Preliminary Full wwPDB X-ray Structure Validation Report (i)

PROTEIN DATA BANK

May 3, 2018 – 04:22 PM EDT

Deposition ID : D_1000234324 PDB ID : (not yet assigned)

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/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 :	(1.7.3 (157068), CSD as 539 be (2018))
Xtriage (Phenix) :	1.13
EDS :	rb-20031021
Percentile statistics :	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac :	5.8.0158
CCP4 :	7.0 (Gargrove)
Ideal geometry (proteins) :	Engh & Huber (2001)
Ideal geometry (DNA, RNA) :	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :	rb-20031021

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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.



Motrio	Whole archive	Similar resolution
Metric	(# Entries)	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	122126	3110(2.60-2.60)
Ramachandran outliers	120053	3062(2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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	522 👗	87%	12%	
2	С	522	87%	13%	-
3	В	522	88%	12%	-

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	3347	-	-	-	Х



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1/1975 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	522	Total 3956	С 2470	N 669	O 788 2	S 29	0	0	0

• Molecule 2 is a protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	С	522	Total C 3962 24	D N 73 668	O S 792 29	0	0	0

• Molecule 3 is a protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
3	В	522	Total 3962	C N 2473 668	O S 792 29)	0	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	W	95	Total O 95 95	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 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.



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Data and refinement statistics (i) 4

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	198.22Å 117.60Å 115.21Å	Depertur
a, b, c, α , β , γ	90.00° 123.79° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\lambda})$	48.99 - 2.60	Depositor
Resolution (A)	48.99 - 2.60	EDS
% Data completeness	96.7 (48.99-2.60)	Depositor
(in resolution range)	97.1 (48.99-2.60)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.98 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1 2575: ???)	Depositor
B B c	0.237 , 0.276	Depositor
	0.238 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
	88.7	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29 , 79.0	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	$\begin{array}{c} & (2^{2}h-1/2^{2}k, (1/2^{2}h+1/2^{2}k, (1/2^{2}h+1/2^{2}k)) \\ & (2^{2}h-1/2^{2}k) \\ & (2^{2}h+1/2^{2}k) \\ & (2^{2}h+1/2^{2}k$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (A^2)	120.0	wwPDB-VP

¹Intensities estimated from amplitudes. ²Theoretical 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.



Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mal Chain		lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5/	
1	А	0.25	0/3955	0.46	0/5387	
2	С	0.25	0/3950	0.45	0/5380	
3	В	0.25	0/3950	0.46	0/5380	
All	All	0.25	0/11855	0.46	0/16147	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Plana rity outliers
1	А	0	
2	С	0	1
3	В	0 ~	
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ALA	Peptide
3	В	279	ALA	Peptide
2	С	279	ALA	Peptide



Too-close contacts (i) 5.2

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	А	3956	0	3830	43	0
2	С	3962	0	3834	44	0
3	В	3962	0	3834	42	0
4	W	95	0	0	6	0
All	All	11975	0	11498	/113	0
					/	

The all-atom clashscore is defined as the number of clashes found per 1,000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:348:ARG:NH1	2:C:436:SER:Ó	2.14	0.79
1:A:348:ARG:NH1	1:A:436:SER:O	2.17	0.76
3:B:348:ARG:NH1	3:B:436:SER:O	2.18	0.75
3:B:129:LEU:HB2	3:B:208:ALA:HB3	1.68	0.74
3:B:515:CYS:SG	4:W:50:HOH:O	2.48	0.72
1:A:129:LEU:HB2	1:A:208:ALA:HB3	1,72	0.71
3:B:162:GLY:O	3:B:377:ARG:NH1	2.26	0.69
2:C:129:LEU:HB2	2;C:208:ALA:HB3	1.75	0.68
1:A:162:GLY:O	1:A:377:ARG:NH1	2.28	0.67
1:A:280:PRO:O	4:W:96:HOH:O	2.13	0.66
2:C:162:GLY:O	2:C:377:ARG:NH1	2.30	0.64
3:B:138:ASP:HB2	3:B:377:ARG:HH12	1.61	0.64
3:B:302:LEU:HD13	3:B:453:VAL:HG22	1.82	0.62
1:A:138:ASP:HB2	1:A:377:ARG:HH12	1.63	0.61
2:C:138:ASP:HB2	2:C:377:ARG/HH12	1.63	0.61
2:C:312:MET:HE3	2:C:443:SER:HB3	1.83	0.61
2:C:302/LEU:HD13	2:C:453:VAL:HG22	1.84	0.58
1:A:274:PHE:HB3	2:C:41:GLU:HG3	1.84	0.58
1;A:133:ASN:O	1:A:203:ARG:NH2	2.31	0.58
1:A:312:MET:HE3	1:A:443:SER:HB3	1.85	0.56
3:B:234:ILE:HB	3/B:286:LEU:HB2	1.88	0.55
3:B:196:PRO:HG2	3:B:197:LEU:HD12	1.88	0.55
1:A:510:LEU:HD13	1:A:560:LEU:HD13	1.88	0.55
		Continue	ed on next page
	w	_O R L D W I D E	



