



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2016 – 02:54 PM EDT

PDB ID : 5JW4  
Title : Structure of MEDI8852 Fab Fragment in Complex with H5 HA  
Authors : Neu, U.; Collins, P.J.; Walker, P.A.; Vorlaender, M.K.; Ogrodowicz, R.W.;  
Martin, S.R.; Gamblin, S.J.; Skehel, J.J.  
Deposited on : 2016-05-11  
Resolution : 3.70 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

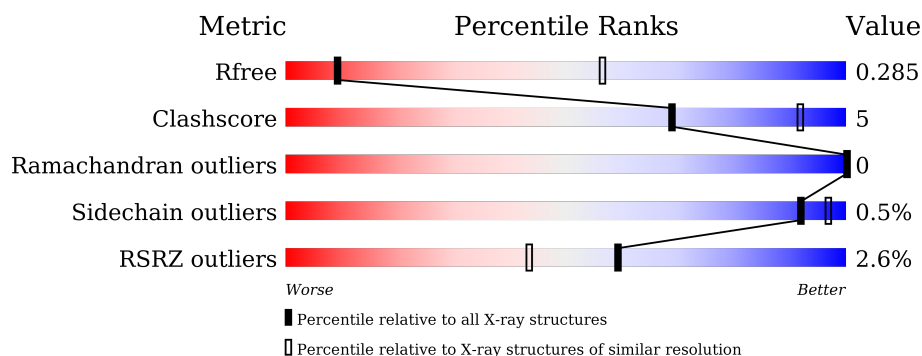
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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.



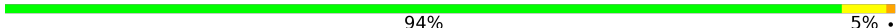


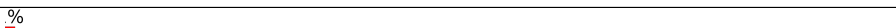
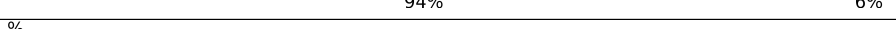
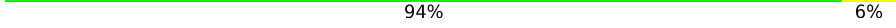
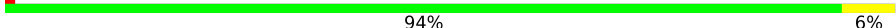


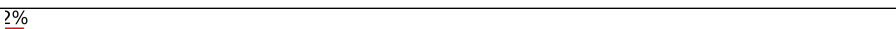
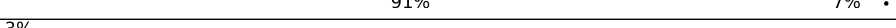
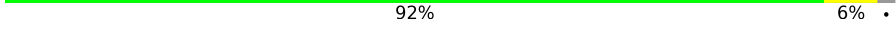



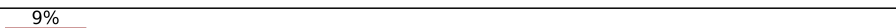


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	321	<div> <div>4%</div> <div>96%</div> <div>.</div> </div>
1	C	321	<div> <div>%</div> <div>93%</div> <div>7%</div> <div>.</div> </div>
1	E	321	<div> <div>%</div> <div>93%</div> <div>6%</div> </div>
1	G	321	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>
1	I	321	<div> <div>9%</div> <div>94%</div> <div>6%</div> </div>
1	K	321	<div> <div>5%</div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	162	 94% 5% .
2	D	162	 94% 6% .
2	F	162	 93% 7% .
2	H	162	 94% 6% .
2	J	162	 94% 6% .
2	L	162	 94% 6% .
3	M	227	 91% 6% ..
3	O	227	 89% 8% .
3	S	227	 91% 7% .
3	U	227	 92% 6% .
3	W	227	 90% 8% .
4	N	206	 88% 12% .
4	P	206	 90% 9% .
4	T	206	 87% 12% .
4	V	206	 91% 8% .
4	X	206	 92% 8% .
5	Q	231	 69% 7% 23% .
6	R	210	 58% 11% 30% .

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
7	NAG	B	201	X	-	-	-
7	NAG	D	201	X	-	-	-
7	NAG	E	402	-	-	X	-
7	NAG	F	201	X	-	-	-
7	NAG	G	401	-	-	-	X
7	NAG	H	201	X	-	-	-
7	NAG	J	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	L	201	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 42466 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	C	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	E	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	G	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	I	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			
1	K	321	Total	C	N	O	S	0	1	0
			2551	1613	439	484	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	LYS	ASN	engineered mutation	UNP Q6DQ34
C	182	LYS	ASN	engineered mutation	UNP Q6DQ34
E	182	LYS	ASN	engineered mutation	UNP Q6DQ34
G	182	LYS	ASN	engineered mutation	UNP Q6DQ34
I	182	LYS	ASN	engineered mutation	UNP Q6DQ34
K	182	LYS	ASN	engineered mutation	UNP Q6DQ34

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	D	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	F	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	J	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			
2	L	162	Total	C	N	O	S	0	0	0
			1312	819	226	259	8			

- Molecule 3 is a protein called MEDI8852 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	O	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	S	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	U	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			
3	W	223	Total	C	N	O	S	0	1	0
			1697	1071	285	335	6			

- Molecule 4 is a protein called MEDI8852 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	P	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	T	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	V	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			
4	X	206	Total	C	N	O	S	0	0	0
			1577	980	270	322	5			

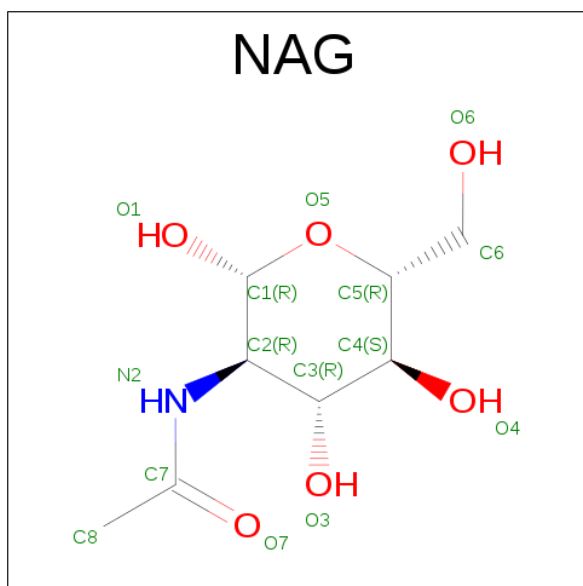
- Molecule 5 is a protein called MEDI8852 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	177	Total	C	N	O	S	0	0	0
			1369	867	230	267	5			

- Molecule 6 is a protein called MEDI8852 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	148	Total	C	N	O	S	0	0	0
			1129	701	193	230	5			

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



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

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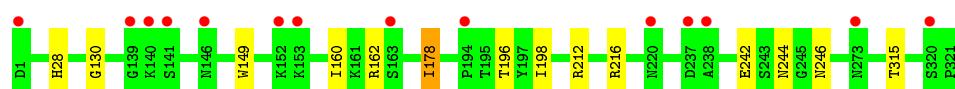
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		



### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

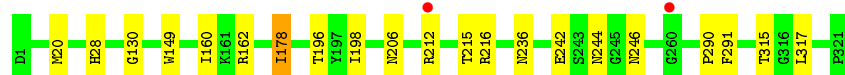
#### • Molecule 1: Hemagglutinin



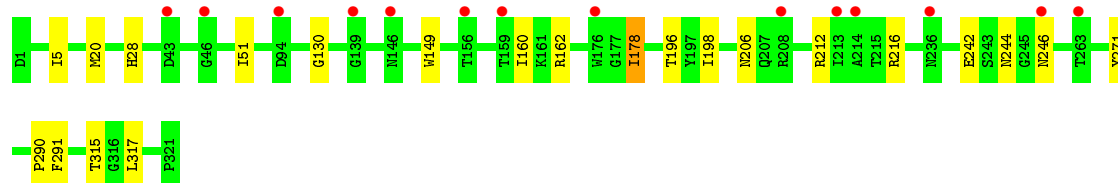
#### • Molecule 1: Hemagglutinin



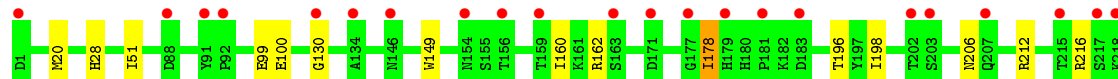
#### • Molecule 1: Hemagglutinin

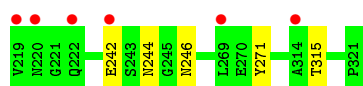


#### • Molecule 1: Hemagglutinin

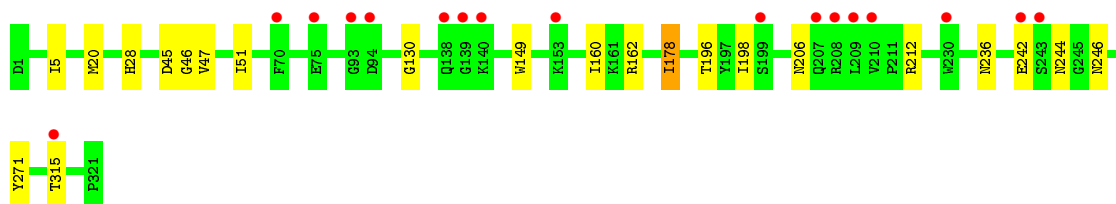
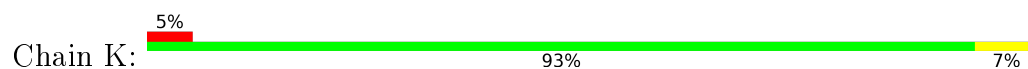


#### • Molecule 1: Hemagglutinin





- Molecule 1: Hemagglutinin



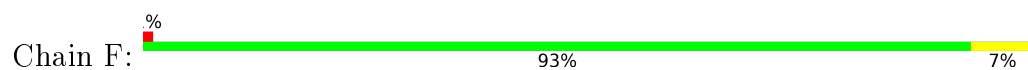
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



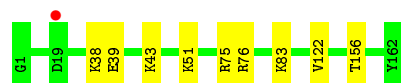
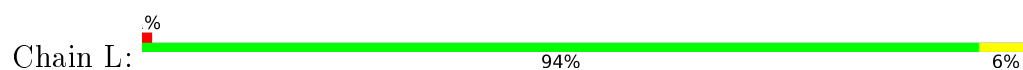
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



