



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:18 AM GMT

PDB ID : 2WMK
Title : Crystal structure of the catalytic module of a family 98 glycoside hydrolase from *Streptococcus pneumoniae* SP3-BS71 (Sp3GH98) in complex with the A-LewisY pentasaccharide blood group antigen.
Authors : Higgins, M.A.; Whitworth, G.E.; El Warry, N.; Randrianntsoa, M.; Samain, E.; Burke, R.D.; Vocadlo, D.J.; Boraston, A.B.
Deposited on : 2009-06-30
Resolution : 1.90 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 ⓘ](#)) 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

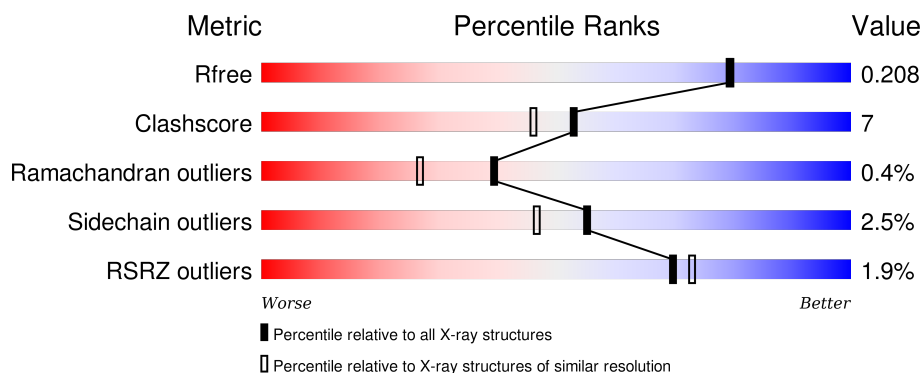
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


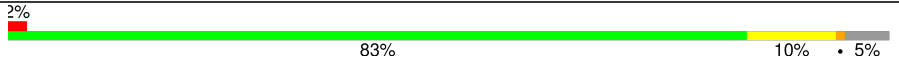
The reported resolution of this entry is 1.90 Å.

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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 $\leq 5\%$. 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	606	 2% 81% 11% • 6%
1	B	606	 2% 83% 10% • 5%

