



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:47 PM GMT

PDB ID : 1QLR  
Title : CRYSTAL STRUCTURE OF THE FAB FRAGMENT OF A HUMAN MON-  
OCLONAL IGM COLD AGGLUTININ  
Authors : Carvalho, J.G.; Cauerhff, A.; Goldbaum, F.; Leoni, J.; Polikarpov, I.  
Deposited on : 1999-09-11  
Resolution : 2.83 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

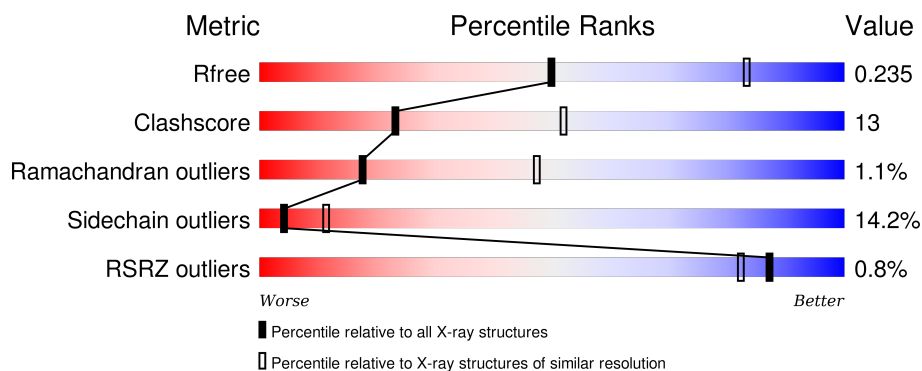
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.83 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))
$R_{free}$	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	215	<div> <div>62%</div> <div>27%</div> <div>8%</div> <div>•</div> </div>
1	C	215	<div> <div>62%</div> <div>28%</div> <div>7%</div> <div>•</div> </div>
2	B	232	<div> <div>51%</div> <div>31%</div> <div>6%</div> <div>•</div> <div>10%</div> </div>
2	D	232	<div> <div>52%</div> <div>29%</div> <div>7%</div> <div>•</div> <div>10%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	B	302	X	-	-	-
3	FUC	D	302	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6540 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 IGM KAPPA CHAIN V-III (KAU COLD AGGLUTININ).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1638	1023	275	335	5			
1	C	215	Total	C	N	O	S	0	0	0
			1638	1023	275	335	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	CYS	GLY	CONFLICT	PIR A23746
C	23	CYS	GLY	CONFLICT	PIR A23746
A	88	CYS	GLY	CONFLICT	PIR A23746
C	88	CYS	GLY	CONFLICT	PIR A23746
A	134	CYS	GLY	CONFLICT	PIR A23746
C	134	CYS	GLY	CONFLICT	PIR A23746
A	194	CYS	GLY	CONFLICT	PIR A23746
C	194	CYS	GLY	CONFLICT	PIR A23746
A	214	CYS	GLY	CONFLICT	PIR A23746
C	214	CYS	GLY	CONFLICT	PIR A23746

- Molecule 2 is a protein called IGM FAB REGION IV-J(H4)-C (KAU COLD AGGLUTININ).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1608	1024	271	308	5			
2	D	209	Total	C	N	O	S	0	0	0
			1608	1024	271	308	5			

There are 2 discrepancies between the modelled and reference sequences:

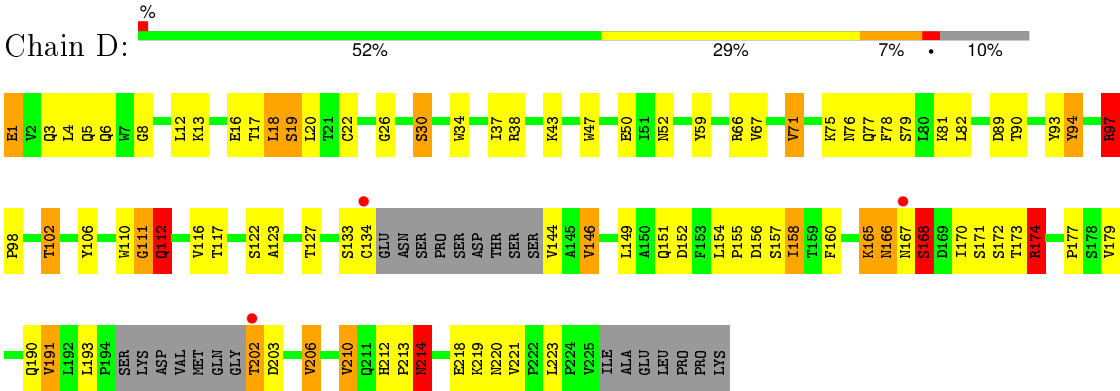
Chain	Residue	Modelled	Actual	Comment	Reference
B	22	CYS	GLY	CONFLICT	PIR B23746
D	22	CYS	GLY	CONFLICT	PIR B23746

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	2	Total	C	N	O	0	0
			24	14	1	9		
3	D	2	Total	C	N	O	0	0
			24	14	1	9		



● Molecule 2: IGM FAB REGION IV-J(H4)-C (KAU COLD AGGLUTININ)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.66Å 115.66Å 174.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	13.10 – 2.83 13.12 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.8 (13.10-2.83) 96.8 (13.12-2.84)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.84Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.265 0.189 , 0.235	Depositor DCC
$R_{free}$ test set	1578 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.6	EDS
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31328 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAG, FUC

