



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:48 PM GMT

PDB ID : 4JJJ  
Title : The structure of T. fusca GH48 D224N mutant  
Authors : Alahuhta, P.M.; Lunin, V.V.  
Deposited on : 2013-03-07  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

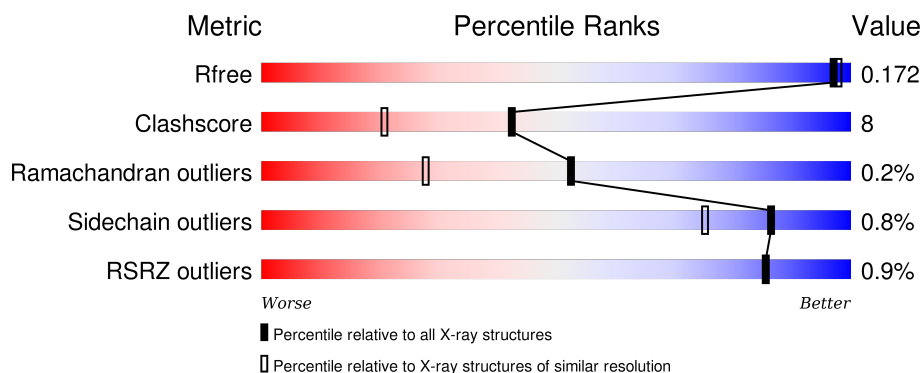
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	642	<div> <div></div> <div>86%</div> <div>11% ..</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
5	CA	A	707	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	A	727	-	-	-	X
8	ZN	A	730[A]	-	-	-	X
8	ZN	A	730[B]	-	-	-	X
8	ZN	A	732	-	-	-	X
8	ZN	A	734	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6750 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.

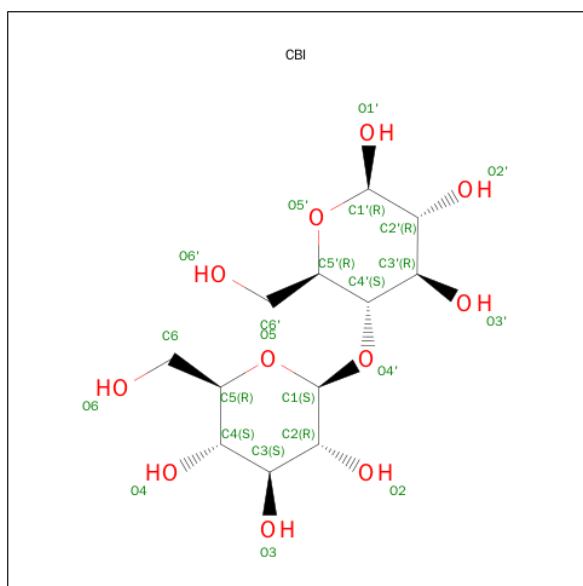
- Molecule 1 is a protein called Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	636	5415	3426	901	1066	22	0	43	0

There is a discrepancy between the modelled and reference sequences:

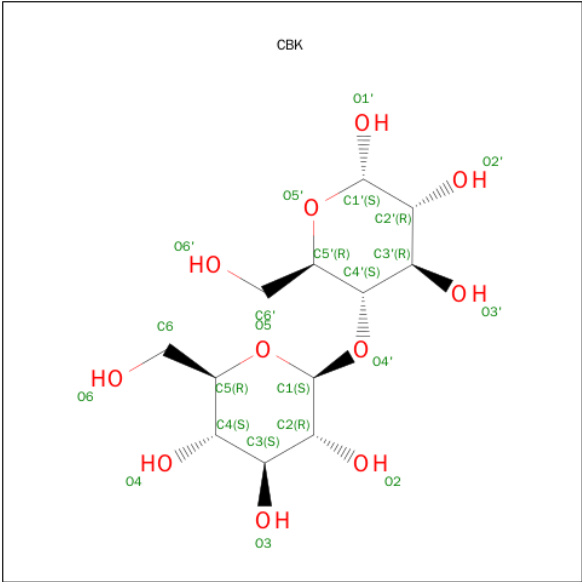
Chain	Residue	Modelled	Actual	Comment	Reference
A	224	ASN	ASP	ENGINEERED MUTATION	UNP Q47NH7

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula:  $C_{12}H_{22}O_{11}$ ).



