Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:43 PM BST

PDB ID	:	2FBJ
Title	:	REFINED CRYSTAL STRUCTURE OF THE GALACTAN-BINDING IMMUNOGLOBULIN FAB J539 AT 1.95-ANGSTROMS RESOLUTION
Authors	:	Bhat, T.N.; Padlan, E.A.; Davies, D.R.
Deposited on	:	1989-08-18
Resolution	:	1.95 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 ①) were used in the production of this report:

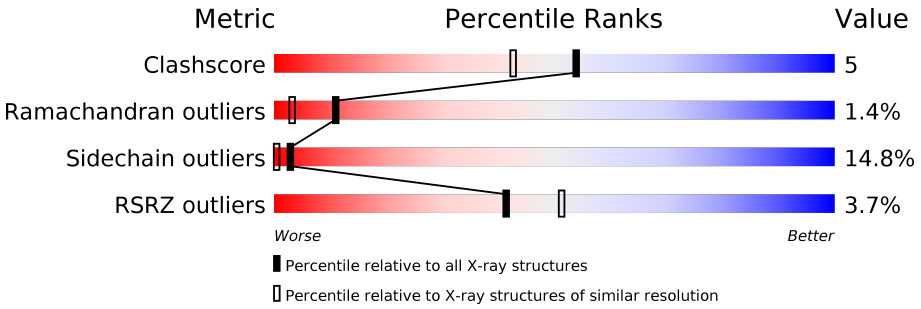
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	L	213	4%, 64%, 26%, 7%
2	H	220	3%, 67%, 24%, 7%
3	A	2	50%, 50%
4	B	3	33%, 67%

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
4	FUC	B	3	X	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3761 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 IGA-KAPPA J539 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1636	1024	270	335	7			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ILE	LEU	conflict	GB 437099
L	11	THR	MET	conflict	GB 437099
L	12	ALA	SER	conflict	GB 437099
L	15	LEU	PRO	conflict	GB 437099
L	?	-	ARG	deletion	GB 437099
L	?	-	PHE	deletion	GB 437099
L	41	THR	ALA	conflict	GB 437099
L	45	PRO	LEU	conflict	GB 437099
L	49	GLU	ASP	conflict	GB 437099
L	50	ILE	THR	conflict	GB 437099
L	55	SER	PRO	conflict	GB 437099
L	75	ASN	SER	conflict	GB 437099
L	76	THR	SER	conflict	GB 437099
L	84	ILE	SER	conflict	GB 437099
L	86	TYR	PHE	conflict	GB 437099
L	88	GLN	HIS	conflict	GB 437099
L	?	-	SER	deletion	GB 437099
L	91	THR	SER	conflict	GB 437099
L	95	ILE	-	insertion	GB 437099

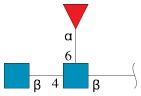
- Molecule 2 is a protein called IGA-KAPPA J539 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1683	1067	279	327	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

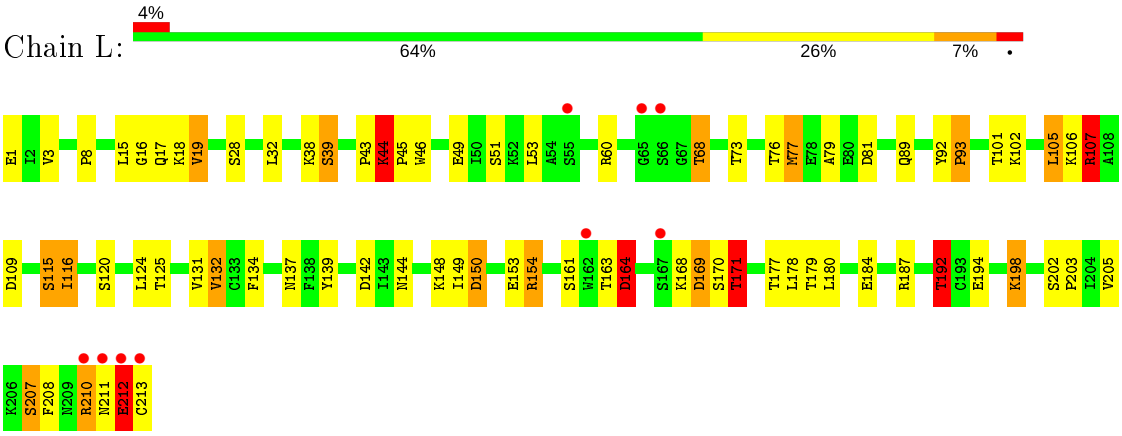
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	193	Total	O	0	0
			193	193		
6	H	182	Total	O	0	0
			182	182		

