Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 03:29 PM GMT

PDB ID	:	4CDH
Title	:	Crystallographic structure of the Human Igg1 alpha 2-6 sialilated Fc-Fragment
Authors	:	Silva-Martin, N.; Bartual, S.G.; Hermoso, J.A.
Deposited on	:	2013-10-31
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

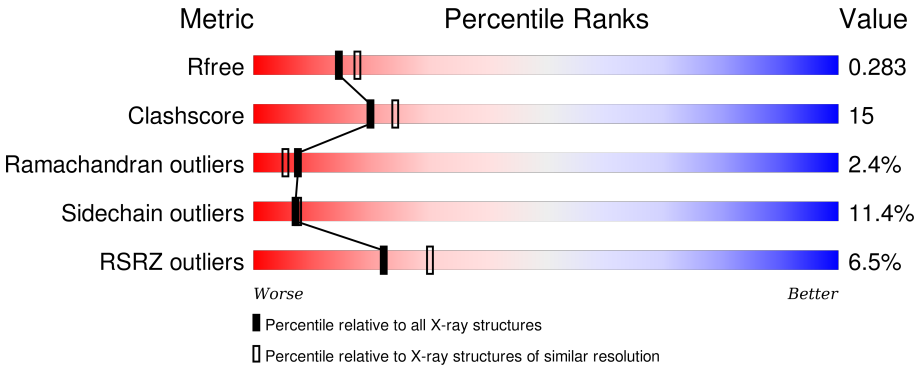
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	A	255	62% 17% • 19%
1	B	255	11% 47% 25% 9% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3619 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 IG GAMMA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1654	1054	278	316	6			
1	B	208	Total	C	N	O	S	0	0	0
			1662	1058	280	318	6			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	EXPRESSION TAG	UNP P01857
A	-25	LYS	-	EXPRESSION TAG	UNP P01857
A	-24	LYS	-	EXPRESSION TAG	UNP P01857
A	-23	THR	-	EXPRESSION TAG	UNP P01857
A	-22	ALA	-	EXPRESSION TAG	UNP P01857
A	-21	ILE	-	EXPRESSION TAG	UNP P01857
A	-20	ALA	-	EXPRESSION TAG	UNP P01857
A	-19	ILE	-	EXPRESSION TAG	UNP P01857
A	-18	ALA	-	EXPRESSION TAG	UNP P01857
A	-17	VAL	-	EXPRESSION TAG	UNP P01857
A	-16	ALA	-	EXPRESSION TAG	UNP P01857
A	-15	LEU	-	EXPRESSION TAG	UNP P01857
A	-14	ALA	-	EXPRESSION TAG	UNP P01857
A	-13	GLY	-	EXPRESSION TAG	UNP P01857
A	-12	PHE	-	EXPRESSION TAG	UNP P01857
A	-11	ALA	-	EXPRESSION TAG	UNP P01857
A	-10	THR	-	EXPRESSION TAG	UNP P01857
A	-9	VAL	-	EXPRESSION TAG	UNP P01857
A	-8	ALA	-	EXPRESSION TAG	UNP P01857
A	-7	GLN	-	EXPRESSION TAG	UNP P01857
A	-6	ALA	-	EXPRESSION TAG	UNP P01857
A	-5	ASP	-	EXPRESSION TAG	UNP P01857
A	-4	VAL	-	EXPRESSION TAG	UNP P01857
A	-3	GLU	-	EXPRESSION TAG	UNP P01857
A	-2	SER	-	EXPRESSION TAG	UNP P01857