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
2	NAG	A	2008	-	-	-	X
2	NAG	B	2008	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10453 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 FUCOLECTIN-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4677	3007	783	874	13			
1	B	573	Total	C	N	O	S	0	0	0
			4682	3010	784	875	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	MET	-	EXPRESSION TAG	UNP A5LBQ0
A	399	GLY	-	EXPRESSION TAG	UNP A5LBQ0
A	400	SER	-	EXPRESSION TAG	UNP A5LBQ0
A	401	SER	-	EXPRESSION TAG	UNP A5LBQ0
A	402	HIS	-	EXPRESSION TAG	UNP A5LBQ0
A	403	HIS	-	EXPRESSION TAG	UNP A5LBQ0
A	404	HIS	-	EXPRESSION TAG	UNP A5LBQ0
A	405	HIS	-	EXPRESSION TAG	UNP A5LBQ0
A	406	HIS	-	EXPRESSION TAG	UNP A5LBQ0
A	407	HIS	-	EXPRESSION TAG	UNP A5LBQ0
A	408	SER	-	EXPRESSION TAG	UNP A5LBQ0
A	409	SER	-	EXPRESSION TAG	UNP A5LBQ0
A	410	GLY	-	EXPRESSION TAG	UNP A5LBQ0
A	411	LEU	-	EXPRESSION TAG	UNP A5LBQ0
A	412	VAL	-	EXPRESSION TAG	UNP A5LBQ0
A	413	PRO	-	EXPRESSION TAG	UNP A5LBQ0
A	414	ARG	-	EXPRESSION TAG	UNP A5LBQ0
A	415	GLY	-	EXPRESSION TAG	UNP A5LBQ0
A	416	SER	-	EXPRESSION TAG	UNP A5LBQ0
A	417	HIS	-	EXPRESSION TAG	UNP A5LBQ0
A	418	MET	-	EXPRESSION TAG	UNP A5LBQ0
A	419	ALA	-	EXPRESSION TAG	UNP A5LBQ0
A	420	SER	-	EXPRESSION TAG	UNP A5LBQ0
A	558	ALA	GLU	ENGINEERED MUTATION	UNP A5LBQ0
B	398	MET	-	EXPRESSION TAG	UNP A5LBQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	399	GLY	-	EXPRESSION TAG	UNP A5LBQ0
B	400	SER	-	EXPRESSION TAG	UNP A5LBQ0
B	401	SER	-	EXPRESSION TAG	UNP A5LBQ0
B	402	HIS	-	EXPRESSION TAG	UNP A5LBQ0
B	403	HIS	-	EXPRESSION TAG	UNP A5LBQ0
B	404	HIS	-	EXPRESSION TAG	UNP A5LBQ0
B	405	HIS	-	EXPRESSION TAG	UNP A5LBQ0
B	406	HIS	-	EXPRESSION TAG	UNP A5LBQ0
B	407	HIS	-	EXPRESSION TAG	UNP A5LBQ0
B	408	SER	-	EXPRESSION TAG	UNP A5LBQ0
B	409	SER	-	EXPRESSION TAG	UNP A5LBQ0
B	410	GLY	-	EXPRESSION TAG	UNP A5LBQ0
B	411	LEU	-	EXPRESSION TAG	UNP A5LBQ0
B	412	VAL	-	EXPRESSION TAG	UNP A5LBQ0
B	413	PRO	-	EXPRESSION TAG	UNP A5LBQ0
B	414	ARG	-	EXPRESSION TAG	UNP A5LBQ0
B	415	GLY	-	EXPRESSION TAG	UNP A5LBQ0
B	416	SER	-	EXPRESSION TAG	UNP A5LBQ0
B	417	HIS	-	EXPRESSION TAG	UNP A5LBQ0
B	418	MET	-	EXPRESSION TAG	UNP A5LBQ0
B	419	ALA	-	EXPRESSION TAG	UNP A5LBQ0
B	420	SER	-	EXPRESSION TAG	UNP A5LBQ0
B	558	ALA	GLU	ENGINEERED MUTATION	UNP A5LBQ0

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			60	34	2	24		
2	B	5	Total	C	N	O	0	0
			60	34	2	24		

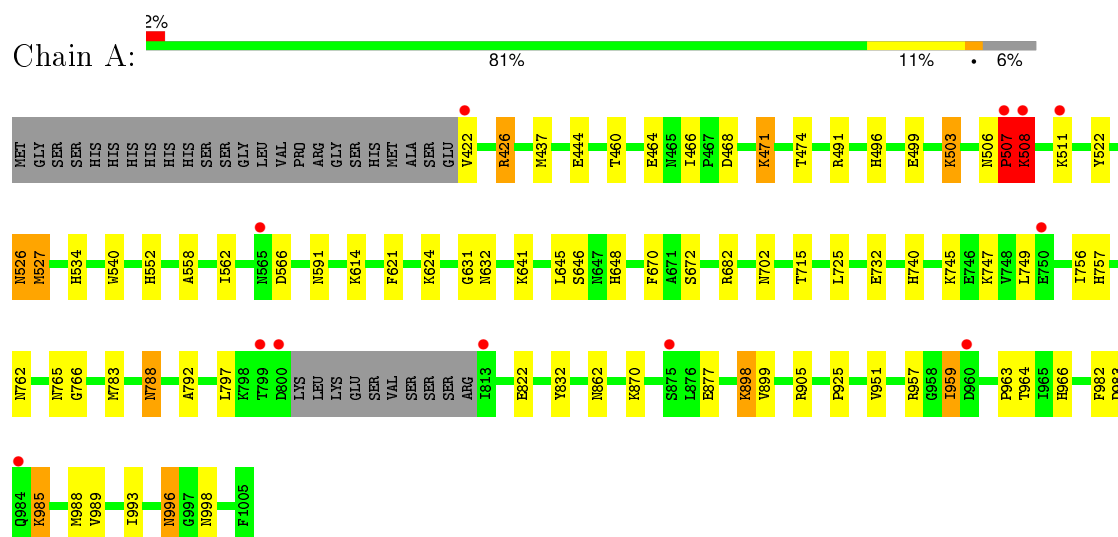
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	453	Total	O	0	0
			453	453		
3	B	521	Total	O	0	0
			521	521		