Atom 2 distance (Å) overlap (Å) LA:63:GLU:HC2 L:A:462:THR:HC23 1.89 0.54 2:C:274:PHE:HB3 3:B:41:GLU:HG3 1.89 0.54 1:A:196:PRO:HG2 1:A:197:LEU:HD12 1.89 0.54 2:C:274:PHE:HB 2:C:286:LEU:HB2 1.89 0.53 1:A:14:GLU:HG3 3:B:274:PHE:HB3 1.91 0.63 2:C:360:FRO:HG2 2:C:190:FEU:HD13 1.91 0.63 2:C:196:FRO:HG2 2:C:190:FEU:HD13 1.91 0.63 2:C:196:FRO:HG2 2:C:190:FEU:HD13 1.92 0.51 2:C:196:FRO:HG2 2:C:190:FEU:HD13 1.92 0.51 2:C:360:LU:HG2 3:B:462:THR:HG23 1.92 0.51 2:C:360:LU:HG2 3:B:564:ARG:NH2 2.43 0.51 1:A:74:SER:HB2 1:A:93:ARG:HE 1.76 0.51 2:C:124:PRO:HD2 2:C:39:ARG:HE 1.77 0.50 2:C:124:PRO:HD2 2:C:39:ARG:HE 1.77 0.50 2:C:124:PRO:HD2 2:C:39:ARG:HE 1.94 0.50	Atom-1		Atom_2	Interatomic	Clash	
1:A:63:GU:HG2 1:A:462:THR:HG23 1.89 0.54 2:C:274:PHE:HB3 3:B:41:GU:HG3 1.88 0.54 1:A:1967:EU:HD12 1.89 0.53 1:A:197:EU:HD13 1.89 0.53 1:A:14:GL:HG3 3:B:274:PHE:HB3 1.90 0.53 2:C:300:LEU:HD13 1.91 0.63 2:C:510:LEU:HD13 1.91 0.63 2:C:510:LEU:HD13 1.92 0.51 3:B:510:LEU:HD13 2:B:66:THR:HG23 1.92 0.51 3:B:510:LEU:HD13 3:B:560:LEU:HD13 1.92 0.51 3:B:5510:LEU:HD13 3:B:560:LEU:HD13 1.92 0.51 3:B:5510:LEU:HD13 3:B:560:LEU:HD13 1.92 0.51 3:B:561:EH:B2 1:A:93:ARG:HE 1.76 0.51 2:C:74:PHE:HB2 2:C:39:ARG:HE 1.76 0.50 2:C:74:PHE:HB2 2:C:39:ARG:HE 1.76 0.50 1:A:27:EE:HB2 2:C:39:ARG:HE 1.76 0.50 1:A:27:EE:HB2 2:C:39:ARG:HE 1.94 0.49 1:A:28:GE:EH:HG3 2:C:39:ARG:HE 1.76 0.50 2:		Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:C:274:PHE:HB3 3:B:41:GLU:HG3 1.88 0.54 1:A:196:PRO:HG2 1:A:197:LEU:HD12 1.89 0.53 2:C:234:ILE:HB 2:C:286:LEU:HB2 1.89 0.53 1:A:342:ASP:N 4:W:33:HOH:O 2.41 0.53 2:C:196:PRO:HG2 2:C:197:LEU:HD13 1.91 0.53 2:C:196:PRO:HG2 2:C:197:LEU:HD13 1.91 0.53 2:C:196:PRO:HG2 2:C:197:LEU:HD13 1.91 0.53 2:C:196:PRO:HG2 2:C:197:LEU:HD13 1.92 0.51 3:B:50:LEU:HD13 3:B:462:THR:HG23 1.92 0.51 3:B:50:LEU:HD13 3:B:560:LEU:HD13 1.92 0.51 3:B:50:LEU:HD13 3:B:560:LEU:HD13 1.92 0.51 3:B:50:LEU:HD13 1.92 0.51 3:B:561:ARG:NH2 2.43 0.51 2:C:124:PRO:IID2 2:C:39:ARG:HE 1.76 0.50 1:A:74:SER:HB2 2:C:39:ARG:HE 1.77 0.50 1:A:24:PHE:HB2 2:C:37:ARG:HE 1.94 0.49 1:A:30:ASP:HA 1.95 0.48 1:A:25:ILE:HG23 2:C:71:HR:HG21 1.94 0.49 1:A:44:RE:HA </td <td></td> <td>1:A:63:GLU:HG2</td> <td>1:A:462:THR:HG23</td> <td>1.89</td> <td>0.54</td> <td></td>		1:A:63:GLU:HG2	1:A:462:THR:HG23	1.89	0.54	
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1:A:561:TYR:CD2 2 2:C:97:ALA:HB1 2 1:A:470:THR:N 2 2:C:587:HIS:O 3:B:79:CYS:HB3 2:C:348:ARG:HA 2 1:A:105:LYS:HE3 1 1:A:491:ARG:HD3 1 1:A:475:CYS:HA 2 2:C:309:ASP:HA 2 2:C:470:THR:N 3 3:B:509:THR:HB 3 1:A:72:LEU:O 1 1:A:234:ILE:HB 2 2:C:491:ARG:HD3 2 2:C:561:TYR:CD2 3 :A:288:LEU:HD23 2 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:57:HIS:O 3:B:475:CYS:HA	2:C:294:LEU:HD11 2:C:239:PRO:HG2 1:A:497:ASN:O 2:C:588:HIS:ND1 3:B:80:PRO:HD3 2:C:351:TRP:CD1 1:A:230:PHE:CD2 1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{c} 2.51 \\ 1.98 \\ 2.50 \\ 2.51 \\ 1.99 \\ 2.52 \\ 2.53 \\ 2.52 \\ 2.00 \\ 2.00 \\ 2.00 \\ 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \end{array}$	$\begin{array}{c c} 0.45 \\ \hline 0.45 \\ \hline 0.44 \\ \hline 0.43 \\ \hline 0.44 \\ \hline 0.44 \\ \hline 0.4$
2:C:97:ALA:HB1 2 1:A:470:THR:N 2 1:A:470:THR:N 2 2:C:587:HIS:O 3 3:B:79:CYS:HB3 2 2:C:348:ARG:HA 2 1:A:105:LYS:HE3 1 1:A:491:ARG:HD3 1 1:A:475:CYS:HA 2 2:C:309:ASP:HA 2 2:C:470:THR:N 3 3:B:509:THR:HB 3 1:A:234:ILE:HB 3 3:B:72:LEU:HB2 2 2:C:491:ARG:HD3 2 2:C:561:TYR:CD2 3 :A:288:LEU:HD23 3 :A:288:LEU:HD23 3 :A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O 3:B:475:CYS:HA	2:C:239:PRO:HG2 1:A:497:ASN:O 2:C:588:HIS:ND1 3:B:80:PRO:HD3 2:C:351:TRP:CD1 1:A:230:PHE:CD2 1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU;HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{c} 1.98 \\ 2.50 \\ 2.51 \\ 1.99 \\ 2.52 \\ 2.53 \\ 2.52 \\ 2.00 \\ 2.00 \\ 2.00 \\ 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \end{array}$	$\begin{array}{c ccccc} 0.45 \\ \hline 0.44 \\ \hline 0.43 \\ \hline$
