



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8EXZ / pdb_00008exz
Title : Structure of GDAP1 containing CMT mutant T157P
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Deposited on : 2022-10-26
Resolution : 2.82 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

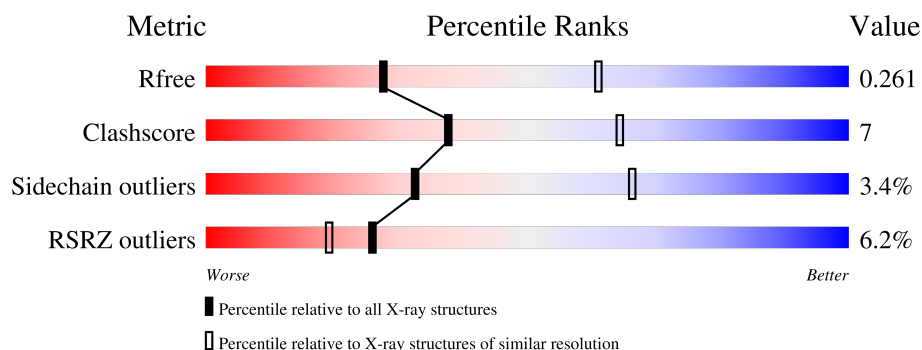
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	358	4% 52% 9% 38%
1	B	358	4% 52% 11% 37%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7332 atoms, of which 3634 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	221	Total	C	H	N	O	S	0	0	0
			3624	1164	1796	317	338	9			
1	B	227	Total	C	H	N	O	S	0	0	0
			3708	1191	1838	328	342	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	PRO	THR	engineered mutation	UNP O88741
B	157	PRO	THR	engineered mutation	UNP O88741

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.59Å 80.06Å 85.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.86 – 2.82 55.86 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.1 (55.86-2.82) 87.7 (55.86-2.82)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.255 , 0.279 (Not available) , 0.261	Depositor DCC
R_{free} test set	991 reflections (7.90%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtrriage
Anisotropy	0.821	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7332	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.73 % 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 3.0307e-05. 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

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	0.14	0/1872	0.28	0/2536
1	B	0.23	0/1916	0.32	0/2597
All	All	0.19	0/3788	0.30	0/5133

There are no bond length outliers.

There are no bond angle outliers.

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	1828	1796	1794	25	0
1	B	1870	1838	1836	26	0
All	All	3698	3634	3630	51	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 7.

