



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:39 AM UTC

PDB ID : 3WDP / pdb_00003wdp
Title : Structural analysis of a beta-glucosidase mutant derived from a hyperthermophilic tetrameric structure
Authors : Nakabayashi, M.; Kataoka, M.; Ishikawa, K.
Deposited on : 2013-06-19
Resolution : 1.70 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

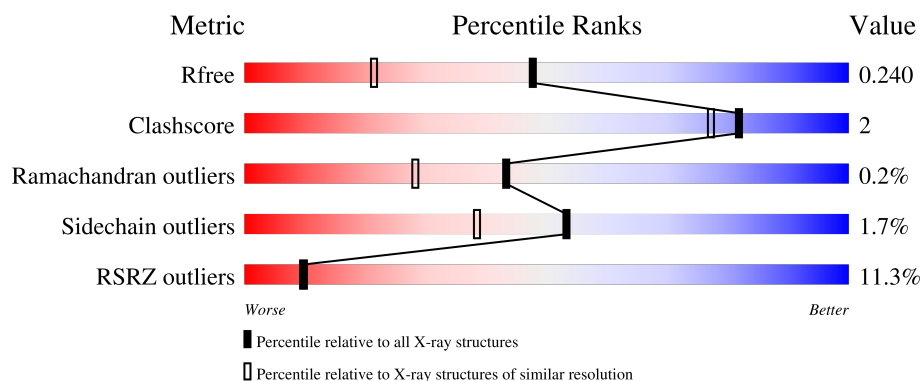
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	P	473	6% 94% 6%
1	Q	473	6% 93% 6%
1	R	473	17% 94% 5%
1	S	473	16% 92% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17178 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-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	472	Total	C	N	O	S	0	0	0
			3858	2512	631	702	13			
1	Q	472	Total	C	N	O	S	0	3	0
			3878	2528	631	706	13			
1	R	472	Total	C	N	O	S	0	2	0
			3868	2519	631	704	14			
1	S	472	Total	C	N	O	S	0	2	0
			3870	2520	633	704	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	0	MET	-	expression tag	UNP Q51723
P	1	ALA	-	expression tag	UNP Q51723
P	170	ALA	ARG	engineered mutation	UNP Q51723
P	220	ALA	ARG	engineered mutation	UNP Q51723
P	227	PHE	TYR	engineered mutation	UNP Q51723
Q	0	MET	-	expression tag	UNP Q51723
Q	1	ALA	-	expression tag	UNP Q51723
Q	170	ALA	ARG	engineered mutation	UNP Q51723
Q	220	ALA	ARG	engineered mutation	UNP Q51723
Q	227	PHE	TYR	engineered mutation	UNP Q51723
R	0	MET	-	expression tag	UNP Q51723
R	1	ALA	-	expression tag	UNP Q51723
R	170	ALA	ARG	engineered mutation	UNP Q51723
R	220	ALA	ARG	engineered mutation	UNP Q51723
R	227	PHE	TYR	engineered mutation	UNP Q51723
S	0	MET	-	expression tag	UNP Q51723
S	1	ALA	-	expression tag	UNP Q51723
S	170	ALA	ARG	engineered mutation	UNP Q51723
S	220	ALA	ARG	engineered mutation	UNP Q51723
S	227	PHE	TYR	engineered mutation	UNP Q51723

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	P	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		
3	S	1	Total	O	P	0	0
			5	4	1		

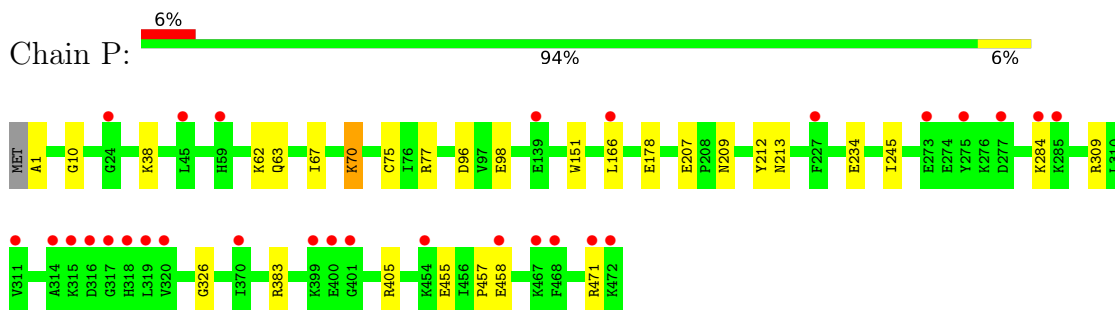
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	452	Total 452	O 452	0	0
4	Q	456	Total 456	O 456	0	0
4	R	344	Total 344	O 344	0	0
4	S	326	Total 326	O 326	0	0

