Full wwPDB X-ray Structure Validation Report

Feb 21, 2017 – 08:51 PM EST

PDB ID	:	5TOJ
Title	:	Crystal structure of the RSV F glycoprotein in complex with the neutralizing single-domain antibody F-VHH-4
Authors	:	Gilman, M.S.A.; Kabeche, S.C.; McLellan, J.S.
Deposited on	:	2016-10-17
Resolution	:	3.30 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:

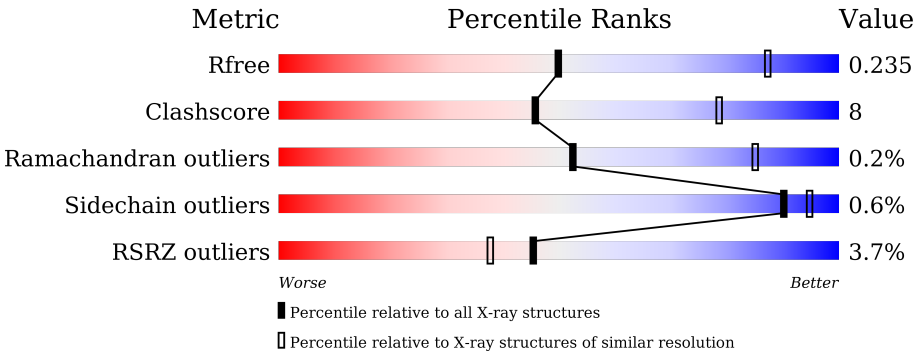
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	550	3% 71% 16% 12%
1	B	550	3% 71% 17% • 12%
1	C	550	2% 71% 16% 13%
2	D	131	% 87% 9% •
2	E	131	13% 81% 13% 6%
2	F	131	3% 81% 15% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14124 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 Fusion glycoprotein F0, Fibritin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3739	2368	616	732	23			
1	B	485	Total	C	N	O	S	0	0	0
			3753	2378	618	734	23			
1	C	481	Total	C	N	O	S	0	0	0
			3727	2360	614	730	23			

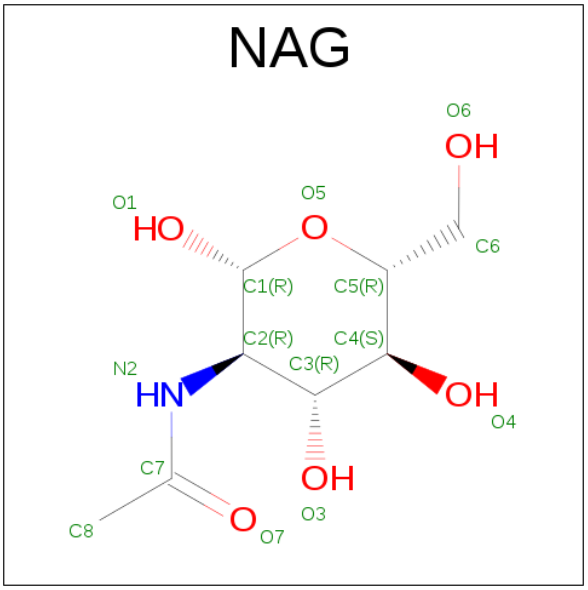
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	conflict	UNP P03420
A	155	CYS	SER	engineered mutation	UNP P03420
A	190	PHE	SER	engineered mutation	UNP P03420
A	207	LEU	VAL	engineered mutation	UNP P03420
A	290	CYS	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	engineered mutation	UNP P03420
A	447	VAL	MET	engineered mutation	UNP P03420
B	102	ALA	PRO	conflict	UNP P03420
B	155	CYS	SER	engineered mutation	UNP P03420
B	190	PHE	SER	engineered mutation	UNP P03420
B	207	LEU	VAL	engineered mutation	UNP P03420
B	290	CYS	SER	engineered mutation	UNP P03420
B	379	VAL	ILE	engineered mutation	UNP P03420
B	447	VAL	MET	engineered mutation	UNP P03420
C	102	ALA	PRO	conflict	UNP P03420
C	155	CYS	SER	engineered mutation	UNP P03420
C	190	PHE	SER	engineered mutation	UNP P03420
C	207	LEU	VAL	engineered mutation	UNP P03420
C	290	CYS	SER	engineered mutation	UNP P03420
C	379	VAL	ILE	engineered mutation	UNP P03420
C	447	VAL	MET	engineered mutation	UNP P03420

- Molecule 2 is a protein called Single-domain antibody F-VHH-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	126	Total	C	N	O	S	0	0	0
			965	604	166	189	6			
2	E	123	Total	C	N	O	S	0	0	0
			943	592	161	184	6			
2	F	125	Total	C	N	O	S	0	0	0
			955	598	163	188	6			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