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-26	MET	-	EXPRESSION TAG	UNP P01857
B	-25	LYS	-	EXPRESSION TAG	UNP P01857
B	-24	LYS	-	EXPRESSION TAG	UNP P01857
B	-23	THR	-	EXPRESSION TAG	UNP P01857
B	-22	ALA	-	EXPRESSION TAG	UNP P01857
B	-21	ILE	-	EXPRESSION TAG	UNP P01857
B	-20	ALA	-	EXPRESSION TAG	UNP P01857
B	-19	ILE	-	EXPRESSION TAG	UNP P01857
B	-18	ALA	-	EXPRESSION TAG	UNP P01857
B	-17	VAL	-	EXPRESSION TAG	UNP P01857
B	-16	ALA	-	EXPRESSION TAG	UNP P01857
B	-15	LEU	-	EXPRESSION TAG	UNP P01857
B	-14	ALA	-	EXPRESSION TAG	UNP P01857
B	-13	GLY	-	EXPRESSION TAG	UNP P01857
B	-12	PHE	-	EXPRESSION TAG	UNP P01857
B	-11	ALA	-	EXPRESSION TAG	UNP P01857
B	-10	THR	-	EXPRESSION TAG	UNP P01857
B	-9	VAL	-	EXPRESSION TAG	UNP P01857
B	-8	ALA	-	EXPRESSION TAG	UNP P01857
B	-7	GLN	-	EXPRESSION TAG	UNP P01857
B	-6	ALA	-	EXPRESSION TAG	UNP P01857
B	-5	ASP	-	EXPRESSION TAG	UNP P01857
B	-4	VAL	-	EXPRESSION TAG	UNP P01857
B	-3	GLU	-	EXPRESSION TAG	UNP P01857
B	-2	SER	-	EXPRESSION TAG	UNP P01857

- Molecule 2 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	10	Total	C	N	O	0	0
			121	68	4	49		

- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	8	Total	C	N	O	0	0
			100	56	4	40		

- Molecule 4 is water.

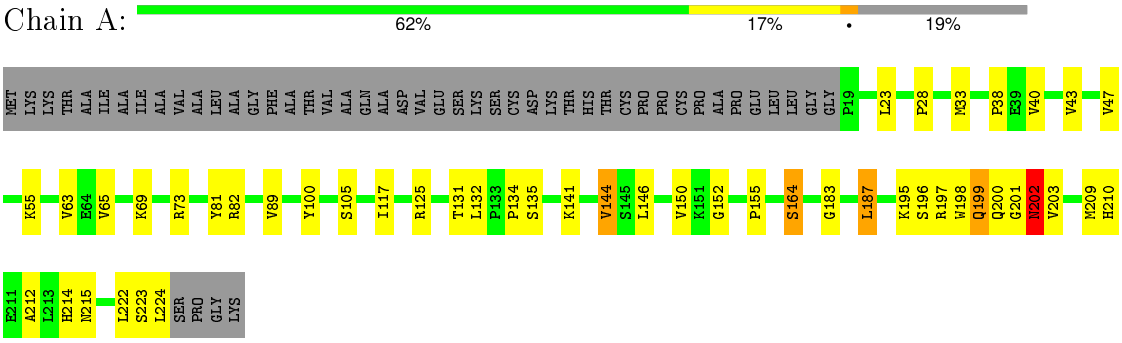
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	49	Total O 49 49	0	0
4	B	33	Total O 33 33	0	0

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.

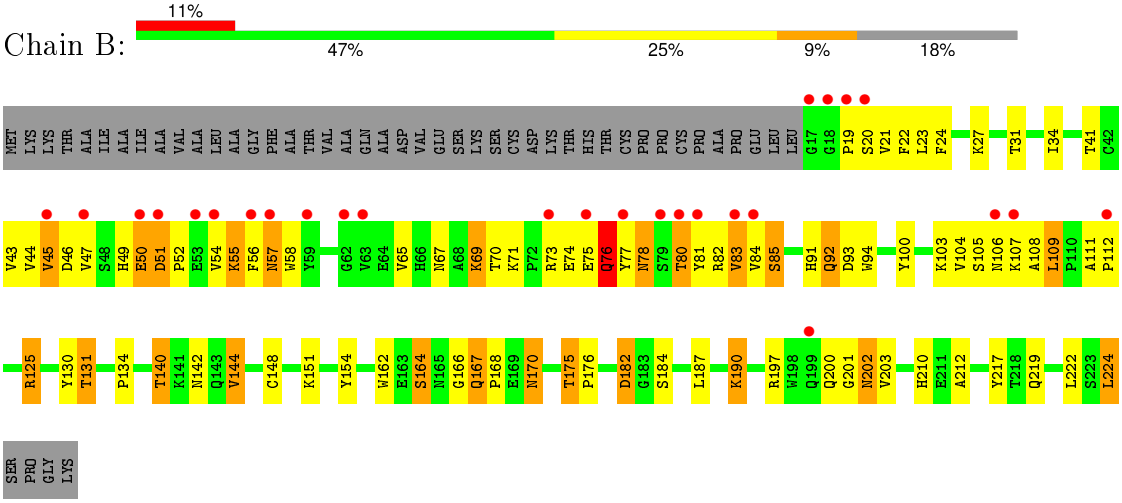
- Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain A:



