Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

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
http://wwpdb.org/validation/2016/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:

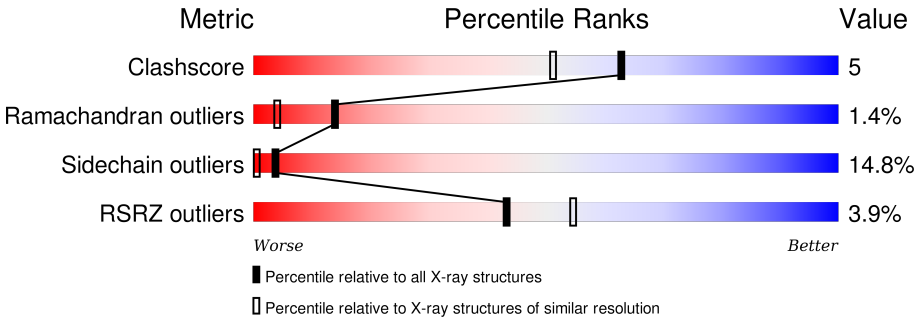
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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. 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	5% 64% 26% 7%
2	H	220	3% 67% 24% 7%

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
3	NAG	H	221	-	-	-	X
4	NAG	H	223	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	H	224	X	-	-	-

2 Entry composition

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

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	3	Total	C	N	O	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.

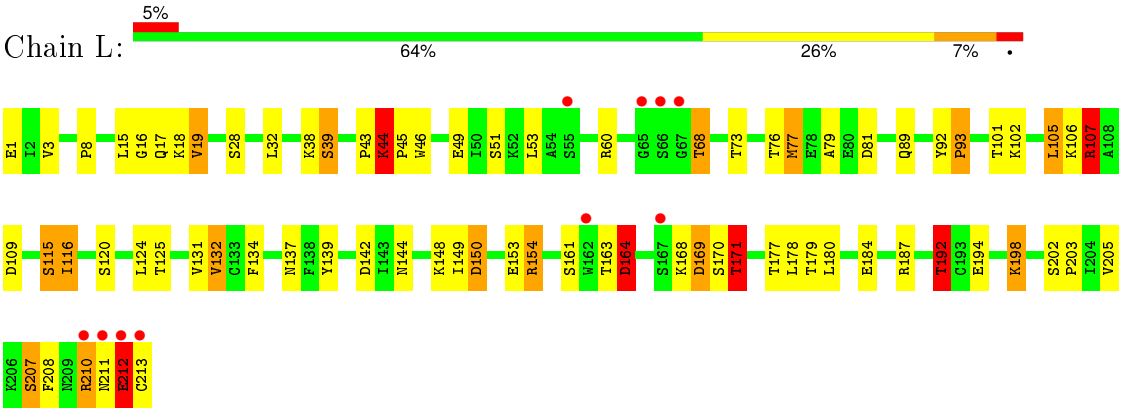
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	182	Total	O	0	0
			182	182		
6	L	193	Total	O	0	0
			193	193		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

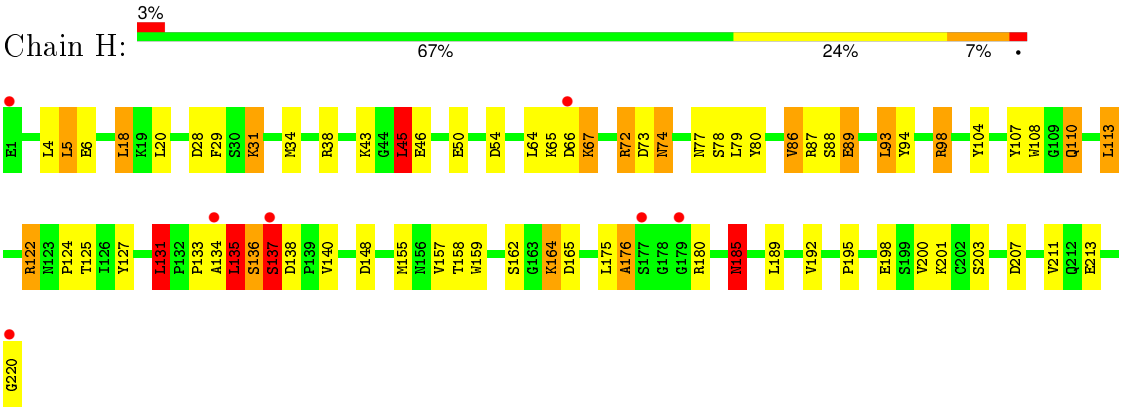
- Molecule 1: IGA-KAPPA J539 FAB (LIGHT CHAIN)

Chain L:



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

Chain H:



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.	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 28312 reflections	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, 0.375 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: 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%)

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
4	H	2	0

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	224	FUC	C5,C1

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	H	28	0	23	1	0
4	H	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
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:H:221:NAG:H3	1.72	0.70
2:H:203:SER:HB3	4:H:223: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:H:223: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	34 21
2	H	218/220 (99%)	202 (93%)	11 (5%)	5 (2%)	8 1
All	All	429/433 (99%)	404 (94%)	19 (4%)	6 (1%)	14 4

