



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 08:54 PM EDT

PDB ID : 6AW3
Title : Crystal structure of the HopQ-CEACAM3 L44Q complex
Authors : Bonsor, D.A.; Sundberg, E.J.
Deposited on : 2017-09-05
Resolution : 2.66 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

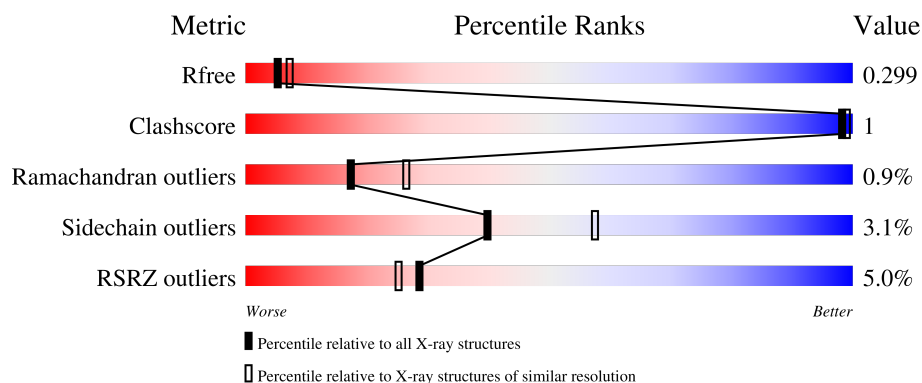
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	B	439	<div> <div>4%</div> <div>77%</div> <div>20%</div> </div>
2	A	109	<div> <div>4%</div> <div>94%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3375 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 HopQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	351	Total	C	N	O	S	0	0	0
			2524	1539	442	532	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	MET	-	initiating methionine	UNP H6A3H4
B	5	GLY	-	expression tag	UNP H6A3H4
B	6	SER	-	expression tag	UNP H6A3H4
B	7	SER	-	expression tag	UNP H6A3H4
B	8	HIS	-	expression tag	UNP H6A3H4
B	9	HIS	-	expression tag	UNP H6A3H4
B	10	HIS	-	expression tag	UNP H6A3H4
B	11	HIS	-	expression tag	UNP H6A3H4
B	12	HIS	-	expression tag	UNP H6A3H4
B	13	HIS	-	expression tag	UNP H6A3H4
B	14	SER	-	expression tag	UNP H6A3H4
B	15	GLN	-	expression tag	UNP H6A3H4
B	16	ASP	-	expression tag	UNP H6A3H4
B	17	PRO	-	expression tag	UNP H6A3H4

- Molecule 2 is a protein called Carcinoembryonic antigen-related cell adhesion molecule 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	108	Total	C	N	O	S	0	0	0
			843	538	139	165	1			

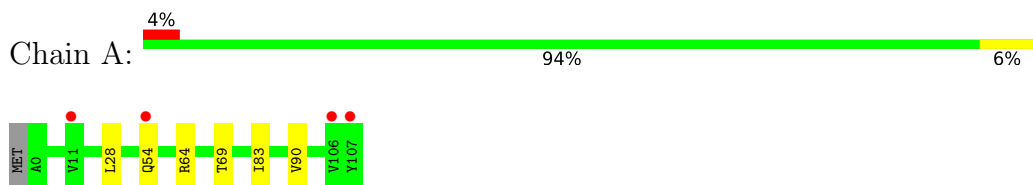
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P40198
A	44	GLN	LEU	engineered mutation	UNP P40198

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	O 4	0	0
3	A	4	Total 4	O 4	0	0

- Molecule 1: HopQ



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	38.83Å 102.59Å 112.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.59 – 2.66 37.93 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.2 (102.59-2.66) 99.3 (37.93-2.66)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.242 , 0.297 0.243 , 0.299	Depositor DCC
R_{free} test set	661 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3375	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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	B	0.37	0/2554	0.54	0/3475
2	A	0.41	0/860	0.60	0/1169
All	All	0.38	0/3414	0.55	0/4644

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	B	2524	0	2356	3	0
2	A	843	0	829	1	0
3	A	4	0	0	0	2
3	B	4	0	0	0	0
All	All	3375	0	3185	4	2

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 1.

All (4) 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:172:ILE:HG23	1:B:216:THR:HG21	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:28:LEU:HD22	2:A:90:VAL:CG1	2.46	0.46
1:B:268:ASN:HB3	1:B:271:GLU:HB2	2.03	0.41
1:B:262:THR:O	1:B:263:ALA:CB	2.69	0.40

All (2) 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:203:HOH:O	3:A:203:HOH:O[4_555]	1.34	0.86
3:A:202:HOH:O	3:A:202:HOH:O[3_454]	2.01	0.19

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	B	341/439 (78%)	320 (94%)	17 (5%)	4 (1%)	13	19
2	A	106/109 (97%)	100 (94%)	6 (6%)	0	100	100
All	All	447/548 (82%)	420 (94%)	23 (5%)	4 (1%)	17	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	379	ASN
1	B	263	ALA
1	B	264	GLY
1	B	265	GLY

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	B	265/368 (72%)	258 (97%)	7 (3%)	46	64
2	A	91/92 (99%)	87 (96%)	4 (4%)	28	43
All	All	356/460 (77%)	345 (97%)	11 (3%)	40	57

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	221	GLN
1	B	271	GLU
1	B	296	GLN
1	B	319	LEU
1	B	363	ASP
1	B	406	THR
2	A	54	GLN
2	A	64	ARG
2	A	69	THR
2	A	83	ILE

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

Mol	Chain	Res	Type
1	B	137	ASN
1	B	221	GLN
1	B	292	GLN
1	B	410	ASN
1	B	413	GLN
2	A	53	GLN
2	A	89	GLN

5.3.3 RNA ⓘ

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	351/439 (79%)	0.14	19 (5%) 25 23	38, 51, 94, 107	0
2	A	108/109 (99%)	0.13	4 (3%) 41 38	43, 53, 84, 93	0
All	All	459/548 (83%)	0.14	23 (5%) 28 25	38, 51, 93, 107	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	THR	6.6
1	B	412	ALA	4.2
1	B	323	ALA	4.0
1	B	309	HIS	3.6
1	B	319	LEU	3.6
2	A	107	TYR	3.2
1	B	316	PRO	3.2
1	B	370	THR	3.1
1	B	324	GLN	3.1
1	B	53	ALA	3.1
1	B	377	GLN	3.0
1	B	126	ASN	2.8
1	B	246	SER	2.6
1	B	414	ASN	2.6
2	A	11	VAL	2.5
2	A	54	GLN	2.5
1	B	416	ALA	2.4
1	B	407	PRO	2.3
2	A	106	VAL	2.3
1	B	54	GLN	2.1
1	B	244	LYS	2.1
1	B	122	ASP	2.1
1	B	262	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.