



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2016 – 04:50 PM EDT

PDB ID : 5DMY  
Title : Beta-galactosidase - construct 33-930  
Authors : Watson, K.A.; Lazidou, A.  
Deposited on : 2015-09-09  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

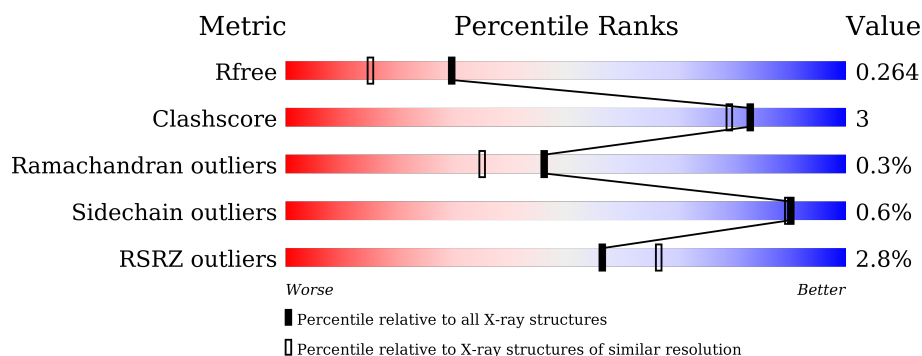
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	904	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 90%, yellow 90%, yellow 95%, green 95%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>90%</span> <span>5%</span> <span>5%</span> </div> </div>
1	B	904	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, orange 4%, orange 86%, yellow 86%, yellow 94%, green 94%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>86%</span> <span>8%</span> <span>5%</span> </div> </div>
1	C	904	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 86%, yellow 86%, yellow 94%, green 94%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>86%</span> <span>8%</span> <span>5%</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21901 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	855	Total	C	N	O	S	13	6	0
			6492	4064	1112	1303	13			
1	B	858	Total	C	N	O	S	0	0	0
			6466	4046	1104	1303	13			
1	C	855	Total	C	N	O	S	5	3	0
			6457	4042	1104	1298	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP D4QAP3
A	-4	HIS	-	expression tag	UNP D4QAP3
A	-3	HIS	-	expression tag	UNP D4QAP3
A	-2	HIS	-	expression tag	UNP D4QAP3
A	-1	HIS	-	expression tag	UNP D4QAP3
A	0	HIS	-	expression tag	UNP D4QAP3
B	-5	HIS	-	expression tag	UNP D4QAP3
B	-4	HIS	-	expression tag	UNP D4QAP3
B	-3	HIS	-	expression tag	UNP D4QAP3
B	-2	HIS	-	expression tag	UNP D4QAP3
B	-1	HIS	-	expression tag	UNP D4QAP3
B	0	HIS	-	expression tag	UNP D4QAP3
C	-5	HIS	-	expression tag	UNP D4QAP3
C	-4	HIS	-	expression tag	UNP D4QAP3
C	-3	HIS	-	expression tag	UNP D4QAP3
C	-2	HIS	-	expression tag	UNP D4QAP3
C	-1	HIS	-	expression tag	UNP D4QAP3
C	0	HIS	-	expression tag	UNP D4QAP3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

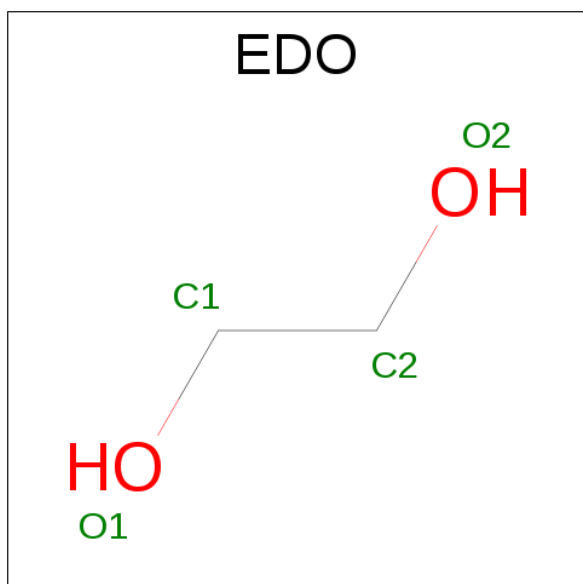
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	2	Total Na 2 2	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0

