Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	8VPL / pdb_00008vpl
Title	:	Glutaminyl cyclase ApgG, diamond shape
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Deposited on	:	2024-01-16
Resolution	:	1.84 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:

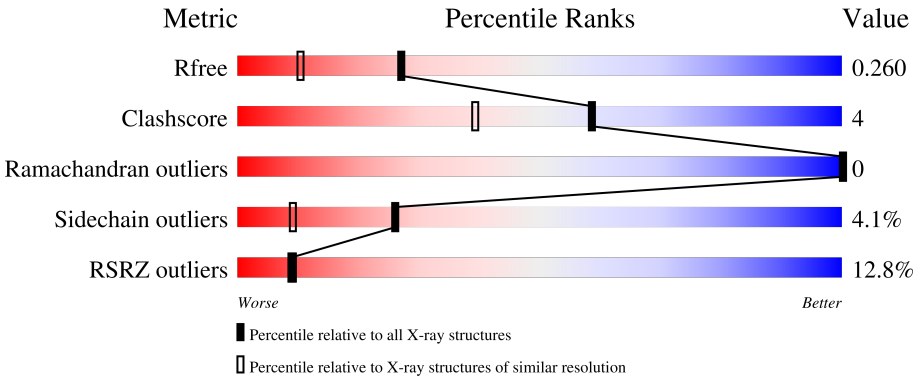
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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 <=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	353	12% 86% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2731 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 Peptide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	2	0
			2700	1717	463	516	4			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7U2MGR8
A	348	HIS	-	expression tag	UNP A0A7U2MGR8
A	349	HIS	-	expression tag	UNP A0A7U2MGR8
A	350	HIS	-	expression tag	UNP A0A7U2MGR8
A	351	HIS	-	expression tag	UNP A0A7U2MGR8
A	352	HIS	-	expression tag	UNP A0A7U2MGR8
A	353	HIS	-	expression tag	UNP A0A7U2MGR8

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

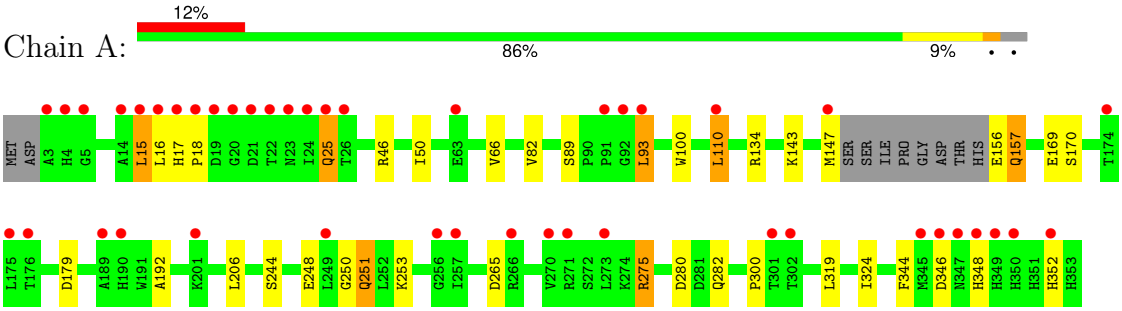
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		

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: Peptide hydrolase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	70.27Å 70.27Å 145.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.63 – 1.84 46.63 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.63-1.84) 99.8 (46.63-1.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.240 , 0.260 0.240 , 0.260	Depositor DCC
R_{free} test set	1864 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2731	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	0.57	2/2779 (0.1%)	0.79	2/3794 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352[A]	HIS	C-O	7.10	1.31	1.23
1	A	352[B]	HIS	C-O	7.10	1.31	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352[A]	HIS	CA-C-O	6.11	127.66	120.20
1	A	352[B]	HIS	CA-C-O	6.11	127.66	120.20

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	2700	0	2608	23	0
2	A	1	0	0	0	0
3	A	30	0	0	0	0
All	All	2731	0	2608	23	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 4.