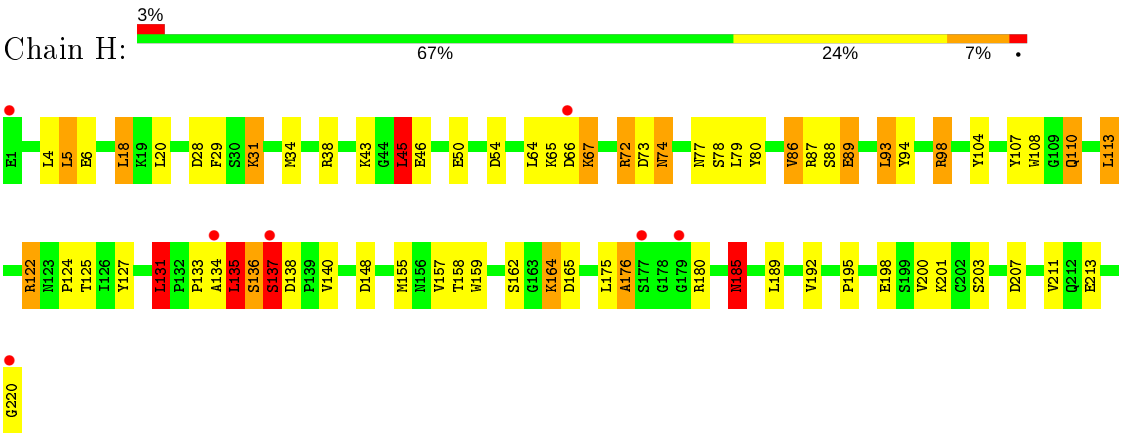
3 Residue-property plots (i)

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: IGA-KAPPA J539 FAB (LIGHT CHAIN)



• Molecule 2: IGA-KAPPA J539 FAB (HEAVY CHAIN)



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.02Å 74.29Å 131.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.95 8.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.95) 72.9 (8.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.194 , (Not available) 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3761	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	L	0.76	0/1674	2.03	59/2277 (2.6%)
2	H	0.72	0/1728	2.01	69/2353 (2.9%)
All	All	0.74	0/3402	2.02	128/4630 (2.8%)

There are no bond length outliers.

