

# wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 01:03 am GMT

PDB ID : 5FU6

Title: NOT module of the human CCR4-NOT complex (Crystallization mutant)
Authors: Raisch, T.; Bhandari, D.; Sabath, K.; Helms, S.; Valkov, E.; Weichenrieder,

O.; Izaurralde, E.

Deposited on : 2016-01-21

Resolution : 2.90 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 (i) 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 (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$ 

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

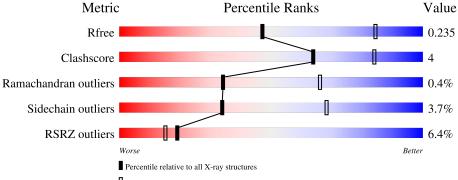
Validation Pipeline (wwPDB-VP) : 2.36

# 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 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.



Percentile relative to X-ray structures of similar resolution

Metric	Whole archive	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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	
-			5%	
1	A	535	79%	16% • •
			5%	
1	D	535	80%	16% •
			17%	
2	В	197	86%	11% •
			8%	
2	$\mathbf{E}$	197	85%	11% • •
			4%	
3	С	148	86%	14%

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Mol	Chain	Length	Quality of chain	
3	F	148	93%	7%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14109 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 CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	515	Total 4186	C 2709	N 718	O 735	S 24	0	0	0
1	D	516	Total	C	N	O	S	0	0	0
1	D	310	4193	2712	719	738	24	0		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1827	GLY	=	expression tag	UNP A5YKK6
A	1828	PRO	-	expression tag	UNP A5YKK6
A	1829	HIS	-	expression tag	UNP A5YKK6
A	1830	MET	-	expression tag	UNP A5YKK6
A	1831	LEU	-	expression tag	UNP A5YKK6
A	1832	GLU	-	expression tag	UNP A5YKK6
A	2344	GLU	HIS	engineered mutation	UNP A5YKK6
A	2345	GLU	CYS	engineered mutation	UNP A5YKK6
A	2346	GLU	ALA	engineered mutation	UNP A5YKK6
D	1827	GLY	-	expression tag	UNP A5YKK6
D	1828	PRO	-	expression tag	UNP A5YKK6
D	1829	HIS	-	expression tag	UNP A5YKK6
D	1830	MET	-	expression tag	UNP A5YKK6
D	1831	LEU	-	expression tag	UNP A5YKK6
D	1832	GLU	-	expression tag	UNP A5YKK6
D	2344	GLU	HIS	engineered mutation	UNP A5YKK6
D	2345	GLU	CYS	engineered mutation	UNP A5YKK6
D	2346	GLU	ALA	engineered mutation	UNP A5YKK6

• Molecule 2 is a protein called CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	D	192	Total	С	N	О	S	0	0	0
	D	192	1578	1019	264	288	7	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Е	191	Total 1566	C 1010	N 263	O 285	S 8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	344	GLY	-	expression tag	UNP Q9NZN8
В	345	PRO	-	expression tag	UNP Q9NZN8
В	346	HIS	-	expression tag	UNP Q9NZN8
В	347	MET	-	expression tag	UNP Q9NZN8
В	348	LEU	-	expression tag	UNP Q9NZN8
В	349	GLU	-	expression tag	UNP Q9NZN8
E	344	GLY	-	expression tag	UNP Q9NZN8
E	345	PRO	-	expression tag	UNP Q9NZN8
E	346	HIS	-	expression tag	UNP Q9NZN8
E	347	MET	-	expression tag	UNP Q9NZN8
E	348	LEU	_	expression tag	UNP Q9NZN8
E	349	GLU	_	expression tag	UNP Q9NZN8

• Molecule 3 is a protein called CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	148	Total 1293		N 216	O 230	S 7	0	0	0
3	F	148	Total 1293			O 230	S 7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

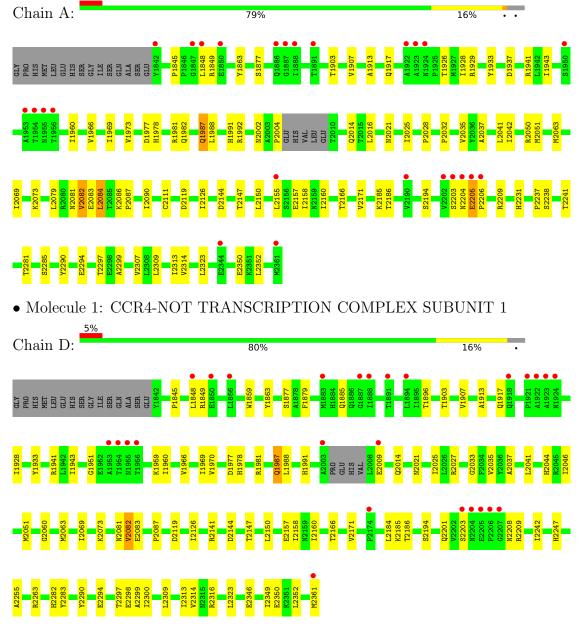
Chain	Residue	Modelled	Actual	Comment	Reference
С	601	GLY	-	expression tag	UNP O75175
С	602	PRO	-	expression tag	UNP O75175
С	603	HIS	-	expression tag	UNP O75175
С	604	MET	-	expression tag	UNP 075175
С	605	LEU	-	expression tag	UNP 075175
С	606	GLU	-	expression tag	UNP O75175
F	601	GLY	-	expression tag	UNP 075175
F	602	PRO	-	expression tag	UNP O75175
F	603	HIS	-	expression tag	UNP 075175
F	604	MET	-	expression tag	UNP O75175
F	605	LEU	-	expression tag	UNP O75175
F	606	GLU	-	expression tag	UNP O75175



