



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:29 am GMT

PDB ID : 2OVW  
Title : ENDOGLUCANASE I COMPLEXED WITH CELLOBIOSE  
Authors : Sulzenbacher, G.; Davies, G.J.; Schulein, M.  
Deposited on : 1997-04-04  
Resolution : 2.30 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

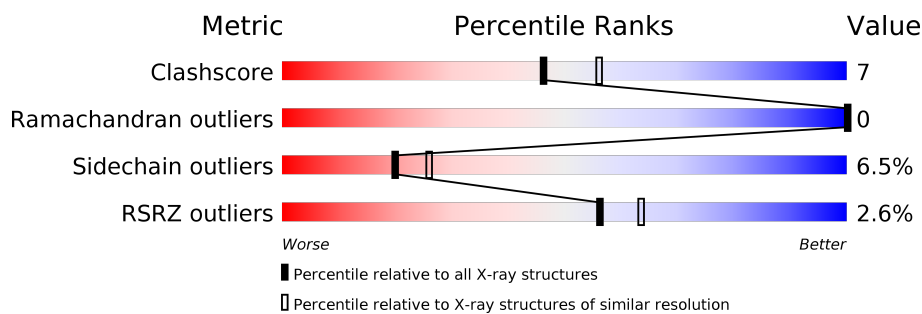
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	411	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>• •</div> </div>
1	B	411	<div> <div>4%</div> <div>75%</div> <div>19%</div> <div>• •</div> </div>
1	C	411	<div> <div>2%</div> <div>74%</div> <div>19%</div> <div>• •</div> </div>
1	D	411	<div> <div>%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	412	-	-	-	X

## 2 Entry composition [i](#)

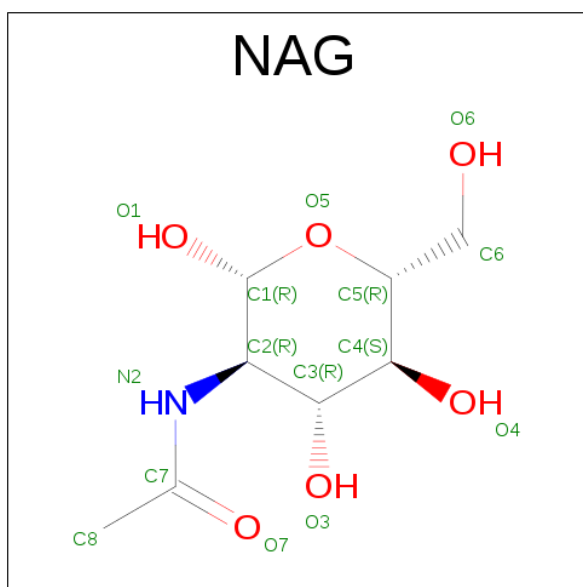
There are 4 unique types of molecules in this entry. The entry contains 13393 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDOGLUCANASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			
1	B	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			
1	C	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			
1	D	398	Total	C	N	O	S	0	0	0
			3022	1870	534	589	29			

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



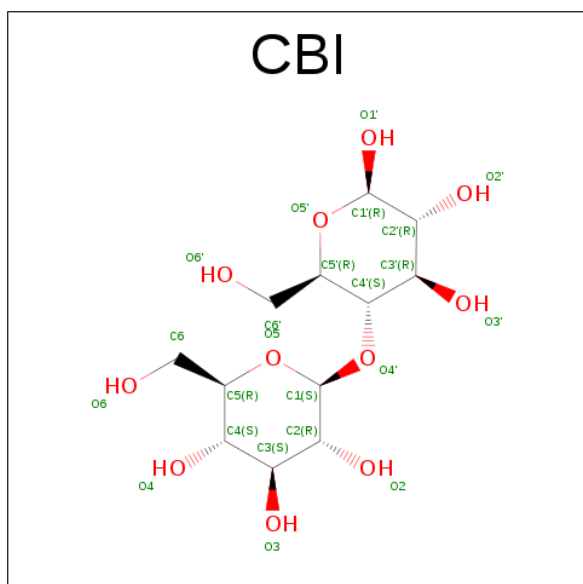
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is SUGAR (LACTOSE) (three-letter code: CBI) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		

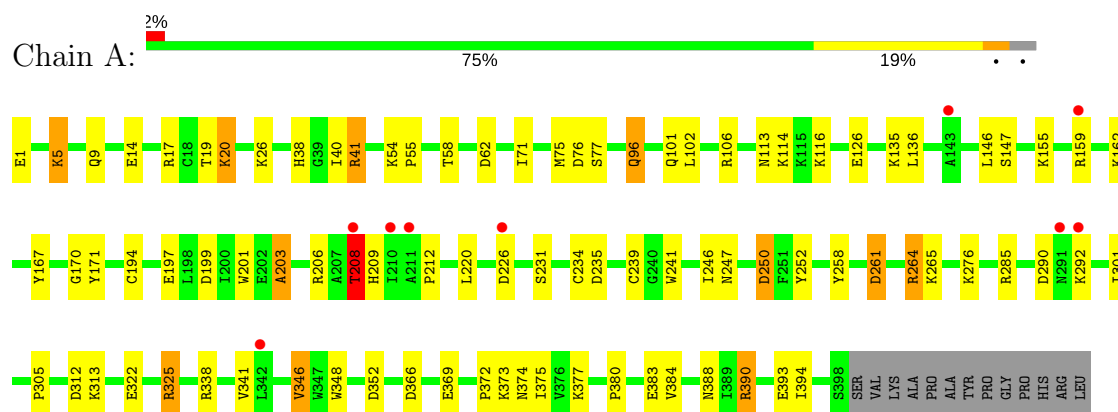
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total 277	O 277	0	0
4	B	268	Total 268	O 268	0	0
4	C	268	Total 268	O 268	0	0
4	D	288	Total 288	O 288	0	0

