



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 08:32 AM EDT

PDB ID : 2NT1 / pdb_00002nt1
Title : Structure of acid-beta-glucosidase at neutral pH
Authors : Lieberman, R.L.; Petsko, G.A.; Ringe, D.
Deposited on : 2006-11-06
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

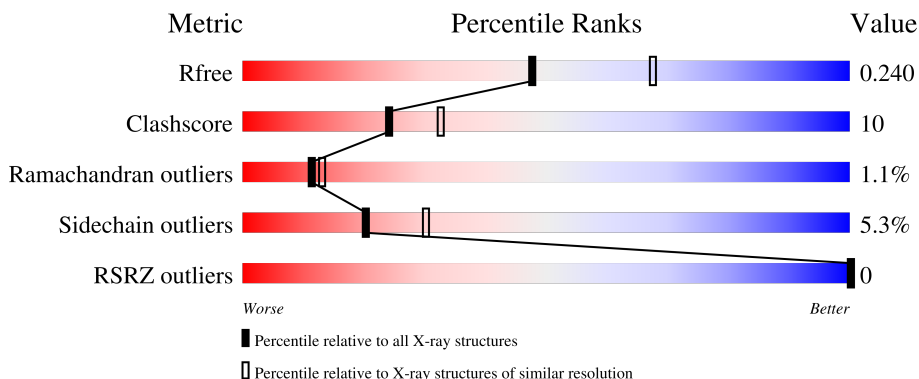
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	497	 79% 17% ..
1	B	497	 82% 15% .
1	C	497	 78% 18% ..
1	D	497	 77% 20% ..

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
3	PO4	A	499	-	X	-	-
3	PO4	A	502	-	-	X	-
3	PO4	A	514	-	-	X	-
3	PO4	A	515	-	-	X	-
3	PO4	A	518	-	-	X	-
3	PO4	B	502	-	-	X	-
3	PO4	B	503	-	-	X	-
3	PO4	C	501	-	-	X	-
3	PO4	C	517	-	-	X	-
3	PO4	C	518	-	-	X	-
3	PO4	C	520	-	-	X	-
3	PO4	D	503	-	-	X	-
3	PO4	D	507	-	-	X	-
3	PO4	D	514	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17510 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3930	2532	671	711	16	0	0	0
1	B	497	3930	2532	671	711	16	0	0	0
1	C	497	3930	2532	671	711	16	0	0	0
1	D	497	3930	2532	671	711	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

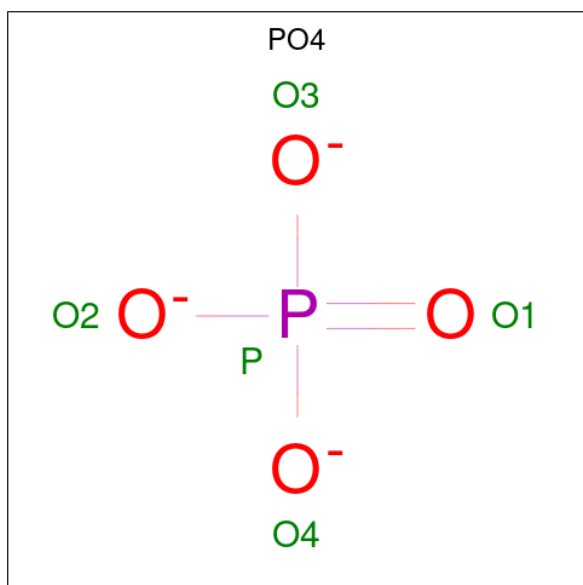
Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	conflict	UNP P04062
B	495	HIS	ARG	conflict	UNP P04062
C	495	HIS	ARG	conflict	UNP P04062
D	495	HIS	ARG	conflict	UNP P04062