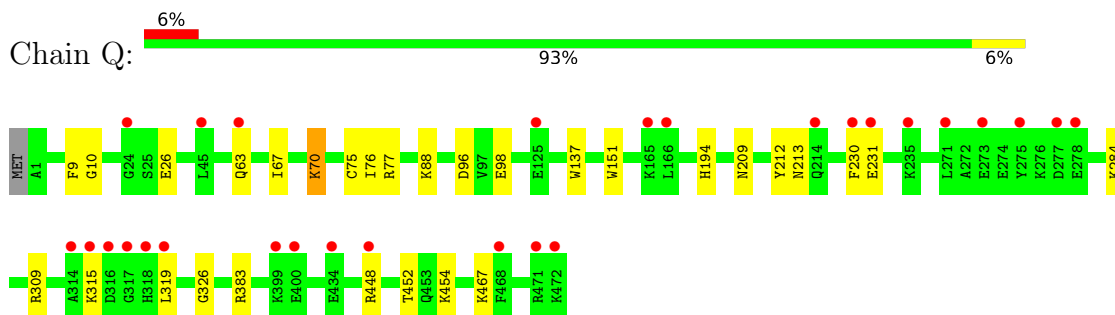
3 Residue-property plots [i](#)

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.

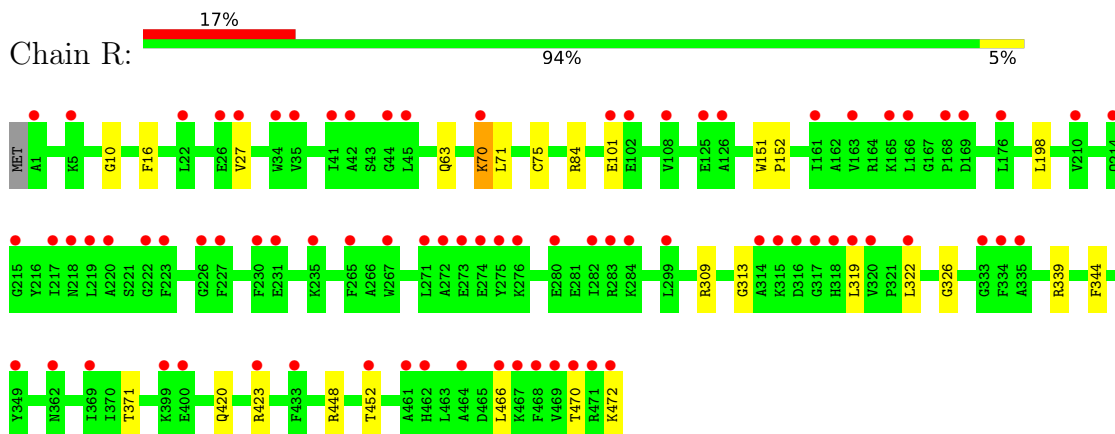
- Molecule 1: Beta-glucosidase



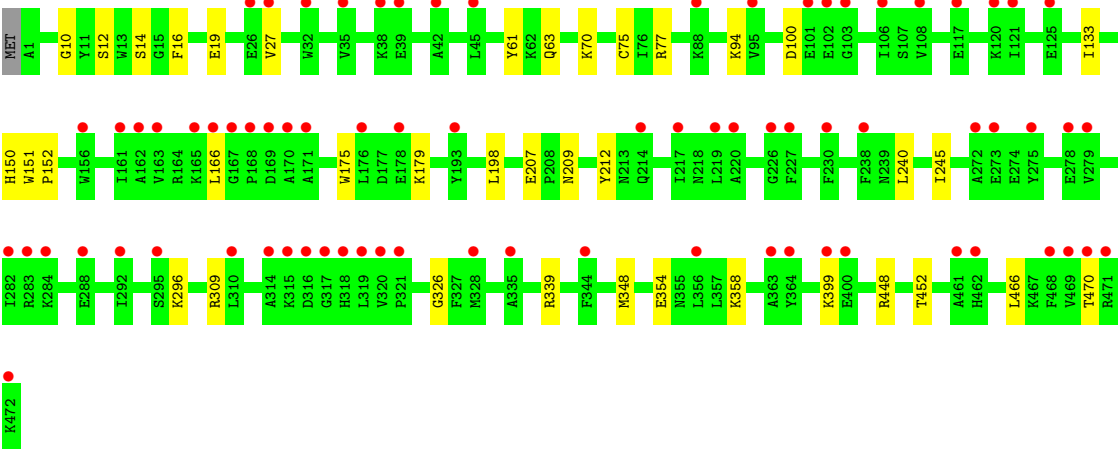
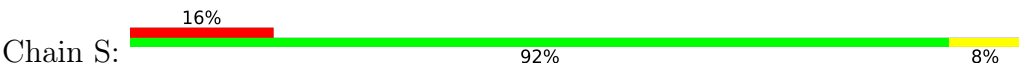
- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase



- Molecule 1: Beta-glucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.15Å 161.15Å 183.82Å 90.00° 108.38° 90.00°	Depositor
Resolution (Å)	47.05 – 1.70 47.05 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.05-1.70) 99.3 (47.05-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.212 , 0.233 0.221 , 0.240	Depositor DCC
R_{free} test set	18527 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17178	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GOL, PO4

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	P	0.80	0/3981	0.88	2/5399 (0.0%)
