



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2017 – 11:52 PM EST

PDB ID : 5N2J  
Title : UDP-Glucose Glycoprotein Glucosyltransferase from *Chaetomium thermophilum* (closed form)  
Authors : Roversi, P.; Caputo, A.T.; Hill, J.; Alonzi, D.S.; Zitzmann, N.  
Deposited on : unknown  
Resolution : 4.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345



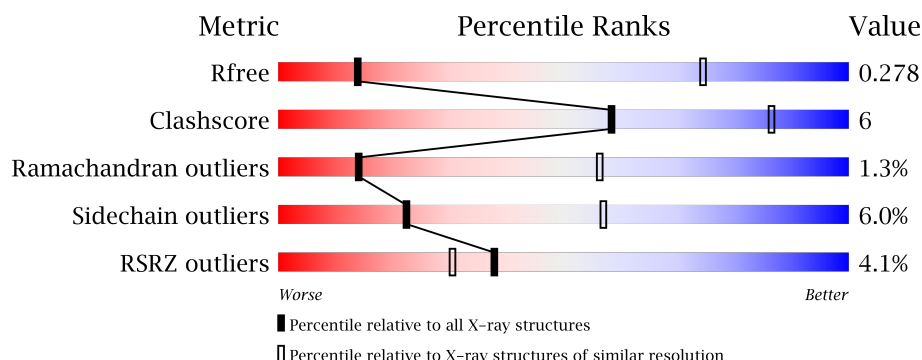
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.40 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))
$R_{free}$	100719	1024 (5.08-3.62)
Clashscore	112137	1021 (5.08-3.70)
Ramachandran outliers	110173	1018 (5.08-3.66)
Sidechain outliers	110143	1000 (5.08-3.66)
RSRZ outliers	101464	1007 (5.08-3.64)

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  $\geq 3$ , 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	1494	<div> <div>4%</div> <div>75%</div> <div>16%</div> <div>8%</div> </div>
1	B	1494	<div> <div>4%</div> <div>74%</div> <div>17%</div> <div>8%</div> </div>

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
2	NAG	A	1601	-	-	-	X
2	NAG	B	1606	-	-	-	X
2	NAG	B	1610	-	-	-	X
5	CA	B	1613	-	-	-	X
6	EDO	A	1614	-	-	-	X



## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 44580 atoms, of which 22133 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 UDP-glucose-glycoprotein glucosyltransferase-like protein.

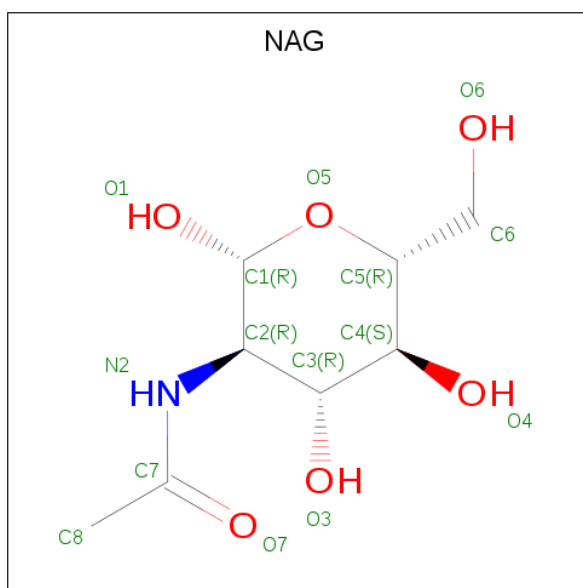
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1373	Total	C	H	N	O	S	0	0	0
			21929	7057	10895	1880	2065	32			
1	B	1381	Total	C	H	N	O	S	0	0	0
			22060	7098	10964	1889	2077	32			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	-	expression tag	UNP G0SB58
A	22	THR	-	expression tag	UNP G0SB58
A	23	GLY	-	expression tag	UNP G0SB58
A	1506	GLY	-	expression tag	UNP G0SB58
A	1507	THR	-	expression tag	UNP G0SB58
A	1508	LYS	-	expression tag	UNP G0SB58
A	1509	HIS	-	expression tag	UNP G0SB58
A	1510	HIS	-	expression tag	UNP G0SB58
A	1511	HIS	-	expression tag	UNP G0SB58
A	1512	HIS	-	expression tag	UNP G0SB58
A	1513	HIS	-	expression tag	UNP G0SB58
A	1514	HIS	-	expression tag	UNP G0SB58
B	21	GLU	-	expression tag	UNP G0SB58
B	22	THR	-	expression tag	UNP G0SB58
B	23	GLY	-	expression tag	UNP G0SB58
B	1506	GLY	-	expression tag	UNP G0SB58
B	1507	THR	-	expression tag	UNP G0SB58
B	1508	LYS	-	expression tag	UNP G0SB58
B	1509	HIS	-	expression tag	UNP G0SB58
B	1510	HIS	-	expression tag	UNP G0SB58
B	1511	HIS	-	expression tag	UNP G0SB58
B	1512	HIS	-	expression tag	UNP G0SB58
B	1513	HIS	-	expression tag	UNP G0SB58
B	1514	HIS	-	expression tag	UNP G0SB58



- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		

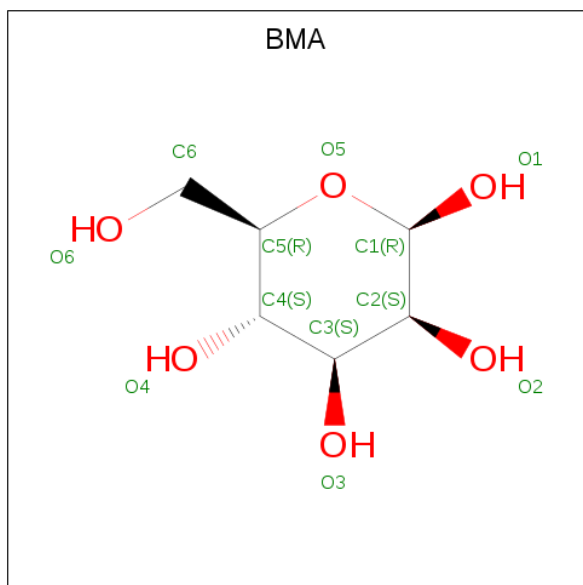
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
2	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

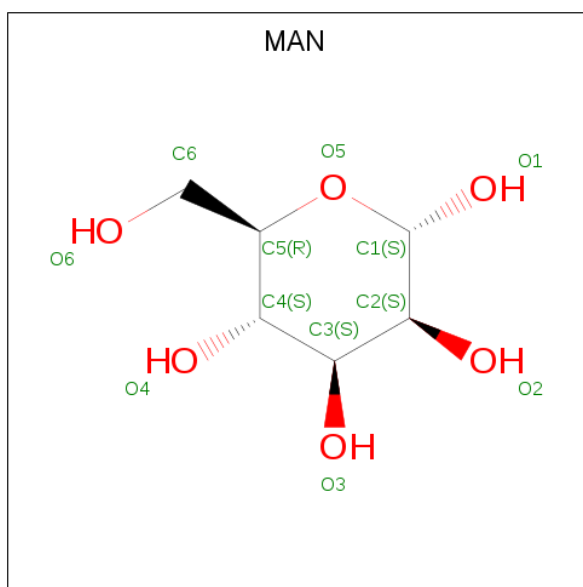
- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			21	6	10	5		
3	A	1	Total	C	H	O	0	0
			20	6	9	5		
3	B	1	Total	C	H	O	0	0
			21	6	10	5		
3	B	1	Total	C	H	O	0	0
			20	6	9	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			20	6	9	5		
4	A	1	Total	C	H	O	0	0
			21	6	10	5		
4	B	1	Total	C	H	O	0	0
			20	6	9	5		
4	B	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0

- Molecule 7 is water.

