



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:40 PM UTC

PDB ID : 5DMY / pdb_00005dmy
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

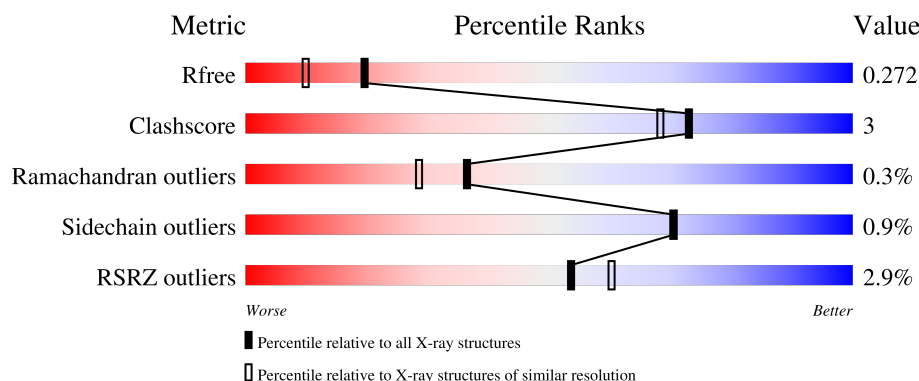
1 Overall quality at a glance

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	2% 89% 5% 5%
1	B	904	5% 86% 8% 5%
1	C	904	2% 85% 9% 5%

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 (CCD ID: MG) (formula: Mg).

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

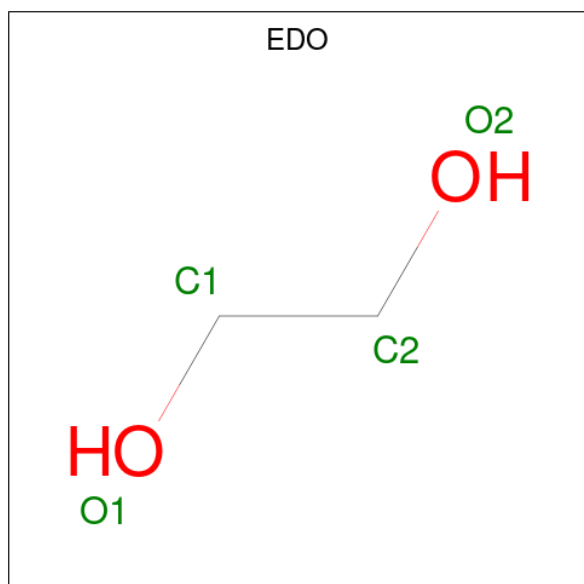
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

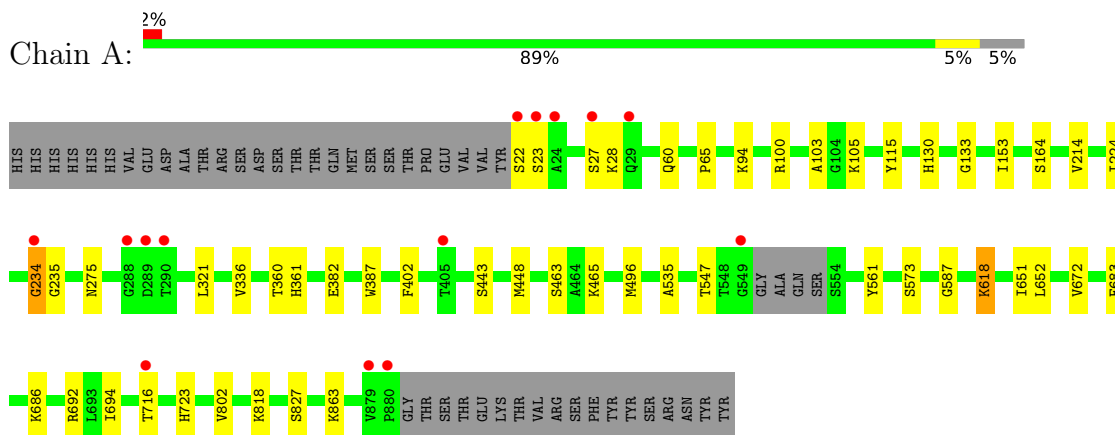
- Molecule 6 is water.

