



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GQI  
Title : STRUCTURE OF PSEUDOMONAS CELLULOSA ALPHA-D-GLUCURON  
IDASE  
Authors : Nurizzo, D.; Nagy, T.; Gilbert, H.J.; Davies, G.J.  
Deposited on : 2001-11-26  
Resolution : 1.48 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

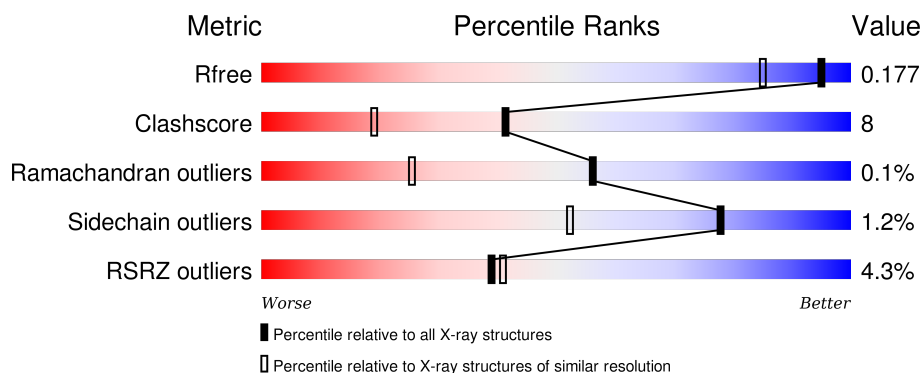
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 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	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (1.50-1.46)

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	708	<div> <div>4%</div> <div>89%</div> <div>10%</div> </div>
1	B	708	<div> <div>5%</div> <div>89%</div> <div>10%</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	EDO	A	1716	-	-	X	-
2	EDO	A	1717	-	-	-	X
2	EDO	A	1718	-	-	-	X
2	EDO	B	1716	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13339 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 ALPHA-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	22	0
			5759	3677	1019	1044	19			
1	B	708	Total	C	N	O	S	0	24	0
			5756	3673	1018	1045	20			

- Molecule 2 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
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Co 4 4	0	4
3	A	4	Total Co 4 4	0	4

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0

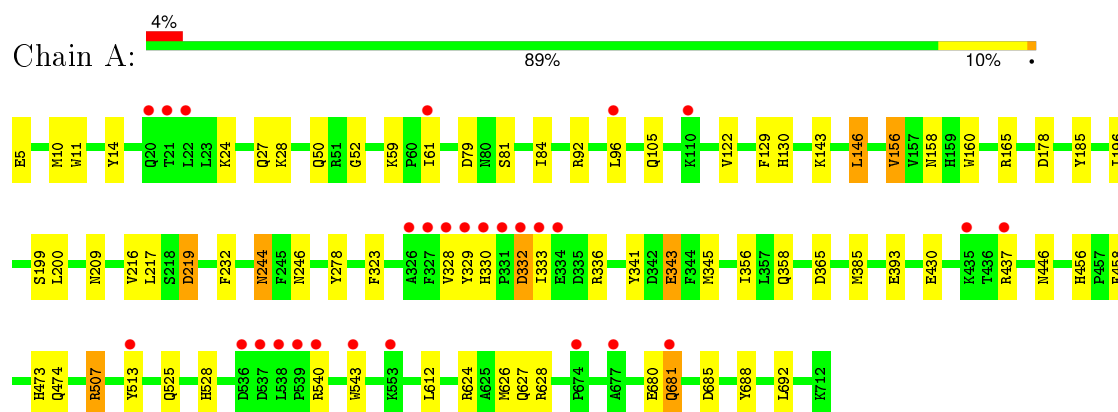
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	890	Total O 890 890	0	68
5	B	876	Total O 876 876	0	46