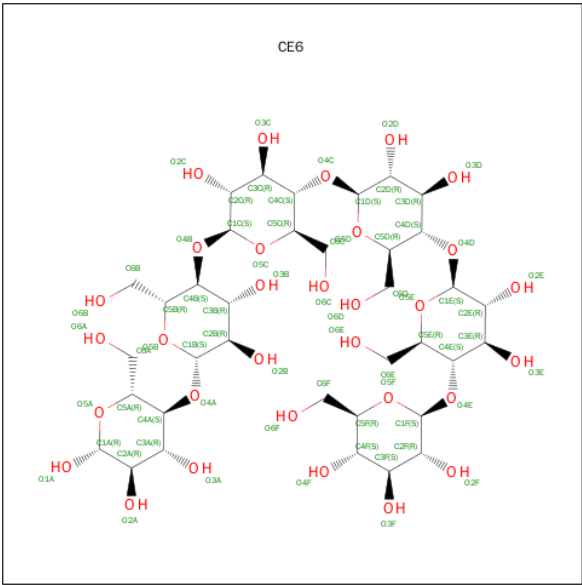
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	23	12	11	0	1

- Molecule 3 is SUGAR (4-O-BETA-D-GLUCOPYRANOSYL-ALPHA-D-GLUCOPYRANOSE) (three-letter code: CBK) (formula:  $C_{12}H_{22}O_{11}$ ).



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

- Molecule 4 is SUGAR (CELLOHEXAOSE) (three-letter code: CE6) (formula:  $C_{36}H_{62}O_{31}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			68	36	32		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Ca 4 4	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Na 3 3	0	0

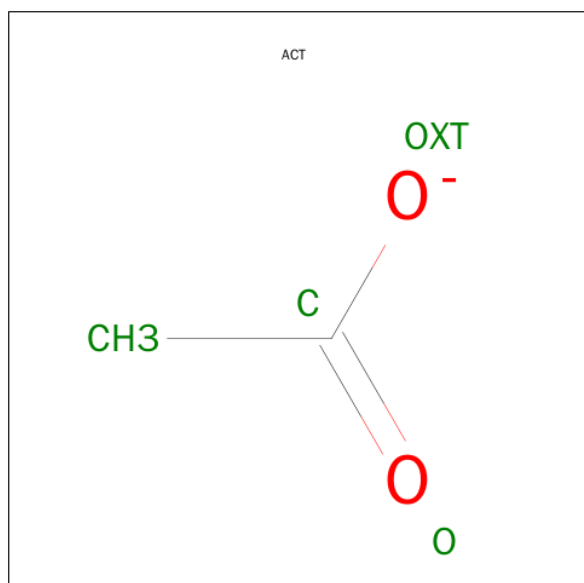
- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total Fe 5 5	0	1

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	21	Total Zn 22 22	0	1

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



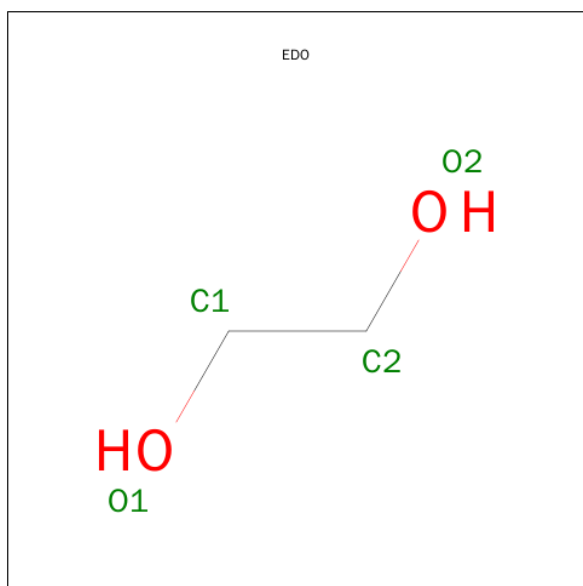
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		

