



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:38 PM GMT

PDB ID : 1UH0
Title : Crystal structure of jacalin- Me-alpha-GalNAc complex
Authors : Jeyapraakash, A.A.; Katiyar, S.; Swaminathan, C.P.; Sekar, K.; Surolia, A.;
Vijayan, M.
Deposited on : 2003-06-23
Resolution : 2.80 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

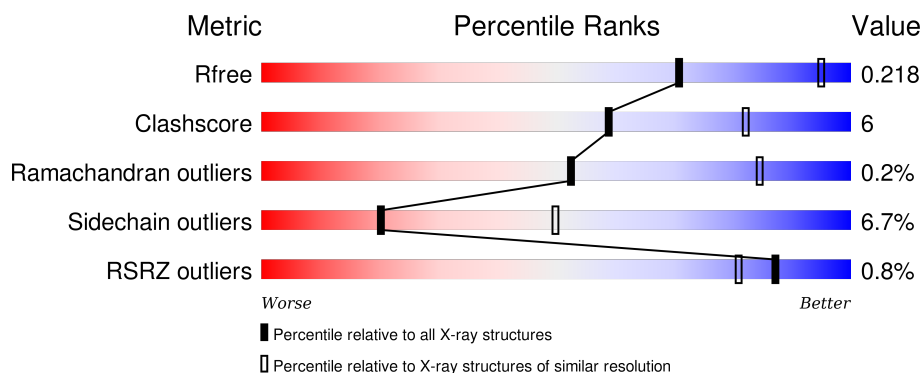
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 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	133	
1	C	133	
1	E	133	
1	G	133	
2	B	20	

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Mol	Chain	Length	Quality of chain
2	D	20	<div><div></div><div>55%15%5%25%</div></div>
2	F	20	<div><div>5%</div><div>55%20%25%</div></div>
2	H	20	<div><div>5%</div><div>55%15%5%25%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4757 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 Agglutinin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
1	C	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
1	E	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			
1	G	133	Total	C	N	O	S	0	0	0
			1040	679	160	199	2			

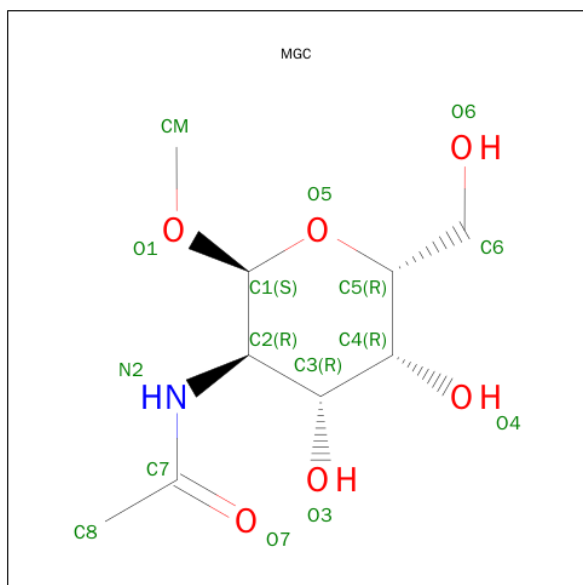
- Molecule 2 is a protein called Agglutinin beta-3 chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			106	68	19	19			
2	D	15	Total	C	N	O	0	0	0
			106	68	19	19			
2	F	15	Total	C	N	O	0	0	0
			106	68	19	19			
2	H	15	Total	C	N	O	0	0	0
			106	68	19	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	LYS	ILE	CONFLICT	UNP P18673
D	6	LYS	ILE	CONFLICT	UNP P18673
F	6	LYS	ILE	CONFLICT	UNP P18673
H	6	LYS	ILE	CONFLICT	UNP P18673

- Molecule 3 is METHYL 2-(ACETYLAMINO)-2-DEOXY-ALPHA-D-GALACTOPYRANO SIDURONIC ACID (three-letter code: MGC) (formula: C₉H₁₇NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	9	1	6		
3	C	1	Total	C	N	O	0	0
			16	9	1	6		
3	E	1	Total	C	N	O	0	0
			16	9	1	6		
3	G	1	Total	C	N	O	0	0
			16	9	1	6		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	3	Total	O	0	0
			3	3		
4	C	25	Total	O	0	0
			25	25		
4	D	2	Total	O	0	0
			2	2		
4	E	27	Total	O	0	0
			27	27		
4	F	5	Total	O	0	0
			5	5		
4	G	22	Total	O	0	0
			22	22		
4	H	4	Total	O	0	0
			4	4		

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: Agglutinin alpha chain

Chain A:  84% 15% .




