Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 AM GMT

PDB ID	:	2J61
Title	:	L-FICOLIN COMPLEXED TO N-ACETYLGLUCOSAMINE (FORME C)
Authors	:	Garlatti, V.; Gaboriaud, C.
Deposited on	:	2006-09-21
Resolution	:	2.70 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:

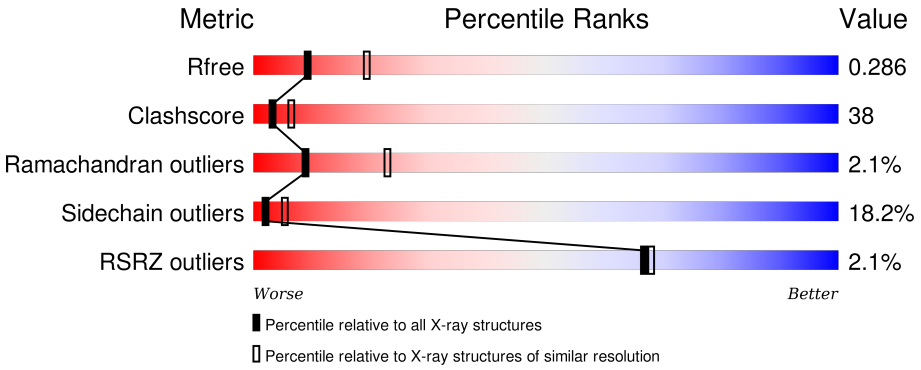
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	218	% 38% 48% 13% ••
2	B	218	3% 36% 50% 12% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1290	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3553 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 FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	1	0
			1738	1094	306	329	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	THR	VAL	CONFLICT	UNP Q15485
A	186	ARG	LYS	CONFLICT	UNP Q15485
A	247	THR	VAL	CONFLICT	UNP Q15485

- Molecule 2 is a protein called FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	1	0
			1736	1094	304	329	9			

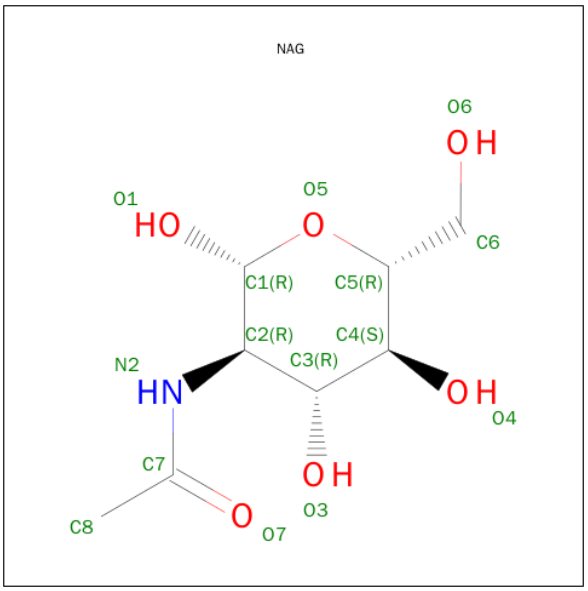
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	168	THR	VAL	CONFLICT	UNP Q15485
B	247	THR	VAL	CONFLICT	UNP Q15485

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 8 1 6	0	0

- Molecule 5 is water.

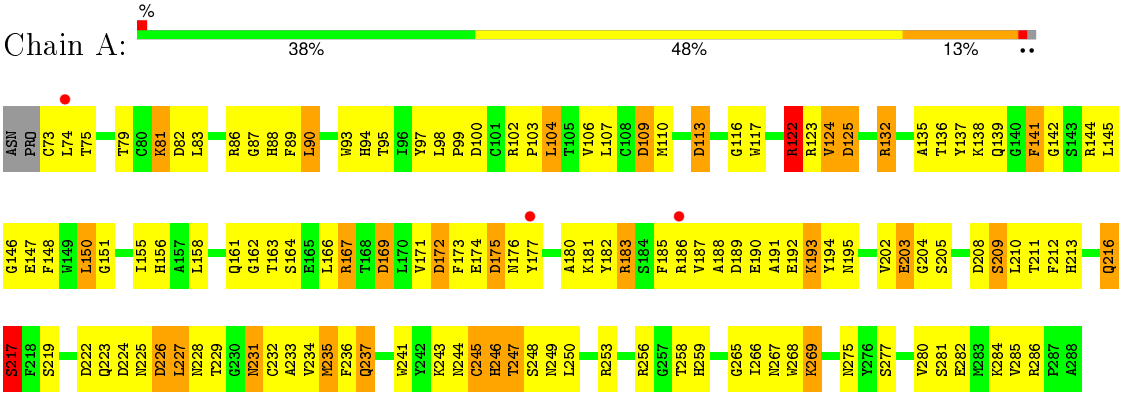
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	29	Total O 29 29	0	0
5	B	33	Total O 33 33	0	0

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.

