



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2020 – 10:53 AM EDT

PDB ID : 6JST  
Title : Structure of Geobacillus kaustophilus lactonase, Y99P/D266N double mutant with bound 3-oxo-C8-HSL  
Authors : Xue, B.; Yew, W.S.  
Deposited on : 2019-04-08  
Resolution : 1.73 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.10.1  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
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) : 2.10.1

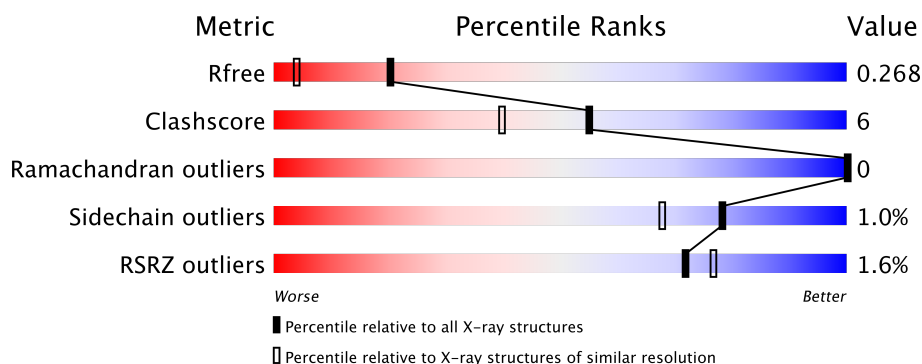
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 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))
$R_{free}$	111664	4894 (1.74-1.70)
Clashscore	122126	5296 (1.74-1.70)
Ramachandran outliers	120053	5219 (1.74-1.70)
Sidechain outliers	120020	5219 (1.74-1.70)
RSRZ outliers	108989	4804 (1.74-1.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	330	 % 88% 9% .
1	B	330	 % 88% 9% .
1	C	330	 2% 81% 17% .
1	D	330	 2% 79% 18% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10942 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 Phosphotriesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2538	1613	436	473	16			
1	B	323	Total	C	N	O	S	0	0	0
			2538	1613	436	473	16			
1	C	323	Total	C	N	O	S	0	0	0
			2538	1613	436	473	16			
1	D	323	Total	C	N	O	S	0	0	0
			2538	1613	436	473	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q5KZU5
A	-2	SER	-	expression tag	UNP Q5KZU5
A	-1	HIS	-	expression tag	UNP Q5KZU5
A	0	ASN	-	expression tag	UNP Q5KZU5
A	99	PRO	TYR	engineered mutation	UNP Q5KZU5
A	266	ASN	ASP	engineered mutation	UNP Q5KZU5
B	-3	GLY	-	expression tag	UNP Q5KZU5
B	-2	SER	-	expression tag	UNP Q5KZU5
B	-1	HIS	-	expression tag	UNP Q5KZU5
B	0	ASN	-	expression tag	UNP Q5KZU5
B	99	PRO	TYR	engineered mutation	UNP Q5KZU5
B	266	ASN	ASP	engineered mutation	UNP Q5KZU5
C	-3	GLY	-	expression tag	UNP Q5KZU5
C	-2	SER	-	expression tag	UNP Q5KZU5
C	-1	HIS	-	expression tag	UNP Q5KZU5
C	0	ASN	-	expression tag	UNP Q5KZU5
C	99	PRO	TYR	engineered mutation	UNP Q5KZU5
C	266	ASN	ASP	engineered mutation	UNP Q5KZU5
D	-3	GLY	-	expression tag	UNP Q5KZU5
D	-2	SER	-	expression tag	UNP Q5KZU5
D	-1	HIS	-	expression tag	UNP Q5KZU5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ASN	-	expression tag	UNP Q5KZU5
D	99	PRO	TYR	engineered mutation	UNP Q5KZU5
D	266	ASN	ASP	engineered mutation	UNP Q5KZU5

