



Full wwPDB X-ray Structure Validation Report

Sep 25, 2014 – 07:42 PM EDT

PDB ID : 4U4J
Title : Crystal structure of Salmonella alpha-2-macroglobulinmutant Y1175G
Authors : Wong, S.G.; Dessen, A.
Deposited on : 2014-07-23
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

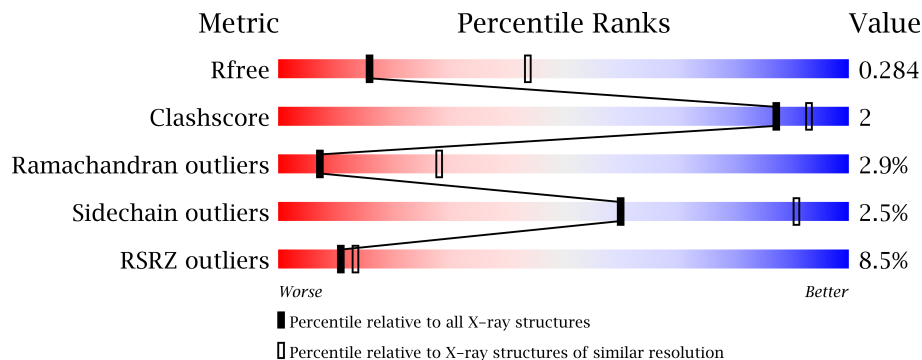
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1647	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23627 atoms, of which 11754 are hydrogens and 0 are deuterium.

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 Putative inner membrane lipoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1538	23627	7480	11754	2091	2279	23	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q8ZN46
A	-1	GLY	-	expression tag	UNP Q8ZN46
A	0	SER	-	expression tag	UNP Q8ZN46
A	1	SER	-	expression tag	UNP Q8ZN46
A	2	HIS	-	expression tag	UNP Q8ZN46
A	3	HIS	-	expression tag	UNP Q8ZN46
A	4	HIS	-	expression tag	UNP Q8ZN46
A	5	HIS	-	expression tag	UNP Q8ZN46
A	6	HIS	-	expression tag	UNP Q8ZN46
A	7	HIS	-	expression tag	UNP Q8ZN46
A	8	SER	-	expression tag	UNP Q8ZN46
A	9	SER	-	expression tag	UNP Q8ZN46
A	10	GLY	-	expression tag	UNP Q8ZN46
A	11	LEU	-	expression tag	UNP Q8ZN46
A	12	VAL	-	expression tag	UNP Q8ZN46
A	13	PRO	-	expression tag	UNP Q8ZN46
A	14	ARG	-	expression tag	UNP Q8ZN46
A	15	GLY	-	expression tag	UNP Q8ZN46
A	16	SER	-	expression tag	UNP Q8ZN46
A	17	HIS	-	expression tag	UNP Q8ZN46
A	18	MET	-	expression tag	UNP Q8ZN46
A	98	ALA	LYS	engineered mutation	UNP Q8ZN46
A	99	ALA	LYS	engineered mutation	UNP Q8ZN46
A	1175	GLY	TYR	engineered mutation	UNP Q8ZN46