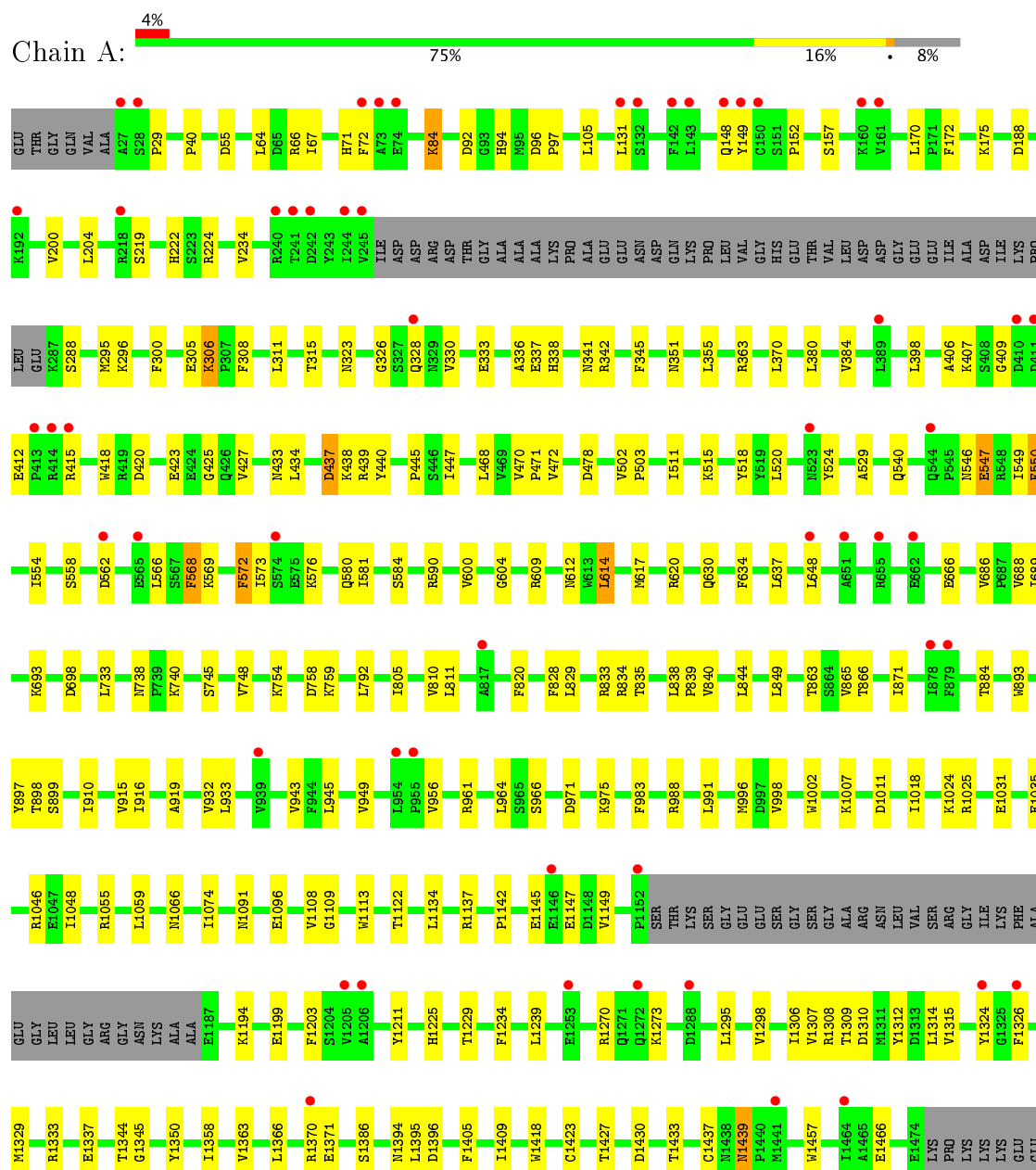
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	B	1	Total O 1 1	0	0



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: UDP-glucose-glycoprotein glucosyltransferase-like protein

