wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 05:33 PM EDT

PDB ID	:	3IIO
Title	:	Evolutionary optimization of computationally designed enzymes: Kemp eliminases of the KE07 series
Authors	:	Khersonsky, O.; Dym, O.; Tawfik, D.S.
Deposited on	:	2009-08-03
Resolution	:	2.25 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:

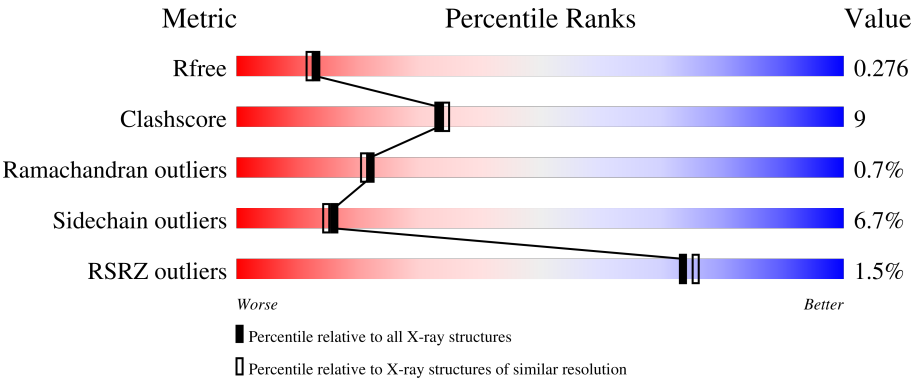
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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
1	A	262	79% 15% • 5%
1	B	262	% 77% 16% • 5%
1	C	262	75% 15% • • 5%
1	D	262	% 76% 16% • 5%
1	E	262	5% 67% 26% • 5%

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Mol	Chain	Length	Quality of chain
1	F	262	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11835 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 KE07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1934	1232	332	366	4			
1	B	250	Total	C	N	O	S	0	0	0
			1947	1241	334	368	4			
1	C	248	Total	C	N	O	S	0	0	0
			1934	1232	332	366	4			
1	D	250	Total	C	N	O	S	0	0	0
			1947	1241	334	368	4			
1	E	248	Total	C	N	O	S	0	0	0
			1934	1232	332	366	4			
1	F	248	Total	C	N	O	S	0	0	0
			1934	1232	332	366	4			

- Molecule 2 is water.

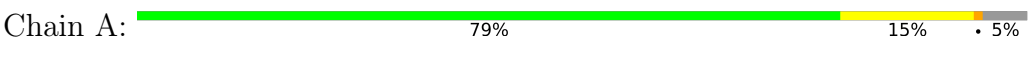
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	43	Total	O	0	0
			43	43		
2	B	36	Total	O	0	0
			36	36		
2	C	58	Total	O	0	0
			58	58		
2	D	41	Total	O	0	0
			41	41		
2	E	12	Total	O	0	0
			12	12		
2	F	15	Total	O	0	0
			15	15		

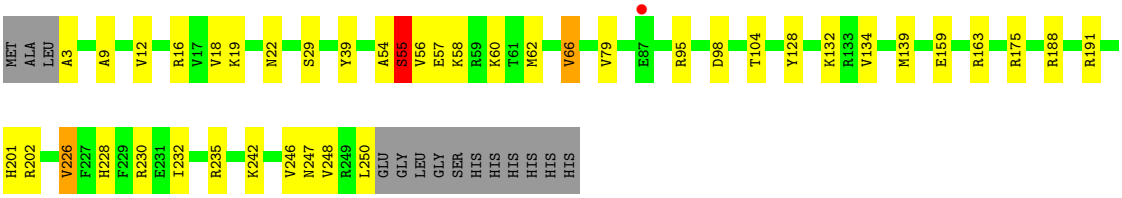
3 Residue-property plots (i)

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: KE07

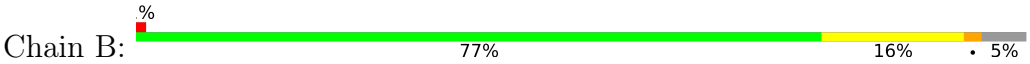
Chain A:

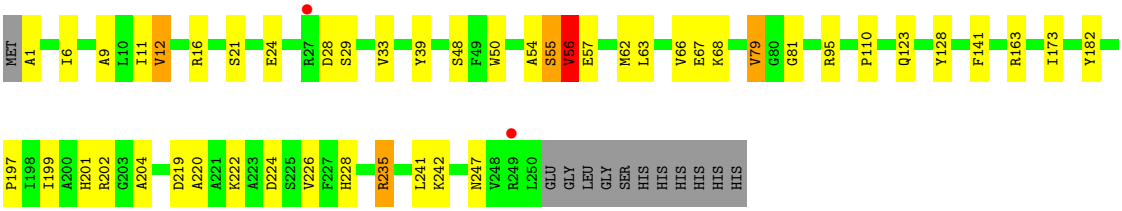




- Molecule 1: KE07

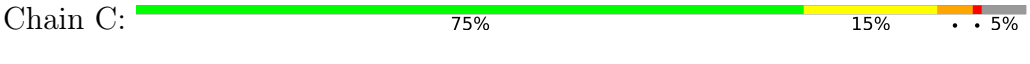
Chain B:

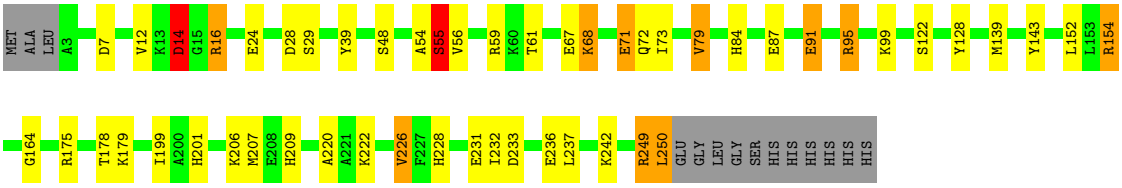




- Molecule 1: KE07

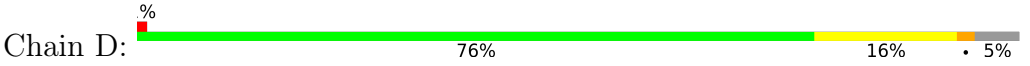
Chain C:



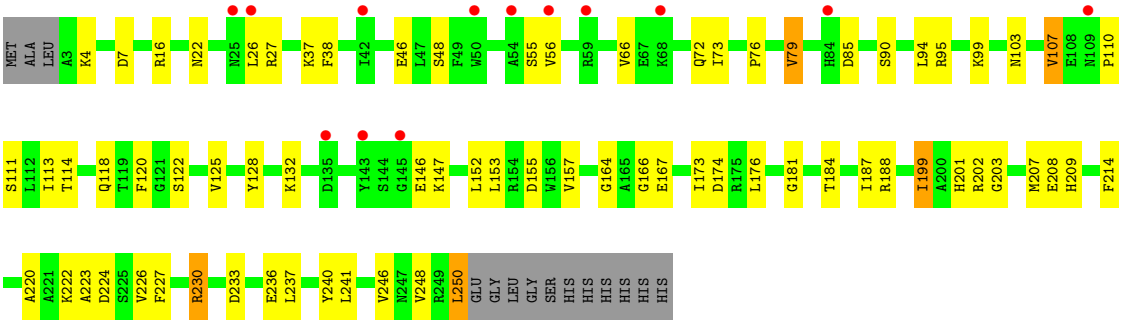


- Molecule 1: KE07

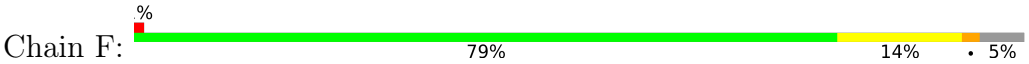
Chain D:

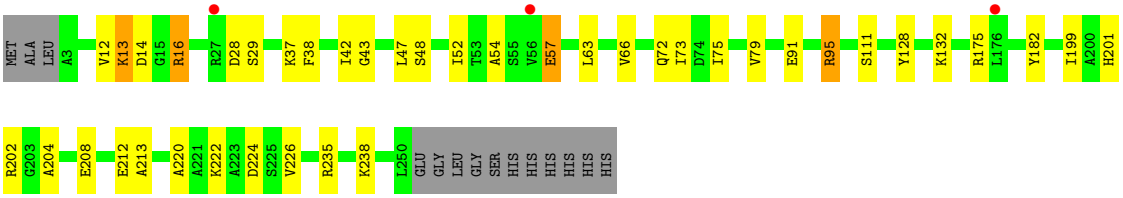


• Molecule 1: KE07



• Molecule 1: KE07





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	106.58Å 106.58Å 128.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.25 49.24 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.25) 99.1 (49.24-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.278 0.214 , 0.276	Depositor DCC
R_{free} test set	3874 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 10.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.328 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11835	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	A	0.77	0/1965	0.80	3/2649 (0.1%)
1	B	0.71	0/1978	0.79	1/2667 (0.0%)
1	C	0.74	0/1965	0.80	1/2649 (0.0%)
1	D	0.68	1/1978 (0.1%)	0.73	0/2667
1	E	0.59	0/1965	0.68	1/2649 (0.0%)
1	F	0.67	0/1965	0.69	0/2649
All	All	0.70	1/11816 (0.0%)	0.75	6/15930 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	GLU	CG-CD	6.37	1.61	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	79	VAL	CB-CA-C	-7.06	97.98	111.40
1	A	188	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	188	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	E	250	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	191	ARG	NE-CZ-NH2	-5.17	117.71	120.30

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	A	1934	0	1956	27	0
1	B	1947	0	1975	32	0
1	C	1934	0	1956	38	0
1	D	1947	0	1975	38	0
1	E	1934	0	1956	49	0
1	F	1934	0	1956	18	0
2	A	43	0	0	2	0
2	B	36	0	0	2	0
2	C	58	0	0	2	0
2	D	41	0	0	5	0
2	E	12	0	0	6	0
2	F	15	0	0	1	0
All	All	11835	0	11774	200	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 9.

The worst 5 of 200 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:55:SER:HB3	1:B:56:VAL:CA	1.71	1.18
1:B:55:SER:CB	1:B:56:VAL:HA	1.77	1.15
1:D:55:SER:HB3	1:D:56:VAL:HA	1.19	1.11
1:F:13:LYS:HG3	1:F:52:ILE:HG13	1.31	1.11
1:A:55:SER:HB2	1:A:56:VAL:HA	1.37	1.03

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	246/262 (94%)	236 (96%)	8 (3%)	2 (1%)	19 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	248/262 (95%)	240 (97%)	5 (2%)	3 (1%)	13 9
1	C	246/262 (94%)	237 (96%)	7 (3%)	2 (1%)	19 17
1	D	248/262 (95%)	233 (94%)	13 (5%)	2 (1%)	19 17
1	E	246/262 (94%)	230 (94%)	15 (6%)	1 (0%)	34 37
1	F	246/262 (94%)	232 (94%)	13 (5%)	1 (0%)	34 37
All	All	1480/1572 (94%)	1408 (95%)	61 (4%)	11 (1%)	22 21

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	B	55	SER
1	C	14	ASP
1	C	55	SER
1	D	55	SER

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	204/215 (95%)	192 (94%)	12 (6%)	19 19
1	B	205/215 (95%)	195 (95%)	10 (5%)	25 27
1	C	204/215 (95%)	186 (91%)	18 (9%)	10 8
1	D	205/215 (95%)	190 (93%)	15 (7%)	14 12
1	E	204/215 (95%)	190 (93%)	14 (7%)	15 14
1	F	204/215 (95%)	191 (94%)	13 (6%)	17 16
All	All	1226/1290 (95%)	1144 (93%)	82 (7%)	16 15

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	79	VAL

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Mol	Chain	Res	Type
1	F	14	ASP
1	E	95	ARG
1	E	224	ASP
1	F	73	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	123	GLN
1	E	118	GLN
1	D	228	HIS
1	E	201	HIS
1	B	228	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 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

6.1 Protein, DNA and RNA chains

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>2	OWAB(Å^2)	Q<0.9
1	A	248/262 (94%)	-0.34	1 (0%) 92 93	13, 26, 41, 51	0
1	B	250/262 (95%)	-0.33	2 (0%) 86 87	16, 28, 44, 59	0
1	C	248/262 (94%)	-0.41	0 100 100	14, 25, 38, 49	0
1	D	250/262 (95%)	-0.26	3 (1%) 79 81	17, 30, 48, 64	0
1	E	248/262 (94%)	0.26	13 (5%) 27 30	32, 49, 72, 79	0
1	F	248/262 (94%)	-0.11	3 (1%) 79 81	27, 41, 58, 75	0
All	All	1492/1572 (94%)	-0.20	22 (1%) 73 75	13, 33, 60, 79	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	135	ASP	4.1
1	E	54	ALA	4.0
1	B	249	ARG	4.0
1	E	25	ASN	3.6
1	F	56	VAL	3.3

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.