



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:00 PM GMT

PDB ID : 3QNF  
Title : Crystal structure of the open state of human endoplasmic reticulum aminopeptidase 1 ERAP1  
Authors : Vollmar, M.; Kochan, G.; Krojer, T.; Harvey, D.; Chaikuad, A.; Allerston, C.; Muniz, J.R.C.; Raynor, J.; Ugochukwu, E.; Berridge, G.; Wordsworth, B.P.; von DELFT, F.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Kavanagh, K.; Oppermann, U.; Structural Genomics Consortium (SGC)  
Deposited on : 2011-02-08  
Resolution : 3.00 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 (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

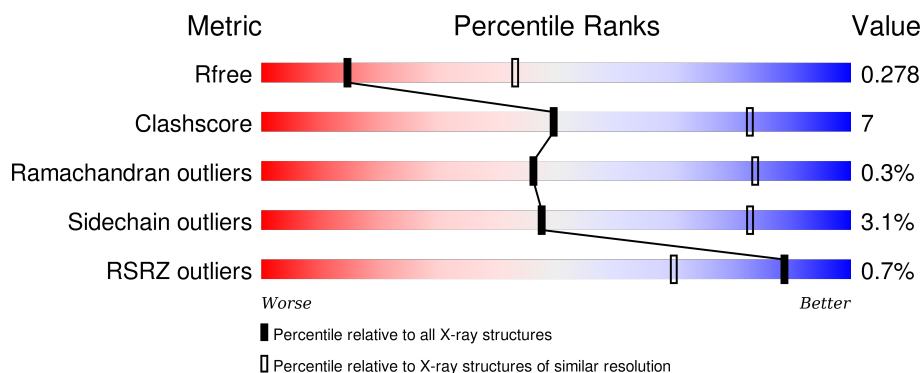
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	954	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>9%</div> <div>27%</div> </div> </div>
1	B	954	<div> <div></div> <div>69%</div> <div>14%</div> <div>•</div> <div>16%</div> </div>
1	C	954	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>16%</div> </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
3	MAN	A	1005	X	-	-	X
4	NAG	B	1154	X	-	-	-
4	NAG	C	1070	-	-	-	X
4	NAG	C	1154	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17682 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	1	0
			5284	3422	863	975	24			
1	B	802	Total	C	N	O	S	0	2	0
			6178	4011	1005	1133	29			
1	C	800	Total	C	N	O	S	0	2	0
			6072	3936	998	1109	29			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	EXPRESSION TAG	UNP Q9NZ08
A	-4	ARG	-	EXPRESSION TAG	UNP Q9NZ08
A	-3	ARG	-	EXPRESSION TAG	UNP Q9NZ08
A	-2	ARG	-	EXPRESSION TAG	UNP Q9NZ08
A	-1	TYR	-	EXPRESSION TAG	UNP Q9NZ08
A	0	THR	-	EXPRESSION TAG	UNP Q9NZ08
A	942	ALA	-	EXPRESSION TAG	UNP Q9NZ08
A	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
A	944	ASN	-	EXPRESSION TAG	UNP Q9NZ08
A	945	LEU	-	EXPRESSION TAG	UNP Q9NZ08
A	946	TYR	-	EXPRESSION TAG	UNP Q9NZ08
A	947	PHE	-	EXPRESSION TAG	UNP Q9NZ08
A	948	GLN	-	EXPRESSION TAG	UNP Q9NZ08
B	-5	LEU	-	EXPRESSION TAG	UNP Q9NZ08
B	-4	ARG	-	EXPRESSION TAG	UNP Q9NZ08
B	-3	ARG	-	EXPRESSION TAG	UNP Q9NZ08
B	-2	ARG	-	EXPRESSION TAG	UNP Q9NZ08
B	-1	TYR	-	EXPRESSION TAG	UNP Q9NZ08
B	0	THR	-	EXPRESSION TAG	UNP Q9NZ08
B	942	ALA	-	EXPRESSION TAG	UNP Q9NZ08
B	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
B	944	ASN	-	EXPRESSION TAG	UNP Q9NZ08
B	945	LEU	-	EXPRESSION TAG	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	946	TYR	-	EXPRESSION TAG	UNP Q9NZ08
B	947	PHE	-	EXPRESSION TAG	UNP Q9NZ08
B	948	GLN	-	EXPRESSION TAG	UNP Q9NZ08
C	-5	LEU	-	EXPRESSION TAG	UNP Q9NZ08
C	-4	ARG	-	EXPRESSION TAG	UNP Q9NZ08
C	-3	ARG	-	EXPRESSION TAG	UNP Q9NZ08
C	-2	ARG	-	EXPRESSION TAG	UNP Q9NZ08
C	-1	TYR	-	EXPRESSION TAG	UNP Q9NZ08
C	0	THR	-	EXPRESSION TAG	UNP Q9NZ08
C	942	ALA	-	EXPRESSION TAG	UNP Q9NZ08
C	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
C	944	ASN	-	EXPRESSION TAG	UNP Q9NZ08
C	945	LEU	-	EXPRESSION TAG	UNP Q9NZ08
C	946	TYR	-	EXPRESSION TAG	UNP Q9NZ08
C	947	PHE	-	EXPRESSION TAG	UNP Q9NZ08
C	948	GLN	-	EXPRESSION TAG	UNP Q9NZ08