- Molecule 1: IG GAMMA-1 CHAIN C REGION

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	49.59Å 80.15Å 140.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.10 – 2.30 42.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.10-2.30) 100.0 (42.17-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.234 , 0.282 0.238 , 0.283	Depositor DCC
R_{free} test set	1299 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 25579 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3619	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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: GAL, FUL, BMA, NAG, MAN

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	0.77	0/1700	0.86	0/2316
1	B	0.81	0/1708	0.93	1/2327 (0.0%)
All	All	0.79	0/3408	0.90	1/4643 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	182	ASP	CB-CA-C	-5.78	98.84	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1654	0	1623	35	0
1	B	1662	0	1628	68	0
2	A	121	0	103	1	0
3	B	100	0	85	4	0
4	A	49	0	0	2	0
4	B	33	0	0	5	0
All	All	3619	0	3439	103	0

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 15.

All (103) 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:41:THR:HG21	3:B:1005:NAG:O6	1.67	0.94
1:B:131:THR:HG23	1:B:222:LEU:HD13	1.60	0.82
1:B:201:GLY:HA2	1:B:224:LEU:HD11	1.61	0.81
1:B:76:GLN:HE22	1:B:82:ARG:HG3	1.46	0.81
1:B:91:HIS:HA	4:B:2010:HOH:O	1.80	0.80
1:A:164:SER:OG	1:A:203:VAL:O	2.01	0.78
1:B:75:GLU:O	1:B:76:GLN:HB2	1.85	0.76
1:B:164:SER:OG	1:B:203:VAL:O	2.04	0.75
1:B:92:GLN:N	4:B:2010:HOH:O	2.15	0.73
1:A:198:TRP:O	1:A:224:LEU:HD11	1.89	0.72
1:A:33:MET:CE	1:A:209:MET:SD	2.77	0.72
1:B:41:THR:HG21	3:B:1005:NAG:HO6	1.55	0.71
1:A:125:ARG:HG3	1:A:152:GLY:O	1.89	0.71
1:B:210:HIS:HD2	1:B:212:ALA:H	1.39	0.70
1:A:198:TRP:O	1:A:224:LEU:CD1	2.39	0.70
1:A:195:LYS:O	1:A:199:GLN:HG2	1.93	0.68
1:B:20:SER:O	1:B:44:VAL:O	2.10	0.68
1:B:81:TYR:HB3	4:B:2008:HOH:O	1.92	0.68
1:A:33:MET:HE2	1:A:209:MET:SD	2.36	0.65
1:A:33:MET:HE3	1:A:209:MET:SD	2.38	0.63
1:A:125:ARG:CG	1:A:152:GLY:O	2.47	0.63
1:A:134:PRO:HG3	1:A:144:VAL:HG13	1.82	0.61
1:A:150:VAL:HB	1:A:187:LEU:CD2	2.32	0.60
1:B:41:THR:CG2	3:B:1005:NAG:O6	2.46	0.60
1:B:224:LEU:H	1:B:224:LEU:HD12	1.67	0.60
1:A:135:SER:HB2	1:B:130:TYR:HB3	1.85	0.59
1:B:140:THR:OG1	1:B:140:THR:O	2.20	0.59
1:A:210:HIS:CD2	1:A:212:ALA:H	2.21	0.58
1:B:21:VAL:O	1:B:22:PHE:CD1	2.56	0.58
1:B:182:ASP:HB3	1:B:184:SER:H	1.68	0.58
1:B:190:LYS:HD2	4:B:2024:HOH:O	2.03	0.58
1:A:201:GLY:CA	1:A:202:ASN:HB2	2.33	0.58
1:A:89:VAL:HG22	1:A:100:TYR:CZ	2.40	0.57
1:A:134:PRO:HG3	1:A:144:VAL:CG1	2.37	0.55
1:B:19:PRO:HB3	1:B:46:ASP:O	2.06	0.55
1:A:155:PRO:O	1:A:210:HIS:HE1	1.90	0.54
1:A:89:VAL:HG22	1:A:100:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NH1	2:A:1002:NAG:O7	2.40	0.54