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	254.24Å 82.16Å 98.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.99 – 2.90 58.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.99-2.90) 99.9 (58.99-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.244 , 0.284 0.244 , 0.284	Depositor DCC
R_{free} test set	2338 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 46790 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23627	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.23	0/12113	0.43	1/16503 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	316	LEU	CA-CB-CG	7.46	132.47	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	LYS	Peptide
1	A	808	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11873	11754	18	59	0
All	All	11873	11754	18	59	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:87:GLN:N	1:A:87:GLN:OE1	2.19	0.76
1:A:1366:GLU:O	1:A:1368:GLN:N	2.19	0.75
1:A:1368:GLN:OE1	1:A:1369:TRP:N	2.30	0.65
1:A:463:LEU:O	1:A:465:ARG:NH1	2.34	0.60
1:A:317:ASN:O	1:A:319:LYS:N	2.33	0.60
1:A:1091:GLN:NE2	1:A:1110:GLN:OE1	2.36	0.58
1:A:1181:GLU:OE1	1:A:1416:THR:OG1	2.22	0.57
1:A:337:GLU:N	1:A:337:GLU:OE1	2.37	0.57
1:A:1294:GLN:OE1	1:A:1328:GLN:NE2	2.38	0.57
1:A:829:ARG:O	1:A:831:ALA:N	2.38	0.57
1:A:84:ASP:HB2	1:A:136:LYS:HE3	1.88	0.55
1:A:1566:GLU:N	1:A:1566:GLU:OE1	2.40	0.55
1:A:922:ASP:OD2	1:A:924:TYR:N	2.40	0.54
1:A:349:LYS:O	1:A:351:GLU:N	2.41	0.53
1:A:663:ARG:NH2	1:A:710:TRP:O	2.40	0.53
1:A:784:SER:O	1:A:786:GLY:N	2.41	0.53
1:A:555:LEU:O	1:A:557:LYS:N	2.42	0.53
1:A:1105:ASP:OD1	1:A:1106:ALA:N	2.42	0.53
1:A:1181:GLU:O	1:A:1184:THR:N	2.42	0.52
1:A:1583:GLU:OE2	1:A:1585:ARG:NE	2.42	0.52
1:A:137:ALA:O	1:A:140:ASN:N	2.43	0.52
1:A:1241:GLU:OE2	1:A:1278:TYR:OH	2.19	0.51
1:A:758:ASN:ND2	1:A:758:ASN:O	2.42	0.51
1:A:555:LEU:C	1:A:555:LEU:HD23	2.31	0.51
1:A:1289:TYR:OH	1:A:1578:ASP:OD2	2.22	0.49
1:A:320:GLY:O	1:A:321:GLN:NE2	2.45	0.49
1:A:1227:ARG:NH1	1:A:1241:GLU:OE1	2.46	0.49
1:A:1347:ASP:OD2	1:A:1350:ARG:NH1	2.45	0.49
1:A:983:ASP:OD1	1:A:1109:LYS:NZ	2.47	0.47
1:A:1494:ASN:O	1:A:1496:LEU:N	2.47	0.47
1:A:204:SER:OG	1:A:319:LYS:O	2.27	0.46
1:A:103:VAL:HG22	1:A:104:ASP:H	1.80	0.46
1:A:1251:ASP:OD1	1:A:1310:ARG:NH1	2.50	0.45
1:A:486:GLN:O	1:A:488:THR:N	2.50	0.45
1:A:557:LYS:HG2	1:A:558:GLY:H	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:LYS:HG3	1:A:255:GLN:HB2	1.98	0.45
1:A:1610:VAL:HG23	1:A:1611:THR:N	2.32	0.44
1:A:134:ALA:O	1:A:136:LYS:N	2.51	0.44
1:A:136:LYS:HE2	1:A:138:LEU:HA	2.00	0.44
1:A:251:ILE:HG23	1:A:253:PRO:HD2	2.00	0.43
1:A:84:ASP:HB2	1:A:136:LYS:HD3	2.01	0.43
1:A:134:ALA:C	1:A:136:LYS:H	2.21	0.43
1:A:1411:GLN:O	1:A:1413:TRP:N	2.52	0.43
1:A:1364:GLN:OE1	1:A:1364:GLN:N	2.49	0.42
1:A:604:ASP:OD1	1:A:604:ASP:N	2.52	0.42
1:A:881:PRO:O	1:A:882:LYS:HB2	2.19	0.42
1:A:1333:LEU:HB3	1:A:1334:PRO:HD3	2.02	0.42
1:A:136:LYS:HE2	1:A:137:ALA:C	2.40	0.42
1:A:136:LYS:HG3	1:A:137:ALA:N	2.35	0.42
1:A:957:VAL:O	1:A:958:ASN:CB	2.68	0.42
1:A:136:LYS:HZ1	1:A:137:ALA:CA	2.33	0.41
1:A:193:ARG:NH2	1:A:256:GLN:OE1	2.53	0.41
1:A:420:LYS:HB2	1:A:421:PRO:HD2	2.02	0.41
1:A:1094:ILE:HB	1:A:1107:GLN:HB2	2.01	0.41
1:A:1288:ARG:NH2	1:A:1289:TYR:OH	2.54	0.41
1:A:1242:GLU:OE1	1:A:1373:TYR:OH	2.31	0.41
1:A:810:TRP:CD1	1:A:810:TRP:N	2.89	0.41
1:A:1368:GLN:N	1:A:1368:GLN:CD	2.73	0.41
1:A:477:GLU:O	1:A:479:MET:N	2.54	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	1526/1647 (93%)	1375 (90%)	106 (7%)	45 (3%)	7	28