- Molecule 1: Agglutinin alpha chain

Chain C:  82% 15% .




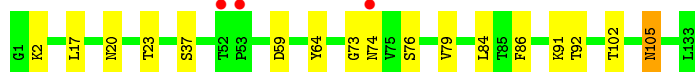
- Molecule 1: Agglutinin alpha chain

Chain E:  83% 16% ..



- Molecule 1: Agglutinin alpha chain

Chain G:  2% 87% 12% .



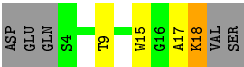
- Molecule 2: Agglutinin beta-3 chain

Chain B:  50% 25% 25%

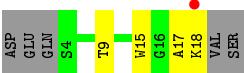


- Molecule 2: Agglutinin beta-3 chain

Chain D:  55% 15% 5% 25%



● Molecule 2: Agglutinin beta-3 chain



● Molecule 2: Agglutinin beta-3 chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.81Å 129.81Å 158.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.99-2.80) 97.6 (19.99-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.218 0.194 , 0.218	Depositor DCC
R_{free} test set	769 reflections (3.95%)	DCC
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 19485 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4757	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MGC

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	1.13	12/1069 (1.1%)	0.92	6/1449 (0.4%)
1	C	1.24	13/1069 (1.2%)	1.05	8/1449 (0.6%)
1	E	1.15	11/1069 (1.0%)	1.27	6/1449 (0.4%)
1	G	1.02	8/1069 (0.7%)	0.88	5/1449 (0.3%)
2	B	0.47	0/108	0.65	0/145
2	D	0.42	0/108	0.64	0/145
2	F	0.42	0/108	0.65	0/145
2	H	0.45	0/108	0.65	0/145
All	All	1.09	44/4708 (0.9%)	1.01	25/6376 (0.4%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	86	PHE	CE2-CZ	-13.49	1.11	1.37
1	A	86	PHE	CE1-CZ	-13.37	1.11	1.37
1	C	86	PHE	CE1-CZ	-13.29	1.12	1.37
1	A	86	PHE	CE2-CZ	-12.89	1.12	1.37
1	G	86	PHE	CE1-CZ	-12.70	1.13	1.37
1	E	86	PHE	CE1-CZ	-12.61	1.13	1.37
1	E	86	PHE	CE2-CZ	-12.59	1.13	1.37
1	C	122	TYR	CE1-CZ	-12.32	1.22	1.38
1	C	86	PHE	CE2-CZ	-12.18	1.14	1.37
1	C	122	TYR	CE2-CZ	-12.08	1.22	1.38
1	E	22	GLU	CD-OE2	11.47	1.38	1.25
1	C	122	TYR	CG-CD2	-11.44	1.24	1.39
1	G	64	TYR	CE2-CZ	-11.36	1.23	1.38
1	E	64	TYR	CE2-CZ	-10.64	1.24	1.38
1	C	64	TYR	CE2-CZ	-10.24	1.25	1.38
1	A	64	TYR	CE2-CZ	-10.09	1.25	1.38
1	C	64	TYR	CE1-CZ	-9.55	1.26	1.38
1	E	64	TYR	CE1-CZ	-9.44	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	122	TYR	CG-CD1	-9.08	1.27	1.39
1	A	64	TYR	CG-CD2	-8.98	1.27	1.39
1	G	64	TYR	CG-CD1	-8.88	1.27	1.39
1	A	64	TYR	CG-CD1	-8.75	1.27	1.39
1	G	64	TYR	CE1-CZ	-8.74	1.27	1.38
1	E	64	TYR	CG-CD1	-8.58	1.28	1.39
1	E	22	GLU	CB-CG	-8.55	1.35	1.52