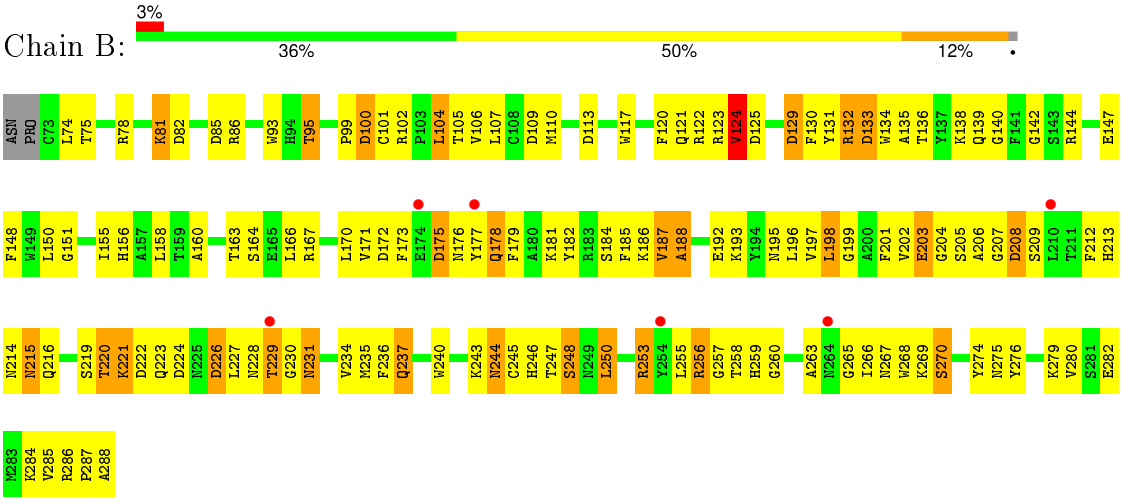
- Molecule 1: FICOLIN-2

Chain A:



- Molecule 2: FICOLIN-2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	79.59Å 79.59Å 172.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.70 19.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.70) 99.8 (19.39-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.291 0.204 , 0.286	Depositor DCC
R_{free} test set	990 reflections (6.25%)	DCC
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.6	EDS
Estimated twinning fraction	0.309 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 16877 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3553	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: CA, NAG

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	0.97	1/1790 (0.1%)	1.17	14/2423 (0.6%)
2	B	0.87	0/1788	1.12	13/2420 (0.5%)
All	All	0.92	1/3578 (0.0%)	1.15	27/4843 (0.6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	PHE	CE1-CZ	6.87	1.50	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	109	ASP	CB-CG-OD2	9.46	126.81	118.30
1	A	175	ASP	CB-CG-OD2	8.46	125.91	118.30
1	A	169	ASP	CB-CG-OD2	7.73	125.26	118.30
1	A	113	ASP	CB-CG-OD2	7.70	125.22	118.30
2	B	226	ASP	CB-CG-OD2	7.49	125.04	118.30
2	B	133	ASP	CB-CG-OD2	7.38	124.94	118.30
2	B	222	ASP	CB-CG-OD2	7.23	124.81	118.30
2	B	129	ASP	CB-CG-OD2	6.95	124.56	118.30
2	B	109	ASP	CB-CG-OD2	6.75	124.37	118.30
2	B	224	ASP	CB-CG-OD2	6.68	124.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	100	ASP	CB-CG-OD2	6.27	123.94	118.30
2	B	208	ASP	CB-CG-OD2	6.21	123.89	118.30
2	B	125	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	107	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	245	CYS	CA-CB-SG	-5.97	103.26	114.00
2	B	175	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	226	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	158	LEU	CA-CB-CG	5.83	128.71	115.30
2	B	150	LEU	CA-CB-CG	5.62	128.23	115.30
2	B	113	ASP	CB-CG-OD2	5.55	123.30	118.30
2	B	107	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	122	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	A	90	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	125	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	167	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	227	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	169	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	PHE	Peptide

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	1738	0	1604	116	0
2	B	1736	0	1604	132	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	15	5	0
5	A	29	0	0	1	0
5	B	33	0	0	2	0
All	All	3553	0	3223	251	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 38.

