



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:06 PM GMT

PDB ID : 4WSG  
Title : Crystal Structure of Soluble WR PIV5 F-GCNt  
Authors : Poor, T.A.; Song, A.S.; Welch, B.D.; Kors, C.A.; Jardetzky, T.S.; Lamb, R.A.  
Deposited on : 2014-10-27  
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

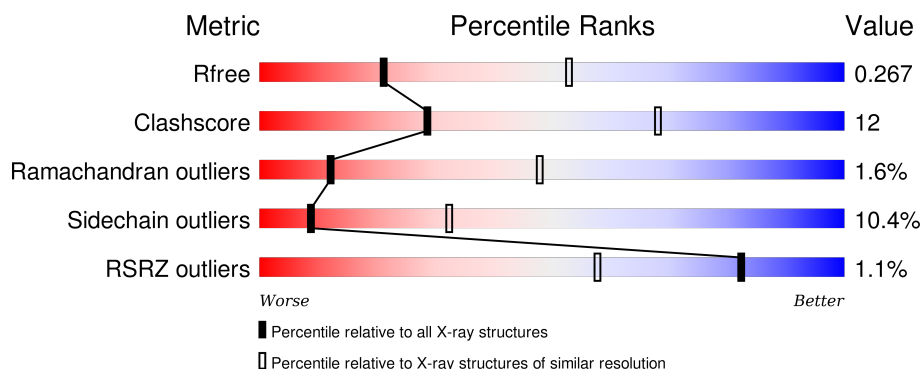
# 1 Overall quality at a glance

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	497	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>.</div> <div>.</div> </div> </div>
1	B	497	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>.</div> <div>.</div> </div> </div>
1	C	497	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>.</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10735 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3567	2258	593	695	21			
1	B	477	Total	C	N	O	S	0	0	0
			3532	2236	584	691	21			
1	C	479	Total	C	N	O	S	0	0	0
			3580	2272	591	696	21			

There are 129 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP Q9YZA2
A	?	-	ARG	deletion	UNP Q9YZA2
A	478	GLU	-	expression tag	UNP Q9YZA2
A	479	ASP	-	expression tag	UNP Q9YZA2
A	480	LYS	-	expression tag	UNP Q9YZA2
A	481	ILE	-	expression tag	UNP Q9YZA2
A	482	GLU	-	expression tag	UNP Q9YZA2
A	483	GLU	-	expression tag	UNP Q9YZA2
A	484	ILE	-	expression tag	UNP Q9YZA2
A	485	LEU	-	expression tag	UNP Q9YZA2
A	486	SER	-	expression tag	UNP Q9YZA2
A	487	LYS	-	expression tag	UNP Q9YZA2
A	488	ILE	-	expression tag	UNP Q9YZA2
A	489	TYR	-	expression tag	UNP Q9YZA2
A	490	HIS	-	expression tag	UNP Q9YZA2
A	491	ILE	-	expression tag	UNP Q9YZA2
A	492	GLU	-	expression tag	UNP Q9YZA2
A	493	ASN	-	expression tag	UNP Q9YZA2
A	494	GLU	-	expression tag	UNP Q9YZA2
A	495	ILE	-	expression tag	UNP Q9YZA2
A	496	ALA	-	expression tag	UNP Q9YZA2
A	497	ARG	-	expression tag	UNP Q9YZA2
A	498	ILE	-	expression tag	UNP Q9YZA2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	499	LYS	-	expression tag	UNP Q9YZA2
A	500	LYS	-	expression tag	UNP Q9YZA2
A	501	LEU	-	expression tag	UNP Q9YZA2
A	502	ILE	-	expression tag	UNP Q9YZA2
A	503	GLY	-	expression tag	UNP Q9YZA2
A	504	GLU	-	expression tag	UNP Q9YZA2
A	505	ALA	-	expression tag	UNP Q9YZA2
A	506	PRO	-	expression tag	UNP Q9YZA2
A	507	GLY	-	expression tag	UNP Q9YZA2
A	508	GLY	-	expression tag	UNP Q9YZA2
A	509	ILE	-	expression tag	UNP Q9YZA2
A	510	GLU	-	expression tag	UNP Q9YZA2
A	511	GLY	-	expression tag	UNP Q9YZA2
A	512	ARG	-	expression tag	UNP Q9YZA2
A	513	HIS	-	expression tag	UNP Q9YZA2
A	514	HIS	-	expression tag	UNP Q9YZA2
A	515	HIS	-	expression tag	UNP Q9YZA2
A	516	HIS	-	expression tag	UNP Q9YZA2
A	517	HIS	-	expression tag	UNP Q9YZA2
A	518	HIS	-	expression tag	UNP Q9YZA2
B	?	-	ARG	deletion	UNP Q9YZA2
B	?	-	ARG	deletion	UNP Q9YZA2
B	478	GLU	-	expression tag	UNP Q9YZA2
B	479	ASP	-	expression tag	UNP Q9YZA2
B	480	LYS	-	expression tag	UNP Q9YZA2
B	481	ILE	-	expression tag	UNP Q9YZA2
B	482	GLU	-	expression tag	UNP Q9YZA2
B	483	GLU	-	expression tag	UNP Q9YZA2
B	484	ILE	-	expression tag	UNP Q9YZA2
B	485	LEU	-	expression tag	UNP Q9YZA2
B	486	SER	-	expression tag	UNP Q9YZA2
B	487	LYS	-	expression tag	UNP Q9YZA2
B	488	ILE	-	expression tag	UNP Q9YZA2
B	489	TYR	-	expression tag	UNP Q9YZA2
B	490	HIS	-	expression tag	UNP Q9YZA2
B	491	ILE	-	expression tag	UNP Q9YZA2
B	492	GLU	-	expression tag	UNP Q9YZA2
B	493	ASN	-	expression tag	UNP Q9YZA2
B	494	GLU	-	expression tag	UNP Q9YZA2
B	495	ILE	-	expression tag	UNP Q9YZA2
B	496	ALA	-	expression tag	UNP Q9YZA2
B	497	ARG	-	expression tag	UNP Q9YZA2