1:A:470:THR:N 2:C:587:HIS:O 3:B:79:CYS:HB3 2:C:348:ARG:HA 2:C:348:ARG:HA 1:A:105:LYS:HE3 1:A:491:ARG:HD3 1:A:475:CYS:HA 2:C:309:ASP:HA 2:C:470:THR:N 3:B:509:THR:HB 3:B:509:THR:HB 3:B:72:LEU:O 1:A:234:ILE:HB 2:C:491:ARG:HD3 2:C:561:TYR:CD2 3:A:288:LEU:HD23 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA	1:A:497:ASN:O 2:C:588:HIS:ND1 3:B:80:PRO:HD3 2:C:351:TRP:CD1 1:A:230:PHE:CD2 1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{c} 2.50\\ \hline 2.51\\ \hline 1.99\\ \hline 2.52\\ \hline 2.53\\ \hline 2.52\\ \hline 2.00\\ \hline 2.00\\ \hline 2.00\\ \hline 2.48\\ \hline 1.99\\ \hline 2.17\\ \hline 1.99\\ \hline 2.17\\ \hline 1.99\\ \hline 2.01\\ \hline 2.53\\ \hline 2.53\\ \hline 2.00\\ \hline 2.52\\ \end{array}$	$\begin{array}{c ccccc} 0.44 \\ \hline 0.43 \\ \hline$
2:C:587:HIS:O 3:B:79:CYS:HB3 2:C:348:ARG:HA 1:A:105:LYS:HE3 1:A:491:ARG:HD3 1:A:491:ARG:HD3 1:A:491:ARG:HD3 1:A:491:ARG:HD3 1:A:491:ARG:HD3 1:A:475:CYS:HA 2:C:309:ASP:HA 2:C:470:THR:N 3:B:509:THR:HB 1:A:72:LEU:O 1:A:234:ILE:HB 3:B:72:LEU:HB2 2:C:491:ARG:HD3 2:C:561:TYR:CD2 3:A:288:LEU:HD23 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA	2:C:588:HIS:ND1 3:B:80:PRO:HD3 2:C:351:TRP:CD1 1:A:230:PHE:CD2 1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU;HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{c} 2.51 \\ 1.99 \\ 2.52 \\ 2.53 \\ 2.52 \\ 2.00 \\ 2.00 \\ 2.00 \\ 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \end{array}$	$\begin{array}{c c} 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array}$
3:B:79:CYS:HB3 2:C:348:ARG:HA 1:A:105:LYS:HE3 1:A:491:ARG:HD3 1:A:491:ARG:HD3 1:A:475:CYS:HA 2:C:309:ASP:HA 2:C:470:THR:N 3:B:509:THR:HB 1:A:72:LEU:O 1:A:234:ILE:HB 2:C:561:TYR:CD2 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA	3:B:80:PRO:HD3 2:C:351:TRP:CD1 1:A:230:PHE:CD2 1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{c c} 1.99 \\ \hline 2.52 \\ \hline 2.53 \\ \hline 2.52 \\ \hline 2.00 \\ \hline 2.00 \\ \hline 2.00 \\ \hline 2.48 \\ \hline 1.99 \\ \hline 2.17 \\ \hline 1.99 \\ \hline 2.01 \\ \hline 2.53 \\ \hline 2.53 \\ \hline 2.00 \\ \hline 2.52 \\ \end{array}$	$\begin{array}{c} 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array}$
2:C:348:ARG:HA 2 1:A:105:LYS:HE3 1 1:A:491:ARG:HD3 1 1:A:491:ARG:HD3 1 1:A:491:ARG:HD3 1 1:A:475:CYS:HA 2 2:C:309:ASP:HA 2 2:C:470:THR:N 3 3:B:509:THR:HB 3 1:A:72:LEU:O 1 1:A:234:ILE:HB 1 3:B:72:LEU:HB2 2 2:C:491:ARG:HD3 2 2:C:561:TYR:CD2 3 1:A:288:LEU:HD23 1 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O 3:B:475:CYS:HA	2:C:351:TRP:CD1 1:A:230:PHE:CD2 1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{r} 2.52 \\ 2.53 \\ 2.52 \\ 2.00 \\ 2.00 \\ 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \\ \end{array}$	$\begin{array}{c} 0.44\\ 0.44\\ 0.44\\ 0.44\\ 0.44\\ 0.44\\ 0.44\\ 0.44\\ 0.44\\ 0.43\\$
1:A:105:LYS:HE3 1 1:A:491:ARG:HD3 1 1:A:475:CYS:HA 1 2:C:309:ASP:HA 1 2:C:470:THR:N 1 3:B:509:THR:HB 1 1:A:72:LEU:O 1 1:A:234:ILE:HB 1 3:B:72:LEU:HB2 1 2:C:561:TYR:CD2 3 1:A:288:LEU:HD23 1 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O 1	1:A:230:PHE:CD2 1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{r} 2.53 \\ 2.52 \\ 2.00 \\ 2.00 \\ 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \end{array}$	$\begin{array}{c cccc} 0.44 \\ \hline 0.43 \\ \hline $
1:A:491:ARG:HD3 1:A:475:CYS:HA 2:C:309:ASP:HA 2:C:470:THR:N 3:B:509:THR:HB 3:B:509:THR:HB 1:A:72:LEU:O 1:A:234:ILE:HB 3:B:72:LEU:HB2 2:C:491:ARG:HD3 2:C:561:TYR:CD2 3:A:288:LEU:HD23 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA	1:A:544:TYR:CZ 1:A:482:CYS:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{r} 2.52 \\ 2.00 \\ 2.00 \\ 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \end{array}$	$\begin{array}{c c} 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array}$
1:A:475:CYS:HA 2:C:309:ASP:HA 2:C:470:THR:N 3:B:509:THR:HB 3:B:509:THR:HB 1:A:72:LEU:O 1:A:72:LEU:HB 2:C:491:ARG:HD3 2:C:561:TYR:CD2 3:A:288:LEU:HD23 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA	1:A:482:CYS:HA 2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{r} 2.00\\ \hline 2.00\\ \hline 2.48\\ \hline 1.99\\ \hline 2.17\\ \hline 1.99\\ \hline 2.01\\ \hline 2.53\\ \hline 2.53\\ \hline 2.00\\ \hline 2.52\\ \end{array}$	$\begin{array}{c c} 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array}$