1	Q	0.80	0/4011	0.88	3/5439 (0.1%)
1	R	0.66	0/3997	0.80	0/5420
1	S	0.67	1/4000 (0.0%)	0.80	1/5425 (0.0%)
All	All	0.74	1/15989 (0.0%)	0.84	6/21683 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	207	GLU	C-O	-8.54	1.20	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	383	ARG	CA-C-N	-5.91	112.49	119.05
1	Q	383	ARG	C-N-CA	-5.91	112.49	119.05
1	Q	194	HIS	N-CA-C	5.79	118.81	111.69
1	S	19	GLU	N-CA-C	5.75	117.55	111.28
1	P	383	ARG	CA-C-N	-5.01	113.49	119.05
1	P	383	ARG	C-N-CA	-5.01	113.49	119.05

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	P	3858	0	3712	17	0
1	Q	3878	0	3733	17	0
1	R	3868	0	3725	23	0
1	S	3870	0	3723	18	0
2	P	24	0	32	1	0
2	Q	18	0	24	0	0
2	R	18	0	24	0	0
2	S	6	0	8	0	0
3	P	20	0	0	1	0
3	Q	20	0	0	1	0
3	R	15	0	0	0	0
3	S	5	0	0	0	0
4	P	452	0	0	8	3
4	Q	456	0	0	5	2
4	R	344	0	0	12	0
4	S	326	0	0	2	0
All	All	17178	0	14981	75	4

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 2.