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	180	ARG	NE-CZ-NH1	15.27	127.94	120.30
1	L	210	ARG	CD-NE-CZ	14.98	144.57	123.60
1	L	154	ARG	NE-CZ-NH1	14.46	127.53	120.30
2	H	38	ARG	NE-CZ-NH2	-12.50	114.05	120.30
2	H	87	ARG	NE-CZ-NH1	12.09	126.34	120.30
2	H	38	ARG	NE-CZ-NH1	12.01	126.30	120.30
2	H	131	LEU	CA-CB-CG	11.73	142.29	115.30
1	L	210	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	L	107	ARG	CA-CB-CG	11.20	138.04	113.40
2	H	98	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	L	163	THR	C-N-CA	9.81	146.23	121.70
1	L	169	ASP	CB-CG-OD1	9.36	126.73	118.30
1	L	187	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	L	68	THR	CA-CB-CG2	9.13	125.19	112.40
1	L	212	GLU	CA-CB-CG	9.07	133.36	113.40
1	L	169	ASP	CB-CG-OD2	-8.84	110.34	118.30
2	H	136	SER	C-N-CA	8.59	143.16	121.70
1	L	142	ASP	CB-CG-OD2	-8.39	110.75	118.30
2	H	98	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	L	109	ASP	CB-CG-OD2	8.11	125.60	118.30
1	L	210	ARG	CA-CB-CG	8.07	131.16	113.40
2	H	98	ARG	CD-NE-CZ	8.04	134.85	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	163	THR	CA-CB-CG2	8.01	123.62	112.40
2	H	80	TYR	CB-CG-CD2	-7.96	116.23	121.00
2	H	4	LEU	CA-CB-CG	7.89	133.46	115.30
2	H	93	LEU	CA-CB-CG	7.88	133.43	115.30
1	L	107	ARG	CD-NE-CZ	7.80	134.52	123.60
1	L	134	PHE	CB-CG-CD2	7.67	126.17	120.80
1	L	134	PHE	CB-CG-CD1	-7.64	115.45	120.80
2	H	98	ARG	CA-CB-CG	7.50	129.89	113.40
1	L	187	ARG	CD-NE-CZ	7.41	133.97	123.60
2	H	192	VAL	CA-CB-CG1	7.40	122.00	110.90
1	L	60	ARG	CD-NE-CZ	7.33	133.86	123.60
2	H	158	THR	CA-CB-CG2	7.31	122.64	112.40
1	L	180	LEU	CA-CB-CG	7.28	132.05	115.30
2	H	122	ARG	CD-NE-CZ	7.23	133.72	123.60
2	H	88	SER	C-N-CA	7.20	139.71	121.70
2	H	86	VAL	CB-CA-C	7.17	125.03	111.40
2	H	72	ARG	NE-CZ-NH2	7.11	123.85	120.30
2	H	113	LEU	CA-CB-CG	6.94	131.27	115.30
2	H	185	ASN	CB-CA-C	6.91	124.23	110.40
2	H	45	LEU	CA-CB-CG	6.84	131.03	115.30
2	H	86	VAL	CA-CB-CG1	6.83	121.15	110.90
2	H	137	SER	C-N-CA	6.64	138.31	121.70
2	H	80	TYR	CB-CG-CD1	6.64	124.98	121.00
1	L	198	LYS	CA-CB-CG	6.61	127.93	113.40
2	H	189	LEU	CA-CB-CG	6.60	130.47	115.30
1	L	125	THR	CA-CB-CG2	6.56	121.58	112.40
1	L	142	ASP	CB-CG-OD1	6.53	124.18	118.30
2	H	6	GLU	OE1-CD-OE2	-6.53	115.46	123.30
2	H	89	GLU	CA-CB-CG	6.52	127.73	113.40
2	H	73	ASP	CB-CG-OD2	-6.45	112.50	118.30
2	H	31	LYS	CA-CB-CG	6.41	127.50	113.40
1	L	171	THR	N-CA-CB	-6.39	98.17	110.30
1	L	205	VAL	CA-CB-CG1	6.37	120.46	110.90
2	H	74	ASN	N-CA-CB	6.35	122.03	110.60
2	H	87	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	L	53	LEU	CA-CB-CG	6.35	129.90	115.30
1	L	109	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	L	150	ASP	CB-CG-OD2	6.30	123.97	118.30
2	H	5	LEU	CA-CB-CG	6.26	129.70	115.30
2	H	175	LEU	CA-CB-CG	6.25	129.68	115.30
2	H	18	LEU	CA-CB-CG	6.24	129.65	115.30