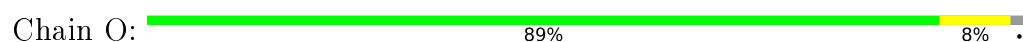
- Molecule 2: Hemagglutinin



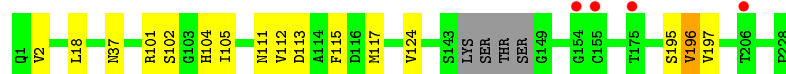
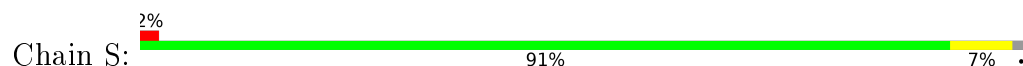
- Molecule 3: MEDI8852 heavy chain



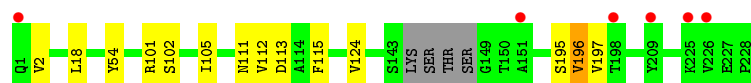
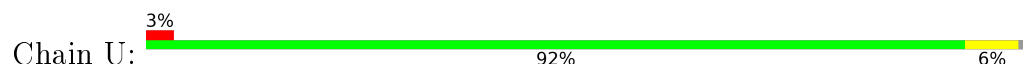
- Molecule 3: MEDI8852 heavy chain



- Molecule 3: MEDI8852 heavy chain



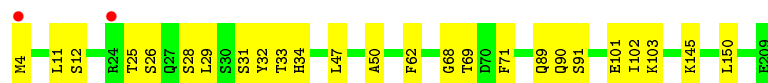
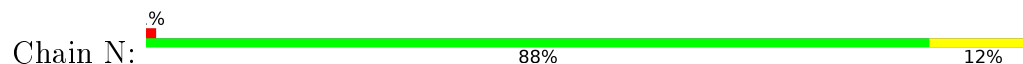
- Molecule 3: MEDI8852 heavy chain



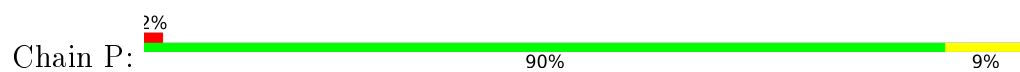
- Molecule 3: MEDI8852 heavy chain



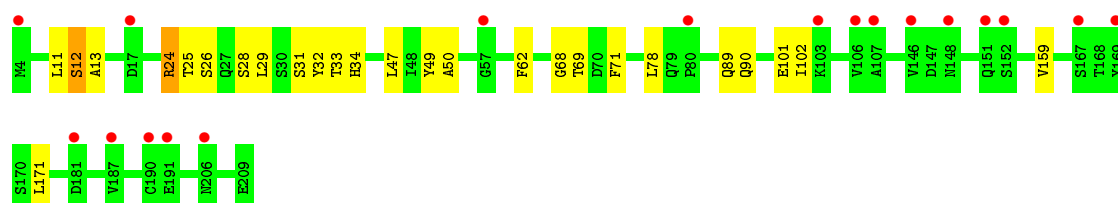
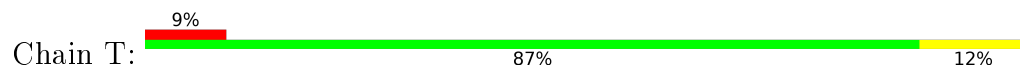
- Molecule 4: MEDI8852 light chain



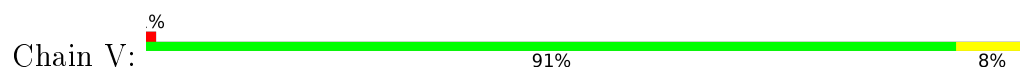
- Molecule 4: MEDI8852 light chain



- Molecule 4: MEDI8852 light chain



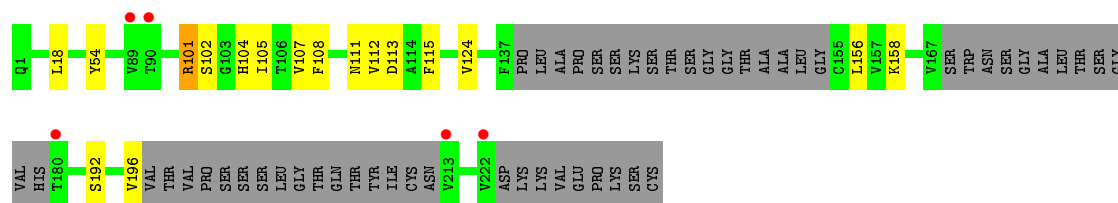
- Molecule 4: MEDI8852 light chain



- Molecule 4: MEDI8852 light chain



- Molecule 5: MEDI8852 heavy chain



- Molecule 6: MEDI8852 light chain



THR	LYS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	SER	GLN	E157	Q162	D166	Y169	S172	SER	THR	LEU	THR	LEU	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	C190	Q195	G196	LEU	SER	SER	PRO	V201	T202	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.26Å 386.36Å 165.86Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	29.80 – 3.70 29.80 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.80-3.70) 97.6 (29.80-3.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 3.75Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.274 , 0.285 0.274 , 0.285	Depositor DCC
$R_{free}$ test set	4768 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	136.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 79.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	42466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/2616	0.58	0/3553
1	C	0.58	1/2616 (0.0%)	0.62	3/3553 (0.1%)
1	E	0.43	0/2616	0.58	0/3553
1	G	0.40	0/2616	0.58	0/3553
1	I	0.40	0/2616	0.58	0/3553
1	K	0.50	1/2616 (0.0%)	0.62	3/3553 (0.1%)
2	B	0.48	0/1339	0.60	0/1802
2	D	0.50	0/1339	0.61	0/1802
2	F	0.51	0/1339	0.61	0/1802
2	H	0.49	0/1339	0.60	0/1802
2	J	0.49	0/1339	0.62	1/1802 (0.1%)
2	L	0.48	0/1339	0.61	0/1802
3	M	0.75	4/1738 (0.2%)	0.78	4/2374 (0.2%)
3	O	0.59	3/1738 (0.2%)	0.75	4/2374 (0.2%)
3	S	0.61	3/1738 (0.2%)	0.73	1/2374 (0.0%)
3	U	0.62	5/1738 (0.3%)	0.73	3/2374 (0.1%)
3	W	0.79	1/1738 (0.1%)	1.03	4/2374 (0.2%)
4	N	0.56	0/1610	0.72	0/2182
4	P	0.49	0/1610	0.70	0/2182
4	T	0.70	1/1610 (0.1%)	0.77	3/2182 (0.1%)
4	V	0.55	0/1610	0.73	1/2182 (0.0%)
4	X	0.53	0/1610	0.70	0/2182
5	Q	0.57	0/1401	0.79	1/1908 (0.1%)
6	R	0.99	1/1147 (0.1%)	0.95	4/1547 (0.3%)
All	All	0.56	20/43018 (0.0%)	0.69	32/58365 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	103	LYS	C-N	26.41	1.94	1.34
3	W	195	SER	C-N	25.07	1.91	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	GLY	C-N	19.65	1.79	1.34
4	T	24	ARG	C-N	19.10	1.77	1.34
3	M	115	PHE	C-N	17.29	1.73	1.34
1	K	46	GLY	C-N	14.37	1.67	1.34
3	M	195	SER	CA-C	-7.26	1.34	1.52
3	U	196[A]	VAL	N-CA	-7.20	1.31	1.46
3	U	196[B]	VAL	N-CA	-7.20	1.31	1.46
3	S	196[A]	VAL	N-CA	-6.74	1.32	1.46
3	S	196[B]	VAL	N-CA	-6.74	1.32	1.46
3	U	195	SER	CA-C	-6.74	1.35	1.52
3	M	196[A]	VAL	N-CA	-6.62	1.33	1.46
3	M	196[B]	VAL	N-CA	-6.62	1.33	1.46
3	S	195	SER	CA-C	-6.14	1.36	1.52
3	O	195	SER	CA-C	-6.13	1.36	1.52
3	O	196[A]	VAL	N-CA	-6.00	1.34	1.46
3	O	196[B]	VAL	N-CA	-6.00	1.34	1.46
3	U	196[A]	VAL	CA-CB	-5.15	1.44	1.54
3	U	196[B]	VAL	CA-CB	-5.15	1.44	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	195	SER	O-C-N	-22.98	85.93	122.70
3	W	195	SER	CA-C-N	-22.98	66.65	117.20
3	W	195	SER	C-N-CA	-19.06	74.06	121.70
6	R	103	LYS	O-C-N	-14.20	99.97	122.70
6	R	103	LYS	C-N-CA	11.06	149.34	121.70
1	K	46	GLY	CA-C-N	-8.88	97.66	117.20
6	R	103	LYS	CA-C-N	8.80	136.56	117.20
4	T	24	ARG	CA-C-N	-8.61	98.26	117.20
1	C	46	GLY	C-N-CA	-7.84	102.11	121.70
4	T	24	ARG	O-C-N	7.55	134.79	122.70
3	M	195	SER	C-N-CA	-7.43	103.11	121.70
4	T	24	ARG	C-N-CA	-7.43	103.12	121.70
1	K	46	GLY	C-N-CA	-7.40	103.20	121.70
1	C	46	GLY	CA-C-N	-7.22	101.31	117.20
5	Q	101	ARG	NE-CZ-NH1	7.19	123.90	120.30
2	J	37	ASP	CB-CG-OD1	7.09	124.68	118.30
3	O	195	SER	N-CA-C	-6.96	92.21	111.00
3	M	195	SER	CB-CA-C	-6.34	98.06	110.10
1	K	46	GLY	O-C-N	5.90	132.15	122.70
3	U	195	SER	N-CA-C	-5.74	95.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	195	SER	C-N-CA	-5.62	107.66	121.70
4	V	32	TYR	CB-CG-CD1	5.52	124.31	121.00
3	M	115	PHE	CA-C-N	-5.42	105.27	117.20
3	U	195	SER	CA-C-O	5.41	131.46	120.10
3	O	195	SER	CA-C-O	5.26	131.14	120.10
6	R	92	ARG	NE-CZ-NH2	-5.21	117.70	120.30
3	M	115	PHE	O-C-N	5.20	131.02	122.70
3	W	45	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	46	GLY	O-C-N	5.13	130.91	122.70
3	O	196[A]	VAL	CG1-CB-CG2	5.13	119.11	110.90
3	O	196[B]	VAL	CG1-CB-CG2	5.13	119.11	110.90
3	S	195	SER	C-N-CA	-5.05	109.08	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2551	0	2501	10	0
1	C	2551	0	2500	22	2
1	E	2551	0	2501	27	0
1	G	2551	0	2501	19	0
1	I	2551	0	2500	15	0
1	K	2551	0	2500	19	0
2	B	1312	0	1218	7	0
2	D	1312	0	1218	10	0
2	F	1312	0	1218	14	0
2	H	1312	0	1218	10	0
2	J	1312	0	1218	9	0
2	L	1312	0	1218	8	0
3	M	1697	0	1648	31	0
3	O	1697	0	1649	20	2
3	S	1697	0	1649	14	0
3	U	1697	0	1649	15	0
3	W	1697	0	1647	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	1577	0	1531	28	0
4	P	1577	0	1531	19	0
4	T	1577	0	1530	27	0
4	V	1577	0	1531	23	0
4	X	1577	0	1531	16	0
5	Q	1369	0	1324	18	0
6	R	1129	0	1089	35	0
7	A	42	0	39	1	0
7	B	28	0	25	0	0
7	C	42	0	39	1	0
7	D	14	0	13	0	0
7	E	56	0	50	12	0
7	F	28	0	25	0	0
7	G	42	0	39	1	0
7	H	28	0	25	0	0
7	I	42	0	39	1	0
7	J	28	0	25	0	0
7	K	56	0	50	6	0
7	L	14	0	13	0	0
All	All	42466	0	41002	387	2