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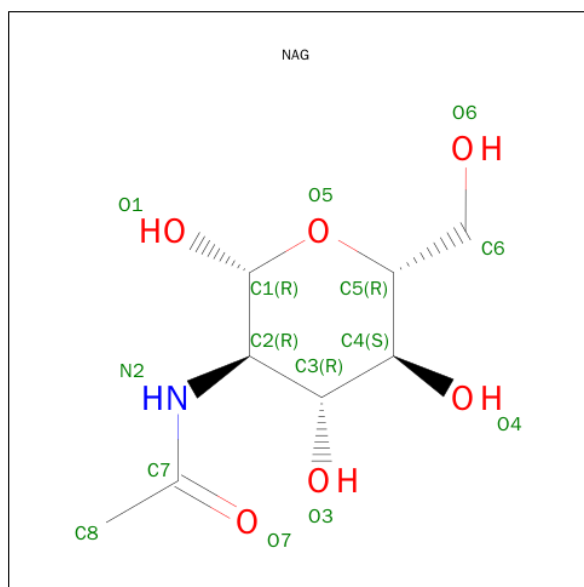
Chain	Residue	Modelled	Actual	Comment	Reference
B	498	ILE	-	expression tag	UNP Q9YZA2
B	499	LYS	-	expression tag	UNP Q9YZA2
B	500	LYS	-	expression tag	UNP Q9YZA2
B	501	LEU	-	expression tag	UNP Q9YZA2
B	502	ILE	-	expression tag	UNP Q9YZA2
B	503	GLY	-	expression tag	UNP Q9YZA2
B	504	GLU	-	expression tag	UNP Q9YZA2
B	505	ALA	-	expression tag	UNP Q9YZA2
B	506	PRO	-	expression tag	UNP Q9YZA2
B	507	GLY	-	expression tag	UNP Q9YZA2
B	508	GLY	-	expression tag	UNP Q9YZA2
B	509	ILE	-	expression tag	UNP Q9YZA2
B	510	GLU	-	expression tag	UNP Q9YZA2
B	511	GLY	-	expression tag	UNP Q9YZA2
B	512	ARG	-	expression tag	UNP Q9YZA2
B	513	HIS	-	expression tag	UNP Q9YZA2
B	514	HIS	-	expression tag	UNP Q9YZA2
B	515	HIS	-	expression tag	UNP Q9YZA2
B	516	HIS	-	expression tag	UNP Q9YZA2
B	517	HIS	-	expression tag	UNP Q9YZA2
B	518	HIS	-	expression tag	UNP Q9YZA2
C	?	-	ARG	deletion	UNP Q9YZA2
C	?	-	ARG	deletion	UNP Q9YZA2
C	478	GLU	-	expression tag	UNP Q9YZA2
C	479	ASP	-	expression tag	UNP Q9YZA2
C	480	LYS	-	expression tag	UNP Q9YZA2
C	481	ILE	-	expression tag	UNP Q9YZA2
C	482	GLU	-	expression tag	UNP Q9YZA2
C	483	GLU	-	expression tag	UNP Q9YZA2
C	484	ILE	-	expression tag	UNP Q9YZA2
C	485	LEU	-	expression tag	UNP Q9YZA2
C	486	SER	-	expression tag	UNP Q9YZA2
C	487	LYS	-	expression tag	UNP Q9YZA2
C	488	ILE	-	expression tag	UNP Q9YZA2
C	489	TYR	-	expression tag	UNP Q9YZA2
C	490	HIS	-	expression tag	UNP Q9YZA2
C	491	ILE	-	expression tag	UNP Q9YZA2
C	492	GLU	-	expression tag	UNP Q9YZA2
C	493	ASN	-	expression tag	UNP Q9YZA2
C	494	GLU	-	expression tag	UNP Q9YZA2
C	495	ILE	-	expression tag	UNP Q9YZA2
C	496	ALA	-	expression tag	UNP Q9YZA2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	497	ARG	-	expression tag	UNP Q9YZA2
C	498	ILE	-	expression tag	UNP Q9YZA2
C	499	LYS	-	expression tag	UNP Q9YZA2
C	500	LYS	-	expression tag	UNP Q9YZA2
C	501	LEU	-	expression tag	UNP Q9YZA2
C	502	ILE	-	expression tag	UNP Q9YZA2
C	503	GLY	-	expression tag	UNP Q9YZA2
C	504	GLU	-	expression tag	UNP Q9YZA2
C	505	ALA	-	expression tag	UNP Q9YZA2
C	506	PRO	-	expression tag	UNP Q9YZA2
C	507	GLY	-	expression tag	UNP Q9YZA2
C	508	GLY	-	expression tag	UNP Q9YZA2
C	509	ILE	-	expression tag	UNP Q9YZA2
C	510	GLU	-	expression tag	UNP Q9YZA2
C	511	GLY	-	expression tag	UNP Q9YZA2
C	512	ARG	-	expression tag	UNP Q9YZA2
C	513	HIS	-	expression tag	UNP Q9YZA2
C	514	HIS	-	expression tag	UNP Q9YZA2
C	515	HIS	-	expression tag	UNP Q9YZA2
C	516	HIS	-	expression tag	UNP Q9YZA2
C	517	HIS	-	expression tag	UNP Q9YZA2
C	518	HIS	-	expression tag	UNP Q9YZA2