- Molecule 5 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
5	A	1	Total C O 4 2 2	0	0

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

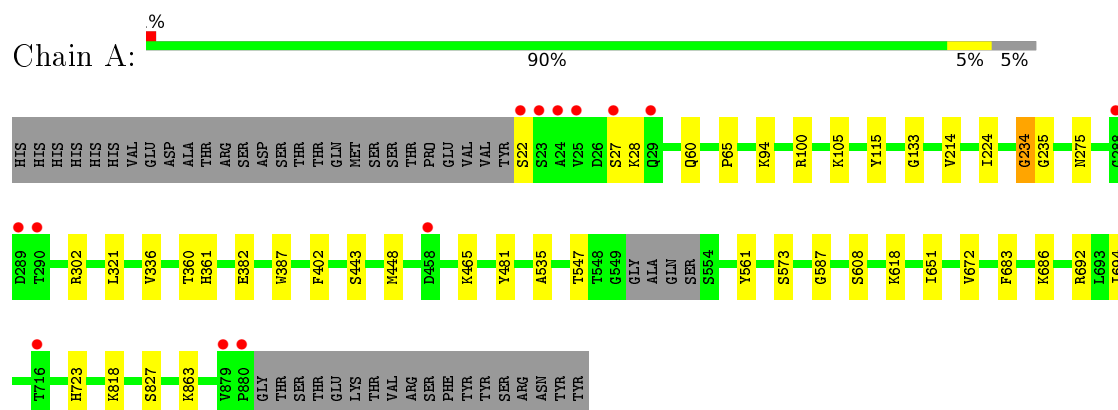
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	985	Total	O	0	0
			985	985		
6	B	716	Total	O	0	0
			716	716		
6	C	768	Total	O	0	0
			768	768		

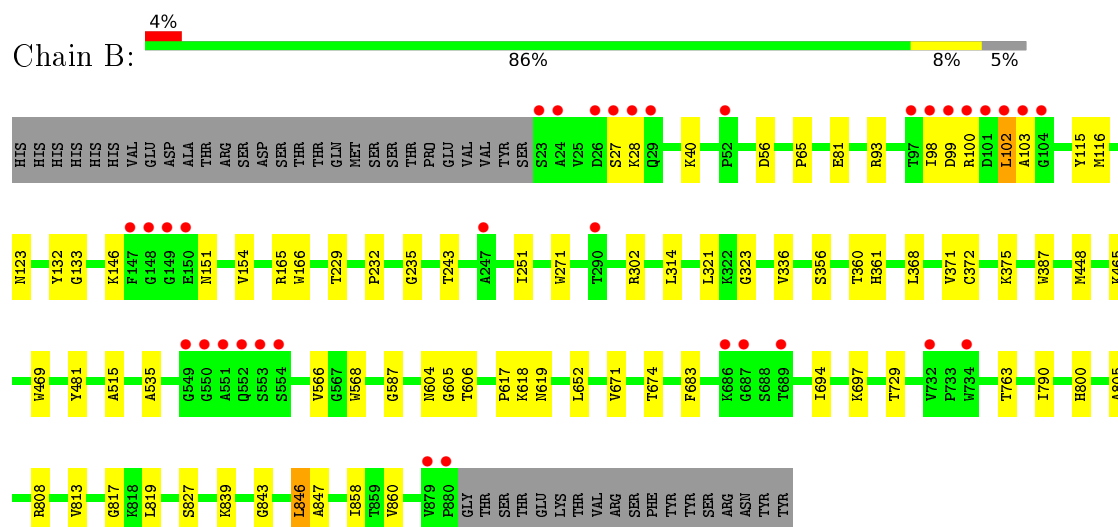
### 3 Residue-property plots

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.

