



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2017 – 08:42 AM EST

PDB ID : 5CMJ
Title : GTA mutant with mercury - E303Q
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Deposited on : 2015-07-16
Resolution : 1.73 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

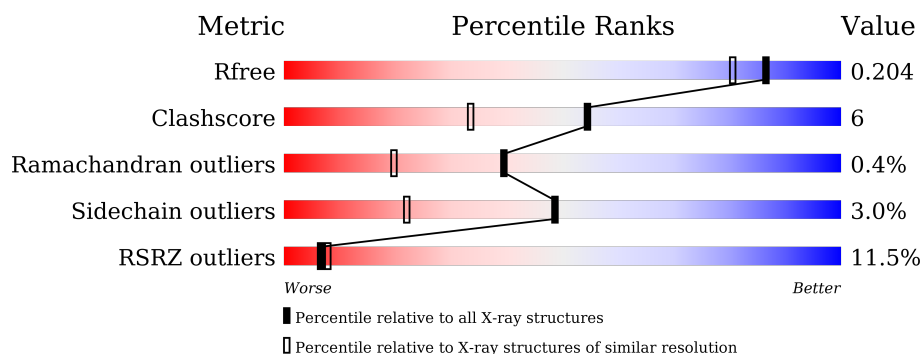
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	91344	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	294	<div> <div>11%</div> <div>80%</div> <div>11%</div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2383 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 Histo-blood group ABO system transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	1	0
			2200	1433	375	382	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	PHE	-	expression tag	UNP P16442
A	63	MET	-	expression tag	UNP P16442
A	303	GLN	GLU	engineered mutation	UNP P16442
A	355	GLU	-	expression tag	UNP P16442

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

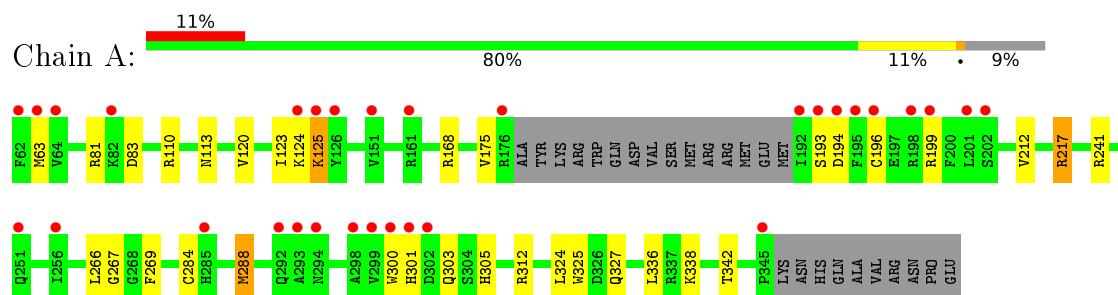
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Hg	0	0
			5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		

i

- Molecule 1: Histo-blood group ABO system transferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	52.70 Å 148.91 Å 79.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.54 – 1.73 19.90 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.2 (74.54-1.73) 99.3 (19.90-1.73)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 1.73 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.173 , 0.200 0.184 , 0.204	Depositor DCC
R_{free} test set	1662 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2383	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: HG

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	0.81	0/2263	0.95	7/3077 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	MET	CG-SD-CE	11.82	119.11	100.20
1	A	241	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	241	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	168	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	83	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	81	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	217	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2200	0	2175	28	0
2	A	5	0	0	0	0
3	A	178	0	0	6	1
All	All	2383	0	2175	28	1

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 6.