# 3 Residue-property plots (i)

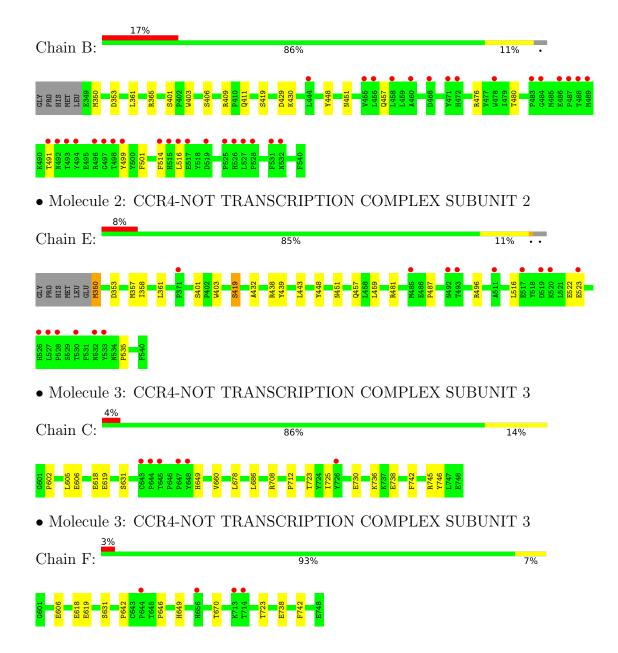
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1



• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	75.98Å 135.32Å 101.33Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $107.67^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	48.24 - 2.90	Depositor
Resolution (A)	48.24 - 2.90	EDS
% Data completeness	99.6 (48.24-2.90)	Depositor
(in resolution range)	99.6 (48.24-2.90)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) > 1$	2.19 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
D D.	0.181 , 0.221	Depositor
$R, R_{free}$	0.192 , $0.235$	DCC
$R_{free}$ test set	2200 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.9	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 70.1	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.23% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.53	0/4294	0.70	0/5839	
1	D	0.52	0/4300	0.69	0/5846	
2	В	0.50	0/1626	0.71	0/2211	
2	Е	0.49	0/1613	0.70	0/2193	
3	С	0.48	0/1344	0.65	0/1819	
3	F	0.48	0/1344	0.65	0/1819	
All	All	0.51	0/14521	0.69	0/19727	

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 (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	4186	0	4205	44	0
1	D	4193	0	4206	48	0
2	В	1578	0	1514	7	0
2	Ε	1566	0	1508	12	0
3	С	1293	0	1207	12	0
3	F	1293	0	1207	8	0
All	All	14109	0	13847	116	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.



The worst 5 of 116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ ( ext{Å}) \end{aligned}$
1:D:2184:LEU:HD22	1:D:2247:HIS:HD2	1.35	0.91
3:C:602:PRO:HB2	3:C:605:LEU:HD23	1.51	0.90
1:D:2147:THR:HG23	1:D:2150:LEU:HB2	1.71	0.73
1:A:2147:THR:HG23	1:A:2150:LEU:HB2	1.71	0.72
2:B:501:PHE:CD1	2:B:514:PHE:HZ	2.10	0.69

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	Perce	ntiles
1	A	511/535~(96%)	490 (96%)	19 (4%)	2 (0%)	34	66
1	D	512/535~(96%)	493 (96%)	18 (4%)	1 (0%)	47	78
2	В	190/197 (96%)	180 (95%)	9 (5%)	1 (0%)	29	61
2	E	189/197~(96%)	178 (94%)	9 (5%)	2 (1%)	14	42
3	С	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
3	F	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
All	All	1694/1760~(96%)	1623 (96%)	65 (4%)	6 (0%)	34	66

#### 5 of 6 Ramachandran outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type
1	A	2082	VAL
1	A	2205	GLU
2	В	353	ASP
1	D	2082	VAL
2	Е	353	ASP



#### 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	462/479~(96%)	445 (96%)	17 (4%)	34 68
1	D	462/479 (96%)	446 (96%)	16 (4%)	36 70
2	В	167/172 (97%)	156 (93%)	11 (7%)	16 44
2	E	166/172 (96%)	158 (95%)	8 (5%)	25 58
3	С	136/136 (100%)	134 (98%)	2 (2%)	65 87
3	F	136/136 (100%)	134 (98%)	2 (2%)	65 87
All	All	1529/1574 (97%)	1473 (96%)	56 (4%)	34 68

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	С	631	SER
3	F	742	PHE
1	D	2027	ARG
3	F	631	SER
2	Е	403	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2201	GLN
3	F	649	HIS
1	D	2247	HIS
1	D	1919	HIS
1	D	2175	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 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,  $95^{th}$  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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	515/535~(96%)	0.10	25 (4%) 29 26	40, 69, 121, 143	0
1	D	516/535 (96%)	0.21	26 (5%) 28 25	39, 77, 130, 159	0
2	В	192/197 (97%)	0.81	34 (17%) 1 1	51, 96, 165, 179	0
2	Е	191/197 (96%)	0.40	15 (7%) 12 10	47, 90, 146, 163	0
3	С	148/148 (100%)	0.17	6 (4%) 37 32	42, 84, 122, 140	0
3	F	148/148 (100%)	0.16	4 (2%) 54 50	47, 75, 108, 118	0
All	All	1710/1760 (97%)	0.26	110 (6%) 19 15	39, 80, 133, 179	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	492	ASN	7.4
1	D	2204	ASN	7.3
2	В	516	LEU	7.2
2	В	493	THR	7.1
1	D	1887	GLY	7.1

# 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.