2:C:309:ASP:HA 2:C:470:THR:N 3:B:509:THR:HB 3:B:509:THR:HB 1:A:72:LEU:O 1:A:234:ILE:HB 3:B:72:LEU:HB2 2:C:491:ARG:HD3 2:C:561:TYR:CD2 3:A:288:LEU:HD23 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O	2:C:447:SER:HA 2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{r} 2.00 \\ 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \end{array}$	$\begin{array}{c} 0.44 \\ 0.44 \\ 0.44 \\ 0.44 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array}$
2:C:470:THR:N 3:B:509:THR:HB 1:A:72:LEU:O 1:A:72:LEU:O 1:A:234:ILE:HB 3:B:72:LEU:HB2 2:C:491:ARG:HD3 2:C:561:TYR:CD2 3:A:288:LEU:HD23 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O	2:C:497:ASN:O 3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU;HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$\begin{array}{r} 2.48 \\ 1.99 \\ 2.17 \\ 1.99 \\ 2.01 \\ 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \end{array}$	$\begin{array}{c c} 0.44 \\ 0.44 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array}$
3:B:509:THR:HB 3 1:A:72:LEU:O 1 1:A:234:ILE:HB 1 3:B:72:LEU:HB2 1 2:C:491:ARG:HD3 2 2:C:561:TYR:CD2 3 1:A:288:LEU:HD23 1 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O 1	3:B:561:TYR:HB2 1:A:93:ARG:HB3 1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$ \begin{array}{r} 1.99\\ 2.17\\ 1.99\\ 2.01\\ 2.53\\ 2.53\\ 2.00\\ 2.52\\ \end{array} $	$\begin{array}{r} 0.44 \\ 0.44 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array}$
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1:A:234:ILE:HB 1 3:B:72:LEU:HB2 2 2:C:491:ARG:HD3 2 2:C:561:TYR:CD2 3 1:A:288:LEU:HD23 1 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O 1	1:A:286:LEU:HB2 3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$ \begin{array}{r} 1.99\\ 2.01\\ 2.53\\ 2.53\\ 2.00\\ 2.52\\ \end{array} $	$\begin{array}{r c} 0.43 \\ \hline \end{array}$
3:B:72:LEU:HB2 2:C:491:ARG:HD3 2 2:C:561:TYR:CD2 3 :A:288:LEU:HD23 2 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O 1	3:B:94:ASP:HB2 2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	2.01 2.53 2.53 2,00 2.52	$ \begin{array}{r} 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array} $
2:C:491:ARG:HD3 2 2:C:561:TYR:CD2 3 1:A:288:LEU:HD23 2 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O 1	2:C:544:TYR:CE2 3:B:294:LEU:HD11 1:A:306:LEU;HB2 3:B:111:SER:O 1:A:588:HIS:ND1	$ \begin{array}{r} 2.53 \\ 2.53 \\ 2.00 \\ 2.52 \\ \end{array} $	$ \begin{array}{r} 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \\ 0.43 \end{array} $
2:C:561:TYR:CD2 3 ::A:288:LEU:HD23 2 2:C:520:ARG:NH2 1 1:A:587:HIS:O 3:B:475:CYS:HA 3 3:B:587:HIS:O	3:B:294:LEU:HD11 1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	2.53 2,00 2.52	0.43 0.43 0.43
:A:288:LEU:HD23 2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O	1:A:306:LEU:HB2 3:B:111:SER:O 1:A:588:HIS:ND1	2.00 2.52	0.43
2:C:520:ARG:NH2 1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O	3:B:111:SER:O 1:A:588:HIS:ND1	2.52	0.43
1:A:587:HIS:O 3:B:475:CYS:HA 3:B:587:HIS:O	1:A:588:HIS:ND1		0.10
3:B:475:CYS:HA 3:B:587:HIS:O		2.52	0.43
3.B.587.HIS.O	3:B:482:CYS:HA	2.00	0.43
0.0.001.110.0	3:B:588:HIS:ND1	2.52	0.42
L:A:294:LEU:HD11 3	3:B:561:TYR:CD2	2.54	0.42
2:C:319:ILE:HB 2	2:C:353:LEU:HD21	2.02	0.42
3:B:348:ARG:HA	3:B:351:TRP:CD1	2.54	0.42
2:C:126:GLU:HB3 / 2	2:C:388:GLN:OE1	2.20	0.42
2:C:475:CYS:HA	2:C:482:CYS:HA	2.00	0.42
3:B:491:ARG:HD3	3:B:544:TYR:CZ	2.54	0.42
3:B:550:ALA:HB2 3	3:B:579:ALA:HB2	2.01	0.42
:B:554:ARG:HH11 3	3:B:577:THR:HG21	1.85	0.42
1:A:347:ASN:HB3	1:A:348:ARG:H	1.77	0.41
2:C:550:ALA:HB2	2:C:579:ALA:HB2	2.02	0.41
2:C:464:ARG:O	3:B:37:GLY:N	2.43	0.41
3:B:236:VAL:HG21 3	3:B:302;LEU:HD23	2.02	0.41
3:B:491:ARG:HD3	3:B:544:TYR:CE2	2.55	0.41
2:C:491:ARG:HD3	2:C:544:TYR:CZ	2.56	0.41
2:C:509:THR:HB 2	2:C:561:TYR:HB2	2.02	0.41
2:C:25:ILE:HG23 3	3:B:51:THR:HG21	2.02	0.41
3:B:74:SER:HB2	3:B:93:ARG:HE	1.85	0.41

