



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:20 AM GMT

PDB ID : 3ORW  
Title : Crystal structure of thermophilic phosphotriesterase from *Geobacillus kaustophilus* HTA426  
Authors : Zheng, B.S.; Yu, S.S.; Zhang, Y.; Lou, Z.Y.; Feng, Y.  
Deposited on : 2010-09-07  
Resolution : 2.40 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

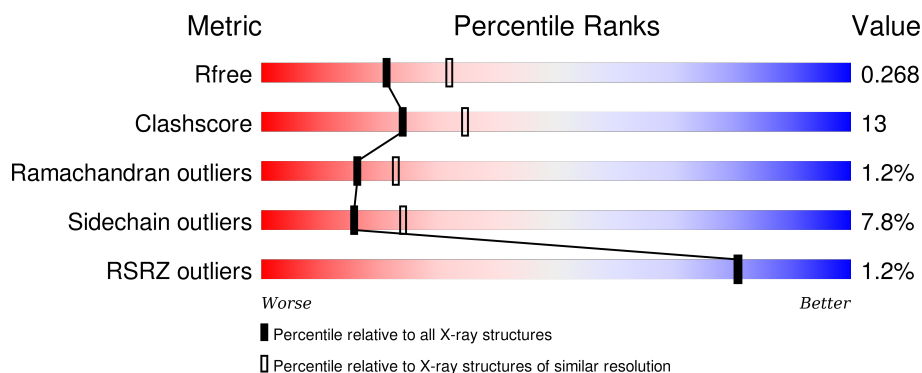
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	326	 72% 24% • •
1	B	326	 2% 64% 27% 8% • •

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5101 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	324	Total	C	N	O	S	0	0	0
			2548	1620	436	476	16			
1	B	324	Total	C	N	O	S	0	0	0
			2548	1620	436	476	16			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Co	0	0
			2	2		
2	A	2	Total	Co	0	0
			2	2		

- Molecule 3 is water.

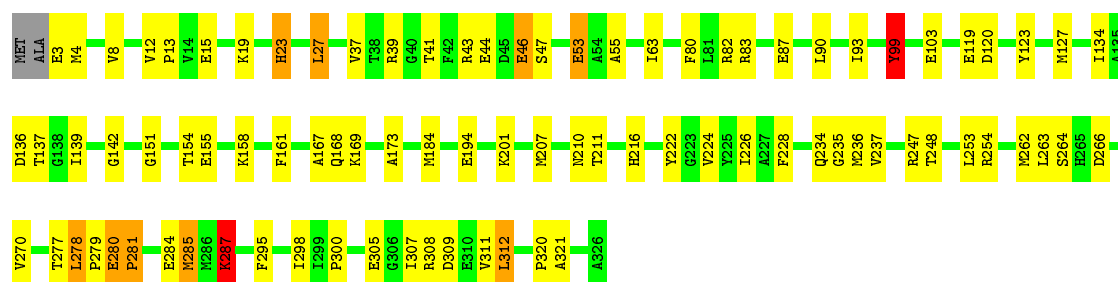
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		

### 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 errors 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.

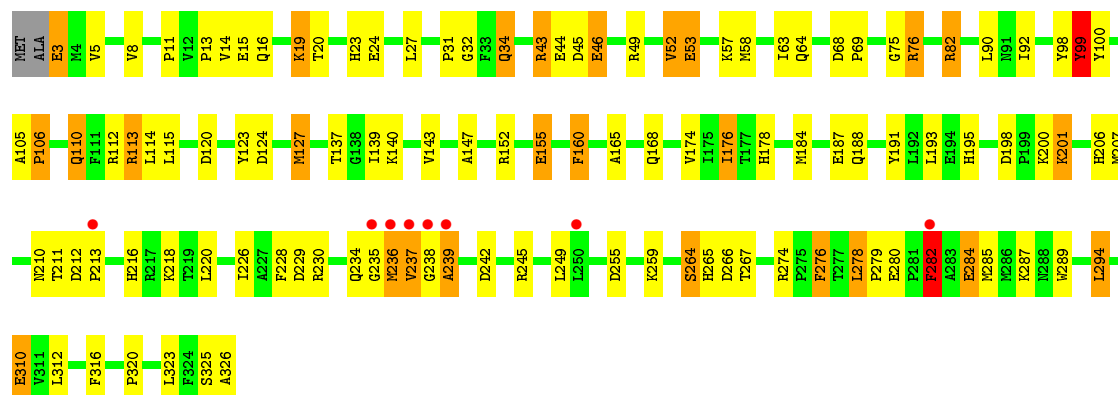
#### • Molecule 1: Phosphotriesterase

Chain A: 



#### • Molecule 1: Phosphotriesterase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.32Å 88.88Å 89.38Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	47.15 – 2.40 47.15 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.15-2.40) 96.2 (47.15-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.268 0.199 , 0.268	Depositor DCC
$R_{free}$ test set	1502 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 29.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29878 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CO, KCX

