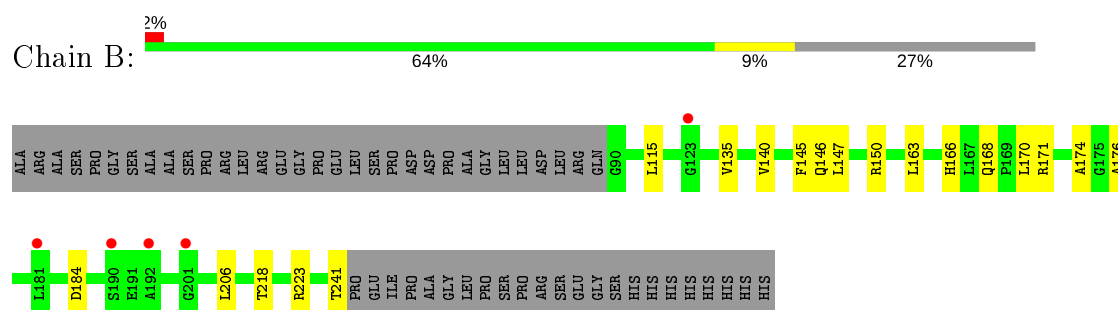
3 Residue-property plots [i](#)

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.

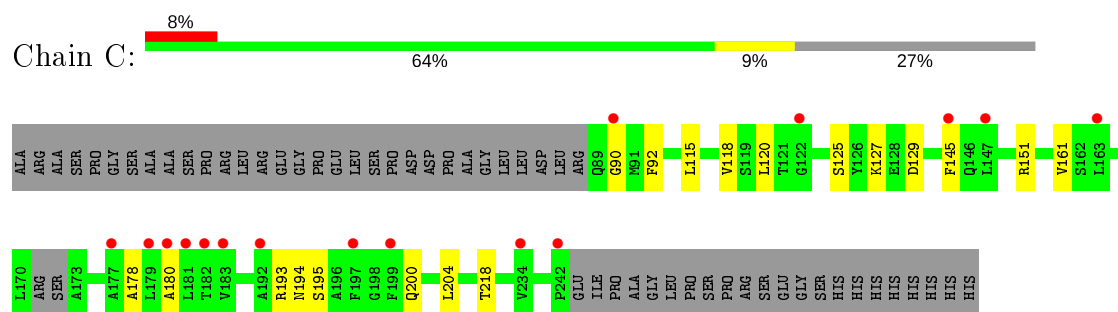
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



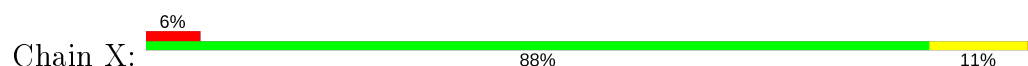
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



- Molecule 1: Tumor necrosis factor ligand superfamily member 9

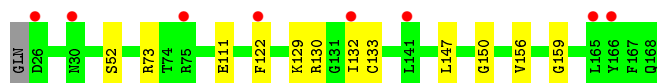
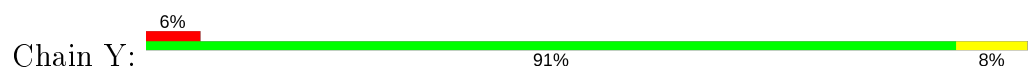


- Molecule 2: Tumor necrosis factor receptor superfamily member 9

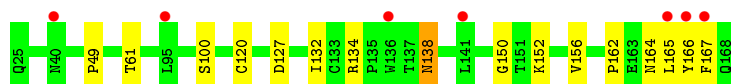
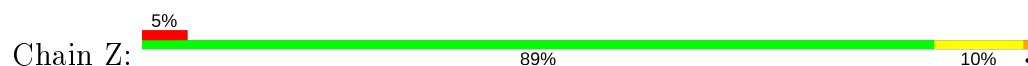




- Molecule 2: Tumor necrosis factor receptor superfamily member 9



- Molecule 2: Tumor necrosis factor receptor superfamily member 9



- Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.01Å 229.38Å 114.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.13 48.91 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.91-2.13) 81.9 (48.91-2.13)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.60 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.217 , 0.250 0.217 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	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	0.95	EDS
Total number of atoms	6717	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: FUC, GOL, NAG, ACT

