Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2020 – 11:56 AM BST

PDB ID	:	3ZGC
Title	:	crystal structure of the KEAP1-NEH2 complex
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Deposited on	:	2012-12-17
Resolution	:	2.20 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 (i) symbol.

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

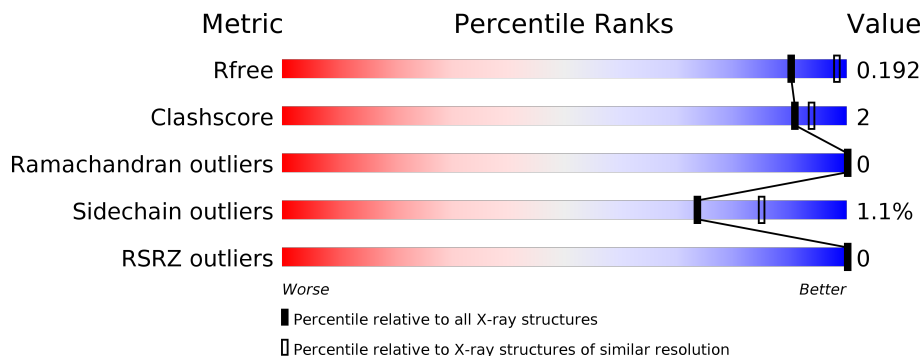|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.20 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	Percentile Ranks	Value
Rfree		0.192
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		0

Worse　　　　　　　　　　　　　　　　　Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 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	310	88%　　　　　　　　　　　　　　•　8%
1	B	310	87%　　　　　　　　　　　　　5%　8%
2	C	7	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5012 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 KELCH-LIKE ECH-ASSOCIATED PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2186	1359	397	415	15			
1	B	285	Total	C	N	O	S	0	0	0
			2186	1359	397	415	15			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	-	expression tag	UNP Q14145
A	301	GLY	-	expression tag	UNP Q14145
A	302	SER	-	expression tag	UNP Q14145
A	303	SER	-	expression tag	UNP Q14145
A	304	HIS	-	expression tag	UNP Q14145
A	305	HIS	-	expression tag	UNP Q14145
A	306	HIS	-	expression tag	UNP Q14145
A	307	HIS	-	expression tag	UNP Q14145
A	308	HIS	-	expression tag	UNP Q14145
A	309	HIS	-	expression tag	UNP Q14145
A	310	SER	-	expression tag	UNP Q14145
A	311	SER	-	expression tag	UNP Q14145
A	312	GLY	-	expression tag	UNP Q14145
A	313	LEU	-	expression tag	UNP Q14145
A	314	VAL	-	expression tag	UNP Q14145
A	315	PRO	-	expression tag	UNP Q14145
A	316	ARG	-	expression tag	UNP Q14145
A	317	GLY	-	expression tag	UNP Q14145
A	318	SER	-	expression tag	UNP Q14145
A	319	HIS	-	expression tag	UNP Q14145
A	320	MET	-	expression tag	UNP Q14145
A	540	ALA	GLU	engineered mutation	UNP Q14145
A	542	ALA	GLU	engineered mutation	UNP Q14145
B	300	MET	-	expression tag	UNP Q14145
B	301	GLY	-	expression tag	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	SER	-	expression tag	UNP Q14145
B	303	SER	-	expression tag	UNP Q14145
B	304	HIS	-	expression tag	UNP Q14145
B	305	HIS	-	expression tag	UNP Q14145
B	306	HIS	-	expression tag	UNP Q14145
B	307	HIS	-	expression tag	UNP Q14145
B	308	HIS	-	expression tag	UNP Q14145
B	309	HIS	-	expression tag	UNP Q14145
B	310	SER	-	expression tag	UNP Q14145
B	311	SER	-	expression tag	UNP Q14145
B	312	GLY	-	expression tag	UNP Q14145
B	313	LEU	-	expression tag	UNP Q14145
B	314	VAL	-	expression tag	UNP Q14145
B	315	PRO	-	expression tag	UNP Q14145
B	316	ARG	-	expression tag	UNP Q14145
B	317	GLY	-	expression tag	UNP Q14145
B	318	SER	-	expression tag	UNP Q14145
B	319	HIS	-	expression tag	UNP Q14145
B	320	MET	-	expression tag	UNP Q14145
B	540	ALA	GLU	engineered mutation	UNP Q14145
B	542	ALA	GLU	engineered mutation	UNP Q14145

- Molecule 2 is a protein called NUCLEAR FACTOR ERYTHROID 2-RELATED FACTOR 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			50	27	7	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	76	GLY	LEU	engineered mutation	UNP Q16236

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	284	Total 284	O 284	0	0
4	B	262	Total 262	O 262	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	4	Total O 4 4		0	0

3 Residue-property plots ⓘ

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: KELCH-LIKE ECH-ASSOCIATED PROTEIN 1

Chain A:
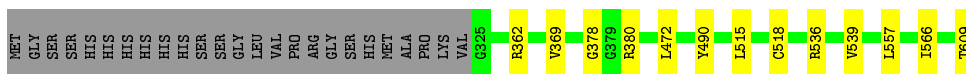
• Molecule 1: KELCH-LIKE ECH-ASSOCIATED PROTEIN 1

Chain B:

• Molecule 2: NUCLEAR FACTOR ERYTHROID 2-RELATED FACTOR 2

Chain C:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.10Å 76.06Å 207.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 38.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.20) 99.8 (38.03-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.51 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.172 , 0.188 0.174 , 0.192	Depositor DCC
R_{free} test set	3097 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.7	EDS
L-test for twinning [2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5012	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.42	0/2239	0.65	0/3048
1	B	0.43	0/2239	0.67	0/3048
2	C	0.35	0/49	0.59	0/64
All	All	0.42	0/4527	0.66	0/6160

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	2186	0	2082	6	0
1	B	2186	0	2082	8	0
2	C	50	0	34	0	0
3	A	16	0	12	0	0
3	B	24	0	18	1	0
4	A	284	0	0	1	0
4	B	262	0	0	0	0
4	C	4	0	0	0	0
All	All	5012	0	4228	14	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 2.