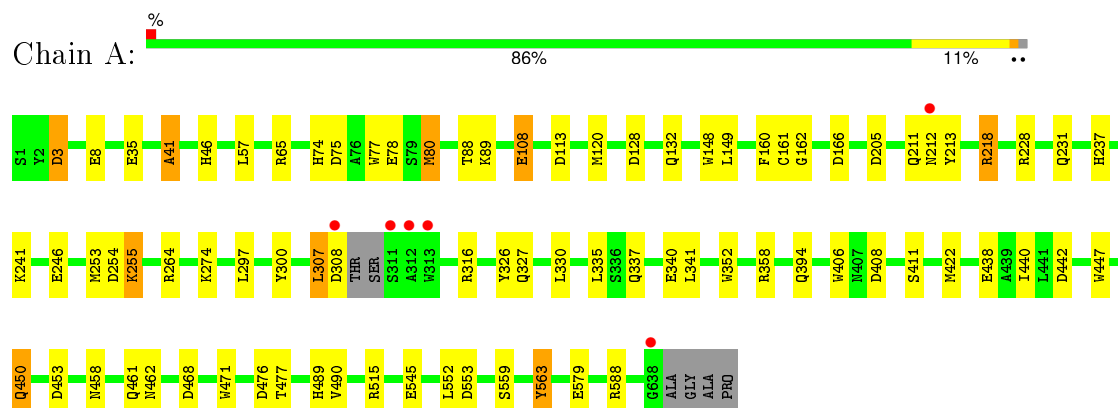
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1136	Total	O	0	39
			1175	1175		

### 3 Residue-property plots

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

- Molecule 1: Cellulose 1,4-beta-cellobiosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.46 Å   88.49 Å   66.75 Å 90.00°   113.72°   90.00°	Depositor
Resolution (Å)	25.00 – 1.60 44.06 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-1.60) 99.4 (44.06-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 1.60 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.121 , 0.164 0.134 , 0.172	Depositor DCC
$R_{free}$ test set	4002 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.4	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 78696 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NA, CA, CBI, EDO, CE6, FE, ACT, CBK

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	1.18	7/5596 (0.1%)	1.17	25/7652 (0.3%)