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%)	4 1
2	H	186/186 (100%)	157 (84%)	29 (16%)	3 0
All	All	372/372 (100%)	317 (85%)	55 (15%)	4 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

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

5.5 Carbohydrates

5 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	H	221	3,2	14,14,15	0.92	1 (7%)	15,19,21	5.52	7 (46%)
3	NAG	H	222	3	14,14,15	0.94	0	15,19,21	6.09	6 (40%)
4	NAG	H	223	2,4	14,14,15	0.97	1 (7%)	15,19,21	4.13	6 (40%)
4	FUC	H	224	4	10,10,11	0.91	0	14,14,16	1.83	3 (21%)
4	NAG	H	225	4	14,14,15	0.90	0	15,19,21	6.39	8 (53%)

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	H	221	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	222	3	-	1/6/23/26	0/1/1/1
4	NAG	H	223	2,4	-	0/6/23/26	0/1/1/1
4	FUC	H	224	4	2/2/4/5	0/0/17/20	0/1/1/1
4	NAG	H	225	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	221	NAG	C8-C7	2.05	1.54	1.50
4	H	223	NAG	C8-C7	2.05	1.54	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	223	NAG	C4-C3-C2	-7.82	99.07	111.23
3	H	222	NAG	C4-C3-C2	-4.73	103.88	111.23
4	H	225	NAG	C4-C3-C2	-4.50	104.24	111.23
3	H	221	NAG	C4-C3-C2	-3.30	106.10	111.23
3	H	221	NAG	C6-C5-C4	-3.10	105.36	113.02
4	H	223	NAG	C3-C4-C5	-2.73	105.43	110.20
4	H	225	NAG	C3-C4-C5	-2.47	105.89	110.20
3	H	221	NAG	O7-C7-C8	-2.25	117.93	122.06
3	H	222	NAG	O4-C4-C5	-2.22	103.34	109.24
3	H	221	NAG	O5-C5-C6	2.01	111.69	107.35
4	H	224	FUC	C1-C2-C3	2.05	111.97	109.54
4	H	224	FUC	O5-C5-C6	2.06	109.54	106.13
4	H	225	NAG	O5-C5-C6	2.10	111.91	107.35
3	H	221	NAG	O4-C4-C3	2.19	115.27	110.34
4	H	225	NAG	O3-C3-C4	2.22	115.33	110.34
4	H	225	NAG	C3-C2-N2	2.26	115.97	110.56
4	H	223	NAG	O3-C3-C4	2.82	116.69	110.34
4	H	225	NAG	O4-C4-C3	2.87	116.79	110.34
4	H	223	NAG	C3-C2-N2	3.20	118.22	110.56
3	H	222	NAG	O4-C4-C3	3.32	117.81	110.34
4	H	223	NAG	O4-C4-C3	3.57	118.38	110.34
3	H	222	NAG	O5-C5-C6	3.82	115.61	107.35
4	H	224	FUC	C1-O5-C5	5.61	121.04	112.38
3	H	221	NAG	C1-O5-C5	8.15	122.59	112.25
3	H	222	NAG	C1-O5-C5	11.56	126.92	112.25
4	H	223	NAG	C1-O5-C5	11.94	127.40	112.25
4	H	225	NAG	C1-O5-C5	15.08	131.38	112.25
4	H	225	NAG	C2-N2-C7	18.18	146.39	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	221	NAG	C2-N2-C7	18.63	146.97	123.04
3	H	222	NAG	C2-N2-C7	18.83	147.24	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	224	FUC	C5
4	H	224	FUC	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	222	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	221	NAG	1	0
4	H	223	NAG	2	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%)	-0.02	10 (4%) 35 46	13, 25, 44, 73	0
2	H	220/220 (100%)	0.00	7 (3%) 51 61	13, 24, 48, 55	0
All	All	433/433 (100%)	-0.01	17 (3%) 43 54	13, 24, 46, 73	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	213	CYS	8.7
1	L	211	ASN	3.9
2	H	134	ALA	3.7
2	H	137	SER	3.2
1	L	167	SER	3.1
1	L	66	SER	3.1
2	H	177	SER	2.9
2	H	220	GLY	2.9
1	L	212	GLU	2.8
1	L	210	ARG	2.5
1	L	65	GLY	2.4
1	L	162	TRP	2.4
2	H	179	GLY	2.4
2	H	66	ASP	2.3
1	L	55	SER	2.2
2	H	1	GLU	2.2
1	L	67	GLY	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 (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^{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	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	H	221	14/15	0.63	0.38	9.58	42,51,52,56	0
4	NAG	H	223	14/15	0.69	0.35	9.50	56,59,64,65	0
4	NAG	H	225	14/15	0.63	0.36	-	65,66,68,68	0
3	NAG	H	222	14/15	0.55	0.39	-	60,62,63,64	0
4	FUC	H	224	10/11	0.53	0.48	-	65,65,66,67	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. 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^{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	LLDF	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.