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

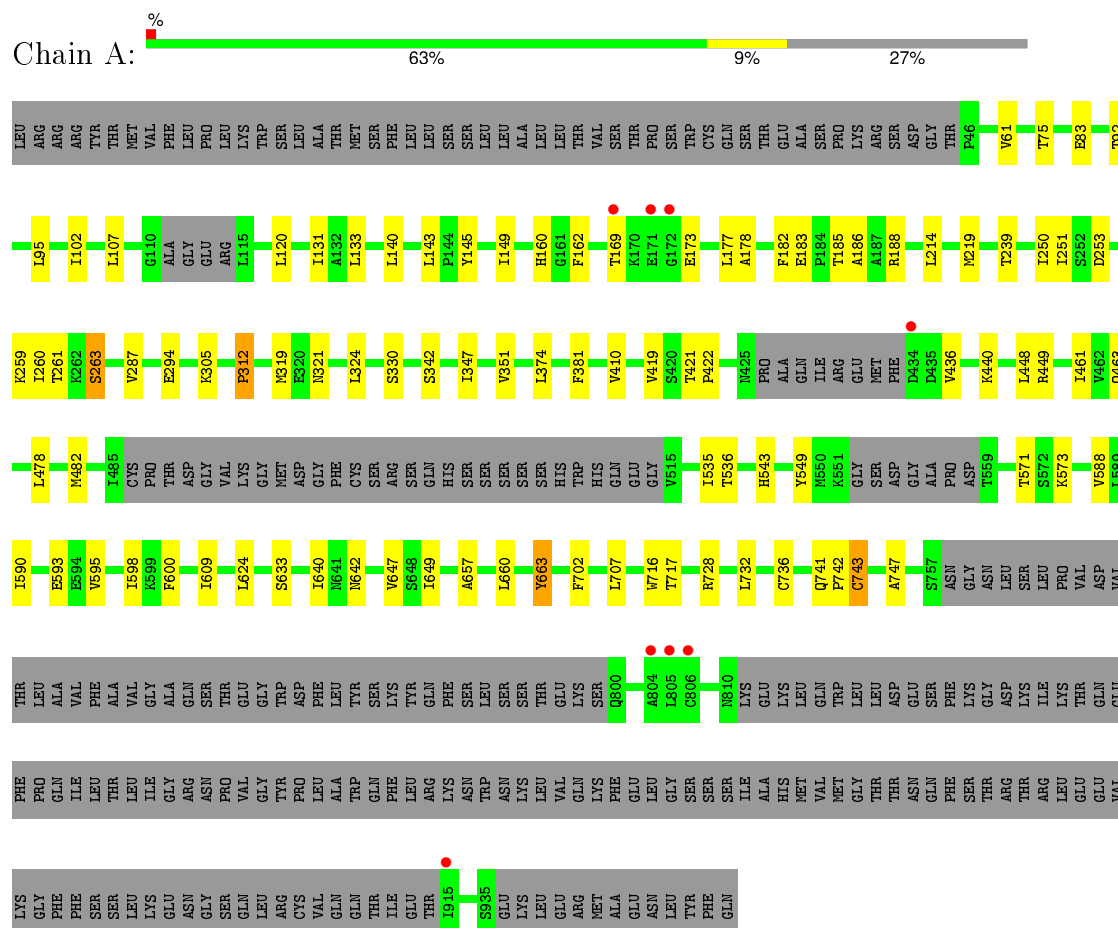
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	B	19	Total	O	0	0
			19	19		
5	C	12	Total	O	0	0
			12	12		

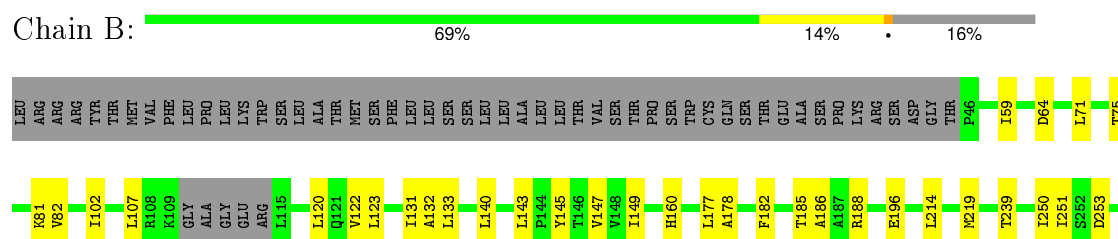
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