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		

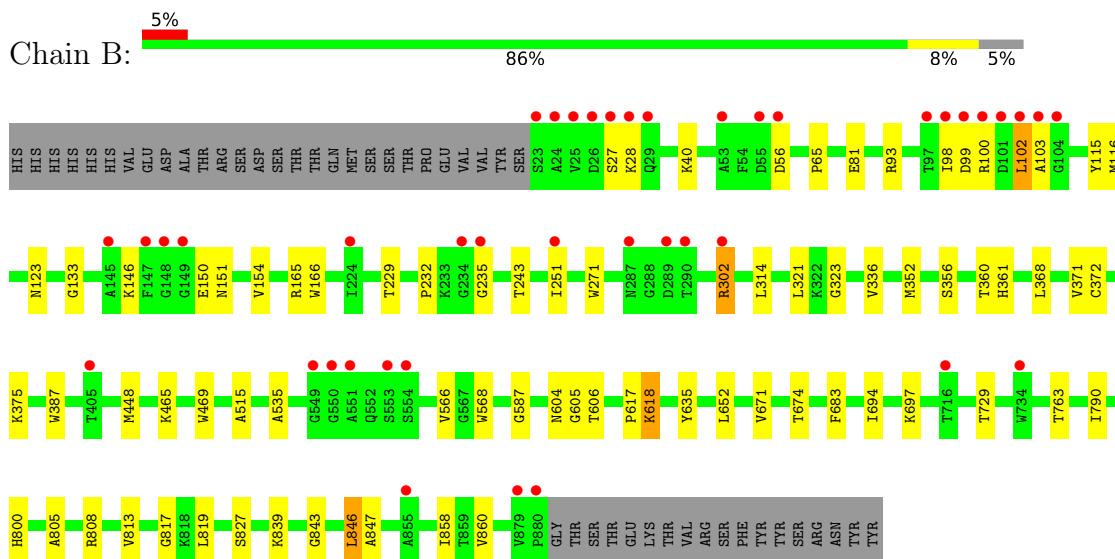
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ($RSRZ > 2$). 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.

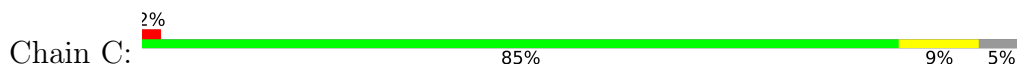
• Molecule 1: Beta-galactosidase

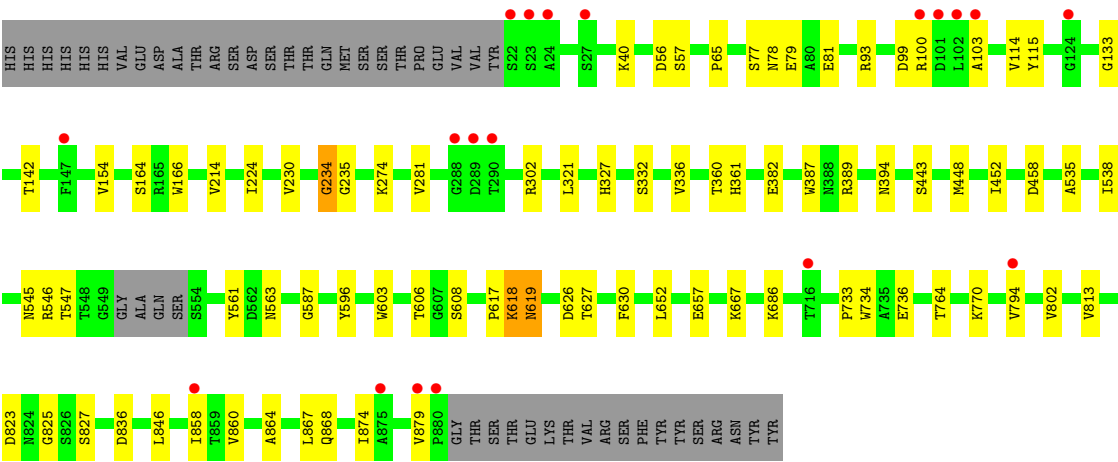


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.264 0.210 , 0.272	Depositor DCC
R_{free} test set	8539 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, NI, NA, MG