All (23) 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:25:GLN:HE21	1:A:25:GLN:H	1.31	0.77
1:A:17:HIS:CG	1:A:18:PRO:HD2	2.36	0.61
1:A:25:GLN:H	1:A:25:GLN:NE2	1.99	0.59
1:A:280:ASP:HB3	1:A:282:GLN:OE1	2.08	0.53
1:A:17:HIS:CD2	1:A:18:PRO:HD2	2.47	0.50
1:A:143:LYS:HB2	1:A:344:PHE:CD2	2.47	0.49
1:A:319:LEU:HD22	1:A:324:ILE:HD11	1.95	0.48
1:A:192:ALA:HB2	1:A:206:LEU:HD22	1.94	0.48
1:A:93:LEU:HD11	1:A:157:GLN:HG3	1.96	0.47
1:A:66:VAL:HG22	1:A:82:VAL:HG13	1.98	0.46
1:A:275:ARG:NH2	1:A:300:PRO:HB2	2.32	0.45
1:A:265:ASP:OD2	1:A:275:ARG:HD3	2.17	0.45
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.79	0.44
1:A:244:SER:O	1:A:248:GLU:HG3	2.17	0.44
1:A:248:GLU:C	1:A:250:GLY:H	2.26	0.43
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.69	0.43
1:A:251:GLN:HE21	1:A:251:GLN:HB3	1.57	0.42
1:A:89:SER:HB3	1:A:100:TRP:HH2	1.85	0.42
1:A:248:GLU:C	1:A:250:GLY:N	2.79	0.41
1:A:147:MET:SD	1:A:156:GLU:HB2	2.61	0.41
1:A:170:SER:HB3	1:A:179:ASP:OD2	2.20	0.41
1:A:110:LEU:HD23	1:A:169:GLU:HB3	2.02	0.40
1:A:46:ARG:O	1:A:50:ILE:HD12	2.22	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	341/353 (97%)	334 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	295/303 (97%)	283 (96%)	12 (4%)	26 9

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	16	LEU
1	A	25	GLN
1	A	93	LEU
1	A	110	LEU
1	A	134	ARG
1	A	157	GLN
1	A	251	GLN
1	A	253	LYS
1	A	275	ARG
1	A	346	ASP
1	A	348	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	77	GLN
1	A	161	GLN
1	A	251	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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, 95^{th} 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	343/353 (97%)	0.93	44 (12%) 9 9	24, 44, 71, 80	2 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	LEU	7.1
1	A	3	ALA	6.6
1	A	348	HIS	4.6
1	A	19	ASP	4.6
1	A	349	HIS	4.4
1	A	257	ILE	4.2
1	A	347	ASN	4.1
1	A	4	HIS	4.1
1	A	18	PRO	4.1
1	A	175	LEU	3.9
1	A	147	MET	3.7
1	A	15	LEU	3.7
1	A	350	HIS	3.5
1	A	17	HIS	3.4
1	A	14	ALA	3.4
1	A	5	GLY	3.4
1	A	301	THR	3.1
1	A	302	THR	3.1
1	A	174	THR	3.0
1	A	271	ARG	2.8
1	A	22	THR	2.6
1	A	24	ILE	2.6
1	A	110	LEU	2.5
1	A	266	ARG	2.5
1	A	249	LEU	2.4
1	A	345	MET	2.4
1	A	256	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	176	THR	2.4
1	A	23	ASN	2.4
1	A	189	ALA	2.4
1	A	93	LEU	2.3
1	A	92	GLY	2.3
1	A	352[A]	HIS	2.3
1	A	346	ASP	2.3
1	A	21	ASP	2.3
1	A	25	GLN	2.2
1	A	26	THR	2.2
1	A	270	VAL	2.1
1	A	63	GLU	2.1
1	A	91	PRO	2.1
1	A	201	LYS	2.1
1	A	273	LEU	2.1
1	A	20	GLY	2.1
1	A	190	HIS	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 monosaccharides 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, 95^{th} 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	ZN	A	401	1/1	0.98	0.05	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.