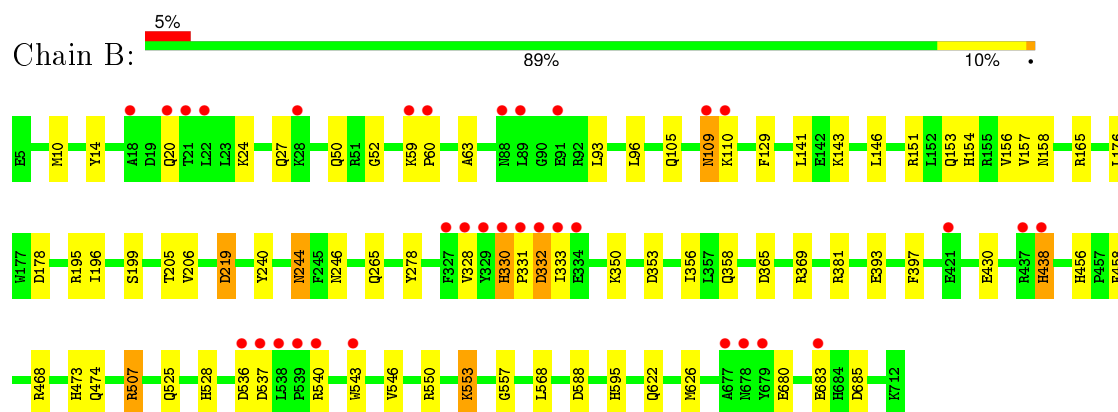
### 3 Residue-property plots

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: ALPHA-GLUCURONIDASE



#### • Molecule 1: ALPHA-GLUCURONIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.91Å 74.68Å 87.59Å 115.18° 93.14° 109.33°	Depositor
Resolution (Å)	20.00 – 1.48 29.43 – 1.48	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-1.48) 80.0 (29.43-1.48)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.133 , 0.168 0.156 , 0.177	Depositor DCC
$R_{free}$ test set	1885 reflections (0.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 235655 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: MG, CO, EDO

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	0.73	3/6035 (0.0%)	0.87	13/8206 (0.2%)
1	B	0.71	0/6045	0.88	16/8219 (0.2%)
All	All	0.72	3/12080 (0.0%)	0.88	29/16425 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156[A]	VAL	CB-CG2	-5.39	1.41	1.52
1	A	156[B]	VAL	CB-CG2	-5.39	1.41	1.52
1	A	626	MET	SD-CE	-5.12	1.49	1.77