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

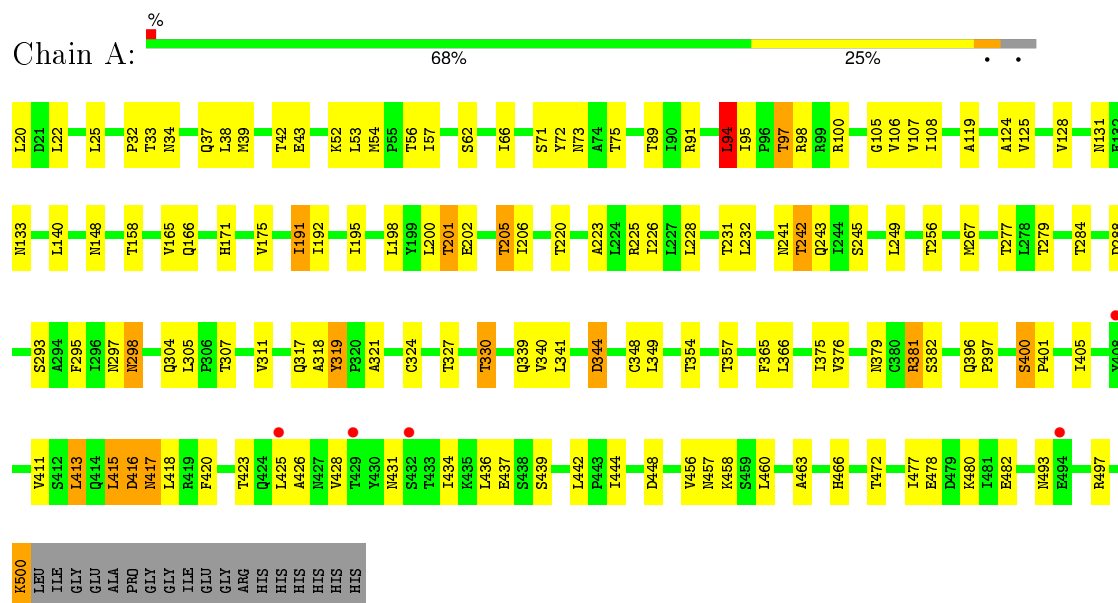


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

### 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.

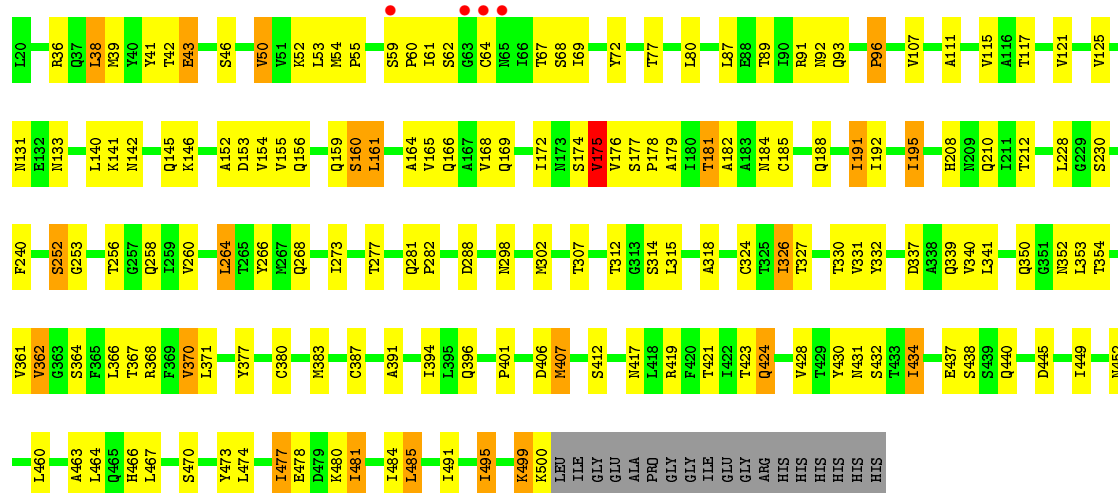
#### • Molecule 1: Fusion glycoprotein F0



#### • Molecule 1: Fusion glycoprotein F0



● Molecule 1: Fusion glycoprotein F0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.53Å 155.52Å 157.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.85 – 3.00 34.85 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.85-3.00) 88.5 (34.85-2.98)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 3.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.230 , 0.281 0.205 , 0.267	Depositor DCC
$R_{free}$ test set	1813 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.0	Xtriage
Anisotropy	0.973	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.4	EDS
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 40999 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/3611	0.64	3/4939 (0.1%)
1	B	0.42	0/3574	0.63	0/4889
1	C	0.45	0/3626	0.66	0/4957
All	All	0.44	0/10811	0.64	3/14785 (0.0%)