All (251) 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)
2:B:235:MET:CE	2:B:235:MET:SD	2.01	1.48
2:B:172:ASP:OD2	2:B:176:ASN:HB3	1.31	1.31
2:B:132:ARG:HG2	2:B:132:ARG:HH11	1.14	1.09
2:B:132:ARG:HH11	2:B:132:ARG:CG	1.70	1.04
2:B:124:VAL:HG23	2:B:280:VAL:HG22	1.05	1.02
2:B:124:VAL:CG2	2:B:280:VAL:HG22	1.91	1.01
1:A:216:GLN:HG2	1:A:243:LYS:HD3	1.42	0.99
1:A:132:ARG:HG3	1:A:136:THR:HG21	1.44	0.97
2:B:156:HIS:HA	2:B:187:VAL:HG23	1.46	0.96
2:B:132:ARG:HG2	2:B:132:ARG:NH1	1.68	0.96
2:B:124:VAL:HG23	2:B:280:VAL:CG2	1.96	0.94
2:B:122:ARG:HD2	2:B:282:GLU:OE2	1.68	0.93
1:A:169:ASP:OD1	1:A:177[A]:TYR:OH	1.88	0.92
2:B:182:TYR:CD2	2:B:198:LEU:HD11	2.05	0.91
1:A:216:GLN:HE21	1:A:243:LYS:NZ	1.70	0.88
2:B:212:PHE:CE2	2:B:243:LYS:HB2	2.08	0.88
1:A:162:GLY:O	1:A:163:THR:HG23	1.72	0.88
2:B:166:LEU:HB2	2:B:185:PHE:HB2	1.58	0.85
2:B:259:HIS:O	2:B:275:ASN:OD1	1.95	0.84
1:A:282:GLU:OE2	4:A:1290:NAG:H1	1.79	0.83
1:A:162:GLY:O	1:A:163:THR:CG2	2.27	0.82
2:B:214:ASN:O	2:B:243:LYS:NZ	2.13	0.81
1:A:93:TRP:CE2	1:A:144:ARG:HG2	2.15	0.81
2:B:134:TRP:HE3	2:B:220:THR:HG1	1.29	0.81
1:A:172:ASP:OD1	1:A:174:GLU:N	2.13	0.80
2:B:227:LEU:O	2:B:244:ASN:ND2	2.15	0.80
1:A:208:ASP:OD2	1:A:211:THR:OG1	2.00	0.80
1:A:213:HIS:ND1	1:A:241:TRP:O	2.17	0.78
1:A:156:HIS:HD2	1:A:187:VAL:O	1.67	0.78
1:A:209:SER:HB2	1:A:268:TRP:CE2	2.18	0.78
2:B:209:SER:HB2	2:B:268:TRP:CE2	2.20	0.77
1:A:228:ASN:HB2	1:A:244:ASN:ND2	2.00	0.76
2:B:216:GLN:HE21	2:B:243:LYS:HD3	1.51	0.76
2:B:207:GLY:HA3	2:B:270:SER:OG	1.86	0.75
1:A:82:ASP:O	1:A:86:ARG:HG3	1.87	0.74
1:A:102:ARG:HG3	1:A:103:PRO:HD2	1.71	0.73
1:A:132:ARG:HG3	1:A:136:THR:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:TYR:CD2	2:B:198:LEU:CD1	2.73	0.71
1:A:231:ASN:C	1:A:235:MET:HE2	2.11	0.71
2:B:182:TYR:CE2	2:B:198:LEU:HD11	2.26	0.70
2:B:231:ASN:CG	2:B:234:VAL:HG23	2.11	0.69
4:A:1290:NAG:H83	4:A:1290:NAG:H3	1.74	0.69
2:B:237:GLN:NE2	2:B:253:ARG:HE	1.89	0.69
1:A:216:GLN:HE21	1:A:243:LYS:HZ3	1.38	0.69
1:A:228:ASN:HD22	1:A:244:ASN:ND2	1.90	0.69
1:A:132:ARG:HB2	1:A:137:TYR:CE2	2.28	0.68
2:B:172:ASP:OD2	2:B:176:ASN:CB	2.26	0.68
2:B:201:PHE:HB2	2:B:208:ASP:OD2	1.93	0.67
2:B:173:PHE:CZ	2:B:256:ARG:HA	2.29	0.67
1:A:188:ALA:HB3	1:A:195:ASN:N	2.09	0.67
2:B:237:GLN:HE21	2:B:253:ARG:HE	1.41	0.66
1:A:265:GLY:H	1:A:267:ASN:HD21	1.42	0.66
2:B:227:LEU:HB2	2:B:244:ASN:HB2	1.79	0.65
2:B:212:PHE:CZ	2:B:243:LYS:HB2	2.30	0.65
2:B:172:ASP:HB2	2:B:276:TYR:OH	1.96	0.65
2:B:199:GLY:O	5:B:2020:HOH:O	2.15	0.65
1:A:228:ASN:HB2	1:A:244:ASN:HD22	1.61	0.65
2:B:122:ARG:HG3	2:B:282:GLU:CG	2.26	0.64
1:A:188:ALA:O	1:A:194:TYR:HA	1.97	0.64
1:A:189:ASP:OD2	1:A:191:ALA:HB3	1.97	0.64
2:B:209:SER:O	2:B:248:SER:OG	2.12	0.64
1:A:259:HIS:O	1:A:275:ASN:OD1	2.14	0.64
2:B:236:PHE:HE2	2:B:245:CYS:SG	2.19	0.64