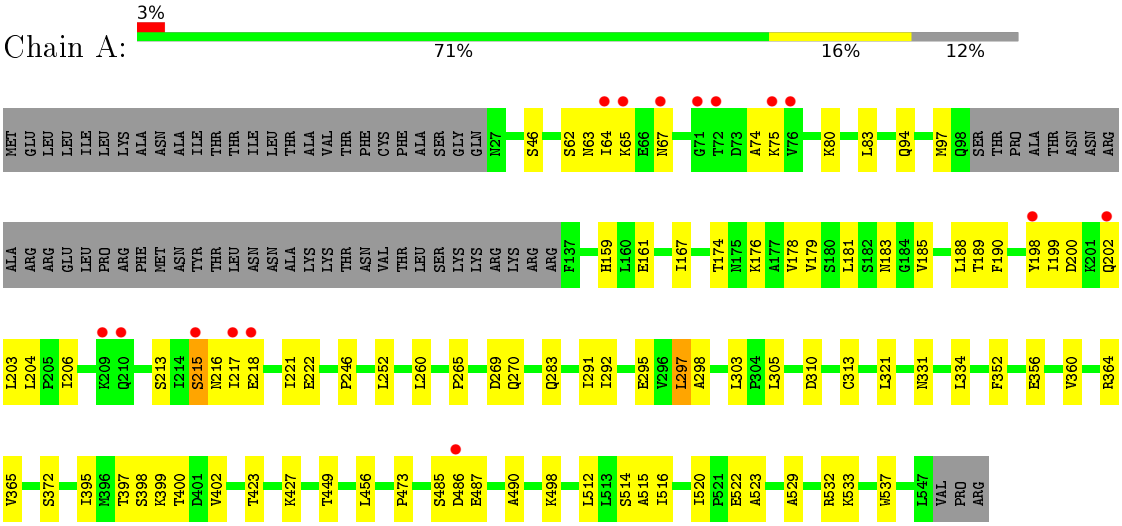
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

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.

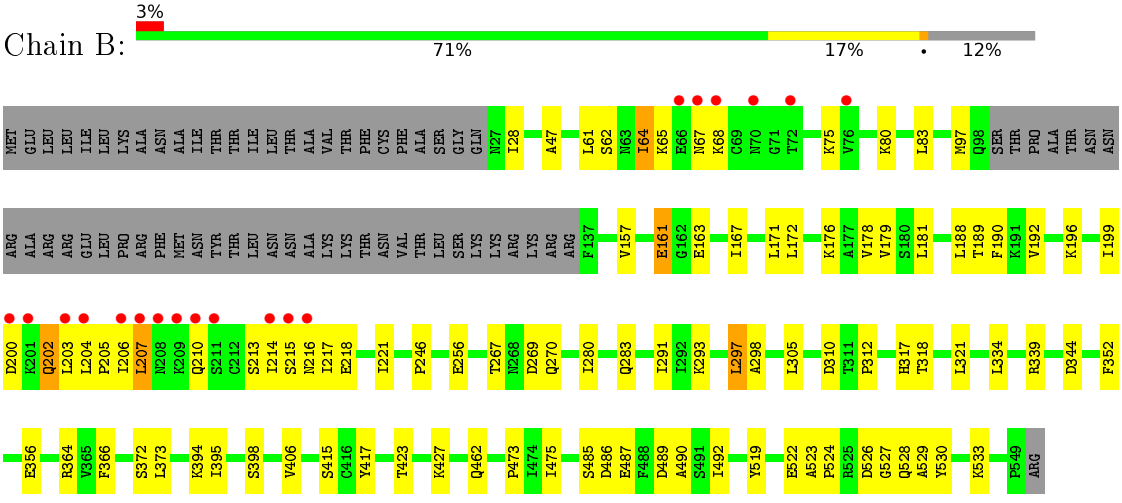
- Molecule 1: Fusion glycoprotein F0, Fibritin chimera

Chain A:



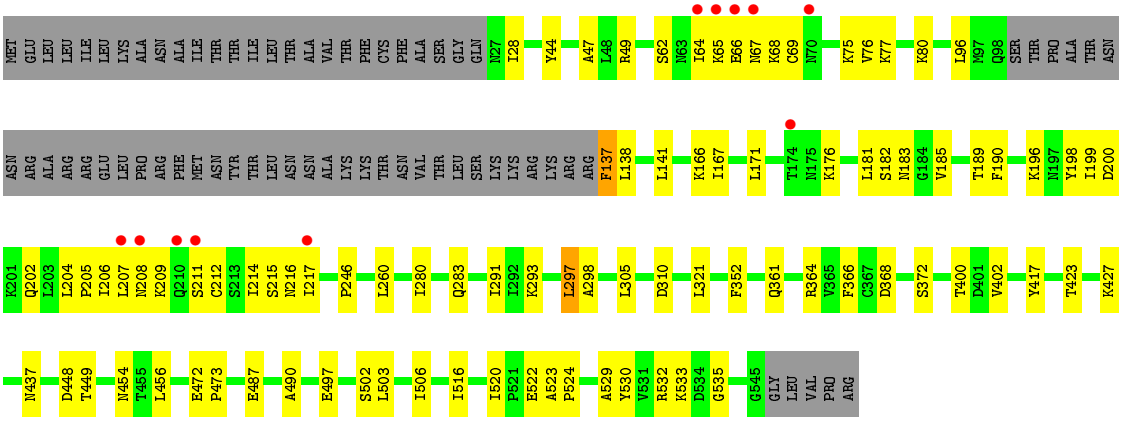
- Molecule 1: Fusion glycoprotein F0, Fibritin chimera

Chain B:

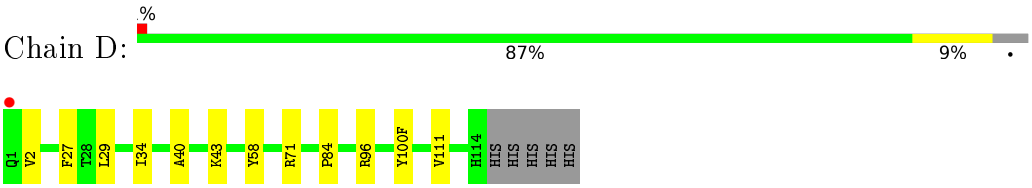


- Molecule 1: Fusion glycoprotein F0, Fibritin chimera

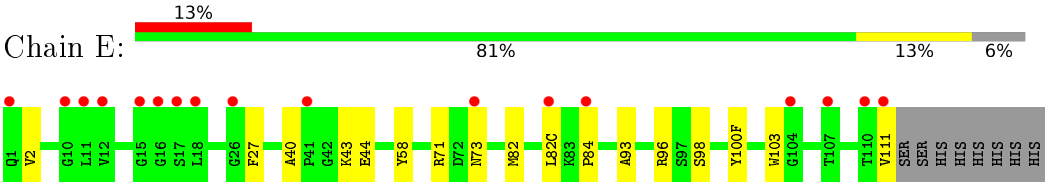
Chain C:



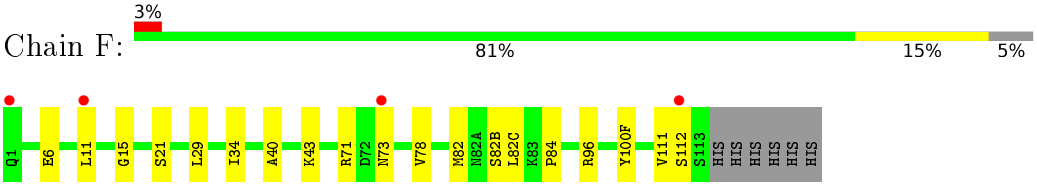
• Molecule 2: Single-domain antibody F-VHH-4



• Molecule 2: Single-domain antibody F-VHH-4



• Molecule 2: Single-domain antibody F-VHH-4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.19Å 173.19Å 153.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.96 – 3.30 37.96 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.96-3.30) 100.0 (37.96-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.234 0.186 , 0.235	Depositor DCC
R_{free} test set	2021 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	85.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14124	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.29	0/3796	0.57	0/5143
1	B	0.30	0/3811	0.62	3/5165 (0.1%)
1	C	0.31	0/3784	0.62	0/5127
2	D	0.31	0/989	0.58	0/1339
2	E	0.27	0/966	0.54	0/1308
2	F	0.28	0/978	0.58	0/1324
All	All	0.30	0/14324	0.60	3/19406 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	207	LEU	CA-CB-CG	-7.08	99.02	115.30
1	B	207	LEU	N-CA-C	5.38	125.54	111.00
1	B	64	ILE	CB-CA-C	-5.14	101.33	111.60

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	3739	0	3777	66	0
1	B	3753	0	3793	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3727	0	3763	65	1
2	D	965	0	912	11	0
2	E	943	0	895	15	0
2	F	955	0	905	13	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
All	All	14124	0	14084	216	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 8.