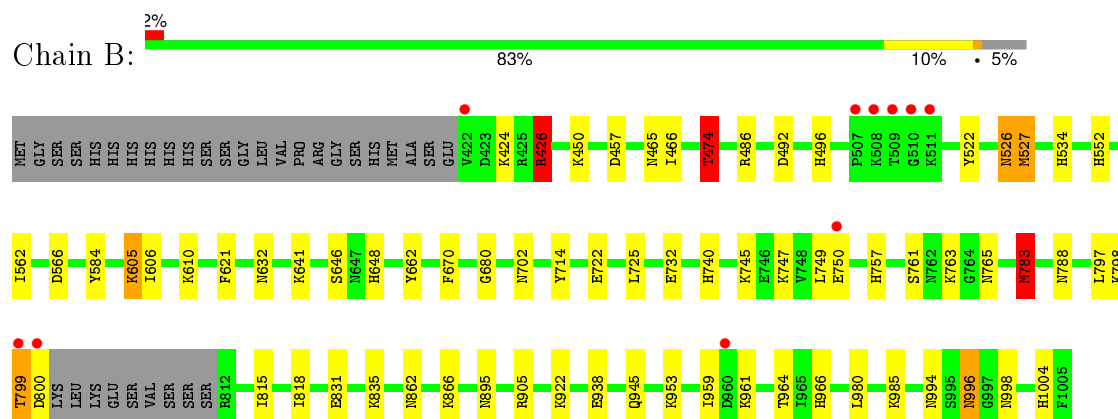
3 Residue-property plots [i](#)

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: FUCOLECTIN-RELATED PROTEIN



• Molecule 1: FUCOLECTIN-RELATED PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.90Å 153.70Å 90.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.12 – 1.90 29.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.12-1.90) 99.0 (29.12-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.162 , 0.210 0.163 , 0.208	Depositor DCC
R_{free} test set	5368 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 107462 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10453	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3948e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FUC, GAL, NAG, A2G

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	0.89	0/4809	0.80	6/6515 (0.1%)
1	B	0.94	0/4814	0.85	12/6522 (0.2%)
All	All	0.91	0/9623	0.83	18/13037 (0.1%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	B	426	ARG	NE-CZ-NH1	12.65	126.63	120.30
1	A	426	ARG	NE-CZ-NH2	-12.55	114.02	120.30
1	B	783	MET	CG-SD-CE	-11.42	81.93	100.20
1	A	426	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	B	486	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	B	486	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	783	MET	CG-SD-CE	5.61	109.17	100.20
1	A	471	LYS	CD-CE-NZ	5.54	124.44	111.70
1	B	527	MET	CG-SD-CE	5.53	109.05	100.20
1	B	745	LYS	CD-CE-NZ	5.51	124.39	111.70
1	B	492	ASP	CB-CG-OD1	5.39	123.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	PRO	N-CA-C	5.31	125.90	112.10
1	B	474	THR	N-CA-CB	-5.30	100.22	110.30
1	B	426	ARG	CD-NE-CZ	5.14	130.80	123.60
1	B	457	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	474	THR	OG1-CB-CG2	5.09	121.72	110.00
1	A	527	MET	CG-SD-CE	5.09	108.34	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	507	PRO	Peptide
1	B	798	LYS	Peptide

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	4677	0	4521	66	0
1	B	4682	0	4523	57	0
2	A	60	0	54	0	0
2	B	60	0	54	0	0
3	A	453	0	0	12	3
3	B	521	0	0	17	3
All	All	10453	0	9152	123	3

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 7.