2:B:134:TRP:HE3	2:B:220:THR:OG1	1.80	0.64
2:B:207:GLY:HA3	2:B:270:SER:HG	1.62	0.64
2:B:163:THR:OG1	2:B:288:ALA:HB3	1.97	0.64
2:B:247:THR:O	2:B:269:LYS:HB2	1.98	0.63
1:A:169:ASP:OD2	1:A:284:LYS:HE3	1.99	0.63
1:A:216:GLN:HE21	1:A:243:LYS:HZ2	1.45	0.62
1:A:193:LYS:NZ	1:A:225:ASN:HD21	1.97	0.62
1:A:166:LEU:HD22	1:A:185:PHE:CD1	2.35	0.61
1:A:156:HIS:CD2	1:A:187:VAL:O	2.50	0.61
1:A:188:ALA:HB3	1:A:195:ASN:H	1.64	0.61
2:B:257:GLY:O	2:B:259:HIS:HD2	1.84	0.60
1:A:93:TRP:HA	1:A:106:VAL:O	2.02	0.60
1:A:183:ARG:HG2	1:A:202:VAL:CG2	2.32	0.60
2:B:216:GLN:HE22	2:B:227:LEU:HD21	1.67	0.60
1:A:93:TRP:CD2	1:A:144:ARG:HG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:CYS:O	1:A:74:LEU:HB2	2.02	0.60
1:A:132:ARG:HB2	1:A:137:TYR:HE2	1.66	0.59
2:B:195:ASN:OD1	2:B:215:ASN:HA	2.03	0.59
1:A:193:LYS:HB3	1:A:217:SER:OG	2.02	0.59
2:B:123:ARG:HG3	2:B:123:ARG:NH1	2.17	0.59
1:A:113:ASP:OD2	1:A:181:LYS:NZ	2.35	0.59
1:A:216:GLN:CG	1:A:243:LYS:HD3	2.24	0.59
2:B:263:ALA:HB2	2:B:274:TYR:HB3	1.85	0.59
1:A:246:HIS:CD2	1:A:246:HIS:C	2.76	0.58
1:A:209:SER:O	1:A:248:SER:HB3	2.02	0.58
1:A:228:ASN:HD22	1:A:244:ASN:HD21	1.49	0.58
1:A:93:TRP:CZ2	1:A:144:ARG:HG2	2.37	0.58
2:B:213:HIS:NE2	2:B:247:THR:HG22	2.18	0.58
2:B:202:VAL:HG12	2:B:203:GLU:HG3	1.85	0.58
2:B:202:VAL:HG12	2:B:203:GLU:CG	2.33	0.58
2:B:123:ARG:HG3	2:B:123:ARG:HH11	1.68	0.58
1:A:202:VAL:HG12	1:A:203:GLU:CG	2.34	0.57
2:B:135:ALA:O	2:B:138:LYS:HB3	2.05	0.56
2:B:122:ARG:CD	2:B:282:GLU:OE2	2.49	0.56
2:B:123:ARG:HA	2:B:147:GLU:HG2	1.88	0.56
1:A:106:VAL:HG12	1:A:150:LEU:HD11	1.86	0.56
2:B:93:TRP:HE3	2:B:105:THR:HG22	1.70	0.56
1:A:174:GLU:O	1:A:175:ASP:HB2	2.06	0.56
1:A:265:GLY:N	1:A:267:ASN:HD21	2.03	0.56
2:B:207:GLY:CA	2:B:270:SER:OG	2.54	0.56
2:B:221:LYS:N	5:B:2023:HOH:O	2.33	0.56
2:B:204:GLY:O	2:B:205:SER:C	2.43	0.55
2:B:104:LEU:HD13	2:B:106:VAL:HG12	1.89	0.55
2:B:240:TRP:CH2	2:B:250:LEU:HB2	2.41	0.55
1:A:88:HIS:O	1:A:110:MET:HG3	2.06	0.55
1:A:135:ALA:O	1:A:139:GLN:HG2	2.07	0.55
1:A:109:ASP:HB3	1:A:117:TRP:HB2	1.89	0.55
2:B:100:ASP:OD1	2:B:102:ARG:N	2.39	0.55
1:A:93:TRP:CZ2	1:A:144:ARG:HA	2.42	0.54
2:B:122:ARG:HG3	2:B:282:GLU:HG2	1.88	0.54
1:A:173:PHE:CE1	1:A:256:ARG:HA	2.43	0.54
1:A:97:TYR:CE2	1:A:103:PRO:HB3	2.43	0.54
1:A:193:LYS:CB	1:A:217:SER:OG	2.56	0.53
2:B:269:LYS:HG3	2:B:274:TYR:CZ	2.44	0.53
1:A:202:VAL:HG12	1:A:203:GLU:HG3	1.89	0.53
1:A:100:ASP:OD1	1:A:102:ARG:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HB2	1:A:185:PHE:HB2	1.91	0.53
2:B:151:GLY:O	2:B:155:ILE:HG13	2.09	0.53
1:A:269:LYS:HD3	1:A:269:LYS:C	2.29	0.53
1:A:231:ASN:O	1:A:235:MET:HG3	2.08	0.52
1:A:79:THR:O	1:A:82:ASP:HB2	2.09	0.52
2:B:236:PHE:HE2	2:B:245:CYS:CB	2.22	0.52
2:B:186:LYS:HB3	2:B:197:VAL:HB	1.92	0.52
2:B:163:THR:O	2:B:287:PRO:HA	2.09	0.51
4:A:1290:NAG:C8	4:A:1290:NAG:H3	2.38	0.51