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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	LEU	CB-CG-CD2	-6.17	100.51	111.00
1	A	94	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	415	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	96	PRO	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	3567	0	3661	92	0
1	B	3532	0	3614	88	1
1	C	3580	0	3685	101	1
2	A	28	0	26	9	0
2	B	14	0	13	6	0
2	C	14	0	13	1	0
All	All	10735	0	11012	251	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (251) 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:457:ASN:HD21	2:A:602:NAG:C1	1.04	1.67
1:B:73:ASN:HD21	2:B:601:NAG:C1	0.96	1.58
1:A:73:ASN:HD21	2:A:601:NAG:C1	1.28	1.47
1:A:457:ASN:ND2	2:A:602:NAG:C1	1.81	1.41
1:B:73:ASN:ND2	2:B:601:NAG:C1	1.74	1.41
1:A:73:ASN:ND2	2:A:601:NAG:C1	1.97	1.24
1:B:166:GLN:HG3	1:B:169:GLN:HB2	1.52	0.92
1:B:52:LYS:HB3	1:B:166:GLN:HB2	1.52	0.90
1:B:73:ASN:HD21	2:B:601:NAG:C2	1.83	0.90
1:B:368:ARG:HD3	1:B:383:MET:HB2	1.54	0.89
1:A:457:ASN:CG	2:A:602:NAG:C1	2.45	0.85
1:B:275:LEU:HD12	1:B:276:PRO:HD2	1.63	0.80
1:B:52:LYS:O	1:B:166:GLN:NE2	2.15	0.79
1:C:430:TYR:HB3	1:C:431:ASN:HA	1.66	0.78
1:B:180:ILE:HA	1:B:184:ASN:HD22	1.51	0.76
1:A:94:LEU:HD12	1:A:95:ILE:H	1.51	0.76
1:C:353:LEU:HD12	1:C:434:ILE:HG21	1.69	0.75
1:A:97:THR:O	1:A:98:ARG:NH1	2.21	0.73
1:A:480:LYS:HD3	1:C:481:ILE:HD11	1.71	0.73
1:B:219:ILE:HD11	1:B:259:ILE:HG13	1.69	0.72
1:C:302:MET:HG3	1:C:361:VAL:HG11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ALA:HB1	1:A:324:CYS:HB2	1.73	0.70
1:B:73:ASN:CG	2:B:601:NAG:C1	2.58	0.70
1:C:168:VAL:HB	1:C:195:ILE:HD11	1.73	0.69
1:A:420:PHE:HA	1:B:107:VAL:H	1.58	0.69
1:A:365:PHE:HD2	1:A:366:LEU:HD23	1.58	0.68
1:A:437:GLU:HG3	1:A:439:SER:H	1.59	0.68
1:C:176:VAL:HA	1:C:188:GLN:HE22	1.58	0.68
1:C:176:VAL:HA	1:C:188:GLN:NE2	2.10	0.66
1:B:91:ARG:NH2	1:B:260:VAL:O	2.29	0.65
1:B:42:THR:HG22	1:B:43:GLU:HG3	1.79	0.65
1:A:53:LEU:HB2	1:A:267:MET:HB3	1.78	0.64
1:A:43:GLU:O	1:A:277:THR:OG1	2.15	0.64
1:B:165:VAL:HG21	1:B:228:LEU:HG	1.79	0.64
1:C:155:VAL:HG22	1:C:160:SER:HA	1.80	0.63
1:A:37:GLN:NE2	1:A:284:THR:O	2.32	0.63
1:B:491:ILE:HD11	1:C:491:ILE:HG21	1.81	0.63
1:C:318:ALA:HB3	1:C:339:GLN:HB2	1.79	0.62
1:C:177:SER:H	1:C:188:GLN:HE22	1.48	0.62
1:A:460:LEU:HD12	1:C:460:LEU:HD13	1.80	0.62
1:A:457:ASN:OD1	2:A:602:NAG:C1	2.47	0.62
1:A:477:ILE:HD11	1:C:478:GLU:HG3	1.82	0.62
1:A:344:ASP:OD2	1:A:344:ASP:N	2.34	0.61
1:A:107:VAL:HG21	1:A:125:VAL:HG22	1.83	0.61
1:C:165:VAL:HG21	1:C:228:LEU:HD22	1.82	0.60
1:A:128:VAL:O	1:A:131:ASN:HB2	2.01	0.60
1:C:89:THR:HG23	1:C:93:GLN:HE21	1.66	0.60
1:C:477:ILE:O	1:C:481:ILE:HG23	2.00	0.60
1:A:52:LYS:HB2	1:A:166:GLN:HG2	1.83	0.59
1:B:96:PRO:HD3	1:B:128:VAL:HG22	1.84	0.59
1:A:477:ILE:HD13	1:C:477:ILE:HD11	1.84	0.59
1:C:166:GLN:HB3	1:C:169:GLN:HB2	1.83	0.59
1:B:281:GLN:OE1	1:B:282:PRO:HD2	2.02	0.59
1:A:297:ASN:ND2	1:A:297:ASN:O	2.36	0.59
1:A:463:ALA:HB2	1:C:464:LEU:HD21	1.85	0.58
1:C:430:TYR:CB	1:C:431:ASN:HA	2.30	0.58
1:A:416:ASP:OD1	1:A:416:ASP:N	2.36	0.58
1:B:467:LEU:HD21	1:C:467:LEU:HB3	1.85	0.58
1:C:364:SER:H	1:C:367:THR:CG2	2.16	0.58
1:C:68:SER:OG	1:C:69:ILE:N	2.37	0.58
1:A:405:ILE:HG21	1:A:413:LEU:HD11	1.85	0.58
1:A:434:ILE:HG22	1:A:436:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD12	1:A:39:MET:H	1.70	0.57
1:C:368:ARG:HD3	1:C:383:MET:HB2	1.86	0.57
1:A:97:THR:HG23	1:A:98:ARG:H	1.68	0.57
1:A:317:GLN:HE22	1:C:362:VAL:HG11	1.70	0.57
1:B:297:ASN:ND2	1:B:297:ASN:O	2.38	0.57
1:B:371:LEU:HD13	1:C:121:VAL:HG21	1.87	0.56
1:C:152:ALA:HB3	1:C:164:ALA:HB3	1.88	0.56
1:A:175:VAL:HB	1:A:191:ILE:HD11	1.86	0.56
1:A:25:LEU:HD11	1:A:349:LEU:HA	1.87	0.56
1:C:140:LEU:HD11	1:C:156:GLN:OE1	2.06	0.56
1:A:318:ALA:HB3	1:A:339:GLN:HB2	1.88	0.55
1:A:71:SER:OG	1:A:72:TYR:N	2.40	0.55
1:A:165:VAL:HG21	1:A:228:LEU:HD22	1.89	0.55