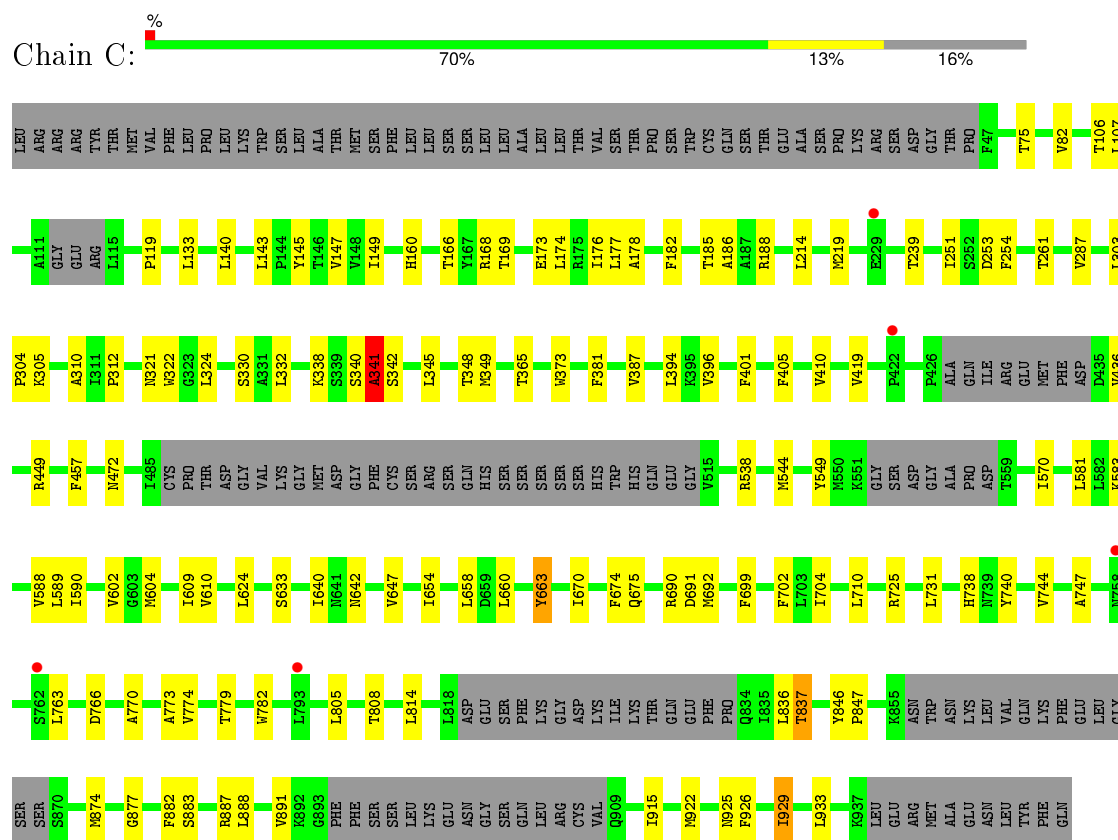
- Molecule 1: Endoplasmic reticulum aminopeptidase 1



- Molecule 1: Endoplasmic reticulum aminopeptidase 1



- Molecule 1: Endoplasmic reticulum aminopeptidase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.25Å 132.82Å 233.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.99-3.00) 97.6 (19.99-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.229 , 0.283 0.228 , 0.278	Depositor DCC
$R_{free}$ test set	3019 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 59669 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 0.375 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: ZN, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.40	0/5419	0.55	0/7396
1	B	0.40	0/6343	0.55	0/8661
1	C	0.40	0/6229	0.54	0/8502
All	All	0.40	0/17991	0.55	0/24559

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
3	A	1	0
All	All	1	2

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1005	MAN	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	736	CYS	Peptide
1	C	341	ALA	Peptide

## 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	5284	0	4868	52	0
1	B	6178	0	5791	96	0
1	C	6072	0	5618	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	50	0	43	1	0
4	B	28	0	26	0	0
4	C	28	0	26	0	0
5	A	8	0	0	0	0
5	B	19	0	0	1	0
5	C	12	0	0	0	0
All	All	17682	0	16372	240	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 7.