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219[A]	ASP	CB-CG-OD1	8.56	126.00	118.30
1	B	219[B]	ASP	CB-CG-OD1	8.56	126.00	118.30
1	B	397	PHE	CB-CG-CD1	7.44	126.01	120.80
1	A	626	MET	CG-SD-CE	-7.44	88.30	100.20
1	A	178	ASP	CB-CG-OD2	7.37	124.93	118.30
1	B	328[A]	VAL	CG1-CB-CG2	6.83	121.83	110.90
1	B	328[B]	VAL	CG1-CB-CG2	6.83	121.83	110.90
1	A	165	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	332	ASP	CB-CG-OD2	6.36	124.03	118.30
1	B	438	HIS	O-C-N	-6.27	112.67	122.70
1	A	79	ASP	CB-CG-OD2	6.13	123.81	118.30
1	A	122[A]	VAL	CG1-CB-CG2	5.90	120.34	110.90
1	A	122[B]	VAL	CG1-CB-CG2	5.90	120.34	110.90
1	B	397	PHE	CB-CG-CD2	-5.84	116.72	120.80
1	A	685	ASP	CB-CG-OD2	5.79	123.52	118.30
1	B	165	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	178	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	685	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	369	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	353	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	343[A]	GLU	CA-CB-CG	5.26	124.97	113.40
1	A	343[B]	GLU	CA-CB-CG	5.26	124.97	113.40
1	B	588	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	195	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	219[A]	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	219[B]	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	232	PHE	CB-CG-CD1	5.09	124.37	120.80
1	B	468	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	5759	0	5608	93	0
1	B	5756	0	5600	101	0
2	A	24	0	36	6	0
2	B	24	0	36	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	890	0	0	21	1
5	B	876	0	0	16	0
All	All	13339	0	11280	194	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 (194) 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:330[B]:HIS:CE1	1:A:333:ILE:CG2	1.89	1.52
1:A:330[B]:HIS:CE1	1:A:333:ILE:HG21	1.48	1.40
1:B:10[B]:MET:SD	1:B:10[B]:MET:CE	1.15	1.24
1:B:330[A]:HIS:CE1	1:B:332:ASP:HB3	1.76	1.21
1:B:10[B]:MET:HE3	1:B:10[B]:MET:SD	1.74	1.10
1:B:10[B]:MET:SD	1:B:10[B]:MET:HE1	1.74	1.09
1:B:10[B]:MET:SD	1:B:10[B]:MET:HE2	1.74	1.08
1:B:219[B]:ASP:OD2	1:B:278:TYR:OH	1.72	1.08
1:A:330[B]:HIS:CE1	1:A:333:ILE:HG23	1.63	1.07
1:A:681:GLN:HG2	5:A:2830:HOH:O	1.55	1.04
1:B:540:ARG:HD3	1:B:543:TRP:CE2	1.95	1.01
1:A:219[B]:ASP:OD2	1:A:278:TYR:OH	1.78	1.01
1:B:330[B]:HIS:NE2	1:B:333:ILE:CG2	2.24	1.00
1:B:10[B]:MET:CE	1:B:10[B]:MET:CG	2.39	0.99
1:B:151:ARG:HH12	1:B:474:GLN:HE21	1.11	0.97
1:B:540:ARG:HD3	1:B:543:TRP:NE1	1.85	0.92
1:A:11:TRP:HZ2	1:A:200[B]:LEU:HD21	1.37	0.88
1:A:5:GLU:N	5:A:2007[A]:HOH:O	2.07	0.87