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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:C:145:PRO:HG2	2:C:148:GLY:H	1.86	0.41
2:C:347:ASN:HB3	2:C:348:ARG:H	1.45	0.41
1:A:126:GLU:HB3	1:A:388:GLN:OE1	2.21	0.40
1:A:309:ASP:OD1	1:A:447:SER:HB3	2.21	0.40
1:A:58:GLN:NE2	1:A:103:LEU:O	2.54	0.40
1:A:307:LEU:HD21	3:B:23:GLU:HG2	2.03	0.40
3:B:277:PRO:HA	3:B:278:PRO:HD3	1.97	0.40
3:B:105:LYS:HE3	3:B:230:PHE:CD2	2.56	0.40

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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	Perce	ntiles
1	А	505/522~(97%)	477 (94%)	27 (5%)	1 (0%)	49	74
2	С	504/522~(97%)	476 (94%)	27 (5%)	1 (0%)	49	74
3	В	504/522 (97%)	476 (94%)	28 (6%)	0	100	100
All	All	1513/1566~(97%)	1429~(94%)	82 (5%)	2(0%)	53	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res Type
1	A	71 CYS
2	C	71 CYS
	/	

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	Perce	ntiles
1	А	430/430~(100%)	426~(99%)	4 (1%)	81	92
2	С	430/430~(100%)	427~(99%)	3 (1%)	85	95
3	В	430/430~(100%)	427~(99%)	3 (1%)	85	95
All	All	1290/1290~(100%)	1280~(99%)	10 (1%)	83	93