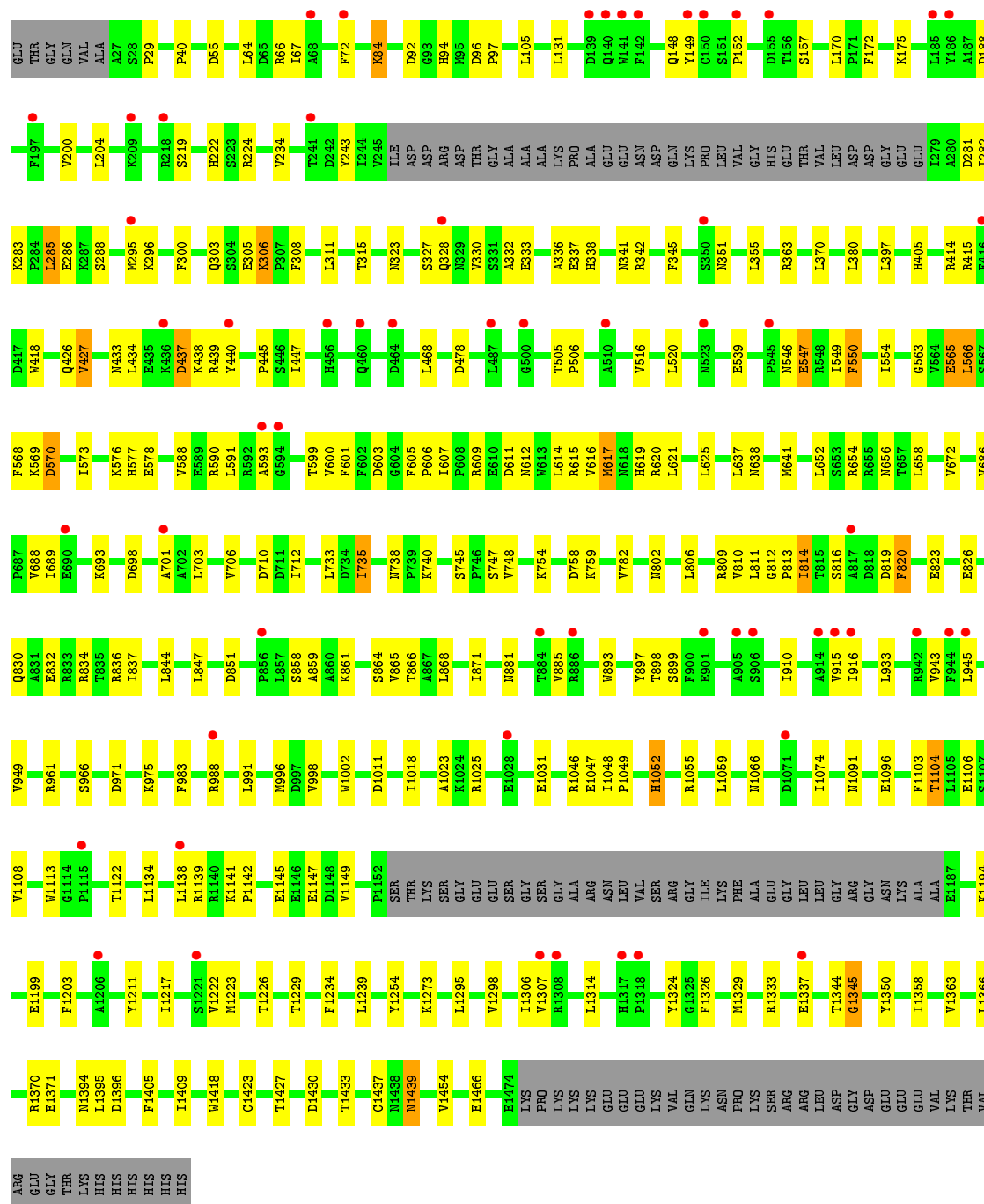




GLU  
LYS  
VAL  
GLN  
LYS  
ASN  
PRO  
LYS  
SER  
ARG  
ARG  
LEU  
ASP  
GLY  
ASP  
GLU  
GLU  
GLU  
VAL  
LYS  
THR  
VAL  
ARG  
GLU  
GLY  
THR  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 1: UDP-glucose-glycoprotein glucosyltransferase-like protein

Chain B: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.60Å 148.60Å 179.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.59 – 4.40 114.59 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (114.59-4.40) 100.0 (114.59-4.30)	Depositor EDS
$R_{merge}$	0.78	Depositor
$R_{sym}$	0.81	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 4.30Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.201 , 0.259 0.220 , 0.278	Depositor DCC
$R_{free}$ test set	1282 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	126.7	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 245.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.167 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	44580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	243.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MAN, CA, BMA, NAG, EDO

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	0.49	0/11298	0.74	2/15323 (0.0%)
1	B	0.55	0/11361	0.77	3/15409 (0.0%)
All	All	0.52	0/22659	0.75	5/30732 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	GLU	C-N-CA	5.80	136.21	121.70
1	B	305	GLU	C-N-CA	5.80	136.21	121.70
1	B	565	GLU	C-N-CA	5.52	135.50	121.70
1	B	306	LYS	N-CA-C	-5.42	96.38	111.00
1	A	306	LYS	N-CA-C	-5.29	96.70	111.00

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	11034	10895	10898	144	0
1	B	11096	10964	10966	105	0
2	A	112	99	99	0	0
2	B	112	99	99	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	19	19	0	0
3	B	22	19	19	0	0
4	A	22	19	19	0	0
4	B	22	19	19	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	1	0
7	B	1	0	0	0	0
All	All	22447	22133	22138	247	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 6.