1:A:11:TRP:CZ2	1:A:200[B]:LEU:HD21	2.10	0.86
1:A:540:ARG:HD3	1:A:543:TRP:CE2	2.11	0.86
1:A:681:GLN:CG	5:A:2830:HOH:O	2.16	0.85
1:A:525:GLN:HE22	1:A:528:HIS:HE1	1.22	0.85
1:B:330[A]:HIS:CD2	1:B:331:PRO:HD2	2.12	0.85
1:B:154:HIS:HE1	1:B:438:HIS:HD2	1.22	0.84
1:B:330[A]:HIS:CE1	1:B:332:ASP:CB	2.61	0.84
1:B:330[B]:HIS:NE2	1:B:333:ILE:HG23	1.91	0.84
1:A:5:GLU:N	5:A:2003:HOH:O	2.11	0.84
1:B:59:LYS:HE3	5:B:2050:HOH:O	1.77	0.84
1:B:330[B]:HIS:CD2	1:B:333:ILE:HG23	2.13	0.83
1:A:196:ILE:HD11	2:A:1716:EDO:H22	1.61	0.82
1:B:330[A]:HIS:HE1	1:B:332:ASP:HB3	1.41	0.82
1:A:330[B]:HIS:HE1	1:A:333:ILE:HG21	0.84	0.82
1:A:328:VAL:HG13	5:A:2438:HOH:O	1.79	0.82
1:B:330[A]:HIS:NE2	1:B:332:ASP:HB3	1.94	0.81
1:B:154:HIS:HE1	1:B:438:HIS:CD2	1.98	0.81
1:B:456:HIS:HD2	1:B:458:PHE:H	1.30	0.80
1:B:330[B]:HIS:CE1	1:B:333:ILE:HG21	2.18	0.79
1:B:525:GLN:HE22	1:B:528:HIS:HE1	1.25	0.78
1:B:553:LYS:HB2	1:B:553:LYS:NZ	1.98	0.78
1:A:680[A]:GLU:OE1	5:A:2829:HOH:O	2.02	0.78
1:B:153[B]:GLN:HE22	1:B:438:HIS:CD2	2.02	0.76
1:A:456:HIS:HD2	1:A:458:PHE:H	1.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ILE:HD11	2:B:1716:EDO:H22	1.66	0.76
1:B:553:LYS:HB2	1:B:553:LYS:HZ3	1.52	0.74
1:A:525:GLN:NE2	1:A:528:HIS:HE1	1.85	0.74
1:A:105:GLN:NE2	1:A:143:LYS:H	1.87	0.72
1:A:680[A]:GLU:OE1	5:A:2826:HOH:O	2.07	0.72
1:B:525:GLN:NE2	1:B:528:HIS:HE1	1.88	0.72
1:B:105:GLN:NE2	1:B:143:LYS:H	1.89	0.71
1:A:330[A]:HIS:CD2	1:A:343[A]:GLU:OE2	2.44	0.70
1:A:330[B]:HIS:ND1	1:A:333:ILE:HG23	2.03	0.70
1:B:330[A]:HIS:HD2	1:B:331:PRO:HD2	1.51	0.70
1:A:328:VAL:CG1	5:A:2438:HOH:O	2.38	0.68
1:A:24:LYS:NZ	1:A:27:GLN:HE22	1.92	0.68
1:A:216:VAL:HG23	1:A:217[B]:LEU:HD22	1.76	0.67
1:B:154:HIS:CE1	1:B:438:HIS:HD2	2.10	0.66
1:B:330[B]:HIS:CE1	1:B:333:ILE:CG2	2.76	0.66
1:B:680:GLU:OE1	5:B:2816:HOH:O	2.15	0.64
1:A:330[B]:HIS:NE2	1:A:333:ILE:CG2	2.54	0.64
1:A:196:ILE:HD11	2:A:1716:EDO:C2	2.27	0.64
1:B:540:ARG:CD	1:B:543:TRP:CE2	2.79	0.63
1:A:540:ARG:HD3	1:A:543:TRP:CZ2	2.33	0.63
1:A:92:ARG:O	1:A:96[A]:LEU:CD1	2.47	0.62
1:A:628[B]:ARG:NH2	5:A:2768:HOH:O	2.30	0.62
1:A:160:TRP:H	1:A:446:ASN:ND2	1.98	0.62
1:B:176[B]:LEU:CD2	5:B:2251:HOH:O	2.48	0.61
1:A:196:ILE:CD1	2:A:1716:EDO:H22	2.30	0.61
1:B:330[B]:HIS:HE2	1:B:333:ILE:CG2	2.12	0.61
1:B:536[B]:ASP:OD2	1:B:537:ASP:N	2.33	0.60
1:A:146:LEU:C	1:A:146:LEU:HD12	2.22	0.60
1:B:473:HIS:HD2	5:B:2598:HOH:O	1.84	0.60
1:B:330[A]:HIS:CE1	1:B:332:ASP:H	2.20	0.60
1:B:50[A]:GLN:NE2	5:B:2088:HOH:O	2.32	0.59
1:B:196:ILE:CD1	2:B:1716:EDO:H22	2.32	0.59
1:A:50:GLN:HG3	1:A:61:ILE:O	2.03	0.58