1:B:326:ILE:HG12	1:B:331:VAL:HG22	1.87	0.55
1:C:177:SER:O	1:C:179:ALA:N	2.40	0.54
1:A:376:VAL:HB	1:A:405:ILE:HB	1.90	0.54
1:A:94:LEU:CD1	1:A:95:ILE:H	2.18	0.54
1:C:77:THR:HG23	1:C:264:LEU:HB3	1.90	0.54
1:B:252:SER:HB3	1:C:208:HIS:HE1	1.73	0.54
1:C:92:ASN:O	1:C:96:PRO:HB3	2.08	0.53
1:C:326:ILE:HG23	1:C:331:VAL:HG22	1.90	0.53
1:C:364:SER:H	1:C:367:THR:HG22	1.72	0.53
1:A:37:GLN:HE21	1:A:38:LEU:H	1.57	0.53
1:C:407:MET:HG3	1:C:423:THR:HA	1.90	0.53
1:B:480:LYS:O	1:B:484:ILE:HG12	2.09	0.53
1:A:457:ASN:ND2	2:A:602:NAG:O5	2.17	0.53
1:B:39:MET:HB3	1:B:278:LEU:HB3	1.90	0.53
1:A:75:THR:HG22	1:A:200:LEU:HD11	1.91	0.52
1:B:494:GLU:O	1:B:495:ILE:HB	2.09	0.52
1:A:119:ALA:HB2	1:C:366:LEU:HD22	1.92	0.52
1:C:43:GLU:O	1:C:277:THR:OG1	2.22	0.52
1:C:166:GLN:OE1	1:C:168:VAL:N	2.43	0.51
1:B:140:LEU:O	1:B:144:ILE:HG13	2.10	0.51
1:C:281:GLN:HG3	1:C:282:PRO:HD2	1.93	0.51
1:C:437:GLU:O	1:C:440:GLN:HB2	2.10	0.51
1:A:94:LEU:HD22	1:A:128:VAL:HG13	1.91	0.51
1:B:487:LYS:O	1:B:491:ILE:HG23	2.10	0.51
1:A:478:GLU:O	1:A:482:GLU:HG2	2.11	0.51
1:A:379:ASN:ND2	1:A:382:SER:HB2	2.26	0.51
1:A:52:LYS:CB	1:A:166:GLN:HG2	2.41	0.50
1:C:42:THR:O	1:C:43:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PRO:HD2	1:B:178:PRO:O	2.12	0.50
1:B:153:ASP:OD2	1:B:155:VAL:HG13	2.12	0.50
1:A:420:PHE:HB3	1:B:107:VAL:HG12	1.94	0.50
1:A:477:ILE:HG21	1:C:477:ILE:HD11	1.93	0.49
1:C:324:CYS:HB3	1:C:332:TYR:O	2.11	0.49
1:B:73:ASN:O	1:B:77:THR:OG1	2.23	0.49
1:A:397:PRO:HG2	1:A:400:SER:HB2	1.95	0.49
1:B:368:ARG:HB3	1:B:383:MET:HE2	1.95	0.49
1:C:153:ASP:OD1	1:C:154:VAL:N	2.46	0.48
1:C:327:THR:OG1	1:C:330:THR:HB	2.13	0.48
1:C:50:VAL:HG13	1:C:164:ALA:HA	1.94	0.48
1:B:252:SER:OG	1:B:254:LEU:HD12	2.13	0.48
1:B:67:THR:N	1:B:189:ASP:OD1	2.46	0.48
1:A:228:LEU:HB3	1:A:231:THR:OG1	2.13	0.48
1:A:242:THR:OG1	1:A:243:GLN:N	2.47	0.48
1:A:225:ARG:HG2	1:A:232:LEU:HD22	1.96	0.48
1:C:240:PHE:HZ	1:C:273:ILE:HG22	1.78	0.48
1:B:444:ILE:H	1:B:444:ILE:HD12	1.78	0.48
1:B:221:ILE:O	1:B:225:ARG:HG3	2.14	0.47
1:B:365:PHE:HD2	1:B:366:LEU:HD12	1.78	0.47
1:C:318:ALA:HB2	1:C:341:LEU:HD21	1.96	0.47
1:A:171:HIS:CE1	1:A:195:ILE:HG12	2.50	0.47
1:A:375:ILE:HD13	1:A:426:ALA:HB2	1.96	0.47
1:A:91:ARG:HA	1:A:94:LEU:CD2	2.45	0.47
1:A:39:MET:HG3	1:A:330:THR:HG23	1.94	0.47
1:A:171:HIS:ND1	1:A:195:ILE:HG12	2.28	0.47
1:A:318:ALA:HB2	1:A:341:LEU:HD21	1.96	0.47
1:B:72:TYR:CD1	1:B:196:LEU:HB3	2.49	0.47
1:A:198:LEU:O	1:A:201:THR:HG22	2.15	0.47
1:A:293:SER:O	1:A:379:ASN:HB2	2.15	0.47
1:C:315:LEU:HA	1:C:315:LEU:HD12	1.72	0.47
1:C:91:ARG:NH2	1:C:260:VAL:O	2.47	0.47
1:C:188:GLN:O	1:C:192:ILE:HG12	2.15	0.47
1:B:166:GLN:OE1	1:B:168:VAL:HG22	2.15	0.46
1:C:208:HIS:HD2	1:C:210:GLN:HG3	1.78	0.46
1:B:464:LEU:HD21	1:C:463:ALA:HB2	1.96	0.46
1:C:142:ASN:HA	1:C:266:TYR:HE2	1.80	0.46
1:A:418:LEU:HD11	1:B:125:VAL:HG21	1.97	0.46
1:B:390:PRO:O	1:B:392:ALA:N	2.48	0.46
1:A:381:ARG:HB2	1:A:396:GLN:HB3	1.98	0.46
1:A:108:ILE:HG12	1:C:421:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:HB2	1:B:82:PRO:HD3	1.98	0.46
1:A:33:THR:HA	1:B:115:VAL:HG11	1.97	0.46
1:C:352:ASN:OD1	1:C:354:THR:OG1	2.25	0.46
1:C:337:ASP:O	1:C:339:GLN:NE2	2.49	0.46
1:B:51:VAL:HG23	1:B:269:MET:HB3	1.97	0.46
1:B:495:ILE:HD11	1:C:495:ILE:HD11	1.97	0.45
1:C:417:ASN:OD1	1:C:417:ASN:N	2.47	0.45
1:A:416:ASP:HB2	1:A:417:ASN:H	1.51	0.45
1:A:97:THR:HG22	1:A:106:VAL:H	1.82	0.45
1:B:96:PRO:HB2	1:B:97:THR:HA	1.99	0.45
1:B:96:PRO:O	1:B:107:VAL:HA	2.16	0.45
1:B:453:LEU:HD21	1:C:452:ASN:HB3	1.98	0.45
1:A:304:GLN:OE1	1:A:444:ILE:HD13	2.17	0.45
1:A:66:ILE:HD13	1:A:192:ILE:HD12	1.99	0.45
1:C:380:CYS:N	1:C:396:GLN:OE1	2.50	0.45
1:B:485:LEU:HD11	1:C:484:ILE:HD11	1.99	0.45
1:C:38:LEU:HD23	1:C:281:GLN:HB3	1.99	0.45
1:C:59:SER:HA	1:C:60:PRO:HD3	1.73	0.45
1:B:90:ILE:O	1:B:94:LEU:HB2	2.16	0.45
1:A:460:LEU:HD21	1:B:459:SER:HB3	1.99	0.45
1:A:124:ALA:O	1:A:128:VAL:HG23	2.16	0.44