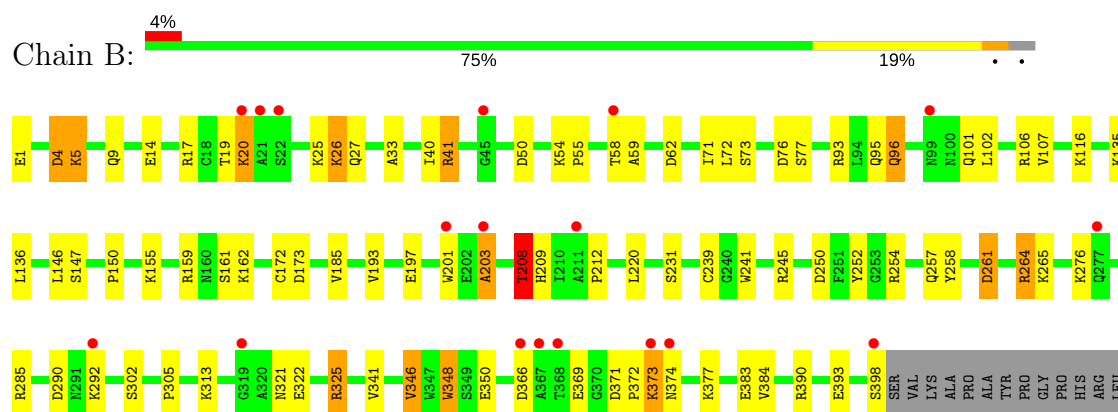
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

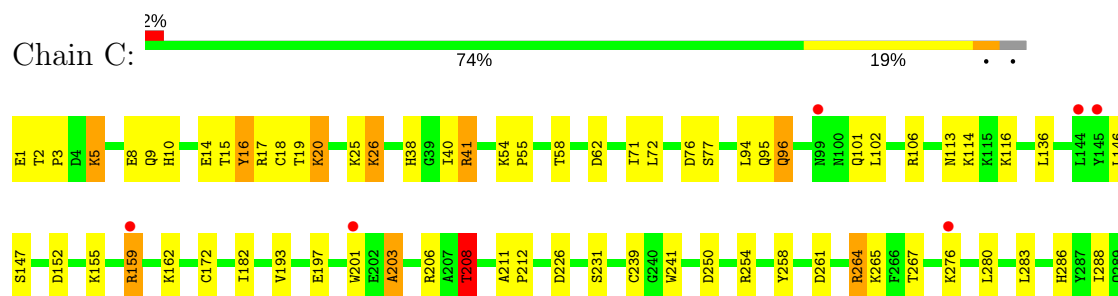
#### • Molecule 1: ENDOGLUCANASE I

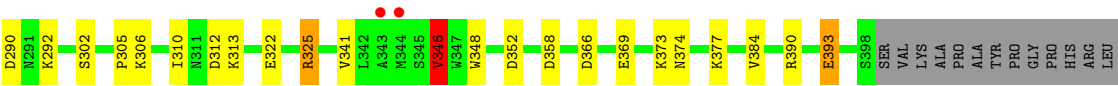


#### • Molecule 1: ENDOGLUCANASE I

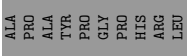
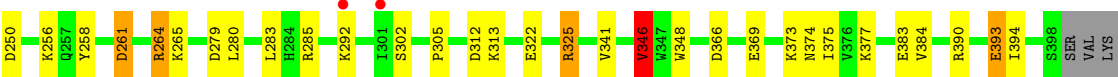
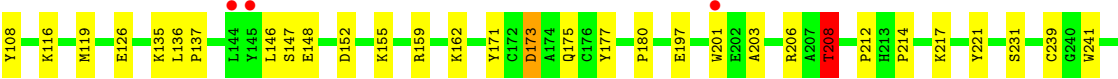


#### • Molecule 1: ENDOGLUCANASE I





● Molecule 1: ENDOGLUCANASE I





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.93Å 78.31Å 142.47Å 90.00° 96.98° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 29.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.4 (15.00-2.30) 86.5 (29.84-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.209 , (Not available) 0.195 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.25% 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: PCA, NAG, CBI