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	0.78	0/1673	2.06	55/2273 (2.4%)
1	C	0.79	2/1673 (0.1%)	2.09	55/2273 (2.4%)
2	B	0.76	1/1654 (0.1%)	1.82	42/2259 (1.9%)
2	D	0.76	0/1654	1.90	42/2259 (1.9%)
All	All	0.77	3/6654 (0.0%)	1.97	194/9064 (2.1%)

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	2
1	C	0	3
3	B	1	0
3	D	1	0
All	All	2	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	TYR	CE2-CZ	-6.25	1.30	1.38
2	B	27	GLY	N-CA	5.50	1.54	1.46
1	C	49	TYR	CE1-CZ	-5.33	1.31	1.38

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ARG	NE-CZ-NH2	-23.10	108.75	120.30
1	A	54	ARG	NE-CZ-NH2	-21.46	109.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	ARG	NE-CZ-NH2	-16.70	111.95	120.30
1	C	49	TYR	CD1-CG-CD2	-14.71	101.72	117.90
1	C	49	TYR	CB-CG-CD2	14.42	129.65	121.00
1	C	45	ARG	NE-CZ-NH2	-14.14	113.23	120.30
1	C	36	TYR	CB-CG-CD2	13.94	129.36	121.00
2	D	30	SER	CA-C-N	12.84	145.45	117.20
1	C	77	ARG	CD-NE-CZ	12.79	141.50	123.60
1	A	36	TYR	CB-CG-CD1	12.67	128.60	121.00
1	A	77	ARG	CD-NE-CZ	12.53	141.14	123.60
1	A	36	TYR	CD1-CG-CD2	-12.52	104.13	117.90
1	C	36	TYR	CD1-CG-CD2	-12.40	104.26	117.90
1	C	54	ARG	NH1-CZ-NH2	12.38	133.02	119.40
1	C	36	TYR	CZ-CE2-CD2	12.34	130.90	119.80
2	B	30	SER	CA-C-N	12.31	144.29	117.20
2	B	97	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	C	42	GLN	OE1-CD-NE2	12.05	149.62	121.90
2	B	50	GLU	OE1-CD-OE2	-11.98	108.92	123.30
1	A	49	TYR	CD1-CE1-CZ	11.62	130.25	119.80
2	B	1	GLU	CG-CD-OE2	11.48	141.26	118.30
1	A	54	ARG	NH1-CZ-NH2	11.31	131.85	119.40
1	A	49	TYR	CD1-CG-CD2	-10.94	105.86	117.90
1	A	49	TYR	CB-CG-CD2	10.81	127.48	121.00
2	D	1	GLU	CG-CD-OE2	10.63	139.56	118.30
1	A	61	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	36	TYR	CB-CG-CD2	10.39	127.24	121.00
1	C	49	TYR	CB-CG-CD1	10.30	127.18	121.00
1	A	45	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	61	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	A	36	TYR	CG-CD2-CE2	10.21	129.47	121.30
1	A	18	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	A	108	ARG	NE-CZ-NH1	10.06	125.33	120.30
2	D	50	GLU	OE1-CD-OE2	-10.01	111.28	123.30
2	D	156	ASP	CB-CG-OD1	9.93	127.24	118.30
1	C	21	LEU	CA-CB-CG	9.78	137.78	115.30
1	C	45	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	C	36	TYR	CG-CD1-CE1	9.70	129.06	121.30
2	B	66	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	A	49	TYR	CG-CD2-CE2	9.39	128.81	121.30
2	D	26	GLY	CA-C-N	9.38	134.96	116.20
1	C	49	TYR	CG-CD2-CE2	9.32	128.75	121.30
2	B	31	ASP	CB-CG-OD2	9.30	126.67	118.30
2	B	26	GLY	CA-C-N	9.28	134.76	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	THR	N-CA-CB	9.26	127.89	110.30
1	C	49	TYR	CG-CD1-CE1	9.16	128.62	121.30
1	A	49	TYR	CE1-CZ-CE2	-9.11	105.22	119.80
2	B	1	GLU	OE1-CD-OE2	-9.09	112.40	123.30
1	C	36	TYR	CB-CG-CD1	8.93	126.36	121.00
2	B	30	SER	CA-C-O	-8.87	101.48	120.10
2	D	97	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	A	36	TYR	CE1-CZ-CE2	-8.74	105.82	119.80
1	A	49	TYR	CB-CG-CD1	8.71	126.23	121.00
1	A	36	TYR	CD1-CE1-CZ	8.66	127.60	119.80
1	C	36	TYR	CE1-CZ-CE2	-8.53	106.15	119.80
1	C	49	TYR	CE1-CZ-CE2	-8.46	106.27	119.80
1	A	36	TYR	CG-CD1-CE1	8.43	128.04	121.30
2	D	30	SER	CA-C-O	-8.43	102.40	120.10
2	D	174	ARG	CD-NE-CZ	8.37	135.32	123.60
2	B	156	ASP	CB-CG-OD1	8.27	125.74	118.30
2	D	1	GLU	OE1-CD-OE2	-8.23	113.42	123.30
1	A	211	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	A	21	LEU	CA-CB-CG	8.16	134.08	115.30
1	C	42	GLN	CG-CD-OE1	-7.96	105.67	121.60
1	A	82	ASP	CB-CG-OD1	7.95	125.45	118.30
1	C	49	TYR	CD1-CE1-CZ	7.87	126.88	119.80
1	C	56	THR	N-CA-CB	7.81	125.14	110.30
1	C	77	ARG	NE-CZ-NH1	7.79	124.19	120.30
2	D	106	TYR	CB-CG-CD2	-7.78	116.33	121.00
1	C	108	ARG	NE-CZ-NH1	7.75	124.18	120.30
2	D	26	GLY	O-C-N	-7.71	110.09	123.20
1	C	18	ARG	CD-NE-CZ	7.69	134.37	123.60
1	A	211	ARG	CD-NE-CZ	7.67	134.34	123.60
2	D	156	ASP	CB-CG-OD2	-7.60	111.46	118.30
2	D	112	GLN	CB-CG-CD	7.37	130.77	111.60
1	C	102	THR	CA-CB-CG2	7.32	122.65	112.40
1	A	135	LEU	N-CA-CB	-7.32	95.77	110.40
1	C	135	LEU	N-CA-CB	-7.27	95.87	110.40
2	D	30	SER	O-C-N	-7.14	111.27	122.70
1	A	92	GLY	O-C-N	-7.08	111.38	122.70
2	D	111	GLY	O-C-N	-7.03	111.45	122.70
1	C	46	LEU	CA-CB-CG	6.99	131.37	115.30
1	A	49	TYR	CZ-CE2-CD2	6.99	126.09	119.80
1	C	137	ASN	CB-CA-C	-6.96	96.47	110.40
1	A	45	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	18	ARG	NE-CZ-NH2	-6.92	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ASP	CB-CG-OD1	6.91	124.52	118.30
2	D	94	TYR	CB-CA-C	-6.72	96.96	110.40
2	B	102	THR	N-CA-CB	-6.71	97.55	110.30
1	A	142	ARG	NE-CZ-NH1	-6.70	116.95	120.30