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	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	GLU	CD-OE1	-6.77	1.18	1.25
1	A	8	GLU	CD-OE2	6.43	1.32	1.25
1	A	108	GLU	CD-OE2	6.24	1.32	1.25
1	A	559	SER	CB-OG	-5.80	1.34	1.42
1	A	108	GLU	CD-OE1	5.45	1.31	1.25
1	A	545	GLU	CB-CG	-5.35	1.42	1.52
1	A	447	TRP	CZ3-CH2	5.16	1.48	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	515	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	65	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	453	ASP	CB-CG-OD2	-8.63	110.54	118.30
1	A	65	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	326	TYR	CB-CG-CD2	-7.61	116.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	476	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	442	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	3	ASP	CB-CG-OD1	-6.96	112.03	118.30
1	A	442	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	563	TYR	CB-CG-CD1	-6.69	116.99	121.00
1	A	128	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	408	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	A	228	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	358	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	255[A]	LYS	CD-CE-NZ	-5.77	98.42	111.70
1	A	255[B]	LYS	CD-CE-NZ	-5.77	98.42	111.70
1	A	108	GLU	OE1-CD-OE2	5.54	129.94	123.30
1	A	588	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	316	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	218	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	80[A]	MET	CG-SD-CE	-5.08	92.07	100.20
1	A	80[B]	MET	CG-SD-CE	-5.08	92.07	100.20
1	A	264	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	LEU	Peptide
1	A	41	ALA	Peptide
1	A	46	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5415	0	4888	84	0
2	A	23	0	22	1	0
3	A	23	0	22	0	0
4	A	68	0	6	1	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	3	0	0	0	0
7	A	5	0	0	0	0
8	A	22	0	0	3	0
9	A	8	0	6	0	0
10	A	4	0	6	0	0
11	A	1175	0	0	53	1
All	All	6750	0	4950	88	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 8.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337[B]:GLN:NE2	11:A:1700:HOH:O	1.58	1.27
1:A:74[B]:HIS:CE1	11:A:1910:HOH:O	1.87	1.25
8:A:733:ZN:ZN	11:A:1930:HOH:O	0.56	1.24
1:A:450[B]:GLN:OE1	11:A:1133:HOH:O	1.56	1.22
1:A:458[A]:ASN:OD1	11:A:1131:HOH:O	1.57	1.17
1:A:77[B]:TRP:CE3	1:A:80[B]:MET:CE	2.29	1.16
1:A:477[C]:THR:CG2	11:A:1139:HOH:O	1.92	1.15
1:A:468[A]:ASP:OD2	11:A:1930:HOH:O	1.68	1.11
1:A:132[B]:GLN:NE2	11:A:1824:HOH:O	1.83	1.09
1:A:468[B]:ASP:OD2	11:A:1283:HOH:O	1.68	1.09
1:A:77[B]:TRP:CZ3	1:A:80[B]:MET:CE	2.35	1.08
1:A:255[A]:LYS:NZ	11:A:1107:HOH:O	1.84	1.08
1:A:78[B]:GLU:OE1	11:A:1898:HOH:O	1.74	1.06
1:A:253[B]:MET:CE	1:A:340[B]:GLU:HB2	1.86	1.05
1:A:77[B]:TRP:CZ3	1:A:80[B]:MET:HE3	1.90	1.04
1:A:253[B]:MET:HE1	1:A:340[B]:GLU:HB2	1.37	1.04
1:A:253[B]:MET:HE2	1:A:340[B]:GLU:HB3	1.41	1.03
1:A:75[B]:ASP:OD1	11:A:1893:HOH:O	1.77	1.00
1:A:253[B]:MET:CE	1:A:340[B]:GLU:CB	2.39	1.00
2:A:701[A]:CBI:O1'	11:A:1114[A]:HOH:O	1.84	0.96
1:A:89[A]:LYS:NZ	11:A:1451:HOH:O	1.77	0.94
1:A:477[C]:THR:HG22	11:A:1139:HOH:O	1.61	0.94
8:A:731:ZN:ZN	11:A:1910:HOH:O	1.16	0.94
