



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:45 PM GMT

PDB ID : 4MMY
Title : Integrin AlphaVBeta3 ectodomain bound to the tenth domain of Fibronectin with the IAKGDWND motif
Authors : van Agthoven, J.; Xiong, J.; Arnaout, M.A.
Deposited on : 2013-09-09
Resolution : 3.18 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

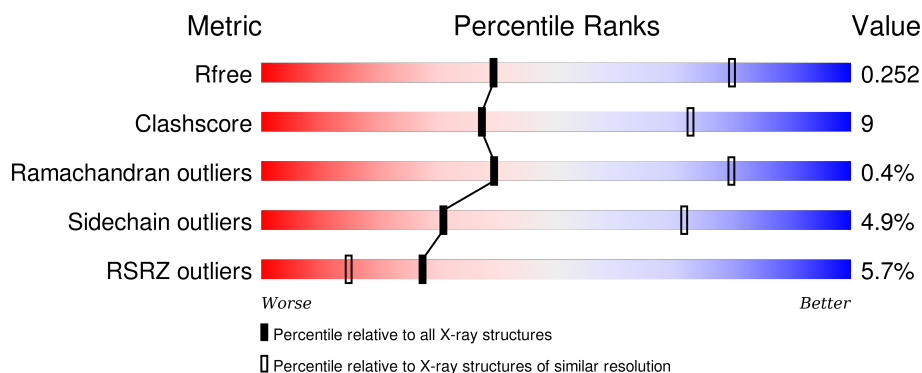
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


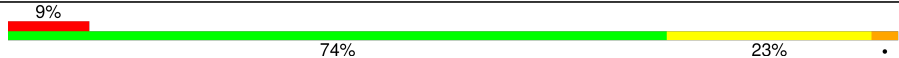
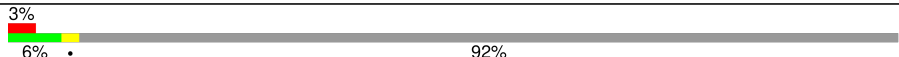
The reported resolution of this entry is 3.18 Å.

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	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

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	959	 3% 74% 21% • •
2	B	692	 9% 74% 23% •
3	C	98	 3% 6% 92% •

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13000 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7196	4556	1221	1384	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	690	Total	C	N	O	S	0	0	0
			5294	3250	904	1070	70			

- Molecule 3 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			65	41	13	11			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1491	ILE	THR	ENGINEERED MUTATION	UNP P02751
C	1492	ALA	GLY	ENGINEERED MUTATION	UNP P02751
C	1496	TRP	SER	ENGINEERED MUTATION	UNP P02751
C	1497	ASN	PRO	ENGINEERED MUTATION	UNP P02751
C	1498	ASP	ALA	ENGINEERED MUTATION	UNP P02751
C	1499	GLY	SER	ENGINEERED MUTATION	UNP P02751
C	1510	GLY	-	EXPRESSION TAG	UNP P02751
C	1511	LYS	-	EXPRESSION TAG	UNP P02751
C	1512	LYS	-	EXPRESSION TAG	UNP P02751
C	1513	GLY	-	EXPRESSION TAG	UNP P02751
C	1514	LYS	-	EXPRESSION TAG	UNP P02751

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			50	28	2	20		
4	A	4	Total	C	N	O	0	0
			50	28	2	20		

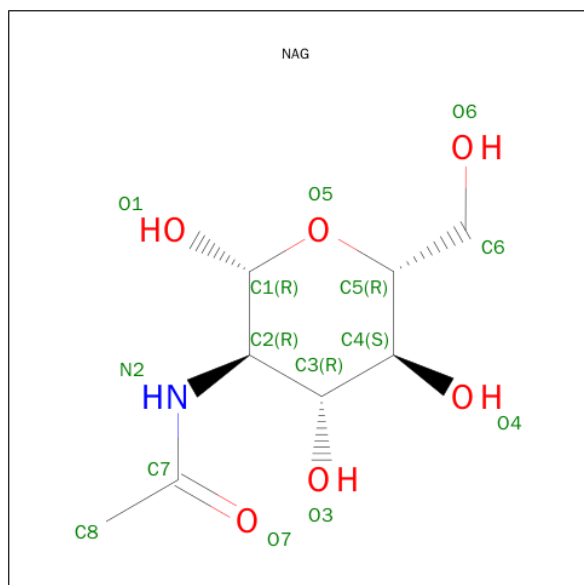
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	3	Total C N O 39 22 2 15	0	0
8	B	3	Total C N O 39 22 2 15	0	0

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	3	Total Mn 3 3	0	0
9	A	5	Total Mn 5 5	0	0