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 5.

All (387) 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)
7:K:401:NAG:O3	7:K:402:NAG:C1	1.64	1.43
3:W:195:SER:C	3:W:196[A]:VAL:C	1.76	1.42
3:M:115:PHE:C	3:M:116:ASP:N	1.73	1.41
7:E:401:NAG:O3	7:E:402:NAG:C1	1.65	1.41
3:W:195:SER:N	3:W:196[B]:VAL:N	1.64	1.40
1:C:46:GLY:C	1:C:47:VAL:N	1.79	1.34
4:T:24:ARG:C	4:T:25:THR:N	1.78	1.34
3:W:195:SER:C	3:W:196[A]:VAL:O	1.68	1.24
1:E:236:ASN:HD21	7:E:402:NAG:C8	1.51	1.23
6:R:103:LYS:C	6:R:104:ARG:N	1.94	1.18
3:W:195:SER:CA	3:W:196[B]:VAL:N	2.01	1.17
3:W:195:SER:O	3:W:196[A]:VAL:CA	1.95	1.15
3:W:194:SER:HB3	3:W:196[B]:VAL:HG13	1.16	1.13
3:W:194:SER:CB	3:W:196[B]:VAL:HG13	1.81	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:194:SER:HB3	3:W:196[B]:VAL:CG1	1.88	1.03
3:W:194:SER:C	3:W:196[B]:VAL:N	2.13	1.02
1:E:236:ASN:HD21	7:E:402:NAG:C7	1.75	1.00
2:J:38:LYS:HD2	4:V:32:TYR:HE2	1.25	0.99
3:W:195:SER:C	3:W:196[A]:VAL:CA	2.04	0.97
3:W:195:SER:O	3:W:196[A]:VAL:C	2.03	0.96
4:T:78:LEU:HD21	4:T:102:ILE:HG13	1.46	0.96
1:E:236:ASN:ND2	7:E:402:NAG:C7	2.29	0.96
3:U:112:VAL:HG23	4:V:32:TYR:CD1	2.01	0.95
3:M:196[A]:VAL:C	3:M:197:VAL:N	2.20	0.95
3:S:196[B]:VAL:C	3:S:197:VAL:N	2.21	0.94
3:S:196[A]:VAL:C	3:S:197:VAL:N	2.22	0.92
3:M:196[B]:VAL:C	3:M:197:VAL:N	2.22	0.92
2:J:38:LYS:HD2	4:V:32:TYR:CE2	2.05	0.90
4:N:25:THR:OG1	4:N:90:GLN:NE2	2.05	0.90
1:E:236:ASN:ND2	7:E:402:NAG:C8	2.37	0.87
3:U:196[B]:VAL:C	3:U:197:VAL:N	2.28	0.86
1:E:236:ASN:HD21	7:E:402:NAG:H81	1.40	0.84
1:C:28:HIS:CD2	1:C:315:THR:OG1	2.30	0.84
1:A:28:HIS:CD2	1:A:315:THR:OG1	2.31	0.84
1:K:28:HIS:CD2	1:K:315:THR:OG1	2.31	0.83
3:U:196[A]:VAL:C	3:U:197:VAL:N	2.32	0.83
1:I:28:HIS:CD2	1:I:315:THR:OG1	2.31	0.83
2:F:19:ASP:OD2	6:R:92:ARG:NH2	2.12	0.83
3:W:139:LEU:CD1	3:W:196[B]:VAL:HG12	2.10	0.82
5:Q:101:ARG:NH1	5:Q:104:HIS:ND1	2.28	0.81
1:E:28:HIS:CD2	1:E:315:THR:OG1	2.33	0.81
1:G:28:HIS:CD2	1:G:315:THR:OG1	2.33	0.81
2:D:38:LYS:HD2	4:P:32:TYR:CE1	2.16	0.80
3:W:181:PHE:HE1	3:W:196[A]:VAL:CG1	1.95	0.79
3:W:195:SER:O	3:W:196[A]:VAL:HA	1.69	0.77
4:T:24:ARG:C	4:T:25:THR:CA	2.53	0.77
4:X:25:THR:HG1	4:X:90:GLN:CD	1.89	0.76
4:T:24:ARG:CA	4:T:25:THR:N	2.48	0.76
3:M:195:SER:O	3:M:196[B]:VAL:CG1	2.35	0.75
6:R:29:LEU:HD13	6:R:32:TYR:CD2	2.22	0.74
4:T:25:THR:O	4:T:69:THR:HB	1.86	0.74
1:C:46:GLY:C	1:C:47:VAL:CA	2.55	0.74
6:R:101:GLU:OE1	6:R:169:TYR:OH	2.07	0.72
4:V:28:SER:HB2	4:V:68:GLY:O	1.90	0.72
5:Q:107:VAL:HG12	5:Q:108:PHE:CD2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:153:LEU:O	3:M:196[A]:VAL:CG2	2.38	0.71
3:M:154:GLY:HA3	3:M:196[B]:VAL:HG12	1.73	0.71
1:C:206:ASN:O	1:E:212:ARG:NH2	2.24	0.71
6:R:32:TYR:O	6:R:34:HIS:CD2	2.44	0.70
6:R:29:LEU:HD13	6:R:32:TYR:HD2	1.56	0.70
3:O:196[A]:VAL:C	3:O:197:VAL:N	2.45	0.70
3:W:139:LEU:HD13	3:W:196[B]:VAL:HG12	1.71	0.70
6:R:32:TYR:O	6:R:34:HIS:NE2	2.25	0.69
5:Q:101:ARG:HH12	5:Q:104:HIS:CE1	2.10	0.69
1:E:236:ASN:ND2	7:E:402:NAG:O7	2.24	0.69
1:C:46:GLY:CA	1:C:47:VAL:N	2.56	0.68
3:W:181:PHE:HE1	3:W:196[B]:VAL:CG2	2.06	0.68
3:M:153:LEU:O	3:M:196[A]:VAL:HG23	1.95	0.67
3:S:112:VAL:HG21	4:T:31:SER:O	1.95	0.67
2:L:38:LYS:HD2	4:X:32:TYR:CE1	2.30	0.66
3:O:196[B]:VAL:C	3:O:197:VAL:N	2.49	0.66
3:W:181:PHE:CE1	3:W:196[A]:VAL:CG1	2.77	0.66
1:C:28:HIS:HD2	1:C:315:THR:OG1	1.78	0.66
6:R:102:ILE:C	6:R:103:LYS:N	2.49	0.66
2:B:38:LYS:HD2	4:N:32:TYR:CE1	2.31	0.65
3:U:112:VAL:HG23	4:V:32:TYR:HD1	1.55	0.65
1:K:28:HIS:HD2	1:K:315:THR:OG1	1.80	0.65
1:A:28:HIS:HD2	1:A:315:THR:OG1	1.80	0.65
7:K:401:NAG:H82	7:K:401:NAG:O3	1.97	0.64
3:M:195:SER:C	3:M:196[B]:VAL:HG13	2.17	0.64
5:Q:101:ARG:NH1	5:Q:104:HIS:CG	2.66	0.64
1:I:28:HIS:HD2	1:I:315:THR:OG1	1.80	0.64
2:D:39:GLU:O	2:D:43:LYS:HG2	1.98	0.64
2:J:39:GLU:O	2:J:43:LYS:HG2	1.98	0.64
3:M:195:SER:C	3:M:196[B]:VAL:CG1	2.65	0.64
4:N:25:THR:OG1	4:N:90:GLN:CD	2.37	0.63
2:L:39:GLU:O	2:L:43:LYS:HG2	1.99	0.63
3:O:181:PHE:HE1	3:O:196[B]:VAL:CG2	2.11	0.63
6:R:12:SER:HB3	6:R:103:LYS:CA	2.29	0.63
2:B:39:GLU:O	2:B:43:LYS:HG2	1.99	0.63
4:N:28:SER:HB2	4:N:68:GLY:O	1.99	0.63
4:X:25:THR:HG22	4:X:69:THR:O	1.99	0.63
2:D:106:ARG:NH1	2:F:105:GLU:OE1	2.32	0.62
3:M:196[A]:VAL:HG22	3:M:197:VAL:N	2.13	0.62
6:R:12:SER:CB	6:R:103:LYS:HB2	2.30	0.62
3:M:115:PHE:CA	3:M:116:ASP:N	2.60	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:12:SER:HB3	6:R:103:LYS:N	2.15	0.61
3:M:154:GLY:HA3	3:M:196[A]:VAL:HG23	1.83	0.61
1:C:206:ASN:OD1	1:E:216:ARG:NH1	2.34	0.60
1:E:28:HIS:HD2	1:E:315:THR:OG1	1.82	0.60
3:W:181:PHE:CE1	3:W:196[A]:VAL:HG12	2.35	0.60
7:E:401:NAG:H82	7:E:401:NAG:O3	2.01	0.60
1:G:28:HIS:HD2	1:G:315:THR:OG1	1.83	0.60
3:O:111:ASN:OD1	3:O:113:ASP:N	2.22	0.60
3:O:181:PHE:HE1	3:O:196[B]:VAL:HG22	1.67	0.60
4:T:34:HIS:ND1	4:T:49:TYR:HA	2.16	0.60
3:W:194:SER:HB2	3:W:196[B]:VAL:HG13	1.81	0.60
5:Q:112:VAL:HG21	6:R:31:SER:O	2.02	0.59
5:Q:196:VAL:HG21	6:R:131:LEU:HD22	1.84	0.59
3:M:153:LEU:O	3:M:196[A]:VAL:HG22	2.02	0.59
6:R:12:SER:HB2	6:R:103:LYS:HB2	1.84	0.59
2:B:51:LYS:HE3	1:C:20:MET:HE2	1.85	0.59
2:F:39:GLU:O	2:F:43:LYS:HG2	2.03	0.59
2:H:39:GLU:O	2:H:43:LYS:HG2	2.03	0.59
4:T:28:SER:HB2	4:T:68:GLY:O	2.03	0.58
2:H:38:LYS:HD2	4:T:32:TYR:CZ	2.39	0.58
4:T:34:HIS:CE1	4:T:50:ALA:H	2.21	0.57
1:K:236:ASN:HD21	7:K:402:NAG:H81	1.70	0.57
3:M:112:VAL:HG21	4:N:31:SER:O	2.05	0.57
2:B:18:VAL:HG21	3:M:54:TYR:CE2	2.40	0.57
3:W:194:SER:HB3	3:W:196[A]:VAL:HB	1.86	0.56
3:W:181:PHE:HE1	3:W:196[A]:VAL:HG11	1.70	0.56
3:S:111:ASN:OD1	3:S:113:ASP:N	2.23	0.56
3:M:18:LEU:HD12	3:M:124:VAL:HG11	1.88	0.56
3:W:181:PHE:CE1	3:W:196[B]:VAL:HG22	2.40	0.56
5:Q:111:ASN:OD1	5:Q:113:ASP:N	2.26	0.56