All (216) 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:64:ILE:HD11	1:B:199:ILE:HG21	1.49	0.94
1:B:75:LYS:HD2	1:B:216:ASN:HA	1.50	0.92
1:C:423:THR:OG1	2:E:96:ARG:NH1	2.08	0.87
1:C:64:ILE:HD11	1:C:199:ILE:HG21	1.57	0.86
1:A:334:LEU:HD11	1:A:395:ILE:HD12	1.61	0.83
1:A:64:ILE:HD11	1:A:199:ILE:HG21	1.60	0.82
1:B:206:ILE:HG13	1:B:207:LEU:HG	1.61	0.82
1:A:423:THR:OG1	2:F:96:ARG:NH1	2.12	0.81
1:A:218:GLU:HG3	1:C:217:ILE:HD13	1.60	0.80
1:B:75:LYS:HG2	1:B:217:ILE:HG23	1.68	0.75
1:B:423:THR:OG1	2:D:96:ARG:NH1	2.19	0.75
1:B:206:ILE:HG22	1:B:213:SER:O	1.88	0.73
1:B:519:TYR:OH	1:C:516:ILE:O	2.05	0.73
1:A:67:ASN:HD22	1:A:83:LEU:HD23	1.56	0.69
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.72	0.69
1:B:334:LEU:HD11	1:B:395:ILE:HD12	1.72	0.69
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.73	0.69
1:C:215:SER:OG	1:C:216:ASN:N	2.24	0.69
1:A:221:ILE:HD12	1:C:217:ILE:HD11	1.76	0.67
1:C:190:PHE:CE2	1:C:260:LEU:HG	2.30	0.66
1:B:200:ASP:HA	1:B:204:LEU:HD12	1.77	0.65
1:B:321:LEU:HD11	1:B:473:PRO:HB3	1.80	0.64
2:D:29:LEU:HD12	2:D:71:ARG:HE	1.63	0.63
1:C:503:LEU:HD23	1:C:506:ILE:HD11	1.81	0.62
1:B:269:ASP:OD1	1:B:270:GLN:N	2.32	0.62
1:B:161:GLU:CD	1:B:161:GLU:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:CG2	1:B:215:SER:H	2.12	0.62
1:A:398:SER:HA	1:A:485:SER:O	2.00	0.62
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.83	0.60
1:A:269:ASP:OD1	1:A:270:GLN:N	2.34	0.60
1:A:321:LEU:HD11	1:A:473:PRO:HB3	1.82	0.60
1:B:202:GLN:HB3	1:B:203:LEU:HD12	1.84	0.59
2:F:84:PRO:HA	2:F:111:VAL:HB	1.83	0.59
1:A:427:LYS:O	2:F:100(F):TYR:HA	2.03	0.58
1:A:216:ASN:HB2	1:A:218:GLU:OE1	2.02	0.58
2:E:43:LYS:NZ	2:E:44:GLU:O	2.37	0.58
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.84	0.58
1:B:524:PRO:HG2	1:B:530:TYR:CZ	2.39	0.58
1:A:520:ILE:HD11	1:B:522:GLU:HA	1.86	0.57
1:B:427:LYS:O	2:D:100(F):TYR:HA	2.04	0.57
2:D:40:ALA:HB3	2:D:43:LYS:HE3	1.86	0.57
1:C:321:LEU:HD11	1:C:473:PRO:HB3	1.87	0.56
1:A:486:ASP:OD1	1:A:486:ASP:N	2.38	0.56
2:E:84:PRO:HA	2:E:111:VAL:HB	1.86	0.56
1:C:206:ILE:HG13	1:C:207:LEU:HG	1.88	0.56
1:B:202:GLN:O	1:B:205:PRO:HD2	2.06	0.56
1:C:138:LEU:HB3	1:C:141:LEU:HD12	1.86	0.56
1:A:399:LYS:NZ	1:C:497:GLU:OE1	2.37	0.55
1:B:267:THR:HA	2:E:58:TYR:HB2	1.88	0.55
1:B:67:ASN:HB3	1:B:80:LYS:HE3	1.88	0.55
1:C:200:ASP:HA	1:C:204:LEU:HG	1.89	0.54
1:B:487:GLU:HB3	1:B:490:ALA:HB2	1.90	0.54
1:A:190:PHE:CE2	1:A:260:LEU:HG	2.41	0.54
1:A:529:ALA:HA	1:C:533:LYS:HB2	1.90	0.53
1:C:69:CYS:O	1:C:80:LYS:NZ	2.37	0.53
1:C:183:ASN:OD1	1:C:185:VAL:HG12	2.09	0.53
2:E:40:ALA:HB3	2:E:43:LYS:HE3	1.89	0.53
1:C:427:LYS:O	2:E:100(F):TYR:HA	2.09	0.53
1:B:157:VAL:HG11	1:B:181:LEU:HB3	1.91	0.52
1:A:218:GLU:HG2	1:C:75:LYS:HG3	1.92	0.52
1:B:310:ASP:OD1	1:B:364:ARG:NH1	2.30	0.52
1:A:97:MET:SD	1:A:291:ILE:HA	2.51	0.51
1:C:454:ASN:HA	2:E:98:SER:HB2	1.93	0.51
1:A:203:LEU:O	1:A:206:ILE:HG12	2.10	0.51
1:B:533:LYS:HB2	1:C:529:ALA:HA	1.93	0.51
1:A:533:LYS:HB2	1:B:529:ALA:HA	1.90	0.51
1:B:167:ILE:HD13	1:B:179:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ILE:HG23	1:C:189:THR:HG21	1.92	0.51
1:B:318:THR:OG1	1:B:339:ARG:HD3	2.11	0.50
1:A:183:ASN:OD1	1:A:185:VAL:HG12	2.12	0.50
1:A:75:LYS:HD2	1:A:215:SER:O	2.11	0.50