All (240) 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:410:VAL:HG11	1:A:436:VAL:HG21	1.50	0.94
1:B:624:LEU:CD1	1:B:660:LEU:HD21	1.98	0.93
1:C:341:ALA:HB3	1:C:725:ARG:CZ	2.09	0.82
1:C:107:LEU:HD11	1:C:145:TYR:HB3	1.62	0.80
1:C:410:VAL:HG11	1:C:436:VAL:HG21	1.63	0.79
1:B:624:LEU:HD13	1:B:660:LEU:HD21	1.64	0.78
1:B:609:ILE:HG23	1:B:642:ASN:OD1	1.86	0.75
1:A:609:ILE:HG23	1:A:642:ASN:OD1	1.88	0.74
1:C:770:ALA:O	1:C:773:ALA:HB3	1.88	0.73
1:A:640:ILE:HD11	1:A:663:TYR:HE2	1.52	0.73
1:B:261:THR:HG22	1:B:287:VAL:HG13	1.71	0.72
1:B:677:LEU:HD21	1:B:707:LEU:CD1	2.19	0.72
1:B:345:LEU:HA	1:B:394:LEU:HD13	1.71	0.72
1:A:410:VAL:CG1	1:A:436:VAL:HG21	2.20	0.72
1:B:853:LEU:HD23	1:B:853:LEU:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:ARG:CB	1:C:692:MET:HE2	2.20	0.71
1:B:410:VAL:HG11	1:B:436:VAL:HG21	1.72	0.70
1:C:405:PHE:CD2	1:C:675:GLN:NE2	2.60	0.70
1:B:196:GLU:OE1	5:B:960:HOH:O	2.09	0.68
1:A:140:LEU:HD12	1:A:143:LEU:HD22	1.75	0.68
1:B:345:LEU:HD11	1:B:396:VAL:HG12	1.76	0.68
1:C:624:LEU:CD1	1:C:660:LEU:HD21	2.23	0.67
1:A:261:THR:HG22	1:A:287:VAL:HG13	1.75	0.67
1:B:704:ILE:HD11	1:B:738:HIS:HB2	1.77	0.67
1:B:640:ILE:HD11	1:B:663:TYR:HE2	1.60	0.65
1:C:410:VAL:CG1	1:C:436:VAL:HG21	2.28	0.64
1:B:219:MET:HG2	1:B:239:THR:HG22	1.81	0.63
1:B:677:LEU:HD21	1:B:707:LEU:HD11	1.80	0.62
1:B:182:PHE:HA	1:B:186:ALA:HB3	1.82	0.62
1:C:782:TRP:CE2	1:C:805:LEU:HD22	2.35	0.62
1:A:716:TRP:CZ3	1:A:732:LEU:HD13	2.34	0.62
1:C:725:ARG:HG3	1:C:766:ASP:OD2	2.00	0.61
1:B:102:ILE:HD11	1:B:131:ILE:HD13	1.81	0.61
1:B:570:ILE:HG23	1:B:602:VAL:HG21	1.81	0.61
1:A:640:ILE:HD11	1:A:663:TYR:CE2	2.34	0.60
1:A:609:ILE:HG23	1:A:642:ASN:CG	2.22	0.60
1:B:604:MET:HG3	1:B:638:SER:HB2	1.82	0.60
1:B:737:VAL:HG11	1:B:807:ARG:NH2	2.16	0.60
1:B:140:LEU:HD12	1:B:143:LEU:HD22	1.83	0.60
1:A:219:MET:HG2	1:A:239:THR:HG22	1.82	0.60
1:C:261:THR:HG22	1:C:287:VAL:HG13	1.83	0.59
1:C:182:PHE:HA	1:C:186:ALA:HB3	1.84	0.59
1:A:743:CYS:O	1:A:747:ALA:CB	2.50	0.59
1:B:853:LEU:C	1:B:853:LEU:HD23	2.24	0.58
1:C:624:LEU:HD13	1:C:660:LEU:HD21	1.86	0.58
1:C:690:ARG:HG3	1:C:692:MET:HE2	1.86	0.57
1:C:140:LEU:HD12	1:C:143:LEU:HD22	1.85	0.57
1:A:461:ILE:HD13	1:A:478:LEU:HD11	1.86	0.57
1:C:740:TYR:O	1:C:744:VAL:HG23	2.04	0.57
1:B:590:ILE:N	1:B:590:ILE:HD12	2.20	0.57
1:B:321:ASN:HB2	1:B:324:LEU:O	2.04	0.57
1:C:888:LEU:HD21	1:C:915:ILE:HG22	1.86	0.56
1:C:341:ALA:HB3	1:C:725:ARG:NH2	2.21	0.56
1:C:647:VAL:HG11	1:C:654:ILE:HD13	1.86	0.56
1:C:405:PHE:CE2	1:C:675:GLN:NE2	2.73	0.56
1:A:549:TYR:CE2	1:A:649:ILE:HD13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:LYS:HD3	1:A:595:VAL:HG12	1.87	0.56
1:C:690:ARG:CG	1:C:692:MET:HE2	2.36	0.55
1:C:888:LEU:HD21	1:C:915:ILE:CG2	2.37	0.55
1:B:107:LEU:HB2	1:B:120:LEU:HD21	1.87	0.55
1:B:883:SER:OG	1:B:922:MET:HG3	2.06	0.55
1:C:690:ARG:HB2	1:C:692:MET:HE2	1.87	0.55
1:A:624:LEU:CD1	1:A:660:LEU:HD21	2.36	0.55
1:B:879:THR:HG22	1:B:882:PHE:HE2	1.71	0.55
1:A:182:PHE:HA	1:A:186:ALA:HB3	1.89	0.55
1:C:782:TRP:CD2	1:C:805:LEU:HD22	2.41	0.55
1:C:219:MET:HG2	1:C:239:THR:HG22	1.87	0.55
1:A:178:ALA:HB3	1:A:251:ILE:HB	1.89	0.55
1:A:107:LEU:HD11	1:A:145:TYR:HB3	1.88	0.54
1:C:349:MET:SD	1:C:396:VAL:HG23	2.46	0.54
1:B:624:LEU:HD12	1:B:660:LEU:HD21	1.86	0.53
1:C:710:LEU:HG	1:C:731:LEU:HD11	1.91	0.53
1:C:704:ILE:HD11	1:C:738:HIS:ND1	2.24	0.53
1:C:106:THR:HG22	1:C:119:PRO:HA	1.91	0.53
1:C:883:SER:CB	1:C:922:MET:HG3	2.39	0.52
1:C:692:MET:SD	1:C:926:PHE:CE1	3.03	0.52
1:C:808:THR:O	1:C:814:LEU:HD11	2.09	0.52
1:C:401:PHE:CG	1:C:604:MET:HE3	2.44	0.52
1:B:133:LEU:HD11	1:B:149:ILE:HD11	1.91	0.52
1:B:647:VAL:HG11	1:B:654:ILE:HD12	1.92	0.52
1:B:604:MET:HE2	1:B:634:ASN:O	2.10	0.51