1:A:241[A]:LYS:NZ	11:A:1780:HOH:O	1.91	0.91
1:A:253[B]:MET:HE2	1:A:340[B]:GLU:CB	1.98	0.90
1:A:77[B]:TRP:CE3	1:A:80[B]:MET:HE3	2.02	0.90
1:A:77[B]:TRP:CZ3	1:A:80[B]:MET:HE1	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254[A]:ASP:OD2	11:A:1929:HOH:O	1.88	0.89
1:A:477[A]:THR:HG21	11:A:1067:HOH:O	1.77	0.83
1:A:253[B]:MET:HE1	1:A:340[B]:GLU:CB	2.03	0.83
1:A:74[B]:HIS:HE1	11:A:1910:HOH:O	1.39	0.83
1:A:57:LEU:HD11	1:A:80[A]:MET:HE1	1.60	0.81
1:A:450[B]:GLN:NE2	11:A:1076:HOH:O	2.17	0.77
1:A:132[B]:GLN:CD	11:A:1824:HOH:O	2.18	0.75
1:A:297:LEU:H	1:A:327:GLN:HE22	1.31	0.73
1:A:74[B]:HIS:NE2	11:A:1910:HOH:O	2.09	0.70
1:A:77[B]:TRP:CE3	1:A:80[B]:MET:HE1	2.21	0.68
1:A:88:THR:OG1	11:A:965[A]:HOH:O	2.13	0.67
8:A:735:ZN:ZN	11:A:1936:HOH:O	1.42	0.67
1:A:120[B]:MET:SD	11:A:1683:HOH:O	2.53	0.67
1:A:212[B]:ASN:OD1	11:A:1803[B]:HOH:O	2.12	0.66
1:A:77[B]:TRP:CE3	1:A:80[B]:MET:HE2	2.28	0.65
1:A:477[C]:THR:HG23	11:A:1139:HOH:O	1.74	0.65
1:A:394:GLN:N	1:A:477[A]:THR:HG22	2.12	0.63
1:A:253[B]:MET:CE	1:A:340[B]:GLU:HB3	2.10	0.61
1:A:132[B]:GLN:OE1	11:A:1824:HOH:O	2.14	0.61
1:A:237[B]:HIS:HB2	1:A:253[B]:MET:SD	2.40	0.61
1:A:212[A]:ASN:HB2	11:A:1619:HOH:O	2.01	0.60
1:A:462:ASN:ND2	11:A:1131:HOH:O	2.36	0.59
1:A:246[B]:GLU:HG3	11:A:1460:HOH:O	2.04	0.58
1:A:461:GLN:HG3	11:A:1326:HOH:O	2.03	0.58
1:A:35:GLU:HB2	11:A:1879:HOH:O	2.05	0.56
1:A:77[B]:TRP:CH2	1:A:80[B]:MET:HE1	2.40	0.56
1:A:300:TYR:CE2	4:A:703[B]:CE6:H6B2	2.41	0.55
1:A:274:LYS:HE3	11:A:1903:HOH:O	2.07	0.55
1:A:308:ASP:HB2	11:A:1859:HOH:O	2.08	0.54
1:A:162:GLY:HA2	11:A:1294[B]:HOH:O	2.08	0.54
1:A:237[B]:HIS:HD2	11:A:1314:HOH:O	1.90	0.53
1:A:166[A]:ASP:OD2	11:A:1110:HOH:O	2.18	0.53
1:A:231:GLN:HG3	1:A:330:LEU:HD12	1.91	0.52
1:A:57:LEU:CD1	1:A:80[A]:MET:HE1	2.35	0.51
1:A:579:GLU:OE1	11:A:1744:HOH:O	2.19	0.51
1:A:246[B]:GLU:HG2	11:A:1684:HOH:O	2.11	0.49
1:A:489:HIS:CE1	11:A:1660:HOH:O	2.65	0.49
1:A:74[A]:HIS:HD2	11:A:1895:HOH:O	1.94	0.49
1:A:205:ASP:HB3	1:A:213:TYR:CZ	2.49	0.48
1:A:212[B]:ASN:HA	11:A:1803[B]:HOH:O	2.14	0.47
1:A:422[B]:MET:HG2	11:A:1459:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HD13	1:A:352:TRP:CE2	2.50	0.46
1:A:422[B]:MET:HE1	1:A:440:ILE:HG22	1.98	0.46
1:A:237[A]:HIS:ND1	11:A:1314:HOH:O	2.32	0.45
1:A:406:TRP:HB2	1:A:411:SER:HB3	1.99	0.45
1:A:253[A]:MET:HE3	1:A:341:LEU:HG	1.99	0.45
1:A:3:ASP:HB3	11:A:1049:HOH:O	2.17	0.44
1:A:160:PHE:O	1:A:161[B]:CYS:C	2.54	0.44
1:A:3:ASP:CB	11:A:1049:HOH:O	2.66	0.43
1:A:80[A]:MET:HB2	1:A:80[A]:MET:HE2	1.55	0.42
1:A:553:ASP:CG	11:A:988:HOH:O	2.57	0.42
1:A:108:GLU:OE1	11:A:1221:HOH:O	2.21	0.42
1:A:113:ASP:HA	1:A:563:TYR:CE2	2.54	0.42
1:A:148:TRP:CE2	1:A:149:LEU:HB2	2.55	0.42
1:A:308:ASP:N	11:A:1297:HOH:O	2.37	0.41
1:A:108:GLU:OE2	11:A:979[A]:HOH:O	2.21	0.41
1:A:471:TRP:CZ3	1:A:490:VAL:HB	2.56	0.41
1:A:330:LEU:HD13	1:A:330:LEU:C	2.42	0.41
1:A:307:LEU:O	1:A:308:ASP:HB2	2.21	0.40
1:A:89[A]:LYS:HG2	11:A:1451:HOH:O	2.21	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)
11:A:1470:HOH:O	11:A:1872:HOH:O[2_747]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	677/642 (106%)	659 (97%)	17 (2%)	1 (0%)	56 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ALA