4:A:2033:HOH:O	1:B:190:LYS:HD3	2.07	0.54
1:B:125:ARG:HG3	1:B:154:TYR:HB3	1.90	0.54
1:A:183:GLY:HA2	4:A:2043:HOH:O	2.07	0.53
1:B:91:HIS:CA	4:B:2010:HOH:O	2.48	0.53
1:B:71:LYS:HB3	1:B:84:VAL:HG22	1.90	0.52
1:B:47:VAL:O	1:B:80:THR:HG22	2.09	0.52
1:B:45:VAL:HG12	1:B:46:ASP:H	1.75	0.52
1:B:175:THR:HG23	1:B:176:PRO:O	2.11	0.51
1:B:109:LEU:HD22	1:B:111:ALA:O	2.11	0.51
1:A:131:THR:HG21	1:A:222:LEU:HB2	1.92	0.51
1:A:201:GLY:HA3	1:A:202:ASN:HB2	1.92	0.51
1:A:23:LEU:HD11	1:A:40:VAL:CG1	2.41	0.51
1:A:131:THR:HG22	1:A:222:LEU:HD22	1.94	0.50
1:B:47:VAL:H	1:B:80:THR:HB	1.76	0.49
1:B:77:TYR:O	1:B:78:ASN:HB3	2.12	0.49
1:A:55:LYS:HB3	1:A:105:SER:HB2	1.92	0.49
1:B:91:HIS:O	1:B:92:GLN:HB2	2.13	0.49
1:A:43:VAL:HG11	1:A:82:ARG:NH1	2.28	0.49
1:B:210:HIS:CD2	1:B:212:ALA:H	2.25	0.48
1:A:131:THR:O	1:A:132:LEU:HD12	2.14	0.48
3:B:1001:NAG:H82	3:B:1001:NAG:O3	2.15	0.47
1:B:47:VAL:N	1:B:80:THR:HB	2.29	0.47
1:B:111:ALA:HB1	1:B:112:PRO:HD2	1.97	0.47
1:B:70:THR:HA	1:B:85:SER:HA	1.97	0.47
1:A:210:HIS:HD2	1:A:212:ALA:H	1.62	0.46
1:B:56:PHE:HZ	1:B:83:VAL:O	1.99	0.46
1:B:106:ASN:OD1	1:B:108:ALA:N	2.47	0.46
1:B:58:TRP:HE1	1:B:85:SER:HG	1.64	0.45
1:B:71:LYS:HB3	1:B:84:VAL:CG2	2.46	0.45
1:B:24:PHE:CD1	1:B:24:PHE:N	2.85	0.45
1:B:91:HIS:CD2	1:B:91:HIS:H	2.35	0.44
1:A:134:PRO:HD3	1:A:146:LEU:HD23	2.00	0.44
1:B:134:PRO:HB3	1:B:144:VAL:HG22	1.98	0.44
1:B:202:ASN:N	1:B:202:ASN:OD1	2.51	0.44
1:B:51:ASP:OD1	1:B:108:ALA:HB2	2.18	0.44
1:B:170:ASN:C	1:B:170:ASN:OD1	2.55	0.44
1:B:69:LYS:HA	1:B:69:LYS:CE	2.48	0.43
1:A:38:PRO:HG2	1:A:89:VAL:O	2.18	0.43
1:B:54:VAL:HG12	1:B:55:LYS:N	2.33	0.43
1:B:201:GLY:CA	1:B:224:LEU:HD11	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:O	1:B:81:TYR:HB2	2.19	0.43
1:A:201:GLY:CA	1:A:202:ASN:CB	2.97	0.43
1:B:45:VAL:HG12	1:B:46:ASP:N	2.33	0.43
1:B:175:THR:HG22	1:B:187:LEU:HB2	2.01	0.43
1:B:57:ASN:HB2	1:B:103:LYS:HB3	2.00	0.43
1:B:166:GLY:C	1:B:167:GLN:HE21	2.22	0.43
1:A:214:HIS:O	1:A:215:ASN:HB2	2.18	0.43
1:B:187:LEU:C	1:B:187:LEU:HD12	2.39	0.42
1:B:50:GLU:C	1:B:52:PRO:HD3	2.39	0.42
1:B:77:TYR:O	1:B:78:ASN:CB	2.67	0.42
1:B:104:VAL:HG12	1:B:105:SER:N	2.35	0.42
1:B:167:GLN:HA	1:B:168:PRO:HD3	1.89	0.42
1:B:69:LYS:HE2	1:B:69:LYS:HA	2.02	0.42
1:A:131:THR:C	1:A:132:LEU:HD12	2.39	0.41
1:B:55:LYS:HB3	1:B:105:SER:HB2	2.02	0.41
1:B:182:ASP:CB	1:B:184:SER:H	2.33	0.41
1:B:175:THR:CG2	1:B:176:PRO:O	2.68	0.41
1:B:148:CYS:HB2	1:B:162:TRP:CZ2	2.55	0.41
1:B:71:LYS:HD3	1:B:84:VAL:HG21	2.03	0.41
1:B:217:TYR:CE1	1:B:219:GLN:HG3	2.55	0.41
1:B:93:ASP:HB3	1:B:100:TYR:OH	2.21	0.41
1:B:31:THR:HG21	1:B:94:TRP:CD1	2.56	0.41
1:A:134:PRO:HD3	1:A:146:LEU:CD2	2.51	0.40
1:A:47:VAL:HB	1:A:81:TYR:HB2	2.02	0.40
1:B:200:GLN:CG	1:B:202:ASN:OD1	2.70	0.40