1:C:76:VAL:HG23	1:C:214:ILE:HG23	1.92	0.50
1:A:178:VAL:HG22	1:A:188:LEU:HD23	1.92	0.50
1:A:487:GLU:HB3	1:A:490:ALA:HB2	1.94	0.50
2:F:82:MET:HB3	2:F:82(C):LEU:HD21	1.93	0.50
1:B:526:ASP:O	1:B:528:GLN:N	2.43	0.49
2:F:29:LEU:HD12	2:F:71:ARG:NH2	2.27	0.49
1:A:174:THR:HG22	1:A:176:LYS:H	1.77	0.49
1:C:66:GLU:OE2	1:C:68:LYS:HE2	2.12	0.49
2:F:71:ARG:HH21	2:F:73:ASN:HA	1.78	0.49
1:B:267:THR:HG23	1:B:269:ASP:OD1	2.13	0.49
1:A:200:ASP:HA	1:A:204:LEU:HB2	1.95	0.48
1:C:310:ASP:OD1	1:C:364:ARG:NH1	2.38	0.48
1:C:423:THR:HG1	2:E:96:ARG:NH1	2.10	0.48
1:A:352:PHE:CE2	1:A:372:SER:HB3	2.49	0.47
1:A:498:LYS:NZ	1:B:486:ASP:OD1	2.35	0.47
1:C:208:ASN:O	1:C:209:LYS:HG3	2.14	0.47
1:C:522:GLU:HG3	1:C:523:ALA:O	2.14	0.47
1:C:215:SER:OG	1:C:216:ASN:OD1	2.32	0.47
1:A:62:SER:OG	1:A:64:ILE:HG13	2.13	0.47
1:A:260:LEU:HD13	1:A:303:LEU:HD11	1.96	0.47
1:B:214:ILE:HG22	1:B:215:SER:H	1.79	0.47
1:C:62:SER:HB2	1:C:196:LYS:HA	1.95	0.47
1:A:360:VAL:HG22	1:A:365:VAL:HG22	1.97	0.47
1:B:394:LYS:NZ	1:C:400:THR:HG21	2.29	0.47
1:B:398:SER:HA	1:B:485:SER:O	2.14	0.47
2:F:11:LEU:HD11	2:F:112:SER:HB3	1.95	0.47
1:B:178:VAL:HG22	1:B:188:LEU:HD23	1.96	0.47
1:B:217:ILE:O	1:B:221:ILE:HG13	2.15	0.47
1:C:171:LEU:HD11	1:C:189:THR:HG22	1.97	0.47
1:B:394:LYS:NZ	1:B:489:ASP:OD1	2.48	0.47
1:C:198:TYR:O	1:C:202:GLN:HB2	2.15	0.47
1:B:394:LYS:HZ2	1:C:400:THR:HG21	1.80	0.47
1:B:62:SER:OG	1:B:64:ILE:HG13	2.14	0.46
1:C:524:PRO:HG2	1:C:530:TYR:CZ	2.50	0.46
2:E:71:ARG:NH1	2:E:73:ASN:OD1	2.48	0.46
2:F:40:ALA:HB3	2:F:43:LYS:HE3	1.96	0.46
1:B:334:LEU:HB2	1:B:475:ILE:HD13	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ALA:HB2	1:B:364:ARG:HD2	1.97	0.46
1:C:212:CYS:O	1:C:214:ILE:HG13	2.16	0.46
1:C:427:LYS:N	1:C:448:ASP:OD2	2.45	0.46
1:B:62:SER:HB3	1:B:199:ILE:HD12	1.97	0.46
1:C:49:ARG:HE	1:C:368:ASP:CG	2.19	0.46
1:C:176:LYS:HG2	1:C:190:PHE:CE1	2.51	0.46
1:C:352:PHE:CE2	1:C:372:SER:HB3	2.51	0.46
1:B:214:ILE:CG2	1:B:215:SER:N	2.77	0.46
1:B:207:LEU:HD23	1:B:207:LEU:HA	1.69	0.46
1:B:352:PHE:CE2	1:B:372:SER:HB3	2.50	0.46
1:A:532:ARG:O	1:B:530:TYR:N	2.44	0.45
1:B:526:ASP:C	1:B:528:GLN:H	2.19	0.45
1:C:47:ALA:HB2	1:C:364:ARG:HD2	1.99	0.45
1:A:97:MET:HB2	1:A:97:MET:HE2	1.80	0.45
1:C:202:GLN:O	1:C:205:PRO:HD2	2.16	0.45
1:A:159:HIS:CE1	1:A:291:ILE:HG23	2.51	0.45
1:B:214:ILE:HG22	1:B:215:SER:N	2.32	0.45
1:B:395:ILE:HD13	1:B:492:ILE:HD13	1.98	0.45
1:C:28:ILE:HD13	1:C:44:TYR:CZ	2.51	0.45
1:A:206:ILE:HB	1:A:213:SER:O	2.16	0.45
1:A:512:LEU:O	1:A:516:ILE:HG13	2.17	0.45
1:B:297:LEU:HD12	1:B:298:ALA:N	2.31	0.45
1:A:167:ILE:HD13	1:A:179:VAL:HG21	1.98	0.45
1:B:176:LYS:HE2	1:B:190:PHE:CE2	2.52	0.45
1:B:67:ASN:ND2	1:B:83:LEU:HD23	2.32	0.45
1:C:280:ILE:HG21	1:C:366:PHE:CG	2.52	0.45
1:A:222:GLU:OE1	1:C:77:LYS:NZ	2.48	0.45
1:C:198:TYR:CE1	1:C:202:GLN:HG3	2.52	0.45
1:B:522:GLU:HG3	1:B:523:ALA:O	2.17	0.45
2:E:93:ALA:HB2	2:E:103:TRP:CE3	2.52	0.45
1:C:297:LEU:HD12	1:C:298:ALA:N	2.32	0.44
1:C:185:VAL:HG23	2:F:100(F):TYR:CZ	2.52	0.44
2:F:34:ILE:HG21	2:F:78:VAL:HG21	1.99	0.44
1:A:252:LEU:HD21	1:A:260:LEU:HD12	1.99	0.44
1:A:94:GLN:HA	1:A:97:MET:HE2	1.99	0.44
1:C:166:LYS:NZ	1:C:182:SER:HB3	2.31	0.44
2:D:84:PRO:HA	2:D:111:VAL:HB	2.00	0.44
1:B:317:HIS:HB3	1:B:406:VAL:HG11	1.99	0.44