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	1.45	19/2594 (0.7%)	1.13	6/3510 (0.2%)
1	B	1.44	16/2594 (0.6%)	1.21	11/3510 (0.3%)
All	All	1.45	35/5188 (0.7%)	1.17	17/7020 (0.2%)

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
1	B	0	2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	TYR	CD2-CE2	-8.47	1.26	1.39
1	A	53	GLU	CG-CD	8.39	1.64	1.51
1	A	305	GLU	CG-CD	7.30	1.62	1.51
1	A	161	PHE	CE1-CZ	7.24	1.51	1.37
1	B	155	GLU	CG-CD	7.02	1.62	1.51
1	B	19	LYS	CD-CE	6.99	1.68	1.51
1	A	224	VAL	CB-CG1	6.67	1.66	1.52
1	A	46	GLU	CG-CD	6.61	1.61	1.51
1	B	228	PHE	CE1-CZ	6.34	1.49	1.37
1	B	310	GLU	CG-CD	6.26	1.61	1.51
1	B	3	GLU	CG-CD	6.14	1.61	1.51
1	A	15	GLU	CG-CD	6.11	1.61	1.51
1	A	53	GLU	CD-OE1	5.99	1.32	1.25
1	A	136	ASP	CB-CG	5.88	1.64	1.51
1	A	15	GLU	CB-CG	5.84	1.63	1.52
1	A	119	GLU	CD-OE2	5.63	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	PHE	CE1-CZ	5.49	1.47	1.37
1	B	15	GLU	CD-OE2	5.49	1.31	1.25
1	A	169	LYS	CE-NZ	5.44	1.62	1.49
1	B	276	PHE	CE1-CZ	5.43	1.47	1.37
1	B	99	TYR	CG-CD1	5.29	1.46	1.39
1	A	19	LYS	CD-CE	5.28	1.64	1.51
1	A	305	GLU	CD-OE1	5.21	1.31	1.25
1	B	53	GLU	CG-CD	5.19	1.59	1.51
1	B	187	GLU	CB-CG	5.19	1.62	1.52
1	B	52	VAL	CB-CG2	5.12	1.63	1.52
1	B	165	ALA	CA-CB	-5.11	1.41	1.52
1	A	311	VAL	CB-CG2	5.10	1.63	1.52
1	A	99	TYR	CG-CD1	5.10	1.45	1.39
1	B	160	PHE	CD2-CE2	5.07	1.49	1.39
1	B	76	ARG	CZ-NH2	5.05	1.39	1.33
1	A	321	ALA	CA-CB	5.05	1.63	1.52
1	B	46	GLU	CG-CD	5.04	1.59	1.51
1	A	37	VAL	CB-CG1	5.02	1.63	1.52
1	A	46	GLU	CB-CG	5.01	1.61	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ARG	NE-CZ-NH1	-11.33	114.63	120.30
1	B	274	ARG	NE-CZ-NH1	-7.39	116.61	120.30
1	B	127	MET	CG-SD-CE	-7.31	88.51	100.20
1	B	120	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	43	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	45	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	B	45	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	294	LEU	CA-CB-CG	6.49	130.22	115.30
1	A	120	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	312	LEU	CA-CB-CG	-5.87	101.81	115.30
1	A	278	LEU	CA-CB-CG	5.83	128.70	115.30
1	B	218	LYS	CD-CE-NZ	5.62	124.63	111.70
1	B	114	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	198	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	280	GLU	C-N-CD	5.27	139.46	128.40
1	A	43	ARG	CG-CD-NE	-5.15	100.98	111.80
1	A	247	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	GLN	Peptide
1	B	239	ALA	Peptide

## 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	2548	0	2491	58	0
1	B	2548	0	2492	75	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	B	1	0	0	0	0
All	All	5101	0	4983	132	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 13.