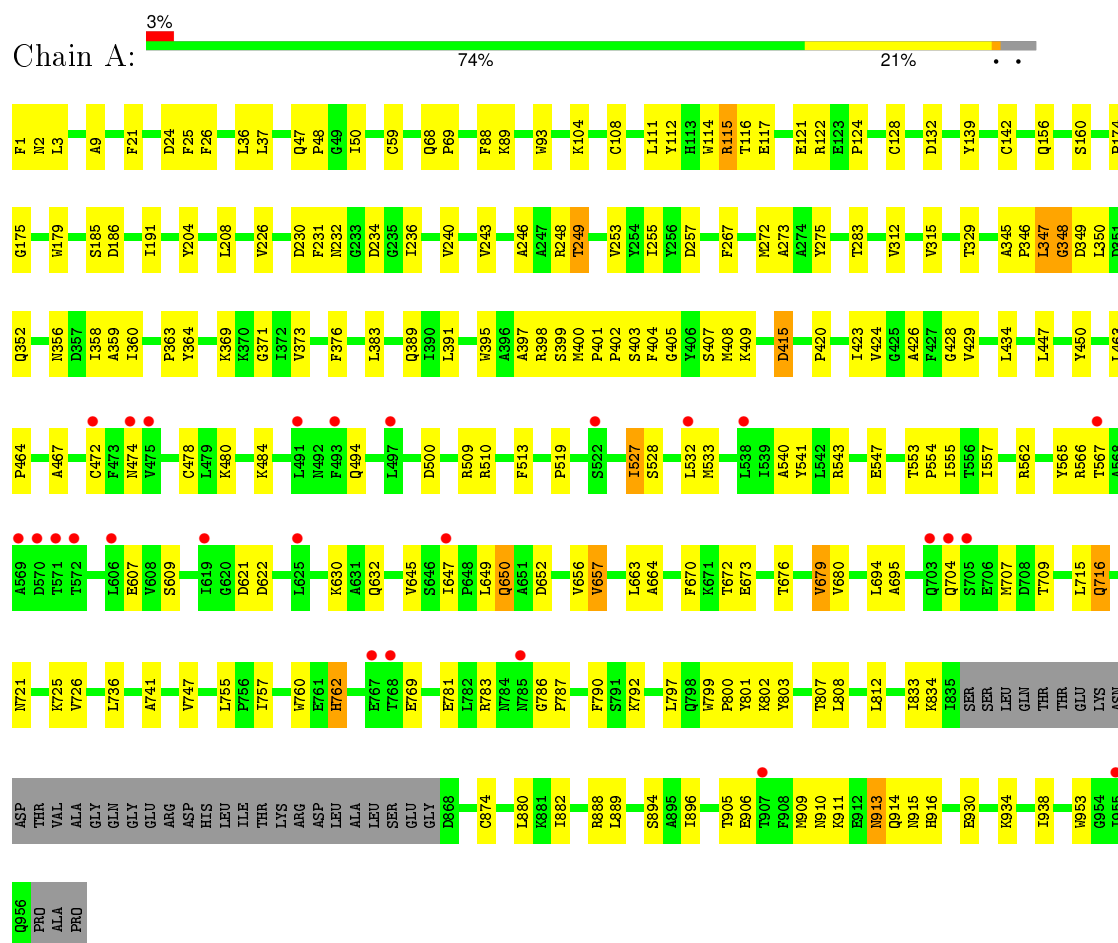
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	3	Total O 3 3	0	0
10	B	2	Total O 2 2	0	0

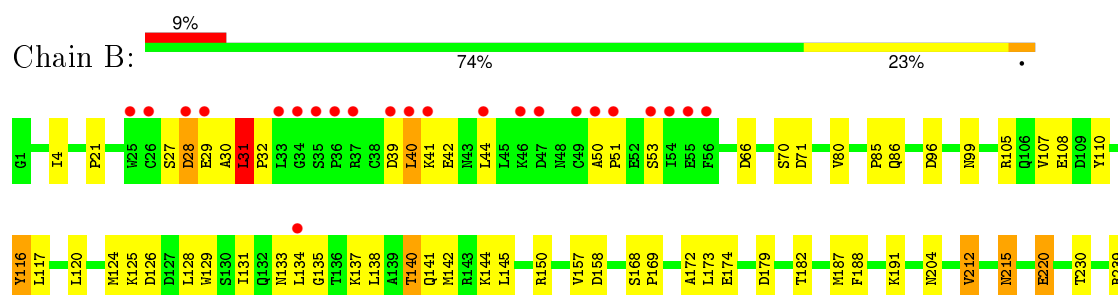
3 Residue-property plots [i](#)

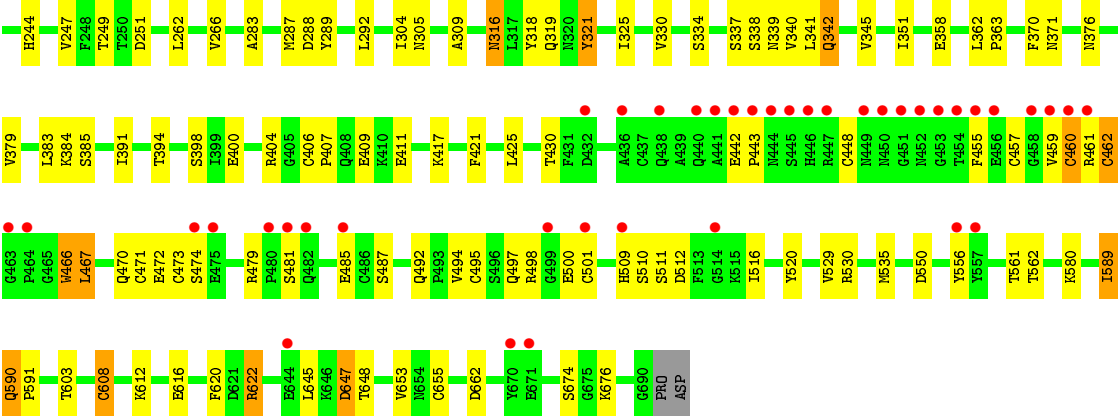
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Integrin alpha-V



• Molecule 2: Integrin beta-3





● Molecule 3: Fibronectin



SER	ASP	VAL	PRO	VAL	ASP	ASP	LEU	GLU	VAL	VAL	ALA	ALA	THR	PRO	THR	SER	LEU	LEU	ILE	SER	TRP	ASP	ALA	PRO	ALA	VAL	THR	VAL	ARG	TYR	TYR	ARG	ILE	TYR	THR	GLY	GLU	THR	GLY	GLY	ASN	SER	SER	PRO	VAL	GLN	GLU	PHE	THR	VAL	PRO	PRO	GLY	SER	LYS	SER	THR	THR	ALA	THR	THR	ILE	SER	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
LEU	LYS	PRO	GLY	VAL	ASP	ASP	TYR	THR	ILE	THR	VAL	TYR	ALA	V1490	I1491	A1492	R1493	G1494	D1495	V1496	I1497	ASP	GLY	SER	LYS	PRO	ILE	ILE	ILE	ASN	TYR	ARG	THR	GLY	LYS	GLY	LYS	LYS	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.02Å 130.02Å 308.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.02 – 3.18 49.69 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.02-3.18) 99.4 (49.69-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.211 , 0.252 0.211 , 0.252	Depositor DCC
R_{free} test set	2536 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.8	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 51179 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13000	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MN, 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	0.23	0/7352	0.44	0/9967
2	B	0.22	0/5390	0.47	0/7289
3	C	0.17	0/66	0.49	0/89
All	All	0.23	0/12808	0.45	0/17345

There are no bond length outliers.