1:B:93:LEU:CD2	1:B:96:LEU:HD12	2.34	0.58
1:B:356:ILE:HD11	1:B:438:HIS:HB3	1.85	0.58
1:A:681:GLN:OE1	5:A:2831:HOH:O	2.16	0.57
1:A:473:HIS:HD2	5:A:2559:HOH:O	1.87	0.57
1:B:196:ILE:HD11	2:B:1716:EDO:C2	2.32	0.57
1:A:196:ILE:O	1:A:200[B]:LEU:CD2	2.53	0.56
1:B:330[B]:HIS:NE2	1:B:333:ILE:HG21	2.11	0.56
1:B:93:LEU:HD23	1:B:96:LEU:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ILE:CD1	1:B:438:HIS:HB3	2.36	0.56
1:B:24:LYS:NZ	1:B:27:GLN:HE22	2.04	0.56
1:B:557:GLY:O	1:B:595:HIS:HD2	1.88	0.56
1:B:10[A]:MET:SD	1:B:196:ILE:HD13	2.46	0.56
1:B:109:ASN:O	1:B:110:LYS:HB3	2.05	0.56
1:A:437:ARG:HG3	5:A:2499:HOH:O	2.05	0.56
1:B:393:GLU:OE2	1:B:528:HIS:HD2	1.87	0.55
1:A:92:ARG:O	1:A:96[A]:LEU:HD13	2.06	0.55
1:A:329:TYR:N	1:A:329:TYR:CD2	2.75	0.55
1:B:176[B]:LEU:HD23	5:B:2251:HOH:O	2.07	0.55
1:A:160:TRP:H	1:A:446:ASN:HD21	1.53	0.55
1:B:59:LYS:NZ	5:B:2104:HOH:O	2.36	0.54
1:A:199:SER:OG	1:A:200[B]:LEU:HD22	2.07	0.54
1:B:536[B]:ASP:OD1	1:B:546:VAL:HG21	2.08	0.54
1:A:158:ASN:HD21	1:A:358:GLN:HE22	1.55	0.54
1:A:330[A]:HIS:NE2	1:A:343[A]:GLU:OE2	2.41	0.54
1:B:158:ASN:HD21	1:B:358:GLN:HE22	1.56	0.54
1:A:196:ILE:HG13	2:A:1716:EDO:H11	1.90	0.54
1:B:176[B]:LEU:HD22	5:B:2251:HOH:O	2.08	0.54
1:A:393:GLU:OE2	1:A:528:HIS:HD2	1.91	0.54
1:B:24:LYS:NZ	5:B:2048:HOH:O	2.41	0.54
1:A:330[B]:HIS:HE1	1:A:333:ILE:CG2	1.62	0.53
1:A:430:GLU:OE1	1:A:473:HIS:HE1	1.92	0.53
1:B:550:ARG:NE	5:B:2664:HOH:O	2.41	0.53
1:B:330[A]:HIS:NE2	1:B:332:ASP:CB	2.67	0.52
1:A:216:VAL:CG2	1:A:217[B]:LEU:HD22	2.39	0.52
1:B:330[B]:HIS:HE1	5:B:2485:HOH:O	1.91	0.52
1:B:153[B]:GLN:NE2	1:B:438:HIS:CD2	2.74	0.52
1:B:350[B]:LYS:NZ	5:B:2498:HOH:O	2.43	0.52
1:B:157:VAL:HG22	1:B:205[B]:THR:HG22	1.90	0.52
1:A:244:ASN:ND2	1:A:246:ASN:H	2.08	0.52
1:B:430:GLU:OE1	1:B:473:HIS:HE1	1.93	0.51
1:A:196:ILE:O	1:A:200[B]:LEU:HD23	2.11	0.51
1:B:93:LEU:HD23	1:B:96:LEU:HD12	1.91	0.51
1:B:265:GLN:NE2	5:B:2419:HOH:O	2.44	0.51
1:A:244:ASN:HD22	1:A:246:ASN:H	1.58	0.51
1:B:330[A]:HIS:CE1	1:B:332:ASP:CA	2.95	0.50
1:A:59:LYS:HE2	5:A:2104:HOH:O	2.12	0.50
1:B:244:ASN:ND2	1:B:246:ASN:H	2.09	0.50
1:A:513:TYR:C	1:A:513:TYR:CD1	2.85	0.49
1:B:59:LYS:CE	5:B:2050:HOH:O	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:CG2	1:B:205[B]:THR:HG22	2.42	0.49
1:A:456:HIS:HE1	5:A:2547:HOH:O	1.96	0.49
1:A:330[B]:HIS:CE1	5:A:2478:HOH:O	2.66	0.48
1:A:24:LYS:HZ2	1:A:27:GLN:HE22	1.61	0.48
1:A:92:ARG:O	1:A:96[A]:LEU:HD11	2.12	0.48
1:B:456:HIS:HE1	5:B:2540:HOH:O	1.95	0.48
1:B:146:LEU:C	1:B:146:LEU:HD12	2.34	0.48
1:A:81:SER:HB3	1:A:84[B]:ILE:HG13	1.96	0.48