1:K:5:ILE:HD11	2:L:122:VAL:HG21	1.87	0.55
1:E:236:ASN:ND2	7:E:402:NAG:H81	2.15	0.55
3:U:18:LEU:HD12	3:U:124:VAL:HG11	1.88	0.55
3:S:18:LEU:HD12	3:S:124:VAL:HG11	1.88	0.55
3:M:179:HIS:O	3:M:196[A]:VAL:HG12	2.06	0.55
3:O:112:VAL:HG21	4:P:31:SER:O	2.07	0.55
2:F:38:LYS:HD2	6:R:32:TYR:CE2	2.41	0.55
3:W:18:LEU:HD12	3:W:124:VAL:HG11	1.87	0.55
4:N:12:SER:OG	4:N:103:LYS:HB2	2.07	0.55
3:O:35:VAL:HG21	3:O:111:ASN:HD22	1.71	0.55
6:R:101:GLU:HB2	6:R:162:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:25:THR:HG22	4:T:69:THR:O	2.06	0.55
5:Q:112:VAL:HG23	6:R:32:TYR:CD1	2.42	0.55
6:R:29:LEU:CD1	6:R:32:TYR:HD2	2.20	0.55
3:W:181:PHE:CE1	3:W:196[B]:VAL:CG2	2.90	0.54
4:P:102:ILE:HD12	4:P:102:ILE:N	2.23	0.54
5:Q:18:LEU:HD12	5:Q:124:VAL:HG11	1.89	0.54
4:V:25:THR:HG22	4:V:69:THR:O	2.07	0.54
3:O:18:LEU:HD12	3:O:124:VAL:HG11	1.88	0.54
2:F:18:VAL:HG12	5:Q:111:ASN:HB3	1.89	0.54
3:O:105:ILE:O	3:O:105:ILE:HG13	2.08	0.54
2:H:156:THR:HG22	2:H:156:THR:O	2.07	0.54
4:N:33:THR:HA	4:N:89:GLN:O	2.08	0.54
4:P:25:THR:HG22	4:P:69:THR:O	2.08	0.53
2:B:156:THR:HG22	2:B:156:THR:O	2.08	0.53
2:J:18:VAL:HG21	3:U:54:TYR:CE2	2.43	0.53
2:L:156:THR:O	2:L:156:THR:HG22	2.08	0.53
3:M:112:VAL:CG2	4:N:32:TYR:HA	2.39	0.53
3:O:181:PHE:CE1	3:O:196[B]:VAL:HG22	2.43	0.53
3:W:194:SER:HB3	3:W:196[B]:VAL:N	2.23	0.53
3:U:2:VAL:HG21	3:U:101:ARG:NH1	2.24	0.53
3:M:195:SER:OG	3:M:196[A]:VAL:N	2.39	0.53
4:N:25:THR:HG22	4:N:69:THR:O	2.09	0.53
2:D:156:THR:HG22	2:D:156:THR:O	2.09	0.53
4:T:25:THR:N	4:T:69:THR:O	2.41	0.53
1:E:236:ASN:HD21	7:E:402:NAG:H82	1.60	0.52
2:J:156:THR:HG22	2:J:156:THR:O	2.08	0.52
2:F:156:THR:O	2:F:156:THR:HG22	2.09	0.52
3:W:103:GLY:CA	3:W:111:ASN:OD1	2.57	0.52
4:V:33:THR:HA	4:V:89:GLN:O	2.09	0.52
3:M:195:SER:O	3:M:196[B]:VAL:HG12	2.10	0.52
4:P:33:THR:HA	4:P:89:GLN:O	2.10	0.52
4:V:25:THR:OG1	4:V:90:GLN:OE1	2.23	0.52
4:X:33:THR:HA	4:X:89:GLN:O	2.10	0.52
5:Q:105:ILE:O	5:Q:105:ILE:HG13	2.10	0.51
5:Q:112:VAL:HG22	6:R:32:TYR:HA	1.92	0.51
2:F:38:LYS:HD2	6:R:32:TYR:CZ	2.46	0.51
3:U:112:VAL:CG2	4:V:32:TYR:CD1	2.87	0.51
4:X:102:ILE:HD12	4:X:102:ILE:N	2.26	0.51
3:W:181:PHE:CD1	3:W:196[A]:VAL:HG12	2.46	0.51
4:T:33:THR:HA	4:T:89:GLN:O	2.11	0.51
3:U:105:ILE:O	3:U:105:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:102:ILE:HD12	4:V:102:ILE:N	2.26	0.51
2:F:38:LYS:NZ	6:R:91:SER:OG	2.43	0.51
1:K:236:ASN:HD21	7:K:402:NAG:C8	2.23	0.51
3:O:102:SER:HB3	3:O:115:PHE:CD1	2.45	0.51
3:W:105:ILE:HG13	3:W:105:ILE:O	2.10	0.51
4:N:145:LYS:CG	4:N:150:LEU:HD23	2.41	0.51
5:Q:107:VAL:HG12	5:Q:108:PHE:HD2	1.72	0.51
2:D:124:LEU:HD22	2:F:134:GLY:HA2	1.94	0.50
4:N:102:ILE:N	4:N:102:ILE:HD12	2.27	0.50
6:R:33:THR:HA	6:R:89:GLN:O	2.12	0.50
4:P:11:LEU:O	4:P:101:GLU:HG2	2.12	0.50
4:T:11:LEU:O	4:T:101:GLU:HG2	2.12	0.50
7:E:401:NAG:O3	7:E:402:NAG:C2	2.54	0.50
3:S:105:ILE:HG13	3:S:105:ILE:O	2.11	0.50
1:A:216:ARG:NH1	1:E:206:ASN:OD1	2.43	0.50
3:M:2:VAL:HG21	3:M:101:ARG:NH1	2.26	0.50
3:O:196[A]:VAL:HG21	4:P:131:LEU:HD22	1.93	0.50
7:C:401:NAG:H82	7:C:401:NAG:O3	2.11	0.49
1:E:178:ILE:HD12	1:E:198:ILE:CD1	2.42	0.49
1:K:178:ILE:HD12	1:K:198:ILE:CD1	2.42	0.49
3:M:111:ASN:OD1	3:M:113:ASP:N	2.28	0.49
3:M:195:SER:OG	3:M:196[B]:VAL:N	2.43	0.49
4:X:11:LEU:O	4:X:101:GLU:HG2	2.12	0.49
4:N:11:LEU:O	4:N:101:GLU:HG2	2.12	0.49
3:O:102:SER:HB3	3:O:115:PHE:HD1	1.77	0.49
6:R:83:PHE:HB2	6:R:102:ILE:CD1	2.42	0.49
3:M:105:ILE:HG13	3:M:105:ILE:O	2.11	0.49
1:A:178:ILE:HD12	1:A:198:ILE:CD1	2.42	0.49
5:Q:112:VAL:CG2	6:R:32:TYR:HA	2.42	0.49
2:H:18:VAL:HG12	3:S:111:ASN:HB3	1.94	0.49
1:C:28:HIS:CD2	3:O:108:PHE:HA	2.48	0.49
4:P:4:MET:SD	4:P:90:GLN:HB2	2.52	0.49
3:W:112:VAL:HG21	4:X:31:SER:O	2.12	0.49
1:C:178:ILE:HD12	1:C:198:ILE:CD1	2.42	0.49
1:I:178:ILE:HD12	1:I:198:ILE:CD1	2.42	0.49
1:G:178:ILE:HD12	1:G:198:ILE:CD1	2.42	0.49
4:N:34:HIS:HD2	4:N:50:ALA:H	1.61	0.49
4:V:11:LEU:O	4:V:101:GLU:HG2	2.13	0.49
1:G:290:PRO:HG3	2:H:56:ILE:HG12	1.94	0.48
5:Q:156:LEU:HG	5:Q:158:LYS:HG2	1.95	0.48
1:I:206:ASN:O	1:K:212:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:32:TYR:CD2	4:P:32:TYR:N	2.81	0.48
3:O:37:ASN:ND2	3:O:102:SER:OG	2.36	0.48
3:W:37:ASN:ND2	3:W:102:SER:OG	2.38	0.48
3:M:195:SER:O	3:M:196[A]:VAL:HB	2.04	0.48
3:S:112:VAL:CG2	4:T:32:TYR:HA	2.44	0.48
3:W:112:VAL:CG2	4:X:32:TYR:HA	2.44	0.48
1:G:206:ASN:O	1:I:212:ARG:NH2	2.46	0.47
3:S:101:ARG:NH2	3:S:104:HIS:CD2	2.82	0.47
4:N:32:TYR:CD2	4:N:32:TYR:N	2.81	0.47
4:T:78:LEU:HD21	4:T:102:ILE:CG1	2.33	0.47
2:D:110:PHE:CD2	1:E:20:MET:HE1	2.50	0.47
1:G:212:ARG:NH2	1:K:206:ASN:O	2.47	0.47
4:T:24:ARG:HA	4:T:25:THR:N	2.30	0.47
1:C:240:ASN:HB2	1:E:215:THR:O	2.15	0.47
1:G:206:ASN:OD1	1:I:216:ARG:NH1	2.47	0.47
2:J:51:LYS:HE3	1:K:20:MET:HE2	1.95	0.47
7:K:401:NAG:O3	7:K:402:NAG:C2	2.56	0.47
6:R:47:LEU:HD11	6:R:62:PHE:CD1	2.49	0.47
2:B:42:GLN:HG2	4:N:29:LEU:HA	1.96	0.47
1:E:178:ILE:HD12	1:E:198:ILE:HD12	1.97	0.47
1:I:99:GLU:HB3	2:L:76:ARG:HD3	1.97	0.47
3:S:112:VAL:HG22	4:T:32:TYR:HA	1.97	0.47
1:K:28:HIS:CD2	3:W:108:PHE:HA	2.50	0.47
1:C:5:ILE:HD11	2:D:122:VAL:HG21	1.97	0.47
3:M:112:VAL:HG22	4:N:32:TYR:HA	1.95	0.47
4:P:32:TYR:HD2	4:P:32:TYR:N	2.12	0.47
1:A:178:ILE:HD12	1:A:198:ILE:HD12	1.97	0.47
2:F:38:LYS:HB3	6:R:29:LEU:HD13	1.97	0.47
1:I:178:ILE:HD12	1:I:198:ILE:HD12	1.97	0.47
1:C:290:PRO:HG3	2:D:56:ILE:HG12	1.97	0.46
1:G:178:ILE:HD12	1:G:198:ILE:HD12	1.97	0.46
4:N:32:TYR:HD2	4:N:32:TYR:N	2.13	0.46
1:G:5:ILE:HD11	2:H:122:VAL:HG21	1.96	0.46
1:G:196:THR:OG1	1:G:246:ASN:ND2	2.48	0.46
4:P:102:ILE:CD1	4:P:102:ILE:N	2.79	0.46
6:R:29:LEU:CD1	6:R:32:TYR:CD2	2.95	0.46
1:E:196:THR:OG1	1:E:246:ASN:ND2	2.49	0.46