There are no bond angle outliers.

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	7196	0	7013	129	0
2	B	5294	0	5024	109	0
3	C	65	0	60	1	0
4	A	100	0	86	0	0
5	A	84	0	75	1	0
5	B	28	0	25	2	0
6	A	72	0	61	0	0
7	A	42	0	39	0	0
7	B	28	0	26	2	0
8	A	39	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	39	0	34	0	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	A	3	0	0	0	0
10	B	2	0	0	0	0
All	All	13000	0	12477	237	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 9.

All (237) 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:346:PRO:C	1:A:347:LEU:HD23	1.66	1.15
1:A:347:LEU:N	1:A:347:LEU:HD23	1.50	1.08
2:B:27:SER:O	2:B:28:ASP:HB2	1.30	1.07
2:B:30:ALA:O	2:B:31:LEU:HD23	1.61	1.00
1:A:347:LEU:N	1:A:347:LEU:CD2	2.30	0.94
2:B:27:SER:HB2	2:B:53:SER:HB2	1.50	0.91
2:B:27:SER:O	2:B:28:ASP:CB	2.16	0.91
2:B:30:ALA:O	2:B:31:LEU:HB3	1.79	0.83
2:B:28:ASP:O	2:B:29:GLU:HB2	1.77	0.83
2:B:30:ALA:O	2:B:31:LEU:CB	2.30	0.80
2:B:510:SER:HB3	2:B:511:SER:HA	1.65	0.78
2:B:31:LEU:HD12	2:B:31:LEU:O	1.84	0.77
2:B:30:ALA:O	2:B:31:LEU:CD2	2.32	0.76
2:B:455:PHE:HA	2:B:460:CYS:HA	1.69	0.74
1:A:415:ASP:OD1	1:A:415:ASP:N	2.16	0.73
1:A:707:MET:HG2	1:A:934:LYS:H	1.53	0.73
1:A:609:SER:HB2	1:A:630:LYS:HB3	1.70	0.73
1:A:348:GLY:O	1:A:356:ASN:CB	2.36	0.73
2:B:141:GLN:HE21	2:B:345:VAL:HG23	1.53	0.73
1:A:664:ALA:HB3	1:A:695:ALA:HB2	1.73	0.71
1:A:348:GLY:O	1:A:356:ASN:HB3	1.90	0.70
2:B:616:GLU:HG3	2:B:622:ARG:HB3	1.75	0.68
2:B:169:PRO:HD2	2:B:172:ALA:HB2	1.76	0.68
1:A:645:VAL:HB	1:A:679:VAL:HG13	1.78	0.66
1:A:402:PRO:HA	1:A:428:GLY:HA3	1.78	0.66
2:B:498:ARG:HD3	2:B:516:ILE:HD13	1.77	0.66
1:A:565:TYR:O	1:A:566:ARG:NH1	2.28	0.64
1:A:371:GLY:HA3	1:A:404:PHE:HB3	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ALA:H	1:A:786:GLY:HA3	1.61	0.64
2:B:417:LYS:NZ	2:B:421:PHE:O	2.29	0.64
2:B:404:ARG:NH1	2:B:550:ASP:OD1	2.28	0.64
1:A:650:GLN:HE21	1:A:704:GLN:HB2	1.62	0.64
2:B:487:SER:HB2	2:B:492:GLN:HB3	1.80	0.63
2:B:292:LEU:HD22	2:B:325:ILE:HD11	1.81	0.63
1:A:348:GLY:O	1:A:356:ASN:HA	2.00	0.61
2:B:28:ASP:O	2:B:29:GLU:CB	2.48	0.61
1:A:348:GLY:O	1:A:356:ASN:CA	2.49	0.61
1:A:725:LYS:HG3	1:A:726:VAL:HG13	1.81	0.61
2:B:473:CYS:SG	2:B:474:SER:N	2.71	0.60
2:B:383:LEU:HG	2:B:385:SER:H	1.66	0.60
1:A:346:PRO:C	1:A:347:LEU:CD2	2.58	0.60
1:A:248:ARG:NH1	1:A:272:MET:SD	2.74	0.60
1:A:345:ALA:O	1:A:347:LEU:HD21	2.02	0.59
1:A:402:PRO:HB3	1:A:429:VAL:HG13	1.85	0.59
2:B:30:ALA:O	2:B:31:LEU:CG	2.51	0.59
2:B:137:LYS:HB3	2:B:341:LEU:HD21	1.85	0.59
2:B:318:TYR:HA	2:B:321:TYR:HB2	1.85	0.58
1:A:3:LEU:HG	1:A:350:LEU:HD21	1.85	0.58
1:A:802:LYS:HG2	1:A:807:THR:HA	1.84	0.58
2:B:134:LEU:O	2:B:137:LYS:N	2.37	0.58
2:B:129:TRP:HZ3	2:B:339:ASN:HD21	1.52	0.58
1:A:395:TRP:HB3	1:A:429:VAL:HG11	1.86	0.57
2:B:411:GLU:HG2	2:B:430:THR:HG22	1.86	0.57
1:A:543:ARG:NH1	1:A:547:GLU:OE1	2.34	0.57
2:B:99:ASN:HD22	7:B:701:NAG:H62	1.69	0.57
1:A:909:MET:HA	1:A:914:GLN:HA	1.87	0.56
1:A:645:VAL:HG22	1:A:715:LEU:HD22	1.88	0.56
2:B:31:LEU:CD1	2:B:31:LEU:O	2.52	0.55
1:A:114:TRP:CD2	1:A:116:THR:HA	2.42	0.55
1:A:114:TRP:CE2	1:A:116:THR:HA	2.41	0.55
2:B:674:SER:HB3	2:B:676:LYS:HG3	1.89	0.55
2:B:31:LEU:CG	2:B:31:LEU:O	2.55	0.54
1:A:397:ALA:HB2	1:A:402:PRO:HD3	1.90	0.54
1:A:913:ASN:ND2	1:A:913:ASN:O	2.40	0.54
2:B:510:SER:H	2:B:511:SER:HB3	1.73	0.54
2:B:288:ASP:OD1	2:B:289:TYR:N	2.40	0.54
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.89	0.54
1:A:450:TYR:HB2	1:A:474:ASN:HB2	1.89	0.54
1:A:253:VAL:HB	1:A:267:PHE:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:GLU:O	2:B:30:ALA:C	2.47	0.53
1:A:621:ASP:OD1	1:A:622:ASP:N	2.40	0.53
2:B:608:CYS:O	2:B:612:LYS:N	2.41	0.53
2:B:31:LEU:H	2:B:32:PRO:HD3	1.73	0.53
2:B:459:VAL:HG12	2:B:461:ARG:H	1.74	0.53
2:B:620:PHE:HB3	2:B:622:ARG:HE	1.75	0.52
1:A:315:VAL:HG21	1:A:360:ILE:HD13	1.91	0.52
1:A:915:ASN:HA	1:A:953:TRP:CD1	2.44	0.52
1:A:124:PRO:HB2	1:A:156:GLN:HG2	1.91	0.52
2:B:120:LEU:HD12	2:B:188:PHE:HZ	1.75	0.52
1:A:607:GLU:OE1	1:A:632:GLN:NE2	2.42	0.52
2:B:530:ARG:HG2	2:B:535:MET:HA	1.90	0.52
2:B:144:LYS:HG3	2:B:145:LEU:HD13	1.91	0.52
1:A:349:ASP:O	1:A:420:PRO:HG3	2.09	0.52
2:B:580:LYS:HG2	2:B:589:ILE:HD11	1.92	0.52
1:A:906:GLU:O	1:A:910:ASN:ND2	2.42	0.51
2:B:529:VAL:HG11	2:B:556:TYR:HE1	1.76	0.51
1:A:231:PHE:CD2	1:A:231:PHE:N	2.77	0.51
2:B:133:ASN:O	2:B:204:ASN:ND2	2.43	0.51
2:B:494:VAL:HG22	2:B:495:CYS:H	1.75	0.51
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.93	0.51
1:A:21:PHE:HE1	2:B:266:VAL:HG11	1.75	0.51
2:B:316:ASN:HB3	7:B:702:NAG:H82	1.93	0.51
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.93	0.51
1:A:345:ALA:O	1:A:347:LEU:CD2	2.59	0.51
1:A:510:ARG:NH2	1:A:553:THR:O	2.25	0.50
2:B:215:ASN:O	3:C:1495:ASP:HB3	2.12	0.50
2:B:50:ALA:N	2:B:51:PRO:HD2	2.27	0.49
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.94	0.49
1:A:185:SER:HB3	1:A:208:LEU:HB2	1.95	0.49
1:A:649:LEU:HD13	1:A:704:GLN:HG3	1.94	0.49
1:A:104:LYS:HD3	1:A:132:ASP:HB2	1.93	0.49
1:A:232:ASN:ND2	1:A:257:ASP:OD1	2.45	0.49
1:A:24:ASP:OD1	1:A:25:PHE:N	2.45	0.49
1:A:26:PHE:HB2	1:A:37:LEU:HG	1.93	0.49
1:A:909:MET:HA	1:A:914:GLN:HG3	1.94	0.49
1:A:513:PHE:HA	1:A:540:ALA:HA	1.95	0.49
1:A:408:MET:HG2	1:A:424:VAL:HG22	1.94	0.49
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.95	0.49
2:B:362:LEU:HD12	2:B:363:PRO:HD2	1.94	0.48
2:B:442:GLU:HG3	2:B:443:PRO:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ILE:HG12	1:A:434:LEU:HD23	1.94	0.48
2:B:400:GLU:HB2	5:B:703:NAG:H83	1.94	0.48
2:B:358:GLU:N	2:B:417:LYS:O	2.42	0.48
2:B:124:MET:HG2	2:B:251:ASP:HB2	1.95	0.48
1:A:249:THR:HG23	1:A:273:ALA:H	1.79	0.48
1:A:349:ASP:O	1:A:420:PRO:CG	2.61	0.48
1:A:2:ASN:OD1	1:A:2:ASN:N	2.47	0.47
2:B:338:SER:HB3	2:B:342:GLN:HB2	1.96	0.47
2:B:608:CYS:HB3	2:B:655:CYS:HB3	1.58	0.47
5:B:703:NAG:H62	5:B:704:NAG:H83	1.96	0.47