1:C:590:ILE:HD12	1:C:590:ILE:N	2.25	0.51
1:C:345:LEU:HA	1:C:394:LEU:HD13	1.92	0.51
1:A:321:ASN:HB2	1:A:324:LEU:O	2.11	0.51
1:A:571:THR:HG22	1:A:598:ILE:HG13	1.91	0.51
1:C:699:PHE:HA	1:C:933:LEU:HD21	1.92	0.51
1:C:405:PHE:CE2	1:C:604:MET:SD	3.03	0.51
1:B:640:ILE:HD11	1:B:663:TYR:CE2	2.44	0.51
1:B:886:THR:HG22	1:B:887:ARG:N	2.25	0.51
1:B:884:THR:O	1:B:919:ILE:HD11	2.10	0.51
1:C:710:LEU:HG	1:C:731:LEU:CD1	2.41	0.51
1:A:741:GLN:HB3	1:A:742:PRO:HD3	1.92	0.50
1:A:381:PHE:HZ	1:A:449:ARG:HD3	1.76	0.50
1:C:888:LEU:CD2	1:C:915:ILE:CG2	2.89	0.50
1:C:303:LEU:HD11	1:C:322:TRP:CG	2.46	0.50
1:C:133:LEU:HD11	1:C:149:ILE:HD11	1.93	0.50
1:B:410:VAL:CG1	1:B:436:VAL:HG21	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:640:ILE:HD11	1:C:663:TYR:HE2	1.76	0.50
1:C:581:LEU:HD23	1:C:583:LYS:HE3	1.93	0.50
1:B:345:LEU:CD1	1:B:396:VAL:HG12	2.40	0.50
1:A:743:CYS:O	1:A:747:ALA:HB2	2.10	0.50
1:A:590:ILE:N	1:A:590:ILE:HD12	2.26	0.50
1:A:250:ILE:HD12	1:A:324:LEU:HD11	1.93	0.50
1:A:448:LEU:HD21	1:A:482:MET:HG2	1.93	0.50
1:B:624:LEU:CD1	1:B:660:LEU:CD2	2.81	0.49
1:B:808:THR:HG23	1:B:814:LEU:HG	1.93	0.49
1:C:887:ARG:O	1:C:891:VAL:HG23	2.12	0.49
1:B:387:VAL:HB	1:B:396:VAL:HG11	1.95	0.49
1:B:919:ILE:HG22	1:B:920:GLY:N	2.27	0.49
1:B:667:GLU:OE2	1:B:669:GLU:N	2.41	0.49
1:A:347:ILE:O	1:A:351:VAL:HG23	2.13	0.49
1:B:782:TRP:HZ2	1:B:817:LEU:HD11	1.78	0.49
1:B:879:THR:OG1	1:B:911:THR:HG21	2.13	0.48
1:B:846:TYR:N	1:B:847:PRO:CD	2.76	0.48
1:C:692:MET:HE1	1:C:922:MET:HE2	1.95	0.48
1:C:837:THR:HG23	1:C:877:GLY:HA3	1.95	0.48
1:B:690:ARG:CD	1:B:884:THR:HG22	2.44	0.48
1:C:321:ASN:HB2	1:C:324:LEU:O	2.13	0.48
1:B:740:TYR:O	1:B:744:VAL:HG23	2.14	0.47
1:B:710:LEU:HD12	1:B:731:LEU:CD1	2.45	0.47
1:B:609:ILE:HG23	1:B:642:ASN:CG	2.34	0.47
1:C:658:LEU:HD11	1:C:929:ILE:HD13	1.97	0.47
1:B:348:THR:HG22	1:B:387:VAL:HG22	1.95	0.47
1:A:419:VAL:HG23	1:A:440:LYS:HD3	1.97	0.47
1:A:183:GLU:OE1	1:A:319:MET:SD	2.73	0.47
1:C:882:PHE:O	1:C:915:ILE:HG23	2.15	0.47
1:B:177:LEU:HD21	1:B:312:PRO:HG2	1.97	0.47
1:A:624:LEU:HD13	1:A:660:LEU:HD21	1.96	0.46
1:B:381:PHE:HZ	1:B:449:ARG:HD3	1.79	0.46
1:B:764:PRO:O	1:B:767:VAL:HG22	2.15	0.46
1:C:166:THR:HG22	1:C:176:ILE:HG12	1.97	0.46
1:C:549:TYR:CD2	1:C:609:ILE:HD12	2.50	0.46
1:B:879:THR:HG22	1:B:882:PHE:CE2	2.50	0.46
1:B:621:THR:HG23	1:B:660:LEU:HA	1.98	0.46
1:B:660:LEU:O	1:B:660:LEU:HD23	2.14	0.46
1:B:122:VAL:HG22	1:B:133:LEU:HD22	1.96	0.46
1:C:690:ARG:HG3	1:C:692:MET:CE	2.45	0.46
1:B:604:MET:CE	1:B:634:ASN:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:SER:OG	1:A:294:GLU:OE1	2.27	0.46
1:C:381:PHE:HZ	1:C:449:ARG:HD3	1.81	0.46
1:B:107:LEU:HD11	1:B:145:TYR:HB3	1.97	0.45
1:B:788:LYS:O	1:B:792:SER:CB	2.64	0.45
1:B:177:LEU:HD21	1:B:312:PRO:HD2	1.98	0.45
1:C:609:ILE:HG22	1:C:610:VAL:N	2.31	0.45
1:B:782:TRP:CE2	1:B:805:LEU:HD22	2.51	0.45
1:A:102:ILE:HD11	1:A:131:ILE:HD13	1.99	0.45
1:C:836:LEU:HD23	1:C:874:MET:CB	2.46	0.45
1:B:695:VAL:HG21	1:B:926:PHE:CE1	2.52	0.45
1:B:677:LEU:CD2	1:B:707:LEU:HD11	2.47	0.45
1:C:365:THR:HB	1:C:472:ASN:ND2	2.31	0.45
1:B:549:TYR:CD2	1:B:609:ILE:HD12	2.50	0.45
1:B:704:ILE:HD11	1:B:738:HIS:CB	2.46	0.45
1:B:250:ILE:HD12	1:B:324:LEU:HD11	1.97	0.45
1:C:654:ILE:HG12	1:C:929:ILE:HD11	1.99	0.44
1:A:535:ILE:HD12	1:A:600:PHE:CE1	2.52	0.44
1:C:925:ASN:O	1:C:926:PHE:C	2.56	0.44
1:A:716:TRP:CE3	1:A:732:LEU:HD13	2.52	0.44
1:C:373:TRP:CE3	1:C:419:VAL:HG11	2.52	0.44
1:B:636:ARG:NH1	1:B:667:GLU:OE1	2.50	0.44
1:C:169:THR:HG22	1:C:173:GLU:O	2.17	0.44
1:A:185:THR:HB	1:A:188:ARG:CZ	2.46	0.44
1:B:365:THR:O	1:B:472:ASN:HA	2.17	0.44
1:C:846:TYR:CD1	1:C:847:PRO:HD3	2.52	0.44
1:B:260:ILE:HG22	1:B:261:THR:O	2.18	0.44
1:C:888:LEU:CD2	1:C:915:ILE:HG21	2.48	0.43
