

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 03:42 am BST

PDB ID : 4BQ7

Title : Crystal structure of the RGMB-Neo1 complex form 2

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Deposited on : 2013-05-30

Resolution : 6.60 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 following versions of software and data (see references (1)) were used in the production of this report:

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

EDS : 2.11

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

Refmac: 5.8.0158

 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

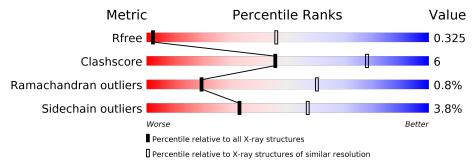
Validation Pipeline (wwPDB-VP) : 2.11

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 6.60 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$\mid \; (\# ext{Entries}, ext{resolution range}(ext{Å})) \; \mid \;$
R_{free}	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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 <=5%

Mol	Chain	Length	Quality of chain					
1	A	264	64%	11%	• 23%			
1	В	264	67%	8%	• 23%			
2	С	122	10%	88%				
2	Е	122	10% ••	88%				
3	D	251	50%	8%	41%			
3	F	251	51%	7%	41%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5714 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 NEOGENIN.

	\mathbf{Mol}	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	Trace	
	1	Λ	202	Total	С	N	О	S	0	0	0
	1	A	202	1591	1017	270	298	6	U	U	0
ĺ	1	D	202	Total	С	N	О	S	0	0	0
	1	Б	202	1591	1017	270	298	6	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	GLU	-	expression tag	UNP P97798
A	881	THR	-	expression tag	UNP P97798
A	882	GLY	-	expression tag	UNP P97798
A	1134	ASN	=	expression tag	UNP P97798
A	1135	GLY	_	expression tag	UNP P97798
A	1136	THR	=	expression tag	UNP P97798
A	1137	LYS	=	expression tag	UNP P97798
A	1138	HIS	_	expression tag	UNP P97798
A	1139	HIS	_	expression tag	UNP P97798
A	1140	HIS	_	expression tag	UNP P97798
A	1141	HIS	_	expression tag	UNP P97798
A	1142	HIS	=	expression tag	UNP P97798
A	1143	HIS	_	expression tag	UNP P97798
В	880	GLU	=	expression tag	UNP P97798
В	881	THR	=	expression tag	UNP P97798
В	882	GLY	=	expression tag	UNP P97798
В	1134	ASN	_	expression tag	UNP P97798
В	1135	GLY	=	expression tag	UNP P97798
В	1136	THR	-	expression tag	UNP P97798
В	1137	LYS	-	expression tag	UNP P97798
В	1138	HIS	-	expression tag	UNP P97798
В	1139	HIS	=	expression tag	UNP P97798
В	1140	HIS	-	expression tag	UNP P97798
В	1141	HIS	ı	expression tag	UNP P97798
В	1142	HIS	-	expression tag	UNP P97798

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Chain	Residue	Modelled	Actual	Comment	Reference
В	1143	HIS	_	expression tag	UNP P97798

• Molecule 2 is a protein called RGM DOMAIN FAMILY MEMBER B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	C	15	Total	С	N	O S	0	0		
2		15	118	79	16	21	2	U	0	
9	Г	15	Total	al C N O S	0	0				
2	E	15	118	79	16	21	2	U	U	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
С	47	GLU	-	expression tag	UNP Q6NW40
С	48	THR	-	expression tag	UNP Q6NW40
С	49	GLY	-	expression tag	UNP Q6NW40
Е	47	GLU	-	expression tag	UNP Q6NW40
Е	48	THR	_	expression tag	UNP Q6NW40
Е	49	GLY	=	expression tag	UNP Q6NW40

• Molecule 3 is a protein called RGM DOMAIN FAMILY MEMBER B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	148		C 721	N 197	O 223	S 7	0	0	0
3	F	148	Total 1148			O 223	S 7	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	411	GLY	-	expression tag	UNP Q6NW40
D	412	THR	_	expression tag	UNP Q6NW40
D	413	LYS	-	expression tag	UNP Q6NW40
D	414	HIS	_	expression tag	UNP Q6NW40
D	415	HIS	-	expression tag	UNP Q6NW40
D	416	HIS	-	expression tag	UNP Q6NW40
D	417	HIS	_	expression tag	UNP Q6NW40
D	418	HIS	_	expression tag	UNP Q6NW40
D	419	HIS	_	expression tag	UNP Q6NW40
D	225	GLY	GLU	conflict	UNP Q6NW40
F	411	GLY	-	expression tag	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
F	412	THR	_	expression tag	UNP Q6NW40
F	413	LYS	-	expression tag	UNP Q6NW40
F	414	HIS	_	expression tag	UNP Q6NW40
F	415	HIS	_	expression tag	UNP Q6NW40
F	416	HIS	_	expression tag	UNP Q6NW40
F	417	HIS	-	expression tag	UNP Q6NW40
F	418	HIS	_	expression tag	UNP Q6NW40
F	419	HIS	_	expression tag	UNP Q6NW40
F	225	GLY	GLU	conflict	UNP Q6NW40