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	0.31	0/1120	0.56	0/1526
1	B	0.31	0/1154	0.55	0/1572
1	C	0.30	0/1147	0.51	0/1563
2	X	0.31	0/1058	0.49	0/1430
2	Y	0.28	0/1043	0.49	0/1412
2	Z	0.39	0/1045	0.56	0/1412
All	All	0.32	0/6567	0.53	0/8915

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1097	0	1081	10	0
1	B	1130	0	1120	13	0
1	C	1123	0	1112	12	0
2	X	1040	0	897	11	0
2	Y	1024	0	880	7	0
2	Z	1027	0	893	9	0
3	D	48	0	43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	48	0	43	1	0
3	F	48	0	43	1	0
4	A	8	0	6	2	0
4	C	4	0	3	0	0
4	X	4	0	3	1	0
4	Y	4	0	3	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	Z	12	0	16	0	0
6	A	14	0	0	0	0
6	B	20	0	0	0	0
6	C	14	0	0	1	0
6	X	10	0	0	0	0
6	Y	16	0	0	0	0
6	Z	14	0	0	1	0
All	All	6717	0	6159	56	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 (56) 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:Z:162:PRO:O	2:Z:167:PHE:HB2	1.87	0.74
1:C:118:VAL:O	6:C:401:HOH:O	2.08	0.71
1:A:179:LEU:HD21	1:A:202:ARG:HG2	1.75	0.69
2:X:113:THR:HG23	2:X:115:LYS:H	1.62	0.65
1:C:161:VAL:HG22	1:C:218:THR:HG23	1.81	0.63
1:A:200:GLN:NE2	1:B:146:GLN:OE1	2.34	0.61
2:X:78:CYS:HB3	2:X:84:ALA:HB2	1.82	0.61
2:Z:127:ASP:OD1	2:Z:134:ARG:NH2	2.35	0.59
1:B:166:HIS:ND1	1:B:176:ALA:O	2.36	0.57
2:X:150:GLY:H	2:X:156:VAL:HG12	1.69	0.57
1:B:241:THR:HG21	1:C:90:GLY:H	1.69	0.55
1:B:115:LEU:HD22	2:Y:52:SER:HB3	1.90	0.54
2:Y:147:LEU:HG	2:Y:159:GLY:HA3	1.88	0.54
2:Z:138:ASN:ND2	6:Z:301:HOH:O	2.39	0.54
2:Y:111:GLU:HB2	2:Y:133:CYS:SG	2.49	0.53
1:B:147:LEU:HD22	1:B:163:LEU:HG	1.90	0.52
1:B:170:LEU:HD12	1:B:171:ARG:H	1.75	0.52
2:X:74:THR:HG21	2:X:77:GLU:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:113:THR:HG22	2:X:116:GLY:O	2.09	0.52
1:A:100:VAL:HG22	4:A:301:ACT:H3	1.92	0.51
2:Z:150:GLY:H	2:Z:156:VAL:HG12	1.75	0.51
1:A:129:ASP:OD1	1:A:129:ASP:N	2.46	0.49
2:Z:132:ILE:O	2:Z:134:ARG:NH1	2.46	0.49
1:B:168:GLN:HA	1:B:168:GLN:HE21	1.79	0.47
1:C:151:ARG:HB3	1:C:194:ASN:HB3	1.97	0.47
1:A:165:LEU:HD11	1:A:212:LEU:HB3	1.96	0.46
1:B:184:ASP:CG	1:C:193:ARG:HE	2.18	0.46
2:Y:111:GLU:OE2	2:Y:132:ILE:HG13	2.15	0.46
2:Z:164:ASN:O	2:Z:166:TYR:N	2.48	0.45
1:B:218:THR:OG1	1:B:223:ARG:HD3	2.16	0.45
1:B:135:VAL:HG11	1:B:206:LEU:HD13	1.98	0.44
1:A:115:LEU:CD2	2:X:52:SER:HB3	2.47	0.44
1:A:168:GLN:HA	1:A:169:PRO:C	2.37	0.44
1:A:119:SER:HB2	4:A:302:ACT:H1	1.99	0.44
1:C:180:ALA:O	1:C:200:GLN:NE2	2.49	0.44
1:C:178:ALA:HB1	1:C:204:LEU:HD21	2.00	0.44
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.72	0.43
2:X:150:GLY:N	2:X:156:VAL:HG12	2.33	0.43
2:Y:150:GLY:H	2:Y:156:VAL:HG12	1.83	0.43
1:B:171:ARG:NH1	1:B:174:ALA:HB2	2.34	0.43
2:X:126:ASN:HA	2:X:134:ARG:NH2	2.34	0.43
1:A:167:LEU:O	1:A:170:LEU:HA	2.18	0.43
2:X:39:ASN:HB2	4:X:205:ACT:H3	1.99	0.43
1:A:168:GLN:HA	1:A:170:LEU:N	2.34	0.42
2:Z:120:CYS:HB2	2:Z:152:LYS:HB2	2.01	0.42
2:X:95:LEU:HD23	2:X:95:LEU:HA	1.89	0.42
2:Y:129:LYS:HE3	2:Y:130:ARG:NH1	2.35	0.42
2:Y:73:ARG:HB2	2:Y:73:ARG:HE	1.67	0.42
1:C:115:LEU:HD21	2:Z:49:PRO:HB2	2.02	0.41
3:F:1:NAG:H61	3:F:4:FUC:H5	2.02	0.41
1:C:120:LEU:HD21	1:C:125:SER:HA	2.02	0.41
1:B:171:ARG:NH2	2:Z:61:THR:OG1	2.54	0.41
2:X:109:GLY:HA2	2:X:152:LYS:O	2.21	0.41
1:C:193:ARG:NH1	1:C:195:SER:O	2.54	0.41
3:E:1:NAG:H62	3:E:4:FUC:H2	1.87	0.41
1:B:140:VAL:HG21	1:C:92:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/207 (70%)	141 (97%)	4 (3%)	1 (1%)	22	14
1	B	151/207 (73%)	149 (99%)	2 (1%)	0	100	100
1	C	149/207 (72%)	145 (97%)	4 (3%)	0	100	100
2	X	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
2	Y	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
2	Z	142/144 (99%)	141 (99%)	0	1 (1%)	22	14
All	All	871/1053 (83%)	853 (98%)	16 (2%)	2 (0%)	47	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	PRO
2	Z	165	LEU