7:I:401:NAG:O3	7:I:401:NAG:H82	2.16	0.46
3:W:194:SER:CB	3:W:196[B]:VAL:CG1	2.66	0.46
7:G:401:NAG:H82	7:G:401:NAG:O3	2.16	0.46
3:O:194:SER:HB3	3:O:196[B]:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HD12	1:C:198:ILE:HD12	1.98	0.46
1:E:236:ASN:CG	7:E:402:NAG:C7	2.83	0.46
6:R:28:SER:HB2	6:R:68:GLY:O	2.15	0.46
1:G:290:PRO:HB3	2:H:56:ILE:HG23	1.97	0.46
1:I:196:THR:OG1	1:I:246:ASN:ND2	2.49	0.46
6:R:47:LEU:HG	6:R:48:ILE:HG12	1.98	0.46
4:T:32:TYR:O	4:T:90:GLN:HA	2.15	0.46
1:A:196:THR:OG1	1:A:246:ASN:ND2	2.49	0.46
1:E:160:ILE:O	1:E:242:GLU:HA	2.16	0.46
4:N:25:THR:HG1	4:N:90:GLN:NE2	2.12	0.46
7:A:401:NAG:H82	7:A:401:NAG:O3	2.15	0.45
1:C:196:THR:OG1	1:C:246:ASN:ND2	2.49	0.45
3:W:194:SER:HB3	3:W:196[A]:VAL:N	2.32	0.45
1:K:236:ASN:ND2	7:K:402:NAG:O7	2.49	0.45
3:O:2:VAL:HG21	3:O:101:ARG:NH1	2.31	0.45
6:R:47:LEU:HD11	6:R:62:PHE:CG	2.51	0.45
3:O:181:PHE:HE1	3:O:196[B]:VAL:HG21	1.82	0.45
1:K:196:THR:OG1	1:K:246:ASN:ND2	2.49	0.45
4:P:12:SER:OG	4:P:101:GLU:OE2	2.35	0.45
4:T:33:THR:HG1	4:T:90:GLN:HE21	1.62	0.45
1:K:51:ILE:HD12	1:K:271:TYR:HB2	1.98	0.45
4:N:32:TYR:O	4:N:90:GLN:HA	2.17	0.45
1:A:160:ILE:O	1:A:242:GLU:HA	2.17	0.45
1:K:160:ILE:O	1:K:242:GLU:HA	2.17	0.45
6:R:33:THR:O	6:R:34:HIS:ND1	2.50	0.45
3:S:37:ASN:ND2	3:S:102:SER:OG	2.36	0.45
4:T:25:THR:HG21	4:T:71:PHE:HE1	1.81	0.45
3:U:102:SER:HB3	3:U:115:PHE:CD1	2.52	0.45
3:U:112:VAL:CG2	4:V:32:TYR:HD1	2.25	0.45
3:W:102:SER:HB3	3:W:115:PHE:CD1	2.51	0.45
2:F:18:VAL:HG21	5:Q:54:TYR:CE2	2.52	0.45
3:M:179:HIS:O	3:M:196[B]:VAL:HG22	2.16	0.45
3:O:112:VAL:CG2	4:P:32:TYR:HA	2.47	0.45
3:M:115:PHE:C	3:M:116:ASP:CA	2.78	0.45
4:T:78:LEU:CD2	4:T:102:ILE:HG13	2.32	0.45
2:B:22:TYR:HD2	2:B:40:SER:OG	2.00	0.44
1:K:178:ILE:HD12	1:K:198:ILE:HD12	1.98	0.44
3:U:111:ASN:OD1	3:U:113:ASP:N	2.30	0.44
1:C:160:ILE:O	1:C:242:GLU:HA	2.17	0.44
2:J:18:VAL:HG12	3:U:111:ASN:HB3	1.99	0.44
3:W:111:ASN:ND2	3:W:113:ASP:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:28:SER:O	4:X:29:LEU:HD23	2.17	0.44
2:H:110:PHE:CD2	1:I:20:MET:HE1	2.52	0.44
2:J:66:VAL:HG21	2:L:83:LYS:HE2	1.99	0.44
1:G:160:ILE:O	1:G:242:GLU:HA	2.17	0.44
1:I:160:ILE:O	1:I:242:GLU:HA	2.17	0.44
4:P:89:GLN:NE2	4:P:91:SER:O	2.45	0.44
1:A:212:ARG:NH2	1:E:206:ASN:O	2.50	0.44
1:E:291:PHE:HZ	2:F:59:MET:HG3	1.82	0.44
1:G:291:PHE:HZ	2:H:59:MET:HG3	1.83	0.44
4:P:28:SER:HB2	4:P:68:GLY:O	2.17	0.44
1:E:317:LEU:HB3	2:F:111:HIS:CG	2.53	0.44
4:X:25:THR:HG21	4:X:71:PHE:HE1	1.82	0.44
1:G:216:ARG:NH1	1:K:206:ASN:OD1	2.51	0.44
3:W:103:GLY:HA3	3:W:111:ASN:OD1	2.17	0.44
1:C:51:ILE:HD12	1:C:271:TYR:HB2	1.99	0.44
6:R:28:SER:O	6:R:29:LEU:HD23	2.18	0.44
4:V:25:THR:HG1	4:V:90:GLN:CD	2.19	0.44
4:N:28:SER:O	4:N:29:LEU:HD23	2.18	0.44
6:R:104:ARG:HD2	6:R:166:ASP:O	2.17	0.44
4:V:102:ILE:CD1	4:V:102:ILE:N	2.81	0.43
1:G:51:ILE:HD12	1:G:271:TYR:HB2	2.00	0.43
1:K:45:ASP:C	1:K:47:VAL:H	2.22	0.43
4:V:12:SER:OG	4:V:101:GLU:OE2	2.35	0.43
3:W:2:VAL:HG21	3:W:101:ARG:CZ	2.48	0.43
1:E:196:THR:HG22	1:E:244:ASN:HB3	2.00	0.43
4:X:102:ILE:CD1	4:X:102:ILE:N	2.82	0.43
4:X:32:TYR:N	4:X:32:TYR:CD2	2.87	0.43
1:C:46:GLY:N	1:C:47:VAL:N	2.67	0.43
4:T:12:SER:OG	4:T:101:GLU:OE2	2.35	0.43
1:A:130:GLY:HA3	1:A:149:TRP:HB3	2.01	0.43
1:G:196:THR:HG22	1:G:244:ASN:HB3	2.00	0.43
1:A:196:THR:HG22	1:A:244:ASN:HB3	2.01	0.43
4:N:89:GLN:NE2	4:N:91:SER:O	2.42	0.43
4:P:28:SER:O	4:P:29:LEU:HD23	2.19	0.43
3:U:112:VAL:CG2	4:V:32:TYR:HA	2.48	0.43
4:V:28:SER:HB2	4:V:68:GLY:C	2.39	0.43
3:M:154:GLY:CA	3:M:196[A]:VAL:HG23	2.47	0.42
4:N:102:ILE:CD1	4:N:102:ILE:N	2.82	0.42
2:J:19:ASP:OD2	4:V:92:ARG:NH2	2.52	0.42
3:M:195:SER:O	3:M:196[B]:VAL:HG13	2.15	0.42
4:X:47:LEU:HD11	4:X:62:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLY:HA3	1:C:149:TRP:HB3	2.01	0.42
1:C:240:ASN:HB3	1:E:215:THR:HB	2.01	0.42
4:N:4:MET:HE1	4:N:90:GLN:HG3	2.02	0.42
3:S:2:VAL:HG21	3:S:101:ARG:NH1	2.35	0.42
1:I:100:GLU:OE1	2:L:75:ARG:N	2.42	0.42
4:P:47:LEU:HD11	4:P:62:PHE:CG	2.55	0.42
3:S:102:SER:HB3	3:S:115:PHE:CD1	2.55	0.42
1:C:196:THR:HG22	1:C:244:ASN:HB3	2.00	0.42
2:D:38:LYS:HD2	4:P:32:TYR:HE1	1.79	0.42
4:V:32:TYR:O	4:V:90:GLN:HA	2.20	0.42
4:X:12:SER:OG	4:X:101:GLU:OE2	2.36	0.42
1:I:196:THR:HG22	1:I:244:ASN:HB3	2.00	0.42
5:Q:102:SER:HB3	5:Q:115:PHE:CD1	2.54	0.42
4:V:29:LEU:HD13	4:V:32:TYR:CD2	2.55	0.42
6:R:12:SER:CB	6:R:103:LYS:CB	2.97	0.41
4:T:13:ALA:O	4:T:102:ILE:HG23	2.20	0.41
1:E:290:PRO:HG3	2:F:56:ILE:HG12	2.02	0.41
1:G:130:GLY:HA3	1:G:149:TRP:HB3	2.01	0.41
1:K:196:THR:HG22	1:K:244:ASN:HB3	2.01	0.41
1:E:130:GLY:HA3	1:E:149:TRP:HB3	2.02	0.41
4:X:32:TYR:O	4:X:90:GLN:HA	2.20	0.41
3:U:112:VAL:HG21	4:V:31:SER:O	2.21	0.41
1:C:291:PHE:HZ	2:D:59:MET:HG3	1.86	0.41
4:N:47:LEU:HD11	4:N:62:PHE:CG	2.56	0.41
3:O:181:PHE:HE1	3:O:196[A]:VAL:CG1	2.34	0.41
3:S:102:SER:HB3	3:S:115:PHE:HD1	1.86	0.41
1:G:20:MET:HE2	2:L:51:LYS:HE3	2.03	0.41
4:T:47:LEU:HD11	4:T:62:PHE:CG	2.55	0.41
4:V:28:SER:O	4:V:29:LEU:HD23	2.21	0.41
1:G:317:LEU:HB3	2:H:111:HIS:CG	2.56	0.41
4:T:28:SER:O	4:T:29:LEU:HD23	2.21	0.41
1:I:130:GLY:HA3	1:I:149:TRP:HB3	2.02	0.41
4:N:25:THR:OG1	4:N:90:GLN:OE1	2.38	0.41
4:X:32:TYR:N	4:X:32:TYR:HD2	2.18	0.41
3:M:2:VAL:HG21	3:M:101:ARG:CZ	2.52	0.40
4:N:145:LYS:HG2	4:N:150:LEU:HD23	2.01	0.40
4:P:32:TYR:O	4:P:90:GLN:HA	2.20	0.40
4:V:47:LEU:HD11	4:V:62:PHE:CG	2.56	0.40
1:I:51:ILE:HD12	1:I:271:TYR:HB2	2.03	0.40
1:K:130:GLY:HA3	1:K:149:TRP:HB3	2.02	0.40
5:Q:158:LYS:HD2	5:Q:192:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:25:THR:HG22	6:R:69:THR:O	2.22	0.40
4:T:159:VAL:HG22	4:T:171:LEU:HD12	2.04	0.40
4:N:145:LYS:HE2	4:N:150:LEU:HD21	2.03	0.40
4:N:25:THR:HG21	4:N:71:PHE:HE1	1.87	0.40