All (75) 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:Q:454:LYS:HD3	4:Q:769:HOH:O	1.67	0.94
1:Q:454:LYS:HD3	4:Q:770:HOH:O	1.82	0.79
1:P:245:ILE:HD13	4:P:852:HOH:O	1.83	0.78
1:R:71:LEU:HB3	4:R:782:HOH:O	1.85	0.75
1:Q:454:LYS:CD	4:Q:770:HOH:O	2.33	0.74
1:P:63:GLN:NE2	4:P:710:HOH:O	2.22	0.73
1:R:448:ARG:HG2	4:R:865:HOH:O	1.89	0.70
1:P:62:LYS:NZ	4:P:951:HOH:O	2.24	0.69
1:P:234:GLU:OE1	4:P:850:HOH:O	2.12	0.66
1:R:27:VAL:HG11	1:R:84:ARG:HG2	1.79	0.65
1:P:38:LYS:HD3	4:P:753:HOH:O	1.97	0.63
1:R:71:LEU:CB	4:R:782:HOH:O	2.45	0.63
1:P:207:GLU:OE1	2:P:504:GOL:H11	2.00	0.62
1:P:405:ARG:HD2	4:P:885:HOH:O	2.01	0.60
1:P:63:GLN:HG3	4:P:709:HOH:O	2.01	0.59
1:R:420:GLN:NE2	4:R:943:HOH:O	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:466:LEU:O	1:S:470:THR:HG23	2.02	0.58
1:R:448:ARG:O	1:R:452:THR:HG23	2.04	0.57
1:R:466:LEU:O	1:R:470:THR:HG23	2.06	0.55
1:S:339:ARG:HE	1:S:470:THR:HG21	1.71	0.55
1:S:63:GLN:HG3	4:S:825:HOH:O	2.07	0.55
1:R:448:ARG:CG	4:R:865:HOH:O	2.53	0.53
1:S:309:ARG:O	1:S:326:GLY:HA3	2.08	0.53
1:R:10:GLY:HA3	1:R:75:CYS:O	2.09	0.53
1:P:67:ILE:HG23	1:P:70:LYS:HE2	1.92	0.52
1:R:339:ARG:HD3	1:R:470:THR:HG22	1.92	0.51
1:S:10:GLY:HA3	1:S:75:CYS:O	2.10	0.51
1:S:448:ARG:O	1:S:452:THR:HG23	2.11	0.51
1:S:339:ARG:HD3	1:S:470:THR:HG22	1.92	0.51
1:R:309:ARG:O	1:R:326:GLY:HA3	2.11	0.50
1:R:313:GLY:HA3	1:R:322:LEU:HD11	1.93	0.50
1:Q:70:LYS:O	1:Q:448:ARG:HD3	2.12	0.49
1:R:420:GLN:O	1:R:423:ARG:HG2	2.11	0.49
1:S:198:LEU:HD23	4:S:848:HOH:O	2.12	0.49
1:R:448:ARG:CA	4:R:782:HOH:O	2.60	0.48
1:Q:96:ASP:OD1	1:Q:98:GLU:OE2	2.31	0.48
1:P:209:ASN:HA	1:P:212:TYR:CZ	2.49	0.48
1:R:423:ARG:HB3	4:R:883:HOH:O	2.14	0.48
1:R:63:GLN:NE2	4:R:641:HOH:O	2.37	0.47
1:R:71:LEU:HD22	4:R:782:HOH:O	2.14	0.47
1:R:448:ARG:N	4:R:782:HOH:O	2.48	0.47
1:Q:26[A]:GLU:CG	4:Q:772:HOH:O	2.63	0.46
1:R:27:VAL:HG11	1:R:84:ARG:CG	2.45	0.46
1:Q:230[B]:PHE:CD2	1:Q:231:GLU:N	2.82	0.45
1:Q:209:ASN:HA	1:Q:212:TYR:CZ	2.52	0.45
1:P:10:GLY:HA3	1:P:75:CYS:O	2.17	0.44
1:P:96:ASP:OD1	1:P:98:GLU:OE2	2.36	0.44
1:S:175:TRP:CE2	1:S:240:LEU:HD21	2.51	0.44
1:Q:448:ARG:O	1:Q:452:THR:HG23	2.18	0.43
1:Q:26[A]:GLU:CD	4:Q:772:HOH:O	2.62	0.43
1:Q:67:ILE:O	1:Q:70:LYS:HD2	2.19	0.43
1:Q:76:ILE:HG13	1:Q:137:TRP:CE2	2.53	0.43
1:Q:67:ILE:HG23	1:Q:70:LYS:HE2	2.00	0.43
1:R:70:LYS:N	1:R:70:LYS:HD3	2.34	0.43
1:R:71:LEU:CA	4:R:782:HOH:O	2.67	0.43
1:S:12:SER:HA	1:S:77:ARG:O	2.19	0.43
1:Q:309:ARG:O	1:Q:326:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:9:PHE:CE2	1:Q:454:LYS:HE3	2.53	0.42
1:Q:10:GLY:HA3	1:Q:75:CYS:O	2.18	0.42
1:P:213:ASN:OD1	3:P:507:PO4:O1	2.38	0.42
1:R:198:LEU:HD23	4:R:709:HOH:O	2.20	0.42
1:S:16:PHE:HB2	1:S:152:PRO:HG2	2.02	0.42
1:P:209:ASN:HA	1:P:212:TYR:CE2	2.54	0.42
1:P:1:ALA:N	4:P:922:HOH:O	2.38	0.41
1:P:455:GLU:O	1:P:457:PRO:HD3	2.21	0.41
1:S:209:ASN:HA	1:S:212:TYR:CZ	2.56	0.41
1:S:245:ILE:HD11	1:S:296:LYS:HD2	2.02	0.41
1:S:354:GLU:HG2	1:S:358:LYS:HE2	2.02	0.41
1:R:16:PHE:HB2	1:R:152:PRO:HG2	2.03	0.40
1:S:14:SER:HB3	1:S:150:HIS:CE1	2.56	0.40
1:S:348:MET:HE2	1:S:348:MET:HB3	1.93	0.40
1:P:309:ARG:O	1:P:326:GLY:HA3	2.22	0.40
1:Q:213:ASN:OD1	3:Q:507:PO4:O1	2.39	0.40
1:S:61:TYR:CG	1:S:133:ILE:HG12	2.57	0.40
1:S:100:ASP:OD1	1:S:100:ASP:C	2.64	0.40