2:B:479:ARG:O	2:B:481:SER:N	2.45	0.47
2:B:116:TYR:HA	2:B:247:VAL:HG13	1.97	0.47
2:B:133:ASN:ND2	2:B:137:LYS:HE3	2.29	0.47
1:A:480:LYS:HB3	1:A:533:MET:HG2	1.96	0.47
2:B:66:ASP:HB3	2:B:85:PRO:HB3	1.97	0.47
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.96	0.47
2:B:134:LEU:O	2:B:138:LEU:N	2.39	0.46
1:A:792:LYS:HB2	1:A:930:GLU:HG2	1.97	0.46
1:A:405:GLY:C	1:A:407:SER:H	2.19	0.46
1:A:243:VAL:HG22	1:A:246:ALA:HB2	1.97	0.46
2:B:158:ASP:HB3	2:B:187:MET:HE1	1.98	0.46
1:A:447:LEU:HD21	1:A:557:ILE:HG22	1.98	0.46
2:B:157:VAL:O	2:B:220:GLU:HG3	2.16	0.46
2:B:135:GLY:HA2	2:B:138:LEU:HB2	1.97	0.46
1:A:108:CYS:HA	1:A:128:CYS:HA	1.98	0.46
2:B:137:LYS:O	2:B:140:THR:HG22	2.16	0.45
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.98	0.45
1:A:400:MET:HB2	1:A:401:PRO:HD2	1.96	0.45
1:A:527:ILE:HG22	1:A:528:SER:H	1.82	0.45
1:A:803:TYR:HB2	1:A:808:LEU:HD11	1.98	0.45
1:A:797:LEU:HD23	1:A:882:ILE:HD12	1.98	0.45
1:A:139:TYR:OH	1:A:186:ASP:OD2	2.31	0.45
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.98	0.45
2:B:41:LYS:HD2	2:B:41:LYS:HA	1.69	0.45
2:B:590:GLN:CD	2:B:591:PRO:HD2	2.36	0.45
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.98	0.45
1:A:652:ASP:N	1:A:652:ASP:OD1	2.50	0.45
1:A:472:CYS:HA	1:A:541:TYR:HA	1.99	0.45
2:B:371:ASN:HB2	2:B:398:SER:OG	2.17	0.45
2:B:305:ASN:HB3	2:B:351:ILE:HD13	1.98	0.45
1:A:160:SER:HB2	1:A:226:VAL:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TRP:CD1	1:A:111:LEU:HD22	2.52	0.45
2:B:249:THR:HA	2:B:309:ALA:O	2.17	0.45
1:A:494:GLN:HB2	1:A:562:ARG:HB3	1.99	0.45
2:B:133:ASN:HD22	2:B:137:LYS:HE3	1.82	0.44
1:A:769:GLU:HG2	1:A:812:LEU:HD21	1.99	0.44
2:B:244:HIS:HB2	2:B:304:ILE:HA	1.99	0.44
1:A:352:GLN:O	1:A:484:LYS:NZ	2.49	0.44
1:A:350:LEU:HA	1:A:350:LEU:HD12	1.74	0.44
1:A:500:ASP:HB2	1:A:555:ILE:HG23	1.98	0.44
1:A:888:ARG:HD2	1:A:888:ARG:HA	1.73	0.44
2:B:105:ARG:HB2	2:B:394:THR:HG23	1.98	0.44
1:A:364:TYR:HB3	1:A:369:LYS:HE3	2.00	0.44
1:A:398:ARG:HG3	1:A:399:SER:H	1.82	0.44
2:B:125:LYS:HG3	2:B:212:VAL:HG21	1.99	0.44
2:B:21:PRO:HB3	2:B:96:ASP:HB2	2.00	0.44
1:A:175:GLY:HA2	1:A:179:TRP:CD1	2.53	0.44
2:B:497:GLN:HB3	2:B:498:ARG:H	1.54	0.43
1:A:799:TRP:HA	1:A:800:PRO:HD3	1.79	0.43
1:A:762:HIS:ND1	1:A:906:GLU:OE1	2.46	0.43
2:B:494:VAL:HG21	2:B:500:GLU:HB2	1.99	0.43
2:B:466:TRP:CD2	2:B:471:CYS:HB3	2.53	0.43
1:A:783:ARG:HG3	1:A:894:SER:HB2	1.99	0.43
1:A:347:LEU:HD11	1:A:359:ALA:HB2	1.99	0.43
2:B:173:LEU:O	2:B:174:GLU:HB3	2.18	0.43
5:A:1018:NAG:H4	5:A:1019:NAG:H2	1.83	0.43
1:A:88:PHE:CE2	1:A:122:ARG:HG2	2.54	0.43
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.88	0.43
2:B:462:CYS:HB3	2:B:467:LEU:H	1.83	0.43
2:B:141:GLN:O	2:B:144:LYS:HG2	2.17	0.43
2:B:407:PRO:HB2	2:B:409:GLU:HG2	2.00	0.43
1:A:509:ARG:HH11	1:A:519:PRO:HB2	1.83	0.43
2:B:131:ILE:HA	2:B:131:ILE:HD12	1.87	0.43
2:B:86:GLN:O	2:B:425:LEU:HD12	2.19	0.43
1:A:747:VAL:HG13	2:B:603:THR:HB	2.01	0.43
2:B:39:ASP:HB3	2:B:40:LEU:H	1.59	0.43
1:A:234:ASP:HB2	1:A:236:ILE:HD12	2.00	0.43
1:A:347:LEU:O	1:A:349:ASP:N	2.51	0.43
2:B:647:ASP:OD1	2:B:647:ASP:N	2.52	0.43
2:B:70:SER:HB2	2:B:107:VAL:HG11	2.01	0.43
2:B:188:PHE:CZ	2:B:191:LYS:HE3	2.53	0.42
1:A:364:TYR:O	1:A:369:LYS:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:HD3	1:A:115:ARG:O	2.19	0.42
2:B:150:ARG:HG3	2:B:239:ARG:CZ	2.49	0.42
2:B:4:ILE:HD12	2:B:4:ILE:H	1.84	0.42
2:B:108:GLU:HG2	2:B:391:ILE:HG22	2.01	0.42
1:A:346:PRO:HA	1:A:358:ILE:HG13	2.02	0.42
2:B:137:LYS:O	2:B:141:GLN:HG2	2.18	0.42
2:B:134:LEU:HA	2:B:134:LEU:HD12	1.92	0.42
1:A:68:GLN:HA	1:A:69:PRO:HD3	1.92	0.42
1:A:716:GLN:HB2	1:A:716:GLN:HE21	1.62	0.42
2:B:71:ASP:OD1	2:B:71:ASP:N	2.45	0.42
1:A:709:THR:O	1:A:736:LEU:HB2	2.20	0.42
1:A:174:PRO:HB2	2:B:262:LEU:HD21	2.02	0.42
1:A:621:ASP:HB2	1:A:787:PRO:HB3	2.02	0.41
2:B:80:VAL:HG11	2:B:110:TYR:HE1	1.85	0.41
1:A:403:SER:O	1:A:426:ALA:HA	2.20	0.41
1:A:230:ASP:OD1	1:A:234:ASP:O	2.38	0.41
2:B:334:SER:OG	2:B:337:SER:OG	2.37	0.41
1:A:911:LYS:C	1:A:913:ASN:H	2.22	0.41
2:B:406:CYS:HA	2:B:407:PRO:HD3	1.81	0.41
2:B:141:GLN:HG3	2:B:142:MET:H	1.85	0.41
1:A:464:PRO:HG2	1:A:467:ALA:HB3	2.01	0.41
1:A:191:ILE:HA	1:A:204:TYR:CE2	2.54	0.41
1:A:760:TRP:CZ2	1:A:905:THR:HB	2.56	0.41
1:A:112:TYR:O	1:A:124:PRO:HA	2.21	0.41
1:A:553:THR:HA	1:A:554:PRO:HD3	1.93	0.41
2:B:283:ALA:HB1	2:B:287:MET:HG2	2.02	0.41
1:A:373:VAL:HB	1:A:391:LEU:HB2	2.02	0.41
1:A:647:ILE:HD11	1:A:670:PHE:HE1	1.86	0.41
1:A:376:PHE:HB3	1:A:383:LEU:HD11	2.02	0.41
1:A:790:PHE:CZ	1:A:889:LEU:HB2	2.55	0.41
1:A:721:ASN:O	1:A:725:LYS:HE2	2.20	0.41
2:B:495:CYS:HB3	2:B:520:TYR:O	2.21	0.41
1:A:755:LEU:HD23	1:A:757:ILE:HD13	2.03	0.41
1:A:781:GLU:HG3	1:A:896:ILE:HG13	2.03	0.41
2:B:126:ASP:OD1	2:B:126:ASP:N	2.52	0.41
1:A:115:ARG:HA	1:A:121:GLU:HB2	2.03	0.41
1:A:657:VAL:HG21	1:A:663:LEU:HD13	2.03	0.41
1:A:232:ASN:N	1:A:232:ASN:OD1	2.53	0.40
1:A:478:CYS:HB3	1:A:533:MET:HB2	2.03	0.40
1:A:363:PRO:HA	1:A:404:PHE:O	2.21	0.40
2:B:117:LEU:HA	2:B:117:LEU:HD23	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:ARG:CZ	2:B:239:ARG:HD3	2.51	0.40
2:B:370:PHE:CG	2:B:384:LYS:HG2	2.56	0.40
1:A:797:LEU:HB3	1:A:882:ILE:HB	2.02	0.40
1:A:673:GLU:O	1:A:676:THR:OG1	2.31	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	920/959 (96%)	853 (93%)	65 (7%)	2 (0%)	52	88
2	B	688/692 (99%)	595 (86%)	89 (13%)	4 (1%)	30	74
3	C	6/98 (6%)	5 (83%)	1 (17%)	0	100	100
All	All	1614/1749 (92%)	1453 (90%)	155 (10%)	6 (0%)	39	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	28	ASP
2	B	31	LEU
1	A	833	ILE
2	B	457	CYS
1	A	348	GLY
2	B	379	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	784/813 (96%)	756 (96%)	28 (4%)	42	79
2	B	612/614 (100%)	572 (94%)	40 (6%)	21	60
3	C	6/81 (7%)	5 (83%)	1 (17%)	3	12
All	All	1402/1508 (93%)	1333 (95%)	69 (5%)	31	72