1:C:168:ARG:CZ	1:C:174:LEU:HB2	2.48	0.43
1:C:405:PHE:CZ	1:C:604:MET:SD	3.12	0.43
1:B:655:GLU:OE2	1:B:928:LYS:HD3	2.18	0.43
1:C:888:LEU:HD23	1:C:915:ILE:HG21	2.00	0.43
1:C:178:ALA:HB3	1:C:251:ILE:HB	2.00	0.43
1:A:536:THR:O	1:A:543[B]:HIS:HB2	2.18	0.43
1:B:604:MET:CE	1:B:634:ASN:CB	2.97	0.43
1:C:449:ARG:HD2	1:C:457:PHE:CD2	2.53	0.43
1:B:387:VAL:CG1	1:B:396:VAL:HG11	2.48	0.43
1:C:185:THR:HB	1:C:188:ARG:CZ	2.48	0.43
1:B:102:ILE:HG23	1:B:149:ILE:HG23	2.01	0.43
1:B:624:LEU:HD12	1:B:660:LEU:CD2	2.47	0.42
1:B:925:ASN:O	1:B:929:ILE:HG13	2.18	0.42
1:A:177:LEU:HD21	1:A:312:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:TYR:CD1	1:B:700:LYS:HE2	2.54	0.42
1:B:604:MET:HE2	1:B:634:ASN:HB3	2.01	0.42
1:A:133:LEU:HD11	1:A:149:ILE:HD11	2.00	0.42
1:C:348:THR:HG22	1:C:387:VAL:HG22	2.01	0.42
1:C:690:ARG:O	1:C:692:MET:N	2.52	0.42
1:C:692:MET:CE	1:C:922:MET:HE2	2.49	0.42
1:B:303:LEU:HD11	1:B:322:TRP:CG	2.54	0.42
1:B:591:LEU:HD11	1:B:598:ILE:HD12	2.01	0.42
1:B:82:VAL:HG13	1:B:147:VAL:HB	2.02	0.42
1:C:570:ILE:HG23	1:C:602:VAL:HG21	2.01	0.42
1:B:813:LYS:O	1:B:816:TRP:HB3	2.18	0.42
1:A:140:LEU:HD12	1:A:143:LEU:CD2	2.46	0.42
1:C:373:TRP:CD2	1:C:419:VAL:CG1	3.02	0.42
1:B:334:PHE:HB2	1:B:347:ILE:CD1	2.49	0.42
1:C:82:VAL:HG13	1:C:147:VAL:HB	2.01	0.42
1:C:310:ALA:HB2	1:C:332:LEU:HD23	2.00	0.42
3:A:1004:MAN:H61	3:A:1005:MAN:H2	1.75	0.42
1:C:747:ALA:HB1	1:C:774:VAL:HB	2.01	0.42
1:C:624:LEU:HD12	1:C:660:LEU:HD21	1.98	0.42
1:B:844:VAL:HG23	1:B:844:VAL:O	2.21	0.41
1:C:340:SER:O	1:C:342:SER:N	2.48	0.41
1:A:107:LEU:HB2	1:A:120:LEU:HD21	2.01	0.41
1:C:731:LEU:HD23	1:C:731:LEU:HA	1.92	0.41
1:C:303:LEU:HB3	1:C:304:PRO:HD2	2.02	0.41
1:B:185:THR:HB	1:B:188:ARG:CZ	2.50	0.41
1:B:364:VAL:HG21	1:B:465:LEU:HA	2.01	0.41
1:A:61:VAL:HG12	1:A:83:GLU:O	2.19	0.41
1:B:933:LEU:O	1:B:935:SER:N	2.54	0.41
1:B:282:ALA:HB1	1:B:332:LEU:CD1	2.50	0.41
1:A:647:VAL:HG21	1:A:657:ALA:CB	2.51	0.41
1:C:177:LEU:HD22	1:C:254:PHE:CZ	2.55	0.41
1:C:763:LEU:HA	1:C:763:LEU:HD23	1.88	0.41
1:C:341:ALA:HB3	1:C:725:ARG:NH1	2.35	0.41
1:B:282:ALA:HB1	1:B:332:LEU:HD11	2.02	0.41
1:C:670:ILE:CG1	1:C:674:PHE:CE2	3.03	0.41
1:B:449:ARG:O	1:B:452:LEU:O	2.38	0.41
1:C:177:LEU:HD22	1:C:254:PHE:CE1	2.56	0.41
1:B:123:LEU:HB2	1:B:132:ALA:HB3	2.02	0.41
1:A:421:THR:HG22	1:A:422:PRO:O	2.21	0.41
1:B:342:SER:HB3	1:B:722:VAL:HG22	2.03	0.41
1:A:260:ILE:HG22	1:A:261:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:MET:HE1	1:C:589:LEU:HD23	2.02	0.41
1:B:178:ALA:HB3	1:B:251:ILE:HB	2.03	0.41
1:B:64:ASP:HB3	1:B:81:LYS:HB2	2.03	0.41
1:A:169:THR:HG22	1:A:173:GLU:O	2.21	0.41
1:A:162:PHE:CE1	1:A:178:ALA:HB1	2.55	0.41
1:A:95:LEU:HD11	1:A:131:ILE:HD11	2.03	0.41
1:B:303:LEU:HB3	1:B:304:PRO:HD2	2.03	0.41
1:C:670:ILE:HG12	1:C:674:PHE:CD2	2.56	0.41
1:A:717:THR:O	1:A:728:ARG:NE	2.54	0.41
1:B:624:LEU:HD13	1:B:660:LEU:CD2	2.43	0.40
1:A:140:LEU:HB2	1:A:143:LEU:HD22	2.03	0.40
1:B:549:TYR:CE2	1:B:609:ILE:HD12	2.57	0.40
1:C:710:LEU:CD2	1:C:731:LEU:HD11	2.51	0.40
1:C:640:ILE:HD11	1:C:663:TYR:CE2	2.56	0.40
1:C:609:ILE:HG23	1:C:642:ASN:OD1	2.21	0.40
1:A:647:VAL:HG21	1:A:657:ALA:HB2	2.01	0.40
1:B:731:LEU:HA	1:B:731:LEU:HD23	1.94	0.40
1:C:670:ILE:HD11	1:C:674:PHE:CE2	2.57	0.40
1:A:259:LYS:HD3	1:A:287:VAL:HG21	2.03	0.40
1:A:660:LEU:HD23	1:A:660:LEU:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	683/954 (72%)	642 (94%)	40 (6%)	1 (0%)	56 90
1	B	788/954 (83%)	741 (94%)	46 (6%)	1 (0%)	56 90
1	C	786/954 (82%)	736 (94%)	46 (6%)	4 (0%)	34 76
All	All	2257/2862 (79%)	2119 (94%)	132 (6%)	6 (0%)	46 84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	LYS
1	C	691	ASP
1	C	341	ALA
1	C	312	PRO
1	A	312	PRO
1	B	312	PRO