All (4) 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)
4:P:840:HOH:O	4:P:840:HOH:O[2_555]	2.04	0.16
4:P:800:HOH:O	4:P:800:HOH:O[2_555]	2.05	0.15
4:P:732:HOH:O	4:Q:824:HOH:O[3_555]	2.14	0.06
4:Q:861:HOH:O	4:Q:861:HOH:O[2_555]	2.14	0.06

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	P	470/473 (99%)	463 (98%)	6 (1%)	1 (0%)	43	28
1	Q	473/473 (100%)	462 (98%)	10 (2%)	1 (0%)	43	28
1	R	472/473 (100%)	463 (98%)	8 (2%)	1 (0%)	43	28
1	S	472/473 (100%)	464 (98%)	7 (2%)	1 (0%)	43	28
All	All	1887/1892 (100%)	1852 (98%)	31 (2%)	4 (0%)	43	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	151	TRP
1	Q	151	TRP
1	R	151	TRP
1	S	151	TRP

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	P	398/399 (100%)	391 (98%)	7 (2%)	51	36
1	Q	401/399 (100%)	393 (98%)	8 (2%)	48	32
1	R	400/399 (100%)	394 (98%)	6 (2%)	57	43
1	S	400/399 (100%)	394 (98%)	6 (2%)	57	43
All	All	1599/1596 (100%)	1572 (98%)	27 (2%)	53	38

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	70	LYS
1	P	77	ARG
1	P	166	LEU
1	P	178	GLU
1	P	284	LYS
1	P	458	GLU
1	P	471	ARG

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Mol	Chain	Res	Type
1	Q	63	GLN
1	Q	70	LYS
1	Q	77	ARG
1	Q	88	LYS
1	Q	284	LYS
1	Q	315	LYS
1	Q	319	LEU
1	Q	467	LYS
1	R	70	LYS
1	R	101	GLU
1	R	319	LEU
1	R	344	PHE
1	R	371	THR
1	R	472	LYS
1	S	27	VAL
1	S	70	LYS
1	S	94	LYS
1	S	166	LEU
1	S	179	LYS
1	S	399	LYS

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

Mol	Chain	Res	Type
1	P	59	HIS
1	P	214	GLN
1	P	218	ASN
1	P	373	ASN
1	Q	63	GLN
1	Q	213	ASN
1	Q	214	GLN
1	Q	218	ASN
1	Q	239	ASN
1	Q	294	HIS
1	Q	355	ASN
1	Q	373	ASN
1	Q	462	HIS
1	R	17	GLN
1	R	355	ASN
1	R	373	ASN
1	S	63	GLN
1	S	373	ASN