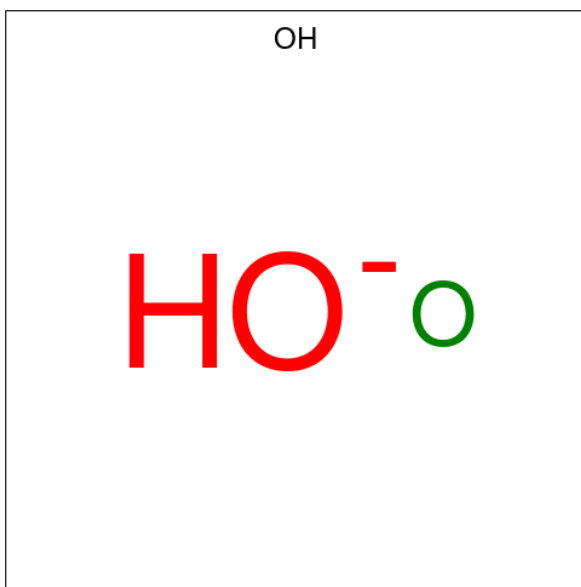
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

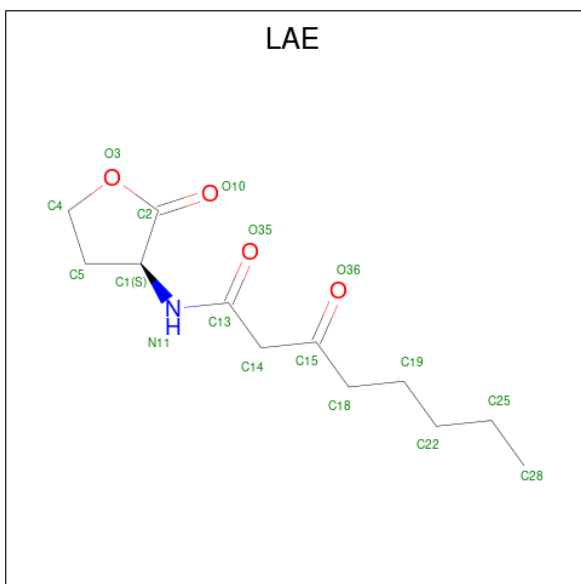
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 5 is 3-OXO-OCTANOIC ACID (2-OXO-TETRAHYDRO-FURAN-3-YL)-AMIDE (three-letter code: LAE) (formula: C<sub>12</sub>H<sub>19</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	12	1	4		

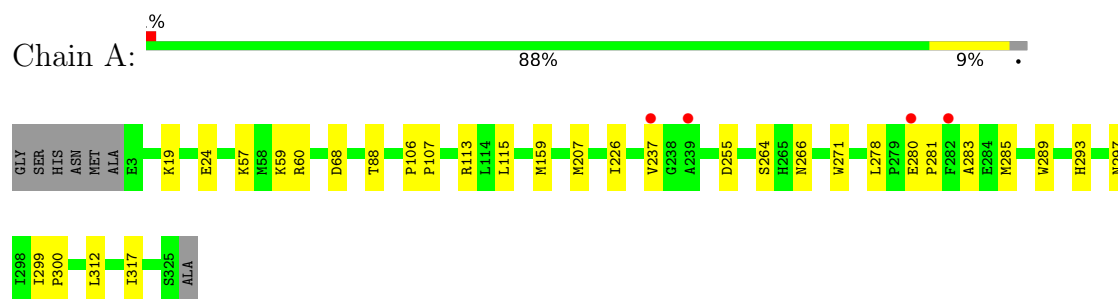
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	270	Total	O	0	0
			270	270		
6	B	252	Total	O	0	0
			252	252		
6	C	127	Total	O	0	0
			127	127		
6	D	113	Total	O	0	0
			113	113		