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

Mol	Chain	\mathbf{Res}	Type
1	А	71	CYS
1	А	141	TRP
1	А	309	ASP
1	А	347	ASN
2	С	71	CYS
2	С	141	TRP
2	С	347	ASN
3	В	71	CYS
3	В	141	TRP
3	В	347	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

20 non-standard protein/DNA/RNA residues 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).



Bond lengths Bond angles Mol Type Chain Res Link Counts RMSZ #|Z| > 2Counts RMSZ #|Z| > 2NAG 3347 1 А 1 14,14,15 0.2817,19,21 0.510 0 NAG 1 А 3497 1 14.14.15 0.280 17,19,21 0.46 0 1 NAG 3498 1 14,14,15 0.240 (17, 19, 21)0.49А Ø BMA 0 1 А 3499 11,11,12 0.5615,15,17 0.750 1 NAG Α 351414,14,15 0.26 0 17,19,21 0.39 0 1 1 NAG 1 А 35781 14,14,15 0.470 17,19,21 0.530 3 NAG В 3347 3 14,14,15 0.29Ń 17, 19, 210 0.533 NAG В 3497 3 14,14,15 0.280 17,19,21 0.460 3 NAG В 34983 14,14,15 0.250 17,19,21 0.470 3 BMA В 34993 11,11,12 0.570 15,15,17 0.910 3 MAN В 35003 11,11,12 0.740 15, 15, 171.202(13%)3 NAG В 3 17,19,21 351414,14,15 0.230 0.420 3 NAG В 35783 14,14,15 0.400 17,19,21 0.530 $\overline{2}$ NAG С 3347 214,14,15 0.340 17,19,21 0.490 2NAG С 214,14,15/ 0.3117,19,21 3497 0 0.450 $\overline{2}$ NAG С 2 3498 14,14,15 0.260 17, 19, 210 0.50 $\overline{2}$ BMA С $\overline{2}$ 3499 11,11,12 0.560 15, 15, 170.890 2MAN С 3500211,11,12 0.720 15, 15, 172(13%)1.19 $\overline{2}$ С $\overline{2}$ NAG 351414,14,15 0.240 17,19,21 0 0.452NAG С 3578214,14,15 0.44 0 17,19,21 0.550