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

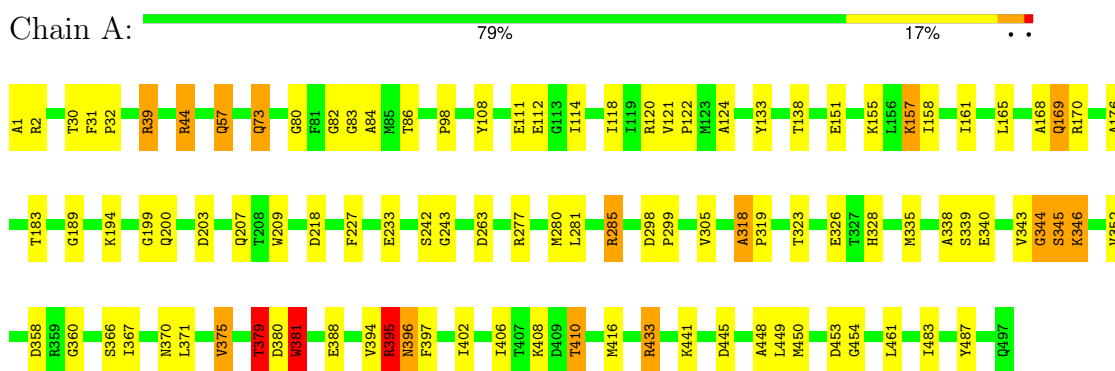
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	364	Total O 364 364	0	0
4	B	293	Total O 293 293	0	0
4	C	377	Total O 377 377	0	0
4	D	310	Total O 310 310	0	0

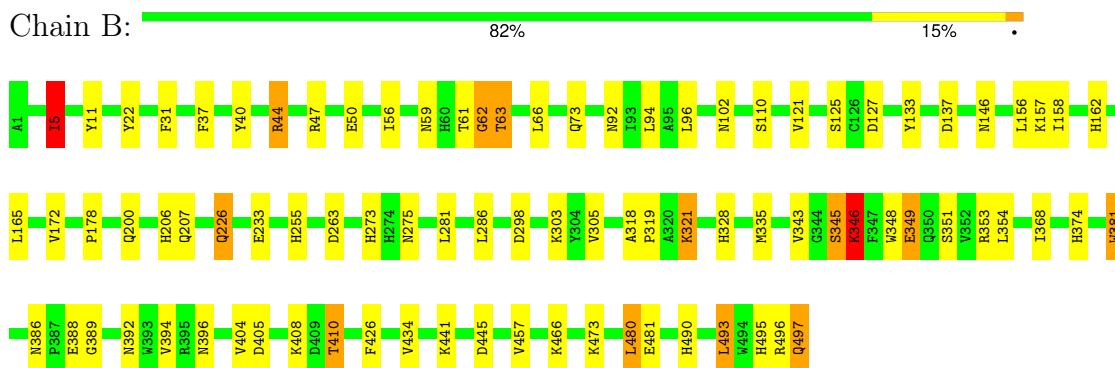
3 Residue-property plots [i](#)

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.

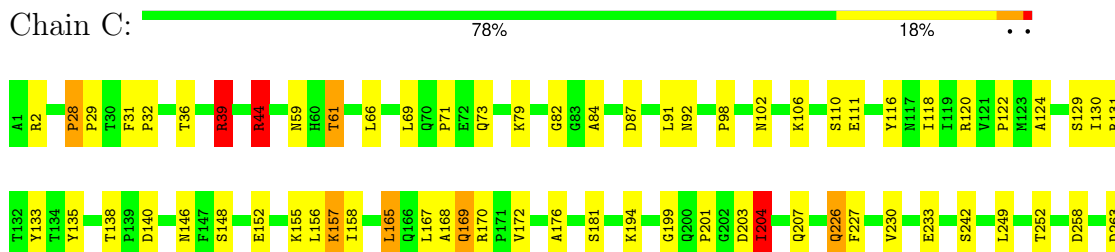
- Molecule 1: Glucosylceramidase

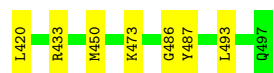
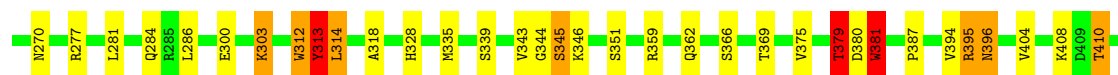