2:D:2:VAL:HG13	2:D:27:PHE:CD2	2.52	0.44
1:A:198:TYR:O	1:A:202:GLN:HB2	2.17	0.44
1:C:137:PHE:C	1:C:137:PHE:CD1	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:HE1	1:A:292:ILE:HB	1.99	0.44
1:B:68:LYS:HB3	1:B:210:GLN:HA	2.00	0.44
1:A:423:THR:HG1	2:F:96:ARG:HH12	1.53	0.44
1:B:427:LYS:HB3	1:B:427:LYS:HE3	1.86	0.44
1:A:217:ILE:HD13	1:B:217:ILE:HD12	2.00	0.43
1:B:83:LEU:HD22	1:B:207:LEU:HD13	2.00	0.43
1:B:61:LEU:O	1:B:196:LYS:HB2	2.17	0.43
2:F:6:GLU:HA	2:F:21:SER:O	2.18	0.43
2:F:15:GLY:HA2	2:F:82(B):SER:HA	2.00	0.43
1:A:331:ASN:O	1:A:399:LYS:HG2	2.17	0.43
2:D:27:PHE:HE1	2:D:29:LEU:HD23	1.83	0.43
2:E:43:LYS:HB3	2:E:43:LYS:HE3	1.87	0.43
2:E:82:MET:HB3	2:E:82(C):LEU:HD21	2.00	0.43
1:B:68:LYS:HD2	1:B:210:GLN:HG3	1.99	0.43
1:B:312:PRO:HG2	1:B:344:ASP:OD2	2.19	0.43
1:C:291:ILE:HD11	1:C:293:LYS:HE2	2.00	0.43
1:A:356:GLU:CD	1:A:356:GLU:H	2.22	0.43
1:A:310:ASP:OD1	1:A:364:ARG:NH1	2.31	0.43
1:A:64:ILE:O	1:A:64:ILE:HG22	2.18	0.43
1:B:291:ILE:HD11	1:B:293:LYS:HE2	1.99	0.43
1:B:356:GLU:CD	1:B:356:GLU:H	2.21	0.43
1:B:64:ILE:O	1:B:64:ILE:HG22	2.18	0.42
1:A:400:THR:HG22	1:A:402:VAL:HG23	2.01	0.42
1:C:487:GLU:HB3	1:C:490:ALA:HB2	2.01	0.42
1:C:62:SER:OG	1:C:64:ILE:HG13	2.19	0.42
1:A:181:LEU:HD12	1:A:185:VAL:HG13	2.02	0.42
1:A:46:SER:HB3	1:A:313:CYS:SG	2.59	0.42
1:A:63:ASN:HB2	1:A:295:GLU:HG2	2.02	0.42
1:A:74:ALA:HB1	1:B:218:GLU:HB3	2.02	0.42
1:B:28:ILE:HD12	1:B:462:GLN:NE2	2.34	0.42
2:D:43:LYS:HE3	2:D:43:LYS:HB3	1.83	0.42
1:A:522:GLU:HG3	1:A:523:ALA:O	2.18	0.42
1:B:192:VAL:HG13	1:B:256:GLU:OE2	2.20	0.42
1:B:415:SER:HB3	1:B:417:TYR:CE2	2.54	0.42
1:B:64:ILE:HD11	1:B:199:ILE:HD13	2.02	0.42
1:B:97:MET:SD	1:B:291:ILE:HA	2.59	0.42
1:A:217:ILE:O	1:A:221:ILE:HG13	2.19	0.42
1:A:265:PRO:HA	2:D:58:TYR:CE1	2.54	0.42
1:C:76:VAL:HG21	1:C:214:ILE:HG12	2.02	0.42
2:D:27:PHE:CE1	2:D:29:LEU:HD23	2.55	0.42
2:E:2:VAL:HG13	2:E:27:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:CD1	1:A:397:THR:HG22	2.50	0.41
1:A:449:THR:HB	1:A:456:LEU:HD11	2.02	0.41
1:A:514:SER:O	1:A:515:ALA:HB3	2.20	0.41
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.80	0.41
1:C:417:TYR:HA	1:C:437:ASN:OD1	2.20	0.41
1:B:373:LEU:HD13	1:C:402:VAL:HG21	2.00	0.41
1:A:67:ASN:O	1:A:80:LYS:HE3	2.20	0.41
1:B:305:LEU:HA	1:B:305:LEU:HD23	1.74	0.41
1:A:537:TRP:HZ2	1:C:520:ILE:HD13	1.86	0.41
1:B:171:LEU:HD11	1:B:189:THR:HG22	2.02	0.41
1:A:297:LEU:HD12	1:A:298:ALA:N	2.35	0.41
1:B:280:ILE:HG21	1:B:366:PHE:CG	2.55	0.41
1:C:449:THR:HB	1:C:456:LEU:HD11	2.01	0.41
2:D:29:LEU:HD22	2:D:34:ILE:HD11	2.03	0.41
1:C:502:SER:O	1:C:506:ILE:HG12	2.20	0.41
1:A:334:LEU:HD12	1:A:397:THR:HG22	2.02	0.41
1:C:181:LEU:HD12	1:C:185:VAL:HG13	2.03	0.41
1:C:454:ASN:CA	2:E:98:SER:HB2	2.51	0.41
1:B:206:ILE:CG1	1:B:207:LEU:HG	2.41	0.40
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.74	0.40
1:C:532:ARG:NH1	1:C:535:GLY:O	2.55	0.40
1:C:96:LEU:HD23	1:C:96:LEU:HA	1.77	0.40
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.73	0.40
1:C:66:GLU:HG2	1:C:67:ASN:N	2.37	0.40
1:B:157:VAL:HG12	1:B:163:GLU:HG2	2.04	0.40
2:E:43:LYS:HG2	2:E:44:GLU:N	2.37	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)
1:C:209:LYS:NZ	1:C:211:SER:O[4_557]	2.08	0.12