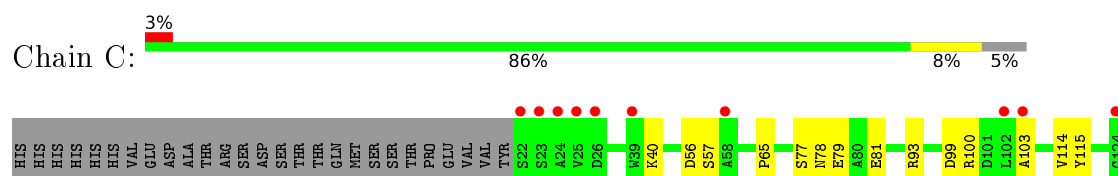
#### • Molecule 1: Beta-galactosidase

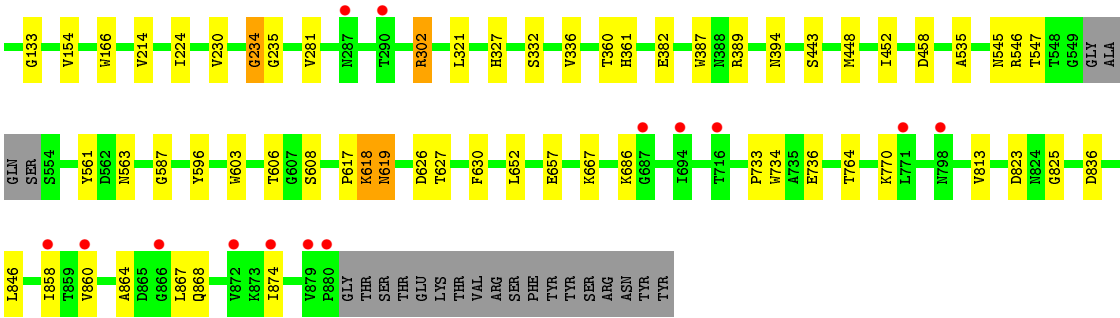


#### • Molecule 1: Beta-galactosidase



#### • Molecule 1: Beta-galactosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.04Å 52.65Å 153.33Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	54.93 – 1.95 54.93 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.0 (54.93-1.95) 95.0 (54.93-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.198 , 0.264 0.198 , 0.264	Depositor DCC
$R_{free}$ test set	8525 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.000 for h,-k,-l 0.026 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.21 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3660e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, EDO, NA

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	0.43	0/6655	0.57	1/9071 (0.0%)
1	B	0.37	0/6612	0.52	0/9016
1	C	0.39	0/6611	0.55	1/9014 (0.0%)
All	All	0.40	0/19878	0.55	2/27101 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLY	N-CA-C	6.36	128.99	113.10
1	C	234	GLY	N-CA-C	5.06	125.76	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6492	0	6176	23	0
1	B	6466	0	6137	46	0
1	C	6457	0	6133	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0
5	A	8	0	12	0	0
6	A	985	0	0	5	2
6	B	716	0	0	8	1
6	C	768	0	0	14	2
All	All	21901	0	18458	117	3

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 3.