1:A:295:PHE:CE2	1:A:298:ASN:HA	2.53	0.44
1:A:202:GLU:HB3	1:A:226:ILE:HG23	1.97	0.44
1:A:357:THR:HG23	1:A:442:LEU:HD13	1.98	0.44
1:B:73:ASN:ND2	2:B:601:NAG:C2	2.61	0.44
1:B:78:LYS:HA	1:B:81:GLN:HG2	1.99	0.44
1:A:57:ILE:HD12	1:A:57:ILE:O	2.17	0.44
1:B:266:TYR:HA	2:B:601:NAG:H82	1.99	0.44
1:A:460:LEU:HD11	1:B:460:LEU:HA	1.99	0.44
1:C:36:ARG:NH1	1:C:288:ASP:OD1	2.50	0.44
1:B:172:ILE:O	1:B:176:VAL:HG12	2.17	0.44
1:C:354:THR:O	1:C:440:GLN:NE2	2.50	0.44
1:C:54:MET:HG2	2:C:601:NAG:H81	1.99	0.44
1:A:54:MET:HG2	2:A:601:NAG:H81	1.99	0.44
1:C:473:TYR:O	1:C:477:ILE:HG23	2.18	0.44
1:B:374:GLY:O	1:B:422:ILE:HG23	2.17	0.44
1:B:326:ILE:O	1:C:210:GLN:HG2	2.18	0.44
1:C:396:GLN:NE2	1:C:401:PRO:O	2.51	0.44
1:C:172:ILE:HG23	1:C:195:ILE:HD13	2.00	0.44
1:B:436:LEU:HD22	1:B:440:GLN:HE22	1.83	0.43
1:B:489:TYR:HD2	1:B:490:HIS:HD1	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:O	1:B:87:LEU:HB2	2.19	0.43
1:C:154:VAL:HG12	1:C:161:LEU:HB2	2.00	0.43
1:A:497:ARG:HB2	1:A:497:ARG:NH1	2.33	0.43
1:A:20:LEU:HD22	1:A:311:VAL:HG21	1.99	0.43
1:B:467:LEU:HD22	1:C:466:HIS:ND1	2.32	0.43
1:C:474:LEU:HA	1:C:474:LEU:HD12	1.62	0.43
1:A:305:LEU:HD21	1:A:348:CYS:SG	2.59	0.43
1:B:33:THR:HA	1:C:115:VAL:HG11	2.00	0.43
1:A:105:GLY:O	1:C:419:ARG:NH1	2.51	0.43
1:C:61:ILE:HG13	1:C:62:SER:N	2.34	0.43
1:B:228:LEU:HD23	1:B:235:VAL:HG11	2.01	0.43
1:B:198:LEU:HA	1:B:198:LEU:HD12	1.76	0.43
1:B:469:GLN:O	1:B:473:TYR:HD2	2.02	0.42
1:C:445:ASP:O	1:C:449:ILE:HG13	2.19	0.42
1:A:206:ILE:HG21	1:A:223:ALA:HA	2.01	0.42
1:C:39:MET:HE2	1:C:39:MET:HB3	1.90	0.42
1:C:142:ASN:OD1	1:C:146:LYS:NZ	2.41	0.42
1:B:476:ALA:O	1:B:477:ILE:HB	2.19	0.42
1:A:319:TYR:HD1	1:A:319:TYR:HA	1.72	0.42
1:B:87:LEU:HD22	1:B:215:ALA:HB1	2.02	0.42
1:B:327:THR:OG1	1:B:330:THR:HG22	2.20	0.42
1:B:141:LYS:HD2	1:B:266:TYR:CD1	2.55	0.42
1:B:96:PRO:CB	1:B:97:THR:HA	2.49	0.42
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.90	0.42
1:C:387:CYS:O	1:C:391:ALA:HA	2.19	0.42
1:B:163:THR:HG21	1:B:235:VAL:HG23	2.02	0.41
1:B:38:LEU:HD12	1:B:331:VAL:O	2.20	0.41
1:C:145:GLN:HB2	1:C:268:GLN:NE2	2.34	0.41
1:C:181:THR:OG1	1:C:182:ALA:N	2.53	0.41
1:A:458:LYS:HB3	1:A:458:LYS:HE3	1.86	0.41
1:C:370:VAL:HG12	1:C:377:TYR:HB2	2.03	0.41
1:B:424:GLN:NE2	1:C:111:ALA:HB2	2.35	0.41
1:C:52:LYS:HG3	1:C:166:GLN:HG2	2.02	0.41
1:C:53:LEU:CD1	1:C:80:LEU:HD11	2.50	0.41
1:B:363:GLY:O	1:B:368:ARG:NH1	2.53	0.41
1:B:321:ALA:HB1	1:B:324:CYS:HB2	2.03	0.41
1:C:252:SER:HB3	1:C:253:GLY:H	1.71	0.41
1:A:205:THR:OG1	1:A:206:ILE:N	2.54	0.41
1:C:485:LEU:HA	1:C:485:LEU:HD12	1.84	0.41
1:C:499:LYS:HB3	1:C:499:LYS:HE2	1.88	0.41
1:B:425:LEU:HA	1:B:425:LEU:HD12	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PHE:CE1	1:A:415:LEU:HD21	2.56	0.41
1:B:155:VAL:HA	1:B:159:GLN:O	2.21	0.41
1:A:245:SER:CB	1:B:78:LYS:HG2	2.51	0.41
1:B:437:GLU:N	1:B:440:GLN:OE1	2.50	0.41
1:B:498:ILE:HG23	1:B:498:ILE:O	2.21	0.41
1:A:73:ASN:CG	2:A:601:NAG:C1	2.80	0.41
1:A:175:VAL:HB	1:A:191:ILE:CD1	2.51	0.41
1:C:54:MET:SD	1:C:55:PRO:HD2	2.61	0.41
1:C:174:SER:O	1:C:175:VAL:HG23	2.21	0.41
1:A:400:SER:HA	1:A:401:PRO:HD3	1.85	0.40
1:B:221:ILE:HD13	1:B:255:LEU:HB2	2.02	0.40
1:B:191:ILE:HD12	1:B:191:ILE:HA	1.86	0.40
1:B:150:ALA:HB2	1:B:170:ASP:OD1	2.21	0.40
1:A:500:LYS:N	1:A:500:LYS:HD2	2.36	0.40
1:C:406:ASP:HB2	1:C:424:GLN:O	2.21	0.40
1:C:68:SER:OG	1:C:69:ILE:HG13	2.21	0.40
1:B:358:PHE:O	1:B:441:ILE:HA	2.21	0.40
1:C:428:VAL:O	1:C:430:TYR:HB2	2.22	0.40
1:A:317:GLN:NE2	1:C:362:VAL:HG11	2.35	0.40
1:C:175:VAL:HG11	1:C:191:ILE:HD11	2.03	0.40
1:C:107:VAL:HG21	1:C:125:VAL:HG22	2.03	0.40
1:A:22:LEU:HD13	1:A:32:PRO:HG3	2.03	0.40
1:C:169:GLN:OE1	1:C:172:ILE:HD11	2.22	0.40
1:B:192:ILE:O	1:B:196:LEU:HG	2.20	0.40
1:C:53:LEU:O	1:C:72:TYR:OH	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:GLU:OE2	1:C:419:ARG:NH2[3_655]	2.19	0.01

