



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 05:49 pm BST

PDB ID : 3FRT
Title : The structure of human CHMP3 (residues 8 - 222).
Authors : Schubert, H.L.; McCullough, J.; Hill, C.P.; Sundquist, W.I.
Deposited on : 2009-01-08
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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	:	2.11
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)	:	2.11

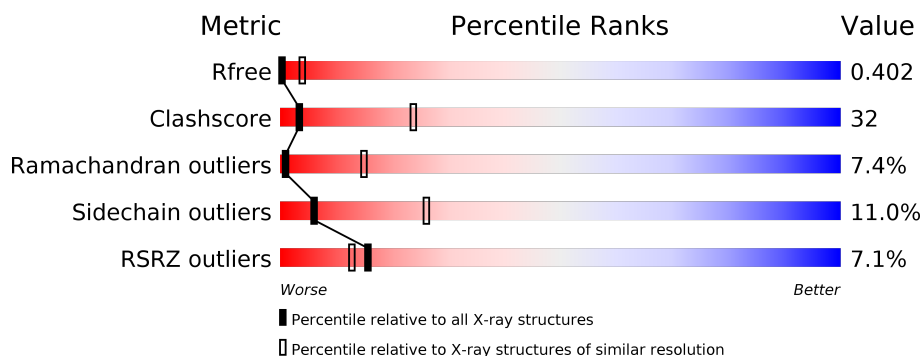
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 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	218	<div> <div>4%</div> <div> <div>29%</div> <div>29%</div> <div>5%</div> <div>35%</div> </div> </div>
1	B	218	<div> <div>5%</div> <div> <div>32%</div> <div>28%</div> <div>35%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2270 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 Charged multivesicular body protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1133	709	203	208	13			
1	B	142	Total	C	N	O	S	0	0	0
			1137	711	204	209	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	EXPRESSION TAG	UNP Q9Y3E7
A	6	HIS	-	EXPRESSION TAG	UNP Q9Y3E7
A	7	MET	-	EXPRESSION TAG	UNP Q9Y3E7
B	5	GLY	-	EXPRESSION TAG	UNP Q9Y3E7
B	6	HIS	-	EXPRESSION TAG	UNP Q9Y3E7
B	7	MET	-	EXPRESSION TAG	UNP Q9Y3E7

These plots are drawn for all protein, RNA and DNA 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.

Chain A:

Sequence logo for Chain A. The y-axis represents information content in bits. The x-axis shows positions 1 to 100. A color key at the bottom identifies amino acids: GLU (blue), ALA (orange), MET (green), THR (red), SER (purple), GLN (brown), GLY (pink), ARG (grey), LEU (light blue), and ASP (dark blue).

Position	Amino Acid	Information Content (bits)
1	GLU	0.5
2	ALA	0.5
3	MET	0.5
4	MET	0.5
5	GLN	0.5
6	SER	0.5
7	ARG	0.5
8	LEU	0.5
9	ALA	0.5
10	ALA	0.5
11	THR	0.5
12	LEU	0.5
13	ARG	0.5
14	SER	0.5
15	GLU	0.5
16	ASP	0.5
17	ASP	0.5
18	GLN	0.5
19	GLY	0.5
20	GLY	0.5
21	THR	0.5
22	THR	0.5
23	THR	0.5
24	THR	0.5
25	THR	0.5
26	THR	0.5
27	THR	0.5
28	THR	0.5
29	THR	0.5
30	THR	0.5
31	THR	0.5
32	THR	0.5
33	THR	0.5
34	THR	0.5
35	THR	0.5
36	THR	0.5
37	THR	0.5
38	THR	0.5
39	THR	0.5
40	THR	0.5
41	THR	0.5
42	THR	0.5
43	THR	0.5
44	THR	0.5
45	THR	0.5
46	THR	0.5
47	THR	0.5
48	THR	0.5
49	THR	0.5
50	THR	0.5
51	THR	0.5
52	THR	0.5
53	THR	0.5
54	THR	0.5
55	THR	0.5
56	THR	0.5
57	THR	0.5
58	THR	0.5
59	THR	0.5
60	THR	0.5
61	THR	0.5
62	THR	0.5
63	THR	0.5
64	THR	0.5
65	THR	0.5
66	THR	0.5
67	THR	0.5
68	THR	0.5
69	THR	0.5
70	THR	0.5
71	THR	0.5
72	THR	0.5
73	THR	0.5
74	THR	0.5
75	THR	0.5
76	THR	0.5
77	THR	0.5
78	THR	0.5
79	THR	0.5
80	THR	0.5
81	THR	0.5
82	THR	0.5
83	THR	0.5
84	THR	0.5
85	THR	0.5
86	THR	0.5
87	THR	0.5
88	THR	0.5
89	THR	0.5
90	THR	0.5
91	THR	0.5
92	THR	0.5
93	THR	0.5
94	THR	0.5
95	THR	0.5
96	THR	0.5
97	THR	0.5
98	THR	0.5
99	THR	0.5
100	THR	0.5