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	106/158 (67%)	104 (98%)	2 (2%)	57	59
1	B	109/158 (69%)	107 (98%)	2 (2%)	59	60
1	C	110/158 (70%)	108 (98%)	2 (2%)	59	60
2	X	115/126 (91%)	113 (98%)	2 (2%)	60	63
2	Y	114/126 (90%)	113 (99%)	1 (1%)	78	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	113/126 (90%)	111 (98%)	2 (2%)	59	60
All	All	667/852 (78%)	656 (98%)	11 (2%)	60	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	A	150	ARG
1	B	145	PHE
1	B	150	ARG
1	C	129	ASP
1	C	145	PHE
2	X	152	LYS
2	X	161	SER
2	Y	122	PHE
2	Z	100	SER
2	Z	138	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	GLN
2	X	39	ASN
2	X	43	GLN
2	X	59	GLN
2	X	104	GLN
2	Z	59	GLN
2	Z	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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
3	NAG	D	1	3,2	14,14,15	0.32	0	17,19,21	0.75	0
3	FUC	D	2	3	10,10,11	0.70	0	14,14,16	1.21	2 (14%)
3	NAG	D	3	3	14,14,15	0.37	0	17,19,21	0.41	0
3	FUC	D	4	3	10,10,11	1.22	1 (10%)	14,14,16	1.03	1 (7%)
3	NAG	E	1	3,2	14,14,15	0.69	1 (7%)	17,19,21	0.72	0
3	FUC	E	2	3	10,10,11	0.77	1 (10%)	14,14,16	1.20	1 (7%)
3	NAG	E	3	3	14,14,15	0.46	0	17,19,21	0.33	0
3	FUC	E	4	3	10,10,11	1.06	0	14,14,16	1.05	0
3	NAG	F	1	3,2	14,14,15	0.68	0	17,19,21	1.50	3 (17%)
3	FUC	F	2	3	10,10,11	1.07	1 (10%)	14,14,16	1.61	3 (21%)
3	NAG	F	3	3	14,14,15	0.53	0	17,19,21	0.36	0
3	FUC	F	4	3	10,10,11	2.11	3 (30%)	14,14,16	1.88	3 (21%)