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	117	GLU
1	A	142	CYS
1	A	249	THR
1	A	275	TYR
1	A	283	THR
1	A	312	VAL
1	A	329	THR
1	A	347	LEU
1	A	415	ASP
1	A	463	LEU
1	A	527	ILE
1	A	532	LEU
1	A	567	THR
1	A	650	GLN
1	A	656	VAL
1	A	657	VAL
1	A	672	THR
1	A	679	VAL
1	A	680	VAL
1	A	694	LEU
1	A	716	GLN
1	A	762	HIS
1	A	834	LYS
1	A	874	CYS
1	A	913	ASN
1	A	916	HIS
1	A	938	ILE
2	B	31	LEU
2	B	40	LEU
2	B	42	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	44	LEU
2	B	116	TYR
2	B	128	LEU
2	B	140	THR
2	B	168	SER
2	B	179	ASP
2	B	182	THR
2	B	212	VAL
2	B	215	ASN
2	B	220	GLU
2	B	316	ASN
2	B	321	TYR
2	B	340	VAL
2	B	342	GLN
2	B	376	ASN
2	B	448	CYS
2	B	460	CYS
2	B	462	CYS
2	B	466	TRP
2	B	467	LEU
2	B	470	GLN
2	B	472	GLU
2	B	485	GLU
2	B	501	CYS
2	B	509	HIS
2	B	512	ASP
2	B	561	THR
2	B	562	THR
2	B	589	ILE
2	B	590	GLN
2	B	608	CYS
2	B	622	ARG
2	B	645	LEU
2	B	647	ASP
2	B	648	THR
2	B	653	VAL
2	B	662	ASP
3	C	1493	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	GLN
2	B	141	GLN