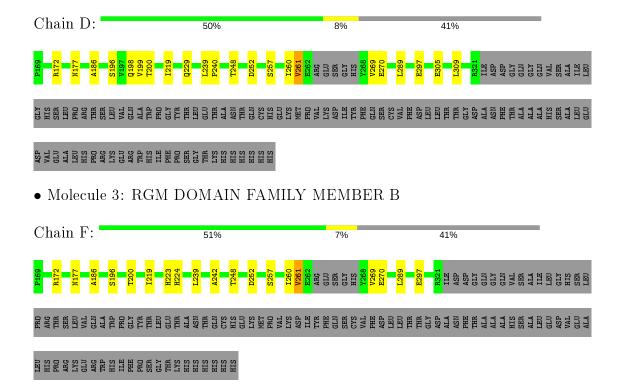
3 Residue-property plots (i)

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. 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. 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: NEOGENIN Chain A: • Molecule 1: NEOGENIN Chain B: 23% • Molecule 2: RGM DOMAIN FAMILY MEMBER B Chain C: 10% ... • Molecule 2: RGM DOMAIN FAMILY MEMBER B Chain E: 10%

• Molecule 3: RGM DOMAIN FAMILY MEMBER B







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants	109.69Å 109.69Å 187.93Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.78 - 6.60	Depositor
Resolution (A)	94.99 - 6.60	EDS
% Data completeness	97.2 (84.78-6.60)	Depositor
(in resolution range)	97.3 (94.99-6.60)	EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.72 (at 6.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D.	0.254 , 0.280	Depositor
R, R_{free}	0.306 , 0.325	DCC
R_{free} test set	231 reflections (9.27%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 152.8	EDS
L-test for twinning ²	$< L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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		Boı	nd lengths	Bond angles		
WIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.68	$1/1635 \ (0.1\%)$	0.80	$4/2234 \ (0.2\%)$	
1	В	0.82	1/1635~(0.1%)	0.71	$1/2234 \ (0.0\%)$	
2	С	0.46	0/122	1.01	1/162~(0.6%)	
2	Е	0.46	0/122	1.01	1/162~(0.6%)	
3	D	0.51	0/1170	0.73	0/1590	
3	F	0.51	0/1170	0.74	0/1590	
All	All	0.65	$2/5854 \ (0.0\%)$	0.76	7/7972~(0.1%)	

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
2	С	0	1
2	E	0	1
All	All	0	2

All (2) bond length outliers are listed below:

\mathbf{Mol}	Chain	${f Res}$	Type	Atoms	\mathbf{Z}	${f Observed(\AA)}$	Ideal(A)
1	В	983	LEU	C-N	26.18	1.94	1.34
1	A	983	LEU	C-N	-18.64	0.91	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	983	LEU	O-C-N	13.56	144.39	122.70
1	A	983	LEU	CA-C-N	-9.95	95.31	117.20
2	Е	167	GLY	C-N-CA	8.68	143.40	121.70
2	С	167	GLY	C-N-CA	8.63	143.28	121.70
1	A	983	LEU	C-N-CA	-6.70	104.95	121.70



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	С	167	GLY	Peptide
2	Е	167	GLY	Peptide

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	1591	0	1585	46	0
1	В	1591	0	1585	16	0
2	С	118	0	101	1	0
2	Е	118	0	101	1	0
3	D	1148	0	1122	33	1
3	F	1148	0	1122	14	0
All	All	5714	0	5616	72	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.

The worst 5 of 72 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:983:LEU:C	1:B:984:VAL:N	1.94	1.21
1:A:1009:GLN:HG3	3:D:200:THR:OG1	1.68	0.94
1:A:991:ASP:OD2	3:D:200:THR:HG21	1.68	0.93
1:A:1009:GLN:HG3	3:D:200:THR:HG1	1.35	0.92
1:A:1009:GLN:HG2	3:D:186:ALA:HB2	1.55	0.86

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	$egin{array}{ll} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
3:D:305:GLU:OE1	3:D:305:GLU:OE1[4_445]	1.91	0.29



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	\mathbf{ntiles}
1	A	200/264~(76%)	187 (94%)	10 (5%)	3 (2%)	10	46
1	В	200/264 (76%)	187 (94%)	10 (5%)	3 (2%)	10	46
2	С	11/122 (9%)	11 (100%)	0	0	100	100
2	E	11/122 (9%)	11 (100%)	0	0	100	100
3	D	144/251 (57%)	134 (93%)	10 (7%)	0	100	100
3	F	144/251 (57%)	133 (92%)	11 (8%)	0	100	100
All	All	710/1274 (56%)	663 (93%)	41 (6%)	6 (1%)	19	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	912	LYS
1	A	913	HIS
1	В	912	LYS
1	В	913	HIS
1	В	966	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	A	178/232 (77%)	173 (97%)	5 (3%)	43 65
1	В	178/232 (77%)	173 (97%)	5 (3%)	43 65
2	С	13/103 (13%)	12 (92%)	1 (8%)	13 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	13/103 (13%)	12 (92%)	1 (8%)	13 37
3	D	128/215 (60%)	122 (95%)	6 (5%)	26 51
3	F	128/215 (60%)	122 (95%)	6 (5%)	26 51
All	All	638/1100 (58%)	614 (96%)	24 (4%)	33 57

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	С	168	ASP
3	D	252	ASP
3	F	261	VAL
3	D	172	ARG
3	D	177	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1009	GLN
3	D	229	GLN
3	F	224	HIS

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)

The following chains have linkage breaks:

\mathbf{Mol}	Chain	Number of breaks	
1	В	1	
1	A	1	

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	$oxed{f Distance (\AA)}$
1	В	983:LEU	С	984:VAL	N	1.94
1	A	983:LEU	С	984:VAL	N	0.91



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