All (117) 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:368:LEU:O	6:B:1001:HOH:O	1.83	0.95
1:B:515:ALA:O	6:B:1002:HOH:O	1.86	0.92
1:C:394:ASN:OD1	6:C:1001:HOH:O	1.91	0.87
1:B:40:LYS:HD3	1:B:56:ASP:HB3	1.59	0.85
1:C:618:LYS:NZ	1:C:619[B]:ASN:OD1	2.14	0.81
1:A:105:LYS:NZ	6:A:1002:HOH:O	2.19	0.75
1:A:65:PRO:HB2	1:A:336:VAL:HG13	1.71	0.72
1:C:545:ASN:OD1	1:C:546:ARG:NH1	2.22	0.72
1:C:79:GLU:OE1	6:C:1001:HOH:O	2.07	0.71
1:B:65:PRO:HG2	1:B:336:VAL:HG13	1.74	0.70
1:C:736:GLU:HG3	1:C:764:THR:HG21	1.73	0.69
1:A:275:ASN:ND2	6:A:1006:HOH:O	2.26	0.68
1:C:458:ASP:OD1	6:C:1002:HOH:O	2.13	0.67
1:B:371:VAL:N	6:B:1001:HOH:O	2.29	0.65
1:C:545:ASN:ND2	6:C:1010:HOH:O	2.31	0.64
1:B:387:TRP:CE2	1:B:448:MET:HG2	2.33	0.64
1:A:100:ARG:NH1	6:A:1010:HOH:O	2.31	0.64
1:B:99:ASP:OD1	1:B:100:ARG:N	2.31	0.63
1:B:56:ASP:OD1	1:B:93:ARG:NE	2.32	0.62
1:A:321:LEU:HB2	1:A:587:GLY:HA3	1.83	0.60
1:B:229:THR:HG23	1:B:243:THR:HG22	1.83	0.60
1:A:387:TRP:CE2	1:A:448:MET:HG2	2.37	0.59
1:A:683:PHE:HB2	1:A:694:ILE:HD11	1.84	0.59
1:C:387:TRP:CE2	1:C:448:MET:HG2	2.39	0.58
1:B:683:PHE:HB2	1:B:694:ILE:HD11	1.86	0.57
1:C:382:GLU:HA	1:C:443:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:ASP:OD2	6:C:1003:HOH:O	2.17	0.57
1:C:389:ARG:NH1	6:C:1018:HOH:O	2.36	0.57
1:A:22:SER:N	1:A:94:LYS:HZ1	2.02	0.57
1:C:858:ILE:N	1:C:874:ILE:O	2.37	0.56
1:C:99:ASP:OD1	1:C:100:ARG:N	2.38	0.56
1:B:674:THR:N	6:B:1009:HOH:O	2.30	0.55
1:B:321:LEU:HB2	1:B:587:GLY:HA3	1.89	0.55
1:C:93:ARG:HG2	1:C:154:VAL:HG22	1.89	0.55
1:C:667:LYS:NZ	1:C:733:PRO:HD3	2.22	0.54
1:A:115:TYR:CD2	1:A:133:GLY:HA3	2.42	0.54
1:C:65:PRO:HB2	1:C:336:VAL:HG13	1.90	0.54
1:A:382:GLU:HA	1:A:443:SER:HB3	1.90	0.54
1:B:617:PRO:HB2	6:B:1010:HOH:O	2.07	0.54
1:C:81:GLU:HG3	1:C:606:THR:HA	1.91	0.52
1:B:697:LYS:NZ	1:B:729:THR:O	2.43	0.52
1:B:652:LEU:HD11	1:B:671:VAL:HB	1.92	0.51
1:C:214:VAL:HG11	1:C:224:ILE:HD13	1.91	0.51
1:C:234:GLY:N	1:C:235:GLY:HA3	2.25	0.51
1:B:93:ARG:HG2	1:B:154:VAL:HG22	1.93	0.51
1:C:77:SER:O	1:C:608[A]:SER:OG	2.26	0.51
1:C:667:LYS:HZ2	1:C:733:PRO:HD3	1.76	0.51
1:C:230:VAL:HG22	1:C:281:VAL:HG22	1.94	0.50
1:C:813:VAL:HG22	1:C:860:VAL:HG22	1.93	0.50
1:C:321:LEU:HB2	1:C:587:GLY:HA3	1.93	0.50
1:B:302:ARG:HG3	1:B:314:LEU:HD11	1.94	0.49
1:C:452:ILE:N	6:C:1014:HOH:O	2.34	0.49
1:C:545:ASN:N	6:C:1036:HOH:O	2.43	0.49
1:C:563:ASN:ND2	6:C:1038:HOH:O	2.44	0.49
1:B:805:ALA:HB3	1:B:843:GLY:HA2	1.96	0.48
1:C:40:LYS:HD2	1:C:56:ASP:HB3	1.95	0.48
1:B:372:CYS:N	6:B:1001:HOH:O	1.94	0.47
1:B:808:ARG:HA	1:B:839:LYS:HA	1.95	0.47