1:B:330[A]:HIS:CD2	1:B:332:ASP:H	2.32	0.47
1:A:525:GLN:NE2	1:A:528:HIS:CE1	2.74	0.47
1:A:146:LEU:O	1:A:146:LEU:HD12	2.14	0.47
1:B:332:ASP:CG	1:B:332:ASP:O	2.53	0.47
1:B:381:ARG:HG3	1:B:381:ARG:HH11	1.79	0.47
1:B:540:ARG:HG3	1:B:543:TRP:CG	2.51	0.46
1:B:196:ILE:HG13	2:B:1716:EDO:H11	1.96	0.46
1:B:393:GLU:OE2	1:B:528:HIS:CD2	2.68	0.46
1:A:130:HIS:CE1	2:A:1715:EDO:H12	2.51	0.46
1:A:333:ILE:HD11	1:A:336:ARG:HA	1.98	0.45
1:A:217[B]:LEU:CD2	5:A:2387:HOH:O	2.64	0.45
1:A:185:TYR:CD2	2:A:1717:EDO:H22	2.51	0.45
1:B:330[A]:HIS:CD2	1:B:331:PRO:CD	2.91	0.45
1:A:24:LYS:HZ3	1:A:27:GLN:HE22	1.65	0.45
1:B:59:LYS:CE	5:B:2104:HOH:O	2.64	0.45
1:A:680[A]:GLU:CG	5:A:2826:HOH:O	2.65	0.45
1:A:160:TRP:HA	1:A:209:ASN:HA	1.99	0.45
1:B:330[A]:HIS:CE1	1:B:332:ASP:N	2.83	0.45
1:A:688:TYR:CE1	1:A:692:LEU:HD11	2.51	0.45
1:A:393:GLU:OE2	1:A:528:HIS:CD2	2.70	0.45
1:B:525:GLN:NE2	1:B:528:HIS:CE1	2.78	0.45
1:A:216:VAL:HG23	1:A:217[B]:LEU:CD2	2.46	0.44
1:B:622:GLN:O	1:B:626[A]:MET:HG3	2.17	0.44
1:B:507:ARG:HD3	1:B:507:ARG:C	2.37	0.44
1:B:244:ASN:HD22	1:B:246:ASN:H	1.66	0.44
1:A:24:LYS:HD3	1:A:27:GLN:NE2	2.32	0.44
1:A:129:PHE:CG	1:A:199:SER:HA	2.53	0.43
1:B:59:LYS:HB2	1:B:60:PRO:HD2	2.00	0.43
1:B:93:LEU:HD23	1:B:96:LEU:HD11	2.00	0.43
1:A:219[B]:ASP:CG	1:A:278:TYR:OH	2.52	0.43
1:B:93:LEU:HD22	1:B:96:LEU:HD12	2.00	0.43
1:A:24:LYS:HA	1:A:24:LYS:HD3	1.81	0.42
1:B:50[A]:GLN:NE2	1:B:63:ALA:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LYS:HD3	1:B:24:LYS:HA	1.69	0.42
1:A:323:PHE:CE1	1:A:385[B]:MET:HE1	2.54	0.42
1:A:341:TYR:CZ	1:A:345:MET:HG3	2.55	0.42
1:B:206:VAL:HG22	1:B:240:TYR:HB2	2.02	0.42
1:B:24:LYS:HD3	1:B:27:GLN:NE2	2.34	0.42
1:B:20:GLN:O	1:B:24:LYS:HG2	2.19	0.41
1:A:28:LYS:HB3	5:A:2064:HOH:O	2.20	0.41
1:B:129:PHE:CG	1:B:199:SER:HA	2.55	0.41
1:A:507:ARG:C	1:A:507:ARG:HD3	2.41	0.41
1:A:474:GLN:CD	5:A:2605:HOH:O	2.58	0.41
1:A:612:LEU:HD23	1:A:612:LEU:C	2.41	0.41
1:A:680[A]:GLU:CD	5:A:2828:HOH:O	2.59	0.41
1:A:356:ILE:HG21	1:A:385[B]:MET:HE3	2.03	0.41
1:A:624:ARG:HA	1:A:627:GLN:HE21	1.86	0.41
1:A:10[A]:MET:SD	1:A:196:ILE:HD13	2.61	0.41
1:A:217[B]:LEU:HD23	5:A:2387:HOH:O	2.21	0.41
1:B:110:LYS:O	1:B:110:LYS:HG2	2.20	0.41
1:B:14:TYR:CG	1:B:52:GLY:HA2	2.56	0.41
1:A:105:GLN:HE22	1:A:143:LYS:H	1.68	0.40
1:B:93:LEU:HA	1:B:93:LEU:HD23	1.98	0.40
1:B:27:GLN:HG2	1:B:59:LYS:HE2	2.02	0.40
1:A:14:TYR:CG	1:A:52:GLY:HA2	2.56	0.40
1:B:568:LEU:HD23	1:B:568:LEU:HA	1.90	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)
5:A:2136:HOH:O	5:A:2825:HOH:O[1_455]	2.10	0.10