1	C	64	TYR	CG-CD1	-8.45	1.28	1.39
1	C	64	TYR	CG-CD2	-7.70	1.29	1.39
1	E	64	TYR	CG-CD2	-7.62	1.29	1.39
1	A	86	PHE	CG-CD2	-7.46	1.27	1.38
1	C	86	PHE	CG-CD2	-7.46	1.27	1.38
1	G	64	TYR	CG-CD2	-7.34	1.29	1.39
1	A	64	TYR	CE1-CZ	-7.34	1.29	1.38
1	G	86	PHE	CG-CD1	-7.13	1.28	1.38
1	E	86	PHE	CG-CD2	-7.00	1.28	1.38
1	C	2	LYS	CE-NZ	-6.89	1.31	1.49
1	G	86	PHE	CG-CD2	-6.68	1.28	1.38
1	E	86	PHE	CG-CD1	-6.55	1.28	1.38
1	A	86	PHE	CG-CD1	-6.47	1.29	1.38
1	A	22	GLU	CB-CG	-6.28	1.40	1.52
1	C	86	PHE	CG-CD1	-6.25	1.29	1.38
1	A	22	GLU	CD-OE2	5.89	1.32	1.25
1	E	22	GLU	CD-OE1	5.80	1.32	1.25
1	A	71	TYR	CD2-CE2	5.65	1.47	1.39
1	A	64	TYR	CD1-CE1	5.33	1.47	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	59	ASP	CB-CG-OD1	26.29	141.96	118.30
1	E	59	ASP	CB-CG-OD2	-22.83	97.76	118.30
1	C	2	LYS	CD-CE-NZ	-11.19	85.97	111.70
1	C	5	ASP	CB-CG-OD1	-10.20	109.12	118.30
1	C	59	ASP	CB-CG-OD1	8.58	126.02	118.30
1	G	59	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	G	59	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	59	ASP	CB-CG-OD1	8.40	125.86	118.30
1	C	59	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	59	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	C	122	TYR	CB-CG-CD2	7.58	125.55	121.00
1	E	22	GLU	CA-CB-CG	-6.40	99.32	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	PHE	CB-CG-CD1	6.04	125.03	120.80
1	C	5	ASP	CB-CG-OD2	5.92	123.63	118.30
1	G	2	LYS	CD-CE-NZ	-5.87	98.20	111.70
1	E	2	LYS	CD-CE-NZ	-5.82	98.32	111.70
1	A	2	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	C	86	PHE	CB-CG-CD1	5.64	124.75	120.80
1	C	122	TYR	CA-CB-CG	5.54	123.93	113.40
1	E	76	SER	N-CA-CB	-5.50	102.26	110.50
1	G	86	PHE	CB-CG-CD2	5.43	124.61	120.80
1	A	22	GLU	CA-CB-CG	-5.39	101.55	113.40
1	E	86	PHE	CB-CG-CD1	5.34	124.54	120.80
1	A	86	PHE	CD1-CG-CD2	-5.16	111.59	118.30
1	G	86	PHE	CD1-CG-CD2	-5.05	111.74	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1040	0	1009	10	0
1	C	1040	0	1009	16	0
1	E	1040	0	1009	13	0
1	G	1040	0	1009	9	0
2	B	106	0	110	6	1
2	D	106	0	110	4	0
2	F	106	0	110	4	0
2	H	106	0	110	5	0
3	A	16	0	17	0	0
3	C	16	0	17	0	0
3	E	16	0	17	0	0
3	G	16	0	16	0	0
4	A	21	0	0	0	0
4	B	3	0	0	0	0
4	C	25	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	27	0	0	0	0
4	F	5	0	0	0	0
4	G	22	0	0	0	0
4	H	4	0	0	0	0
All	All	4757	0	4543	53	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 6.