Chain B:

5% 32% 28% 35%

ALA THR LEU ARG SER E158 E159 E160 A161 E162 M163 E164 I165 D166 R167 L168 L169 F170 E171 I172 THR ALA GLY ALA LEU LEU GLY LYS ALA PRO PRO SER LYS VAL THR ASP ALA LEU PRO PRO PRO GLY ALA MET ALA ALA SER LEU GLU MET GLN SER LEU

M91 Q94 W97 L98 ARG VAL G102 S103 Q104 Q105 K106 S107 T108 E109 V110 M111 M114 L117 V118 K119 P120 I121 E122 I123 Q124 A125 T126 M127 L130 S131 M134 M135 K136 I139 I140 GLU ASP MET LEU GLU ASP THR PHE GLU LEU SER MET ASP ASP GLN GLU M97

GLY HIS MET GLN GLU LYS PRO P12 K13 E14 E18 W19 S20 L21 K22 M27 R28 V29 V30 D31 R32 Q33 V44 V48 A51 K54 G55 Q56 K57 D58 V59 C60 I61 V62 L63 A64 K65 E66 M67 I68 R69 V74 L77 S80 M84 N85 L88 M89 C90

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.47Å 131.51Å 48.51Å 90.00° 108.06° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 37.76 – 3.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-4.00) 78.5 (37.76-3.99)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 3.99Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.383 , 0.436 0.402 , 0.402	Depositor DCC
R_{free} test set	126 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	135.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 10.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2270	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.84% 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](#)

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	0.74	3/1137 (0.3%)	0.68	0/1504
1	B	0.74	1/1141 (0.1%)	0.68	0/1509
All	All	0.74	4/2278 (0.2%)	0.68	0/3013

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	MET	CG-SD	5.64	1.95	1.81
1	B	157	MET	CG-SD	5.61	1.95	1.81
1	A	157	MET	CG-SD	5.60	1.95	1.81
1	A	134	MET	CG-SD	5.23	1.94	1.81

There are no bond angle outliers.

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	1133	0	1222	87	0
1	B	1137	0	1225	81	0
All	All	2270	0	2447	153	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 32.

The worst 5 of 153 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:59:VAL:HG22	1:B:62:VAL:CG1	1.83	1.08
1:A:33:GLN:HE22	1:A:122:GLU:HG2	1.16	1.07
1:B:33:GLN:HE22	1:B:122:GLU:HG2	1.16	1.06
1:A:33:GLN:NE2	1:A:122:GLU:HG2	1.74	1.03
1:B:33:GLN:NE2	1:B:122:GLU:HG2	1.74	1.02

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	135/218 (62%)	112 (83%)	13 (10%)	10 (7%)	1	15
1	B	136/218 (62%)	113 (83%)	13 (10%)	10 (7%)	1	15
All	All	271/436 (62%)	225 (83%)	26 (10%)	20 (7%)	1	15

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	SER
1	A	136	LYS
1	B	107	SER
1	B	136	LYS
1	A	118	VAL

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	127/188 (68%)	113 (89%)	14 (11%)	6	26
1	B	127/188 (68%)	113 (89%)	14 (11%)	6	26
All	All	254/376 (68%)	226 (89%)	28 (11%)	6	26

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	ASP
1	B	32	ARG
1	B	159	GLU
1	A	168	ILE
1	B	14	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	94	GLN

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 carbohydrates 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	A	141/218 (64%)	0.15	9 (6%) 19 15	34, 58, 81, 89	0
1	B	142/218 (65%)	0.20	11 (7%) 13 11	34, 59, 82, 90	0
All	All	283/436 (64%)	0.17	20 (7%) 16 13	34, 59, 82, 90	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	ILE	4.0
1	A	122	GLU	3.8
1	A	172	ILE	3.7
1	A	12	PRO	3.6
1	A	120	ILE	3.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.