1:B:123:ASN:OD1	1:B:151:ASN:HA	2.15	0.47
1:A:547:THR:HG22	1:A:561:TYR:CE1	2.50	0.47
1:C:302[B]:ARG:NH2	6:C:1040:HOH:O	2.46	0.46
1:B:817:GLY:HA3	1:B:858:ILE:HD13	1.97	0.46
1:C:458:ASP:HB2	6:C:1231:HOH:O	2.15	0.46
1:A:60:GLN:HG3	6:A:1453:HOH:O	2.16	0.46
1:A:818:LYS:HB3	1:A:818:LYS:HE2	1.68	0.46
1:C:115:TYR:CD2	1:C:133:GLY:HA3	2.50	0.46
1:B:98:ILE:HG23	1:B:102:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:THR:HA	1:C:361:HIS:HA	1.64	0.46
1:C:864:ALA:HB3	1:C:867:LEU:HD12	1.98	0.45
1:C:858:ILE:HB	1:C:874:ILE:HB	1.99	0.45
1:B:813:VAL:HG21	1:B:819:LEU:HB2	1.99	0.45
1:A:692:ARG:NH2	6:A:1049:HOH:O	2.46	0.45
1:B:839:LYS:HE3	1:B:839:LYS:HB2	1.75	0.45
1:C:78:ASN:HB3	6:C:1251:HOH:O	2.17	0.45
1:C:332:SER:HB3	1:C:823:ASP:HB2	1.99	0.45
1:C:603:TRP:CD2	1:C:617:PRO:HG2	2.52	0.45
1:C:114:VAL:O	1:C:133:GLY:HA2	2.16	0.45
1:B:271:TRP:CE3	1:B:302:ARG:HD3	2.53	0.44
1:C:630:PHE:CZ	1:C:846:LEU:HB2	2.53	0.44
1:A:360:THR:HA	1:A:361:HIS:HA	1.69	0.44
1:B:27:SER:HA	1:B:28:LYS:HA	1.72	0.44
1:B:790:ILE:HD13	1:B:860:VAL:HG11	2.00	0.44
1:B:566:VAL:HG21	1:B:568:TRP:CE2	2.51	0.44
1:C:686:LYS:HE2	6:C:1656:HOH:O	2.17	0.44
1:A:573:SER:OG	1:A:723:HIS:ND1	2.46	0.43
1:A:234:GLY:N	1:A:235:GLY:HA3	2.33	0.43
1:A:27:SER:HA	1:A:28:LYS:HA	1.54	0.43
1:B:302:ARG:CZ	6:B:1049:HOH:O	2.66	0.43
1:B:371:VAL:O	1:B:375:LYS:N	2.51	0.43
1:C:657:GLU:HB2	1:C:734:TRP:CH2	2.52	0.43
1:B:360:THR:HA	1:B:361:HIS:HA	1.67	0.43
1:B:232:PRO:O	1:B:235:GLY:HA2	2.18	0.43
1:B:146:LYS:NZ	6:B:1058:HOH:O	2.51	0.43
1:C:547:THR:O	1:C:563:ASN:HB2	2.18	0.43
1:B:465:LYS:HE3	1:B:469:TRP:NE1	2.34	0.42
1:C:770:LYS:HG3	1:C:868:GLN:HB2	2.01	0.42
1:B:604:ASN:OD1	1:B:605:GLY:N	2.53	0.42
1:B:81:GLU:HG3	1:B:606:THR:HA	2.02	0.42
1:B:115:TYR:CD2	1:B:133:GLY:HA3	2.55	0.42
1:B:81:GLU:HG3	1:B:605:GLY:O	2.20	0.42
1:C:627:THR:OG1	1:C:825:GLY:HA2	2.19	0.42
1:B:652:LEU:CD1	1:B:671:VAL:HB	2.50	0.41
1:B:115:TYR:HA	1:B:116:MET:HA	1.90	0.41
1:B:846:LEU:HG	1:B:847:ALA:N	2.35	0.41
1:B:323:GLY:HA2	1:B:356:SER:O	2.20	0.41
1:A:863:LYS:HE2	1:A:863:LYS:HB2	1.83	0.41
1:B:763:THR:HG21	1:B:800:HIS:CE1	2.55	0.41
1:A:651:ILE:HG12	1:A:672:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LYS:HG3	1:A:827:SER:O	2.20	0.41
1:C:626:ASP:HB2	6:C:1357:HOH:O	2.20	0.41
1:C:166:TRP:CD2	1:C:327:HIS:CE1	3.09	0.41
1:C:547:THR:HG22	1:C:561:TYR:CE1	2.55	0.41
1:A:214:VAL:HG11	1:A:224:ILE:HD13	2.03	0.40
1:C:596:TYR:O	1:C:619[B]:ASN:HB2	2.21	0.40
1:B:618:LYS:HG3	1:B:827:SER:O	2.22	0.40
1:B:165:ARG:HB2	1:B:166:TRP:CE3	2.56	0.40
1:A:465:LYS:HE2	1:A:465:LYS:HB3	1.98	0.40