All (51) 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:279:TYR:O	1:B:283:VAL:HG23	1.89	0.73
1:A:146:LEU:HD12	1:A:205:LEU:HD23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:HD21	1:B:137:THR:OG1	1.95	0.67
1:B:80:LEU:HD22	1:B:93:ILE:HG23	1.79	0.65
1:A:42:LEU:HD23	1:A:249:VAL:HG13	1.83	0.59
1:B:143:HIS:ND1	1:B:202:VAL:HG22	2.18	0.58
1:A:71:LEU:CD1	1:A:137:THR:HG21	2.35	0.57
1:A:71:LEU:HD13	1:A:137:THR:HG21	1.86	0.57
1:A:43:VAL:HG13	1:A:109:LEU:HD12	1.85	0.56
1:A:26:LEU:CD2	1:A:82:HIS:CD2	2.89	0.55
1:B:43:VAL:HG13	1:B:109:LEU:HD12	1.89	0.55
1:B:133:MET:O	1:B:137:THR:HG23	2.08	0.54
1:B:146:LEU:HD12	1:B:205:LEU:HD23	1.88	0.54
1:A:26:LEU:HD21	1:A:82:HIS:CD2	2.44	0.52
1:A:217:ASP:O	1:A:221:THR:HG23	2.09	0.52
1:A:35:PHE:CE1	1:A:253:VAL:HG12	2.45	0.52
1:A:133:MET:HE2	1:A:257:ARG:HG2	1.92	0.51
1:A:87:ILE:HD12	1:A:87:ILE:N	2.26	0.51
1:B:124:TYR:O	1:B:128:LEU:HD23	2.09	0.51
1:B:46:GLU:OE1	1:B:109:LEU:HD21	2.11	0.50
1:B:71:LEU:HD21	1:B:137:THR:HG1	1.76	0.50
1:A:26:LEU:HD23	1:A:82:HIS:CD2	2.48	0.48
1:B:71:LEU:HD12	1:B:71:LEU:O	2.14	0.48
1:B:60:LEU:HD23	1:B:60:LEU:O	2.15	0.46
1:A:71:LEU:CD1	1:A:137:THR:CG2	2.93	0.46
1:B:87:ILE:HD12	1:B:87:ILE:N	2.30	0.46
1:A:279:TYR:O	1:A:283:VAL:HG23	2.16	0.46
1:A:77:VAL:O	1:A:77:VAL:HG23	2.16	0.46
1:A:133:MET:HE2	1:A:257:ARG:CG	2.46	0.46
1:B:68:PHE:CD1	1:B:141:ILE:HD11	2.51	0.45
1:A:251:LEU:HD23	1:A:279:TYR:CZ	2.53	0.44
1:B:137:THR:HG22	1:B:261:LEU:HD11	1.99	0.43
1:A:146:LEU:HD12	1:A:205:LEU:CD2	2.44	0.43
1:B:255:LEU:HD22	1:B:268:TRP:CZ3	2.53	0.43
1:B:35:PHE:CE1	1:B:253:VAL:HG12	2.54	0.43
1:A:111:PRO:HG2	1:A:118:TYR:HA	2.00	0.43
1:B:143:HIS:CE1	1:B:202:VAL:HG22	2.54	0.43
1:A:88:CYS:O	1:A:89:GLU:HB2	2.18	0.42
1:B:151:MET:HG3	1:B:260:PHE:HA	2.01	0.42
1:A:140:CYS:SG	1:A:147:THR:HG21	2.58	0.42
1:B:77:VAL:O	1:B:77:VAL:HG23	2.19	0.42
1:B:151:MET:HE2	1:B:297:ASN:HB3	2.03	0.41
1:B:111:PRO:HG2	1:B:118:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:HD3	1:B:287:LYS:H	1.86	0.41
1:A:124:TYR:O	1:A:128:LEU:HD23	2.21	0.41
1:A:70:ARG:O	1:A:70:ARG:CG	2.69	0.41
1:B:146:LEU:HD12	1:B:205:LEU:CD2	2.52	0.40
1:A:146:LEU:CD1	1:A:205:LEU:HD23	2.47	0.40
1:B:251:LEU:HD23	1:B:279:TYR:CZ	2.57	0.40
1:B:280:TYR:CE2	1:B:284:LEU:HD11	2.57	0.40
1:A:106:THR:O	1:A:108:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	204/318 (64%)	200 (98%)	4 (2%)	48	79
1	B	208/318 (65%)	198 (95%)	10 (5%)	23	54
All	All	412/636 (65%)	398 (97%)	14 (3%)	32	66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	140	CYS
1	A	235	ASN
1	A	265	ARG
1	B	50	LYS

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Mol	Chain	Res	Type
1	B	71	LEU
1	B	76	GLU
1	B	104	GLU
1	B	140	CYS
1	B	141	ILE
1	B	145	GLU
1	B	230	THR
1	B	281	GLU
1	B	287	LYS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	221/358 (61%)	0.71	14 (6%) 26 19	31, 60, 92, 121	0
1	B	227/358 (63%)	0.72	14 (6%) 26 19	34, 62, 91, 103	0
All	All	448/716 (62%)	0.71	28 (6%) 26 19	31, 61, 92, 121	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	GLU	4.0
1	B	154	ALA	3.6
1	B	296	VAL	3.3
1	A	150	SER	3.2
1	B	101	PHE	3.0
1	B	199	HIS	2.8
1	A	69	MET	2.7
1	A	25	HIS	2.7
1	B	294	GLY	2.6
1	B	239	LEU	2.5
1	A	199	HIS	2.5
1	B	270	HIS	2.5
1	B	26	LEU	2.4
1	B	46	GLU	2.3
1	B	231	PRO	2.3
1	A	70	ARG	2.3
1	A	73	SER	2.2
1	A	71	LEU	2.2
1	A	112	ASP	2.1
1	B	226	ARG	2.1
1	B	267	ASN	2.1
1	A	64	ASN	2.1
1	A	221	THR	2.1
1	B	86	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	74	ALA	2.1
1	B	240	CYS	2.0
1	A	148	VAL	2.0
1	A	81	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.