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
	1	NAG	A /	3347		- /	0/6/23/26	0/1/1/1
	1	NAG	A	3497	1	-/	0/6/23/26	0/1/1/1
	1	NAG	A	3498	ų	-	0/6/23/26	0/1/1/1
	1	BMA	A	3499	1	/ -	0/2/19/22	0/1/1/1
	1	NAG	A	3514	1	/ -	0/6/23/26	0/1/1/1
	1	NAG	A	3578	1 /	-	0/6/23/26	0/1/1/1
	3	NAG	В	3347	3	-	0/6/23/26	0/1/1/1
	3	NAG	В	3497	3	-	0/6/23/26	0/1/1/1
	3	NAG	В	3498	3	-	0/6/23/26	0/1/1/1
	3	BMA	В	3499	3	_	0/2/19/22	0/1/1/1
	3	MAN	В	3500	3	-	0/2/19/22	1/1/1/1
	3	NAG	В	3514	3	-	0/6/23/26	0/1/1/1
	3	NAG	В	3578	3	-	0/6/23/26	0/1/1/1
/	2	NAG	C /	3347	2	-	0/6/23/26	0/1/1/1
	2	NAG	C	3497	2	-	0/6/23/26	0/1/1/1
							ntinued on ne	ext page



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	С	3498	2	-	0/6/23/26	0/1/1/1
2	BMA	С	3499	2	-	0/2/19/22	0/1/1/1
2	MAN	С	3500	2	-	0/2/19/22	1/1/1/1
2	NAG	С	3514	2	-	0/6/23/26	0/1/1/1
2	NAG	С	3578	2	-	0/6/23/26	0/1/1/1

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There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	3500	MAN	O2-C2-C3	-2.29	105.72	110.19
3	В	3500	MAN	O2-C2-C3	-2.27	105.77	110.19
2	С	3500	MAN	C1-O5-C5	3.40	116.87	112.19
3	В	3500	MAN	C1-O5-C5	3.45	116.93	112.19

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	3500	MAN	C1-C2-C3-C4-C5-O5
2	С	3500	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers i

There are no such residues in this entry.



/

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	В	9
1	А	9
2	С	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	588:HIS	С	3347:NAG	04	59.82
1	A	588:HIS	С	3497:NAG	04	53.89
1	С	588:HIS	С	3497:NAG	04	53.85
1	А	3514:NAG	C1	3347:NAG	04	48.37
1	С	3514:NAG	C1	3347:NAG	04	48.17
1	В	3500:MAN	C1	3514:NAG	04	39.45
1	С	3500:MAN	C1	3514:NAG	04	38.62
1	A	3347:NAG	C1 /	3578:NAG	04	38.11
1	С	3347:NAG	C1 /	3578:NAG	04	38.11
1	А	3499:BMA	C1	3514:NAG	04	35.99
1	В	3514:NAG	Q1	3578:NAG	Ø4	27.74
1	В	3347:NAG	/C1	3497:NAG	/ 04	24.57
1	В	240:THR	C	273:GLN	N	22.62
1	A	240:THR	С	273:GLN	Ν	22.49
1	А	331:ALA	С	342:ASP	Ν	22.08
1	С	240:THR	C	273:GLN	Ν	21.94
1	В	330:PRO	С	342:ASP	Ν	19.74
1	С	330:PRO	C C	342:ASP	Ν	19.61
1	С	83:CYS	C	89:THR	Ν	9.79
1	А	83:CYS	C	89:THR	Ν	9.67
1	В	83:CYS	C /	89:THR	Ν	9.58
1	C	76:ASP	C	79:CYS	Ν	8.63
1	В	76:ASP	С	79:CYS	Ν	8.47
1	Á	76:ASP	Ć	79:CYS	Ν	8.29
1	A	74:SER	C	76:ASP	Ν	4.41
1	C	74:SER	C	76:ASP	Ν	4.39
1 /	B 🚬	74:SER	С	76:ASP	Ν	4.37