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	0.68	0/3076	1.58	41/4155 (1.0%)
1	B	0.68	0/3076	1.59	40/4155 (1.0%)
1	C	0.70	0/3076	1.57	34/4155 (0.8%)
1	D	0.69	0/3076	1.59	44/4155 (1.1%)
All	All	0.69	0/12304	1.58	159/16620 (1.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	ARG	NE-CZ-NH1	18.48	129.54	120.30
1	A	325	ARG	NE-CZ-NH1	16.49	128.55	120.30
1	C	264	ARG	CD-NE-CZ	15.53	145.34	123.60
1	C	325	ARG	CD-NE-CZ	15.48	145.27	123.60
1	C	325	ARG	NE-CZ-NH1	15.23	127.91	120.30
1	A	325	ARG	CD-NE-CZ	15.17	144.84	123.60
1	A	264	ARG	CD-NE-CZ	14.28	143.59	123.60
1	B	325	ARG	CD-NE-CZ	14.08	143.31	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	B	264	ARG	NE-CZ-NH2	-13.55	113.53	120.30
1	A	41	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	B	264	ARG	CD-NE-CZ	13.23	142.13	123.60
1	D	106	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	D	261	ASP	CB-CG-OD1	12.73	129.76	118.30
1	D	325	ARG	CD-NE-CZ	12.33	140.86	123.60
1	C	325	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	D	264	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	B	41	ARG	CD-NE-CZ	12.21	140.70	123.60
1	B	264	ARG	NE-CZ-NH1	12.03	126.31	120.30
1	A	41	ARG	CD-NE-CZ	11.73	140.02	123.60
1	D	41	ARG	CD-NE-CZ	11.39	139.55	123.60
1	C	41	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	C	41	ARG	CD-NE-CZ	11.01	139.01	123.60
1	B	62	ASP	CB-CG-OD1	10.97	128.18	118.30
1	A	226	ASP	CB-CG-OD2	-10.96	108.44	118.30
1	B	325	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	D	264	ARG	CD-NE-CZ	10.25	137.95	123.60
1	C	62	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	C	254	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	A	206	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	C	106	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	C	312	ASP	CB-CG-OD1	9.12	126.51	118.30
1	A	106	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	390	ARG	CD-NE-CZ	9.08	136.31	123.60
1	D	325	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	325	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	C	41	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	B	261	ASP	CB-CG-OD1	8.72	126.15	118.30
1	D	264	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	285	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	264	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	D	41	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	252	TYR	CB-CG-CD1	8.23	125.94	121.00
1	C	264	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	D	261	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	B	17	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	B	254	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	285	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	390	ARG	CD-NE-CZ	7.70	134.38	123.60
1	C	206	ARG	NE-CZ-NH1	7.52	124.06	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ASP	CB-CG-OD1	7.52	125.07	118.30
1	B	261	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	235	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	373	LYS	CA-CB-CG	7.46	129.81	113.40
1	A	390	ARG	CD-NE-CZ	7.44	134.02	123.60
1	D	16	TYR	CB-CG-CD1	-7.44	116.54	121.00
1	D	285	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	D	108	TYR	CB-CG-CD1	-7.20	116.68	121.00
1	A	338	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	17	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	C	358	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	203	ALA	CB-CA-C	-7.08	99.48	110.10
1	A	264	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	226	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	93	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	208	THR	N-CA-CB	6.85	123.32	110.30
1	A	199	ASP	CB-CG-OD1	-6.85	112.14	118.30
1	A	285	ARG	CD-NE-CZ	6.83	133.16	123.60
1	D	62	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	373	LYS	CA-CB-CG	6.75	128.26	113.40
1	D	16	TYR	CB-CG-CD2	6.75	125.05	121.00
1	A	62	ASP	CB-CG-OD1	6.74	124.37	118.30
1	D	312	ASP	CB-CG-OD1	6.74	124.37	118.30
1	D	173	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	B	241	TRP	N-CA-CB	6.74	122.73	110.60
1	C	346	VAL	CB-CA-C	-6.69	98.69	111.40
1	C	264	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	C	208	THR	N-CA-CB	6.56	122.77	110.30
1	A	208	THR	N-CA-CB	6.56	122.76	110.30
1	A	312	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	4	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	241	TRP	N-CA-CB	6.49	122.29	110.60
1	B	285	ARG	CD-NE-CZ	6.49	132.68	123.60
1	A	62	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	226	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	A	261	ASP	CB-CG-OD1	6.45	124.10	118.30
1	D	208	THR	N-CA-CB	6.39	122.45	110.30
1	B	346	VAL	N-CA-CB	6.38	125.53	111.50
1	D	152	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	373	LYS	CB-CA-C	-6.27	97.85	110.40
1	C	286	HIS	N-CA-CB	6.27	121.88	110.60
1	D	4	ASP	CB-CG-OD1	6.25	123.93	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	LYS	CB-CA-C	-6.21	97.99	110.40
1	A	352	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	206	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	167	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	41	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	346	VAL	N-CA-CB	6.08	124.89	111.50
1	D	34	ASP	CB-CG-OD2	6.06	123.76	118.30
1	B	203	ALA	CB-CA-C	-6.04	101.04	110.10
1	D	241	TRP	N-CA-CB	6.03	121.46	110.60
1	B	398	SER	CA-C-O	-6.00	107.50	120.10
1	D	373	LYS	CA-CB-CG	5.99	126.57	113.40
1	C	390	ARG	CD-NE-CZ	5.94	131.91	123.60
1	A	346	VAL	CB-CA-C	-5.93	100.13	111.40
1	B	290	ASP	CB-CG-OD1	-5.93	112.97	118.30
1	D	346	VAL	N-CA-CB	5.89	124.47	111.50
1	A	346	VAL	N-CA-CB	5.88	124.43	111.50
1	B	50	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	93	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	206	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
1	B	41	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	148	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	B	17	ARG	CD-NE-CZ	5.73	131.62	123.60
1	D	312	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	346	VAL	CB-CA-C	-5.71	100.55	111.40
1	D	177	TYR	CB-CG-CD1	5.71	124.42	121.00
1	A	338	ARG	CG-CD-NE	5.69	123.75	111.80
1	D	180	PRO	N-CA-CB	5.67	110.11	103.30
1	D	104	SER	N-CA-CB	-5.66	102.02	110.50
1	B	373	LYS	CB-CA-C	-5.64	99.12	110.40
1	B	173	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	D	119	MET	CG-SD-CE	5.60	109.16	100.20
1	B	373	LYS	CA-CB-CG	5.55	125.62	113.40
1	C	18	CYS	CB-CA-C	-5.54	99.32	110.40
1	A	285	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	241	TRP	N-CA-CB	5.51	120.51	110.60
1	C	16	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	A	250	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	350	GLU	CA-CB-CG	5.42	125.33	113.40
1	B	59	ALA	CB-CA-C	-5.38	102.03	110.10
1	C	116	LYS	CA-CB-CG	5.38	125.23	113.40
1	D	78	ASN	N-CA-CB	-5.38	100.92	110.60
1	D	285	ARG	CD-NE-CZ	5.36	131.11	123.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	ALA	CB-CA-C	-5.35	102.08	110.10
1	B	390	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	C	352	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	214	PRO	N-CA-CB	5.30	109.66	103.30
1	A	17	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	27	GLN	CB-CA-C	-5.24	99.91	110.40
1	B	208	THR	CA-CB-CG2	-5.24	105.06	112.40
1	B	245	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	A	171	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	159	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	D	108	TYR	CB-CG-CD2	5.18	124.11	121.00
1	C	373	LYS	CB-CA-C	-5.17	100.07	110.40
1	B	398	SER	CA-CB-OG	5.16	125.14	111.20
1	D	171	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	106	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	252	TYR	CB-CG-CD1	5.10	124.06	121.00
1	C	15	THR	N-CA-CB	5.10	119.98	110.30
1	C	17	ARG	CD-NE-CZ	5.09	130.72	123.60
1	C	152	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	170	GLY	N-CA-C	5.05	125.73	113.10
1	B	150	PRO	N-CA-CB	5.05	109.36	103.30
1	A	116	LYS	CA-CB-CG	5.04	124.49	113.40
1	D	116	LYS	CA-CB-CG	5.02	124.44	113.40
1	D	346	VAL	CB-CA-C	-5.01	101.87	111.40
1	D	208	THR	CA-CB-CG2	-5.01	105.38	112.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	PCA	Mainchain
1	B	1	PCA	Mainchain
1	C	1	PCA	Mainchain
1	D	1	PCA	Mainchain

## 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	3022	0	2905	36	1
1	B	3022	0	2905	42	1
1	C	3022	0	2905	49	0
1	D	3022	0	2905	47	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	23	0	22	1	0
3	B	23	0	22	1	0
3	C	23	0	22	1	0
3	D	23	0	22	2	0
4	A	277	0	0	2	0
4	B	268	0	0	4	0
4	C	268	0	0	4	0
4	D	288	0	0	5	0
All	All	13393	0	11812	173	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 7.