- Molecule 1: Glucosylceramidase



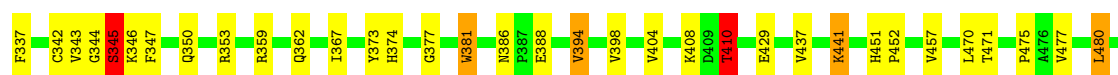
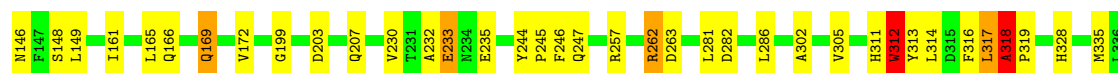
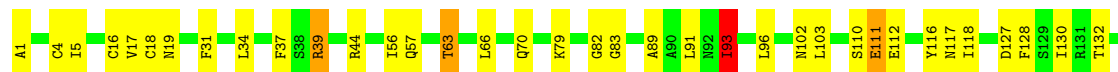
- Molecule 1: Glucosylceramidase





- Molecule 1: Glucosylceramidase

Chain D: 77% 20% ..



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.19Å 91.79Å 153.04Å 90.00° 110.91° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 19.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.94-2.30) 94.8 (19.94-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.30Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.240 0.175 , 0.240	Depositor DCC
R_{free} test set	6021 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.477 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17510	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.27	8/4051 (0.2%)	1.22	22/5523 (0.4%)
1	B	1.24	6/4051 (0.1%)	1.20	17/5523 (0.3%)
1	C	1.27	8/4051 (0.2%)	1.26	29/5523 (0.5%)
1	D	1.26	8/4051 (0.2%)	1.20	12/5523 (0.2%)
All	All	1.26	30/16204 (0.2%)	1.22	80/22092 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	ILE	CA-CB	10.11	1.59	1.54
1	C	158	ILE	CA-CB	9.97	1.59	1.54
1	A	121	VAL	CA-CB	8.22	1.60	1.54
1	A	375	VAL	CA-CB	7.98	1.63	1.54
1	A	158	ILE	CA-CB	6.62	1.57	1.54

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ASN	N-CA-C	-11.06	97.08	112.45
1	B	62	GLY	CA-C-O	-9.45	115.71	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	TYR	CA-C-N	8.87	137.66	121.70
1	C	313	TYR	C-N-CA	8.87	137.66	121.70
1	B	62	GLY	N-CA-C	-8.43	102.84	112.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	345	SER	Peptide
1	C	91	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3930	0	3843	81	0
1	B	3930	0	3843	55	0
1	C	3930	0	3843	96	0
1	D	3930	0	3843	74	0
2	A	14	0	13	1	0
2	B	14	0	13	1	0
2	C	14	0	13	0	0
2	D	14	0	13	2	0
3	A	105	0	0	24	0
3	B	90	0	0	9	0
3	C	115	0	0	32	0
3	D	80	0	0	11	0
4	A	364	0	0	15	0
4	B	293	0	0	15	0
4	C	377	0	0	21	0
4	D	310	0	0	17	0
All	All	17510	0	15424	316	0

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 10.

The worst 5 of 316 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:358:ASP:HB3	4:A:878:HOH:O	1.27	1.25
1:A:120:ARG:HD3	3:A:518:PO4:O2	1.44	1.17
1:A:84:ALA:HB2	3:A:518:PO4:O4	1.45	1.14
1:A:344:GLY:HA2	1:A:345:SER:HB2	1.17	1.14
1:C:204:ILE:HD13	4:C:1138:HOH:O	1.48	1.10

There are no symmetry-related clashes.

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	495/497 (100%)	459 (93%)	29 (6%)	7 (1%)	9	9
1	B	495/497 (100%)	475 (96%)	16 (3%)	4 (1%)	16	20
1	C	495/497 (100%)	465 (94%)	25 (5%)	5 (1%)	12	15
1	D	495/497 (100%)	469 (95%)	21 (4%)	5 (1%)	12	15
All	All	1980/1988 (100%)	1868 (94%)	91 (5%)	21 (1%)	11	13

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	233	GLU
1	D	317	LEU
1	D	345	SER
1	A	124	ALA
1	A	233	GLU

5.3.2 Protein sidechains [i](#)

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	424/424 (100%)	406 (96%)	18 (4%)	26	40
1	B	424/424 (100%)	401 (95%)	23 (5%)	20	29
1	C	424/424 (100%)	402 (95%)	22 (5%)	21	31
1	D	424/424 (100%)	397 (94%)	27 (6%)	16	23
All	All	1696/1696 (100%)	1606 (95%)	90 (5%)	20	30

