



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:59 PM UTC

PDB ID : 8A4K / pdb_00008a4k
Title : Human GDAP1, R282H mutant
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Deposited on : 2022-06-12
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
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

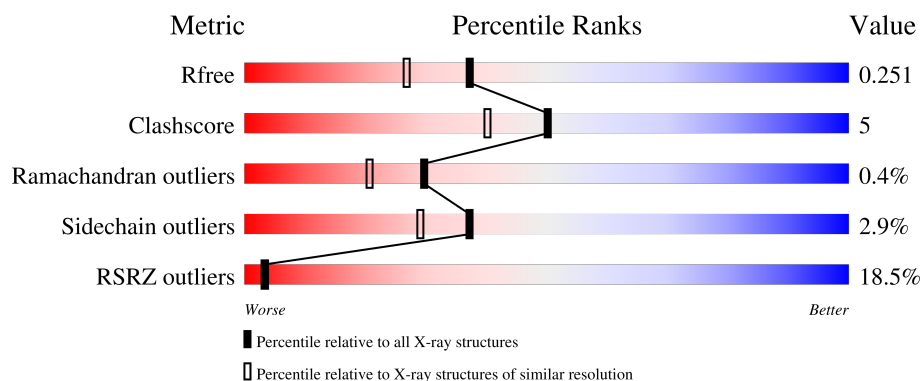
1 Overall quality at a glance

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	280	12% 78% 12% 9%
1	B	280	20% 71% 13% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8214 atoms, of which 4062 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 Ganglioside-induced differentiation-associated protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	H	N	O	S	0	1	0
			4211	1341	2105	368	388	9			
1	B	237	Total	C	H	N	O	S	0	0	0
			3927	1256	1957	344	361	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	HIS	ARG	variant	UNP Q8TB36
B	282	HIS	ARG	variant	UNP Q8TB36

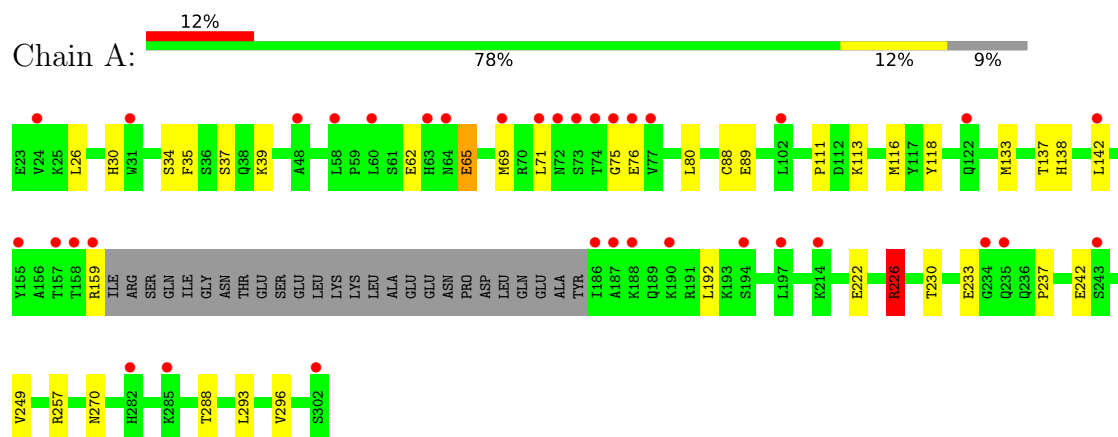
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	54	Total	O	0	0
			54	54		
2	B	22	Total	O	0	0
			22	22		

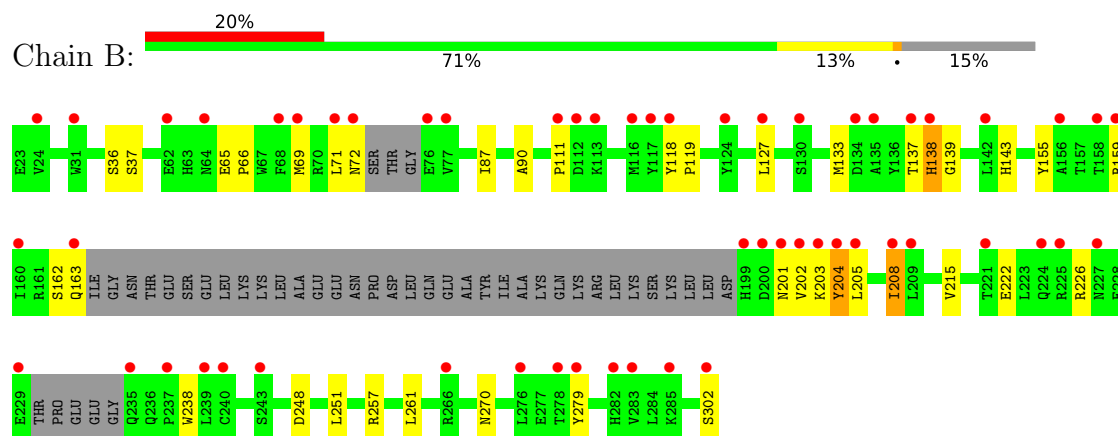
3 Residue-property plots [i](#)