2:B:160:ALA:O	2:B:186:LYS:NZ	2.37	0.51
2:B:123:ARG:HD3	2:B:130:PHE:CE2	2.46	0.51
2:B:82:ASP:O	2:B:86:ARG:HG3	2.11	0.51
2:B:164:SER:HA	2:B:286:ARG:O	2.11	0.51
2:B:133:ASP:OD2	2:B:135:ALA:HB3	2.11	0.51
1:A:166:LEU:HB2	1:A:185:PHE:CB	2.40	0.51
2:B:132:ARG:HH11	2:B:132:ARG:HG3	1.67	0.50
2:B:213:HIS:HA	2:B:243:LYS:HE2	1.92	0.50
1:A:193:LYS:HZ2	1:A:225:ASN:ND2	2.09	0.50
2:B:185:PHE:O	2:B:186:LYS:HB2	2.10	0.50
2:B:255:LEU:HD12	2:B:265:GLY:CA	2.42	0.50
2:B:124:VAL:CG2	2:B:280:VAL:CG2	2.74	0.50
2:B:123:ARG:CD	2:B:130:PHE:CZ	2.95	0.50
1:A:172:ASP:OD1	1:A:173:PHE:N	2.46	0.49
1:A:172:ASP:OD1	1:A:172:ASP:C	2.51	0.49
2:B:172:ASP:CG	2:B:176:ASN:HB3	2.22	0.49
1:A:224:ASP:C	1:A:224:ASP:OD1	2.51	0.49
2:B:142:GLY:HA3	2:B:148:PHE:HA	1.95	0.49
1:A:209:SER:HB2	1:A:268:TRP:NE1	2.28	0.49
2:B:93:TRP:HA	2:B:106:VAL:O	2.12	0.49
1:A:151:GLY:O	1:A:155:ILE:HG13	2.13	0.49
4:A:1290:NAG:C3	4:A:1290:NAG:H83	2.41	0.48
2:B:81:LYS:NZ	2:B:85:ASP:OD1	2.46	0.48
1:A:132:ARG:CB	1:A:137:TYR:CE2	2.96	0.48
1:A:246:HIS:CE1	1:A:249:ASN:HB2	2.49	0.48
1:A:145:LEU:HD12	1:A:145:LEU:N	2.28	0.48
2:B:121:GLN:HE22	2:B:250:LEU:HB3	1.77	0.48
2:B:95:THR:HA	2:B:105:THR:HA	1.95	0.48
1:A:98:LEU:HB3	1:A:99:PRO:HD2	1.94	0.48
2:B:187:VAL:O	2:B:188:ALA:O	2.32	0.48
2:B:120:PHE:HE2	2:B:285:VAL:HG13	1.79	0.48
1:A:138:LYS:HE2	1:A:190:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:ASP:C	2:B:228:ASN:H	2.17	0.48
2:B:246:HIS:HE1	2:B:263:ALA:O	1.96	0.48
1:A:193:LYS:HZ2	1:A:225:ASN:HD21	1.59	0.48
1:A:231:ASN:HB3	1:A:234:VAL:HB	1.95	0.47
1:A:172:ASP:OD2	1:A:176:ASN:HB2	2.14	0.47
1:A:209:SER:HA	1:A:247:THR:HG21	1.96	0.47
1:A:182:TYR:CZ	1:A:210:LEU:HB3	2.49	0.47
1:A:202:VAL:HG12	1:A:203:GLU:HG2	1.96	0.47
1:A:113:ASP:HB2	1:A:167:ARG:NH1	2.30	0.47
2:B:173:PHE:CE2	2:B:279:LYS:HG3	2.49	0.47
2:B:196:LEU:HD12	2:B:197:VAL:N	2.30	0.47
2:B:139:GLN:HG3	2:B:140:GLY:N	2.29	0.47
2:B:231:ASN:ND2	2:B:234:VAL:HG23	2.30	0.46
1:A:191:ALA:C	1:A:193:LYS:H	2.18	0.46
1:A:237:GLN:HE21	1:A:253:ARG:NE	2.14	0.46
1:A:171:VAL:HB	1:A:280:VAL:HB	1.98	0.46
2:B:122:ARG:HG3	2:B:282:GLU:HG3	1.97	0.46
2:B:231:ASN:CG	2:B:234:VAL:CG2	2.83	0.46
1:A:282:GLU:OE2	4:A:1290:NAG:C1	2.58	0.46
2:B:236:PHE:CE2	2:B:245:CYS:CB	2.98	0.46
1:A:232:CYS:HA	1:A:235:MET:HE3	1.98	0.46
1:A:244:ASN:N	1:A:245:CYS:HA	2.31	0.45
2:B:131:TYR:CZ	2:B:221:LYS:HD3	2.52	0.45
1:A:180:ALA:HA	1:A:204:GLY:HA3	1.99	0.45
2:B:166:LEU:HG	2:B:167:ARG:N	2.30	0.45
1:A:246:HIS:CD2	1:A:247:THR:N	2.85	0.45
2:B:93:TRP:CZ2	2:B:144:ARG:HA	2.52	0.45
2:B:248:SER:HA	2:B:267:ASN:O	2.16	0.45
2:B:123:ARG:HD3	2:B:130:PHE:CZ	2.52	0.45
2:B:99:PRO:C	2:B:101:CYS:H	2.20	0.45
1:A:162:GLY:C	1:A:163:THR:HG23	2.33	0.45
2:B:196:LEU:HD12	2:B:197:VAL:H	1.82	0.45
1:A:87:GLY:HA2	1:A:89:PHE:CZ	2.51	0.45
2:B:228:ASN:ND2	2:B:244:ASN:OD1	2.36	0.45