All (247) 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:1225:HIS:ND1	1:A:1308:ARG:HA	1.68	1.07
1:B:243:TYR:O	1:B:285:LEU:HG	1.65	0.96
1:A:1225:HIS:CE1	1:A:1308:ARG:HA	2.04	0.93
1:A:1149:VAL:HG13	1:A:1371:GLU:O	1.71	0.90
1:B:1149:VAL:HG13	1:B:1371:GLU:O	1.73	0.87
1:A:326:GLY:HA2	1:A:330:VAL:HG11	1.59	0.84
1:A:67:ILE:HG22	1:A:72:PHE:CD2	2.16	0.81
1:B:67:ILE:HG22	1:B:72:PHE:CD2	2.18	0.79
1:A:554:ILE:HG23	1:A:558:SER:HB2	1.65	0.77
1:A:1295:LEU:HD21	1:A:1298:VAL:CG2	2.15	0.76
1:B:1295:LEU:HD21	1:B:1298:VAL:CG2	2.17	0.74
1:A:566:LEU:HD13	1:A:568:PHE:CD2	2.24	0.71
1:A:524:TYR:HE2	1:A:558:SER:HG	1.38	0.70
1:A:1225:HIS:ND1	1:A:1308:ARG:CA	2.53	0.70
1:A:1059:LEU:HD11	1:A:1074:ILE:HD11	1.74	0.69
1:A:515:LYS:HG3	1:A:581:ILE:HD11	1.75	0.69
1:B:1059:LEU:HD11	1:B:1074:ILE:HD11	1.76	0.68
1:B:414:ARG:HD2	1:B:652:LEU:HD11	1.76	0.67
1:A:384:VAL:HG23	1:A:865:VAL:HG11	1.77	0.66
1:A:834:ARG:O	1:A:839:PRO:HD3	1.97	0.65
1:A:1048:ILE:HD11	1:A:1137:ARG:HB3	1.78	0.64
1:A:686:VAL:O	1:A:754:LYS:HE2	1.98	0.64
1:A:1329:MET:HG2	1:A:1358:ILE:HD11	1.80	0.64
1:B:447:ILE:HD11	1:B:637:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASP:OD1	1:A:427:VAL:CG1	2.46	0.63
1:A:418:TRP:HE1	1:A:648:LEU:HD11	1.64	0.62
1:B:1329:MET:HG2	1:B:1358:ILE:HD11	1.81	0.62
1:A:515:LYS:CG	1:A:581:ILE:HD11	2.30	0.62
1:B:686:VAL:O	1:B:754:LYS:HE2	1.99	0.62
1:A:447:ILE:HD11	1:A:637:LEU:HB3	1.80	0.62
1:A:398:LEU:CD2	1:A:866:THR:HG22	2.29	0.61
1:B:1306:ILE:HD13	1:B:1454:VAL:HG21	1.83	0.60
1:A:338:HIS:HD2	1:A:898:THR:HG23	1.65	0.60
1:A:338:HIS:O	1:A:341:ASN:HB2	2.02	0.60
1:B:338:HIS:HD2	1:B:898:THR:HG23	1.67	0.59
1:A:295:MET:CE	1:A:949:VAL:HG12	2.32	0.59
1:A:152:PRO:HB3	1:A:200:VAL:HG21	1.85	0.58
1:A:470:VAL:HG23	1:A:600:VAL:HG22	1.85	0.58
1:A:384:VAL:CG2	1:A:865:VAL:HG11	2.33	0.58
1:A:420:ASP:OD1	1:A:427:VAL:HG13	2.04	0.58
1:A:1199:GLU:HG3	1:A:1229:THR:OG1	2.03	0.58
1:B:295:MET:CE	1:B:949:VAL:HG12	2.33	0.58
1:B:152:PRO:HB3	1:B:200:VAL:HG21	1.85	0.58
1:A:311:LEU:O	1:A:315:THR:HG22	2.04	0.58
1:A:420:ASP:HB3	1:A:425:GLY:HA2	1.87	0.57
1:A:829:LEU:O	1:A:833:ARG:HB2	2.04	0.57
1:B:1199:GLU:HG3	1:B:1229:THR:OG1	2.03	0.57
1:A:1307:VAL:HG13	1:A:1433:THR:HG22	1.87	0.57
1:B:338:HIS:O	1:B:341:ASN:HB2	2.04	0.57
1:A:554:ILE:O	1:A:558:SER:HB3	2.05	0.56
1:B:802:ASN:O	1:B:813:PRO:HA	2.05	0.56
1:A:573:ILE:HB	1:A:576:LYS:HB3	1.87	0.56
1:A:67:ILE:HG22	1:A:72:PHE:HD2	1.71	0.56
1:B:1108:VAL:HG12	1:B:1134:LEU:HD22	1.88	0.56
1:A:600:VAL:CG2	1:A:609:ARG:HG2	2.35	0.56
1:A:1108:VAL:HG12	1:A:1134:LEU:HD22	1.87	0.56
1:A:554:ILE:HG23	1:A:558:SER:CB	2.33	0.55
1:B:745:SER:O	1:B:748:VAL:HG22	2.07	0.55
1:A:554:ILE:O	1:A:558:SER:CB	2.54	0.55
1:A:66:ARG:O	1:A:71:HIS:HB3	2.07	0.55
1:B:311:LEU:O	1:B:315:THR:HG22	2.07	0.54
1:A:398:LEU:HD23	1:A:866:THR:HG22	1.89	0.54
1:A:524:TYR:HE2	1:A:558:SER:OG	1.89	0.54
1:B:434:LEU:HD23	1:B:440:TYR:CE2	2.43	0.54
1:A:745:SER:O	1:A:748:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:HB2	1:A:97:PRO:HD2	1.90	0.54
1:B:899:SER:HA	1:B:943:VAL:O	2.08	0.54
1:A:1418:TRP:HE1	1:A:1427:THR:HB	1.73	0.54
1:A:337:GLU:OE1	1:A:897:TYR:CD2	2.61	0.54
1:A:434:LEU:HD23	1:A:440:TYR:CE2	2.43	0.53
1:A:899:SER:HA	1:A:943:VAL:O	2.08	0.53
1:A:1091:ASN:OD1	1:A:1122:THR:HG23	2.09	0.53
1:A:170:LEU:HD11	1:A:172:PHE:CE1	2.43	0.53
1:B:234:VAL:HG22	1:B:996:MET:CE	2.38	0.53
1:A:566:LEU:HD13	1:A:568:PHE:CE2	2.44	0.53
1:B:170:LEU:HD11	1:B:172:PHE:CE1	2.44	0.53
1:A:72:PHE:CE1	1:A:84:LYS:HG3	2.44	0.53
1:A:420:ASP:OD1	1:A:427:VAL:HG12	2.10	0.52
1:B:735:ILE:HD12	1:B:735:ILE:N	2.24	0.52
1:A:234:VAL:HG22	1:A:996:MET:CE	2.38	0.52
1:A:29:PRO:HB2	1:A:1018:ILE:HD13	1.91	0.52
1:A:600:VAL:HG23	1:A:609:ARG:CG	2.40	0.52
1:A:630:GLN:O	1:A:634:PHE:HD1	1.93	0.52
1:B:1418:TRP:HE1	1:B:1427:THR:HB	1.74	0.52
1:B:1091:ASN:OD1	1:B:1122:THR:HG23	2.10	0.52
1:B:333:GLU:CD	1:B:336:ALA:HB2	2.30	0.52
1:B:96:ASP:HB2	1:B:97:PRO:HD2	1.92	0.52
1:B:1103:PHE:HB3	1:B:1138:LEU:HD22	1.92	0.52
1:A:296:LYS:HE2	1:A:330:VAL:HG13	1.92	0.51
1:A:547:GLU:HA	1:A:550:PHE:HB3	1.92	0.51
1:A:1048:ILE:CD1	1:A:1137:ARG:HB3	2.40	0.51
1:A:64:LEU:HD12	1:A:67:ILE:HD11	1.92	0.51
1:B:1222:VAL:O	1:B:1226:THR:HG22	2.10	0.51
1:A:1199:GLU:HB2	1:A:1229:THR:O	2.10	0.51
1:B:64:LEU:HD12	1:B:67:ILE:HD11	1.92	0.51
1:B:355:LEU:HD11	1:B:910:ILE:HG23	1.93	0.51
1:A:333:GLU:CD	1:A:336:ALA:HB2	2.32	0.51
1:A:524:TYR:HE2	1:A:558:SER:CB	2.24	0.50
1:B:337:GLU:OE1	1:B:897:TYR:CD2	2.64	0.50
1:A:1059:LEU:CD1	1:A:1074:ILE:HD11	2.40	0.50
1:B:1059:LEU:CD1	1:B:1074:ILE:HD11	2.41	0.50
1:B:547:GLU:HA	1:B:550:PHE:HB3	1.93	0.50
1:A:1306:ILE:HD11	1:A:1457:TRP:HD1	1.75	0.50
1:B:1104:THR:HG23	1:B:1139:ARG:O	2.12	0.50
1:B:1307:VAL:HG13	1:B:1433:THR:HG22	1.93	0.50
1:B:72:PHE:CE1	1:B:84:LYS:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PRO:HB2	1:B:1018:ILE:HD13	1.93	0.50
1:A:518:TYR:HB3	1:A:580:GLN:OE1	2.12	0.49
1:B:1046:ARG:HA	1:B:1052:HIS:O	2.12	0.49
1:A:468:LEU:HD22	1:A:617:MET:SD	2.53	0.49
1:B:380:LEU:HG	1:B:865:VAL:HG13	1.95	0.49
1:A:472:VAL:O	1:A:503:PRO:HA	2.11	0.49
1:A:511:ILE:HG23	1:A:581:ILE:HD13	1.94	0.49
1:A:355:LEU:HD11	1:A:910:ILE:HG23	1.93	0.49
1:B:590:ARG:O	1:B:654:ARG:HA	2.13	0.48
1:A:1324:TYR:CD1	1:A:1326:PHE:HE1	2.31	0.48
1:B:1199:GLU:HB2	1:B:1229:THR:O	2.11	0.48
1:A:1295:LEU:HD21	1:A:1298:VAL:HG22	1.94	0.48
1:A:1048:ILE:HD11	1:A:1137:ARG:HD2	1.95	0.48
1:A:546:ASN:HB3	1:A:549:ILE:HG22	1.96	0.48
1:A:1324:TYR:CE1	1:A:1409:ILE:HG12	2.48	0.48
1:A:1109:GLY:HA2	7:A:1701:HOH:O	2.14	0.48
1:B:1104:THR:HG22	1:B:1141:LYS:HG3	1.96	0.48
1:B:1048:ILE:HG22	1:B:1049:PRO:HA	1.95	0.48
1:B:1329:MET:SD	1:B:1358:ILE:HD11	2.54	0.48