## 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	477/497 (96%)	434 (91%)	39 (8%)	4 (1%)	24	66
1	B	473/497 (95%)	422 (89%)	41 (9%)	10 (2%)	9	40
1	C	477/497 (96%)	431 (90%)	37 (8%)	9 (2%)	10	43
All	All	1427/1491 (96%)	1287 (90%)	117 (8%)	23 (2%)	12	48

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	THR
1	B	95	ILE
1	B	99	ARG
1	B	391	ALA
1	B	477	ILE
1	B	495	ILE
1	C	43	GLU
1	A	428	VAL
1	A	431	ASN
1	B	150	ALA
1	B	426	ALA
1	C	175	VAL
1	C	178	PRO
1	A	100	ARG
1	C	252	SER
1	C	432	SER
1	C	96	PRO
1	C	131	ASN
1	C	159	GLN
1	C	185	CYS
1	B	298	ASN
1	B	489	TYR
1	B	96	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	401/424 (95%)	359 (90%)	42 (10%)	8	32
1	B	396/424 (93%)	359 (91%)	37 (9%)	11	39
1	C	405/424 (96%)	359 (89%)	46 (11%)	7	28
All	All	1202/1272 (94%)	1077 (90%)	125 (10%)	9	32

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	42	THR
1	A	56	THR
1	A	62	SER
1	A	89	THR
1	A	94	LEU
1	A	133	ASN
1	A	140	LEU
1	A	148	ASN
1	A	158	THR
1	A	191	ILE
1	A	201	THR
1	A	205	THR
1	A	220	THR
1	A	241	ASN
1	A	242	THR
1	A	249	LEU
1	A	256	THR
1	A	279	THR
1	A	288	ASP
1	A	298	ASN
1	A	307	THR
1	A	319	TYR
1	A	327	THR
1	A	330	THR
1	A	340	VAL
1	A	344	ASP
1	A	354	THR
1	A	381	ARG
1	A	400	SER
1	A	411	VAL
1	A	413	LEU