1:A:98:LEU:HB3	1:A:99:PRO:CD	2.47	0.45
1:A:122:ARG:O	1:A:147:GLU:HB3	2.17	0.45
2:B:258:THR:O	2:B:259:HIS:HB3	2.18	0.44
1:A:104:LEU:HD13	1:A:106:VAL:HG13	1.99	0.44
2:B:131:TYR:OH	2:B:234:VAL:HG13	2.17	0.44
2:B:286:ARG:HB2	2:B:287:PRO:CD	2.47	0.44
2:B:93:TRP:CE2	2:B:144:ARG:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLY:O	1:A:286:ARG:HG3	2.17	0.44
1:A:237:GLN:HE21	1:A:253:ARG:HE	1.66	0.44
2:B:179:PHE:O	2:B:206:ALA:HB3	2.18	0.44
2:B:286:ARG:HB2	2:B:287:PRO:HD3	1.99	0.44
1:A:164:SER:HB3	1:A:285:VAL:HB	1.99	0.44
2:B:213:HIS:O	2:B:216:GLN:HB2	2.17	0.44
1:A:269:LYS:HD3	1:A:269:LYS:O	2.18	0.44
1:A:81:LYS:HD3	1:A:81:LYS:HA	1.83	0.44
1:A:233:ALA:O	1:A:237:GLN:N	2.46	0.43
2:B:187:VAL:C	2:B:188:ALA:O	2.56	0.43
2:B:250:LEU:HD12	2:B:266:ILE:HG22	2.00	0.43
1:A:146:GLY:HA3	5:A:2014:HOH:O	2.18	0.43
2:B:123:ARG:HD2	2:B:123:ARG:HA	1.83	0.43
1:A:162:GLY:O	1:A:163:THR:HG22	2.15	0.43
2:B:117:TRP:HB3	2:B:284:LYS:HB2	2.00	0.43
2:B:198:LEU:O	2:B:214:ASN:ND2	2.42	0.43
2:B:186:LYS:O	2:B:197:VAL:N	2.46	0.43
2:B:129:ASP:O	2:B:132:ARG:HD3	2.19	0.43
1:A:211:THR:O	1:A:213:HIS:N	2.52	0.43
2:B:155:ILE:HA	2:B:158:LEU:HD12	2.01	0.43
1:A:83:LEU:HD13	1:A:94:HIS:HB2	2.00	0.43
2:B:282:GLU:HB3	2:B:284:LYS:CE	2.49	0.43
2:B:226:ASP:OD2	2:B:228:ASN:O	2.37	0.42
1:A:193:LYS:HD3	1:A:193:LYS:HA	1.61	0.42
1:A:123:ARG:HA	1:A:123:ARG:HD2	1.88	0.42
2:B:246:HIS:CE1	2:B:263:ALA:O	2.72	0.42
1:A:211:THR:O	1:A:212:PHE:C	2.57	0.42
2:B:120:PHE:CD1	2:B:155:ILE:HD13	2.54	0.42
2:B:171:VAL:HG22	2:B:177[B]:TYR:CG	2.55	0.42
2:B:212:PHE:CZ	2:B:243:LYS:CB	3.02	0.42
2:B:132:ARG:NH1	2:B:132:ARG:CG	2.37	0.42
2:B:212:PHE:HB3	2:B:247:THR:HG21	2.01	0.42
2:B:104:LEU:HD13	2:B:106:VAL:CG1	2.49	0.41
2:B:132:ARG:NH1	2:B:136:THR:HG21	2.36	0.41
1:A:188:ALA:HB1	1:A:192:GLU:HB2	2.01	0.41
1:A:253:ARG:O	1:A:266:ILE:HG13	2.20	0.41
2:B:178:GLN:HB2	2:B:206:ALA:HB2	2.03	0.41
1:A:136:THR:HG22	1:A:141:PHE:CD2	2.56	0.41
2:B:247:THR:O	2:B:269:LYS:N	2.49	0.41
2:B:100:ASP:C	2:B:100:ASP:OD1	2.59	0.41
1:A:142:GLY:HA3	1:A:148:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASN:ND2	1:A:244:ASN:HD21	2.16	0.41
1:A:228:ASN:ND2	1:A:244:ASN:ND2	2.64	0.41
2:B:228:ASN:O	2:B:230:GLY:O	2.39	0.41
1:A:193:LYS:HZ3	1:A:225:ASN:HD21	1.66	0.41
1:A:243:LYS:HB2	1:A:244:ASN:H	1.53	0.41
2:B:205:SER:O	2:B:207:GLY:N	2.54	0.41
2:B:173:PHE:CE1	2:B:257:GLY:N	2.89	0.40
1:A:183:ARG:CG	1:A:202:VAL:CG2	2.99	0.40
2:B:202:VAL:HG12	2:B:203:GLU:HG2	2.01	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	215/218 (99%)	183 (85%)	29 (14%)	3 (1%)	14 35
2	B	215/218 (99%)	180 (84%)	29 (14%)	6 (3%)	6 15
All	All	430/436 (99%)	363 (84%)	58 (14%)	9 (2%)	9 23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	SER
2	B	188	ALA
1	A	124	VAL
2	B	124	VAL
1	A	125	ASP
2	B	192	GLU
2	B	244	ASN
2	B	229	THR
2	B	260	GLY