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 ⓘ

28 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	$\# Z > 2$
4	NAG	A	1001	1,4	14,14,15	0.54	0	15,19,21	0.37	0
4	NAG	A	1002	4	14,14,15	0.17	0	15,19,21	0.29	0
4	BMA	A	1003	4	11,11,12	0.60	0	14,15,17	0.72	0
4	MAN	A	1004	4	11,11,12	0.70	0	14,15,17	1.06	2 (14%)
5	NAG	A	1005	1,5	14,14,15	0.24	0	15,19,21	0.32	0
5	NAG	A	1006	5	14,14,15	0.22	0	15,19,21	0.33	0
6	NAG	A	1007	1,6	14,14,15	0.29	0	15,19,21	0.30	0
6	NAG	A	1008	6	14,14,15	0.19	0	15,19,21	0.38	0
6	BMA	A	1009	6	11,11,12	0.66	0	14,15,17	0.71	0
6	MAN	A	1010	6	11,11,12	0.67	0	14,15,17	1.08	2 (14%)
6	BMA	A	1011	6	11,11,12	1.30	2 (18%)	14,15,17	1.18	1 (7%)
6	MAN	A	1012	6	11,11,12	0.70	0	14,15,17	1.02	2 (14%)
4	NAG	A	1013	1,4	14,14,15	0.36	0	15,19,21	0.30	0
4	NAG	A	1014	4	14,14,15	0.32	0	15,19,21	0.30	0
4	BMA	A	1015	4	11,11,12	0.77	0	14,15,17	1.03	2 (14%)
4	MAN	A	1016	4	11,11,12	0.80	0	14,15,17	1.02	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1018	1,5	14,14,15	0.18	0	15,19,21	0.38	0
5	NAG	A	1019	5	14,14,15	0.24	0	15,19,21	0.28	0
5	NAG	A	1022	1,5	14,14,15	0.27	0	15,19,21	0.42	0
5	NAG	A	1023	5	14,14,15	0.50	0	15,19,21	0.70	1 (6%)
8	NAG	A	1024	1,8	14,14,15	0.24	0	15,19,21	0.37	0
8	NAG	A	1025	8	14,14,15	0.73	1 (7%)	15,19,21	0.95	1 (6%)
8	BMA	A	1026	8	11,11,12	1.25	2 (18%)	14,15,17	1.80	3 (21%)
5	NAG	B	703	2,5	14,14,15	0.23	0	15,19,21	0.29	0
5	NAG	B	704	5	14,14,15	0.71	1 (7%)	15,19,21	0.98	1 (6%)
8	NAG	B	705	8,2	14,14,15	0.27	0	15,19,21	0.40	0
8	NAG	B	706	8	14,14,15	0.68	1 (7%)	15,19,21	0.96	1 (6%)
8	BMA	B	707	8	11,11,12	0.77	0	14,15,17	1.24	2 (14%)