All (123) 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:B:831:GLU:O	1:B:835:LYS:HE2	1.50	1.12
1:A:437:MET:HG3	1:A:474:THR:CG2	2.04	0.87
1:B:496:HIS:HD2	3:B:3025:HOH:O	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ARG:H	1:A:996:ASN:HD21	1.22	0.82
1:B:905:ARG:H	1:B:996:ASN:HD21	1.25	0.81
1:A:757:HIS:HE1	1:A:797:LEU:O	1.62	0.80
1:A:670:PHE:H	1:A:862:ASN:HD21	1.31	0.78
1:B:670:PHE:H	1:B:862:ASN:HD21	1.33	0.76
1:B:670:PHE:H	1:B:862:ASN:ND2	1.86	0.74
1:B:998:ASN:CB	3:B:3508:HOH:O	2.35	0.74
1:B:527:MET:CE	3:B:3075:HOH:O	2.36	0.73
1:A:437:MET:CG	1:A:474:THR:HG23	2.19	0.72
1:A:437:MET:CG	1:A:474:THR:CG2	2.69	0.71
1:B:641:LYS:NZ	1:B:788:ASN:ND2	2.39	0.70
1:B:750:GLU:OE1	3:B:3271:HOH:O	2.09	0.70
1:B:466:ILE:HG21	1:B:474:THR:HG21	1.74	0.70
1:B:964:THR:OG1	1:B:966:HIS:HE1	1.76	0.69
1:B:998:ASN:HB3	3:B:3508:HOH:O	1.92	0.69
1:B:740:HIS:HE1	3:B:3257:HOH:O	1.75	0.69
1:B:938:GLU:HG3	3:B:3447:HOH:O	1.94	0.67
1:A:632:ASN:ND2	1:A:765:ASN:HB3	2.10	0.67
1:A:499:GLU:O	1:A:503:LYS:HG2	1.95	0.66
1:A:496:HIS:HD2	3:A:3026:HOH:O	1.78	0.66
1:A:670:PHE:H	1:A:862:ASN:ND2	1.93	0.66
1:A:762:ASN:ND2	3:A:3255:HOH:O	2.29	0.65
1:B:605:LYS:HE3	3:B:3141:HOH:O	1.95	0.65
1:A:444:GLU:HG3	3:A:3054:HOH:O	1.96	0.64
1:B:424:LYS:HE2	1:B:584:TYR:CZ	2.32	0.64
1:A:646:SER:OG	1:A:648:HIS:HD2	1.81	0.64
1:A:702:ASN:HD21	1:A:788:ASN:HB2	1.63	0.63
1:A:466:ILE:HD13	1:A:474:THR:HG21	1.81	0.63
1:B:757:HIS:HE1	1:B:797:LEU:O	1.82	0.62
1:B:922:LYS:HE2	3:B:3205:HOH:O	1.98	0.62
1:A:740:HIS:HE1	3:A:3241:HOH:O	1.83	0.62
1:B:641:LYS:NZ	1:B:788:ASN:HD22	1.98	0.60
1:A:964:THR:OG1	1:A:966:HIS:HE1	1.84	0.60
1:A:983:ASP:OD1	1:A:985:LYS:HG3	2.02	0.60
1:A:496:HIS:HE1	3:A:3078:HOH:O	1.86	0.57
1:A:426:ARG:HE	1:A:552:HIS:HD2	1.50	0.57
1:B:641:LYS:NZ	1:B:702:ASN:HD22	2.04	0.56