All (2) 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:C:169:GLN:CG	3:O:219:ASN:OD1[2_655]	1.93	0.27
1:C:252:TYR:CE1	3:O:79:LYS:CE[2_655]	2.05	0.15

## 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	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	C	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	E	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	G	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	I	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
1	K	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
2	B	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	D	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	F	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	H	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	J	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	L	160/162 (99%)	156 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	217/227 (96%)	210 (97%)	7 (3%)	0	100	100
3	O	217/227 (96%)	211 (97%)	6 (3%)	0	100	100
3	S	217/227 (96%)	212 (98%)	5 (2%)	0	100	100
3	U	217/227 (96%)	211 (97%)	6 (3%)	0	100	100
3	W	217/227 (96%)	210 (97%)	7 (3%)	0	100	100
4	N	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	P	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	T	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	V	204/206 (99%)	200 (98%)	4 (2%)	0	100	100
4	X	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
5	Q	167/231 (72%)	163 (98%)	4 (2%)	0	100	100
6	R	136/210 (65%)	133 (98%)	3 (2%)	0	100	100
All	All	5288/5504 (96%)	5151 (97%)	137 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	290/289 (100%)	288 (99%)	2 (1%)	88	95
1	C	290/289 (100%)	288 (99%)	2 (1%)	88	95
1	E	290/289 (100%)	288 (99%)	2 (1%)	88	95
1	G	290/289 (100%)	288 (99%)	2 (1%)	88	95
1	I	290/289 (100%)	288 (99%)	2 (1%)	88	95
1	K	290/289 (100%)	288 (99%)	2 (1%)	88	95
2	B	138/138 (100%)	137 (99%)	1 (1%)	88	95
2	D	138/138 (100%)	138 (100%)	0	100	100
2	F	138/138 (100%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	138/138 (100%)	138 (100%)	0	100	100
2	J	138/138 (100%)	138 (100%)	0	100	100
2	L	138/138 (100%)	138 (100%)	0	100	100
3	M	195/198 (98%)	195 (100%)	0	100	100
3	O	195/198 (98%)	195 (100%)	0	100	100
3	S	195/198 (98%)	194 (100%)	1 (0%)	92	97
3	U	195/198 (98%)	195 (100%)	0	100	100
3	W	195/198 (98%)	195 (100%)	0	100	100
4	N	181/181 (100%)	180 (99%)	1 (1%)	90	96
4	P	181/181 (100%)	179 (99%)	2 (1%)	80	92
4	T	181/181 (100%)	179 (99%)	2 (1%)	80	92
4	V	181/181 (100%)	179 (99%)	2 (1%)	80	92
4	X	181/181 (100%)	179 (99%)	2 (1%)	80	92
5	Q	157/201 (78%)	157 (100%)	0	100	100
6	R	130/185 (70%)	128 (98%)	2 (2%)	72	90
All	All	4735/4843 (98%)	4710 (100%)	25 (0%)	92	97

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ARG
1	A	178	ILE
2	B	22	TYR
1	C	162	ARG
1	C	178	ILE
1	E	162	ARG
1	E	178	ILE
1	G	162	ARG
1	G	178	ILE
1	I	162	ARG
1	I	178	ILE
1	K	162	ARG
1	K	178	ILE
4	N	26	SER
4	P	12	SER
4	P	26	SER
6	R	26	SER

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Mol	Chain	Res	Type
6	R	92	ARG
3	S	117	MET
4	T	12	SER
4	T	26	SER
4	V	12	SER
4	V	26	SER
4	X	12	SER
4	X	26	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	246	ASN
1	C	28	HIS
1	C	246	ASN
2	D	79	ASN
1	E	28	HIS
1	E	236	ASN
1	E	246	ASN
2	F	79	ASN
1	G	28	HIS
1	G	246	ASN
2	H	79	ASN
1	I	28	HIS
1	I	246	ASN
2	J	79	ASN
1	K	28	HIS
1	K	236	ASN
1	K	246	ASN
4	N	90	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