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	479/550 (87%)	465 (97%)	13 (3%)	1 (0%)	52 85
1	B	481/550 (88%)	467 (97%)	12 (2%)	2 (0%)	39 76
1	C	477/550 (87%)	454 (95%)	22 (5%)	1 (0%)	52 85
2	D	124/131 (95%)	118 (95%)	6 (5%)	0	100 100
2	E	121/131 (92%)	118 (98%)	3 (2%)	0	100 100
2	F	123/131 (94%)	120 (98%)	3 (2%)	0	100 100
All	All	1805/2043 (88%)	1742 (96%)	59 (3%)	4 (0%)	52 85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	B	65	LYS
1	C	65	LYS
1	B	527	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	435/494 (88%)	432 (99%)	3 (1%)	88 94
1	B	437/494 (88%)	434 (99%)	3 (1%)	88 94
1	C	434/494 (88%)	430 (99%)	4 (1%)	84 92
2	D	103/108 (95%)	103 (100%)	0	100 100
2	E	100/108 (93%)	100 (100%)	0	100 100
2	F	102/108 (94%)	102 (100%)	0	100 100
All	All	1611/1806 (89%)	1601 (99%)	10 (1%)	90 95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	GLU
1	A	215	SER
1	A	297	LEU
1	B	161	GLU
1	B	202	GLN
1	B	297	LEU
1	C	137	PHE
1	C	297	LEU
1	C	361	GLN
1	C	472	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	225	GLN
1	B	317	HIS
1	C	460	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