2	B	30	SER	N-CA-C	6.65	128.95	111.00
1	A	42	GLN	OE1-CD-NE2	6.64	137.17	121.90
1	A	45	ARG	N-CA-CB	-6.53	98.84	110.60
2	B	181	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	54	ARG	CG-CD-NE	-6.51	98.14	111.80
1	C	42	GLN	CB-CG-CD	-6.51	94.68	111.60
2	B	22	CYS	CA-CB-SG	6.46	125.63	114.00
2	D	71	VAL	CB-CA-C	-6.42	99.21	111.40
1	A	81	GLU	CA-CB-CG	6.40	127.49	113.40
2	B	29	PHE	CA-C-O	6.39	133.53	120.10
1	C	54	ARG	CG-CD-NE	-6.38	98.40	111.80
1	A	18	ARG	CD-NE-CZ	6.37	132.51	123.60
2	D	214	ASN	CA-C-O	-6.37	106.72	120.10
1	A	42	GLN	CB-CG-CD	-6.36	95.06	111.60
1	A	56	THR	CB-CA-C	-6.34	94.47	111.60
1	C	94	SER	CB-CA-C	-6.34	98.06	110.10
1	C	199	GLN	CA-C-N	6.32	128.83	116.20
2	B	174	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	D	19	SER	N-CA-CB	-6.21	101.18	110.50
2	B	26	GLY	O-C-N	-6.18	112.69	123.20
2	B	174	ARG	CD-NE-CZ	6.17	132.24	123.60
2	B	1	GLU	CG-CD-OE1	-6.14	106.01	118.30
2	D	38	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	42	GLN	O-C-N	6.13	132.51	122.70
1	C	49	TYR	CZ-CE2-CD2	6.12	125.31	119.80
2	B	97	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	B	74	SER	N-CA-CB	-6.05	101.43	110.50
1	C	213	GLU	CA-CB-CG	6.04	126.69	113.40
1	A	90	GLN	CA-CB-CG	6.03	126.66	113.40
2	B	110	TRP	O-C-N	-5.97	113.05	123.20
2	B	97	ARG	CA-CB-CG	5.95	126.50	113.40
2	D	110	TRP	O-C-N	-5.88	113.20	123.20
2	D	30	SER	N-CA-C	5.88	126.88	111.00
1	A	18	ARG	NH1-CZ-NH2	5.81	125.79	119.40
2	B	214	ASN	CA-C-N	5.81	127.81	116.20
2	D	151	GLN	OE1-CD-NE2	5.80	135.24	121.90
2	D	1	GLU	CG-CD-OE1	-5.79	106.72	118.30
1	C	91	TYR	CB-CG-CD2	5.77	124.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	218	GLU	CA-CB-CG	5.77	126.08	113.40
2	B	94	TYR	CB-CA-C	-5.76	98.87	110.40
2	D	97	ARG	CA-CB-CG	5.74	126.03	113.40
2	B	71	VAL	CB-CA-C	-5.71	100.56	111.40
1	A	137	ASN	CB-CA-C	-5.69	99.03	110.40
2	B	96	ALA	N-CA-CB	-5.68	102.15	110.10
1	C	88	CYS	CA-CB-SG	5.65	124.18	114.00
1	C	56	THR	CB-CA-C	-5.65	96.34	111.60
2	D	152	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	B	181	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	B	211	GLN	CA-CB-CG	5.64	125.81	113.40
1	A	36	TYR	CZ-CE2-CD2	5.62	124.86	119.80
1	C	91	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	C	70	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	46	LEU	CA-CB-CG	5.61	128.20	115.30
2	B	23	ALA	CB-CA-C	-5.60	101.70	110.10
1	C	5	THR	CA-CB-CG2	5.56	120.19	112.40
2	D	59	TYR	CB-CG-CD2	5.56	124.33	121.00
2	B	30	SER	O-C-N	-5.53	113.85	122.70
2	B	1	GLU	CA-C-O	-5.50	108.55	120.10
2	B	93	TYR	CB-CG-CD1	5.47	124.28	121.00
1	A	55	ALA	CA-C-O	-5.46	108.62	120.10
2	D	3	GLN	N-CA-CB	5.46	120.44	110.60
1	C	36	TYR	CD1-CE1-CZ	5.46	124.72	119.80
2	B	72	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	54	ARG	N-CA-CB	-5.45	100.79	110.60
1	C	42	GLN	CG-CD-NE2	-5.43	103.67	116.70
2	B	66	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	21	LEU	CB-CG-CD2	5.40	120.18	111.00
2	B	181	ARG	CA-CB-CG	5.40	125.28	113.40
1	C	165	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	A	165	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	203	SER	N-CA-CB	5.39	118.59	110.50
2	D	79	SER	CA-CB-OG	-5.38	96.68	111.20
2	D	151	GLN	CG-CD-OE1	-5.38	110.85	121.60
2	B	62	SER	O-C-N	-5.37	114.11	122.70
1	C	75	ILE	N-CA-C	-5.34	96.58	111.00
2	D	97	ARG	N-CA-CB	-5.34	100.99	110.60
2	B	112	GLN	CB-CG-CD	5.34	125.47	111.60
2	B	27	GLY	O-C-N	-5.30	114.22	122.70
1	A	60	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	C	211	ARG	NE-CZ-NH1	5.28	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	LEU	CA-CB-CG	5.28	127.43	115.30
1	A	45	ARG	CD-NE-CZ	-5.24	116.27	123.60
2	D	112	GLN	CG-CD-OE1	-5.23	111.13	121.60
2	D	37	ILE	CA-C-O	-5.21	109.16	120.10
1	C	38	GLN	N-CA-CB	5.21	119.97	110.60
2	B	29	PHE	CB-CG-CD1	5.20	124.44	120.80
1	C	142	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	C	17	GLU	OE1-CD-OE2	5.17	129.50	123.30
2	B	216	ASN	O-C-N	-5.16	114.44	122.70
2	D	106	TYR	CG-CD1-CE1	-5.16	117.17	121.30
2	D	174	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	45	ARG	CD-NE-CZ	-5.15	116.40	123.60
2	D	93	TYR	CA-C-N	5.15	128.52	117.20
1	A	46	LEU	CA-C-O	-5.13	109.33	120.10
1	C	211	ARG	CD-NE-CZ	5.13	130.78	123.60
2	D	106	TYR	CG-CD2-CE2	-5.11	117.21	121.30
1	A	77	ARG	CG-CD-NE	5.10	122.51	111.80
1	A	199	GLN	CA-C-N	5.09	126.38	116.20
2	D	158	ILE	CB-CA-C	5.08	121.77	111.60
1	C	96	LEU	CA-C-N	5.07	128.36	117.20
2	D	210	VAL	CB-CA-C	-5.07	101.76	111.40
2	D	202	THR	C-N-CA	5.06	134.36	121.70
1	C	21	LEU	CB-CG-CD2	5.06	119.60	111.00
2	B	5	GLN	CB-CA-C	-5.05	100.31	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	302	FUC	C1
3	D	302	FUC	C1