All (173) 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:B:203:ALA:HB2	1:B:208:THR:HG23	1.42	1.00
1:C:203:ALA:HB2	1:C:208:THR:HG23	1.47	0.95
1:D:203:ALA:HB2	1:D:208:THR:HG23	1.48	0.94
1:C:5:LYS:HE2	1:C:5:LYS:H	1.34	0.93
1:B:5:LYS:HE2	1:B:5:LYS:H	1.35	0.91
1:D:5:LYS:HE2	1:D:5:LYS:H	1.35	0.91
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.52	0.89
1:A:5:LYS:HE2	1:A:5:LYS:H	1.38	0.85
1:D:197:GLU:OE2	3:D:414:CBI:H1'	1.82	0.79
1:A:197:GLU:OE2	3:A:414:CBI:H1'	1.86	0.74
1:C:201:TRP:CZ3	1:C:208:THR:HG21	2.24	0.72
1:B:54:LYS:HB2	1:B:55:PRO:HD2	1.71	0.72
1:B:261:ASP:OD2	1:B:264:ARG:HD3	1.91	0.71
1:D:201:TRP:CZ3	1:D:208:THR:HG21	2.26	0.70
1:D:261:ASP:OD2	1:D:264:ARG:HD3	1.92	0.69
1:A:54:LYS:HB2	1:A:55:PRO:HD2	1.75	0.69
1:A:261:ASP:OD2	1:A:264:ARG:HD3	1.92	0.68
1:B:116:LYS:HD3	4:B:658:HOH:O	1.94	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TRP:CZ3	1:B:208:THR:HG21	2.28	0.67
1:B:366:ASP:OD1	1:B:369:GLU:HG2	1.94	0.67
1:D:54:LYS:HB2	1:D:55:PRO:HD2	1.76	0.67
1:C:197:GLU:OE2	3:C:414:CBI:H1'	1.96	0.65
1:A:201:TRP:CZ3	1:A:208:THR:HG21	2.31	0.65
1:D:14:GLU:OE1	1:D:26:LYS:HD2	1.98	0.64
1:D:305:PRO:HG3	1:D:313:LYS:HG2	1.80	0.64
1:A:19:THR:HA	1:A:393:GLU:HG2	1.80	0.63
1:C:54:LYS:HB2	1:C:55:PRO:HD2	1.81	0.62
1:B:197:GLU:OE2	3:B:414:CBI:H1'	2.00	0.61
1:D:96:GLN:HE21	1:D:96:GLN:HA	1.66	0.60
1:D:256:LYS:HE2	4:D:1098:HOH:O	2.02	0.60
1:C:261:ASP:OD2	1:C:264:ARG:HD3	2.01	0.60
1:D:279:ASP:OD2	4:D:1023:HOH:O	2.16	0.59
1:C:20:LYS:HG3	1:C:393:GLU:HG3	1.85	0.59
1:C:9:GLN:OE1	1:C:76:ASP:HB2	2.02	0.59
1:B:19:THR:HA	1:B:393:GLU:HG2	1.86	0.58
1:C:305:PRO:HG3	1:C:313:LYS:HG2	1.84	0.58
1:A:96:GLN:HE21	1:A:96:GLN:HA	1.68	0.58
1:A:20:LYS:HG3	1:A:393:GLU:HG3	1.86	0.57
1:B:305:PRO:HG3	1:B:313:LYS:HG2	1.86	0.57
1:B:20:LYS:HG3	1:B:393:GLU:HG3	1.87	0.56
1:B:54:LYS:HB2	1:B:55:PRO:CD	2.36	0.56
1:C:96:GLN:HE21	1:C:96:GLN:HA	1.70	0.56
1:D:9:GLN:OE1	1:D:76:ASP:HB2	2.05	0.56
1:D:54:LYS:HG2	4:D:793:HOH:O	2.05	0.55
1:A:366:ASP:OD1	1:A:369:GLU:HG2	2.06	0.55
1:B:136:LEU:HD11	1:B:384:VAL:HB	1.88	0.55
1:C:366:ASP:CG	1:C:369:GLU:HG2	2.27	0.55
1:D:136:LEU:HD11	1:D:384:VAL:HB	1.89	0.55
1:C:366:ASP:OD1	1:C:369:GLU:HG2	2.06	0.54
1:D:20:LYS:HG3	1:D:393:GLU:HG3	1.89	0.54
1:C:322:GLU:OE1	1:C:325:ARG:NH1	2.37	0.54
1:D:366:ASP:OD1	1:D:369:GLU:HG2	2.08	0.54
1:C:94:LEU:HB3	1:C:346:VAL:HG22	1.90	0.53
1:C:54:LYS:HG2	4:C:565:HOH:O	2.08	0.53
1:A:136:LEU:HD11	1:A:384:VAL:HB	1.89	0.53
1:B:374:ASN:HA	1:B:377:LYS:HE2	1.89	0.53
1:C:136:LEU:HD11	1:C:384:VAL:HB	1.91	0.53
1:D:19:THR:HA	1:D:393:GLU:HG2	1.89	0.53
1:B:366:ASP:CG	1:B:369:GLU:HG2	2.29	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:HG2	4:B:523:HOH:O	2.08	0.53
1:B:96:GLN:HA	1:B:96:GLN:HE21	1.74	0.52
1:D:135:LYS:HD3	1:D:383:GLU:HG2	1.91	0.52
1:A:305:PRO:HG3	1:A:313:LYS:HG2	1.92	0.51
1:B:172:CYS:HB3	1:B:193:VAL:HG12	1.91	0.51
1:D:77:SER:HB2	4:D:1081:HOH:O	2.11	0.50
1:B:208:THR:HG22	1:B:209:HIS:H	1.76	0.50
1:A:322:GLU:OE1	1:A:325:ARG:NH1	2.42	0.50
1:A:194:CYS:HB3	1:A:234:CYS:SG	2.52	0.50
1:B:33:ALA:HA	1:B:107:VAL:HG12	1.93	0.50
1:C:203:ALA:CB	1:C:208:THR:HG23	2.32	0.49
1:A:9:GLN:OE1	1:A:76:ASP:HB2	2.12	0.49
1:D:203:ALA:CB	1:D:208:THR:HG23	2.33	0.49
1:D:374:ASN:HA	1:D:377:LYS:HE2	1.94	0.49
1:B:116:LYS:HE2	4:B:647:HOH:O	2.13	0.49
1:C:19:THR:HA	1:C:393:GLU:HG2	1.94	0.49
1:A:372:PRO:HA	1:A:375:ILE:HD12	1.94	0.49
1:A:388:ASN:OD1	1:A:390:ARG:NE	2.46	0.49
1:D:5:LYS:HE2	1:D:5:LYS:N	2.18	0.49
1:B:135:LYS:HD3	1:B:383:GLU:HG2	1.95	0.49
1:C:16:TYR:CE2	1:C:26:LYS:HG3	2.47	0.48
1:A:374:ASN:HA	1:A:377:LYS:HE2	1.95	0.48
1:C:201:TRP:CH2	1:C:208:THR:HG21	2.49	0.48
1:A:247:ASN:HB2	1:A:301:ILE:HG23	1.96	0.48
1:C:40:ILE:HA	1:C:71:ILE:O	2.14	0.48
1:D:322:GLU:OE1	1:D:325:ARG:NH1	2.44	0.48
1:A:54:LYS:HB2	1:A:55:PRO:CD	2.44	0.48