1:B:1324:TYR:CE1	1:B:1409:ILE:HG12	2.49	0.48
1:A:524:TYR:CD2	1:A:558:SER:HA	2.49	0.47
1:A:835:THR:O	1:A:839:PRO:HD2	2.14	0.47
1:A:840:VAL:HG21	1:A:863:THR:HA	1.96	0.47
1:B:554:ILE:HG21	1:B:568:PHE:CE2	2.49	0.47
1:A:1350:TYR:O	1:A:1405:PHE:HZ	1.97	0.47
1:A:345:PHE:HB3	1:A:893:TRP:CZ2	2.50	0.47
1:A:370:LEU:HD13	1:A:933:LEU:HD11	1.96	0.47
1:A:468:LEU:HD11	1:A:600:VAL:CG1	2.45	0.47
1:B:1047:GLU:HG2	1:B:1052:HIS:HB2	1.96	0.47
1:A:614:LEU:HD12	1:A:617:MET:CE	2.45	0.47
1:B:296:LYS:HG2	1:B:330:VAL:HG13	1.95	0.47
1:A:433:ASN:O	1:A:437:ASP:HB2	2.15	0.47
1:A:471:PRO:HA	1:A:502:VAL:O	2.14	0.47
1:A:200:VAL:O	1:A:204:LEU:HG	2.14	0.47
1:A:338:HIS:CD2	1:A:898:THR:HG23	2.48	0.47
1:A:1329:MET:CG	1:A:1358:ILE:HD11	2.44	0.47
1:A:600:VAL:HG23	1:A:609:ARG:HG2	1.95	0.47
1:B:546:ASN:HB3	1:B:549:ILE:HG22	1.97	0.47
1:B:370:LEU:HD13	1:B:933:LEU:HD11	1.97	0.47
1:A:380:LEU:HG	1:A:865:VAL:HG13	1.98	0.46
1:B:810:VAL:HG12	1:B:811:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:MET:SD	1:A:1358:ILE:HD11	2.56	0.46
1:A:1333:ARG:HG2	1:A:1423:CYS:C	2.35	0.46
1:A:407:LYS:NZ	1:A:884:THR:HB	2.30	0.46
1:A:961:ARG:HG2	1:A:983:PHE:CE2	2.50	0.46
1:B:345:PHE:HB3	1:B:893:TRP:CZ2	2.51	0.46
1:A:92:ASP:HB2	1:A:94:HIS:CD2	2.51	0.46
1:B:1046:ARG:NH2	1:B:1113:TRP:O	2.49	0.46
1:B:961:ARG:HG2	1:B:983:PHE:CE2	2.51	0.46
1:B:1329:MET:CG	1:B:1358:ILE:HD11	2.45	0.46
1:B:686:VAL:O	1:B:688:VAL:HG23	2.16	0.46
1:A:998:VAL:HG22	1:A:1002:TRP:HB2	1.98	0.46
1:B:1223:MET:HG3	1:B:1254:TYR:HB3	1.98	0.46
1:B:1324:TYR:CD1	1:B:1326:PHE:HE1	2.34	0.46
1:A:1046:ARG:NH2	1:A:1113:TRP:O	2.50	0.45
1:A:1314:LEU:HG	1:A:1363:VAL:CG2	2.47	0.45
1:A:188:ASP:OD1	1:A:219:SER:HB3	2.16	0.45
1:B:1295:LEU:HD21	1:B:1298:VAL:HG22	1.95	0.45
1:B:1333:ARG:HG2	1:B:1423:CYS:C	2.37	0.45
1:B:92:ASP:HB2	1:B:94:HIS:CD2	2.52	0.45
1:A:415:ARG:HA	1:A:604:GLY:O	2.17	0.45
1:A:520:LEU:HD23	1:A:529:ALA:HA	1.99	0.45
1:A:573:ILE:CG2	1:B:1023:ALA:O	2.65	0.45
1:A:738:ASN:HD22	1:A:792:LEU:HD11	1.82	0.45
1:B:67:ILE:HG22	1:B:72:PHE:HD2	1.74	0.45
1:A:1309:THR:HG22	1:A:1310:ASP:O	2.17	0.45
1:A:326:GLY:CA	1:A:330:VAL:HG11	2.38	0.45
1:A:418:TRP:NE1	1:A:648:LEU:HD11	2.30	0.45
1:A:600:VAL:CG2	1:A:609:ARG:CG	2.94	0.44
1:B:1366:LEU:O	1:B:1370:ARG:HG3	2.17	0.44
1:B:433:ASN:O	1:B:437:ASP:HB2	2.17	0.44
1:B:812:GLY:CA	1:B:814:ILE:HD13	2.47	0.44
1:A:686:VAL:O	1:A:688:VAL:HG23	2.17	0.44
1:A:1366:LEU:O	1:A:1370:ARG:HG3	2.16	0.44
1:A:573:ILE:HG22	1:B:1023:ALA:O	2.17	0.44
1:B:658:LEU:HD22	1:B:814:ILE:HD12	1.99	0.44
1:A:406:ALA:HB2	1:A:839:PRO:HG2	1.99	0.44
1:A:370:LEU:HD13	1:A:933:LEU:CD1	2.48	0.44
1:B:998:VAL:HG22	1:B:1002:TRP:HB2	2.00	0.44
1:B:1314:LEU:HG	1:B:1363:VAL:CG2	2.48	0.44
1:B:397:LEU:HD21	1:B:866:THR:CG2	2.48	0.44
1:B:131:LEU:HD11	1:B:148:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:PHE:CD2	1:A:572:PHE:N	2.85	0.44
1:B:812:GLY:HA2	1:B:814:ILE:HD13	1.99	0.44
1:A:149:TYR:CE1	1:A:157:SER:HB3	2.52	0.44
1:A:351:ASN:HA	1:A:915:VAL:O	2.18	0.44
1:B:370:LEU:HD13	1:B:933:LEU:CD1	2.48	0.43
1:B:188:ASP:OD1	1:B:219:SER:HB3	2.18	0.43
1:A:105:LEU:HD13	1:A:966:SER:HA	2.00	0.43
1:A:844:LEU:HD12	1:A:849:LEU:HB2	1.99	0.43
1:B:105:LEU:HD13	1:B:966:SER:HA	2.00	0.43
1:B:588:VAL:HG13	1:B:593:ALA:O	2.18	0.43
1:B:295:MET:HE3	1:B:949:VAL:HG12	2.01	0.43
1:A:1234:PHE:HB3	1:A:1239:LEU:HD11	2.01	0.43
1:B:1048:ILE:HD12	1:B:1106:GLU:OE1	2.19	0.43
1:B:338:HIS:CD2	1:B:898:THR:HG23	2.49	0.43
1:B:351:ASN:HA	1:B:915:VAL:O	2.19	0.43
1:B:505:THR:N	1:B:506:PRO:HD3	2.34	0.43
1:A:689:ILE:HD12	1:A:733:LEU:HD23	2.01	0.42
1:B:1395:LEU:HD12	1:B:1396:ASP:N	2.34	0.42
1:B:149:TYR:CE1	1:B:157:SER:HB3	2.54	0.42
1:A:811:LEU:HD11	1:A:828:PHE:CE1	2.54	0.42
1:A:131:LEU:HD11	1:A:148:GLN:OE1	2.18	0.42
1:A:40:PRO:HB3	1:A:224:ARG:HD2	2.01	0.42
1:B:591:LEU:HD22	1:B:601:PHE:CZ	2.55	0.42
1:A:427:VAL:CG2	1:A:584:SER:HA	2.50	0.42
1:A:1011:ASP:CG	1:A:1025:ARG:HH22	2.22	0.42
1:B:689:ILE:HD12	1:B:733:LEU:HD23	2.01	0.42
1:A:1314:LEU:HG	1:A:1363:VAL:HG22	2.02	0.42
1:A:916:ILE:O	1:A:945:LEU:HA	2.19	0.42
1:A:919:ALA:O	1:A:956:VAL:HG23	2.20	0.42
1:A:1395:LEU:HD12	1:A:1396:ASP:N	2.34	0.42
1:B:1234:PHE:HB3	1:B:1239:LEU:HD11	2.01	0.42
1:B:617:MET:SD	1:B:617:MET:N	2.93	0.42
1:B:916:ILE:O	1:B:945:LEU:HA	2.20	0.42
1:A:600:VAL:HG23	1:A:609:ARG:HG3	2.02	0.42
1:B:599:THR:CG2	1:B:606:PRO:HB2	2.50	0.42
1:A:805:ILE:HG12	1:A:810:VAL:HG22	2.01	0.42
1:B:600:VAL:N	1:B:607:ILE:O	2.53	0.42
1:A:838:LEU:HD23	1:A:838:LEU:HA	1.80	0.41
1:B:988:ARG:HA	1:B:1018:ILE:HB	2.00	0.41
1:B:40:PRO:HB3	1:B:224:ARG:HD2	2.02	0.41
1:A:1312:TYR:O	1:A:1315:VAL:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:LYS:HG3	1:A:1035:GLU:HB2	2.02	0.41
1:B:327:SER:O	1:B:330:VAL:HB	2.20	0.41
1:A:1108:VAL:CG1	1:A:1134:LEU:HD22	2.51	0.41
1:A:1344:THR:HG22	1:A:1345:GLY:N	2.35	0.41
1:B:814:ILE:HG21	1:B:820:PHE:HB2	2.02	0.41
1:B:1011:ASP:CG	1:B:1025:ARG:HH22	2.23	0.41
1:B:1344:THR:HG22	1:B:1345:GLY:N	2.36	0.41
1:B:380:LEU:HD11	1:B:868:LEU:HB2	2.03	0.41
1:A:932:VAL:HG11	1:A:964:LEU:HG	2.03	0.41
1:A:1270:ARG:HD2	1:A:1386:SER:OG	2.20	0.41
1:B:672:VAL:HG23	1:B:864:SER:OG	2.20	0.41
1:A:524:TYR:CE2	1:A:558:SER:HA	2.56	0.41
1:B:568:PHE:O	1:B:570:ASP:N	2.52	0.41
1:B:836:ARG:C	1:B:837:ILE:HD12	2.41	0.41
1:A:423:GLU:OE1	1:A:590:ARG:NH1	2.54	0.41
1:B:303:GLN:HE22	1:B:330:VAL:HA	1.86	0.41
1:B:1350:TYR:O	1:B:1405:PHE:HZ	2.04	0.40
1:A:149:TYR:HE1	1:A:157:SER:HB3	1.87	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	1367/1494 (92%)	1297 (95%)	59 (4%)	11 (1%)	22	67
1	B	1375/1494 (92%)	1265 (92%)	84 (6%)	26 (2%)	9	49
All	All	2742/2988 (92%)	2562 (93%)	143 (5%)	37 (1%)	14	56