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASN	Mainchain
1	A	60	ASP	Mainchain
1	C	151	ASP	Mainchain
1	C	5	THR	Mainchain
1	C	94	SER	Mainchain

## 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	1638	0	1586	39	0
1	C	1638	0	1586	39	1
2	B	1608	0	1550	44	1
2	D	1608	0	1550	56	0
3	B	24	0	22	0	0
3	D	24	0	22	1	0
All	All	6540	0	6316	172	1

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 13.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASN:HB3	1:C:138:ASN:HD22	1.28	0.98
1:A:137:ASN:HB3	1:A:138:ASN:HD22	1.28	0.93
1:C:79:GLU:HG3	1:C:80:PRO:HD2	1.64	0.80
1:A:79:GLU:HG3	1:A:80:PRO:HD2	1.65	0.79
2:B:18:LEU:HD12	2:B:19:SER:N	2.03	0.73
2:D:97:ARG:HD3	2:D:98:PRO:O	1.91	0.69
2:B:75:LYS:HB2	2:B:77:GLN:HG3	1.73	0.69
2:B:97:ARG:HD3	2:B:98:PRO:O	1.93	0.68
1:C:119:PRO:HG3	2:D:134:CYS:HB2	1.75	0.68
1:A:197:THR:HG22	1:A:204:PRO:HG3	1.76	0.67
2:B:146:VAL:HG12	2:B:191:VAL:HG23	1.77	0.65
1:A:149:LYS:HE3	1:A:154:LEU:HD23	1.80	0.64
2:D:90:THR:HG23	2:D:117:THR:HA	1.80	0.64
2:D:214:ASN:HD22	2:D:214:ASN:H	1.45	0.64
2:D:146:VAL:HG12	2:D:191:VAL:HG23	1.80	0.63
2:D:1:GLU:N	2:D:1:GLU:CD	2.51	0.63
1:C:125:LEU:HD22	1:C:183:LYS:HG3	1.78	0.63
1:C:137:ASN:HB3	1:C:138:ASN:ND2	2.09	0.63
2:B:90:THR:HG23	2:B:117:THR:HA	1.82	0.61
1:C:79:GLU:HG3	1:C:80:PRO:CD	2.32	0.60
2:D:203:ASP:HB2	3:D:302:FUC:O4	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLU:CD	2:B:1:GLU:N	2.55	0.59
1:A:8:PRO:O	1:A:102:THR:HB	2.02	0.59
2:B:154:LEU:HD12	2:B:155:PRO:HA	1.85	0.59
2:D:6:GLN:H	2:D:112:GLN:HE22	1.51	0.59
2:D:18:LEU:HD12	2:D:19:SER:N	2.18	0.59
1:A:193:ALA:HB2	1:A:208:SER:HB3	1.85	0.58
1:A:79:GLU:HG3	1:A:80:PRO:CD	2.31	0.58
2:D:8:GLY:HA3	2:D:20:LEU:HD23	1.85	0.58
1:A:77:ARG:HH11	1:A:77:ARG:HB2	1.68	0.58
1:A:7:SER:HA	1:A:8:PRO:C	2.23	0.57
2:B:72:ASP:OD1	2:B:74:SER:HB3	2.04	0.57
2:D:6:GLN:HE22	2:D:94:TYR:HA	1.69	0.57
2:D:1:GLU:N	2:D:1:GLU:OE1	2.37	0.57
1:A:125:LEU:HD22	1:A:183:LYS:HG3	1.86	0.57
2:D:1:GLU:H3	2:D:1:GLU:CD	2.08	0.57
2:B:112:GLN:CD	2:B:112:GLN:H	2.08	0.56
2:D:212:HIS:CG	2:D:213:PRO:HD2	2.40	0.56
1:C:6:GLN:HB3	1:C:102:THR:HG22	1.87	0.56
2:B:71:VAL:HG12	2:B:78:PHE:HB3	1.87	0.56
1:C:193:ALA:HB2	1:C:208:SER:HB3	1.87	0.56
1:C:197:THR:HG22	1:C:204:PRO:HG3	1.86	0.56
2:B:18:LEU:HD11	2:B:20:LEU:HG	1.87	0.56
2:D:144:VAL:N	2:D:193:LEU:O	2.39	0.56
1:A:137:ASN:HB3	1:A:138:ASN:ND2	2.11	0.55
1:C:153:ALA:O	1:C:154:LEU:C	2.45	0.55
2:B:1:GLU:CD	2:B:1:GLU:H3	2.09	0.55
1:C:7:SER:HA	1:C:8:PRO:C	2.28	0.54
1:C:149:LYS:HE3	1:C:154:LEU:HD23	1.89	0.54
1:C:13:LEU:HD12	1:C:19:ALA:HB2	1.90	0.54
1:A:155:GLN:HA	1:A:155:GLN:NE2	2.22	0.54
1:C:36:TYR:HE1	1:C:89:GLN:HE21	1.56	0.54