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	$OWAB(A^2)$	Q<0.9
1	А	516/522~(98%)	0.07	16 (3%) 49 41	77, 110, 189, 270	0
2	С	515/522~(98%)	0.11	20 (3%) 39 31	80, 110, 186, 277	0
3	В	515/522~(98%)	0.05	17 (3%) 46 39	78, 110, 189, 291	0
All	All	1546/1566~(98%)	0.08	53 (3%) 45 37	77, 110, 189, 291	0

All (53) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	С	275	LEU	8.6
3	В	274	PHE	8.2
1	А	275	LEU	7.6
2	С	274	PHE	7.2
3	В	275	LEU	6.9
3	В	424	ASP	5.5
2	С	424	ASP	5.3
1	А	200	LEU	5.0
1	А	582	LEU	4.9
3	В	452	SER	4.8
2	С	200	LEU	4.7
2	С	89	THR	4.5
2	C /	426	THR	4.3
2	C	454	ALA	4.3
2	Q	584	HIS	3.8
2	/C	587	HIS	/3.6
2	C	427	LEU	3.4
3 /	В	211	LEU	3.4
2	C	67	PHE	3.3
/3	В	587	HÍS	3.3
2	C	582	LEU	3.2
1	A	424	ASP	3.1
2	C	455	ALA	3.0



	IVIOI	Chain	Res	Type	RSRL	
	1	А	67	PHE	2.9	
	2	С	425	THR	2.8	
	3	В	582	LEU	2.6	
	1	А	89	THR	2.6	
	1	А	587	HIS	2.6	
	2	С	125	LEU	2.6	
	1	А	564	VAL	2.5	
	1	А	346	THR	2.5	
	1	А	203	ARG	2.4	
	3	В	427	LEU	2.4	
	3	В	301	LEU	2.4	
	2	С	586	HIS	2.4	
	1	А	426	THR	2.3	
	3	В	203	ARG	2.3	
	1	А	173	TRP	2.3	
	3	В	200	LEU	2.3	
	1	А	30	LEU	2.3	
	1	А	427	LEU	2.2	
	3	В	564	VAL	2.2	
	3	В	584	HIS	2.2	
	3	В	74	SER	2.1	
	2	С	494	ILE	2.1	
	1	А	150	PHE	/2.1	
	1	А	65	LEU	2.1	
	3	В	537	LEU	2.0	
	3	В	281	SER	2.0	
	2	С	236	VAL	2.0	
	2	С	177	́РНЕ	2.0	
	2	С	203	ARG	2.0	
	3	В	377	ARG	2.0	
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6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
/1	NAG	A	3514	14/?	0.56	0.26	$129,\!157,\!178,\!181$	0
1	NAG	A /	3347	14/?	0.70	0.38	$150,\!177,\!207,\!208$	0
2	NAG	C	3347	14/?	0.75	0.43	$139,\!181,\!195,\!195$	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	MAN	В	3500	11/?	0.81	0.22	221,227,230,232	0
2	NAG	С	3514	14/?	0.81	0.13	$127,\!151,\!162,\!164$	0
2	NAG	С	3578	14/?	0.81	0.16	113, 131, 150, 153	0
3	NAG	В	3347	14/?	0.82	0.30	$136,\!164,\!190,\!193$	0
3	NAG	В	3578	14/?	0.82	0.16	$109,\!126,\!140,\!141$	0
3	NAG	В	3514	14/?	0.85	0.20	142,160,172,174	0
1	BMA	А	3499	11/?	0.87	0.14	$175,\!186,\!198,\!199$	0
1	NAG	А	3578	14/?	0.87	0.17	$106,\!128,\!147,\!148$	0
2	MAN	С	3500	11/?	0.90	0.23	237,243,246,246	0
3	NAG	В	3498	14/?	0.91	0.14	132, 161, 171, 186	0/
1	NAG	А	3498	14/?	0.91	0.17	132,160,165,173	0
3	BMA	В	3499	11/?	0.92	0.10	$199,\!206,\!216,\!219$	0
2	NAG	С	3498	14/?	0.92	0.15	$136,\!164,\!174,\!189$	0
3	NAG	В	3497	14/?	0.93	0.15	84,117,150,151	0
2	BMA	С	3499	11/?	0.93	0.11	204,213,222,230	0
1	NAG	А	3497	14/?	0.94	0.13	$90,\!122,\!150,\!152$	0
2	NAG	С	3497	14/?	0.97	0.11	79,113,154,158	0

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6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