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	1001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1003	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1004	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1005	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1006	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1007	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1008	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1009	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1010	6	-	0/2/19/22	0/1/1/1
6	BMA	A	1011	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1012	6	-	0/2/19/22	0/1/1/1
4	NAG	A	1013	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1014	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1015	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1016	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1018	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1019	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1022	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1023	5	-	0/6/23/26	0/1/1/1
8	NAG	A	1024	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1025	8	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	A	1026	8	-	0/2/19/22	0/1/1/1
5	NAG	B	703	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	704	5	-	0/6/23/26	0/1/1/1
8	NAG	B	705	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	706	8	-	0/6/23/26	0/1/1/1
8	BMA	B	707	8	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1011	BMA	O5-C1	-2.30	1.39	1.43
8	A	1025	NAG	O5-C1	2.20	1.47	1.43
8	B	706	NAG	O5-C1	2.26	1.47	1.43
8	A	1026	BMA	C1-C2	2.29	1.57	1.52
5	B	704	NAG	O5-C1	2.42	1.47	1.43
6	A	1011	BMA	C4-C5	2.65	1.58	1.53
8	A	1026	BMA	C2-C3	3.08	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1016	MAN	O2-C2-C3	-2.31	105.47	110.12
4	A	1004	MAN	O2-C2-C3	-2.29	105.51	110.12
4	A	1015	BMA	C1-C2-C3	-2.25	106.88	109.54
6	A	1012	MAN	O2-C2-C3	-2.23	105.63	110.12
6	A	1010	MAN	O2-C2-C3	-2.19	105.71	110.12
8	B	707	BMA	O5-C1-C2	2.03	114.16	110.86
6	A	1012	MAN	C1-O5-C5	2.12	114.94	112.25
4	A	1004	MAN	C1-O5-C5	2.12	114.94	112.25
6	A	1010	MAN	C1-O5-C5	2.28	115.14	112.25
8	A	1026	BMA	C2-C3-C4	2.31	114.97	111.04
6	A	1011	BMA	C3-C4-C5	2.38	114.34	110.20
4	A	1015	BMA	O3-C3-C2	2.39	114.32	110.00
5	A	1023	NAG	C1-O5-C5	2.64	115.59	112.25
8	B	707	BMA	C1-O5-C5	2.87	115.89	112.25
8	A	1026	BMA	O5-C1-C2	3.05	115.81	110.86
8	B	706	NAG	C1-O5-C5	3.57	116.77	112.25
8	A	1025	NAG	C1-O5-C5	3.61	116.83	112.25
5	B	704	NAG	C1-O5-C5	3.66	116.90	112.25
8	A	1026	BMA	C1-C2-C3	4.62	115.00	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1018	NAG	1	0
5	A	1019	NAG	1	0
5	B	703	NAG	2	0
5	B	704	NAG	1	0