1:C:140:TYR:CG	1:C:141:PRO:HA	2.43	0.53
2:D:4:LEU:O	2:D:112:GLN:OE1	2.25	0.53
2:B:6:GLN:H	2:B:112:GLN:HE22	1.57	0.53
2:D:18:LEU:HD11	2:D:20:LEU:HG	1.89	0.53
2:D:71:VAL:HG12	2:D:78:PHE:HB3	1.91	0.53
2:D:34:TRP:CH2	2:D:97:ARG:HG3	2.43	0.53
1:A:212:GLY:O	1:A:214:CYS:N	2.42	0.53
1:C:209:PHE:HB2	2:D:134:CYS:SG	2.50	0.52
2:B:6:GLN:HE22	2:B:94:TYR:HA	1.74	0.52
2:D:102:THR:O	2:D:102:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:HE1	1:A:89:GLN:HE21	1.57	0.52
2:D:212:HIS:CE1	2:D:214:ASN:HD22	2.28	0.52
2:D:13:LYS:O	2:D:16:GLU:HG3	2.10	0.52
2:B:18:LEU:HD22	2:B:116:VAL:HG11	1.93	0.51
2:D:122:SER:O	2:D:123:ALA:C	2.47	0.51
2:D:12:LEU:HD11	2:D:18:LEU:HB2	1.93	0.51
2:D:67:VAL:HG23	2:D:82:LEU:HD12	1.93	0.51
2:D:170:ILE:HD11	2:D:206:VAL:CG2	2.40	0.51
2:D:154:LEU:HD12	2:D:155:PRO:HA	1.91	0.51
2:B:6:GLN:HE21	2:B:111:GLY:HA3	1.77	0.50
2:D:206:VAL:HB	2:D:223:LEU:HD21	1.93	0.50
1:C:123:GLU:OE2	2:D:219:LYS:HE3	2.11	0.50
1:A:4:LEU:HD23	1:A:25:ALA:HA	1.94	0.50
2:D:167:ASN:O	2:D:168:SER:HB3	2.12	0.50
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.44	0.50
2:D:6:GLN:HE21	2:D:111:GLY:HA3	1.77	0.49
1:A:140:TYR:CG	1:A:141:PRO:HA	2.47	0.49
2:B:144:VAL:N	2:B:193:LEU:O	2.45	0.49
1:C:8:PRO:O	1:C:102:THR:HB	2.13	0.49
1:A:193:ALA:CB	1:A:208:SER:HB3	2.43	0.49
1:C:175:LEU:HD23	1:C:176:SER:N	2.28	0.49
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.95	0.49
1:C:155:GLN:NE2	1:C:155:GLN:HA	2.27	0.48
2:D:112:GLN:H	2:D:112:GLN:CD	2.10	0.48
1:A:153:ALA:O	1:A:154:LEU:C	2.51	0.48
2:B:1:GLU:N	2:B:1:GLU:OE1	2.45	0.48
2:D:123:ALA:HA	2:D:154:LEU:O	2.14	0.48
2:B:67:VAL:HG23	2:B:82:LEU:CD1	2.43	0.48
1:A:28:SER:HA	1:A:69:THR:HG22	1.95	0.48
1:C:77:ARG:HB2	1:C:77:ARG:HH11	1.78	0.48
2:B:212:HIS:CE1	2:B:214:ASN:HD22	2.32	0.48
2:D:67:VAL:HG23	2:D:82:LEU:CD1	2.43	0.47
1:C:162:SER:OG	2:D:177:PRO:HD2	2.15	0.47
2:D:212:HIS:CD2	2:D:213:PRO:HD2	2.48	0.47
1:A:203:SER:HB2	1:A:204:PRO:HD2	1.96	0.47
1:C:77:ARG:HH11	1:C:77:ARG:CB	2.27	0.47
2:D:66:ARG:NH2	2:D:89:ASP:OD2	2.44	0.47
1:A:77:ARG:HH11	1:A:77:ARG:CB	2.27	0.47
1:C:96:LEU:HD12	2:D:47:TRP:CE2	2.50	0.47
1:C:193:ALA:CB	1:C:208:SER:HB3	2.45	0.46
1:C:160:GLN:HB3	2:D:179:VAL:HG11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLY:O	1:A:67:SER:HB3	2.15	0.46
2:D:160:PHE:CD2	2:D:210:VAL:HG12	2.51	0.46
2:D:34:TRP:CZ3	2:D:97:ARG:HG3	2.51	0.46
2:D:214:ASN:ND2	2:D:214:ASN:N	2.63	0.46
1:A:212:GLY:O	1:A:213:GLU:C	2.54	0.46
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.37	0.45
2:B:212:HIS:HE1	2:B:214:ASN:HD22	1.63	0.45
1:A:6:GLN:HB3	1:A:102:THR:HG22	1.98	0.45
2:D:75:LYS:HB2	2:D:77:GLN:HG3	1.98	0.45