### 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	515/851 (60%)	497 (96%)	18 (4%)	43	80
1	B	623/851 (73%)	602 (97%)	21 (3%)	44	81
1	C	591/851 (69%)	576 (98%)	15 (2%)	55	86
All	All	1729/2553 (68%)	1675 (97%)	54 (3%)	47	83

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	92	THR
1	A	160	HIS
1	A	214	LEU
1	A	253	ASP
1	A	263	SER
1	A	305	LYS
1	A	330	SER
1	A	342	SER
1	A	374	LEU
1	A	463	GLN
1	A	588	VAL
1	A	593	GLU
1	A	633	SER
1	A	663	TYR

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Mol	Chain	Res	Type
1	A	702	PHE
1	A	707	LEU
1	A	743	CYS
1	B	59	ILE
1	B	71	LEU
1	B	75	THR
1	B	160	HIS
1	B	214	LEU
1	B	253	ASP
1	B	305	LYS
1	B	330	SER
1	B	340	SER
1	B	538	ARG
1	B	573	LYS
1	B	588	VAL
1	B	633	SER
1	B	654	ILE
1	B	663	TYR
1	B	702	PHE
1	B	710	LEU
1	B	721	SER
1	B	779	THR
1	B	787	SER
1	B	886	THR
1	C	75	THR
1	C	160	HIS
1	C	214	LEU
1	C	253	ASP
1	C	305	LYS
1	C	330	SER
1	C	538[A]	ARG
1	C	538[B]	ARG
1	C	588	VAL
1	C	633	SER
1	C	663	TYR
1	C	702	PHE
1	C	779	THR
1	C	837	THR
1	C	929	ILE