All (14) 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:466:ALA:HB1	1:B:514:VAL:HG23	1.70	0.71
1:B:362:ARG:NH2	1:B:394:ASP:OD2	2.36	0.59
1:B:483:ARG:HD3	3:B:1611:ACT:O	2.07	0.54
1:B:483:ARG:HG2	1:B:508:SER:HB3	1.93	0.50
1:A:362:ARG:HD2	1:A:378:GLY:O	2.13	0.49
1:B:422:ASP:OD1	1:B:470:ARG:NH2	2.46	0.48
1:A:472:LEU:HB3	1:A:490:TYR:HB3	1.96	0.47
1:A:380:ARG:HD2	4:A:2040:HOH:O	2.16	0.45
1:B:369:VAL:HG21	1:B:609:THR:HB	1.98	0.45
1:A:369:VAL:HG21	1:A:609:THR:HB	1.98	0.44
1:B:515:LEU:HD22	1:B:566:ILE:HG13	2.01	0.43
1:B:485:ASN:HB3	1:B:506:ILE:HG13	2.00	0.42
1:A:515:LEU:HD22	1:A:566:ILE:HG13	2.01	0.41
1:A:518:CYS:HB3	1:A:536:ARG:HG3	2.02	0.41

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	283/310 (91%)	277 (98%)	6 (2%)	0	100	100
1	B	283/310 (91%)	276 (98%)	7 (2%)	0	100	100
2	C	5/7 (71%)	5 (100%)	0	0	100	100
All	All	571/627 (91%)	558 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	229/250 (92%)	227 (99%)	2 (1%)	78	88
1	B	229/250 (92%)	226 (99%)	3 (1%)	69	81
2	C	5/5 (100%)	5 (100%)	0	100	100
All	All	463/505 (92%)	458 (99%)	5 (1%)	73	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	539	VAL
1	A	557	LEU
1	B	483	ARG
1	B	539	VAL
1	B	557	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	ACT	B	1611	-	1,3,3	5.45	1 (100%)	0,3,3	0.00	-
3	ACT	B	1615	-	1,3,3	6.13	1 (100%)	0,3,3	0.00	-
3	ACT	B	1612	-	1,3,3	4.57	1 (100%)	0,3,3	0.00	-
3	ACT	B	1610	-	1,3,3	3.67	1 (100%)	0,3,3	0.00	-
3	ACT	A	1612	-	1,3,3	4.97	1 (100%)	0,3,3	0.00	-
3	ACT	B	1614	-	1,3,3	4.96	1 (100%)	0,3,3	0.00	-
3	ACT	A	1611	-	1,3,3	4.24	1 (100%)	0,3,3	0.00	-
3	ACT	B	1613	-	1,3,3	5.26	1 (100%)	0,3,3	0.00	-
3	ACT	A	1613	-	1,3,3	5.39	1 (100%)	0,3,3	0.00	-
3	ACT	A	1610	-	1,3,3	5.30	1 (100%)	0,3,3	0.00	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1615	ACT	CH3-C	6.13	1.56	1.48
3	B	1611	ACT	CH3-C	5.45	1.55	1.48
3	A	1613	ACT	CH3-C	5.39	1.55	1.48
3	A	1610	ACT	CH3-C	5.30	1.55	1.48
3	B	1613	ACT	CH3-C	5.26	1.55	1.48
3	A	1612	ACT	CH3-C	4.97	1.55	1.48
3	B	1614	ACT	CH3-C	4.96	1.55	1.48
3	B	1612	ACT	CH3-C	4.57	1.54	1.48
3	A	1611	ACT	CH3-C	4.24	1.54	1.48
3	B	1610	ACT	CH3-C	3.67	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1611	ACT	1	0

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(Å²)	Q<0.9
1	A	285/310 (91%)	-0.63	0	100	100	26, 37, 55, 70	0
1	B	285/310 (91%)	-0.69	0	100	100	27, 36, 56, 77	0
2	C	7/7 (100%)	-1.02	0	100	100	33, 34, 46, 46	0
All	All	577/627 (92%)	-0.67	0	100	100	26, 37, 56, 77	0

There are no RSRZ outliers to report.

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	ACT	B	1611	4/4	0.95	0.11	27,28,31,33	0
3	ACT	B	1615	4/4	0.95	0.14	40,42,43,44	0
3	ACT	B	1614	4/4	0.96	0.17	45,48,48,59	0
3	ACT	B	1613	4/4	0.96	0.09	44,45,46,46	0
3	ACT	A	1613	4/4	0.96	0.19	43,44,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	B	1612	4/4	0.98	0.09	43,46,46,51	0
3	ACT	A	1611	4/4	0.98	0.13	34,38,40,48	0
3	ACT	B	1610	4/4	0.98	0.07	35,38,39,44	0
3	ACT	A	1612	4/4	0.98	0.17	54,56,58,60	0
3	ACT	A	1610	4/4	0.99	0.05	35,38,38,40	0

6.5 Other polymers (i)

There are no such residues in this entry.