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
3	NAG	D	1	3,2	-	4/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	D	3	3	-	1/6/23/26	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	2/6/23/26	0/1/1/1
3	FUC	E	4	3	-	-	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	3	3	-	0/6/23/26	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	FUC	C1-C2	4.91	1.63	1.52
3	F	4	FUC	C2-C3	3.02	1.57	1.52
3	F	2	FUC	C1-C2	2.85	1.58	1.52
3	F	4	FUC	O5-C1	2.62	1.47	1.43
3	D	4	FUC	O5-C1	-2.56	1.39	1.43
3	E	1	NAG	O5-C1	-2.21	1.40	1.43
3	E	2	FUC	C1-C2	2.08	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-O5-C5	4.73	118.60	112.19
3	F	4	FUC	C1-C2-C3	4.53	115.23	109.67
3	F	4	FUC	C1-O5-C5	3.66	121.06	112.78
3	F	2	FUC	C1-C2-C3	3.65	114.15	109.67
3	F	2	FUC	C1-O5-C5	3.00	119.58	112.78
3	F	2	FUC	O5-C1-C2	2.80	115.10	110.77
3	E	2	FUC	C1-O5-C5	2.62	118.71	112.78
3	D	2	FUC	O5-C5-C4	2.60	114.19	109.52
3	F	4	FUC	O5-C5-C4	2.60	114.18	109.52
3	D	2	FUC	C1-O5-C5	2.59	118.64	112.78
3	F	1	NAG	O3-C3-C4	2.34	115.76	110.35
3	D	4	FUC	O5-C5-C4	2.25	113.57	109.52
3	F	1	NAG	O5-C5-C6	-2.20	103.75	107.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	O7-C7-N2-C2
3	E	3	NAG	C4-C5-C6-O6
3	D	3	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	FUC	1	0
3	F	1	NAG	1	0
3	E	1	NAG	1	0
3	E	4	FUC	1	0

5.6 Ligand geometry

9 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	ACT	X	205	-	1,3,3	1.64	0	0,3,3	0.00	-
5	GOL	Z	206	-	5,5,5	0.38	0	5,5,5	0.30	0
4	ACT	C	302	-	1,3,3	1.13	0	0,3,3	0.00	-
5	GOL	Z	205	-	5,5,5	0.36	0	5,5,5	0.20	0
4	ACT	A	302	-	1,3,3	1.27	0	0,3,3	0.00	-
5	GOL	C	301	-	5,5,5	0.33	0	5,5,5	0.43	0
5	GOL	B	301	-	5,5,5	0.43	0	5,5,5	0.23	0
4	ACT	A	301	-	1,3,3	1.48	0	0,3,3	0.00	-
4	ACT	Y	205	-	1,3,3	1.53	0	0,3,3	0.00	-

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	GOL	B	301	-	-	2/4/4/4	-
5	GOL	Z	205	-	-	4/4/4/4	-
5	GOL	C	301	-	-	2/4/4/4	-
5	GOL	Z	206	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	206	GOL	C1-C2-C3-O3
5	Z	206	GOL	O2-C2-C3-O3
5	Z	205	GOL	O1-C1-C2-C3
5	B	301	GOL	O1-C1-C2-C3
5	Z	206	GOL	O1-C1-C2-C3
5	Z	205	GOL	C1-C2-C3-O3
5	C	301	GOL	O1-C1-C2-C3
5	Z	206	GOL	O1-C1-C2-O2
5	Z	205	GOL	O1-C1-C2-O2
5	Z	205	GOL	O2-C2-C3-O3
5	B	301	GOL	O1-C1-C2-O2
5	C	301	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	205	ACT	1	0
4	A	302	ACT	1	0
4	A	301	ACT	1	0