1:A:527:MET:HE2	3:A:3082:HOH:O	2.05	0.56
1:A:437:MET:HG2	1:A:474:THR:HG23	1.88	0.55
1:B:961:LYS:HE2	3:B:3473:HOH:O	2.06	0.55
1:A:747:LYS:HE2	3:A:3309:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:SER:OG	1:B:648:HIS:HD2	1.89	0.55
1:B:641:LYS:HZ1	1:B:702:ASN:HD22	1.55	0.54
1:B:702:ASN:HD21	1:B:788:ASN:HB2	1.73	0.54
1:A:527:MET:CE	3:A:3082:HOH:O	2.54	0.54
1:B:465:ASN:HB2	3:B:3238:HOH:O	2.07	0.54
1:B:426:ARG:HH21	1:B:552:HIS:HD2	1.56	0.53
1:B:953:LYS:HE2	3:B:3500:HOH:O	2.09	0.53
1:B:566:ASP:N	1:B:566:ASP:OD1	2.30	0.53
1:A:905:ARG:H	1:A:996:ASN:ND2	2.01	0.53
1:A:682:ARG:NH1	1:A:925:PRO:O	2.35	0.52
1:A:522:TYR:HA	1:A:526:ASN:HD21	1.74	0.52
1:A:732:GLU:HG2	3:A:3227:HOH:O	2.09	0.52
1:A:631:GLY:O	1:A:766:GLY:HA3	2.11	0.51
1:B:641:LYS:HZ3	1:B:788:ASN:ND2	2.06	0.51
1:A:757:HIS:CE1	1:A:797:LEU:O	2.54	0.50
1:A:558:ALA:HB2	1:A:624:LYS:HE3	1.94	0.50
1:A:522:TYR:HA	1:A:526:ASN:ND2	2.27	0.50
1:A:963:PRO:HD3	1:A:989:VAL:HG21	1.93	0.50
1:A:468:ASP:OD1	1:A:471:LYS:HE2	2.13	0.49
1:A:566:ASP:N	1:A:566:ASP:OD1	2.35	0.49
1:B:526:ASN:O	1:B:534:HIS:HD2	1.96	0.49
1:A:632:ASN:HD21	1:A:765:ASN:HB3	1.77	0.48
1:B:522:TYR:HA	1:B:526:ASN:HD21	1.77	0.48
1:A:526:ASN:O	1:A:534:HIS:HD2	1.97	0.48
1:A:715:THR:HA	1:A:725:LEU:HD13	1.95	0.48
1:B:450:LYS:HD3	3:B:3019:HOH:O	2.14	0.47
1:A:437:MET:HG3	1:A:474:THR:HG21	1.94	0.47
1:A:506:ASN:OD1	1:A:508:LYS:HB3	2.15	0.47
1:B:424:LYS:HE2	1:B:584:TYR:CE1	2.49	0.47
1:B:895:ASN:O	1:B:1004:HIS:HA	2.15	0.46
1:A:959:ILE:HG21	1:A:989:VAL:HG23	1.98	0.46
1:B:757:HIS:CE1	1:B:797:LEU:O	2.67	0.46
1:B:522:TYR:HA	1:B:526:ASN:ND2	2.31	0.46
1:A:982:PHE:CD1	1:A:989:VAL:HG22	2.51	0.45
1:A:740:HIS:HD2	3:A:3314:HOH:O	1.98	0.45
1:B:606:ILE:HD12	1:B:610:LYS:HE3	1.98	0.45
1:B:426:ARG:HH21	1:B:552:HIS:CD2	2.32	0.45