2:B:165:LYS:HE3	2:B:204:GLU:OE2	2.15	0.45
2:B:125:ALA:HB1	2:B:126:PRO:HD2	1.98	0.45
2:D:202:THR:HB	2:D:203:ASP:H	1.58	0.45
2:B:214:ASN:H	2:B:214:ASN:HD22	1.64	0.45
2:B:174:ARG:HH11	2:B:174:ARG:HG2	1.80	0.45
2:B:163:LYS:NZ	2:B:169:ASP:OD1	2.47	0.45
2:D:174:ARG:HG2	2:D:174:ARG:HH11	1.82	0.45
2:D:214:ASN:N	2:D:214:ASN:HD22	2.13	0.44
2:B:122:SER:O	2:B:123:ALA:C	2.55	0.44
2:B:34:TRP:CH2	2:B:97:ARG:HG3	2.51	0.44
1:A:31:ASN:HD21	1:A:67:SER:CB	2.30	0.44
2:D:166:ASN:O	2:D:167:ASN:C	2.55	0.44
1:A:37:GLN:OE1	1:A:45:ARG:NH1	2.50	0.43
1:A:203:SER:HB2	1:A:204:PRO:CD	2.49	0.43
1:C:4:LEU:HD23	1:C:25:ALA:HA	1.99	0.43
2:D:5:GLN:O	2:D:22:CYS:HA	2.18	0.43
1:C:140:TYR:CD1	1:C:141:PRO:HA	2.54	0.43
2:B:170:ILE:HD11	2:B:206:VAL:CG2	2.49	0.43
1:A:125:LEU:HA	1:A:125:LEU:HD23	1.91	0.43
1:A:31:ASN:HD21	1:A:67:SER:HB3	1.84	0.43
2:B:212:HIS:CG	2:B:213:PRO:HD2	2.53	0.43
1:C:210:ASN:O	1:C:211:ARG:C	2.57	0.43
1:C:28:SER:HA	1:C:69:THR:HG22	2.01	0.43
1:C:130:ALA:N	1:C:181:LEU:O	2.46	0.43
1:A:212:GLY:O	1:A:214:CYS:HB2	2.19	0.43
2:B:214:ASN:N	2:B:214:ASN:ND2	2.66	0.43
1:A:136:LEU:HD22	1:A:196:VAL:HG21	2.01	0.42
1:C:31:ASN:HD21	1:C:67:SER:HB3	1.84	0.42
2:B:18:LEU:HD12	2:B:18:LEU:C	2.39	0.42
2:B:164:TYR:CE2	2:B:170:ILE:HG12	2.54	0.42
2:D:97:ARG:HA	2:D:98:PRO:HD3	1.82	0.42
2:B:102:THR:HG23	2:B:102:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:HIS:HE1	2:D:214:ASN:HD22	1.67	0.42
1:A:130:ALA:N	1:A:181:LEU:O	2.43	0.42
2:B:67:VAL:HG23	2:B:82:LEU:HD12	2.03	0.41
2:D:75:LYS:O	2:D:76:ASN:HB2	2.20	0.41
1:C:198:HIS:O	1:C:199:GLN:C	2.58	0.41
2:B:60:ASN:OD1	2:B:61:PRO:HD2	2.20	0.41
2:B:97:ARG:HA	2:B:98:PRO:HD3	1.85	0.41
1:C:94:SER:HA	1:C:95:PRO:C	2.40	0.41
2:D:212:HIS:HE1	2:D:214:ASN:ND2	2.19	0.41
1:C:36:TYR:OH	1:C:89:GLN:NE2	2.54	0.41
2:D:165:LYS:O	2:D:167:ASN:N	2.54	0.41
1:A:167:ASP:OD1	1:A:169:LYS:N	2.50	0.41
1:A:105:GLU:HG2	1:A:106:ILE:N	2.36	0.41
2:B:51:ILE:HG13	2:B:57:THR:HG22	2.02	0.41
2:B:190:GLN:HE21	2:B:190:GLN:HB2	1.73	0.41
2:B:34:TRP:CZ3	2:B:97:ARG:HG3	2.56	0.41
1:A:28:SER:HA	1:A:68:GLY:O	2.21	0.41
2:B:132:VAL:HG12	2:B:224:PRO:HB3	2.02	0.41
2:D:18:LEU:HD22	2:D:116:VAL:HG11	2.02	0.40
1:A:107:LYS:HE2	1:A:107:LYS:HB3	1.93	0.40
2:D:146:VAL:HG22	2:D:221:VAL:HG11	2.04	0.40
1:C:203:SER:HB2	1:C:204:PRO:HD2	2.04	0.40
1:A:185:ASP:O	1:A:186:TYR:C	2.58	0.40
2:B:148:CYS:HB2	2:B:162:TRP:CZ2	2.57	0.40
1:C:136:LEU:HD22	1:C:196:VAL:HG21	2.03	0.40
1:A:198:HIS:O	1:A:199:GLN:C	2.59	0.40
1:C:7:SER:HB2	1:C:8:PRO:HA	2.04	0.40
1:C:96:LEU:HG	1:C:96:LEU:H	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:GLN:OE1	1:C:27:GLN:NE2[4_456]	2.14	0.06