All (37) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	288	SER
1	A	569	LYS
1	A	1439	ASN
1	B	288	SER
1	B	332	ALA
1	B	426	GLN
1	B	539	GLU
1	B	566	LEU
1	B	603	ASP
1	B	859	ALA
1	B	1439	ASN
1	B	427	VAL
1	B	563	GLY
1	B	569	LYS
1	B	611	ASP
1	B	616	VAL
1	B	710	ASP
1	B	712	ILE
1	B	747	SER
1	B	782	VAL
1	A	568	PHE
1	A	666	GLU
1	A	1337	GLU
1	B	701	ALA
1	B	1337	GLU
1	B	577	HIS
1	B	615	ARG
1	A	306	LYS
1	A	572	PHE
1	A	1142	PRO
1	B	306	LYS
1	B	1142	PRO
1	A	409	GLY
1	B	445	PRO
1	A	445	PRO
1	B	282	ILE
1	B	1345	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1199/1297 (92%)	1150 (96%)	49 (4%)	35	66
1	B	1206/1297 (93%)	1110 (92%)	96 (8%)	14	47
All	All	2405/2594 (93%)	2260 (94%)	145 (6%)	22	57

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	84	LYS
1	A	175	LYS
1	A	222	HIS
1	A	300	PHE
1	A	308	PHE
1	A	323	ASN
1	A	328	GLN
1	A	342	ARG
1	A	363	ARG
1	A	412	GLU
1	A	437	ASP
1	A	438	LYS
1	A	439	ARG
1	A	478	ASP
1	A	540	GLN
1	A	547	GLU
1	A	550	PHE
1	A	562	ASP
1	A	612	ASN
1	A	614	LEU
1	A	620	ARG
1	A	693	LYS
1	A	698	ASP
1	A	740	LYS
1	A	758	ASP
1	A	759	LYS
1	A	820	PHE
1	A	871	ILE
1	A	971	ASP
1	A	975	LYS
1	A	988	ARG
1	A	991	LEU

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Mol	Chain	Res	Type
1	A	1024	LYS
1	A	1031	GLU
1	A	1055	ARG
1	A	1066	ASN
1	A	1096	GLU
1	A	1145	GLU
1	A	1147	GLU
1	A	1194	LYS
1	A	1203	PHE
1	A	1211	TYR
1	A	1273	LYS
1	A	1394	ASN
1	A	1430	ASP
1	A	1437	CYS
1	A	1439	ASN
1	A	1466	GLU
1	B	55	ASP
1	B	66	ARG
1	B	84	LYS
1	B	175	LYS
1	B	204	LEU
1	B	222	HIS
1	B	281	ASP
1	B	283	LYS
1	B	285	LEU
1	B	286	GLU
1	B	300	PHE
1	B	308	PHE
1	B	323	ASN
1	B	328	GLN
1	B	342	ARG
1	B	363	ARG
1	B	405	HIS
1	B	415	ARG
1	B	418	TRP
1	B	427	VAL
1	B	437	ASP
1	B	438	LYS
1	B	439	ARG
1	B	468	LEU
1	B	478	ASP
1	B	516	VAL