There are no symmetry-related clashes.

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	204/255 (80%)	197 (97%)	6 (3%)	1 (0%)	34 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	206/255 (81%)	176 (85%)	21 (10%)	9 (4%)	3 1
All	All	410/510 (80%)	373 (91%)	27 (7%)	10 (2%)	7 5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	45	VAL
1	B	78	ASN
1	B	76	GLN
1	B	80	THR
1	B	85	SER
1	B	92	GLN
1	A	202	ASN
1	B	67	ASN
1	B	50	GLU
1	B	83	VAL

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	193/229 (84%)	177 (92%)	16 (8%)	14 17
1	B	193/229 (84%)	165 (86%)	28 (14%)	4 3
All	All	386/458 (84%)	342 (89%)	44 (11%)	7 7

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	63	VAL
1	A	65	VAL
1	A	69	LYS
1	A	73	ARG
1	A	117	ILE

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Mol	Chain	Res	Type
1	A	141	LYS
1	A	144	VAL
1	A	164	SER
1	A	187	LEU
1	A	196	SER
1	A	197	ARG
1	A	199	GLN
1	A	200	GLN
1	A	202	ASN
1	A	223	SER
1	B	23	LEU
1	B	27	LYS
1	B	34	ILE
1	B	43	VAL
1	B	49	HIS
1	B	51	ASP
1	B	55	LYS
1	B	57	ASN
1	B	65	VAL
1	B	69	LYS
1	B	73	ARG
1	B	76	GLN
1	B	107	LYS
1	B	109	LEU
1	B	125	ARG
1	B	131	THR
1	B	140	THR
1	B	142	ASN
1	B	144	VAL
1	B	151	LYS
1	B	164	SER
1	B	167	GLN
1	B	170	ASN
1	B	175	THR
1	B	190	LYS
1	B	197	ARG
1	B	202	ASN
1	B	224	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	76	GLN
1	A	92	GLN
1	A	199	GLN
1	A	202	ASN
1	A	210	HIS
1	A	219	GLN
1	B	76	GLN
1	B	91	HIS
1	B	142	ASN
1	B	167	GLN
1	B	210	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