### 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	567/525 (108%)	561 (99%)	6 (1%)	80	63

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	218	ARG
1	A	450[A]	GLN
1	A	450[B]	GLN
1	A	552[A]	LEU
1	A	552[B]	LEU

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	4	GLN
1	A	127	GLN
1	A	327	GLN
1	A	407	ASN
1	A	489	HIS
1	A	593	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 34 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	CBI	A	701[A]	-	24,24,24	0.85	1 (4%)	35,35,35	1.12	1 (2%)
3	CBK	A	702[B]	-	24,24,24	1.25	4 (16%)	35,35,35	1.26	3 (8%)
4	CE6	A	703[A]	-	72,72,72	0.99	4 (5%)	107,107,107	1.52	17 (15%)
4	CE6	A	703[B]	-	72,72,72	1.00	4 (5%)	107,107,107	1.57	18 (16%)
9	ACT	A	736	8	1,3,3	2.04	1 (100%)	0,3,3	0.00	-
9	ACT	A	737	8	1,3,3	0.13	0	0,3,3	0.00	-
10	EDO	A	738	-	3,3,3	0.46	0	2,2,2	0.13	0

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	CBI	A	701[A]	-	-	0/8/48/48	0/2/2/2
3	CBK	A	702[B]	-	-	0/8/48/48	0/2/2/2
4	CE6	A	703[A]	-	-	0/32/152/152	0/6/6/6
4	CE6	A	703[B]	-	-	0/32/152/152	0/6/6/6
9	ACT	A	736	8	-	0/0/0/0	0/0/0/0
9	ACT	A	737	8	-	0/0/0/0	0/0/0/0
10	EDO	A	738	-	-	0/1/1/1	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702[B]	CBK	C1'-C2'	-2.55	1.48	1.52
9	A	736	ACT	CH3-C	-2.04	1.46	1.48
4	A	703[A]	CE6	O5F-C5F	2.02	1.49	1.44
4	A	703[B]	CE6	O5F-C5F	2.02	1.49	1.44
3	A	702[B]	CBK	C4-C3	2.07	1.57	1.52
2	A	701[A]	CBI	O1'-C1'	2.14	1.47	1.39
4	A	703[A]	CE6	O3F-C3F	2.19	1.48	1.43
4	A	703[B]	CE6	O3F-C3F	2.19	1.48	1.43
4	A	703[A]	CE6	O4E-C4E	2.40	1.49	1.43
4	A	703[B]	CE6	O4E-C4E	2.40	1.49	1.43
4	A	703[A]	CE6	O5F-C1F	2.62	1.48	1.41
4	A	703[B]	CE6	O5F-C1F	2.62	1.48	1.41
3	A	702[B]	CBK	C4-C5	2.79	1.59	1.53
3	A	702[B]	CBK	O2'-C2'	2.89	1.49	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703[A]	CE6	C1F-O5F-C5F	-4.78	104.46	113.75
4	A	703[B]	CE6	C1F-O5F-C5F	-4.78	104.46	113.75
4	A	703[A]	CE6	O6F-C6F-C5F	-3.63	99.32	111.33
4	A	703[B]	CE6	O6F-C6F-C5F	-3.63	99.32	111.33
4	A	703[A]	CE6	C1F-O4E-C4E	-3.49	108.88	118.01