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	182/183 (100%)	147 (81%)	35 (19%)	2 4
2	B	182/183 (100%)	151 (83%)	31 (17%)	2 6
All	All	364/366 (100%)	298 (82%)	66 (18%)	2 5

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	81	LYS
1	A	90	LEU
1	A	95	THR
1	A	104	LEU
1	A	122	ARG
1	A	124	VAL
1	A	132	ARG
1	A	150	LEU
1	A	161	GLN
1	A	172	ASP
1	A	183	ARG
1	A	186	ARG
1	A	193	LYS
1	A	203	GLU
1	A	205	SER
1	A	209	SER
1	A	216	GLN
1	A	217	SER
1	A	219	SER
1	A	222	ASP
1	A	223	GLN
1	A	226	ASP
1	A	227	LEU
1	A	229	THR
1	A	231	ASN
1	A	235	MET

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Mol	Chain	Res	Type
1	A	237	GLN
1	A	246	HIS
1	A	247	THR
1	A	250	LEU
1	A	258	THR
1	A	269	LYS
1	A	277	SER
1	A	281	SER
2	B	74	LEU
2	B	75	THR
2	B	78	ARG
2	B	81	LYS
2	B	95	THR
2	B	104	LEU
2	B	110	MET
2	B	124	VAL
2	B	132	ARG
2	B	170	LEU
2	B	175	ASP
2	B	178	GLN
2	B	181	LYS
2	B	184	SER
2	B	187	VAL
2	B	193	LYS
2	B	198	LEU
2	B	203	GLU
2	B	215	ASN
2	B	219	SER
2	B	220	THR
2	B	221	LYS
2	B	223	GLN
2	B	229	THR
2	B	231	ASN
2	B	237	GLN
2	B	248	SER
2	B	250	LEU
2	B	253	ARG
2	B	256	ARG
2	B	270	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	216	GLN
1	A	225	ASN
1	A	231	ASN
1	A	237	GLN
1	A	244	ASN
1	A	246	HIS
1	A	267	ASN
1	A	275	ASN
2	B	139	GLN
2	B	231	ASN
2	B	237	GLN
2	B	246	HIS
2	B	259	HIS
2	B	267	ASN
2	B	275	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\|>2$
4	NAG	A	1290	1	15,15,15	0.60	0	17,21,21	2.51	8 (47%)