18 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	NAG	A	1001	1,2	14,14,15	0.42	0	15,19,21	1.85	5 (33%)
2	NAG	A	1002	2	14,14,15	1.00	1 (7%)	15,19,21	1.25	2 (13%)
2	BMA	A	1003	2	11,11,12	1.02	1 (9%)	14,15,17	1.96	3 (21%)
2	MAN	A	1004	2	11,11,12	0.81	0	14,15,17	2.03	6 (42%)
2	NAG	A	1005	2	14,14,15	0.93	1 (7%)	15,19,21	1.99	3 (20%)
2	GAL	A	1006	2	11,11,12	0.89	0	14,15,17	1.72	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	A	1008	2	11,11,12	0.77	0	14,15,17	2.26	7 (50%)
2	NAG	A	1009	2	14,14,15	0.68	0	15,19,21	2.19	6 (40%)
2	GAL	A	1010	2	11,11,12	0.82	0	14,15,17	2.57	4 (28%)
2	FUL	A	1011	2	10,10,11	0.65	0	14,14,16	1.91	4 (28%)
3	NAG	B	1001	1,3	14,14,15	0.68	0	15,19,21	3.12	5 (33%)
3	NAG	B	1002	3	14,14,15	0.66	0	15,19,21	1.22	2 (13%)
3	BMA	B	1003	3	11,11,12	0.77	0	14,15,17	2.29	7 (50%)
3	MAN	B	1004	3	11,11,12	0.65	0	14,15,17	2.10	4 (28%)
3	NAG	B	1005	3	14,14,15	0.77	0	15,19,21	2.31	7 (46%)
3	GAL	B	1006	3	11,11,12	0.65	0	14,15,17	1.98	4 (28%)
3	MAN	B	1008	3	11,11,12	0.55	0	14,15,17	1.72	4 (28%)
3	NAG	B	1009	3	14,14,15	0.65	0	15,19,21	2.10	6 (40%)