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, 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	150/207 (72%)	0.41	5 (3%)	46	54	49, 64, 104, 137	0
1	B	152/207 (73%)	0.38	5 (3%)	46	54	41, 58, 88, 127	0
1	C	152/207 (73%)	0.69	16 (10%)	6	8	46, 64, 110, 125	0
2	X	144/144 (100%)	0.20	8 (5%)	24	30	54, 71, 101, 127	0
2	Y	143/144 (99%)	0.11	8 (5%)	24	30	51, 74, 113, 157	0
2	Z	144/144 (100%)	0.13	7 (4%)	29	36	47, 64, 114, 140	0
All	All	885/1053 (84%)	0.33	49 (5%)	25	31	41, 66, 106, 157	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	166	TYR	7.5
2	X	165	LEU	5.0
2	Z	167	PHE	4.8
2	X	143	GLY	4.7
1	A	169	PRO	4.3
2	Z	165	LEU	4.3
2	Y	122	PHE	3.7
2	X	141	LEU	3.6
2	Z	40	ASN	3.4
1	B	192	ALA	3.4
1	C	90	GLY	3.3
2	X	166	TYR	3.3
1	C	122	GLY	3.2
1	C	242	PRO	3.0
2	Y	165	LEU	3.0
1	A	123	GLY	2.9
1	C	182	THR	2.7
2	Y	132	ILE	2.7
2	X	122	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	181	LEU	2.7
1	A	171	ARG	2.7
1	C	177	ALA	2.6
2	X	167	PHE	2.6
1	C	179	LEU	2.6
2	Y	166	TYR	2.6
1	B	190	SER	2.6
1	B	201	GLY	2.6
1	C	163	LEU	2.6
1	C	192	ALA	2.5
2	X	164	ASN	2.5
1	C	180	ALA	2.4
1	C	145	PHE	2.4
1	C	234	VAL	2.4
2	Z	136	TRP	2.4
1	C	147	LEU	2.4
1	A	234	VAL	2.3
2	Y	30	ASN	2.3
1	B	181	LEU	2.2
1	C	199	PHE	2.2
2	X	163	GLU	2.2
2	Z	141	LEU	2.1
1	C	197	PHE	2.1
1	A	147	LEU	2.1
2	Y	141	LEU	2.0
2	Z	95	LEU	2.0
1	B	123	GLY	2.0
2	Y	75	ARG	2.0
2	Y	26	ASP	2.0
1	C	183	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
3	NAG	D	3	14/15	0.83	0.27	134,139,147,148	0
3	FUC	E	4	10/11	0.84	0.34	123,129,139,142	0
3	FUC	D	2	10/11	0.86	0.13	130,135,140,144	0
3	NAG	F	3	14/15	0.88	0.20	113,126,137,141	0
3	FUC	F	4	10/11	0.89	0.28	115,119,121,121	0
3	FUC	D	4	10/11	0.89	0.30	120,127,129,133	0
3	NAG	D	1	14/15	0.90	0.13	81,92,122,129	0
3	NAG	E	1	14/15	0.90	0.15	67,88,113,123	0
3	NAG	E	3	14/15	0.91	0.30	127,140,150,153	0
3	FUC	F	2	10/11	0.92	0.11	114,120,124,125	0
3	NAG	F	1	14/15	0.93	0.12	81,95,116,117	0
3	FUC	E	2	10/11	0.93	0.14	103,114,119,120	0

6.4 Ligands

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
5	GOL	B	301	6/6	0.40	0.46	101,108,110,111	0
5	GOL	Z	205	6/6	0.68	0.26	90,97,97,98	0
5	GOL	Z	206	6/6	0.76	0.28	91,92,93,96	0
4	ACT	Y	205	4/4	0.81	0.21	95,95,96,96	0
4	ACT	X	205	4/4	0.89	0.14	66,72,76,80	0
4	ACT	A	301	4/4	0.89	0.15	62,65,66,68	0
4	ACT	A	302	4/4	0.89	0.24	92,92,93,94	0
4	ACT	C	302	4/4	0.95	0.12	57,61,61,65	0
5	GOL	C	301	6/6	0.96	0.22	59,63,67,70	0

6.5 Other polymers

There are no such residues in this entry.