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	GLN
1	A	556	ASP
1	A	587	SER
1	A	651	LYS
1	A	758	ASN
1	A	882	LYS
1	A	957	VAL
1	A	1098	ASN
1	A	1367	ARG
1	A	1368	GLN
1	A	1370	ILE
1	A	134	ALA
1	A	137	ALA
1	A	142	THR
1	A	231	ARG
1	A	829	ARG
1	A	830	SER
1	A	958	ASN
1	A	983	ASP
1	A	1347	ASP
1	A	1635	ALA
1	A	135	VAL
1	A	487	LYS
1	A	588	GLY
1	A	876	LYS
1	A	1369	TRP
1	A	1411	GLN
1	A	90	SER
1	A	307	ALA
1	A	319	LYS
1	A	350	GLU
1	A	832	THR
1	A	1104	LEU
1	A	174	ALA
1	A	253	PRO
1	A	831	ALA
1	A	881	PRO
1	A	984	PHE
1	A	1178	GLY
1	A	1206	ASP
1	A	1394	PRO
1	A	929	GLU
1	A	1161	PRO

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Mol	Chain	Res	Type
1	A	103	VAL
1	A	824	PRO

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	1259/1347 (94%)	1227 (98%)	32 (2%)	60	91

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	53	GLN
1	A	70	ASP
1	A	87	GLN
1	A	91	ARG
1	A	136	LYS
1	A	142	THR
1	A	154	ARG
1	A	227	VAL
1	A	248	LEU
1	A	256	GLN
1	A	311	ILE
1	A	319	LYS
1	A	331	GLN
1	A	334	VAL
1	A	350	GLU
1	A	439	ARG
1	A	555	LEU
1	A	586	GLU
1	A	663	ARG
1	A	753	LYS
1	A	766	LYS
1	A	826	ASP
1	A	876	LYS
1	A	926	GLN
1	A	1179	CYS

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Mol	Chain	Res	Type
1	A	1303	TYR
1	A	1321	GLU
1	A	1367	ARG
1	A	1368	GLN
1	A	1378	ARG
1	A	1400	LEU