## 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	213/215 (99%)	195 (92%)	15 (7%)	3 (1%)	14	40
1	C	213/215 (99%)	197 (92%)	15 (7%)	1 (0%)	34	67
2	B	203/232 (88%)	194 (96%)	6 (3%)	3 (2%)	13	38
2	D	203/232 (88%)	185 (91%)	16 (8%)	2 (1%)	19	50
All	All	832/894 (93%)	771 (93%)	52 (6%)	9 (1%)	17	47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLU
2	D	166	ASN
2	D	168	SER
1	A	51	ALA
1	A	154	LEU
2	B	121	GLY
2	B	167	ASN
1	C	154	LEU
2	B	91	ALA

### 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	185/185 (100%)	160 (86%)	25 (14%)	5	13
1	C	185/185 (100%)	159 (86%)	26 (14%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	180/201 (90%)	153 (85%)	27 (15%)	3	10
2	D	180/201 (90%)	154 (86%)	26 (14%)	4	11
All	All	730/772 (95%)	626 (86%)	104 (14%)	4	11

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	20	THR
1	A	21	LEU
1	A	33	LEU
1	A	46	LEU
1	A	56	THR
1	A	72	THR
1	A	77	ARG
1	A	78	LEU
1	A	89	GLN
1	A	102	THR
1	A	105	GLU
1	A	108	ARG
1	A	135	LEU
1	A	136	LEU
1	A	142	ARG
1	A	145	LYS
1	A	152	ASN
1	A	154	LEU
1	A	162	SER
1	A	176	SER
1	A	185	ASP
1	A	190	LYS
1	A	199	GLN
1	A	213	GLU
2	B	17	THR
2	B	18	LEU
2	B	30	SER
2	B	43	LYS
2	B	52	ASN
2	B	71	VAL
2	B	81	LYS
2	B	97	ARG
2	B	102	THR

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Mol	Chain	Res	Type
2	B	112	GLN
2	B	127	THR
2	B	133	SER
2	B	146	VAL
2	B	149	LEU
2	B	157	SER
2	B	158	ILE
2	B	171	SER
2	B	172	SER
2	B	173	THR
2	B	174	ARG
2	B	190	GLN
2	B	191	VAL
2	B	202	THR
2	B	204	GLU
2	B	206	VAL
2	B	214	ASN
2	B	220	ASN
1	C	5	THR
1	C	12	SER
1	C	20	THR
1	C	21	LEU
1	C	30(A)	SER
1	C	46	LEU
1	C	56	THR
1	C	72	THR
1	C	77	ARG
1	C	78	LEU
1	C	89	GLN
1	C	102	THR
1	C	105	GLU
1	C	108	ARG
1	C	135	LEU
1	C	136	LEU
1	C	142	ARG
1	C	145	LYS
1	C	152	ASN
1	C	154	LEU
1	C	162	SER
1	C	176	SER
1	C	190	LYS
1	C	199	GLN