1:A:506:ASN:HA	1:A:507:PRO:HD3	1.73	0.45
1:A:870:LYS:NZ	1:A:877:GLU:OE2	2.43	0.45
1:A:641:LYS:NZ	1:A:702:ASN:HD22	2.15	0.44
1:B:799:THR:HG21	1:B:815:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ASN:HB3	1:A:766:GLY:H	1.56	0.44
1:A:964:THR:OG1	1:A:966:HIS:CE1	2.67	0.44
1:A:614:LYS:NZ	3:A:3150:HOH:O	2.51	0.44
1:A:460:THR:O	1:A:464:GLU:HG3	2.18	0.43
1:B:662:TYR:CD1	1:B:680:GLY:HA2	2.53	0.43
1:B:714:TYR:CZ	1:B:725:LEU:HD12	2.53	0.43
1:B:632:ASN:HD21	1:B:765:ASN:HB3	1.83	0.43
1:B:996:ASN:C	1:B:996:ASN:HD22	2.22	0.43
1:B:632:ASN:ND2	1:B:765:ASN:HB3	2.32	0.43
1:A:957:ARG:NH1	1:A:988:MET:SD	2.91	0.43
1:A:491:ARG:HD2	1:A:540:TRP:CD1	2.53	0.43
1:B:465:ASN:HD21	1:B:722:GLU:HG3	1.82	0.43
1:B:466:ILE:HD13	1:B:474:THR:CG2	2.49	0.43
1:A:822:GLU:HG2	1:A:832:TYR:CD1	2.54	0.43
1:A:745:LYS:O	1:A:749:LEU:HB2	2.18	0.43
1:B:994:ASN:ND2	3:B:3501:HOH:O	2.49	0.42
1:A:444:GLU:CG	3:A:3054:HOH:O	2.60	0.42
1:B:964:THR:OG1	1:B:966:HIS:CE1	2.64	0.42
1:A:898:LYS:HD3	1:A:899:VAL:N	2.35	0.42
1:A:996:ASN:HD22	1:A:996:ASN:C	2.23	0.42
1:A:499:GLU:O	1:A:503:LYS:CG	2.66	0.42
1:B:998:ASN:HB2	3:B:3508:HOH:O	2.13	0.42
1:B:945:GLN:HG3	3:B:3416:HOH:O	2.19	0.42
1:B:783:MET:HG3	1:B:783:MET:H	1.60	0.42
1:B:732:GLU:HG3	3:B:3508:HOH:O	2.18	0.42
1:B:763:LYS:HG3	1:B:818:ILE:HG12	2.01	0.42
1:A:951:VAL:HA	1:A:993:ILE:O	2.20	0.41
1:A:747:LYS:HG3	1:A:747:LYS:O	2.18	0.41
1:A:641:LYS:HZ1	1:A:702:ASN:HD22	1.68	0.41
1:B:606:ILE:CD1	1:B:610:LYS:HE3	2.50	0.41
1:B:761:SER:HA	1:B:765:ASN:OD1	2.20	0.41
1:A:645:LEU:HD22	1:A:749:LEU:HD13	2.03	0.41
1:A:464:GLU:OE2	1:A:507:PRO:HG3	2.20	0.41
1:A:725:LEU:HD23	1:A:725:LEU:O	2.20	0.41
1:A:756:ILE:O	1:A:792:ALA:HA	2.20	0.41
1:B:985:LYS:HE3	1:B:985:LYS:HB2	1.96	0.41
1:A:506:ASN:OD1	1:A:507:PRO:HD2	2.22	0.41
1:B:747:LYS:O	1:B:750:GLU:HG2	2.20	0.40