## 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	728/708 (103%)	711 (98%)	16 (2%)	1 (0%)	56	25
1	B	730/708 (103%)	710 (97%)	19 (3%)	1 (0%)	56	25
All	All	1458/1416 (103%)	1421 (98%)	35 (2%)	2 (0%)	56	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	ASP
1	B	365	ASP

### 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	610/588 (104%)	603 (99%)	7 (1%)	80	56
1	B	612/588 (104%)	602 (98%)	10 (2%)	70	39
All	All	1222/1176 (104%)	1205 (99%)	17 (1%)	78	46

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LEU
1	A	156[A]	VAL
1	A	156[B]	VAL
1	A	244	ASN
1	A	332	ASP
1	A	507	ARG
1	A	681	GLN
1	B	109	ASN
1	B	141	LEU
1	B	156[A]	VAL
1	B	156[B]	VAL
1	B	244	ASN
1	B	330[A]	HIS
1	B	330[B]	HIS

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Mol	Chain	Res	Type
1	B	507	ARG
1	B	553	LYS
1	B	683	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	27	GLN
1	A	32	HIS
1	A	105	GLN
1	A	158	ASN
1	A	244	ASN
1	A	265	GLN
1	A	266	GLN
1	A	446	ASN
1	A	456	HIS
1	A	473	HIS
1	A	512	ASN
1	A	525	GLN
1	A	528	HIS
1	A	600	HIS
1	A	618	GLN
1	A	627	GLN
1	A	633	GLN
1	A	681	GLN
1	B	15	GLN
1	B	27	GLN
1	B	105	GLN
1	B	154	HIS
1	B	158	ASN
1	B	244	ASN
1	B	265	GLN
1	B	266	GLN
1	B	392	GLN
1	B	438	HIS
1	B	456	HIS
1	B	473	HIS
1	B	474	GLN
1	B	512	ASN
1	B	525	GLN
1	B	528	HIS

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Mol	Chain	Res	Type
1	B	595	HIS
1	B	618	GLN
1	B	627	GLN
1	B	681	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 ⓘ