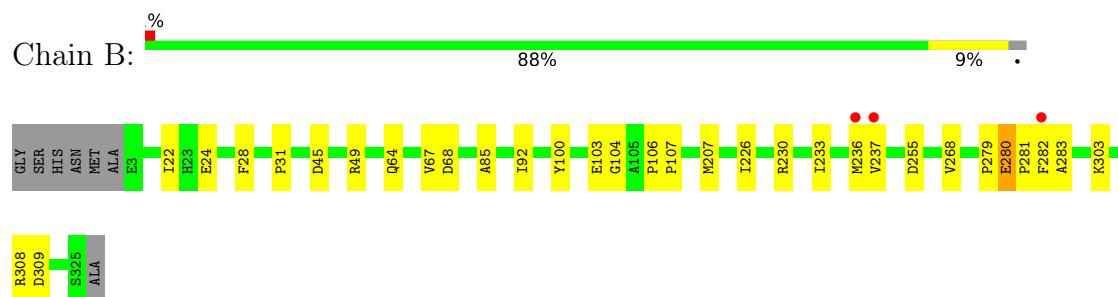
### 3 Residue-property plots

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 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.

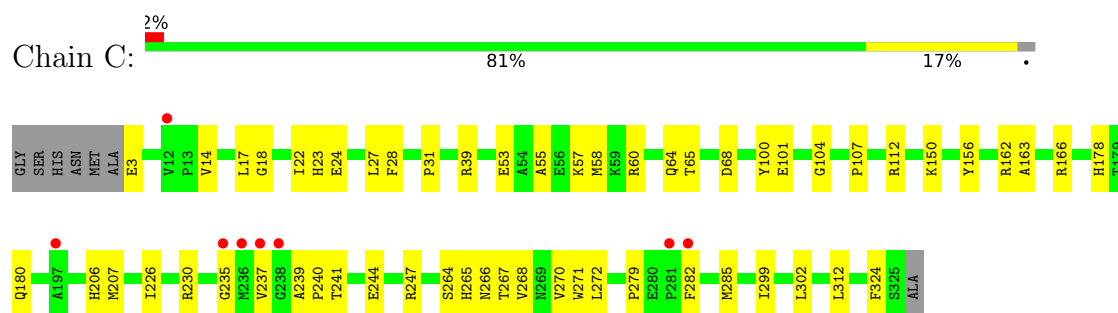
#### • Molecule 1: Phosphotriesterase



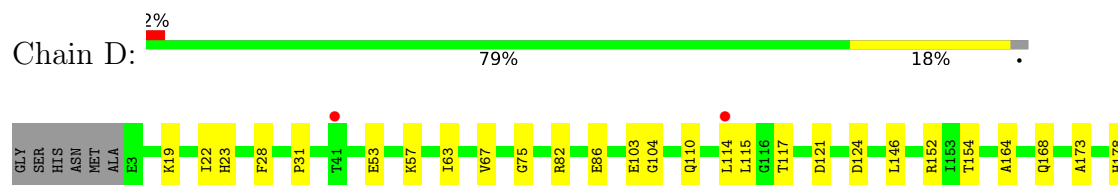
#### • Molecule 1: Phosphotriesterase

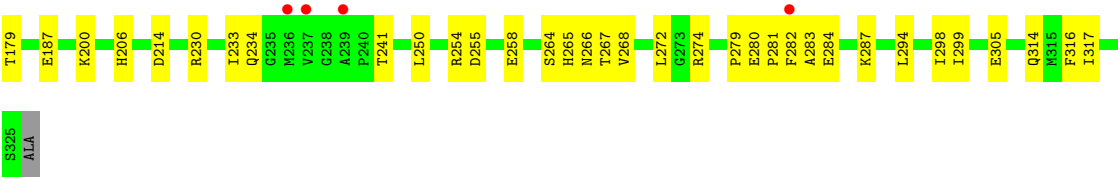


#### • Molecule 1: Phosphotriesterase



#### • Molecule 1: Phosphotriesterase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.99Å 51.19Å 134.47Å 90.99° 91.33° 96.33°	Depositor
Resolution (Å)	19.99 – 1.73 47.81 – 1.73	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-1.73) 93.3 (47.81-1.73)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.219 , 0.264 0.225 , 0.268	Depositor DCC
$R_{free}$ test set	6527 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 21.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.118 for -h,-k,l 0.118 for k,h,-l 0.390 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10942	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: LAE, ZN, KCX, FE, OH