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: Ganglioside-induced differentiation-associated protein 1



- Molecule 1: Ganglioside-induced differentiation-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.28Å 113.37Å 115.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.84 – 1.95 44.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.3 (44.84-1.95) 84.6 (44.84-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.29 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.225 , 0.251 0.225 , 0.251	Depositor DCC
R_{free} test set	1994 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8214	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	1/2154 (0.0%)	0.83	1/2914 (0.0%)
1	B	0.51	0/2014	0.72	0/2724
All	All	0.63	1/4168 (0.0%)	0.78	1/5638 (0.0%)

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	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLU	CB-CG	-6.91	1.31	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	CG-CD-NE	-7.78	94.89	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	ARG	Sidechain
1	A	257	ARG	Sidechain
1	B	257	ARG	Sidechain

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	2106	2105	2102	22	0
1	B	1970	1957	1956	21	0
2	A	54	0	0	1	0
2	B	22	0	0	0	0
All	All	4152	4062	4058	43	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 5.

All (43) 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:222:GLU:OE2	1:B:226:ARG:NH2	1.89	1.05
1:A:222:GLU:OE2	1:A:226:ARG:NH2	2.04	0.89
1:A:138:HIS:NE2	1:A:142:LEU:HD11	2.03	0.73
1:B:133:MET:O	1:B:137:THR:HG23	2.00	0.61
1:B:36:SER:HB2	1:B:90:ALA:HB2	1.86	0.57
1:B:143:HIS:NE2	1:B:201:ASN:OD1	2.38	0.57
1:A:26:LEU:HD22	1:A:80:LEU:HD11	1.87	0.57
1:A:65:GLU:HG2	1:A:159:ARG:NH1	2.21	0.56
1:B:162:SER:O	1:B:163:GLN:HB2	2.05	0.55
1:A:133:MET:O	1:A:137:THR:HG23	2.06	0.55
1:A:65:GLU:HG2	1:A:159:ARG:HH12	1.73	0.54
1:A:34:SER:HB3	1:A:75:GLY:HA3	1.93	0.50
1:A:222:GLU:HG3	1:A:226:ARG:HH21	1.76	0.49
1:B:204:TYR:CE2	1:B:208:ILE:HD11	2.47	0.49
1:B:137:THR:HG22	1:B:261:LEU:HD11	1.96	0.47
1:B:65:GLU:HG2	1:B:159:ARG:NH1	2.30	0.47
1:A:65:GLU:CD	1:A:159:ARG:NH2	2.74	0.46
1:A:113:LYS:HG3	1:A:113:LYS:O	2.16	0.46
1:A:69:MET:HE2	1:A:159:ARG:HH11	1.81	0.46
1:A:138:HIS:CE1	1:A:142:LEU:HD11	2.50	0.46
1:B:87:ILE:HD12	1:B:87:ILE:N	2.31	0.46
1:A:111:PRO:HG2	1:A:118:TYR:HA	1.97	0.45
1:B:127:LEU:HD21	1:B:215:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD23	1:B:279:TYR:CZ	2.51	0.45
1:B:118:TYR:HB3	1:B:119:PRO:HD3	1.98	0.45
1:A:116:MET:O	2:A:401:HOH:O	2.21	0.45
1:A:35:PHE:CE2	1:A:39:LYS:HD2	2.52	0.44
1:B:139:GLY:HA3	1:B:205:LEU:HD21	1.98	0.44
1:B:72:ASN:HB3	1:B:138:HIS:CE1	2.52	0.44
1:B:202:VAL:HG12	1:B:203:LYS:N	2.33	0.43
1:B:238:TRP:HB3	1:B:248:ASP:OD1	2.18	0.43
1:A:230:THR:HG21	1:A:237:PRO:HD3	2.01	0.43
1:B:226:ARG:HD3	1:B:226:ARG:HA	1.78	0.43
1:A:88:CYS:O	1:A:89:GLU:HB2	2.18	0.43
1:A:293:LEU:O	1:A:296:VAL:HG22	2.19	0.42
1:B:65:GLU:HB3	1:B:69:MET:HB2	2.00	0.42
1:B:66:PRO:HD2	1:B:69:MET:HG3	2.01	0.42
1:B:202:VAL:HG12	1:B:204:TYR:H	1.84	0.41
1:A:65:GLU:OE2	1:A:159:ARG:NH2	2.54	0.41
1:A:71:LEU:HD12	1:A:71:LEU:HA	1.90	0.41
1:A:30:HIS:HB2	1:A:37:SER:HB2	2.02	0.41
1:B:155:TYR:CD1	1:B:155:TYR:C	2.97	0.40
1:A:270:ASN:O	1:A:270:ASN:OD1	2.39	0.40