All (3) 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)
3:A:3264:HOH:O	3:B:3057:HOH:O[3_554]	1.73	0.47
3:A:3266:HOH:O	3:B:3057:HOH:O[3_554]	1.85	0.35
3:A:3268:HOH:O	3:B:3057:HOH:O[3_554]	1.92	0.28

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/606 (94%)	543 (96%)	22 (4%)	3 (0%)	34	21
1	B	569/606 (94%)	547 (96%)	20 (4%)	2 (0%)	39	27
All	All	1137/1212 (94%)	1090 (96%)	42 (4%)	5 (0%)	39	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	799	THR
1	A	508	LYS
1	A	562	ILE
1	A	591	ASN
1	B	562	ILE

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	A	501/531 (94%)	488 (97%)	13 (3%)	54	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	501/531 (94%)	489 (98%)	12 (2%)	57	49
All	All	1002/1062 (94%)	977 (98%)	25 (2%)	55	47

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	VAL
1	A	503	LYS
1	A	508	LYS
1	A	511	LYS
1	A	526	ASN
1	A	621	PHE
1	A	672	SER
1	A	788	ASN
1	A	898	LYS
1	A	959	ILE
1	A	985	LYS
1	A	996	ASN
1	A	998	ASN
1	B	426	ARG
1	B	474	THR
1	B	526	ASN
1	B	605	LYS
1	B	621	PHE
1	B	749	LEU
1	B	783	MET
1	B	800	ASP
1	B	866	LYS
1	B	959	ILE
1	B	980	LEU
1	B	996	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	HIS
1	A	448	GLN
1	A	496	HIS
1	A	512	ASN
1	A	526	ASN
1	A	534	HIS

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Mol	Chain	Res	Type
1	A	552	HIS
1	A	581	ASN
1	A	609	GLN
1	A	618	ASN
1	A	632	ASN
1	A	648	HIS
1	A	702	ASN
1	A	740	HIS
1	A	757	HIS
1	A	788	ASN
1	A	862	ASN
1	A	916	GLN
1	A	919	ASN
1	A	926	GLN
1	A	966	HIS
1	A	972	ASN
1	A	994	ASN
1	A	996	ASN
1	A	998	ASN
1	B	465	ASN
1	B	496	HIS
1	B	512	ASN
1	B	526	ASN
1	B	534	HIS
1	B	552	HIS
1	B	581	ASN
1	B	609	GLN
1	B	618	ASN
1	B	632	ASN
1	B	648	HIS
1	B	651	GLN
1	B	702	ASN
1	B	740	HIS
1	B	757	HIS
1	B	788	ASN
1	B	862	ASN
1	B	916	GLN
1	B	966	HIS
1	B	986	ASN
1	B	994	ASN
1	B	996	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 ⓘ

10 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	$\# Z > 2$
2	FUC	A	2006	2	10,10,11	0.75	0	14,14,16	1.26	2 (14%)
2	GAL	A	2007	2	11,11,12	0.87	0	14,15,17	2.01	3 (21%)
2	NAG	A	2008	2	15,15,15	0.91	0	17,21,21	1.50	3 (17%)
2	FUC	A	2009	2	10,10,11	0.62	0	14,14,16	1.56	4 (28%)
2	A2G	A	2010	2	14,14,15	1.16	1 (7%)	15,19,21	1.44	1 (6%)
2	FUC	B	2006	2	10,10,11	0.72	0	14,14,16	1.13	0
2	GAL	B	2007	2	11,11,12	0.80	0	14,15,17	2.37	4 (28%)
2	NAG	B	2008	2	15,15,15	0.89	0	17,21,21	1.43	3 (17%)
2	FUC	B	2009	2	10,10,11	0.74	0	14,14,16	1.72	2 (14%)
2	A2G	B	2010	2	14,14,15	0.95	1 (7%)	15,19,21	1.35	1 (6%)