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	0.47	0/2584	0.63	0/3497
1	B	0.48	0/2584	0.64	0/3497
1	C	0.32	0/2584	0.51	0/3497
1	D	0.30	0/2584	0.50	0/3497
All	All	0.40	0/10336	0.57	0/13988

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	2538	0	2486	21	0
1	B	2538	0	2486	20	0
1	C	2538	0	2486	36	0
1	D	2538	0	2486	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	17	0	19	5	0
6	A	270	0	0	0	0
6	B	252	0	0	1	0
6	C	127	0	0	0	0
6	D	113	0	0	0	0
All	All	10942	0	9963	113	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 6.

All (113) 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:C:60:ARG:O	1:C:60:ARG:NE	1.98	0.96
1:A:278:LEU:HD11	5:A:404:LAE:H222	1.51	0.92
1:C:244:GLU:HG2	1:C:247:ARG:HH21	1.45	0.82
1:A:280:GLU:HA	1:A:283:ALA:HB3	1.63	0.80
1:C:244:GLU:HG2	1:C:247:ARG:NH2	1.99	0.78
1:D:280:GLU:HA	1:D:283:ALA:HB3	1.70	0.72
1:D:19:LYS:HG2	1:D:63:ILE:HD13	1.75	0.69
1:A:59:LYS:NZ	1:A:88:THR:O	2.29	0.64
1:D:265:HIS:HB2	1:D:267:THR:HG23	1.78	0.64
1:C:53:GLU:HG3	1:C:57:LYS:HE2	1.80	0.63
1:C:31:PRO:HG2	1:C:104:GLY:HA2	1.80	0.63
1:C:27:LEU:HD23	1:C:270:VAL:HB	1.81	0.62
1:D:280:GLU:OE1	1:D:284:GLU:HB2	2.00	0.62
1:C:235:GLY:HA3	1:C:285:MET:SD	2.40	0.62
1:C:265:HIS:HB2	1:C:267:THR:HG23	1.83	0.61
1:D:31:PRO:HG2	1:D:104:GLY:HA2	1.83	0.61
1:B:236:MET:HG2	1:B:282:PHE:HD2	1.66	0.61
1:D:258:GLU:HG3	1:D:314:GLN:HG2	1.82	0.61
1:C:163:ALA:HA	1:C:166:ARG:HD3	1.85	0.59
1:B:230:ARG:NH2	1:B:237:VAL:HG11	2.18	0.58
1:D:82:ARG:O	1:D:86:GLU:HG3	2.03	0.58
1:D:230:ARG:HB3	1:D:233:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ARG:NH2	1:D:305:GLU:HG3	2.18	0.57
1:A:237:VAL:HG13	1:A:237:VAL:O	2.05	0.57
1:C:230:ARG:NH1	1:C:237:VAL:HG11	2.18	0.57
1:C:107:PRO:HG3	1:D:103:GLU:HA	1.86	0.56
1:B:303:LYS:NZ	1:B:309:ASP:OD1	2.37	0.56
1:A:113:ARG:HD3	1:A:159:MET:SD	2.46	0.55