1	L	44	LYS	CA-CB-CG	6.22	127.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	19	VAL	CA-CB-CG2	6.21	120.22	110.90
2	H	50	GLU	CG-CD-OE2	-6.13	106.04	118.30
2	H	73	ASP	CB-CG-OD1	6.12	123.81	118.30
1	L	17	GLN	CA-CB-CG	6.12	126.85	113.40
1	L	3	VAL	CA-CB-CG1	6.10	120.05	110.90
1	L	153	GLU	OE1-CD-OE2	6.06	130.57	123.30
1	L	131	VAL	CA-CB-CG2	6.05	119.98	110.90
1	L	184	GLU	CG-CD-OE1	6.05	130.39	118.30
1	L	107	ARG	N-CA-CB	-5.94	99.91	110.60
2	H	87	ARG	CD-NE-CZ	5.94	131.92	123.60
1	L	205	VAL	CG1-CB-CG2	-5.90	101.46	110.90
1	L	168	LYS	C-N-CA	5.89	136.43	121.70
2	H	54	ASP	CB-CA-C	5.87	122.13	110.40
2	H	104	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	L	77	MET	CA-CB-CG	5.71	123.01	113.30
2	H	107	TYR	CB-CG-CD2	-5.68	117.59	121.00
2	H	198	GLU	CG-CD-OE1	5.67	129.64	118.30
1	L	163	THR	CA-C-O	5.66	131.98	120.10
1	L	101	THR	CA-CB-CG2	5.65	120.32	112.40
1	L	164	ASP	CA-CB-CG	5.62	125.76	113.40
2	H	87	ARG	CA-CB-CG	5.60	125.71	113.40
1	L	51	SER	N-CA-CB	-5.59	102.11	110.50
2	H	140	VAL	CA-CB-CG1	5.58	119.28	110.90
1	L	132	VAL	CA-CB-CG1	5.58	119.27	110.90
2	H	207	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	L	115	SER	N-CA-CB	5.53	118.79	110.50
1	L	15	LEU	CB-CA-C	5.52	120.69	110.20
1	L	192	THR	CA-CB-CG2	5.52	120.12	112.40
1	L	49	GLU	CA-C-O	5.50	131.65	120.10
2	H	29	PHE	CB-CG-CD2	-5.49	116.95	120.80
2	H	73	ASP	CB-CA-C	5.49	121.38	110.40
2	H	157	VAL	CA-CB-CG2	5.49	119.13	110.90
2	H	113	LEU	CB-CG-CD2	5.47	120.29	111.00
1	L	81	ASP	CB-CG-OD1	5.46	123.22	118.30
1	L	93	PRO	N-CA-CB	-5.42	96.64	102.60
2	H	176	ALA	CB-CA-C	5.40	118.20	110.10
2	H	64	LEU	CA-CB-CG	5.38	127.66	115.30
1	L	164	ASP	O-C-N	-5.35	114.14	122.70
2	H	28	ASP	CA-CB-CG	5.35	125.17	113.40
2	H	125	THR	N-CA-CB	5.29	120.35	110.30
2	H	46	GLU	CG-CD-OE1	5.23	128.75	118.30
2	H	45	LEU	CB-CG-CD1	5.22	119.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	110	GLN	CB-CG-CD	5.22	125.18	111.60
1	L	179	THR	N-CA-CB	5.22	120.21	110.30
1	L	38	LYS	C-N-CA	5.21	134.73	121.70
2	H	28	ASP	CB-CA-C	5.21	120.82	110.40
2	H	86	VAL	N-CA-CB	-5.21	100.05	111.50
2	H	94	TYR	CB-CG-CD1	5.20	124.12	121.00
2	H	20	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	L	73	THR	CA-CB-CG2	5.15	119.61	112.40
2	H	108	TRP	CA-CB-CG	5.15	123.48	113.70
1	L	184	GLU	CA-CB-CG	5.14	124.71	113.40
2	H	67	LYS	CA-CB-CG	5.14	124.72	113.40
2	H	131	LEU	CB-CA-C	5.11	119.92	110.20
2	H	200	VAL	CA-CB-CG2	5.11	118.57	110.90
2	H	89	GLU	CB-CG-CD	5.10	127.97	114.20
1	L	154	ARG	CD-NE-CZ	5.09	130.72	123.60
1	L	124	LEU	CA-CB-CG	5.06	126.94	115.30
2	H	180	ARG	NH1-CZ-NH2	-5.06	113.84	119.40
2	H	134	ALA	CB-CA-C	5.04	117.67	110.10
2	H	127	TYR	CB-CG-CD1	5.04	124.03	121.00
1	L	139	TYR	CB-CG-CD2	5.04	124.02	121.00
2	H	198	GLU	CA-CB-CG	5.04	124.48	113.40
1	L	212	GLU	CB-CA-C	5.02	120.44	110.40