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Mol	Chain	Res	Type
1	S	415	ASN
1	S	420	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	Q	507	-	4,4,4	0.79	0	6,6,6	0.84	0
3	PO4	R	505	-	4,4,4	0.88	0	6,6,6	0.43	0
3	PO4	Q	504	-	4,4,4	0.89	0	6,6,6	0.36	0
3	PO4	R	506	-	4,4,4	0.91	0	6,6,6	0.40	0
3	PO4	P	507	-	4,4,4	0.79	0	6,6,6	0.87	0
2	GOL	Q	503	-	5,5,5	0.41	0	5,5,5	0.93	0
2	GOL	Q	501	-	5,5,5	0.32	0	5,5,5	0.91	0
3	PO4	R	504	-	4,4,4	0.75	0	6,6,6	0.81	0
2	GOL	S	501	-	5,5,5	0.42	0	5,5,5	0.82	0
3	PO4	Q	505	-	4,4,4	0.80	0	6,6,6	0.62	0
3	PO4	P	508	-	4,4,4	0.89	0	6,6,6	0.52	0
2	GOL	P	501	-	5,5,5	0.30	0	5,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	P	503	-	5,5,5	0.78	0	5,5,5	0.89	0
3	PO4	Q	506	-	4,4,4	0.75	0	6,6,6	0.80	0
2	GOL	R	502	-	5,5,5	0.23	0	5,5,5	0.83	0
3	PO4	P	505	-	4,4,4	0.98	0	6,6,6	0.64	0
2	GOL	Q	502	-	5,5,5	0.36	0	5,5,5	0.23	0
2	GOL	P	504	-	5,5,5	0.52	0	5,5,5	0.78	0
3	PO4	S	502	-	4,4,4	0.77	0	6,6,6	0.95	0
2	GOL	R	501	-	5,5,5	0.24	0	5,5,5	0.59	0
2	GOL	R	503	-	5,5,5	0.41	0	5,5,5	0.36	0
3	PO4	P	506	-	4,4,4	0.62	0	6,6,6	0.83	0
2	GOL	P	502	-	5,5,5	0.29	0	5,5,5	0.55	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	GOL	Q	502	-	-	2/4/4/4	-
2	GOL	Q	503	-	-	4/4/4/4	-
2	GOL	Q	501	-	-	0/4/4/4	-
2	GOL	P	504	-	-	0/4/4/4	-
2	GOL	S	501	-	-	0/4/4/4	-
2	GOL	R	501	-	-	0/4/4/4	-
2	GOL	R	503	-	-	2/4/4/4	-
2	GOL	P	501	-	-	0/4/4/4	-
2	GOL	R	502	-	-	2/4/4/4	-
2	GOL	P	502	-	-	0/4/4/4	-
2	GOL	P	503	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	502	GOL	C1-C2-C3-O3
2	Q	503	GOL	O1-C1-C2-C3
2	Q	503	GOL	C1-C2-C3-O3
2	R	502	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	R	503	GOL	O1-C1-C2-O2
2	R	503	GOL	O1-C1-C2-C3
2	Q	502	GOL	O2-C2-C3-O3
2	Q	503	GOL	O2-C2-C3-O3
2	Q	503	GOL	O1-C1-C2-O2
2	R	502	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	507	PO4	1	0
3	P	507	PO4	1	0
2	P	504	GOL	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

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	P	472/473 (99%)	0.65	29 (6%)	27	29	9, 15, 28, 65	0
1	Q	472/473 (99%)	0.65	28 (5%)	28	31	9, 15, 28, 62	3 (0%)
1	R	472/473 (99%)	1.17	80 (16%)	4	3	9, 21, 37, 59	2 (0%)
1	S	472/473 (99%)	1.25	76 (16%)	4	4	10, 20, 36, 72	2 (0%)
All	All	1888/1892 (99%)	0.93	213 (11%)	10	10	9, 18, 34, 72	7 (0%)