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	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1003	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1004	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1005	2	-	0/6/23/26	0/1/1/1
2	GAL	A	1006	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1008	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1009	2	-	0/6/23/26	0/1/1/1
2	GAL	A	1010	2	-	0/2/19/22	0/1/1/1
2	FUL	A	1011	2	-	0/0/17/20	0/1/1/1
3	NAG	B	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3	-	0/6/23/26	0/1/1/1
3	BMA	B	1003	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1004	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1005	3	-	0/6/23/26	0/1/1/1
3	GAL	B	1006	3	-	0/2/19/22	0/1/1/1
3	MAN	B	1008	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1009	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	NAG	O5-C1	-2.61	1.39	1.43
2	A	1005	NAG	O5-C1	-2.37	1.39	1.43
2	A	1003	BMA	O5-C1	-2.10	1.40	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1010	GAL	C1-C2-C3	-6.55	101.80	109.54
3	B	1003	BMA	O5-C1-C2	-4.96	102.81	110.86
2	A	1008	MAN	O2-C2-C3	-4.26	101.56	110.12
2	A	1004	MAN	C1-O5-C5	-3.88	107.32	112.25
3	B	1003	BMA	O2-C2-C1	-3.84	101.51	109.21
2	A	1010	GAL	O5-C1-C2	-3.73	104.81	110.86
2	A	1011	FUL	O2-C2-C1	-3.40	102.39	109.21
3	B	1005	NAG	O7-C7-C8	-3.39	115.84	122.06
3	B	1006	GAL	O2-C2-C3	-3.28	103.53	110.12
3	B	1004	MAN	C2-C3-C4	-3.09	105.79	111.04
3	B	1008	MAN	C3-C4-C5	-3.08	104.83	110.20
2	A	1005	NAG	C4-C3-C2	-3.00	106.56	111.23
2	A	1006	GAL	O2-C2-C3	-2.97	104.15	110.12
3	B	1005	NAG	O3-C3-C4	-2.91	103.78	110.34
2	A	1006	GAL	C6-C5-C4	-2.86	105.95	113.02
3	B	1001	NAG	O7-C7-C8	-2.82	116.89	122.06
2	A	1009	NAG	C4-C3-C2	-2.73	106.99	111.23
2	A	1005	NAG	O7-C7-C8	-2.72	117.07	122.06
2	A	1004	MAN	O2-C2-C3	-2.67	104.75	110.12
2	A	1002	NAG	C3-C4-C5	-2.66	105.56	110.20
3	B	1006	GAL	C2-C3-C4	-2.62	106.59	111.04
2	A	1008	MAN	C2-C3-C4	-2.55	106.70	111.04
3	B	1002	NAG	C1-O5-C5	-2.49	109.08	112.25
3	B	1003	BMA	O3-C3-C4	-2.48	104.75	110.34
2	A	1011	FUL	O5-C1-C2	-2.43	106.92	110.86
2	A	1006	GAL	C2-C3-C4	-2.40	106.96	111.04
2	A	1003	BMA	O4-C4-C3	-2.35	105.04	110.34
2	A	1002	NAG	C4-C3-C2	-2.33	107.60	111.23
2	A	1008	MAN	O4-C4-C3	-2.27	105.23	110.34
3	B	1008	MAN	O5-C1-C2	-2.26	107.18	110.86
3	B	1004	MAN	O4-C4-C3	-2.24	105.29	110.34
2	A	1001	NAG	C6-C5-C4	-2.23	107.51	113.02
2	A	1004	MAN	C2-C3-C4	-2.16	107.37	111.04
3	B	1009	NAG	O7-C7-C8	-2.14	118.14	122.06
3	B	1003	BMA	C1-O5-C5	-2.12	109.56	112.25
2	A	1001	NAG	C4-C3-C2	-2.07	108.00	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1003	BMA	O3-C3-C4	-2.06	105.71	110.34
3	B	1003	BMA	O6-C6-C5	-2.04	104.61	111.33
2	A	1004	MAN	O4-C4-C5	2.05	114.66	109.24
2	A	1009	NAG	O4-C4-C3	2.06	114.98	110.34
3	B	1003	BMA	C3-C4-C5	2.11	113.88	110.20
3	B	1004	MAN	O5-C1-C2	2.17	114.38	110.86
3	B	1008	MAN	O3-C3-C2	2.18	113.94	110.00
2	A	1009	NAG	O4-C4-C5	2.30	115.32	109.24
2	A	1006	GAL	O2-C2-C1	2.32	113.87	109.21
3	B	1002	NAG	O4-C4-C5	2.41	115.63	109.24
2	A	1008	MAN	O5-C1-C2	2.44	114.82	110.86
3	B	1005	NAG	O3-C3-C2	2.45	113.97	109.11
2	A	1006	GAL	O5-C5-C6	2.46	112.68	107.35
2	A	1008	MAN	C1-C2-C3	2.60	112.62	109.54