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	379	THR
1	D	112	GLU
1	C	396	ASN
1	D	57	GLN
1	D	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	396	ASN
1	D	495	HIS
1	C	169	GLN
1	D	328	HIS
1	C	146	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

82 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
2	NAG	D	498	1	14,14,15	0.76	0	17,19,21	2.52	5 (29%)
3	PO4	C	520	-	4,4,4	1.07	0	6,6,6	0.69	0
3	PO4	C	509	-	4,4,4	0.62	0	6,6,6	0.98	0
3	PO4	C	521	-	4,4,4	0.74	0	6,6,6	0.86	0
3	PO4	C	515	-	4,4,4	0.93	0	6,6,6	0.66	0
3	PO4	C	511	-	4,4,4	0.88	0	6,6,6	0.58	0
3	PO4	C	517	-	4,4,4	1.26	0	6,6,6	0.73	0
3	PO4	D	506	-	4,4,4	0.98	0	6,6,6	0.84	0
3	PO4	D	499	-	4,4,4	1.08	0	6,6,6	1.60	2 (33%)
3	PO4	A	502	-	4,4,4	1.03	0	6,6,6	1.61	2 (33%)
3	PO4	C	513	-	4,4,4	0.84	0	6,6,6	1.03	0
3	PO4	B	503	-	4,4,4	0.91	0	6,6,6	1.36	1 (16%)
3	PO4	A	501	-	4,4,4	1.26	0	6,6,6	1.55	1 (16%)
3	PO4	C	510	-	4,4,4	0.87	0	6,6,6	0.27	0
2	NAG	B	498	1	14,14,15	0.67	0	17,19,21	2.76	4 (23%)
3	PO4	D	510	-	4,4,4	0.86	0	6,6,6	0.81	0
3	PO4	A	505	-	4,4,4	0.74	0	6,6,6	1.29	1 (16%)
3	PO4	B	502	-	4,4,4	1.20	0	6,6,6	1.29	1 (16%)
3	PO4	B	512	-	4,4,4	0.53	0	6,6,6	0.97	0
3	PO4	A	519	-	4,4,4	0.88	0	6,6,6	0.61	0
3	PO4	A	503	-	4,4,4	0.73	0	6,6,6	1.79	2 (33%)
3	PO4	C	504	-	4,4,4	1.08	0	6,6,6	1.00	0
3	PO4	A	514	-	4,4,4	0.94	0	6,6,6	0.62	0
3	PO4	A	510	-	4,4,4	0.88	0	6,6,6	0.77	0
3	PO4	C	503	-	4,4,4	0.99	0	6,6,6	1.25	0
3	PO4	D	511	-	4,4,4	0.82	0	6,6,6	0.98	0
3	PO4	B	509	-	4,4,4	0.78	0	6,6,6	0.51	0
3	PO4	D	512	-	4,4,4	0.57	0	6,6,6	1.03	0
3	PO4	B	515	-	4,4,4	0.96	0	6,6,6	0.61	0
3	PO4	D	513	-	4,4,4	0.92	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	500	-	4,4,4	1.44	1 (25%)	6,6,6	0.67	0
3	PO4	D	503	-	4,4,4	1.11	0	6,6,6	1.40	1 (16%)
3	PO4	D	505	-	4,4,4	0.81	0	6,6,6	0.97	0
3	PO4	D	500	-	4,4,4	1.04	0	6,6,6	0.95	0
3	PO4	C	519	-	4,4,4	0.70	0	6,6,6	0.93	0
3	PO4	C	505	-	4,4,4	1.04	0	6,6,6	1.30	0
3	PO4	C	508	-	4,4,4	0.67	0	6,6,6	1.04	0
3	PO4	C	501	-	4,4,4	1.21	0	6,6,6	1.55	1 (16%)
3	PO4	C	499	-	4,4,4	1.50	0	6,6,6	1.06	0
3	PO4	B	507	-	4,4,4	1.13	0	6,6,6	0.47	0
3	PO4	C	500	-	4,4,4	1.26	0	6,6,6	1.07	0
3	PO4	C	516	-	4,4,4	1.29	0	6,6,6	0.78	0
3	PO4	A	508	-	4,4,4	0.76	0	6,6,6	0.95	0
3	PO4	B	506	-	4,4,4	0.89	0	6,6,6	0.72	0
3	PO4	B	511	-	4,4,4	0.55	0	6,6,6	0.65	0
3	PO4	B	500	-	4,4,4	1.03	0	6,6,6	1.06	0
3	PO4	A	504	-	4,4,4	1.18	0	6,6,6	0.95	0