4	A	703[B]	CE6	C1F-O4E-C4E	-3.49	108.88	118.01
4	A	703[A]	CE6	O4E-C4E-C5E	-3.18	100.97	109.32
4	A	703[B]	CE6	O4E-C4E-C5E	-3.18	100.97	109.32
4	A	703[A]	CE6	O5F-C5F-C4F	-3.05	103.96	109.68
4	A	703[B]	CE6	O5F-C5F-C4F	-3.05	103.96	109.68
4	A	703[A]	CE6	C1B-O5B-C5B	-2.88	108.15	113.75
4	A	703[B]	CE6	C1B-O5B-C5B	-2.88	108.15	113.75
4	A	703[A]	CE6	C1E-O5E-C5E	-2.88	108.15	113.75
4	A	703[B]	CE6	C1E-O5E-C5E	-2.88	108.15	113.75
4	A	703[A]	CE6	O4A-C1B-O5B	-2.79	103.62	110.68
4	A	703[B]	CE6	O4A-C1B-O5B	-2.79	103.62	110.68
4	A	703[A]	CE6	O4E-C1F-C2F	-2.75	101.40	108.10
4	A	703[B]	CE6	O4E-C1F-C2F	-2.75	101.40	108.10
2	A	701[A]	CBI	O2'-C2'-C3'	-2.64	104.39	110.34
3	A	702[B]	CBK	O1'-C1'-C2'	-2.61	102.22	109.21
3	A	702[B]	CBK	O2'-C2'-C3'	-2.53	104.64	110.34
4	A	703[A]	CE6	C3B-C4B-C5B	-2.23	105.79	110.84
4	A	703[B]	CE6	C3B-C4B-C5B	-2.23	105.79	110.84
4	A	703[A]	CE6	C1D-O4C-C4C	-2.18	112.32	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703[B]	CE6	C1D-O4C-C4C	-2.18	112.32	118.01
4	A	703[A]	CE6	O5D-C1D-C2D	-2.15	105.86	110.28
4	A	703[B]	CE6	O5D-C1D-C2D	-2.15	105.86	110.28
4	A	703[A]	CE6	O4A-C4A-C3A	-2.05	101.87	107.17
4	A	703[B]	CE6	O4A-C4A-C3A	-2.05	101.87	107.17
4	A	703[A]	CE6	O2F-C2F-C3F	-2.00	105.83	110.34
4	A	703[B]	CE6	O2F-C2F-C3F	-2.00	105.83	110.34
4	A	703[A]	CE6	C6E-C5E-C4E	2.02	119.11	113.25
4	A	703[B]	CE6	C6E-C5E-C4E	2.02	119.11	113.25
4	A	703[A]	CE6	O5B-C5B-C6B	2.42	112.47	106.36
4	A	703[B]	CE6	O5B-C5B-C6B	2.42	112.47	106.36
3	A	702[B]	CBK	O5-C5-C6	3.19	114.41	106.36
4	A	703[A]	CE6	O5A-C1A-C2A	3.54	115.44	109.80
4	A	703[B]	CE6	O5A-C1A-C2A	3.54	115.44	109.80
4	A	703[B]	CE6	O6B-C6B-C5B	4.05	124.73	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701[A]	CBI	1	0
4	A	703[B]	CE6	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	636/642 (99%)	-0.52	6 (0%) 85 85	4, 9, 19, 54	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	SER	3.8
1	A	308	ASP	3.3
1	A	313	TRP	3.3
1	A	312	ALA	2.5
1	A	212[A]	ASN	2.4
1	A	638	GLY	2.3