30 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	$\# Z  > 2$
7	NAG	A	401	1	14,14,15	0.74	1 (7%)	15,19,21	1.86	4 (26%)
7	NAG	A	402	1	14,14,15	0.47	0	15,19,21	1.22	2 (13%)
7	NAG	A	403	1	14,14,15	0.30	0	15,19,21	1.07	1 (6%)
7	NAG	B	201	2,7	14,14,15	0.63	0	15,19,21	1.87	4 (26%)
7	NAG	B	202	7	14,14,15	0.47	0	15,19,21	0.93	0
7	NAG	C	401	1	14,14,15	0.42	0	15,19,21	1.87	4 (26%)
7	NAG	C	402	1	14,14,15	0.36	0	15,19,21	1.57	2 (13%)
7	NAG	C	403	1	14,14,15	0.31	0	15,19,21	0.78	0
7	NAG	D	201	2	14,14,15	0.38	0	15,19,21	1.89	3 (20%)
7	NAG	E	401	1,7	14,14,15	1.01	2 (14%)	15,19,21	3.19	7 (46%)
7	NAG	E	402	7	14,14,15	1.40	2 (14%)	15,19,21	3.05	6 (40%)
7	NAG	E	403	1	14,14,15	0.40	0	15,19,21	1.28	2 (13%)
7	NAG	E	404	1	14,14,15	1.40	1 (7%)	15,19,21	1.36	3 (20%)
7	NAG	F	201	2,7	14,14,15	1.08	1 (7%)	15,19,21	1.52	4 (26%)
7	NAG	F	202	7	14,14,15	0.37	0	15,19,21	1.13	1 (6%)
7	NAG	G	401	1	14,14,15	0.74	1 (7%)	15,19,21	1.86	5 (33%)
7	NAG	G	402	1	14,14,15	0.37	0	15,19,21	1.28	2 (13%)
7	NAG	G	403	1	14,14,15	0.38	0	15,19,21	0.70	0
7	NAG	H	201	2,7	14,14,15	0.72	1 (7%)	15,19,21	1.36	2 (13%)
7	NAG	H	202	7	14,14,15	0.39	0	15,19,21	1.01	0
7	NAG	I	401	1	14,14,15	0.99	1 (7%)	15,19,21	1.87	3 (20%)
7	NAG	I	402	1	14,14,15	0.26	0	15,19,21	1.30	3 (20%)
7	NAG	I	403	1	14,14,15	0.28	0	15,19,21	0.93	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	J	201	2,7	14,14,15	0.76	0	15,19,21	1.81	3 (20%)
7	NAG	J	202	7	14,14,15	0.47	0	15,19,21	0.97	0
7	NAG	K	401	1	14,14,15	0.79	0	15,19,21	3.12	7 (46%)
7	NAG	K	402	-	14,14,15	1.45	2 (14%)	15,19,21	2.91	2 (13%)
7	NAG	K	403	1	14,14,15	0.37	0	15,19,21	1.52	2 (13%)
7	NAG	K	404	1	14,14,15	0.80	1 (7%)	15,19,21	0.82	0
7	NAG	L	201	2	14,14,15	0.39	0	15,19,21	1.15	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	401	1	-	0/6/23/26	0/1/1/1
7	NAG	A	402	1	-	0/6/23/26	0/1/1/1
7	NAG	A	403	1	-	0/6/23/26	0/1/1/1
7	NAG	B	201	2,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	B	202	7	-	0/6/23/26	0/1/1/1
7	NAG	C	401	1	-	0/6/23/26	0/1/1/1
7	NAG	C	402	1	-	0/6/23/26	0/1/1/1
7	NAG	C	403	1	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	E	401	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	402	7	-	0/6/23/26	0/1/1/1
7	NAG	E	403	1	-	0/6/23/26	0/1/1/1
7	NAG	E	404	1	-	0/6/23/26	0/1/1/1
7	NAG	F	201	2,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	F	202	7	-	0/6/23/26	0/1/1/1
7	NAG	G	401	1	-	0/6/23/26	0/1/1/1
7	NAG	G	402	1	-	0/6/23/26	0/1/1/1
7	NAG	G	403	1	-	0/6/23/26	0/1/1/1
7	NAG	H	201	2,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	H	202	7	-	0/6/23/26	0/1/1/1
7	NAG	I	401	1	-	0/6/23/26	0/1/1/1
7	NAG	I	402	1	-	0/6/23/26	0/1/1/1
7	NAG	I	403	1	-	0/6/23/26	0/1/1/1
7	NAG	J	201	2,7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	J	202	7	-	0/6/23/26	0/1/1/1
7	NAG	K	401	1	-	0/6/23/26	0/1/1/1
7	NAG	K	402	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	403	1	-	0/6/23/26	0/1/1/1
7	NAG	K	404	1	-	0/6/23/26	0/1/1/1
7	NAG	L	201	2	1/1/5/7	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	201	NAG	O5-C1	-3.33	1.38	1.43
7	I	401	NAG	O5-C1	-2.61	1.39	1.43
7	G	401	NAG	C1-C2	-2.52	1.48	1.52
7	E	401	NAG	C3-C2	-2.21	1.47	1.52
7	E	401	NAG	O5-C1	-2.20	1.40	1.43
7	H	201	NAG	O5-C1	-2.19	1.40	1.43
7	K	402	NAG	C2-N2	2.12	1.50	1.46
7	E	402	NAG	C2-N2	2.18	1.50	1.46
7	A	401	NAG	C1-C2	2.29	1.55	1.52
7	K	404	NAG	C1-C2	2.89	1.56	1.52
7	E	402	NAG	C1-C2	4.39	1.58	1.52
7	E	404	NAG	C1-C2	4.67	1.59	1.52
7	K	402	NAG	C1-C2	4.74	1.59	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	401	NAG	O4-C4-C3	-6.54	95.62	110.36
7	E	401	NAG	O4-C4-C3	-6.42	95.89	110.36
7	E	401	NAG	O5-C5-C4	-4.49	102.70	110.13
7	K	401	NAG	O5-C5-C4	-3.65	104.09	110.13
7	G	401	NAG	O5-C5-C4	-3.33	104.62	110.13
7	I	401	NAG	O5-C5-C4	-3.21	104.82	110.13
7	K	401	NAG	O3-C3-C4	-2.94	103.74	110.36
7	G	401	NAG	C1-O5-C5	-2.93	107.83	112.14
7	E	401	NAG	C1-O5-C5	-2.87	107.92	112.14
7	A	401	NAG	O5-C5-C4	-2.76	105.56	110.13
7	C	401	NAG	O7-C7-C8	-2.66	117.18	122.07
7	C	401	NAG	O5-C5-C4	-2.65	105.75	110.13
7	F	202	NAG	O5-C5-C4	-2.61	105.81	110.13
7	H	201	NAG	C4-C3-C2	-2.59	107.31	111.34
7	F	201	NAG	O5-C5-C6	-2.43	102.14	107.34
7	E	401	NAG	O3-C3-C4	-2.42	104.90	110.36
7	A	401	NAG	O7-C7-C8	-2.36	117.73	122.07
7	K	401	NAG	O7-C7-C8	-2.34	117.77	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	401	NAG	O7-C7-C8	-2.30	117.84	122.07
7	E	404	NAG	O5-C5-C4	-2.24	106.42	110.13
7	J	201	NAG	O3-C3-C4	-2.20	105.40	110.36
7	E	402	NAG	C8-C7-N2	-2.17	111.94	116.10
7	B	201	NAG	O7-C7-C8	-2.08	118.24	122.07
7	F	201	NAG	O4-C4-C5	2.00	114.50	109.23
7	F	201	NAG	C2-N2-C7	2.16	125.91	123.11
7	K	403	NAG	C2-N2-C7	2.16	125.92	123.11
7	C	402	NAG	C2-N2-C7	2.17	125.93	123.11
7	H	201	NAG	C2-N2-C7	2.17	125.93	123.11
7	A	403	NAG	C1-O5-C5	2.20	115.38	112.14
7	E	404	NAG	C2-N2-C7	2.26	126.04	123.11
7	E	402	NAG	C2-N2-C7	2.28	126.07	123.11
7	B	201	NAG	C2-N2-C7	2.31	126.10	123.11
7	E	403	NAG	O5-C5-C6	2.36	112.39	107.34
7	G	402	NAG	C2-N2-C7	2.41	126.25	123.11
7	I	402	NAG	O5-C5-C6	2.43	112.55	107.34
7	E	402	NAG	O7-C7-C8	2.46	126.60	122.07
7	I	402	NAG	C1-O5-C5	2.49	115.80	112.14
7	A	402	NAG	C1-O5-C5	2.52	115.85	112.14
7	A	402	NAG	O5-C5-C6	2.55	112.79	107.34
7	L	201	NAG	C8-C7-N2	2.60	121.08	116.10
7	I	402	NAG	C2-N2-C7	2.61	126.50	123.11
7	E	402	NAG	O5-C5-C4	2.63	114.49	110.13
7	G	402	NAG	O5-C5-C6	2.68	113.08	107.34
7	E	404	NAG	C1-O5-C5	2.76	116.20	112.14
7	F	201	NAG	C8-C7-N2	2.77	121.41	116.10
7	J	201	NAG	C8-C7-N2	2.83	121.52	116.10
7	E	402	NAG	C4-C3-C2	2.85	115.77	111.34
7	E	401	NAG	C8-C7-N2	2.87	121.59	116.10
7	D	201	NAG	C2-N2-C7	2.99	126.99	123.11
7	G	401	NAG	C2-N2-C7	2.99	127.00	123.11
7	D	201	NAG	C8-C7-N2	3.01	121.86	116.10
7	E	403	NAG	C2-N2-C7	3.01	127.02	123.11
7	B	201	NAG	C8-C7-N2	3.02	121.88	116.10
7	I	401	NAG	C8-C7-N2	3.14	122.12	116.10
7	K	401	NAG	C8-C7-N2	3.39	122.59	116.10
7	G	401	NAG	C8-C7-N2	3.39	122.60	116.10
7	A	401	NAG	C8-C7-N2	3.46	122.72	116.10
7	C	401	NAG	C8-C7-N2	3.71	123.22	116.10
7	C	401	NAG	C2-N2-C7	3.86	128.12	123.11
7	K	402	NAG	O5-C5-C4	3.96	116.70	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	401	NAG	C2-N2-C7	4.19	128.56	123.11
7	A	401	NAG	C2-N2-C7	4.29	128.68	123.11
7	D	201	NAG	C1-O5-C5	4.37	118.56	112.14
7	E	401	NAG	C2-N2-C7	4.54	129.01	123.11
7	J	201	NAG	C1-O5-C5	4.57	118.86	112.14
7	K	403	NAG	C1-O5-C5	4.64	118.97	112.14
7	K	401	NAG	C2-N2-C7	4.70	129.22	123.11
7	C	402	NAG	C1-O5-C5	4.85	119.27	112.14
7	B	201	NAG	C1-O5-C5	4.91	119.35	112.14
7	K	401	NAG	O4-C4-C5	5.80	124.50	109.23
7	E	401	NAG	O4-C4-C5	6.42	126.15	109.23
7	K	402	NAG	C1-O5-C5	10.23	127.18	112.14
7	E	402	NAG	C1-O5-C5	10.28	127.25	112.14

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	H	201	NAG	C1
7	B	201	NAG	C1
7	J	201	NAG	C1
7	D	201	NAG	C1
7	F	201	NAG	C1
7	L	201	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	401	NAG	1	0
7	C	401	NAG	1	0
7	E	401	NAG	3	0
7	E	402	NAG	11	0
7	G	401	NAG	1	0
7	I	401	NAG	1	0
7	K	401	NAG	3	0
7	K	402	NAG	5	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	W	4
3	M	3
3	U	2
3	O	2
6	R	2
3	S	2
5	Q	1
1	K	1
1	C	1
4	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	196[B]:VAL	C	197:VAL	N	3.54
1	W	196[A]:VAL	C	197:VAL	N	3.43
1	Q	128:SER	C	129:ALA	N	3.05
1	O	196[B]:VAL	C	197:VAL	N	2.49
1	R	102:ILE	C	103:LYS	N	2.49
1	O	196[A]:VAL	C	197:VAL	N	2.45
1	U	196[A]:VAL	C	197:VAL	N	2.32
1	U	196[B]:VAL	C	197:VAL	N	2.28
1	M	196[B]:VAL	C	197:VAL	N	2.22
1	S	196[A]:VAL	C	197:VAL	N	2.22
1	S	196[B]:VAL	C	197:VAL	N	2.21
1	M	196[A]:VAL	C	197:VAL	N	2.20
1	W	195:SER	C	196[B]:VAL	N	2.06
1	R	103:LYS	C	104:ARG	N	1.94
1	W	195:SER	C	196[A]:VAL	N	1.91
1	C	46:GLY	C	47:VAL	N	1.79
1	T	24:ARG	C	25:THR	N	1.78
1	M	115:PHE	C	116:ASP	N	1.73
1	K	46:GLY	C	47:VAL	N	1.67