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
2	FUC	A	2006	2	-	0/0/17/20	0/1/1/1
2	GAL	A	2007	2	-	0/2/19/22	0/1/1/1
2	NAG	A	2008	2	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	A	2009	2	-	0/0/17/20	0/1/1/1
2	A2G	A	2010	2	-	0/6/23/26	0/1/1/1
2	FUC	B	2006	2	-	0/0/17/20	0/1/1/1
2	GAL	B	2007	2	-	0/2/19/22	0/1/1/1
2	NAG	B	2008	2	-	0/6/26/26	0/1/1/1
2	FUC	B	2009	2	-	0/0/17/20	0/1/1/1
2	A2G	B	2010	2	-	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)
2	A	2010	A2G	O-C1	2.22	1.47	1.43
2	B	2010	A2G	C1-C2	2.28	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2010	A2G	C2-N2-C7	-4.84	116.82	123.04
2	A	2010	A2G	C2-N2-C7	-4.06	117.82	123.04
2	A	2008	NAG	O7-C7-C8	-3.22	116.15	122.06
2	B	2009	FUC	C2-C3-C4	-3.10	105.77	111.04
2	A	2009	FUC	C6-C5-C4	-2.80	107.56	113.08
2	B	2007	GAL	O2-C2-C3	-2.09	105.91	110.12
2	A	2007	GAL	O5-C5-C6	-2.07	102.86	107.35
2	B	2008	NAG	C1-O5-C5	2.10	117.35	113.47
2	A	2009	FUC	C1-O5-C5	2.15	115.70	112.38
2	A	2008	NAG	C8-C7-N2	2.22	120.35	116.11
2	A	2008	NAG	O3-C3-C2	2.28	114.30	109.66
2	B	2008	NAG	C4-C3-C2	2.33	113.66	110.43
2	A	2009	FUC	O2-C2-C1	2.36	113.94	109.21
2	A	2009	FUC	O5-C5-C6	2.36	110.03	106.13
2	A	2006	FUC	C1-C2-C3	2.46	112.45	109.54
2	A	2006	FUC	O5-C5-C6	2.64	110.50	106.13
2	B	2008	NAG	C2-N2-C7	2.72	130.08	123.10
2	B	2007	GAL	O5-C1-C2	2.79	115.38	110.86
2	B	2007	GAL	C1-C2-C3	2.87	112.94	109.54
2	A	2007	GAL	C1-C2-C3	3.18	113.31	109.54
2	B	2009	FUC	O5-C5-C6	3.89	112.56	106.13
2	A	2007	GAL	C1-O5-C5	5.67	119.44	112.25
2	B	2007	GAL	C1-O5-C5	7.09	121.25	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	572/606 (94%)	-0.25	12 (2%) 67 70	4, 11, 29, 45	0
1	B	573/606 (94%)	-0.38	10 (1%) 73 76	3, 9, 24, 47	0
All	All	1145/1212 (94%)	-0.32	22 (1%) 70 73	3, 10, 27, 47	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	ASP	4.9
1	B	800	ASP	4.2
1	B	508	LYS	3.8
1	A	508	LYS	3.3
1	B	509	THR	3.3
1	A	422	VAL	3.1
1	A	565	ASN	3.0
1	A	800	ASP	2.9
1	B	960	ASP	2.9
1	A	984	GLN	2.8
1	A	799	THR	2.7
1	B	511	LYS	2.6
1	A	875	SER	2.6
1	B	510	GLY	2.5
1	A	813	ILE	2.4
1	A	507	PRO	2.4
1	A	511	LYS	2.4
1	B	422	VAL	2.3
1	B	507	PRO	2.3
1	B	799	THR	2.3
1	A	750	GLU	2.1
1	B	750	GLU	2.1

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	2008	15/15	0.82	0.22	16.82	17,26,36,37	0
2	NAG	A	2008	15/15	0.79	0.24	7.51	20,28,44,48	0
2	A2G	B	2010	14/15	0.97	0.09	0.69	5,7,22,27	0
2	A2G	A	2010	14/15	0.97	0.08	0.05	6,7,20,25	0
2	FUC	A	2006	10/11	0.99	0.07	-0.82	5,7,9,9	0
2	GAL	A	2007	11/12	0.97	0.06	-1.01	5,9,13,15	0
2	FUC	B	2006	10/11	0.99	0.06	-1.17	5,6,8,9	0
2	GAL	B	2007	11/12	0.98	0.05	-1.40	6,9,11,14	0
2	FUC	A	2009	10/11	0.88	0.23	-	18,29,29,33	0
2	FUC	B	2009	10/11	0.88	0.20	-	15,24,26,26	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.