1:A:212:PRO:HD2	1:A:239:CYS:O	2.14	0.47
1:C:172:CYS:HB3	1:C:193:VAL:HG12	1.96	0.47
1:C:280:LEU:HD21	1:C:283:LEU:HD11	1.96	0.47
1:D:54:LYS:HB2	1:D:55:PRO:CD	2.43	0.47
1:C:211:ALA:HA	1:C:212:PRO:HD2	1.84	0.47
1:D:366:ASP:CG	1:D:369:GLU:HG2	2.34	0.47
1:B:257:GLN:HB3	1:C:377:LYS:O	2.15	0.47
1:D:40:ILE:HA	1:D:71:ILE:O	2.15	0.47
1:B:40:ILE:HA	1:B:71:ILE:O	2.15	0.47
1:C:8:GLU:HG2	1:C:10:HIS:CE1	2.50	0.47
1:A:126:GLU:HB2	1:A:394:ILE:HA	1.96	0.46
1:C:374:ASN:HA	1:C:377:LYS:HE2	1.97	0.46
1:B:14:GLU:OE2	1:B:26:LYS:HD3	2.15	0.46
1:D:137:PRO:HG2	1:D:375:ILE:HG23	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:HA	1:A:341:VAL:O	2.16	0.46
1:A:40:ILE:HA	1:A:71:ILE:O	2.14	0.46
1:B:257:GLN:HG2	1:B:258:TYR:CE2	2.50	0.46
1:C:26:LYS:HE2	1:C:26:LYS:HB3	1.56	0.46
1:D:25:LYS:HA	1:D:25:LYS:HD3	1.76	0.46
1:D:54:LYS:CB	1:D:55:PRO:HD2	2.46	0.46
1:C:212:PRO:HD2	1:C:239:CYS:O	2.15	0.46
1:C:14:GLU:HB3	1:C:26:LYS:HD2	1.98	0.46
1:B:208:THR:HG22	1:B:209:HIS:N	2.30	0.46
1:C:203:ALA:HB2	1:C:208:THR:CG2	2.33	0.45
1:D:33:ALA:HA	1:D:107:VAL:HG12	1.98	0.45
1:D:201:TRP:CH2	1:D:208:THR:HG21	2.52	0.45
1:B:146:LEU:HA	1:B:341:VAL:O	2.16	0.45
1:B:9:GLN:OE1	1:B:76:ASP:HB2	2.17	0.45
1:C:25:LYS:HA	1:C:25:LYS:HD3	1.78	0.45
1:C:72:LEU:HD23	1:C:72:LEU:C	2.37	0.45
1:A:38:HIS:CD2	1:A:75:MET:HG3	2.52	0.45
1:D:280:LEU:HD21	1:D:283:LEU:HD11	1.99	0.44
1:C:182:ILE:HD12	1:C:193:VAL:HG22	2.00	0.44
1:A:54:LYS:HG2	4:A:523:HOH:O	2.17	0.44
1:D:8:GLU:OE2	1:D:38:HIS:NE2	2.31	0.44
1:B:322:GLU:OE1	1:B:325:ARG:NH1	2.47	0.44
1:B:193:VAL:HG13	1:B:220:LEU:HD21	2.00	0.44
1:B:95:GLN:NE2	4:B:608:HOH:O	2.43	0.44
1:A:250:ASP:O	1:A:258:TYR:HA	2.18	0.44
1:A:208:THR:HG22	1:A:209:HIS:H	1.82	0.43
1:B:250:ASP:O	1:B:258:TYR:HA	2.18	0.43
1:C:20:LYS:NZ	1:C:393:GLU:OE2	2.46	0.43
1:A:20:LYS:HE3	4:A:637:HOH:O	2.17	0.43
1:C:14:GLU:HG2	4:C:1035:HOH:O	2.17	0.43
1:B:72:LEU:HD23	1:B:72:LEU:C	2.38	0.43
1:A:113:ASN:O	1:A:114:LYS:HB2	2.18	0.43
1:A:14:GLU:OE1	1:A:26:LYS:HD2	2.19	0.43
1:A:246:ILE:HG13	1:A:246:ILE:H	1.73	0.43
1:B:212:PRO:HD2	1:B:239:CYS:O	2.18	0.43
1:D:212:PRO:HD2	1:D:239:CYS:O	2.19	0.43
1:D:72:LEU:C	1:D:72:LEU:HD23	2.39	0.43
1:C:283:LEU:HB2	1:C:310:ILE:HB	2.00	0.42
1:C:5:LYS:N	1:C:5:LYS:HE2	2.16	0.42
1:D:250:ASP:O	1:D:258:TYR:HA	2.18	0.42
1:C:264:ARG:HH22	1:C:290:ASP:CG	2.22	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HA	1:D:341:VAL:O	2.19	0.42
1:D:10:HIS:HA	1:D:11:PRO:HD3	1.88	0.42
1:D:175:GLN:HG2	3:D:414:CBI:O2'	2.19	0.42
1:D:73:SER:HB3	4:D:889:HOH:O	2.18	0.42
1:B:54:LYS:CB	1:B:55:PRO:CD	2.95	0.42
1:A:135:LYS:HD3	1:A:383:GLU:HG2	2.01	0.42
1:C:267:THR:HB	1:C:288:ILE:HB	2.02	0.42
1:D:217:LYS:HE3	1:D:221:TYR:CE2	2.55	0.42
1:B:348:TRP:CE2	1:B:372:PRO:HB3	2.54	0.42
1:C:20:LYS:HE3	4:C:679:HOH:O	2.19	0.42
1:A:220:LEU:C	1:A:220:LEU:HD23	2.40	0.41
1:D:173:ASP:HB2	1:D:197:GLU:OE1	2.20	0.41
1:B:25:LYS:HD3	1:B:25:LYS:HA	1.88	0.41
1:A:264:ARG:NH2	1:A:290:ASP:OD1	2.53	0.41
1:C:250:ASP:O	1:C:258:TYR:HA	2.20	0.41
1:C:264:ARG:NH2	1:C:290:ASP:OD1	2.53	0.41
1:B:371:ASP:OD1	1:B:373:LYS:HB2	2.19	0.41
1:C:95:GLN:NE2	4:C:650:HOH:O	2.45	0.41
1:D:94:LEU:HB3	1:D:346:VAL:HG22	2.03	0.41
1:C:54:LYS:HB2	1:C:55:PRO:CD	2.48	0.41
1:B:4:ASP:OD2	1:B:73:SER:HA	2.20	0.41
1:B:161:SER:HB2	1:B:185:VAL:HG13	2.03	0.41
1:C:146:LEU:HA	1:C:341:VAL:O	2.21	0.41
1:C:8:GLU:OE2	1:C:38:HIS:NE2	2.37	0.41
1:B:257:GLN:HG2	1:B:258:TYR:CD2	2.56	0.40
1:A:201:TRP:CH2	1:A:208:THR:HG21	2.55	0.40
1:D:126:GLU:HB2	1:D:394:ILE:HA	2.02	0.40
1:C:113:ASN:O	1:C:114:LYS:HB2	2.20	0.40
1:D:31:ILE:HG23	1:D:107:VAL:HB	2.03	0.40
1:D:54:LYS:CB	1:D:55:PRO:CD	2.98	0.40
1:D:98:ILE:O	1:D:99:ASN:C	2.60	0.40
1:C:2:THR:HA	1:C:3:PRO:HD3	1.93	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:A:290:ASP:O	1:B:321:ASN:ND2[2_656]	2.09	0.11