1:B:236:MET:HG2	1:B:282:PHE:CD2	2.42	0.55
1:D:294:LEU:O	1:D:299:ILE:HG12	2.07	0.55
1:C:279:PRO:HD3	1:D:115:LEU:HD12	1.88	0.54
1:D:19:LYS:HG3	1:D:316:PHE:HB3	1.88	0.54
1:A:207:MET:HG3	1:A:226:ILE:HB	1.90	0.54
1:B:230:ARG:HH21	1:B:237:VAL:HG11	1.71	0.54
1:A:266:ASN:HD21	5:A:404:LAE:H42	1.72	0.53
1:D:206:HIS:ND1	1:D:230:ARG:HD2	2.23	0.53
1:C:299:ILE:HD12	1:C:312:LEU:HD22	1.91	0.52
1:B:31:PRO:HG2	1:B:104:GLY:HA2	1.90	0.52
1:D:234:GLN:HG2	1:D:241:THR:HA	1.91	0.52
1:A:57:LYS:HG3	1:A:60:ARG:HH21	1.75	0.51
1:D:187:GLU:OE1	1:D:187:GLU:N	2.41	0.51
1:C:162:ARG:O	1:C:166:ARG:HG3	2.10	0.51
1:C:101:GLU:HG3	1:C:156:TYR:CD2	2.46	0.50
1:A:266:ASN:ND2	5:A:404:LAE:H42	2.26	0.50
1:D:250:LEU:HD13	1:D:305:GLU:HG2	1.91	0.50
1:D:152:ARG:HD2	1:D:154:THR:HG22	1.93	0.50
1:A:299:ILE:N	1:A:300:PRO:CD	2.75	0.50
1:D:250:LEU:CD1	1:D:305:GLU:HG2	2.42	0.50
1:D:284:GLU:OE2	1:D:287:LYS:NZ	2.35	0.50
1:D:53:GLU:HG3	1:D:57:LYS:HE3	1.94	0.49
1:C:299:ILE:HD13	1:C:302:LEU:HD12	1.93	0.49
1:A:281:PRO:O	1:A:285:MET:HE2	2.12	0.49
1:D:19:LYS:HE3	1:D:317:ILE:HD11	1.93	0.48
1:A:115:LEU:HD22	1:B:279:PRO:HD3	1.95	0.48
1:C:39:ARG:HD2	1:D:124:ASP:OD2	2.14	0.48
1:A:299:ILE:HD12	1:A:312:LEU:HD22	1.96	0.48
1:C:282:PHE:O	1:C:285:MET:HG2	2.14	0.47
1:A:280:GLU:N	1:A:281:PRO:HD2	2.30	0.47
1:C:3:GLU:O	1:C:14:VAL:HG23	2.15	0.47
1:B:207:MET:HG3	1:B:226:ILE:HB	1.97	0.47
1:D:206:HIS:CG	1:D:230:ARG:HD2	2.49	0.46
1:C:23:HIS:CD2	1:C:266:ASN:OD1	2.68	0.46
1:D:280:GLU:N	1:D:281:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLU:N	1:B:281:PRO:HD2	2.30	0.46
1:D:179:THR:OG1	1:D:206:HIS:HB2	2.14	0.46
1:C:100:TYR:OH	1:C:180:GLN:NE2	2.48	0.46
1:C:28:PHE:HB3	1:C:268:VAL:HG13	1.98	0.46
1:B:280:GLU:HA	1:B:283:ALA:HB3	1.97	0.46
1:C:150:LYS:HE2	1:C:150:LYS:HB3	1.87	0.46
1:B:85:ALA:HB2	1:B:92:ILE:HD12	1.97	0.46
