Full wwPDB X-ray Structure Validation Report (i)

May 1, 2021 – 05:50 PM EDT

PDB ID	:	5RG7
Title	:	Crystal Structure of Kemp Eliminase HG3.14 in unbound state, 277K
Authors	:	Broom, A.; Rakotoharisoa, R.V.; Thompson, M.C.; Fraser, J.S.; Chica, R.A.
Deposited on	:	2020-03-19
Resolution	:	1.47 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:

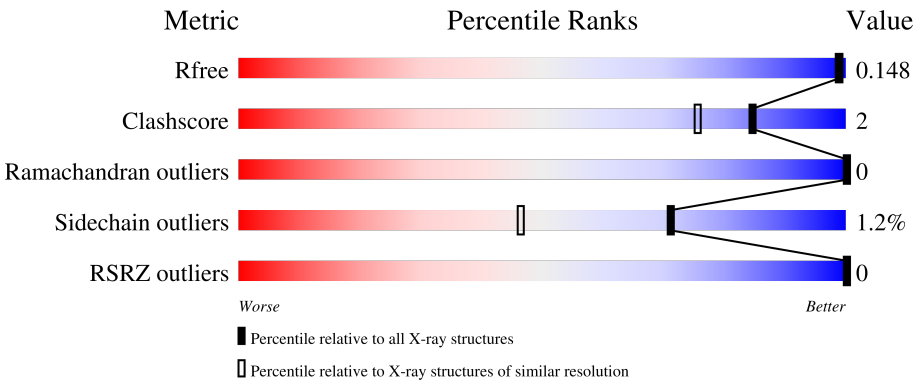
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 1.47 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	318	87% 7% 6%
1	B	318	89% 5% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	402	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11288 atoms, of which 5355 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 Kemp Eliminase HG3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	300	5354	1701	2665	465	508	15	0	84	0
1	B	300	5408	1708	2690	475	520	15	0	90	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P23360
A	0	ALA	-	expression tag	UNP P23360
A	1	GLU	-	expression tag	UNP P23360
A	6	ILE	VAL	engineered mutation	UNP P23360
A	37	LYS	GLN	engineered mutation	UNP P23360
A	42	MET	GLN	engineered mutation	UNP P23360
A	44	TRP	THR	engineered mutation	UNP P23360
A	50	GLN	LYS	engineered mutation	UNP P23360
A	81	GLY	ARG	engineered mutation	UNP P23360
A	82	ALA	GLY	engineered mutation	UNP P23360
A	83	GLY	HIS	engineered mutation	UNP P23360
A	84	CYS	THR	engineered mutation	UNP P23360
A	90	HIS	GLN	engineered mutation	UNP P23360
A	105	ILE	THR	engineered mutation	UNP P23360
A	125	THR	ALA	engineered mutation	UNP P23360
A	130	GLY	ASN	engineered mutation	UNP P23360
A	142	ASN	THR	engineered mutation	UNP P23360
A	172	MET	ASN	engineered mutation	UNP P23360
A	208	MET	THR	engineered mutation	UNP P23360
A	234	SER	ALA	engineered mutation	UNP P23360
A	236	LEU	THR	engineered mutation	UNP P23360
A	237	MET	GLU	engineered mutation	UNP P23360
A	267	PHE	TRP	engineered mutation	UNP P23360
A	279	SER	THR	engineered mutation	UNP P23360
A	300	ASN	ASP	engineered mutation	UNP P23360