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

Mol	Chain	Res	Type
1	A	758	ASN
1	A	956	HIS
1	A	1091	GLN
1	A	1328	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	1538/1647 (93%)	0.67	130 (8%)	11 13	51, 90, 137, 213	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	928	ILE	8.8
1	A	85	PRO	7.2
1	A	588	GLY	6.6
1	A	57	LYS	6.1
1	A	929	GLU	6.0
1	A	930	GLY	6.0
1	A	70	ASP	5.9
1	A	1176	PRO	5.8
1	A	559	GLY	5.8
1	A	191	PHE	5.7
1	A	83	LEU	5.2
1	A	649	GLY	4.9
1	A	314	VAL	4.6
1	A	650	GLU	4.5
1	A	194	VAL	4.5
1	A	1364	GLN	4.5
1	A	75	LEU	4.4
1	A	87	GLN	4.2
1	A	589	GLY	4.1
1	A	937	LEU	4.1
1	A	172	LYS	3.9
1	A	519	LEU	3.9
1	A	551	VAL	3.8
1	A	924	TYR	3.8
1	A	1567	VAL	3.8
1	A	1570	LEU	3.7
1	A	758	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1178	GLY	3.7
1	A	1175	GLY	3.6
1	A	311	ILE	3.6
1	A	1013	VAL	3.6
1	A	228	TYR	3.5
1	A	223	MET	3.5
1	A	118	LEU	3.4
1	A	1101	GLY	3.4
1	A	817	LEU	3.4
1	A	346	LEU	3.4
1	A	1546	LEU	3.3
1	A	927	VAL	3.3
1	A	325	GLN	3.2
1	A	767	LEU	3.2
1	A	851	LEU	3.2
1	A	810	TRP	3.2
1	A	108	GLU	3.2
1	A	768	HIS	3.2
1	A	622	ARG	3.1
1	A	548	LEU	3.1
1	A	808	LYS	3.1
1	A	312	GLU	3.1
1	A	761	PRO	3.0
1	A	1566	GLU	2.9
1	A	474	PHE	2.9
1	A	225	ASP	2.9
1	A	988	LEU	2.9
1	A	1522	LEU	2.9
1	A	1367	ARG	2.9
1	A	515	LEU	2.9
1	A	765	MET	2.9
1	A	1509	ARG	2.9
1	A	295	LEU	2.8
1	A	192	PHE	2.8
1	A	234	LEU	2.8
1	A	809	THR	2.8
1	A	113	LEU	2.8
1	A	262	ALA	2.8
1	A	89	PHE	2.7
1	A	931	GLN	2.7
1	A	674	GLU	2.7
1	A	985	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	587	SER	2.6
1	A	517	GLY	2.6
1	A	358	LEU	2.6
1	A	116	LEU	2.6
1	A	248	LEU	2.6
1	A	823	ARG	2.6
1	A	437	LEU	2.5
1	A	202	PHE	2.5
1	A	254	LEU	2.5
1	A	735	TRP	2.5
1	A	616	LYS	2.5
1	A	1012	PRO	2.5
1	A	107	TRP	2.5
1	A	498	PHE	2.4
1	A	1604	VAL	2.4
1	A	638	ALA	2.4
1	A	349	LYS	2.4
1	A	344	LEU	2.4
1	A	802	LEU	2.4
1	A	766	LYS	2.3
1	A	759	TYR	2.3
1	A	1177	TYR	2.3
1	A	1601	VAL	2.3
1	A	111	PRO	2.3
1	A	189	VAL	2.3
1	A	127	LEU	2.3
1	A	596	VAL	2.3
1	A	173	ILE	2.3
1	A	365	LEU	2.3
1	A	297	ILE	2.2
1	A	754	LEU	2.2
1	A	1582	MET	2.2
1	A	870	ARG	2.2
1	A	1047	ILE	2.2
1	A	560	ARG	2.2
1	A	477	GLU	2.2
1	A	77	LEU	2.2
1	A	355	LEU	2.2
1	A	105	GLY	2.2
1	A	1630	TRP	2.1
1	A	1033	LEU	2.1
1	A	1512	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	79	PHE	2.1
1	A	895	VAL	2.1
1	A	82	PRO	2.1
1	A	261	VAL	2.1
1	A	264	MET	2.1
1	A	493	ALA	2.1
1	A	1536	ALA	2.1
1	A	1179	CYS	2.1
1	A	484	THR	2.1
1	A	174	ALA	2.1
1	A	109	LEU	2.0
1	A	1286	LEU	2.0
1	A	1315	PRO	2.0
1	A	117	ARG	2.0
1	A	84	ASP	2.0
1	A	807	ASP	2.0
1	A	1455	ARG	2.0
1	A	779	ALA	2.0
1	A	400	LEU	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.