1:A:24:GLU:O	1:A:68:ASP:HA	2.16	0.45
1:A:271:TRP:CZ2	5:A:404:LAE:H181	2.51	0.45
1:C:178:HIS:ND1	1:C:206:HIS:HD2	2.01	0.45
1:D:23:HIS:CD2	1:D:266:ASN:OD1	2.69	0.45
1:A:289:TRP:CZ3	5:A:404:LAE:H182	2.51	0.45
1:B:230:ARG:HB3	1:B:233:ILE:HD12	1.99	0.45
1:C:239:ALA:HB1	1:C:240:PRO:HD2	1.97	0.45
1:C:112:ARG:CZ	1:D:274:ARG:HB3	2.47	0.45
1:B:24:GLU:O	1:B:68:ASP:HA	2.17	0.45
1:D:110:GLN:O	1:D:114:LEU:HD12	2.17	0.44
1:A:19:LYS:HG3	1:A:317:ILE:HD11	1.98	0.44
1:D:22:ILE:HD12	1:D:67:VAL:HG21	1.99	0.44
1:D:178:HIS:ND1	1:D:206:HIS:CD2	2.86	0.44
1:D:168:GLN:HG3	1:D:173:ALA:O	2.17	0.44
1:B:308:ARG:HD3	6:B:699:HOH:O	2.16	0.44
1:D:75:GLY:HA3	1:D:272:LEU:CD1	2.48	0.44
1:C:24:GLU:O	1:C:68:ASP:HA	2.18	0.44
1:B:45:ASP:O	1:B:49:ARG:HG3	2.17	0.43
1:A:106:PRO:N	1:A:107:PRO:CD	2.82	0.43
1:C:17:LEU:HD22	1:C:65:THR:HG21	2.00	0.43
1:C:241:THR:O	1:C:244:GLU:HB2	2.19	0.43
1:C:268:VAL:HG11	1:C:271:TRP:CD2	2.53	0.43
1:D:279:PRO:O	1:D:283:ALA:N	2.52	0.43
1:C:18:GLY:HA3	1:C:64:GLN:OE1	2.19	0.43
1:D:146:LEU:HD21	1:D:164:ALA:HB2	2.01	0.43
1:C:27:LEU:HD22	1:C:272:LEU:HD21	2.00	0.42
1:B:22:ILE:O	1:B:67:VAL:HB	2.20	0.42
1:D:117:THR:OG1	1:D:121:ASP:OD2	2.27	0.42
1:B:106:PRO:N	1:B:107:PRO:CD	2.83	0.42
1:C:22:ILE:O	1:C:22:ILE:HG13	2.20	0.42
1:B:28:PHE:HB3	1:B:268:VAL:HG13	2.02	0.41
1:A:293:HIS:ND1	1:A:297:ASN:HB2	2.36	0.41
1:C:55:ALA:HA	1:C:58:MET:HE2	2.03	0.41
1:C:207:MET:HG3	1:C:226:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HG3	1:A:60:ARG:NH2	2.34	0.41
1:D:28:PHE:HB3	1:D:268:VAL:HG13	2.03	0.41
1:D:19:LYS:HE2	1:D:316:PHE:CB	2.51	0.41
1:B:100:TYR:OH	1:B:103:GLU:HG3	2.21	0.41
1:D:19:LYS:HE2	1:D:316:PHE:HB3	2.03	0.40
1:D:294:LEU:HA	1:D:298:ILE:HB	2.03	0.40
1:C:14:VAL:HG11	1:C:324:PHE:HB2	2.04	0.40
1:B:22:ILE:HD12	1:B:67:VAL:HG21	2.03	0.40
1:D:279:PRO:O	1:D:282:PHE:N	2.55	0.40