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	0.54	0/6655	0.82	8/9071 (0.1%)
1	B	0.48	0/6612	0.79	0/9016
1	C	0.49	0/6611	0.81	6/9014 (0.1%)
All	All	0.50	0/19878	0.81	14/27101 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLY	N-CA-C	9.15	128.99	114.90
1	A	23	SER	N-CA-C	-6.94	105.43	114.04
1	A	103	ALA	N-CA-C	6.59	119.02	111.11
1	C	234	GLY	N-CA-C	6.24	125.76	114.46
1	C	164	SER	N-CA-C	5.75	117.85	108.76
1	A	802	VAL	CA-C-N	5.33	124.84	119.19
1	A	802	VAL	C-N-CA	5.33	124.84	119.19
1	C	827	SER	CA-C-N	-5.22	115.51	120.83
1	C	827	SER	C-N-CA	-5.22	115.51	120.83
1	A	164	SER	N-CA-C	5.19	117.13	108.99
1	C	802	VAL	CA-C-N	5.12	124.79	119.56
1	C	802	VAL	C-N-CA	5.12	124.79	119.56
1	A	130	HIS	CA-C-N	5.11	126.23	119.84
1	A	130	HIS	C-N-CA	5.11	126.23	119.84

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	6492	0	6176	24	0
1	B	6466	0	6137	47	0
1	C	6457	0	6133	49	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
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	120	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 (120) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:22:SER:N	1:A:94:LYS:HZ1	2.06	0.53
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: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:C:667:LYS:HZ2	1:C:733:PRO:HD3	1.78	0.48
1:B:805:ALA:HB3	1:B:843:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:360:THR:HA	1:C:361:HIS:HA	1.64	0.46
1:C:858:ILE:HB	1:C:874:ILE:HB	1.99	0.45
1:C:864:ALA:HB3	1:C:867:LEU:HD12	1.98	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:A:463:SER:HB2	1:A:496:MET:HE3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:LYS:HG3	1:C:868:GLN:HB2	2.01	0.42
1:B:81:GLU:HG3	1:B:606:THR:HA	2.02	0.42
1:B:604:ASN:OD1	1:B:605:GLY:N	2.53	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:B:352:MET:HE2	1:B:635:TYR:CD2	2.55	0.41
1:A:863:LYS:HB2	1:A:863:LYS:HE2	1.83	0.41
1:B:763:THR:HG21	1:B:800:HIS:CE1	2.55	0.41
1:A:618:LYS:HG3	1:A:827:SER:O	2.20	0.41
1:A:651:ILE:HG12	1:A:672:VAL:HG22	2.02	0.41
1:C:56:ASP:CG	1:C:93:ARG:HE	2.28	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:HB3	1:A:465:LYS:HE2	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 [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	857/904 (95%)	831 (97%)	24 (3%)	2 (0%)	43	36
1	B	856/904 (95%)	825 (96%)	28 (3%)	3 (0%)	30	21
1	C	854/904 (94%)	821 (96%)	30 (4%)	3 (0%)	30	21
All	All	2567/2712 (95%)	2477 (96%)	82 (3%)	8 (0%)	36	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	103	ALA
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%)	76	76
1	B	675/737 (92%)	670 (99%)	5 (1%)	76	76
1	C	675/737 (92%)	666 (99%)	9 (1%)	61	58
All	All	2029/2211 (92%)	2010 (99%)	19 (1%)	70	70

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ILE
1	A	618	LYS

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Mol	Chain	Res	Type
1	A	652	LEU
1	A	686	LYS
1	A	716	THR
1	B	150	GLU
1	B	251	ILE
1	B	302	ARG
1	B	618	LYS
1	B	846	LEU
1	C	142	THR
1	C	274	LYS
1	C	538	ILE
1	C	618	LYS
1	C	619[A]	ASN
1	C	619[B]	ASN
1	C	652	LEU
1	C	794	VAL
1	C	879	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	499	ASN
1	A	581	GLN
1	A	807	ASN
1	A	850	GLN
1	B	61	GLN
1	B	117	ASN
1	B	144	ASN
1	B	491	ASN
1	B	499	ASN
1	B	850	GLN
1	C	110	ASN
1	C	228	GLN
1	C	345	GLN
1	C	350	GLN
1	C	435	ASN
1	C	499	ASN
1	C	563	ASN
1	C	666	ASN
1	C	807	ASN