3 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	NAG	A	800	1	14,14,15	0.22	0	15,19,21	0.28	0
3	NAG	B	800	1	14,14,15	0.22	0	15,19,21	0.51	0
3	NAG	C	800	1	14,14,15	0.36	0	15,19,21	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	800	1	-	0/6/23/26	0/1/1/1
3	NAG	B	800	1	-	0/6/23/26	0/1/1/1
3	NAG	C	800	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (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	483/550 (87%)	-0.02	15 (3%) 52 46	49, 78, 165, 238	0
1	B	485/550 (88%)	0.08	19 (3%) 43 36	48, 84, 170, 264	0
1	C	481/550 (87%)	0.02	11 (2%) 64 57	50, 82, 159, 239	0
2	D	126/131 (96%)	-0.05	1 (0%) 87 84	58, 77, 109, 151	0
2	E	123/131 (93%)	0.63	17 (13%) 4 3	80, 128, 167, 175	0
2	F	125/131 (95%)	0.19	4 (3%) 51 44	62, 98, 137, 188	0
All	All	1823/2043 (89%)	0.08	67 (3%) 45 38	48, 84, 163, 264	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	SER	12.0
1	B	211	SER	7.1
1	B	210	GLN	7.1
1	B	207	LEU	6.7
1	B	209	LYS	5.8
1	B	208	ASN	5.7
1	B	216	ASN	4.7
1	A	215	SER	4.6
1	B	72	THR	4.3
1	C	208	ASN	4.2
2	F	73	ASN	3.8
1	A	67	ASN	3.7
2	E	1	GLN	3.6
2	E	10	GLY	3.5
1	C	210	GLN	3.5
1	C	67	ASN	3.5
2	E	15	GLY	3.5
2	E	11	LEU	3.4
1	B	206	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	70	ASN	3.4
1	C	207	LEU	3.3
1	C	65	LYS	3.3
2	E	110	THR	3.2
2	E	111	VAL	3.2
1	B	204	LEU	3.1
1	B	68	LYS	3.1
2	F	11	LEU	3.0
2	E	82(C)	LEU	2.9
2	D	1	GLN	2.9
1	B	214	ILE	2.9
1	C	64	ILE	2.8
1	B	67	ASN	2.8
2	F	112	SER	2.7
1	C	66	GLU	2.6
1	B	200	ASP	2.6
2	E	104	GLY	2.5
1	C	217	ILE	2.5
2	E	17	SER	2.5
1	B	66	GLU	2.5
2	E	18	LEU	2.4
1	A	75	LYS	2.4
2	E	16	GLY	2.4
1	A	72	THR	2.4
1	A	202	GLN	2.4
2	E	12	VAL	2.4
1	A	209	LYS	2.4
1	A	65	LYS	2.3
1	A	218	GLU	2.3
2	F	1	GLN	2.3
1	A	198	TYR	2.3
2	E	26	GLY	2.3
2	E	107	THR	2.3
1	A	210	GLN	2.3
2	E	41	PRO	2.2
2	E	84	PRO	2.2
1	B	201	LYS	2.2
1	A	76	VAL	2.1
1	A	64	ILE	2.1
1	A	71	GLY	2.1
1	A	217	ILE	2.1
1	C	211	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	486	ASP	2.1
1	C	174	THR	2.1
1	B	70	ASN	2.1
1	B	76	VAL	2.1
1	B	203	LEU	2.0
2	E	73	ASN	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	800	14/15	0.96	0.24	0.90	71,78,85,87	0
3	NAG	B	800	14/15	0.84	0.32	-	109,118,126,126	0
3	NAG	C	800	14/15	0.93	0.26	-	81,92,99,100	0

6.5 Other polymers (i)

There are no such residues in this entry.