All (53) 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:A:105:ASN:HD21	2:D:15:TRP:HE1	1.29	0.81
1:C:105:ASN:HD22	1:C:105:ASN:C	1.85	0.80
1:E:105:ASN:HD22	1:E:105:ASN:C	1.86	0.78
1:G:105:ASN:HD22	1:G:105:ASN:C	1.86	0.78
1:A:105:ASN:ND2	1:A:105:ASN:O	2.18	0.76
2:B:15:TRP:HE1	1:C:105:ASN:ND2	1.83	0.76
1:E:105:ASN:HD21	2:H:15:TRP:HE1	1.38	0.69
1:A:105:ASN:ND2	2:D:15:TRP:HE1	1.92	0.67
2:H:18:LYS:HA	2:H:18:LYS:HE2	1.75	0.67
2:B:15:TRP:HE1	1:C:105:ASN:HD21	1.37	0.67
1:E:105:ASN:ND2	2:H:15:TRP:HE1	1.94	0.66
2:D:18:LYS:HA	2:D:18:LYS:HE2	1.80	0.64
2:F:15:TRP:HE1	1:G:105:ASN:HD21	1.47	0.63
2:F:15:TRP:HE1	1:G:105:ASN:ND2	1.98	0.62
1:A:105:ASN:C	1:A:105:ASN:ND2	2.54	0.59
1:E:105:ASN:ND2	1:E:105:ASN:O	2.33	0.59
1:E:79:VAL:O	2:F:17:ALA:HB2	2.05	0.56
1:E:105:ASN:ND2	1:E:105:ASN:C	2.58	0.55
1:A:105:ASN:HD22	1:A:105:ASN:C	2.05	0.54
1:A:79:VAL:O	2:B:17:ALA:HB2	2.08	0.53
1:G:105:ASN:ND2	1:G:105:ASN:O	2.36	0.52
1:C:105:ASN:C	1:C:105:ASN:ND2	2.58	0.52
1:C:105:ASN:O	1:C:105:ASN:ND2	2.35	0.51
1:A:5:ASP:OD1	1:A:117:LYS:HE3	2.11	0.50
1:E:21:LYS:O	1:E:98:VAL:HG22	2.13	0.48
1:E:17:LEU:HD12	1:E:17:LEU:C	2.35	0.47
1:G:17:LEU:HD12	1:G:17:LEU:C	2.35	0.47
1:C:17:LEU:HD12	1:C:17:LEU:C	2.35	0.47
1:G:20:ASN:HB3	1:G:23:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:ASN:HB3	1:E:23:THR:OG1	2.15	0.46
1:C:79:VAL:O	2:D:17:ALA:HB2	2.16	0.46
1:G:105:ASN:ND2	1:G:105:ASN:C	2.58	0.44
1:E:73:GLY:O	1:E:79:VAL:HA	2.17	0.44
1:C:5:ASP:OD1	1:C:117:LYS:HB3	2.17	0.44
2:B:13:GLY:O	1:C:107:PRO:HB2	2.18	0.44
2:B:18:LYS:HG2	2:B:18:LYS:O	2.17	0.44
1:A:17:LEU:C	1:A:17:LEU:HD12	2.38	0.43
2:B:15:TRP:NE1	1:C:105:ASN:ND2	2.52	0.43
1:E:107:PRO:HB2	2:H:13:GLY:O	2.18	0.42
1:C:24:ALA:HB1	1:C:82:ARG:HA	2.00	0.42
1:G:73:GLY:O	1:G:79:VAL:HA	2.18	0.42
1:C:20:ASN:HB3	1:C:23:THR:OG1	2.19	0.42
1:C:74:ASN:HD22	1:C:74:ASN:HA	1.53	0.42
1:E:56:ILE:HG23	1:E:93:TYR:CD2	2.55	0.42
1:C:24:ALA:CB	1:C:82:ARG:HA	2.50	0.41
1:C:73:GLY:O	1:C:79:VAL:HA	2.20	0.41
1:A:20:ASN:HB3	1:A:23:THR:OG1	2.20	0.41
1:A:56:ILE:HG23	1:A:93:TYR:CD2	2.54	0.41
1:E:24:ALA:HB1	1:E:82:ARG:HA	2.02	0.41
2:F:18:LYS:O	2:F:18:LYS:HG2	2.21	0.41
1:G:91:LYS:HG2	1:G:92:THR:N	2.36	0.41
1:C:21:LYS:O	1:C:98:VAL:HG22	2.20	0.40
2:H:18:LYS:HA	2:H:18:LYS:CE	2.47	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:18:LYS:NZ	2:B:18:LYS:NZ[10_665]	1.84	0.36