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	A	730[A]	1/1	0.97	0.24	10.92	28,28,28,28	1
8	ZN	A	730[B]	1/1	0.97	0.24	10.48	25,25,25,25	1
8	ZN	A	732	1/1	0.71	0.25	10.29	52,52,52,52	1
5	CA	A	707	1/1	0.98	0.17	7.34	21,21,21,21	1
8	ZN	A	727	1/1	0.83	0.33	6.50	56,56,56,56	1
8	ZN	A	734	1/1	0.97	0.15	4.41	35,35,35,35	1
3	CBK	A	702[B]	23/23	0.98	0.11	1.74	7,9,14,14	23
2	CBI	A	701[A]	23/23	0.97	0.10	1.54	2,3,5,9	23
10	EDO	A	738	4/4	0.85	0.12	0.73	30,35,36,44	0
7	FE	A	714	1/1	1.00	0.12	0.61	16,16,16,16	0
4	CE6	A	703[A]	67/67	0.94	0.09	0.01	4,8,28,31	1
4	CE6	A	703[B]	67/67	0.94	0.09	0.01	4,8,28,31	1
8	ZN	A	723	1/1	1.00	0.05	-0.39	13,13,13,13	1
7	FE	A	711	1/1	0.99	0.04	-1.59	9,9,9,9	1
5	CA	A	704	1/1	1.00	0.04	-1.71	8,8,8,8	0
8	ZN	A	733	1/1	0.99	0.04	-4.66	16,16,16,16	1
8	ZN	A	717	1/1	0.99	0.03	-5.54	13,13,13,13	1
6	NA	A	708	1/1	0.92	0.08	-	35,35,35,35	0
8	ZN	A	728	1/1	0.99	0.05	-	14,14,14,14	1
8	ZN	A	725	1/1	0.99	0.03	-	17,17,17,17	1
8	ZN	A	719	1/1	1.00	0.02	-	8,8,8,8	0
5	CA	A	706	1/1	0.98	0.13	-	31,31,31,31	0
9	ACT	A	736	4/4	0.92	0.10	-	34,38,41,42	0
8	ZN	A	716	1/1	0.99	0.04	-	16,16,16,16	0
8	ZN	A	726	1/1	1.00	0.05	-	15,15,15,15	1
8	ZN	A	718	1/1	0.99	0.05	-	16,16,16,16	0
7	FE	A	712[A]	1/1	0.95	0.06	-	19,19,19,19	1
8	ZN	A	720	1/1	0.99	0.11	-	17,17,17,17	1
8	ZN	A	722	1/1	0.99	0.11	-	18,18,18,18	1
7	FE	A	712[B]	1/1	0.95	0.06	-	29,29,29,29	1
9	ACT	A	737	4/4	0.93	0.13	-	25,29,33,36	0
8	ZN	A	715	1/1	1.00	0.03	-	7,7,7,7	0
7	FE	A	713	1/1	0.66	0.17	-	39,39,39,39	1
8	ZN	A	729	1/1	0.98	0.04	-	31,31,31,31	1
8	ZN	A	735	1/1	0.94	0.05	-	33,33,33,33	1
8	ZN	A	731	1/1	0.96	0.10	-	62,62,62,62	1
8	ZN	A	721	1/1	0.99	0.13	-	22,22,22,22	1
6	NA	A	709	1/1	0.90	0.09	-	27,27,27,27	0
8	ZN	A	724	1/1	0.99	0.07	-	14,14,14,14	1
6	NA	A	710	1/1	0.93	0.25	-	32,32,32,32	0
5	CA	A	705	1/1	0.99	0.06	-	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.