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

### 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 ⓘ

4 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$
3	NAG	A	1001	1,3	14,14,15	0.53	0	15,19,21	0.93	0
3	NAG	A	1002	3	14,14,15	0.50	0	15,19,21	1.50	2 (13%)
3	MAN	A	1004	3	11,11,12	0.71	0	14,15,17	1.30	1 (7%)
3	MAN	A	1005	3	11,11,12	0.62	0	14,15,17	2.11	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3	-	0/6/23/26	0/1/1/1
3	MAN	A	1004	3	-	0/2/19/22	1/1/1/1
3	MAN	A	1005	3	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAG	O4-C4-C3	-2.88	103.85	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	MAN	O6-C6-C5	-2.19	104.09	111.33
3	A	1005	MAN	O2-C2-C1	2.10	113.41	109.21
3	A	1005	MAN	O5-C5-C6	2.61	113.00	107.35
3	A	1005	MAN	C3-C4-C5	3.15	115.69	110.20
3	A	1002	NAG	C1-O5-C5	3.94	117.24	112.25
3	A	1005	MAN	C1-O5-C5	5.93	119.78	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1005	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	MAN	1	0
3	A	1005	MAN	1	0

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	1070	1	14,14,15	0.40	0	15,19,21	0.73	0
4	NAG	B	1154	1	14,14,15	0.65	0	15,19,21	0.95	1 (6%)
4	NAG	C	1070	1	14,14,15	0.44	0	15,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1154	1	14,14,15	0.80	1 (7%)	15,19,21	2.00	5 (33%)

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	B	1070	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1154	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	1070	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1154	1	1/1/5/7	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)
4	C	1154	NAG	C1-C2	2.14	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1154	NAG	O7-C7-C8	-2.17	118.07	122.06
4	C	1154	NAG	O7-C7-N2	2.01	125.95	121.86
4	C	1154	NAG	C4-C3-C2	2.12	114.52	111.23
4	B	1154	NAG	C1-O5-C5	2.38	115.27	112.25
4	C	1154	NAG	C2-N2-C7	3.77	127.88	123.04
4	C	1154	NAG	C1-O5-C5	5.06	118.67	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1154	NAG	C1
4	C	1154	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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<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	696/954 (72%)	-0.41	8 (1%) 82 58	19, 39, 78, 104	0
1	B	802/954 (84%)	-0.51	3 (0%) 93 80	19, 40, 69, 104	0
1	C	800/954 (83%)	-0.42	5 (0%) 90 73	19, 41, 73, 103	0
All	All	2298/2862 (80%)	-0.45	16 (0%) 89 70	19, 40, 74, 104	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	GLY	3.1
1	B	425	ASN	2.8
1	A	169	THR	2.7
1	A	806	CYS	2.7
1	A	434	ASP	2.7
1	C	758	ASN	2.6
1	A	915	ILE	2.4
1	A	805	LEU	2.4
1	A	171	GLU	2.3
1	C	793	LEU	2.3
1	A	804	ALA	2.2
1	C	229	GLU	2.2
1	C	422	PRO	2.1
1	B	793	LEU	2.1
1	B	792	SER	2.0
1	C	762	SER	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 ⓘ

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
3	MAN	A	1005	11/12	0.83	0.35	3.36	66,77,89,92	0
3	NAG	A	1001	14/15	0.96	0.19	-0.22	14,37,46,50	0
3	MAN	A	1004	11/12	0.94	0.20	-	35,45,58,61	0
3	NAG	A	1002	14/15	0.96	0.36	-	30,46,55,64	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, 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
4	NAG	C	1070	14/15	0.90	0.28	2.09	80,88,97,103	0
4	NAG	B	1070	14/15	0.88	0.24	0.89	37,72,96,97	0
2	ZN	A	5000	1/1	0.99	0.04	-3.82	26,26,26,26	0
2	ZN	B	5000	1/1	0.99	0.03	-4.04	25,25,25,25	0
2	ZN	C	5000	1/1	0.99	0.02	-4.19	31,31,31,31	0
4	NAG	C	1154	14/15	0.76	0.38	-	98,107,107,110	0
4	NAG	B	1154	14/15	0.64	0.39	-	80,94,104,105	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.