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	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
1	C	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
1	E	131/133 (98%)	127 (97%)	3 (2%)	1 (1%)	24	58
1	G	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
2	B	13/20 (65%)	13 (100%)	0	0	100	100
2	D	13/20 (65%)	13 (100%)	0	0	100	100
2	F	13/20 (65%)	13 (100%)	0	0	100	100
2	H	13/20 (65%)	13 (100%)	0	0	100	100
All	All	576/612 (94%)	559 (97%)	16 (3%)	1 (0%)	52	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	59	ASP

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	113/113 (100%)	106 (94%)	7 (6%)	23	54
1	C	113/113 (100%)	105 (93%)	8 (7%)	18	46
1	E	113/113 (100%)	107 (95%)	6 (5%)	28	61
1	G	113/113 (100%)	107 (95%)	6 (5%)	28	61
2	B	11/16 (69%)	10 (91%)	1 (9%)	12	33
2	D	11/16 (69%)	9 (82%)	2 (18%)	2	6
2	F	11/16 (69%)	10 (91%)	1 (9%)	12	33
2	H	11/16 (69%)	9 (82%)	2 (18%)	2	6
All	All	496/516 (96%)	463 (93%)	33 (7%)	20	50

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	37	SER
1	A	74	ASN
1	A	76	SER
1	A	84	LEU
1	A	102	THR
1	A	105	ASN
2	B	9	THR
1	C	2	LYS
1	C	37	SER
1	C	74	ASN
1	C	84	LEU
1	C	100	SER
1	C	102	THR
1	C	105	ASN
1	C	131	LEU
2	D	9	THR
2	D	18	LYS
1	E	37	SER
1	E	59	ASP
1	E	74	ASN
1	E	84	LEU
1	E	102	THR
1	E	105	ASN
2	F	9	THR
1	G	37	SER
1	G	74	ASN
1	G	76	SER
1	G	84	LEU
1	G	102	THR
1	G	105	ASN
2	H	9	THR
2	H	18	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	105	ASN
1	C	20	ASN
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	105	ASN
1	E	74	ASN
1	E	105	ASN
1	G	20	ASN
1	G	74	ASN
1	G	105	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MGC	A	1200	-	16,16,16	0.88	0	21,22,22	4.79	5 (23%)
3	MGC	C	2200	-	16,16,16	1.40	2 (12%)	21,22,22	4.20	9 (42%)
3	MGC	E	3200	-	16,16,16	1.10	1 (6%)	21,22,22	4.43	6 (28%)
3	MGC	G	4200	-	16,16,16	3.00	8 (50%)	21,22,22	5.70	9 (42%)