3	PO4	A	512	-	4,4,4	0.90	0	6,6,6	1.34	1 (16%)
3	PO4	A	518	-	4,4,4	1.31	0	6,6,6	0.43	0
2	NAG	C	498	1	14,14,15	1.13	1 (7%)	17,19,21	2.02	5 (29%)
3	PO4	B	505	-	4,4,4	1.07	0	6,6,6	1.11	0
3	PO4	C	507	-	4,4,4	0.70	0	6,6,6	0.65	0
3	PO4	B	508	-	4,4,4	0.74	0	6,6,6	0.93	0
3	PO4	B	501	-	4,4,4	0.70	0	6,6,6	1.44	2 (33%)
3	PO4	A	509	-	4,4,4	0.85	0	6,6,6	0.72	0
3	PO4	D	507	-	4,4,4	0.89	0	6,6,6	0.17	0
2	NAG	A	498	1	14,14,15	1.21	1 (7%)	17,19,21	1.99	6 (35%)
3	PO4	B	504	-	4,4,4	0.99	0	6,6,6	0.60	0
3	PO4	A	507	-	4,4,4	0.60	0	6,6,6	0.96	0
3	PO4	B	499	-	4,4,4	1.45	1 (25%)	6,6,6	1.13	0
3	PO4	C	506	-	4,4,4	0.79	0	6,6,6	0.84	0
3	PO4	D	508	-	4,4,4	0.83	0	6,6,6	0.98	0
3	PO4	D	514	-	4,4,4	1.16	0	6,6,6	0.63	0
3	PO4	D	509	-	4,4,4	0.68	0	6,6,6	0.88	0
3	PO4	A	511	-	4,4,4	0.74	0	6,6,6	1.57	1 (16%)
3	PO4	B	510	-	4,4,4	1.02	0	6,6,6	0.86	0
3	PO4	A	499	-	4,4,4	1.73	1 (25%)	6,6,6	1.91	3 (50%)
3	PO4	B	514	-	4,4,4	0.85	0	6,6,6	0.76	0
3	PO4	A	513	-	4,4,4	0.61	0	6,6,6	1.18	1 (16%)
3	PO4	A	516	-	4,4,4	0.71	0	6,6,6	1.43	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	B	516	-	4,4,4	0.89	0	6,6,6	0.76	0
3	PO4	C	514	-	4,4,4	0.71	0	6,6,6	1.21	1 (16%)
3	PO4	D	501	-	4,4,4	0.95	0	6,6,6	0.98	0
3	PO4	D	504	-	4,4,4	1.01	0	6,6,6	1.00	0
3	PO4	A	515	-	4,4,4	1.16	0	6,6,6	0.57	0
3	PO4	C	518	-	4,4,4	1.08	0	6,6,6	0.60	0
3	PO4	D	502	-	4,4,4	1.10	0	6,6,6	0.96	0
3	PO4	A	506	-	4,4,4	0.62	0	6,6,6	0.62	0
3	PO4	B	513	-	4,4,4	0.68	0	6,6,6	1.52	1 (16%)
3	PO4	A	517	-	4,4,4	1.03	0	6,6,6	1.05	0
3	PO4	C	502	-	4,4,4	1.12	0	6,6,6	1.93	3 (50%)
3	PO4	C	512	-	4,4,4	0.84	0	6,6,6	0.90	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	NAG	B	498	1	-	2/6/23/26	0/1/1/1
2	NAG	D	498	1	-	2/6/23/26	0/1/1/1
2	NAG	C	498	1	-	0/6/23/26	0/1/1/1
2	NAG	A	498	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	498	NAG	C1-C2	2.80	1.56	1.52
2	C	498	NAG	C1-C2	2.74	1.56	1.52
3	A	499	PO4	P-O3	-2.67	1.46	1.54
3	A	500	PO4	P-O2	-2.16	1.48	1.54
3	B	499	PO4	P-O2	-2.00	1.48	1.54

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	498	NAG	C1-O5-C5	8.94	124.17	112.19
2	D	498	NAG	C1-O5-C5	6.60	121.04	112.19
2	C	498	NAG	C1-O5-C5	5.28	119.26	112.19
2	D	498	NAG	C6-C5-C4	-4.37	102.29	113.02
2	B	498	NAG	O5-C5-C6	-3.94	100.00	107.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	498	NAG	O5-C5-C6-O6
2	D	498	NAG	C4-C5-C6-O6
2	B	498	NAG	O5-C5-C6-O6
2	B	498	NAG	C4-C5-C6-O6

There are no ring outliers.