## 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	396/411 (96%)	381 (96%)	15 (4%)	0	100	100
1	B	396/411 (96%)	381 (96%)	15 (4%)	0	100	100
1	C	396/411 (96%)	382 (96%)	14 (4%)	0	100	100
1	D	396/411 (96%)	382 (96%)	14 (4%)	0	100	100
All	All	1584/1644 (96%)	1526 (96%)	58 (4%)	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	323/333 (97%)	303 (94%)	20 (6%)	21	28
1	B	323/333 (97%)	302 (94%)	21 (6%)	20	26
1	C	323/333 (97%)	300 (93%)	23 (7%)	17	22
1	D	323/333 (97%)	303 (94%)	20 (6%)	21	28
All	All	1292/1332 (97%)	1208 (94%)	84 (6%)	20	26

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	20	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	41	ARG
1	A	58	THR
1	A	77	SER
1	A	96	GLN
1	A	101	GLN
1	A	102	LEU
1	A	147	SER
1	A	155	LYS
1	A	159	ARG
1	A	162	LYS
1	A	208	THR
1	A	231	SER
1	A	265	LYS
1	A	276	LYS
1	A	292	LYS
1	A	346	VAL
1	A	348	TRP
1	A	380	PRO
1	B	5	LYS
1	B	20	LYS
1	B	26	LYS
1	B	41	ARG
1	B	58	THR
1	B	77	SER
1	B	96	GLN
1	B	101	GLN
1	B	102	LEU
1	B	147	SER
1	B	155	LYS
1	B	159	ARG
1	B	162	LYS
1	B	208	THR
1	B	231	SER
1	B	265	LYS
1	B	276	LYS
1	B	292	LYS
1	B	302	SER
1	B	346	VAL
1	B	348	TRP
1	C	5	LYS
1	C	20	LYS
1	C	26	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	41	ARG
1	C	58	THR
1	C	77	SER
1	C	96	GLN
1	C	101	GLN
1	C	102	LEU
1	C	147	SER
1	C	155	LYS
1	C	159	ARG
1	C	162	LYS
1	C	208	THR
1	C	231	SER
1	C	265	LYS
1	C	276	LYS
1	C	292	LYS
1	C	302	SER
1	C	306	LYS
1	C	346	VAL
1	C	348	TRP
1	C	393	GLU
1	D	5	LYS
1	D	20	LYS
1	D	41	ARG
1	D	58	THR
1	D	77	SER
1	D	96	GLN
1	D	101	GLN
1	D	102	LEU
1	D	147	SER
1	D	155	LYS
1	D	159	ARG
1	D	162	LYS
1	D	208	THR
1	D	231	SER
1	D	265	LYS
1	D	292	LYS
1	D	302	SER
1	D	346	VAL
1	D	348	TRP
1	D	393	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	B	96	GLN
1	B	331	GLN
1	C	96	GLN
1	C	277	GLN
1	D	96	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PCA	A	1	1	8,8,9	2.02	1 (12%)	9,10,12	1.83	4 (44%)
1	PCA	B	1	1	8,8,9	1.80	1 (12%)	9,10,12	1.74	2 (22%)
1	PCA	C	1	1	8,8,9	1.64	1 (12%)	9,10,12	2.65	4 (44%)
1	PCA	D	1	1	8,8,9	2.19	2 (25%)	9,10,12	2.26	4 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	PCA	CG-CD	2.34	1.57	1.50
1	C	1	PCA	CA-C	2.64	1.53	1.50
1	B	1	PCA	CA-C	4.10	1.55	1.50
1	D	1	PCA	CA-C	4.71	1.56	1.50
1	A	1	PCA	CA-C	4.78	1.56	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	OE-CD-CG	-5.46	116.81	126.86
1	C	1	PCA	O-C-CA	-4.07	115.66	125.15
1	D	1	PCA	OE-CD-CG	-3.87	119.73	126.86
1	D	1	PCA	CB-CA-C	-3.34	108.10	112.70
1	A	1	PCA	OE-CD-CG	-3.08	121.18	126.86
1	D	1	PCA	O-C-CA	-3.06	118.01	125.15
1	B	1	PCA	O-C-CA	-3.01	118.13	125.15
1	C	1	PCA	CA-N-CD	-2.70	104.33	113.58
1	A	1	PCA	OE-CD-N	-2.67	117.96	124.75
1	B	1	PCA	OE-CD-CG	-2.59	122.09	126.86
1	A	1	PCA	O-C-CA	-2.53	119.26	125.15
1	D	1	PCA	CA-N-CD	-2.36	105.50	113.58
1	A	1	PCA	CA-N-CD	-2.18	106.10	113.58
1	C	1	PCA	CB-CA-C	-2.15	109.75	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	412	1	14,14,15	1.26	1 (7%)	15,19,21	1.64	4 (26%)
2	NAG	A	413	1	14,14,15	1.12	1 (7%)	15,19,21	1.65	3 (20%)
3	CBI	A	414	-	24,24,24	1.09	1 (4%)	35,35,35	1.48	4 (11%)
2	NAG	B	412	1	14,14,15	1.25	1 (7%)	15,19,21	1.67	3 (20%)
2	NAG	B	413	1	14,14,15	1.21	1 (7%)	15,19,21	2.16	7 (46%)
3	CBI	B	414	-	24,24,24	1.18	2 (8%)	35,35,35	1.52	5 (14%)
2	NAG	C	412	1	14,14,15	1.21	1 (7%)	15,19,21	2.25	3 (20%)
2	NAG	C	413	1	14,14,15	1.15	1 (7%)	15,19,21	1.60	2 (13%)
3	CBI	C	414	-	24,24,24	1.18	1 (4%)	35,35,35	1.48	4 (11%)
2	NAG	D	412	1	14,14,15	1.34	1 (7%)	15,19,21	1.99	5 (33%)
2	NAG	D	413	1	14,14,15	1.18	1 (7%)	15,19,21	1.92	4 (26%)
3	CBI	D	414	-	24,24,24	1.15	0	35,35,35	1.48	5 (14%)