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	320/330 (97%)	312 (98%)	8 (2%)	0	100	100
1	B	320/330 (97%)	313 (98%)	7 (2%)	0	100	100
1	C	320/330 (97%)	309 (97%)	11 (3%)	0	100	100
1	D	320/330 (97%)	309 (97%)	11 (3%)	0	100	100
All	All	1280/1320 (97%)	1243 (97%)	37 (3%)	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	263/267 (98%)	261 (99%)	2 (1%)	83	75
1	B	263/267 (98%)	260 (99%)	3 (1%)	76	64
1	C	263/267 (98%)	262 (100%)	1 (0%)	92	88
1	D	263/267 (98%)	259 (98%)	4 (2%)	67	51
All	All	1052/1068 (98%)	1042 (99%)	10 (1%)	78	68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ASP
1	A	264	SER
1	B	64	GLN
1	B	255	ASP
1	B	280	GLU
1	C	264	SER
1	D	200	LYS
1	D	214	ASP
1	D	255	ASP
1	D	264	SER

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	KCX	C	145	1,3,2	7,11,12	0.97	1 (14%)	4,12,14	1.04	0
1	KCX	A	145	1,3,2	7,11,12	1.33	1 (14%)	4,12,14	0.95	0
1	KCX	D	145	1,3,2	7,11,12	0.88	1 (14%)	4,12,14	0.76	0
1	KCX	B	145	1,3,2	7,11,12	1.37	1 (14%)	4,12,14	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	145	1,3,2	-	0/7/10/12	-
1	KCX	A	145	1,3,2	-	0/7/10/12	-
1	KCX	D	145	1,3,2	-	0/7/10/12	-
1	KCX	B	145	1,3,2	-	0/7/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	KCX	CE-NZ	2.88	1.51	1.45
1	B	145	KCX	CE-NZ	2.75	1.51	1.45
1	C	145	KCX	CE-NZ	2.23	1.50	1.45
1	D	145	KCX	CE-NZ	2.05	1.50	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic and 3 are modelled with single atom - leaving 1 for Mogul analysis.



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	$\# Z  > 2$
5	LAE	A	404	-	17,17,17	1.23	1 (5%)	16,21,21	1.08	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LAE	A	404	-	-	7/13/23/23	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	LAE	O3-C2	4.39	1.44	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	LAE	C19-C18-C15	-2.12	109.15	114.60

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	LAE	C14-C13-N11-C1
5	A	404	LAE	O35-C13-N11-C1
5	A	404	LAE	C13-C14-C15-O36
5	A	404	LAE	C15-C18-C19-C22
5	A	404	LAE	C18-C19-C22-C25
5	A	404	LAE	C13-C14-C15-C18
5	A	404	LAE	C5-C1-N11-C13

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	LAE	5	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	322/330 (97%)	-0.27	4 (1%) 79 83	8, 18, 39, 58	0
1	B	322/330 (97%)	-0.32	3 (0%) 84 87	7, 17, 39, 63	0
1	C	322/330 (97%)	0.47	8 (2%) 57 62	27, 39, 53, 66	0
1	D	322/330 (97%)	0.33	6 (1%) 66 71	28, 38, 53, 64	0
All	All	1288/1320 (97%)	0.05	21 (1%) 72 77	7, 33, 51, 66	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	VAL	6.8
1	B	237	VAL	5.5
1	C	282	PHE	5.4
1	C	237	VAL	5.1
1	B	282	PHE	4.7
1	D	282	PHE	4.1
1	C	238	GLY	3.9
1	D	237	VAL	3.6
1	C	236	MET	3.5
1	D	114	LEU	3.2
1	D	236	MET	3.2
1	B	236	MET	2.9
1	D	239	ALA	2.9
1	A	282	PHE	2.9
1	A	239	ALA	2.7
1	C	12	VAL	2.6
1	A	280	GLU	2.3
1	C	281	PRO	2.2
1	C	197	ALA	2.2
1	C	235	GLY	2.1
1	D	41	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	D	145	12/13	0.90	0.12	28,32,38,46	0
1	KCX	C	145	12/13	0.92	0.09	28,35,44,45	0
1	KCX	B	145	12/13	0.96	0.07	7,18,29,38	0
1	KCX	A	145	12/13	0.97	0.07	5,15,25,25	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	LAE	A	404	17/17	0.80	0.24	35,41,47,48	17
4	OH	C	403	1/1	0.93	0.08	34,34,34,34	0
4	OH	A	403	1/1	0.95	0.18	20,20,20,20	0
4	OH	B	403	1/1	0.97	0.08	20,20,20,20	0
3	ZN	D	402	1/1	0.98	0.10	31,31,31,31	1
2	FE	A	401	1/1	0.99	0.03	10,10,10,10	0
3	ZN	C	402	1/1	0.99	0.06	35,35,35,35	1
2	FE	D	401	1/1	0.99	0.10	30,30,30,30	0
3	ZN	B	402	1/1	0.99	0.03	21,21,21,21	1
2	FE	B	401	1/1	1.00	0.03	12,12,12,12	0
3	ZN	A	402	1/1	1.00	0.02	16,16,16,16	1
2	FE	C	401	1/1	1.00	0.12	29,29,29,29	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.