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Chain	Residue	Modelled	Actual	Comment	Reference
A	304	GLY	-	expression tag	UNP P23360
A	305	SER	-	expression tag	UNP P23360
A	306	ILE	-	expression tag	UNP P23360
A	307	GLU	-	expression tag	UNP P23360
A	308	GLY	-	expression tag	UNP P23360
A	309	ARG	-	expression tag	UNP P23360
A	310	GLY	-	expression tag	UNP P23360
A	311	HIS	-	expression tag	UNP P23360
A	312	HIS	-	expression tag	UNP P23360
A	313	HIS	-	expression tag	UNP P23360
A	314	HIS	-	expression tag	UNP P23360
A	315	HIS	-	expression tag	UNP P23360
A	316	HIS	-	expression tag	UNP P23360
B	-1	MET	-	initiating methionine	UNP P23360
B	0	ALA	-	expression tag	UNP P23360
B	1	GLU	-	expression tag	UNP P23360
B	6	ILE	VAL	engineered mutation	UNP P23360
B	37	LYS	GLN	engineered mutation	UNP P23360
B	42	MET	GLN	engineered mutation	UNP P23360
B	44	TRP	THR	engineered mutation	UNP P23360
B	50	GLN	LYS	engineered mutation	UNP P23360
B	81	GLY	ARG	engineered mutation	UNP P23360
B	82	ALA	GLY	engineered mutation	UNP P23360
B	83	GLY	HIS	engineered mutation	UNP P23360
B	84	CYS	THR	engineered mutation	UNP P23360
B	90	HIS	GLN	engineered mutation	UNP P23360
B	105	ILE	THR	engineered mutation	UNP P23360
B	125	THR	ALA	engineered mutation	UNP P23360
B	130	GLY	ASN	engineered mutation	UNP P23360
B	142	ASN	THR	engineered mutation	UNP P23360
B	172	MET	ASN	engineered mutation	UNP P23360
B	208	MET	THR	engineered mutation	UNP P23360
B	234	SER	ALA	engineered mutation	UNP P23360
B	236	LEU	THR	engineered mutation	UNP P23360
B	237	MET	GLU	engineered mutation	UNP P23360
B	267	PHE	TRP	engineered mutation	UNP P23360
B	279	SER	THR	engineered mutation	UNP P23360
B	300	ASN	ASP	engineered mutation	UNP P23360
B	304	GLY	-	expression tag	UNP P23360
B	305	SER	-	expression tag	UNP P23360
B	306	ILE	-	expression tag	UNP P23360
B	307	GLU	-	expression tag	UNP P23360

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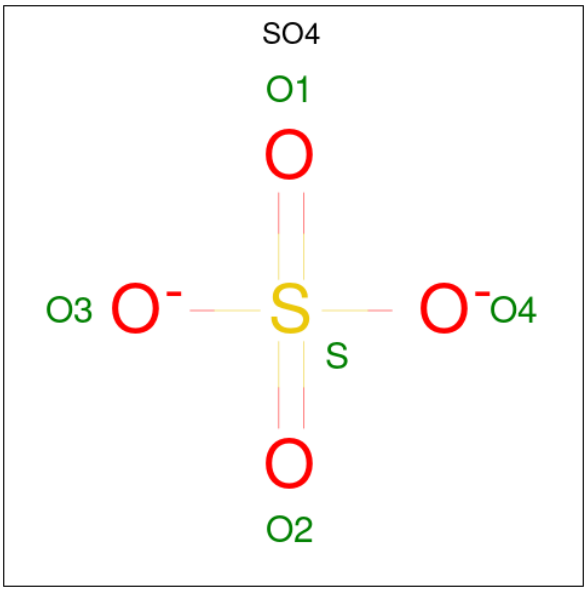
Chain	Residue	Modelled	Actual	Comment	Reference
B	308	GLY	-	expression tag	UNP P23360
B	309	ARG	-	expression tag	UNP P23360
B	310	GLY	-	expression tag	UNP P23360
B	311	HIS	-	expression tag	UNP P23360
B	312	HIS	-	expression tag	UNP P23360
B	313	HIS	-	expression tag	UNP P23360
B	314	HIS	-	expression tag	UNP P23360
B	315	HIS	-	expression tag	UNP P23360
B	316	HIS	-	expression tag	UNP P23360

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0

- Molecule 3 is water.

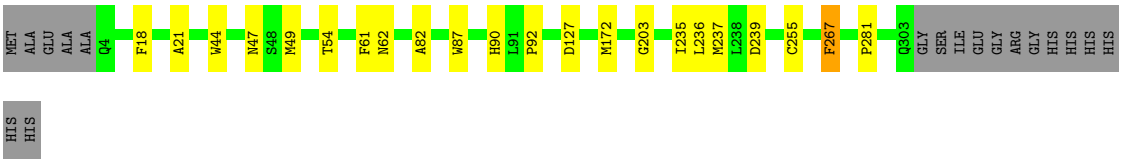
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	261	262	262	0	7
			Total	O		
3	B	249	249	249	0	5

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: Kemp Eliminase HG3

Chain A:



- Molecule 1: Kemp Eliminase HG3

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.31Å 79.83Å 99.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.83 – 1.47 62.17 – 1.47	Depositor EDS
% Data completeness (in resolution range)	99.7 (79.83-1.47) 99.7 (62.17-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.132 , 0.148 0.132 , 0.148	Depositor DCC
R_{free} test set	5255 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	11288	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.44	0/3046	0.65	0/4156
1	B	0.40	0/3089	0.63	0/4213
All	All	0.42	0/6135	0.64	0/8369