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	472	LYS	5.8
1	S	166	LEU	5.7
1	P	472	LYS	5.7
1	S	317	GLY	5.7
1	S	472	LYS	5.6
1	Q	472	LYS	5.3
1	S	165	LYS	4.6
1	Q	315	LYS	4.5
1	P	468	PHE	4.5
1	S	318	HIS	4.4
1	Q	230[A]	PHE	4.4
1	R	230	PHE	4.4
1	R	219	LEU	4.4
1	R	471	ARG	4.3
1	P	317	GLY	4.3
1	P	319	LEU	4.3
1	S	230	PHE	4.2
1	S	319	LEU	4.2
1	S	275	TYR	4.1
1	R	218	ASN	4.1
1	S	315	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	R	317	GLY	4.1
1	R	27	VAL	4.1
1	R	220	ALA	4.0
1	R	217	ILE	4.0
1	R	470	THR	3.9
1	S	470	THR	3.9
1	Q	319	LEU	3.9
1	R	318	HIS	3.8
1	S	170	ALA	3.8
1	Q	317	GLY	3.8
1	P	318	HIS	3.7
1	R	468	PHE	3.7
1	R	166	LEU	3.7
1	S	162	ALA	3.7
1	S	106	ILE	3.7
1	R	314	ALA	3.6
1	P	166	LEU	3.6
1	P	315	LYS	3.6
1	S	468	PHE	3.6
1	R	271	LEU	3.6
1	R	316	ASP	3.6
1	S	399	LYS	3.5
1	Q	318	HIS	3.5
1	S	108	VAL	3.5
1	S	171	ALA	3.4
1	S	27	VAL	3.4
1	S	169	ASP	3.4
1	R	469	VAL	3.4
1	P	400	GLU	3.3
1	R	319	LEU	3.3
1	P	316	ASP	3.3
1	P	273	GLU	3.2
1	R	284	LYS	3.2
1	R	400	GLU	3.2
1	S	101	GLU	3.2
1	Q	314	ALA	3.2
1	R	467	LYS	3.2
1	R	275	TYR	3.1
1	R	462	HIS	3.1
1	Q	468	PHE	3.1
1	Q	275	TYR	3.1
1	S	400	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	S	121	ILE	3.1
1	S	273	GLU	3.1
1	R	334	PHE	3.1
1	Q	24	GLY	3.0
1	S	214	GLN	3.0
1	Q	166	LEU	3.0
1	S	42	ALA	3.0
1	R	333	GLY	3.0
1	S	220	ALA	3.0
1	S	282	ILE	3.0
1	P	314	ALA	2.9
1	P	458	GLU	2.9
1	S	292	ILE	2.9
1	S	471	ARG	2.9
1	S	461	ALA	2.9
1	R	466	LEU	2.9
1	S	227	PHE	2.9
1	S	163	VAL	2.9
1	P	370	ILE	2.9
1	S	335	ALA	2.8
1	Q	316	ASP	2.8
1	S	316	ASP	2.8
1	P	471	ARG	2.8
1	P	320	VAL	2.8
1	R	41	ILE	2.8
1	S	168	PRO	2.8
1	P	467	LYS	2.8
1	R	464	ALA	2.7
1	R	227	PHE	2.7
1	S	39	GLU	2.7
1	S	288	GLU	2.7
1	R	168	PRO	2.7
1	Q	45	LEU	2.7
1	R	165	LYS	2.7
1	P	277	ASP	2.7
1	R	452	THR	2.6
1	R	45	LEU	2.6
1	Q	400	GLU	2.6
1	S	45	LEU	2.6
1	S	95	VAL	2.6
1	S	32	TRP	2.6
1	R	335	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	R	399	LYS	2.6
1	R	222	GLY	2.6
1	R	283	ARG	2.6
1	R	280	GLU	2.6
1	S	125	GLU	2.6
1	R	299	LEU	2.6
1	S	462	HIS	2.6
1	R	315	LYS	2.6
1	S	217	ILE	2.6
1	S	102	GLU	2.6
1	S	278	GLU	2.6
1	P	24	GLY	2.5
1	S	320	VAL	2.5
1	S	321	PRO	2.5
1	Q	63	GLN	2.5
1	S	295	SER	2.5
1	Q	273	GLU	2.5
1	S	176	LEU	2.5
1	P	399	LYS	2.5
1	S	117	GLU	2.5
1	R	461	ALA	2.5
1	S	88	LYS	2.4
1	R	108	VAL	2.4
1	R	26	GLU	2.4
1	R	101	GLU	2.4
1	R	226	GLY	2.4
1	R	1	ALA	2.4
1	R	282	ILE	2.4
1	Q	434	GLU	2.4
1	R	125	GLU	2.4
1	S	178	GLU	2.4