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	L	1636	0	1578	24	0
2	H	1683	0	1625	12	0
3	A	28	0	23	1	0
4	B	38	0	33	2	0
5	H	1	0	0	0	0
6	H	182	0	0	3	3
6	L	193	0	0	7	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3761	0	3259	35	4

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 5.

All (35) 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:L:18:LYS:HE2	6:L:372:HOH:O	0.90	1.07
2:H:220:GLY:HA3	6:H:398:HOH:O	1.61	1.01
1:L:194:GLU:OE2	6:L:382:HOH:O	1.96	0.84
1:L:150:ASP:OD1	6:L:404:HOH:O	1.96	0.82
1:L:192:THR:HB	1:L:207:SER:HB2	1.65	0.78
1:L:16:GLY:HA2	1:L:76:THR:HG23	1.66	0.78
1:L:93:PRO:HG3	3:A:1:NAG:H3	1.72	0.70
2:H:203:SER:HB3	4:B:1:NAG:H81	1.75	0.68
1:L:137:ASN:HD22	1:L:171:THR:HG21	1.62	0.65
2:H:164:LYS:NZ	6:H:394:HOH:O	2.30	0.64
1:L:107:ARG:HG3	1:L:170:SER:HB2	1.79	0.64
1:L:79:ALA:HA	1:L:105:LEU:HD13	1.81	0.62
2:H:159:TRP:HE1	2:H:185:ASN:HD21	1.49	0.60
2:H:220:GLY:CA	6:H:398:HOH:O	2.33	0.60
2:H:201:LYS:HE2	2:H:213:GLU:HB3	1.85	0.58
1:L:148:LYS:HB2	1:L:192:THR:HG23	1.87	0.57
2:H:124:PRO:HG3	2:H:155:MET:HE1	1.85	0.57
2:H:131:LEU:HD12	2:H:135:LEU:HD23	1.88	0.55
1:L:149:ILE:HD11	1:L:178:LEU:HD21	1.87	0.55
2:H:159:TRP:HE1	2:H:185:ASN:ND2	2.04	0.55
1:L:212:GLU:HG2	1:L:213:CYS:H	1.72	0.55
2:H:211:VAL:HG11	4:B:1:NAG:H82	1.88	0.54
1:L:132:VAL:HG22	1:L:177:THR:HG23	1.91	0.53
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.92	0.51
1:L:8:PRO:HA	6:L:392:HOH:O	2.12	0.50
1:L:43:PRO:HG2	2:H:45:LEU:HD11	1.95	0.49
1:L:46:TRP:HH2	6:L:374:HOH:O	1.97	0.48
1:L:137:ASN:HD22	1:L:171:THR:CG2	2.27	0.46
1:L:77:MET:HG3	1:L:105:LEU:HD12	2.00	0.43
1:L:44:LYS:HA	1:L:45:PRO:HD3	1.85	0.43
1:L:116:ILE:HD12	1:L:208:PHE:CD1	2.54	0.43
1:L:202:SER:HA	1:L:203:PRO:HD3	1.83	0.42
1:L:164:ASP:HB2	6:L:379:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:92:TYR:HA	1:L:93:PRO:HA	1.94	0.41
1:L:154:ARG:HD2	6:L:255:HOH:O	2.21	0.40

All (4) 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)
6:L:406:HOH:O	6:H:402:HOH:O[3_545]	1.37	0.83
6:L:404:HOH:O	6:L:405:HOH:O[4_545]	1.42	0.78
6:L:400:HOH:O	6:H:404:HOH:O[3_545]	1.69	0.51
6:L:401:HOH:O	6:H:403:HOH:O[3_545]	2.09	0.11

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	L	211/213 (99%)	202 (96%)	8 (4%)	1 (0%)	29 17
2	H	218/220 (99%)	202 (93%)	11 (5%)	5 (2%)	6 1
All	All	429/433 (99%)	404 (94%)	19 (4%)	6 (1%)	11 3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	39	SER
2	H	74	ASN
2	H	137	SER
2	H	176	ALA
2	H	135	LEU
2	H	138	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	186/186 (100%)	160 (86%)	26 (14%)	3 0
2	H	186/186 (100%)	157 (84%)	29 (16%)	2 0
All	All	372/372 (100%)	317 (85%)	55 (15%)	3 0

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLU
1	L	19	VAL
1	L	28	SER
1	L	32	LEU
1	L	39	SER
1	L	44	LYS
1	L	68	THR
1	L	89	GLN
1	L	102	LYS
1	L	105	LEU
1	L	106	LYS
1	L	107	ARG
1	L	115	SER
1	L	116	ILE
1	L	120	SER
1	L	144	ASN
1	L	161	SER
1	L	164	ASP
1	L	169	ASP
1	L	171	THR
1	L	192	THR
1	L	198	LYS
1	L	207	SER
1	L	210	ARG
1	L	211	ASN
1	L	212	GLU
2	H	5	LEU

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Mol	Chain	Res	Type
2	H	18	LEU
2	H	31	LYS
2	H	43	LYS
2	H	45	LEU
2	H	65	LYS
2	H	66	ASP
2	H	67	LYS
2	H	72	ARG
2	H	77	ASN
2	H	78	SER
2	H	86	VAL
2	H	89	GLU
2	H	93	LEU
2	H	98	ARG
2	H	110	GLN
2	H	113	LEU
2	H	122	ARG
2	H	131	LEU
2	H	133	PRO
2	H	135	LEU
2	H	136	SER
2	H	137	SER
2	H	148	ASP
2	H	162	SER
2	H	164	LYS
2	H	165	ASP
2	H	185	ASN
2	H	195	PRO

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

Mol	Chain	Res	Type
1	L	17	GLN
1	L	89	GLN
1	L	137	ASN
2	H	185	ASN
2	H	206	HIS

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)

5 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	A	1	3,2	14,14,15	0.94	0	17,19,21	4.84	8 (47%)
3	NAG	A	2	3	14,14,15	0.96	0	17,19,21	5.38	7 (41%)
4	NAG	B	1	2,4	14,14,15	0.98	0	17,19,21	3.83	7 (41%)
4	NAG	B	2	4	14,14,15	0.93	0	17,19,21	5.57	7 (41%)
4	FUC	B	3	4	10,10,11	0.89	0	14,14,16	1.33	1 (7%)