All (28) 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:284:CYS:HB3	3:A:666:HOH:O	1.28	1.28
1:A:266:LEU:CD1	1:A:303[B]:GLN:HE22	1.76	0.99
1:A:284:CYS:O	1:A:288:MET:HG3	1.68	0.93
1:A:266:LEU:HD13	1:A:303[B]:GLN:HE22	1.47	0.78
1:A:266:LEU:HD12	1:A:303[B]:GLN:HE22	1.50	0.76
1:A:284:CYS:O	1:A:288:MET:CG	2.36	0.72
1:A:266:LEU:HD12	1:A:303[B]:GLN:NE2	2.05	0.71
1:A:266:LEU:CD1	1:A:303[B]:GLN:NE2	2.53	0.71
1:A:123:ILE:HG22	1:A:124:LYS:HG2	1.78	0.66
1:A:120:VAL:HG22	1:A:212:VAL:HB	1.87	0.56
1:A:338:LYS:HE3	3:A:522:HOH:O	2.08	0.53
1:A:63:MET:HA	1:A:63:MET:HE3	1.93	0.50
1:A:125:LYS:H	1:A:125:LYS:HD2	1.78	0.48
1:A:305:HIS:HD2	3:A:669:HOH:O	1.97	0.47
1:A:300:TRP:O	1:A:303[B]:GLN:HB3	2.15	0.47
1:A:325:TRP:CZ3	1:A:336:LEU:HD11	2.50	0.47
1:A:288:MET:HE1	3:A:666:HOH:O	2.13	0.47
1:A:267:GLY:N	1:A:303[A]:GLN:OE1	2.47	0.46
1:A:217:ARG:HH12	1:A:327:GLN:HE22	1.66	0.44
1:A:217:ARG:HD3	1:A:342:THR:OG1	2.18	0.43
1:A:325:TRP:CE3	1:A:336:LEU:HD11	2.53	0.43
1:A:288:MET:CE	3:A:666:HOH:O	2.67	0.42
1:A:217:ARG:HH22	1:A:327:GLN:HE21	1.67	0.42
1:A:312:ARG:HA	1:A:312:ARG:HD3	1.84	0.41
1:A:175:VAL:HG12	1:A:193:SER:HB3	2.02	0.41
1:A:267:GLY:HA3	1:A:303[A]:GLN:OE1	2.20	0.41
1:A:305:HIS:HE1	3:A:510:HOH:O	2.03	0.40
1:A:110:ARG:HA	1:A:110:ARG:HD2	1.98	0.40

All (1) 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)
3:A:611:HOH:O	3:A:673:HOH:O[3_554]	2.16	0.04

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	266/294 (90%)	259 (97%)	6 (2%)	1 (0%)	39	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	HIS

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	238/262 (91%)	231 (97%)	7 (3%)	50	23

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	125	LYS
1	A	194	ASP
1	A	196	CYS
1	A	199	ARG
1	A	269	PHE
1	A	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	155	GLN
1	A	251	GLN
1	A	286	GLN
1	A	294	ASN
1	A	305	HIS
1	A	327	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are 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, 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	269/294 (91%)	0.56	31 (11%) 6 8	17, 27, 53, 65	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ALA	6.8
1	A	300	TRP	6.5
1	A	299	VAL	5.9
1	A	196	CYS	5.4
1	A	192	ILE	5.4
1	A	195	PHE	5.2
1	A	176	ARG	4.7
1	A	193	SER	4.1
1	A	345	PRO	3.7
1	A	63	MET	3.5
1	A	301	HIS	3.4
1	A	201	LEU	3.3
1	A	293	ALA	3.1
1	A	64	VAL	3.1
1	A	256	ILE	3.0
1	A	125	LYS	3.0
1	A	202	SER	3.0
1	A	161	ARG	3.0
1	A	302	ASP	3.0
1	A	199	ARG	2.7
1	A	194	ASP	2.7
1	A	126	TYR	2.6
1	A	292	GLN	2.6
1	A	285	HIS	2.6
1	A	251	GLN	2.3
1	A	198	ARG	2.2
1	A	62	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	151	VAL	2.1
1	A	82	LYS	2.1
1	A	294	ASN	2.1
1	A	124	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	HG	A	401	1/1	0.97	0.04	-1.83	35,35,35,35	1
2	HG	A	404	1/1	1.00	0.04	-2.38	30,30,30,30	1
2	HG	A	405	1/1	0.90	0.07	-	61,61,61,61	1
2	HG	A	403	1/1	0.97	0.04	-	31,31,31,31	0
2	HG	A	402	1/1	0.97	0.04	-	34,34,34,34	1

6.5 Other polymers [i](#)

There are no such residues in this entry.