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 oligosaccharides 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	0.49	0	2,2,2	0.46	0
5	EDO	A	906	-	3,3,3	0.43	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
5	EDO	A	905	-	-	0/1/1/1	-
5	EDO	A	906	-	-	0/1/1/1	-

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

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, 95th 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 ²)	Q<0.9
1	A	855/904 (94%)	-0.29	14 (1%) 70 77	2, 8, 20, 50	6 (0%)
1	B	858/904 (94%)	0.33	41 (4%) 35 41	7, 17, 33, 59	0
1	C	855/904 (94%)	0.23	19 (2%) 62 69	6, 14, 31, 59	3 (0%)
All	All	2568/2712 (94%)	0.09	74 (2%) 53 60	2, 13, 30, 59	9 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	ALA	5.7
1	A	27	SER	4.8
1	B	27	SER	4.7
1	B	551	ALA	4.6
1	B	102	LEU	4.6
1	B	26	ASP	4.0
1	A	22	SER	3.9
1	B	23	SER	3.9
1	C	22	SER	3.8
1	B	550	GLY	3.7
1	C	880	PRO	3.6
1	A	23	SER	3.6
1	B	25	VAL	3.6
1	B	290	THR	3.6
1	B	879	VAL	3.6
1	A	880	PRO	3.5
1	C	24	ALA	3.5
1	B	29	GLN	3.5
1	B	104	GLY	3.4
1	B	553	SER	3.4
1	B	99	ASP	3.4
1	B	97	THR	3.3
1	C	102	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	101	ASP	3.3
1	B	148	GLY	3.3
1	B	103	ALA	3.3
1	A	289	ASP	3.2
1	C	124	GLY	3.1
1	A	24	ALA	3.0
1	C	879	VAL	3.0
1	B	716	THR	3.0
1	C	289	ASP	3.0
1	B	149	GLY	2.9
1	B	100	ARG	2.8
1	C	858	ILE	2.8
1	B	147	PHE	2.7
1	B	98	ILE	2.7
1	C	27	SER	2.7
1	B	302	ARG	2.7
1	B	234	GLY	2.6
1	C	875	ALA	2.6
1	B	880	PRO	2.6
1	C	23	SER	2.6
1	B	549	GLY	2.5
1	B	251	ILE	2.5
1	B	53	ALA	2.5
1	A	549	GLY	2.4
1	C	103	ALA	2.4
1	C	794	VAL	2.4
1	B	235	GLY	2.4
1	C	147	PHE	2.3
1	B	855	ALA	2.3
1	C	290	THR	2.3
1	B	287	ASN	2.3
1	B	28	LYS	2.3
1	A	879	VAL	2.3
1	A	288	GLY	2.3
1	A	29	GLN	2.2
1	B	734	TRP	2.2
1	A	405	THR	2.2
1	C	716	THR	2.2
1	C	288	GLY	2.2
1	B	289	ASP	2.2
1	A	716	THR	2.1
1	C	100	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	224	ILE	2.1
1	B	55	ASP	2.1
1	A	290	THR	2.1
1	A	234	GLY	2.1
1	C	101	ASP	2.1
1	B	554	SER	2.1
1	B	56	ASP	2.1
1	B	405	THR	2.0
1	B	145	ALA	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	C	902	1/1	0.95	0.06	18,18,18,18	0
3	NA	C	903	1/1	0.95	0.06	15,15,15,15	0
5	EDO	A	906	4/4	0.95	0.07	9,13,16,27	0
2	MG	C	901	1/1	0.98	0.04	9,9,9,9	0
5	EDO	A	905	4/4	0.98	0.04	6,6,7,7	0
2	MG	A	901	1/1	0.98	0.04	8,8,8,8	0
2	MG	B	901	1/1	0.99	0.06	9,9,9,9	0
2	MG	B	902	1/1	0.99	0.03	12,12,12,12	0
4	NI	A	904	1/1	0.99	0.06	24,24,24,24	0
2	MG	A	902	1/1	0.99	0.04	10,10,10,10	0
3	NA	A	903	1/1	0.99	0.06	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.