3	B	1005	NAG	C3-C4-C5	2.63	114.78	110.20
2	A	1001	NAG	C3-C2-N2	2.70	117.02	110.56
2	A	1004	MAN	C1-C2-C3	2.82	112.88	109.54
3	B	1003	BMA	C1-C2-C3	2.87	112.93	109.54
3	B	1001	NAG	C2-N2-C7	2.88	126.75	123.04
2	A	1008	MAN	O4-C4-C5	2.89	116.90	109.24
3	B	1005	NAG	C3-C2-N2	2.91	117.53	110.56
3	B	1009	NAG	O5-C5-C6	2.95	113.72	107.35
2	A	1001	NAG	C2-N2-C7	3.05	126.95	123.04
3	B	1006	GAL	O2-C2-C1	3.10	115.43	109.21
2	A	1011	FUL	C1-C2-C3	3.11	113.22	109.54
2	A	1004	MAN	C6-C5-C4	3.14	120.76	113.02
3	B	1009	NAG	C8-C7-N2	3.16	122.15	116.11
2	A	1009	NAG	C3-C2-N2	3.25	118.34	110.56
2	A	1009	NAG	O3-C3-C4	3.25	117.65	110.34
3	B	1008	MAN	O5-C5-C6	3.25	114.39	107.35
2	A	1008	MAN	O2-C2-C1	3.27	115.75	109.21
3	B	1005	NAG	C8-C7-N2	3.27	122.36	116.11
3	B	1009	NAG	C1-O5-C5	3.30	116.44	112.25
3	B	1009	NAG	C3-C4-C5	3.31	115.97	110.20
3	B	1001	NAG	C3-C4-C5	3.32	115.98	110.20
2	A	1010	GAL	O2-C2-C1	3.63	116.48	109.21
2	A	1001	NAG	C1-O5-C5	3.73	116.99	112.25
3	B	1001	NAG	C8-C7-N2	3.78	123.34	116.11
3	B	1009	NAG	C4-C3-C2	3.93	117.34	111.23
2	A	1011	FUL	C1-O5-C5	4.02	118.59	112.38
2	A	1010	GAL	C3-C4-C5	4.14	117.41	110.20
3	B	1005	NAG	C1-O5-C5	4.18	117.55	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1006	GAL	O5-C5-C6	4.23	116.50	107.35
2	A	1005	NAG	C8-C7-N2	4.42	124.57	116.11
2	A	1009	NAG	C2-N2-C7	4.45	128.75	123.04
2	A	1003	BMA	C1-C2-C3	5.38	115.91	109.54
3	B	1004	MAN	C1-O5-C5	5.45	119.17	112.25
3	B	1001	NAG	C1-O5-C5	9.62	124.46	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	NAG	1	0
3	B	1001	NAG	1	0
3	B	1005	NAG	3	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	206/255 (80%)	-0.02	0 100 100	21, 35, 58, 69	0
1	B	208/255 (81%)	0.64	27 (12%) 5 7	18, 45, 82, 98	0
All	All	414/510 (81%)	0.31	27 (6%) 22 30	18, 39, 77, 98	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	VAL	8.0
1	B	81	TYR	6.2
1	B	54	VAL	3.9
1	B	77	TYR	3.7
1	B	45	VAL	3.6
1	B	18	GLY	3.6
1	B	20	SER	3.4
1	B	107	LYS	3.3
1	B	79	SER	3.2
1	B	47	VAL	3.1
1	B	50	GLU	3.0
1	B	75	GLU	3.0
1	B	19	PRO	2.9
1	B	80	THR	2.7
1	B	17	GLY	2.7
1	B	59	TYR	2.5
1	B	51	ASP	2.5
1	B	62	GLY	2.5
1	B	84	VAL	2.4
1	B	112	PRO	2.3
1	B	106	ASN	2.3
1	B	56	PHE	2.3
1	B	63	VAL	2.2
1	B	53	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	57	ASN	2.1
1	B	73	ARG	2.1
1	B	199	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	GAL	B	1006	11/12	0.89	0.14	-0.28	40,43,52,53	0
2	NAG	A	1005	14/15	0.94	0.12	-0.56	40,46,52,58	0
2	GAL	A	1006	11/12	0.97	0.12	-0.76	30,36,42,51	0
3	NAG	B	1005	14/15	0.91	0.13	-1.37	50,56,66,70	0
3	NAG	B	1009	14/15	0.82	0.22	-	69,78,87,87	0
2	GAL	A	1010	11/12	0.38	0.26	-	69,76,84,85	0
3	BMA	B	1003	11/12	0.84	0.13	-	61,67,71,74	0
2	NAG	A	1009	14/15	0.74	0.29	-	56,77,84,86	0
3	NAG	B	1002	14/15	0.76	0.21	-	68,76,87,90	0
3	NAG	B	1001	14/15	0.62	0.31	-	60,74,86,92	0
2	MAN	A	1004	11/12	0.91	0.10	-	41,47,50,55	0
2	NAG	A	1001	14/15	0.90	0.11	-	42,49,63,66	0
2	FUL	A	1011	10/11	0.86	0.23	-	63,69,72,76	0
2	BMA	A	1003	11/12	0.91	0.12	-	37,44,53,54	0
2	NAG	A	1002	14/15	0.95	0.11	-	34,38,43,46	0
3	MAN	B	1004	11/12	0.87	0.11	-	59,62,64,65	0
3	MAN	B	1008	11/12	0.86	0.14	-	63,67,69,75	0
2	MAN	A	1008	11/12	0.89	0.13	-	60,63,68,68	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.