1	R	423	ARG	2.4
1	Q	214	GLN	2.4
1	P	45	LEU	2.4
1	R	273	GLU	2.4
1	S	120	LYS	2.4
1	S	161	ILE	2.4
1	R	22	LEU	2.3
1	R	272	ALA	2.3
1	R	276	LYS	2.3
1	S	38	LYS	2.3
1	S	103	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	S	284	LYS	2.3
1	Q	125	GLU	2.3
1	R	267	TRP	2.3
1	Q	277	ASP	2.3
1	Q	399	LYS	2.3
1	Q	271	LEU	2.3
1	S	219	LEU	2.3
1	P	275	TYR	2.3
1	S	279	VAL	2.3
1	S	328	MET	2.3
1	R	42	ALA	2.2
1	S	310	LEU	2.2
1	R	70	LYS	2.2
1	R	215	GLY	2.2
1	R	223	PHE	2.2
1	R	265	PHE	2.2
1	S	238	PHE	2.2
1	R	214	GLN	2.2
1	R	433	PHE	2.2
1	Q	448	ARG	2.2
1	R	235	LYS	2.2
1	S	469	VAL	2.2
1	R	126	ALA	2.2
1	P	139	GLU	2.2
1	R	231	GLU	2.2
1	S	226	GLY	2.2
1	P	284	LYS	2.2
1	R	349	TYR	2.2
1	R	369	ILE	2.2
1	S	35	VAL	2.1
1	S	314	ALA	2.1
1	P	401	GLY	2.1
1	S	167	GLY	2.1
1	R	322	LEU	2.1
1	S	356	LEU	2.1
1	P	454	LYS	2.1
1	S	26	GLU	2.1
1	S	193	TYR	2.1
1	Q	471	ARG	2.1
1	S	283	ARG	2.1
1	R	35	VAL	2.1
1	R	210	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	363	ALA	2.1
1	R	362	ASN	2.1
1	Q	231	GLU	2.1
1	R	34	TRP	2.1
1	R	102	GLU	2.1
1	R	169	ASP	2.1
1	P	227	PHE	2.1
1	S	344	PHE	2.1
1	Q	235	LYS	2.1
1	Q	165	LYS	2.1
1	R	5	LYS	2.1
1	R	274	GLU	2.0
1	P	311	VAL	2.0
1	R	163	VAL	2.0
1	R	320	VAL	2.0
1	R	176	LEU	2.0
1	Q	278	GLU	2.0
1	R	44	GLY	2.0
1	S	156	TRP	2.0
1	R	161	ILE	2.0
1	S	364	TYR	2.0
1	S	272	ALA	2.0
1	P	59	HIS	2.0
1	P	285	LYS	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	PO4	P	508	5/5	0.65	0.23	55,56,58,61	0
3	PO4	R	506	5/5	0.72	0.19	66,66,69,71	0
3	PO4	Q	505	5/5	0.74	0.17	45,46,48,52	0
2	GOL	Q	502	6/6	0.74	0.23	18,27,31,33	0
3	PO4	R	505	5/5	0.77	0.15	44,45,50,51	0
2	GOL	P	503	6/6	0.78	0.20	19,26,30,32	0
3	PO4	R	504	5/5	0.78	0.17	37,39,41,42	0
2	GOL	P	502	6/6	0.79	0.18	29,32,36,36	0
3	PO4	P	505	5/5	0.79	0.16	43,44,46,51	0
2	GOL	P	504	6/6	0.79	0.21	20,26,27,32	0
3	PO4	Q	504	5/5	0.79	0.15	50,50,51,52	0
2	GOL	R	503	6/6	0.84	0.18	30,34,36,39	0
2	GOL	R	502	6/6	0.84	0.17	23,28,32,35	0
3	PO4	P	507	5/5	0.84	0.18	22,24,27,30	0
2	GOL	Q	503	6/6	0.86	0.16	18,22,25,27	0
3	PO4	S	502	5/5	0.86	0.14	36,38,40,40	0
2	GOL	R	501	6/6	0.87	0.12	19,20,21,21	0
3	PO4	Q	506	5/5	0.87	0.23	28,29,33,35	0
2	GOL	S	501	6/6	0.88	0.11	19,19,20,20	0
2	GOL	P	501	6/6	0.89	0.12	13,16,17,21	0
3	PO4	Q	507	5/5	0.89	0.18	23,23,27,30	0
3	PO4	P	506	5/5	0.89	0.22	28,28,32,33	0
2	GOL	Q	501	6/6	0.91	0.10	13,15,17,20	0

6.5 Other polymers

There are no such residues in this entry.