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	MGC	A	1200	-	-	0/8/28/28	0/1/1/1
3	MGC	C	2200	-	-	0/8/28/28	0/1/1/1
3	MGC	E	3200	-	-	0/8/28/28	0/1/1/1
3	MGC	G	4200	-	-	0/8/28/28	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4200	MGC	O3-C3	-3.44	1.34	1.43
3	G	4200	MGC	O1-C1	-3.42	1.34	1.40
3	G	4200	MGC	O1-CM	-2.08	1.34	1.42
3	C	2200	MGC	C8-C7	2.11	1.54	1.50
3	E	3200	MGC	C1-C2	2.24	1.57	1.53
3	G	4200	MGC	C4-C3	2.42	1.58	1.52
3	G	4200	MGC	C1-C2	2.80	1.58	1.53
3	G	4200	MGC	C2-N2	3.16	1.51	1.45
3	C	2200	MGC	C3-C2	4.22	1.61	1.53
3	G	4200	MGC	O5-C1	4.28	1.52	1.41
3	G	4200	MGC	C8-C7	7.86	1.66	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4200	MGC	C2-N2-C7	-3.81	113.34	123.10
3	G	4200	MGC	C4-C3-C2	-3.80	105.17	110.43
3	A	1200	MGC	C2-N2-C7	-3.65	113.74	123.10
3	C	2200	MGC	C2-N2-C7	-3.47	114.20	123.10
3	E	3200	MGC	C2-N2-C7	-3.38	114.44	123.10
3	E	3200	MGC	O7-C7-C8	-3.05	116.47	122.06
3	C	2200	MGC	C3-C2-N2	-2.34	105.82	110.66
3	A	1200	MGC	C3-C2-N2	-2.15	106.22	110.66
3	C	2200	MGC	C3-C4-C5	-2.13	106.49	110.20
3	C	2200	MGC	O5-C1-C2	-2.06	106.29	110.78
3	G	4200	MGC	O5-C1-O1	-2.04	105.97	110.88
3	G	4200	MGC	C3-C2-N2	2.08	114.97	110.66
3	G	4200	MGC	O5-C1-C2	2.16	115.48	110.78
3	E	3200	MGC	O5-C5-C6	2.39	112.39	106.36
3	C	2200	MGC	O3-C3-C2	2.41	114.56	109.66
3	C	2200	MGC	C1-O5-C5	4.44	122.36	113.75
3	G	4200	MGC	O4-C4-C3	4.49	120.44	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	G	4200	MGC	O1-C1-C2	7.34	119.95	108.03
3	E	3200	MGC	O1-C1-C2	7.83	120.75	108.03
3	E	3200	MGC	O6-C6-C5	8.12	138.16	111.33
3	C	2200	MGC	O1-C1-C2	8.17	121.29	108.03
3	C	2200	MGC	O6-C6-C5	8.22	138.49	111.33
3	A	1200	MGC	O6-C6-C5	8.41	139.11	111.33
3	G	4200	MGC	O6-C6-C5	8.52	139.48	111.33
3	A	1200	MGC	O1-C1-C2	9.30	123.13	108.03
3	C	2200	MGC	CM-O1-C1	13.30	135.06	113.29
3	E	3200	MGC	CM-O1-C1	15.67	138.94	113.29
3	A	1200	MGC	CM-O1-C1	16.99	141.10	113.29
3	G	4200	MGC	CM-O1-C1	21.82	149.00	113.29

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 [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, 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	133/133 (100%)	-0.52	0 100 100	13, 27, 52, 78	0
1	C	133/133 (100%)	-0.51	0 100 100	15, 26, 51, 78	0
1	E	133/133 (100%)	-0.51	0 100 100	15, 28, 52, 83	0
1	G	133/133 (100%)	-0.17	3 (2%) 64 52	17, 36, 61, 83	0
2	B	15/20 (75%)	-0.52	0 100 100	15, 26, 58, 102	0
2	D	15/20 (75%)	-0.27	0 100 100	16, 25, 54, 101	0
2	F	15/20 (75%)	-0.29	1 (6%) 21 12	18, 27, 69, 97	0
2	H	15/20 (75%)	-0.25	1 (6%) 21 12	19, 34, 62, 103	0
All	All	592/612 (96%)	-0.42	5 (0%) 87 81	13, 29, 58, 103	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	18	LYS	3.1
1	G	74	ASN	3.1
1	G	53	PRO	2.2
1	G	52	THR	2.2
2	F	18	LYS	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](#)

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	MGC	E	3200	16/16	0.93	0.18	0.91	31,31,31,31	0
3	MGC	G	4200	16/16	0.82	0.27	0.71	53,53,53,53	0
3	MGC	A	1200	16/16	0.95	0.16	0.34	28,28,28,28	0
3	MGC	C	2200	16/16	0.94	0.16	-0.02	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.