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	412	1	-	0/6/23/26	0/1/1/1
2	NAG	A	413	1	-	0/6/23/26	0/1/1/1
3	CBI	A	414	-	-	0/8/48/48	0/2/2/2
2	NAG	B	412	1	-	0/6/23/26	0/1/1/1
2	NAG	B	413	1	-	0/6/23/26	0/1/1/1
3	CBI	B	414	-	-	0/8/48/48	0/2/2/2
2	NAG	C	412	1	-	0/6/23/26	0/1/1/1
2	NAG	C	413	1	-	0/6/23/26	0/1/1/1
3	CBI	C	414	-	-	0/8/48/48	0/2/2/2
2	NAG	D	412	1	-	0/6/23/26	0/1/1/1
2	NAG	D	413	1	-	0/6/23/26	0/1/1/1
3	CBI	D	414	-	-	0/8/48/48	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	NAG	O7-C7	-3.78	1.14	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	412	NAG	O7-C7	-3.60	1.14	1.23
2	A	412	NAG	O7-C7	-3.53	1.15	1.23
2	B	413	NAG	O7-C7	-3.40	1.15	1.23
2	B	412	NAG	O7-C7	-3.39	1.15	1.23
2	C	412	NAG	O7-C7	-3.33	1.15	1.23
2	D	413	NAG	O7-C7	-3.12	1.15	1.23
2	C	413	NAG	O7-C7	-3.08	1.16	1.23
3	B	414	CBI	C3'-C2'	2.01	1.57	1.52
3	C	414	CBI	O5-C5	2.14	1.49	1.44
3	B	414	CBI	O5'-C1'	2.38	1.47	1.43
3	A	414	CBI	O5-C5	2.49	1.50	1.44