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	321/321 (100%)	0.18	14 (4%) 38 25	107, 166, 215, 249	0
1	C	321/321 (100%)	0.05	4 (1%) 81 68	106, 154, 211, 232	0
1	E	321/321 (100%)	-0.06	2 (0%) 90 83	101, 145, 164, 177	0
1	G	321/321 (100%)	0.24	14 (4%) 38 25	118, 199, 244, 262	0
1	I	321/321 (100%)	0.45	28 (8%) 13 8	123, 214, 247, 264	0
1	K	321/321 (100%)	0.23	17 (5%) 30 20	125, 193, 231, 253	0
2	B	162/162 (100%)	-0.02	0 100 100	104, 122, 149, 161	0
2	D	162/162 (100%)	0.04	3 (1%) 70 55	104, 118, 136, 142	0
2	F	162/162 (100%)	0.03	2 (1%) 81 68	104, 117, 141, 152	0
2	H	162/162 (100%)	0.03	2 (1%) 81 68	112, 132, 173, 191	0
2	J	162/162 (100%)	0.12	2 (1%) 81 68	125, 138, 174, 189	0
2	L	162/162 (100%)	0.03	1 (0%) 90 83	121, 134, 174, 199	0
3	M	223/227 (98%)	-0.02	0 100 100	105, 134, 161, 179	0
3	O	223/227 (98%)	0.18	1 (0%) 93 88	109, 139, 186, 205	0
3	S	223/227 (98%)	0.27	4 (1%) 71 57	117, 168, 210, 220	0
3	U	223/227 (98%)	0.07	6 (2%) 58 42	112, 134, 161, 174	0
3	W	223/227 (98%)	0.18	4 (1%) 71 57	120, 145, 182, 196	0
4	N	206/206 (100%)	-0.03	2 (0%) 84 72	106, 124, 153, 170	0
4	P	206/206 (100%)	0.26	4 (1%) 70 55	109, 154, 180, 192	0
4	T	206/206 (100%)	0.56	18 (8%) 13 8	134, 188, 231, 238	0
4	V	206/206 (100%)	-0.08	2 (0%) 84 72	115, 131, 155, 166	0
4	X	206/206 (100%)	0.16	1 (0%) 91 86	124, 151, 182, 189	0
5	Q	177/231 (76%)	0.20	5 (2%) 56 41	101, 124, 161, 161	0
6	R	148/210 (70%)	0.19	4 (2%) 58 42	103, 134, 162, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5368/5504 (97%)	0.15	140 (2%) 59 43	101, 144, 223, 264	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	163	SER	6.1
1	K	199	SER	5.0
1	K	242	GLU	4.8
1	A	140	LYS	4.8
1	I	134	ALA	4.7
1	A	163	SER	4.3
1	K	208	ARG	3.7
6	R	130	CYS	3.6
2	L	19	ASP	3.6
4	T	17	ASP	3.6
1	A	1	ASP	3.6
1	A	152	LYS	3.5
1	I	177	GLY	3.5
1	I	218	LYS	3.5
2	D	144	CYS	3.4
3	W	149	GLY	3.4
6	R	195	GLN	3.3
2	J	144	CYS	3.3
1	I	217	SER	3.3
3	W	81	GLN	3.2
4	T	167	SER	3.2
4	T	152	SER	3.2
1	K	139	GLY	3.2
4	T	190	CYS	3.2
1	E	260	GLY	3.2
1	I	159	THR	3.2
2	D	147	GLU	3.1
1	I	146	ASN	3.1
1	I	130	GLY	3.0
1	C	139	GLY	3.0
1	E	212	ARG	3.0
1	I	181	PRO	3.0
5	Q	222	VAL	3.0
1	I	183	ASP	2.9
1	G	156	THR	2.9
1	A	153	LYS	2.9
4	V	149	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	138	GLN	2.9
3	U	226	VAL	2.9
4	P	138	ARG	2.9
1	G	246	ASN	2.8
4	T	4	MET	2.8
4	T	187	VAL	2.8
4	T	107	ALA	2.8
1	K	210	VAL	2.7
4	T	106	VAL	2.7
4	T	146	VAL	2.7
1	A	146	ASN	2.7
1	A	141	SER	2.7
1	I	202	THR	2.6
1	I	1	ASP	2.6
1	C	126	GLU	2.6
4	T	191	GLU	2.6
1	K	207	GLN	2.5
1	I	242	GLU	2.5
5	Q	213	VAL	2.5
1	I	171	ASP	2.5
1	I	179	HIS	2.5
3	U	225	LYS	2.5
3	S	155	CYS	2.5
1	A	237	ASP	2.5
1	K	94	ASP	2.5
3	W	209	TYR	2.5
1	G	43	ASP	2.4
3	U	209	TYR	2.4
1	K	75	GLU	2.4
1	K	209	LEU	2.4
1	I	154	ASN	2.4
3	U	151	ALA	2.4
4	T	181	ASP	2.4
1	G	263	THR	2.4
6	R	190	CYS	2.4
4	P	174	THR	2.4
3	S	206	THR	2.4
3	S	154	GLY	2.4
1	G	146	ASN	2.4
1	G	139	GLY	2.4
1	G	208	ARG	2.4
5	Q	180	THR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	88	ASP	2.3
3	S	175	THR	2.3
1	I	314	ALA	2.3
1	A	320	SER	2.3
2	F	162	TYR	2.3
2	H	162	TYR	2.3
1	I	222	GLN	2.3
4	T	151	GLN	2.3
4	P	4	MET	2.3
1	G	159	THR	2.3
1	K	70	PHE	2.3
1	I	92	PRO	2.3
3	W	80	ASN	2.3
1	I	91	TYR	2.3
6	R	113	ILE	2.3
1	G	176	TRP	2.2
1	I	156	THR	2.2
1	K	93	GLY	2.2
1	A	273	ASN	2.2
3	U	1	GLN	2.2
4	T	57	GLY	2.2
1	A	194	PRO	2.2
1	C	138	GLN	2.2
1	K	140	LYS	2.2
1	G	236	ASN	2.2
1	G	213	ILE	2.2
1	G	214	ALA	2.2
4	N	24	ARG	2.2
4	T	169	TYR	2.2
4	T	80	PRO	2.2
3	U	198	THR	2.2
4	T	103	LYS	2.1
4	T	206	ASN	2.1
1	I	219	VAL	2.1
1	I	215	THR	2.1
5	Q	90	THR	2.1
1	I	269	LEU	2.1
1	I	220	ASN	2.1
1	I	203	SER	2.1
4	X	139	GLU	2.1
1	A	238	ALA	2.1
1	K	153	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	157	TYR	2.1
1	G	94	ASP	2.1
1	A	139	GLY	2.1
1	K	315	THR	2.1
5	Q	89	VAL	2.1
1	A	220	ASN	2.1
2	F	157	TYR	2.1
2	J	70	PHE	2.1
4	N	4	MET	2.1
4	V	4	MET	2.1
4	P	184	LYS	2.0
2	D	145	ASP	2.0
1	G	46	GLY	2.0
1	K	230	TRP	2.0
1	K	243	SER	2.0
1	I	207	GLN	2.0
1	C	219	VAL	2.0
3	O	197	VAL	2.0
4	T	148	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	K	401	14/15	0.91	0.39	0.95	139,139,139,139	0
7	NAG	C	401	14/15	0.70	0.35	0.89	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	G	401	14/15	0.79	0.46	0.57	139,139,139,139	0
7	NAG	I	401	14/15	0.81	0.27	-0.48	139,139,139,139	0
7	NAG	C	402	14/15	0.77	0.33	-	139,139,139,139	0
7	NAG	J	201	14/15	0.81	0.31	-	184,186,187,188	0
7	NAG	I	402	14/15	0.87	0.26	-	139,139,139,139	0
7	NAG	E	404	14/15	0.84	0.26	-	139,139,139,139	0
7	NAG	F	202	14/15	0.87	0.41	-	190,191,194,196	0
7	NAG	B	202	14/15	0.75	0.40	-	182,185,188,188	0
7	NAG	E	401	14/15	0.75	0.52	-	139,139,139,139	0
7	NAG	K	404	14/15	0.85	0.62	-	139,139,139,139	0
7	NAG	K	403	14/15	0.65	0.47	-	139,139,139,139	0
7	NAG	J	202	14/15	0.75	0.29	-	189,190,192,192	0
7	NAG	A	402	14/15	0.79	0.28	-	139,139,139,139	0
7	NAG	E	402	14/15	0.64	0.61	-	139,139,139,139	0
7	NAG	A	401	14/15	0.72	0.38	-	139,139,139,139	0
7	NAG	G	402	14/15	0.88	0.26	-	139,139,139,139	0
7	NAG	G	403	14/15	0.79	0.33	-	139,139,139,139	0
7	NAG	K	402	14/15	0.79	0.49	-	139,139,139,139	0
7	NAG	C	403	14/15	0.88	0.50	-	139,139,139,139	0
7	NAG	H	201	14/15	0.92	0.27	-	188,189,192,192	0
7	NAG	A	403	14/15	0.89	0.30	-	139,139,139,139	0
7	NAG	E	403	14/15	0.82	0.30	-	139,139,139,139	0
7	NAG	I	403	14/15	0.70	0.33	-	139,139,139,139	0
7	NAG	D	201	14/15	0.62	0.42	-	174,176,178,178	0
7	NAG	H	202	14/15	0.83	0.34	-	193,195,196,197	0
7	NAG	F	201	14/15	0.90	0.28	-	182,185,189,189	0
7	NAG	B	201	14/15	0.88	0.41	-	176,178,181,181	0
7	NAG	L	201	14/15	0.71	0.43	-	190,192,195,196	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.