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Mol	Chain	Res	Type
1	B	520	LEU
1	B	547	GLU
1	B	550	PHE
1	B	565	GLU
1	B	566	LEU
1	B	570	ASP
1	B	573	ILE
1	B	576	LYS
1	B	578	GLU
1	B	605	PHE
1	B	609	ARG
1	B	612	ASN
1	B	614	LEU
1	B	617	MET
1	B	619	HIS
1	B	620	ARG
1	B	621	LEU
1	B	625	LEU
1	B	638	ASN
1	B	641	MET
1	B	656	ASN
1	B	693	LYS
1	B	698	ASP
1	B	703	LEU
1	B	706	VAL
1	B	735	ILE
1	B	738	ASN
1	B	740	LYS
1	B	758	ASP
1	B	759	LYS
1	B	806	LEU
1	B	809	ARG
1	B	814	ILE
1	B	816	SER
1	B	819	ASP
1	B	820	PHE
1	B	823	GLU
1	B	826	GLU
1	B	830	GLN
1	B	832	GLU
1	B	834	ARG
1	B	844	LEU

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Mol	Chain	Res	Type
1	B	847	LEU
1	B	851	ASP
1	B	858	SER
1	B	861	LYS
1	B	871	ILE
1	B	881	ASN
1	B	885	VAL
1	B	971	ASP
1	B	975	LYS
1	B	991	LEU
1	B	1031	GLU
1	B	1052	HIS
1	B	1055	ARG
1	B	1066	ASN
1	B	1096	GLU
1	B	1104	THR
1	B	1145	GLU
1	B	1147	GLU
1	B	1194	LYS
1	B	1203	PHE
1	B	1211	TYR
1	B	1217	ILE
1	B	1273	LYS
1	B	1394	ASN
1	B	1430	ASP
1	B	1437	CYS
1	B	1439	ASN
1	B	1466	GLU

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

Mol	Chain	Res	Type
1	A	94	HIS
1	A	513	GLN
1	A	751	GLN
1	A	1058	GLN
1	B	94	HIS
1	B	303	GLN
1	B	323	ASN
1	B	400	HIS
1	B	523	ASN
1	B	738	ASN

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Mol	Chain	Res	Type
1	B	751	GLN
1	B	1058	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 24 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	$\# Z  > 2$
2	NAG	A	1601	1	14,14,15	0.39	0	15,19,21	0.74	0
2	NAG	A	1602	1,2	14,14,15	0.32	0	15,19,21	1.06	1 (6%)
2	NAG	A	1603	3,2	14,14,15	0.48	0	15,19,21	1.69	3 (20%)
3	BMA	A	1604	2	11,11,12	0.49	0	13,15,17	0.87	1 (7%)
2	NAG	A	1605	1,2	14,14,15	0.29	0	15,19,21	2.62	2 (13%)
2	NAG	A	1606	3,2	14,14,15	0.36	0	15,19,21	1.94	2 (13%)
3	BMA	A	1607	2,4	11,11,12	0.32	0	13,15,17	0.57	0
4	MAN	A	1608	3,4	11,11,12	0.46	0	13,15,17	0.96	1 (7%)
4	MAN	A	1609	4	11,11,12	0.40	0	13,15,17	1.18	1 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1610	1,2	14,14,15	0.37	0	15,19,21	0.92	1 (6%)
2	NAG	A	1611	2	14,14,15	0.44	0	15,19,21	1.77	2 (13%)
2	NAG	A	1612	1	14,14,15	0.41	0	15,19,21	2.20	4 (26%)
2	NAG	B	1601	1	14,14,15	0.31	0	15,19,21	0.58	0
2	NAG	B	1602	1,2	14,14,15	0.32	0	15,19,21	0.95	1 (6%)
2	NAG	B	1603	3,2	14,14,15	0.52	0	15,19,21	1.55	2 (13%)
3	BMA	B	1604	2	11,11,12	0.52	0	13,15,17	0.96	1 (7%)
2	NAG	B	1605	1,2	14,14,15	0.23	0	15,19,21	2.65	2 (13%)
2	NAG	B	1606	3,2	14,14,15	0.34	0	15,19,21	2.05	2 (13%)
3	BMA	B	1607	2,4	11,11,12	0.36	0	13,15,17	0.60	0
4	MAN	B	1608	3,4	11,11,12	0.40	0	13,15,17	0.95	1 (7%)
4	MAN	B	1609	4	11,11,12	0.37	0	13,15,17	1.16	1 (7%)
2	NAG	B	1610	1,2	14,14,15	0.36	0	15,19,21	1.01	1 (6%)
2	NAG	B	1611	2	14,14,15	0.45	0	15,19,21	1.85	2 (13%)
2	NAG	B	1612	1	14,14,15	0.45	0	15,19,21	2.20	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1603	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1604	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1605	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1606	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1607	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1608	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1609	4	-	0/2/19/22	1/1/1/1
2	NAG	A	1610	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1611	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1612	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1603	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1604	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1605	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1606	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	B	1607	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1608	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1609	4	-	0/2/19/22	1/1/1/1
2	NAG	B	1610	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1611	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1612	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1602	NAG	O5-C1-C2	-3.38	106.77	111.47
2	B	1602	NAG	O5-C1-C2	-2.41	108.12	111.47
2	A	1603	NAG	O4-C4-C3	-2.05	105.89	110.36
3	B	1604	BMA	C1-C2-C3	2.13	112.34	109.65
2	B	1612	NAG	C2-N2-C7	2.19	126.14	122.94
2	A	1612	NAG	C2-N2-C7	2.19	126.14	122.94
3	A	1604	BMA	C1-O5-C5	2.21	115.21	112.17
2	B	1610	NAG	C1-O5-C5	2.31	115.35	112.17
2	A	1610	NAG	C1-O5-C5	2.39	115.46	112.17
4	B	1608	MAN	C1-C2-C3	2.39	112.68	109.65
2	A	1612	NAG	C3-C4-C5	2.40	114.45	110.22
2	B	1612	NAG	C3-C4-C5	2.46	114.56	110.22
4	A	1608	MAN	C1-C2-C3	2.57	112.91	109.65
2	A	1606	NAG	C1-O5-C5	2.59	115.74	112.17
2	B	1606	NAG	C1-O5-C5	2.87	116.12	112.17
2	A	1603	NAG	O4-C4-C5	3.34	117.70	109.28
2	A	1612	NAG	C1-C2-N2	3.34	116.19	110.49
2	B	1603	NAG	C1-O5-C5	3.46	116.94	112.17
2	B	1612	NAG	C1-C2-N2	3.60	116.64	110.49
4	B	1609	MAN	C1-O5-C5	3.87	117.50	112.17
4	A	1609	MAN	C1-O5-C5	3.94	117.60	112.17
2	B	1603	NAG	O4-C4-C5	4.10	119.61	109.28
2	A	1611	NAG	O5-C1-C2	4.52	117.77	111.47
2	A	1603	NAG	C1-O5-C5	4.64	118.56	112.17
2	B	1611	NAG	O5-C1-C2	4.65	117.94	111.47
2	A	1611	NAG	C1-O5-C5	4.80	118.78	112.17
2	B	1611	NAG	C1-O5-C5	5.12	119.22	112.17
2	A	1605	NAG	O5-C1-C2	5.37	118.94	111.47
2	B	1605	NAG	O5-C1-C2	5.50	119.13	111.47
2	A	1606	NAG	O5-C1-C2	6.46	120.46	111.47
2	B	1612	NAG	C1-O5-C5	6.62	121.29	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1612	NAG	C1-O5-C5	6.79	121.53	112.17
2	B	1606	NAG	O5-C1-C2	6.83	120.98	111.47
2	A	1605	NAG	C1-O5-C5	8.26	123.56	112.17
2	B	1605	NAG	C1-O5-C5	8.27	123.57	112.17