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	412	NAG	C1-O5-C5	-6.97	102.56	112.17
2	D	412	NAG	O5-C1-C2	-4.89	104.67	111.47
2	B	413	NAG	O5-C1-C2	-4.85	104.72	111.47
2	B	412	NAG	C1-O5-C5	-4.65	105.76	112.17
3	A	414	CBI	O3'-C3'-C2'	-4.51	100.55	110.36
3	C	414	CBI	O3'-C3'-C2'	-4.45	100.66	110.36
3	B	414	CBI	O3'-C3'-C2'	-4.41	100.76	110.36
3	D	414	CBI	O2-C2-C1	-4.33	100.96	110.03
2	D	413	NAG	C2-N2-C7	-4.17	116.86	122.94
2	A	413	NAG	O5-C1-C2	-3.96	105.96	111.47
2	D	413	NAG	C4-C3-C2	-3.90	105.30	111.02
3	B	414	CBI	O2-C2-C1	-3.72	102.26	110.03
2	C	412	NAG	O5-C1-C2	-3.70	106.32	111.47
3	D	414	CBI	O3'-C3'-C2'	-3.53	102.67	110.36
3	C	414	CBI	O2-C2-C1	-3.46	102.79	110.03
2	A	412	NAG	O4-C4-C5	-3.18	101.26	109.28
2	D	412	NAG	C2-N2-C7	-3.14	118.37	122.94
3	A	414	CBI	O2-C2-C1	-3.07	103.61	110.03
2	A	412	NAG	C8-C7-N2	-2.70	111.23	116.11
2	D	413	NAG	O5-C1-C2	-2.57	107.90	111.47
2	A	413	NAG	O3-C3-C2	-2.54	103.94	109.39
2	D	412	NAG	C6-C5-C4	-2.46	107.25	113.00
2	A	412	NAG	O5-C1-C2	-2.44	108.08	111.47
2	D	412	NAG	C1-O5-C5	-2.43	108.81	112.17
2	B	412	NAG	C8-C7-N2	-2.40	111.77	116.11
2	B	413	NAG	C8-C7-N2	-2.33	111.89	116.11
2	B	413	NAG	C1-C2-N2	-2.27	106.61	110.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	413	NAG	O3-C3-C4	-2.20	105.56	110.36
2	B	413	NAG	C2-N2-C7	-2.15	119.80	122.94
2	B	413	NAG	C6-C5-C4	-2.15	107.98	113.00
2	C	412	NAG	C4-C3-C2	-2.13	107.89	111.02
2	B	412	NAG	O7-C7-C8	2.02	125.73	122.06
3	C	414	CBI	O5'-C5'-C6'	2.05	111.31	106.41
2	D	412	NAG	C3-C4-C5	2.12	113.95	110.22
3	D	414	CBI	O5-C1-C2	2.12	114.39	110.30
3	D	414	CBI	O5'-C5'-C6'	2.16	111.57	106.41
3	B	414	CBI	O5'-C1'-C2'	2.16	113.63	110.04
3	B	414	CBI	O3-C3-C2	2.20	115.15	110.36
3	D	414	CBI	O5'-C1'-C2'	2.21	113.71	110.04
3	C	414	CBI	O5'-C1'-C2'	2.23	113.74	110.04
2	B	413	NAG	C1-O5-C5	2.27	115.29	112.17
3	B	414	CBI	O5'-C5'-C6'	2.34	112.01	106.41
3	A	414	CBI	O1'-C1'-O5'	2.38	117.25	110.20
2	A	413	NAG	O3-C3-C4	2.46	115.71	110.36
2	A	412	NAG	C3-C4-C5	2.47	114.57	110.22
2	D	413	NAG	O6-C6-C5	2.57	120.00	111.34
2	B	413	NAG	C3-C4-C5	2.83	115.21	110.22
3	A	414	CBI	O5'-C1'-C2'	3.24	115.42	110.04
2	C	413	NAG	C1-O5-C5	4.40	118.24	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	414	CBI	1	0
3	B	414	CBI	1	0
3	C	414	CBI	1	0
3	D	414	CBI	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	397/411 (96%)	-0.18	9 (2%) 61 67	13, 26, 43, 52	0
1	B	397/411 (96%)	0.05	18 (4%) 34 41	14, 27, 44, 51	0
1	C	397/411 (96%)	-0.07	8 (2%) 65 72	12, 27, 44, 53	0
1	D	397/411 (96%)	-0.21	6 (1%) 74 78	14, 25, 42, 51	0
All	All	1588/1644 (96%)	-0.10	41 (2%) 56 63	12, 26, 43, 53	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ARG	3.8
1	C	201	TRP	3.0
1	C	276	LYS	2.9
1	B	368	THR	2.9
1	B	203	ALA	2.9
1	B	374	ASN	2.8
1	B	367	ALA	2.8
1	B	319	GLY	2.8
1	C	145	TYR	2.7
1	C	144	LEU	2.6
1	A	226	ASP	2.4
1	D	145	TYR	2.4
1	D	144	LEU	2.4
1	B	22	SER	2.4
1	D	292	LYS	2.4
1	B	99	ASN	2.4
1	A	342	LEU	2.3
1	B	58	THR	2.3
1	C	344	MET	2.2
1	B	277	GLN	2.2
1	B	21	ALA	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	58	THR	2.2
1	A	292	LYS	2.2
1	B	373	LYS	2.2
1	C	159	ARG	2.2
1	D	301	ILE	2.2
1	A	291	ASN	2.2
1	B	20	LYS	2.2
1	B	398	SER	2.2
1	C	99	ASN	2.2
1	D	201	TRP	2.2
1	C	343	ALA	2.1
1	B	45	GLY	2.1
1	A	143	ALA	2.1
1	A	211	ALA	2.1
1	B	292	LYS	2.1
1	A	208	THR	2.1
1	B	211	ALA	2.1
1	B	201	TRP	2.1
1	A	210	ILE	2.0
1	B	366	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	PCA	D	1	8/9	0.96	0.09	-	23,26,27,28	0
1	PCA	C	1	8/9	0.94	0.11	-	27,29,31,33	0
1	PCA	B	1	8/9	0.96	0.09	-	24,27,29,31	0
1	PCA	A	1	8/9	0.96	0.09	-	23,26,29,31	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	412	14/15	0.87	0.25	2.01	53,55,56,56	0
2	NAG	D	412	14/15	0.88	0.19	0.93	52,54,57,57	0
2	NAG	A	413	14/15	0.82	0.23	0.91	56,59,62,62	0
3	CBI	C	414	23/23	0.88	0.19	0.61	28,35,39,43	0
3	CBI	A	414	23/23	0.92	0.17	0.57	28,34,39,43	0
2	NAG	C	413	14/15	0.88	0.18	0.50	56,58,59,61	0
3	CBI	D	414	23/23	0.92	0.17	0.27	26,34,39,43	0
3	CBI	B	414	23/23	0.91	0.17	0.05	28,34,38,43	0
2	NAG	B	412	14/15	0.87	0.23	-0.04	52,54,55,56	0
2	NAG	C	412	14/15	0.88	0.16	-0.13	52,54,55,55	0
2	NAG	D	413	14/15	0.77	0.27	-	57,59,62,62	0
2	NAG	B	413	14/15	0.81	0.25	-	59,61,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.