All (3) 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)
6:B:1504:HOH:O	6:C:1492:HOH:O[1_565]	2.10	0.10
6:A:1482:HOH:O	6:C:1508:HOH:O[2_556]	2.15	0.05
6:A:1277:HOH:O	6:A:1743:HOH:O[1_545]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	857/904 (95%)	831 (97%)	24 (3%)	2 (0%)	52	43
1	B	856/904 (95%)	825 (96%)	28 (3%)	3 (0%)	39	27
1	C	854/904 (94%)	821 (96%)	30 (4%)	3 (0%)	39	27
All	All	2567/2712 (95%)	2477 (96%)	82 (3%)	8 (0%)	46	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	103	ALA

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Mol	Chain	Res	Type
1	B	103	ALA
1	C	57	SER
1	A	402	PHE
1	A	535	ALA
1	B	102	LEU
1	B	535	ALA
1	C	535	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	679/737 (92%)	674 (99%)	5 (1%)	88	88
1	B	675/737 (92%)	670 (99%)	5 (1%)	88	88
1	C	675/737 (92%)	669 (99%)	6 (1%)	84	83
All	All	2029/2211 (92%)	2013 (99%)	16 (1%)	90	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302[A]	ARG
1	A	302[B]	ARG
1	A	481	TYR
1	A	608	SER
1	A	686	LYS
1	B	132	TYR
1	B	251	ILE
1	B	481	TYR
1	B	619	ASN
1	B	846	LEU
1	C	302[A]	ARG
1	C	302[B]	ARG
1	C	618	LYS
1	C	619[A]	ASN
1	C	619[B]	ASN

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Mol	Chain	Res	Type
1	C	652	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	$\# Z  > 2$
5	EDO	A	905	-	3,3,3	0.50	0	2,2,2	0.49	0
5	EDO	A	906	-	3,3,3	0.44	0	2,2,2	0.63	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
5	EDO	A	905	-	-	0/1/1/1	0/0/0/0
5	EDO	A	906	-	-	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.