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	EDO	A	1713	-	3,3,3	0.34	0	2,2,2	0.45	0
2	EDO	A	1714	-	3,3,3	0.38	0	2,2,2	0.52	0
2	EDO	A	1715	-	3,3,3	0.30	0	2,2,2	1.05	0
2	EDO	A	1716	-	3,3,3	0.56	0	2,2,2	0.92	0
2	EDO	A	1717	-	3,3,3	0.66	0	2,2,2	0.87	0
2	EDO	A	1718	-	3,3,3	0.41	0	2,2,2	0.47	0
2	EDO	B	1713	-	3,3,3	0.60	0	2,2,2	0.51	0
2	EDO	B	1714	-	3,3,3	0.45	0	2,2,2	0.56	0
2	EDO	B	1715	-	3,3,3	0.23	0	2,2,2	0.63	0
2	EDO	B	1716	-	3,3,3	0.55	0	2,2,2	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	B	1717	-	3,3,3	0.40	0	2,2,2	0.50	0
2	EDO	B	1718	-	3,3,3	0.30	0	2,2,2	0.58	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	EDO	A	1713	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1714	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1715	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1716	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1717	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1718	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1713	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1714	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1715	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1716	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1717	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1718	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1715	EDO	1	0
2	A	1716	EDO	4	0
2	A	1717	EDO	1	0
2	B	1716	EDO	4	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	708/708 (100%)	0.31	28 (3%) 42 44	6, 10, 22, 38	0
1	B	708/708 (100%)	0.25	33 (4%) 35 36	6, 10, 24, 38	0
All	All	1416/1416 (100%)	0.28	61 (4%) 39 41	6, 10, 23, 38	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	TYR	10.2
1	A	331	PRO	9.5
1	A	543	TRP	9.1
1	B	437	ARG	8.8
1	A	328	VAL	8.1
1	A	327	PHE	8.1
1	B	543	TRP	7.5
1	A	332	ASP	7.4
1	B	332	ASP	6.9
1	B	328[A]	VAL	6.4
1	A	437	ARG	6.0
1	A	537	ASP	6.0
1	B	330[A]	HIS	5.9
1	A	333	ILE	5.7
1	B	331	PRO	5.6
1	B	329	TYR	5.4
1	A	538	LEU	5.4
1	B	537	ASP	5.3
1	A	330[A]	HIS	5.3
1	B	538	LEU	4.7
1	A	334	GLU	4.6
1	A	435	LYS	4.4
1	A	513	TYR	4.4
1	A	22	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	683	GLU	4.1
1	B	539	PRO	4.1
1	A	539	PRO	3.8
1	B	109	ASN	3.7
1	B	327	PHE	3.5
1	B	22	LEU	3.5
1	B	677	ALA	3.3
1	B	333	ILE	3.1
1	B	678	ASN	3.1
1	A	677	ALA	3.0
1	A	21	THR	2.9
1	B	91	GLU	2.9
1	B	21	THR	2.8
1	B	334	GLU	2.7
1	B	88	ASN	2.7
1	B	679	TYR	2.7
1	B	536[A]	ASP	2.6
1	A	681	GLN	2.6
1	B	540	ARG	2.5
1	B	110	LYS	2.5
1	B	421	GLU	2.4
1	B	60	PRO	2.4
1	B	18	ALA	2.4
1	B	59	LYS	2.4
1	A	540	ARG	2.4
1	B	89	LEU	2.3
1	B	438	HIS	2.3
1	A	61	ILE	2.2
1	A	674	PRO	2.2
1	B	28	LYS	2.2
1	A	553	LYS	2.2
1	A	326	ALA	2.2
1	A	110	LYS	2.2
1	A	96[A]	LEU	2.1
1	A	20	GLN	2.1
1	A	536	ASP	2.1
1	B	20	GLN	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	A	1717	4/4	0.88	0.19	15.41	21,22,22,24	0
2	EDO	A	1718	4/4	0.94	0.20	3.92	10,16,20,23	0
2	EDO	B	1713	4/4	0.98	0.11	1.84	9,9,11,11	0
3	CO	B	1720[A]	1/1	0.99	0.09	1.50	10,10,10,10	1
2	EDO	B	1715	4/4	0.93	0.10	1.35	19,21,22,23	0
2	EDO	B	1718	4/4	0.96	0.09	1.15	16,16,16,17	0
2	EDO	B	1717	4/4	0.83	0.20	0.99	32,33,35,35	0
2	EDO	A	1716	4/4	0.98	0.09	0.05	9,11,11,13	0
2	EDO	B	1716	4/4	0.97	0.10	-0.02	9,12,13,14	0
2	EDO	A	1715	4/4	0.92	0.09	-0.11	16,17,18,19	0
2	EDO	A	1713	4/4	0.98	0.08	-0.60	7,8,10,11	0
3	CO	A	1720[A]	1/1	1.00	0.06	-1.36	10,10,10,10	1
3	CO	B	1719[A]	1/1	1.00	0.06	-1.86	11,11,11,11	1
3	CO	A	1719[A]	1/1	1.00	0.06	-3.07	11,11,11,11	1
4	MG	B	1723	1/1	0.98	0.15	-	18,18,18,18	0
3	CO	A	1721[A]	1/1	0.99	0.10	-	15,15,15,15	1
3	CO	A	1722[A]	1/1	1.00	0.06	-	14,14,14,14	1
4	MG	A	1723	1/1	0.97	0.21	-	23,23,23,23	0
3	CO	B	1722[A]	1/1	0.99	0.10	-	16,16,16,16	1
2	EDO	B	1714	4/4	0.95	0.10	-	11,12,16,17	0
3	CO	B	1721[A]	1/1	1.00	0.07	-	14,14,14,14	1
2	EDO	A	1714	4/4	0.96	0.09	-	11,12,14,16	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.