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Mol	Chain	Res	Type
1	C	213	GLU
1	C	214	CYS
2	D	17	THR
2	D	18	LEU
2	D	30	SER
2	D	43	LYS
2	D	52	ASN
2	D	81	LYS
2	D	97	ARG
2	D	102	THR
2	D	112	GLN
2	D	127	THR
2	D	133	SER
2	D	146	VAL
2	D	149	LEU
2	D	157	SER
2	D	158	ILE
2	D	165	LYS
2	D	168	SER
2	D	171	SER
2	D	172	SER
2	D	173	THR
2	D	174	ARG
2	D	190	GLN
2	D	191	VAL
2	D	206	VAL
2	D	214	ASN
2	D	220	ASN

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	138	ASN
1	A	155	GLN
2	B	6	GLN
2	B	52	ASN
2	B	76	ASN
2	B	167	ASN
2	B	205	HIS
2	B	214	ASN
1	C	89	GLN

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Mol	Chain	Res	Type
1	C	138	ASN
1	C	155	GLN
1	C	199	GLN
2	D	6	GLN
2	D	52	ASN
2	D	76	ASN
2	D	112	GLN
2	D	167	ASN
2	D	205	HIS
2	D	214	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 ⓘ

4 carbohydrates 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	B	301	3,2	14,14,15	1.23	1 (7%)	15,19,21	1.86	4 (26%)
3	FUC	B	302	3	10,10,11	0.83	0	14,14,16	2.25	4 (28%)
3	NAG	D	301	3,2	14,14,15	1.38	2 (14%)	15,19,21	2.62	9 (60%)
3	FUC	D	302	3	10,10,11	0.64	0	14,14,16	1.49	2 (14%)

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	B	301	3,2	-	0/6/23/26	0/1/1/1
3	FUC	B	302	3	1/1/4/5	0/0/17/20	0/1/1/1
3	NAG	D	301	3,2	-	0/6/23/26	0/1/1/1
3	FUC	D	302	3	1/1/4/5	0/0/17/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAG	O7-C7	-3.52	1.15	1.23
3	D	301	NAG	O7-C7	-3.47	1.15	1.23
3	D	301	NAG	C1-C2	2.18	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	NAG	C4-C3-C2	-5.55	102.60	111.23
3	B	301	NAG	C4-C3-C2	-3.86	105.23	111.23
3	D	301	NAG	C6-C5-C4	-3.47	104.47	113.02
3	D	301	NAG	C2-N2-C7	-2.76	119.49	123.04
3	B	301	NAG	C6-C5-C4	-2.35	107.22	113.02
3	B	302	FUC	O2-C2-C1	-2.33	104.54	109.21
3	B	301	NAG	C3-C4-C5	-2.14	106.47	110.20
3	D	301	NAG	O7-C7-N2	-2.07	117.65	121.86
3	D	302	FUC	C1-O5-C5	2.60	116.39	112.38
3	B	302	FUC	O2-C2-C3	2.61	115.37	110.12
3	D	301	NAG	O4-C4-C3	2.64	116.29	110.34
3	D	301	NAG	C8-C7-N2	2.88	121.61	116.11
3	D	301	NAG	C3-C2-N2	2.98	117.70	110.56
3	D	301	NAG	O5-C5-C6	2.99	113.83	107.35
3	D	301	NAG	O6-C6-C5	3.24	122.05	111.33
3	D	302	FUC	O2-C2-C3	3.32	116.80	110.12
3	B	301	NAG	C2-N2-C7	3.42	127.44	123.04
3	B	302	FUC	C2-C3-C4	4.09	117.98	111.04
3	B	302	FUC	C1-C2-C3	5.94	116.57	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	302	FUC	C1
3	B	302	FUC	C1

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
3	D	302	FUC	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/215 (100%)	-0.82	0 <b>100</b> <b>100</b>	16, 39, 76, 94	0
1	C	215/215 (100%)	-0.78	2 (0%) <b>85</b> <b>80</b>	16, 39, 76, 93	0
2	B	209/232 (90%)	-0.60	2 (0%) <b>84</b> <b>78</b>	17, 37, 90, 100	0
2	D	209/232 (90%)	-0.63	3 (1%) <b>78</b> <b>71</b>	17, 37, 90, 100	0
All	All	848/894 (94%)	-0.71	7 (0%) <b>87</b> <b>82</b>	16, 39, 85, 100	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	202	THR	4.4
1	C	214	CYS	3.0
2	D	202	THR	2.9
2	B	204	GLU	2.4
1	C	190	LYS	2.3
2	D	167	ASN	2.2
2	D	134	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FUC	D	302	10/11	0.85	0.36	-	100,100,100,100	0
3	NAG	D	301	14/15	0.80	0.23	-	98,99,100,100	0
3	FUC	B	302	10/11	0.93	0.25	-	99,100,100,100	0
3	NAG	B	301	14/15	0.78	0.28	-	99,99,100,100	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.