No monomer is involved in short contacts.

## 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 ⓘ

### 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	855/904 (94%)	-0.05	13 (1%) 76 84	2, 8, 20, 50	0
1	B	858/904 (94%)	0.31	34 (3%) 42 53	7, 17, 33, 59	0
1	C	855/904 (94%)	0.31	24 (2%) 56 66	7, 14, 31, 59	0
All	All	2568/2712 (94%)	0.19	71 (2%) 56 66	2, 13, 30, 59	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22	SER	9.9
1	B	550	GLY	6.4
1	B	551	ALA	5.4
1	B	24	ALA	5.3
1	C	24	ALA	5.3
1	A	27	SER	5.3
1	B	102	LEU	4.5
1	B	27	SER	4.4
1	B	23	SER	4.3
1	C	858	ILE	4.3
1	A	22	SER	4.2
1	B	290	THR	4.2
1	C	124	GLY	3.9
1	B	26	ASP	3.9
1	B	553	SER	3.8
1	A	23	SER	3.7
1	B	148	GLY	3.7
1	C	290	THR	3.6
1	A	24	ALA	3.5
1	C	103	ALA	3.4
1	C	23	SER	3.3
1	B	29	GLN	3.2
1	C	287	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	686	LYS	2.9
1	B	147	PHE	2.9
1	B	687	GLY	2.9
1	A	879	VAL	2.8
1	B	104	GLY	2.8
1	C	880	PRO	2.8
1	B	101	ASP	2.8
1	B	28	LYS	2.7
1	B	149	GLY	2.7
1	B	879	VAL	2.6
1	B	880	PRO	2.6
1	B	103	ALA	2.6
1	B	549	GLY	2.6
1	B	554	SER	2.6
1	A	288	GLY	2.6
1	C	25	VAL	2.6
1	B	247	ALA	2.6
1	A	880	PRO	2.6
1	C	102	LEU	2.5
1	C	798	ASN	2.5
1	B	97	THR	2.5
1	C	874	ILE	2.5
1	A	289	ASP	2.4
1	C	866	GLY	2.4
1	B	552	GLN	2.4
1	A	29	GLN	2.4
1	A	290	THR	2.4
1	A	458[A]	ASP	2.4
1	B	689	THR	2.4
1	B	98	ILE	2.4
1	A	25	VAL	2.3
1	C	716	THR	2.3
1	C	879	VAL	2.3
1	C	694	ILE	2.2
1	C	771	LEU	2.2
1	C	26	ASP	2.2
1	B	99	ASP	2.2
1	B	52	PRO	2.1
1	B	100	ARG	2.1
1	B	150	GLU	2.1
1	B	732	VAL	2.1
1	C	39	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	58	ALA	2.1
1	C	872	VAL	2.1
1	C	860	VAL	2.0
1	B	734	TRP	2.0
1	C	687	GLY	2.0
1	A	716	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	901	1/1	0.99	0.14	1.97	9,9,9,9	0
5	EDO	A	906	4/4	0.97	0.12	0.41	9,13,16,27	0
2	MG	C	901	1/1	0.99	0.11	-0.22	9,9,9,9	0
2	MG	A	901	1/1	0.99	0.09	-0.81	8,8,8,8	0
3	NA	C	903	1/1	0.95	0.10	-1.15	15,15,15,15	0
5	EDO	A	905	4/4	0.99	0.09	-1.70	6,6,7,7	0
3	NA	A	903	1/1	0.99	0.07	-2.91	10,10,10,10	0
2	MG	A	902	1/1	0.99	0.07	-3.10	10,10,10,10	0
2	MG	B	902	1/1	0.98	0.06	-3.58	12,12,12,12	0
3	NA	C	902	1/1	0.97	0.08	-3.81	18,18,18,18	0
4	NI	A	904	1/1	0.99	0.05	-5.43	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.