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	251/280 (90%)	245 (98%)	5 (2%)	1 (0%)	30	21
1	B	229/280 (82%)	225 (98%)	3 (1%)	1 (0%)	30	21
All	All	480/560 (86%)	470 (98%)	8 (2%)	2 (0%)	30	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	PRO
1	A	76	GLU

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	236/258 (92%)	230 (98%)	6 (2%)	42	34
1	B	221/258 (86%)	214 (97%)	7 (3%)	34	25
All	All	457/516 (89%)	444 (97%)	13 (3%)	37	30

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	192	LEU
1	A	233	GLU
1	A	242	GLU
1	A	249	VAL
1	A	288	THR
1	B	37	SER
1	B	71	LEU
1	B	138	HIS
1	B	204	TYR
1	B	208	ILE
1	B	270	ASN
1	B	302	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	123	HIS
1	A	201	ASN
1	B	30	HIS

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Mol	Chain	Res	Type
1	B	236	GLN
1	B	267	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](#)

There are no ligands in this entry.

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	A	254/280 (90%)	0.90	35 (13%) 6 7	34, 77, 144, 176	1 (0%)
1	B	237/280 (84%)	1.36	56 (23%) 2 2	71, 101, 159, 189	0
All	All	491/560 (87%)	1.12	91 (18%) 3 3	34, 88, 156, 189	1 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	VAL	6.8
1	A	186	ILE	5.9
1	B	160	ILE	4.9
1	B	302	SER	4.8
1	B	71	LEU	4.7
1	A	75	GLY	4.4
1	A	187	ALA	4.2
1	A	74	THR	4.2
1	B	204	TYR	4.1
1	B	221	THR	3.9
1	B	31	TRP	3.9
1	B	76	GLU	3.8
1	B	64	ASN	3.8
1	A	71	LEU	3.7
1	A	58	LEU	3.6
1	B	72	ASN	3.6
1	A	159	ARG	3.5
1	B	158	THR	3.4
1	B	208	ILE	3.4
1	B	205	LEU	3.4
1	B	227	ASN	3.4
1	A	60	LEU	3.3
1	B	77	VAL	3.3
1	B	117	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLU	3.2
1	A	24	VAL	3.2
1	B	111	PRO	3.1
1	B	243	SER	3.1
1	A	197	LEU	3.0
1	B	62	GLU	3.0
1	B	209	LEU	2.9
1	A	234	GLY	2.9
1	A	63	HIS	2.9
1	B	138	HIS	2.9
1	A	142	LEU	2.9
1	B	116	MET	2.9
1	B	203	LYS	2.9
1	B	282	HIS	2.8
1	B	199	HIS	2.8
1	A	282[A]	HIS	2.8
1	B	283	VAL	2.8
1	A	155	TYR	2.7
1	A	235	GLN	2.7
1	B	137	THR	2.7
1	A	158	THR	2.7
1	B	235	GLN	2.7
1	A	64	ASN	2.7
1	A	190	LYS	2.7
1	B	279	TYR	2.7
1	B	200	ASP	2.6
1	B	24	VAL	2.6
1	B	225	ARG	2.6
1	A	157	THR	2.6
1	B	240	CYS	2.6
1	A	102	LEU	2.6
1	B	237	PRO	2.6
1	B	159	ARG	2.6
1	B	163	GLN	2.5
1	B	130	SER	2.5
1	A	122	GLN	2.5
1	A	76	GLU	2.5
1	B	135	ALA	2.4
1	B	127	LEU	2.4
1	B	113	LYS	2.4
1	A	31	TRP	2.4
1	A	188	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	124	TYR	2.3
1	B	156	ALA	2.3
1	A	194	SER	2.3
1	B	134	ASP	2.3
1	B	201	ASN	2.3
1	B	239	LEU	2.3
1	A	48	ALA	2.2
1	A	214	LYS	2.2
1	B	142	LEU	2.2
1	A	72	ASN	2.2
1	B	278	THR	2.2
1	B	224	GLN	2.2
1	B	112	ASP	2.2
1	A	77	VAL	2.2
1	A	69	MET	2.1
1	A	73	SER	2.1
1	B	276	LEU	2.1
1	A	285	LYS	2.1
1	B	285	LYS	2.1
1	B	266	ARG	2.1
1	B	68	PHE	2.1
1	A	243	SER	2.1
1	A	302	SER	2.0
1	B	118	TYR	2.0
1	B	69	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.