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
4	NAG	A	1290	1	-	1/6/26/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1290	NAG	C6-C5-C4	-4.30	102.42	113.02
4	A	1290	NAG	C1-O5-C5	-2.80	108.28	113.47
4	A	1290	NAG	O3-C3-C2	2.04	113.83	109.66
4	A	1290	NAG	O7-C7-C8	2.15	126.00	122.06
4	A	1290	NAG	O5-C5-C4	2.25	113.90	109.68
4	A	1290	NAG	O5-C5-C6	3.60	115.46	106.36
4	A	1290	NAG	C4-C3-C2	4.05	116.05	110.43
4	A	1290	NAG	C3-C4-C5	5.06	119.02	110.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1290	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1290	NAG	5	0

5.7 Other polymers

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	A	216/218 (99%)	0.13	3 (1%)	78 77	32, 52, 70, 78	0
2	B	216/218 (99%)	0.16	6 (2%)	56 57	35, 62, 79, 85	0
All	All	432/436 (99%)	0.15	9 (2%)	67 68	32, 56, 75, 85	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	264	ASN	3.1
2	B	177[A]	TYR	3.0
2	B	229	THR	2.9
2	B	174	GLU	2.9
1	A	177[A]	TYR	2.7
2	B	210	LEU	2.5
2	B	254	TYR	2.3
1	A	186	ARG	2.3
1	A	74	LEU	2.2

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

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, 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
4	NAG	A	1290	15/15	0.69	0.38	2.70	44,74,76,78	0
3	CA	A	1289	1/1	0.95	0.17	1.30	73,73,73,73	0
3	CA	B	1289	1/1	0.83	0.27	1.00	50,50,50,50	1

6.5 Other polymers (i)

There are no such residues in this entry.