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	2689	2665	2369	12	0
1	B	2718	2690	2345	13	0
2	B	15	0	0	2	0
3	A	262	0	0	2	2
3	B	249	0	0	6	1
All	All	5933	5355	4714	25	2

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 (25) 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:74[A]:GLN:NE2	3:B:501:HOH:O	2.28	0.66
1:A:47[A]:ASN:OD1	3:A:401:HOH:O	2.12	0.65
1:B:109[B]:LYS:NZ	2:B:402:SO4:O3	2.23	0.62
1:B:109[B]:LYS:NZ	2:B:402:SO4:S	2.72	0.61
1:B:26[B]:ARG:NE	1:B:46[B]:GLU:OE1	2.30	0.61
1:B:96[B]:SER:HA	1:B:143[B]:VAL:HG21	1.85	0.58
1:B:113[B]:THR:HG22	3:B:636:HOH:O	2.02	0.58
1:B:113[B]:THR:HG21	3:B:514:HOH:O	2.04	0.57
1:A:235[B]:ILE:HD12	1:A:255[B]:CYS:SG	2.47	0.54
1:B:195[B]:ARG:HD2	1:B:230:THR:HG22	1.89	0.53
1:A:21:ALA:HB3	1:A:267[B]:PHE:O	2.10	0.51
1:B:49[B]:MET:SD	1:B:82:ALA:HB1	2.51	0.50
1:A:49[B]:MET:SD	1:A:82:ALA:HB1	2.52	0.49
1:B:143[B]:VAL:HG23	3:B:671:HOH:O	2.13	0.48
1:B:4[A]:GLN:NE2	3:B:504:HOH:O	2.46	0.47
1:A:87[B]:TRP:CZ2	1:A:90[B]:HIS:ND1	2.83	0.47
1:A:127:ASP:OD2	1:A:172[B]:MET:SD	2.74	0.45
1:B:54:THR:O	1:B:61:PHE:HA	2.18	0.43
1:A:54:THR:O	1:A:61[B]:PHE:HA	2.20	0.42
1:B:299[B]:GLN:HG2	3:B:542:HOH:O	2.20	0.41
1:A:236[A]:LEU:HG	1:A:237[A]:MET:HG2	2.01	0.41
1:A:21:ALA:HA	1:A:44[B]:TRP:O	2.20	0.41
1:A:236[B]:LEU:HD11	3:A:414:HOH:O	2.20	0.41
1:A:239[A]:ASP:HB2	1:A:281:PRO:HB2	2.03	0.41

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:437:HOH:O	3:B:589:HOH:O[3_555]	1.94	0.26
3:A:445:HOH:O	3:A:639:HOH:O[2_554]	2.09	0.11

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	381/318 (120%)	374 (98%)	7 (2%)	0	100	100
1	B	389/318 (122%)	381 (98%)	8 (2%)	0	100	100
All	All	770/636 (121%)	755 (98%)	15 (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	322/256 (126%)	316 (98%)	6 (2%)	57	26
1	B	329/256 (128%)	327 (99%)	2 (1%)	86	72
All	All	651/512 (127%)	643 (99%)	8 (1%)	71	46

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	62[A]	ASN
1	A	62[B]	ASN
1	A	92	PRO
1	A	267[A]	PHE
1	A	267[B]	PHE
1	B	18	PHE
1	B	62	ASN

Sometimes 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)

3 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	$\#\|Z\| > 2$
2	SO4	B	403	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	B	402	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	401	-	4,4,4	0.13	0	6,6,6	0.13	0

There are no bond length outliers.

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	SO4	2	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(Å^2)	Q<0.9
1	A	300/318 (94%)	-0.37	0	100	100	12, 18, 29, 53	0
1	B	300/318 (94%)	-0.28	0	100	100	13, 20, 36, 62	0
All	All	600/636 (94%)	-0.33	0	100	100	12, 19, 34, 62	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(Å^2)	Q<0.9
2	SO4	B	403	5/5	0.84	0.15	100,100,103,109	0
2	SO4	B	402	5/5	0.86	0.15	83,90,92,94	5
2	SO4	B	401	5/5	0.88	0.21	47,63,76,83	5

6.5 Other polymers (i)

There are no such residues in this entry.