25 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	498	NAG	2	0
3	C	520	PO4	7	0
3	C	515	PO4	1	0
3	C	517	PO4	14	0
3	A	502	PO4	4	0
3	B	503	PO4	3	0
2	B	498	NAG	1	0
3	B	502	PO4	3	0
3	A	503	PO4	1	0
3	A	514	PO4	4	0
3	D	503	PO4	3	0
3	C	501	PO4	3	0
3	A	508	PO4	1	0
3	A	518	PO4	9	0
3	D	507	PO4	2	0
2	A	498	NAG	1	0
3	B	504	PO4	1	0
3	D	514	PO4	6	0
3	A	511	PO4	1	0
3	B	510	PO4	1	0
3	C	514	PO4	1	0
3	A	515	PO4	4	0
3	C	518	PO4	5	0
3	B	513	PO4	1	0
3	C	502	PO4	1	0

5.7 Other polymers [i](#)

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 [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	497/497 (100%)	-1.61	0 100 100	8, 25, 40, 55	5 (1%)
1	B	497/497 (100%)	-1.58	0 100 100	7, 26, 48, 62	5 (1%)
1	C	497/497 (100%)	-1.62	0 100 100	7, 24, 40, 51	5 (1%)
1	D	497/497 (100%)	-1.59	0 100 100	8, 26, 48, 61	5 (1%)
All	All	1988/1988 (100%)	-1.60	0 100 100	7, 25, 44, 62	20 (1%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	NAG	B	498	14/15	0.98	0.03	32,40,42,42	0
3	PO4	A	507	5/5	0.98	0.04	73,73,74,75	0
3	PO4	A	509	5/5	0.98	0.07	84,85,86,87	0
3	PO4	A	510	5/5	0.98	0.04	93,93,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	519	5/5	0.98	0.05	76,77,78,79	0
3	PO4	B	507	5/5	0.98	0.04	91,92,93,93	0
3	PO4	B	508	5/5	0.98	0.05	83,83,84,84	0
3	PO4	B	509	5/5	0.98	0.04	76,76,78,79	0
3	PO4	B	510	5/5	0.98	0.07	78,78,79,80	0
3	PO4	B	512	5/5	0.98	0.06	75,76,78,78	0
3	PO4	C	510	5/5	0.98	0.04	82,84,85,86	0
3	PO4	C	514	5/5	0.98	0.05	63,64,65,66	0
3	PO4	D	511	5/5	0.98	0.05	73,74,75,75	0
3	PO4	A	512	5/5	0.99	0.04	55,56,58,59	0
3	PO4	A	513	5/5	0.99	0.03	58,60,60,63	0
3	PO4	A	514	5/5	0.99	0.03	63,64,65,66	0
3	PO4	A	515	5/5	0.99	0.06	141,141,142,142	0
3	PO4	A	516	5/5	0.99	0.04	64,64,66,67	0
3	PO4	A	518	5/5	0.99	0.09	256,256,257,257	0
3	PO4	A	501	5/5	0.99	0.02	37,37,40,42	0
3	PO4	B	501	5/5	0.99	0.03	42,45,48,51	0
3	PO4	B	504	5/5	0.99	0.04	70,70,72,72	0
3	PO4	B	505	5/5	0.99	0.04	56,57,60,61	0
3	PO4	B	506	5/5	0.99	0.06	77,78,78,80	0
3	PO4	A	503	5/5	0.99	0.03	52,53,54,59	0
3	PO4	A	505	5/5	0.99	0.04	59,61,61,64	0
3	PO4	A	506	5/5	0.99	0.03	61,62,65,65	0
2	NAG	A	498	14/15	0.99	0.03	23,31,34,35	0
3	PO4	B	511	5/5	0.99	0.05	75,75,76,77	0
3	PO4	A	508	5/5	0.99	0.07	79,80,80,81	0