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	A	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	A	2	3	-	5/6/23/26	0/1/1/1
4	NAG	B	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	B	2	4	-	5/6/23/26	0/1/1/1
4	FUC	B	3	4	2/2/4/5	-	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2	NAG	C2-N2-C7	17.09	147.24	122.90
3	A	1	NAG	C2-N2-C7	16.90	146.97	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2	NAG	C2-N2-C7	16.50	146.39	122.90
4	B	2	NAG	C1-O5-C5	14.17	131.38	112.19
4	B	1	NAG	C1-O5-C5	11.23	127.40	112.19
3	A	2	NAG	C1-O5-C5	10.87	126.92	112.19
4	B	1	NAG	C4-C3-C2	-8.15	99.07	111.02
3	A	1	NAG	C1-O5-C5	7.67	122.59	112.19
3	A	2	NAG	O5-C5-C6	5.36	115.61	107.20
3	A	2	NAG	C4-C3-C2	-4.87	103.88	111.02
4	B	2	NAG	C4-C3-C2	-4.62	104.24	111.02
4	B	3	FUC	C1-O5-C5	3.65	121.04	112.78
4	B	1	NAG	O4-C4-C3	3.47	118.38	110.35
3	A	1	NAG	C4-C3-C2	-3.36	106.10	111.02
4	B	1	NAG	O5-C1-C2	-3.29	106.10	111.29
3	A	1	NAG	C6-C5-C4	-3.27	105.36	113.00
3	A	2	NAG	O4-C4-C3	3.23	117.81	110.35
4	B	2	NAG	O5-C5-C6	3.00	111.91	107.20
3	A	1	NAG	O5-C5-C6	2.86	111.69	107.20
4	B	2	NAG	O4-C4-C3	2.79	116.79	110.35
4	B	1	NAG	O3-C3-C4	2.74	116.69	110.35
4	B	1	NAG	C3-C4-C5	-2.69	105.43	110.24
4	B	1	NAG	O5-C5-C6	2.61	111.30	107.20
4	B	2	NAG	C3-C4-C5	-2.44	105.89	110.24
3	A	2	NAG	O4-C4-C5	-2.40	103.34	109.30
3	A	1	NAG	O5-C1-C2	-2.25	107.74	111.29
3	A	1	NAG	O7-C7-C8	-2.22	117.93	122.06
4	B	2	NAG	O3-C3-C4	2.16	115.33	110.35
3	A	1	NAG	O4-C4-C3	2.13	115.27	110.35
3	A	2	NAG	C6-C5-C4	-2.06	108.17	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	3	FUC	C5
4	B	3	FUC	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
3	A	2	NAG	C8-C7-N2-C2
3	A	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
3	A	1	NAG	O5-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
3	A	1	NAG	O7-C7-N2-C2
3	A	1	NAG	C4-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C3-C2-N2-C7
3	A	2	NAG	O5-C5-C6-O6
3	A	1	NAG	C3-C2-N2-C7
4	B	2	NAG	O5-C5-C6-O6
3	A	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	2	0
3	A	1	NAG	1	0

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	213/213 (100%)	-0.06	9 (4%)	36	45	13, 25, 44, 73	0
2	H	220/220 (100%)	-0.04	7 (3%)	47	57	13, 24, 48, 55	0
All	All	433/433 (100%)	-0.05	16 (3%)	41	51	13, 24, 46, 73	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	213	CYS	8.6
1	L	211	ASN	3.8
2	H	134	ALA	3.6
2	H	137	SER	3.1
1	L	167	SER	3.0
1	L	66	SER	2.9
2	H	177	SER	2.8
2	H	220	GLY	2.7
1	L	212	GLU	2.7
1	L	210	ARG	2.5
1	L	65	GLY	2.4
1	L	162	TRP	2.3
2	H	66	ASP	2.2
2	H	179	GLY	2.2
2	H	1	GLU	2.1
1	L	55	SER	2.1

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 (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	B	3	10/11	0.55	0.47	65,65,66,67	0
3	NAG	A	2	14/15	0.55	0.39	60,62,63,64	0
4	NAG	B	2	14/15	0.63	0.36	65,66,68,68	0
3	NAG	A	1	14/15	0.64	0.38	42,51,52,56	0
4	NAG	B	1	14/15	0.69	0.34	56,59,64,65	0

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	H	226	1/1	0.98	0.03	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.