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Mol	Chain	Res	Type
1	A	416	ASP
1	A	417	ASN
1	A	423	THR
1	A	425	LEU
1	A	448	ASP
1	A	456	VAL
1	A	466	HIS
1	A	472	THR
1	A	493	ASN
1	A	500	LYS
1	B	51	VAL
1	B	52	LYS
1	B	85	GLU
1	B	87	LEU
1	B	95	ILE
1	B	107	VAL
1	B	122	THR
1	B	128	VAL
1	B	140	LEU
1	B	158	THR
1	B	166	GLN
1	B	212	THR
1	B	220	THR
1	B	230	SER
1	B	235	VAL
1	B	241	ASN
1	B	244	ILE
1	B	254	LEU
1	B	256	THR
1	B	279	THR
1	B	284	THR
1	B	297	ASN
1	B	327	THR
1	B	340	VAL
1	B	344	ASP
1	B	364	SER
1	B	371	LEU
1	B	375	ILE
1	B	427	ASN
1	B	444	ILE
1	B	471	ASP
1	B	474	LEU

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Mol	Chain	Res	Type
1	B	490	HIS
1	B	491	ILE
1	B	494	GLU
1	B	498	ILE
1	B	500	LYS
1	C	38	LEU
1	C	41	TYR
1	C	46	SER
1	C	50	VAL
1	C	64	CYS
1	C	67	THR
1	C	87	LEU
1	C	117	THR
1	C	133	ASN
1	C	141	LYS
1	C	160	SER
1	C	161	LEU
1	C	175	VAL
1	C	181	THR
1	C	184	ASN
1	C	191	ILE
1	C	195	ILE
1	C	212	THR
1	C	230	SER
1	C	256	THR
1	C	258	GLN
1	C	264	LEU
1	C	298	ASN
1	C	307	THR
1	C	312	THR
1	C	314	SER
1	C	326	ILE
1	C	340	VAL
1	C	350	GLN
1	C	362	VAL
1	C	370	VAL
1	C	371	LEU
1	C	394	ILE
1	C	407	MET
1	C	412	SER
1	C	424	GLN
1	C	434	ILE

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Mol	Chain	Res	Type
1	C	438	SER
1	C	470	SER
1	C	477	ILE
1	C	480	LYS
1	C	481	ILE
1	C	485	LEU
1	C	495	ILE
1	C	499	LYS
1	C	500	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	73	ASN
1	A	297	ASN
1	A	317	GLN
1	A	457	ASN
1	B	73	ASN
1	B	184	ASN
1	C	93	GLN
1	C	188	GLN
1	C	424	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	601	-	14,14,15	0.74	0	15,19,21	1.66	4 (26%)
2	NAG	A	602	-	14,14,15	0.44	0	15,19,21	1.63	4 (26%)
2	NAG	B	601	-	14,14,15	0.52	0	15,19,21	1.40	2 (13%)
2	NAG	C	601	-	14,14,15	0.53	0	15,19,21	1.16	2 (13%)

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	601	-	-	0/6/23/26	0/1/1/1
2	NAG	A	602	-	-	0/6/23/26	0/1/1/1
2	NAG	B	601	-	-	0/6/23/26	0/1/1/1
2	NAG	C	601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	NAG	C2-N2-C7	-3.26	118.85	123.04
2	A	602	NAG	O7-C7-C8	-2.10	118.21	122.06
2	A	601	NAG	O7-C7-C8	-2.05	118.31	122.06
2	A	602	NAG	C4-C3-C2	-2.03	108.08	111.23
2	B	601	NAG	C1-O5-C5	2.01	114.80	112.25
2	A	602	NAG	C3-C2-N2	2.03	115.43	110.56
2	C	601	NAG	C1-O5-C5	2.38	115.26	112.25
2	A	601	NAG	O4-C4-C5	2.40	115.59	109.24
2	A	601	NAG	C1-O5-C5	2.41	115.31	112.25
2	B	601	NAG	C2-N2-C7	2.63	126.42	123.04
2	A	601	NAG	O3-C3-C2	3.54	116.13	109.11
2	A	602	NAG	C1-O5-C5	4.13	117.49	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	4	0
2	A	602	NAG	5	0
2	B	601	NAG	6	0
2	C	601	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	479/497 (96%)	-0.26	5 (1%) 84 60	57, 80, 125, 167	0
1	B	477/497 (95%)	-0.25	7 (1%) 76 49	59, 83, 116, 168	0
1	C	479/497 (96%)	-0.33	4 (0%) 87 67	55, 74, 115, 153	0
All	All	1435/1491 (96%)	-0.28	16 (1%) 82 58	55, 80, 119, 168	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	PHE	4.4
1	B	104	ALA	4.2
1	B	97	THR	4.0
1	B	96	PRO	3.5
1	C	59	SER	3.4
1	A	429	THR	2.9
1	A	432	SER	2.7
1	A	408	TYR	2.7
1	B	108	ILE	2.5
1	C	64	CYS	2.4
1	A	494	GLU	2.2
1	A	425	LEU	2.1
1	C	63	GLY	2.1
1	B	241	ASN	2.0
1	C	65	ASN	2.0
1	B	95	ILE	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( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	601	14/15	0.90	0.21	0.86	76,82,90,93	0
2	NAG	B	601	14/15	0.84	0.17	-0.44	79,87,92,94	0
2	NAG	A	601	14/15	0.90	0.13	-1.45	61,68,74,74	0
2	NAG	A	602	14/15	0.87	0.20	-	84,93,100,101	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.