3	PO4	B	513	5/5	0.99	0.05	55,56,56,56	0
3	PO4	B	514	5/5	0.99	0.03	61,62,64,67	0
3	PO4	B	515	5/5	0.99	0.06	83,84,85,85	0
3	PO4	B	516	5/5	0.99	0.05	77,78,78,78	0
3	PO4	C	503	5/5	0.99	0.04	49,51,54,55	0
3	PO4	C	505	5/5	0.99	0.08	73,74,75,75	0
3	PO4	C	506	5/5	0.99	0.06	67,69,70,70	0
3	PO4	C	507	5/5	0.99	0.06	84,84,84,85	0
3	PO4	C	508	5/5	0.99	0.04	82,83,84,85	0
3	PO4	C	509	5/5	0.99	0.05	78,79,80,80	0
2	NAG	C	498	14/15	0.99	0.03	30,35,37,38	0
3	PO4	C	511	5/5	0.99	0.04	80,80,82,82	0
3	PO4	C	512	5/5	0.99	0.04	51,53,54,57	0
3	PO4	C	513	5/5	0.99	0.04	63,64,64,65	0
2	NAG	D	498	14/15	0.99	0.03	34,37,38,38	0
3	PO4	C	515	5/5	0.99	0.03	58,59,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	C	516	5/5	0.99	0.03	51,54,55,58	0
3	PO4	C	517	5/5	0.99	0.10	373,373,373,373	0
3	PO4	C	518	5/5	0.99	0.08	163,163,164,164	0
3	PO4	C	519	5/5	0.99	0.04	57,59,61,62	0
3	PO4	C	520	5/5	0.99	0.09	160,161,161,161	0
3	PO4	C	521	5/5	0.99	0.03	69,69,70,72	0
3	PO4	D	501	5/5	0.99	0.03	43,47,51,52	0
3	PO4	D	502	5/5	0.99	0.04	43,45,47,48	0
3	PO4	D	504	5/5	0.99	0.04	65,66,67,67	0
3	PO4	D	505	5/5	0.99	0.04	85,85,87,87	0
3	PO4	D	506	5/5	0.99	0.06	65,66,67,69	0
3	PO4	D	507	5/5	0.99	0.05	72,76,77,77	0
3	PO4	D	508	5/5	0.99	0.04	74,74,76,76	0
3	PO4	D	509	5/5	0.99	0.04	68,70,71,72	0
3	PO4	D	510	5/5	0.99	0.06	59,60,62,62	0
3	PO4	A	511	5/5	0.99	0.03	67,67,69,69	0
3	PO4	D	512	5/5	0.99	0.04	66,66,68,68	0
3	PO4	D	513	5/5	0.99	0.06	68,69,70,71	0
3	PO4	D	514	5/5	0.99	0.08	184,184,184,184	0
3	PO4	B	502	5/5	1.00	0.02	46,47,49,49	0
3	PO4	D	499	5/5	1.00	0.01	25,26,27,29	0
3	PO4	D	500	5/5	1.00	0.02	36,36,39,39	0
3	PO4	B	503	5/5	1.00	0.03	44,48,49,52	0
3	PO4	A	504	5/5	1.00	0.04	47,51,55,56	0
3	PO4	D	503	5/5	1.00	0.02	46,46,48,51	0
3	PO4	A	517	5/5	1.00	0.03	49,49,52,53	0
3	PO4	A	499	5/5	1.00	0.01	21,22,23,26	0
3	PO4	A	502	5/5	1.00	0.02	45,45,47,48	0
3	PO4	C	499	5/5	1.00	0.01	23,23,27,30	0
3	PO4	C	500	5/5	1.00	0.02	35,39,40,40	0
3	PO4	C	501	5/5	1.00	0.02	35,37,40,40	0
3	PO4	C	502	5/5	1.00	0.02	36,36,37,37	0
3	PO4	B	499	5/5	1.00	0.02	26,30,31,33	0
3	PO4	C	504	5/5	1.00	0.04	45,46,48,48	0
3	PO4	B	500	5/5	1.00	0.02	36,36,38,39	0
3	PO4	A	500	5/5	1.00	0.03	31,35,36,36	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.