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1609	MAN	C1-C2-C3-C4-C5-O5
4	B	1609	MAN	C1-C2-C3-C4-C5-O5

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1373/1494 (91%)	0.19	55 (4%) 39 31	169, 248, 284, 297	0
1	B	1381/1494 (92%)	0.25	59 (4%) 36 29	160, 244, 281, 295	0
All	All	2754/2988 (92%)	0.22	114 (4%) 38 30	160, 246, 282, 297	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	6.9
1	A	1206	ALA	6.0
1	B	945	LEU	5.6
1	B	1307	VAL	5.2
1	A	879	PHE	5.0
1	B	150	CYS	5.0
1	A	28	SER	4.8
1	B	72	PHE	4.6
1	B	944	PHE	4.2
1	A	1272	GLN	4.2
1	A	565	GLU	4.2
1	B	1318	PRO	4.1
1	A	241	THR	4.1
1	A	1205	VAL	4.0
1	B	186	TYR	3.9
1	A	574	SER	3.7
1	B	142	PHE	3.7
1	B	886	ARG	3.7
1	B	594	GLY	3.6
1	B	523	ASN	3.6
1	A	143	LEU	3.5
1	B	817	ALA	3.4
1	B	905	ALA	3.4
1	A	132	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	350	SER	3.4
1	A	817	ALA	3.4
1	B	149	TYR	3.3
1	A	149	TYR	3.3
1	B	1221	SER	3.2
1	A	148	GLN	3.2
1	B	510	ALA	3.2
1	B	487	LEU	3.1
1	B	1028	GLU	3.1
1	B	701	ALA	3.1
1	A	562	ASP	3.1
1	B	1317	HIS	3.0
1	A	662	GLU	3.0
1	A	414	ARG	2.9
1	B	942	ARG	2.9
1	A	192	LYS	2.9
1	A	242	ASP	2.9
1	A	955	PRO	2.9
1	A	328	GLN	2.9
1	B	1206	ALA	2.9
1	B	545	PRO	2.9
1	B	185	LEU	2.8
1	A	1288	ASP	2.8
1	A	131	LEU	2.8
1	A	161	VAL	2.8
1	B	906	SER	2.8
1	B	1308	ARG	2.7
1	A	244	ILE	2.7
1	A	410	ASP	2.7
1	A	245	VAL	2.7
1	B	218	ARG	2.7
1	B	1071	ASP	2.7
1	B	197	PHE	2.6
1	A	142	PHE	2.6
1	A	411	ASP	2.6
1	B	139	ASP	2.6
1	A	939	VAL	2.6
1	A	218	ARG	2.6
1	B	593	ALA	2.6
1	A	389	LEU	2.5
1	A	544	GLN	2.5
1	B	68	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1253	GLU	2.5
1	B	1138	LEU	2.5
1	B	295	MET	2.5
1	B	856	PRO	2.5
1	A	73	ALA	2.5
1	A	72	PHE	2.5
1	B	436	LYS	2.5
1	B	690	GLU	2.4
1	B	460	GLN	2.4
1	B	141	TRP	2.4
1	B	1337	GLU	2.4
1	A	1324	TYR	2.4
1	A	150	CYS	2.4
1	B	152	PRO	2.4
1	A	1370	ARG	2.4
1	A	523	ASN	2.4
1	B	464	ASP	2.4
1	A	1441	MET	2.4
1	B	416	PHE	2.4
1	B	328	GLN	2.3
1	A	1146	GLU	2.3
1	B	440	TYR	2.3
1	A	1464	ILE	2.3
1	B	914	ALA	2.2
1	B	155	ASP	2.2
1	A	954	LEU	2.2
1	B	1115	PRO	2.2
1	A	1152	PRO	2.2
1	B	456	HIS	2.2
1	B	916	ILE	2.2
1	B	884	THR	2.2
1	A	651	ALA	2.2
1	B	209	LYS	2.1
1	A	415	ARG	2.1
1	A	648	LEU	2.1
1	A	74	GLU	2.1
1	B	140	GLN	2.1
1	B	915	VAL	2.1
1	A	240	ARG	2.1
1	A	878	ILE	2.1
1	B	500	GLY	2.1
1	B	241	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	988	ARG	2.0
1	A	413	PRO	2.0
1	A	160	LYS	2.0
1	A	1326	PHE	2.0
1	A	655	ARG	2.0
1	B	901	GLU	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	B	1610	14/15	0.44	0.89	6.33	291,292,293,294	0
5	CA	B	1613	1/1	0.47	0.70	3.33	257,257,257,257	0
2	NAG	B	1606	14/15	0.72	0.34	2.71	268,272,277,283	0
6	EDO	A	1614	1/4	0.80	0.53	2.20	110,110,110,110	0
5	CA	A	1613	1/1	0.27	0.39	0.96	277,277,277,277	1
2	NAG	A	1602	14/15	0.62	0.32	0.54	284,291,292,292	0
2	NAG	A	1601	14/15	0.44	0.52	0.33	279,286,289,290	0
2	NAG	A	1606	14/15	0.58	0.34	-0.17	275,288,291,292	0
2	NAG	A	1605	14/15	0.82	0.23	-0.41	263,268,273,281	0
2	NAG	A	1610	14/15	0.62	0.28	-0.44	288,293,295,295	0
2	NAG	B	1602	14/15	0.72	0.29	-0.52	276,285,289,291	0
2	NAG	B	1605	14/15	0.76	0.26	-0.52	256,258,260,264	0
4	MAN	B	1609	11/12	0.77	0.24	-	270,288,293,298	0
2	NAG	A	1603	14/15	0.78	0.25	-	286,294,297,299	0
2	NAG	A	1612	14/15	0.66	0.46	-	296,300,300,300	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	B	1604	11/12	0.55	0.44	-	292,295,297,298	0
2	NAG	B	1612	14/15	0.28	0.84	-	293,296,297,298	0
3	BMA	A	1607	11/12	0.74	0.23	-	296,297,299,299	0
4	MAN	B	1608	11/12	0.88	0.20	-	292,296,299,299	0
2	NAG	B	1603	14/15	0.75	0.26	-	290,294,296,296	0
2	NAG	B	1601	14/15	0.67	0.35	-	276,278,279,281	0
3	BMA	B	1607	11/12	0.69	0.23	-	274,281,296,296	0
4	MAN	A	1608	11/12	0.60	0.68	-	297,299,300,300	0
3	BMA	A	1604	11/12	0.50	0.48	-	289,295,298,299	0
2	NAG	A	1611	14/15	0.67	0.47	-	294,295,295,295	0
4	MAN	A	1609	11/12	0.35	0.39	-	298,299,300,300	0
2	NAG	B	1611	14/15	-0.03	1.12	-	278,290,293,293	0

## 6.5 Other polymers

There are no such residues in this entry.