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	$\# Z > 2$
7	NAG	A	1017	1	14,14,15	0.26	0	15,19,21	0.38	0
7	NAG	A	1020	1	14,14,15	0.25	0	15,19,21	0.40	0
7	NAG	A	1021	1	14,14,15	0.22	0	15,19,21	0.35	0
7	NAG	B	701	2	14,14,15	0.68	1 (7%)	15,19,21	0.88	1 (6%)
7	NAG	B	702	2	14,14,15	0.34	0	15,19,21	0.40	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
7	NAG	A	1017	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1020	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1021	1	-	0/6/23/26	0/1/1/1
7	NAG	B	701	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	701	NAG	O5-C1	2.29	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	701	NAG	C1-O5-C5	3.31	116.45	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	701	NAG	1	0
7	B	702	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	924/959 (96%)	0.16	26 (2%) 56 42	56, 105, 149, 190	0
2	B	690/692 (99%)	0.42	63 (9%) 11 6	58, 118, 211, 259	1 (0%)
3	C	8/98 (8%)	1.76	3 (37%) 0 0	99, 135, 152, 157	0
All	All	1622/1749 (92%)	0.28	92 (5%) 27 15	56, 110, 186, 259	1 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	452	ASN	11.8
2	B	443	PRO	8.7
2	B	456	GLU	7.3
2	B	37	ARG	7.2
2	B	36	PRO	7.1
2	B	454	THR	6.6
2	B	35	SER	6.0
2	B	442	GLU	5.7
2	B	453	GLY	5.7
2	B	459	VAL	4.9
2	B	464	PRO	4.5
2	B	440	GLN	4.4
2	B	474	SER	4.2
2	B	455	PHE	4.2
2	B	444	ASN	3.9
1	A	907	THR	3.8
2	B	29	GLU	3.7
1	A	705	SER	3.7
1	A	570	ASP	3.6
2	B	461	ARG	3.6
3	C	1497	ASN	3.5
2	B	481	SER	3.5
3	C	1491	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	25	TRP	3.5
2	B	41	LYS	3.4
2	B	671	GLU	3.4
2	B	451	GLY	3.3
2	B	50	ALA	3.3
2	B	446	HIS	3.2
2	B	441	ALA	3.2
2	B	644	GLU	3.2
2	B	55	GLU	3.2
2	B	28	ASP	3.2
2	B	449	ASN	3.2
1	A	475	VAL	3.2
1	A	704	GLN	3.1
2	B	475	GLU	3.0
2	B	482	GLN	3.0
2	B	46	LYS	3.0
1	A	785	ASN	3.0
2	B	39	ASP	2.9
1	A	767	GLU	2.8
1	A	567	THR	2.8
2	B	514	GLY	2.7
2	B	49	CYS	2.7
2	B	56	PHE	2.6
1	A	522	SER	2.6
2	B	26	CYS	2.6
2	B	480	PRO	2.6
2	B	53	SER	2.6
2	B	33	LEU	2.6
3	C	1490	VAL	2.6
1	A	955	ILE	2.5
1	A	497	LEU	2.5
1	A	647	ILE	2.5
1	A	472	CYS	2.5
2	B	445	SER	2.5
2	B	458	GLY	2.5
2	B	509	HIS	2.5
2	B	40	LEU	2.5
2	B	501	CYS	2.5
1	A	474	ASN	2.5
2	B	436	ALA	2.4
2	B	557	TYR	2.4
1	A	569	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	670	TYR	2.4
2	B	44	LEU	2.3
2	B	447	ARG	2.3
2	B	432	ASP	2.3
2	B	485	GLU	2.3
2	B	51	PRO	2.3
1	A	571	THR	2.3
2	B	438	GLN	2.3
2	B	134	LEU	2.3
2	B	34	GLY	2.2
1	A	619	ILE	2.2
1	A	625	LEU	2.2
2	B	556	TYR	2.2
2	B	463	GLY	2.2
2	B	47	ASP	2.2
1	A	703	GLN	2.2
2	B	460	CYS	2.2
1	A	538	LEU	2.2
1	A	532	LEU	2.2
2	B	54	ILE	2.1
2	B	499	GLY	2.1
1	A	572	THR	2.1
1	A	491	LEU	2.1
1	A	768	THR	2.1
1	A	493	PHE	2.1
1	A	606	LEU	2.1
2	B	450	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](#)

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
8	NAG	B	705	14/15	0.96	0.21	-0.60	85,104,125,128	0
5	NAG	B	703	14/15	0.92	0.17	-0.64	94,123,132,149	0
4	NAG	A	1001	14/15	0.95	0.16	-0.96	69,87,110,126	0
5	NAG	A	1018	14/15	0.91	0.15	-1.27	128,152,163,163	0
4	NAG	A	1013	14/15	0.89	0.14	-1.56	86,118,158,166	0
6	NAG	A	1007	14/15	0.97	0.14	-2.01	52,69,101,106	0
8	NAG	A	1024	14/15	0.93	0.14	-2.12	86,127,138,145	0
5	NAG	B	704	14/15	0.84	0.18	-	126,167,175,177	0
6	MAN	A	1012	11/12	0.77	0.28	-	147,171,182,182	0
4	MAN	A	1016	11/12	0.78	0.38	-	172,186,195,200	0
8	NAG	A	1025	14/15	0.71	0.29	-	170,192,209,217	0
6	NAG	A	1008	14/15	0.96	0.17	-	66,89,109,133	0
5	NAG	A	1005	14/15	0.92	0.19	-	111,141,164,166	0
4	NAG	A	1002	14/15	0.87	0.24	-	139,158,180,182	0
4	BMA	A	1015	11/12	0.72	0.34	-	169,184,221,228	0
6	BMA	A	1009	11/12	0.88	0.13	-	135,145,154,155	0
6	BMA	A	1011	11/12	0.83	0.17	-	136,153,183,190	0
6	MAN	A	1010	11/12	0.87	0.14	-	126,154,167,169	0
5	NAG	A	1006	14/15	0.84	0.31	-	153,173,179,180	0
4	NAG	A	1014	14/15	0.84	0.36	-	127,164,185,190	0
5	NAG	A	1019	14/15	0.85	0.23	-	119,145,151,154	0
8	NAG	B	706	14/15	0.93	0.18	-	109,115,128,129	0
4	BMA	A	1003	11/12	0.80	0.16	-	175,189,196,198	0
8	BMA	B	707	11/12	0.82	0.15	-	119,129,139,140	0
5	NAG	A	1022	14/15	0.94	0.11	-	107,133,152,163	0
8	BMA	A	1026	11/12	0.17	0.34	-	173,182,211,217	0
4	MAN	A	1004	11/12	0.77	0.15	-	197,201,203,205	0
5	NAG	A	1023	14/15	0.90	0.17	-	144,178,183,183	0

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
7	NAG	A	1021	14/15	0.84	0.26	1.43	92,119,132,144	0
9	MN	A	1027	1/1	0.98	0.14	-0.18	141,141,141,141	0
9	MN	A	1029	1/1	0.96	0.15	-0.26	131,131,131,131	0
9	MN	B	710	1/1	0.93	0.23	-0.35	99,99,99,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	MN	B	708	1/1	1.00	0.15	-0.67	65,65,65,65	0
9	MN	B	709	1/1	0.91	0.10	-0.90	115,115,115,115	0
9	MN	A	1031	1/1	0.97	0.11	-0.99	111,111,111,111	0
9	MN	A	1028	1/1	0.94	0.06	-1.58	123,123,123,123	0
9	MN	A	1030	1/1	0.97	0.11	-1.73	123,123,123,123	0
7	NAG	B	702	14/15	0.93	0.16	-1.93	95,128,144,150	0
7	NAG	A	1020	14/15	0.67	0.26	-	156,182,185,188	0
7	NAG	A	1017	14/15	0.68	0.45	-	143,167,187,187	0
7	NAG	B	701	14/15	0.79	0.39	-	123,162,179,180	0

6.5 Other polymers [i](#)

There are no such residues in this entry.