All (132) 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:A:134:ILE:O	1:A:137:THR:HG22	1.08	1.26
1:A:134:ILE:O	1:A:137:THR:CG2	1.87	1.23
1:A:234:GLN:O	1:A:285:MET:HE3	1.62	0.99
1:A:262:MET:HE3	1:A:320:PRO:HG3	1.45	0.97
1:A:127:MET:CE	1:A:167:ALA:HA	2.08	0.84
1:B:236:MET:HE2	1:B:282:PHE:CZ	2.12	0.84
1:B:123:TYR:CE1	1:B:127:MET:HE1	2.14	0.82
1:B:235:GLY:HA3	1:B:285:MET:SD	2.19	0.81
1:A:127:MET:HE1	1:A:167:ALA:HA	1.64	0.80
1:A:137:THR:HG23	1:A:139:ILE:H	1.47	0.79
1:B:325:SER:O	1:B:326:ALA:HB2	1.83	0.79
1:B:236:MET:CE	1:B:282:PHE:CZ	2.67	0.78
1:B:43:ARG:HH11	1:B:43:ARG:HB2	1.49	0.78
1:B:112:ARG:HA	1:B:115:LEU:HD12	1.65	0.76
1:B:210:ASN:O	1:B:216:HIS:HE1	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:SER:O	1:B:326:ALA:CB	2.34	0.76
1:A:235:GLY:HA3	1:A:285:MET:CE	2.15	0.76
1:A:262:MET:CE	1:A:320:PRO:HG3	2.14	0.76
1:B:236:MET:HE1	1:B:282:PHE:CE2	2.22	0.75
1:A:168:GLN:HG3	1:A:173:ALA:O	1.86	0.75
1:B:110:GLN:HE21	1:B:110:GLN:HA	1.54	0.73
1:B:32:GLY:H	1:B:34:GLN:NE2	1.86	0.73
1:A:262:MET:HE3	1:A:320:PRO:CG	2.20	0.72
1:B:32:GLY:H	1:B:34:GLN:HE21	1.36	0.71
1:B:13:PRO:HG2	1:B:16:GLN:NE2	2.04	0.71
1:A:123:TYR:CE1	1:A:127:MET:HE2	2.25	0.71
1:B:265:HIS:HB2	1:B:267:THR:HG23	1.75	0.69
1:B:113:ARG:CZ	1:B:155:GLU:OE2	2.41	0.69
1:A:207:MET:HG3	1:A:226:ILE:HB	1.76	0.68
1:B:123:TYR:CE1	1:B:127:MET:CE	2.77	0.68
1:A:123:TYR:CE1	1:A:127:MET:CE	2.78	0.66
1:B:210:ASN:O	1:B:216:HIS:CE1	2.49	0.66
1:A:55:ALA:HB1	1:A:90:LEU:HD22	1.78	0.65
1:A:123:TYR:HE1	1:A:127:MET:CE	2.11	0.64
1:B:43:ARG:NH1	1:B:43:ARG:HB2	2.12	0.64
1:A:253:LEU:HD13	1:A:307:ILE:HD12	1.79	0.64
1:B:137:THR:HB	1:B:139:ILE:HD12	1.80	0.64
1:B:236:MET:CE	1:B:282:PHE:CE2	2.82	0.62
1:A:210:ASN:O	1:A:216:HIS:HE1	1.82	0.62
1:A:137:THR:HG23	1:A:139:ILE:N	2.14	0.61
1:B:235:GLY:CA	1:B:285:MET:SD	2.89	0.60
1:A:235:GLY:HA3	1:A:285:MET:HE3	1.84	0.60
1:A:235:GLY:HA3	1:A:285:MET:HE1	1.81	0.60
1:B:13:PRO:HG2	1:B:16:GLN:HE21	1.63	0.60
1:B:284:GLU:O	1:B:287:LYS:HG2	2.02	0.59
1:B:237:VAL:HG12	1:B:237:VAL:O	2.03	0.59
1:A:155:GLU:OE1	1:A:158:LYS:NZ	2.36	0.59
1:B:220:LEU:HD21	1:B:226:ILE:HD13	1.86	0.58
1:A:123:TYR:HE1	1:A:127:MET:HE2	1.69	0.57
1:B:191:TYR:O	1:B:195:HIS:HD2	1.88	0.57
1:A:151:GLY:HA2	1:A:184:MET:HE3	1.86	0.56
1:A:151:GLY:HA2	1:A:184:MET:CE	2.36	0.56
1:B:242:ASP:OD1	1:B:245:ARG:NH1	2.39	0.56
1:B:19:LYS:HB3	1:B:63:ILE:HD13	1.90	0.54
1:A:47:SER:HB2	1:A:270:VAL:HG11	1.89	0.54
1:A:210:ASN:O	1:A:216:HIS:CE1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:TYR:HD2	1:A:103:GLU:O	1.92	0.53
1:B:113:ARG:NH2	1:B:155:GLU:OE2	2.42	0.53
1:B:184:MET:O	1:B:188:GLN:HG3	2.08	0.53
1:B:236:MET:HG3	1:B:239:ALA:HB3	1.90	0.53
1:A:284:GLU:O	1:A:287:LYS:HB2	2.09	0.53
1:B:100:TYR:HB3	1:B:147:ALA:HB1	1.90	0.53
1:B:113:ARG:NH1	1:B:113:ARG:HG2	2.24	0.53
1:B:58:MET:O	1:B:63:ILE:HB	2.09	0.52
1:B:98:TYR:HB2	1:B:160:PHE:CE2	2.44	0.52
1:B:68:ASP:C	1:B:68:ASP:OD1	2.47	0.52
1:A:127:MET:HE2	1:A:167:ALA:HA	1.89	0.51
1:B:82:ARG:HH11	1:B:82:ARG:HG2	1.75	0.51
1:A:280:GLU:HA	1:A:280:GLU:OE2	2.10	0.51
1:A:280:GLU:N	1:A:281:PRO:HD2	2.26	0.51
1:B:106:PRO:O	1:B:110:GLN:HG2	2.11	0.50
1:B:229:ASP:O	1:B:266:ASP:HB2	2.12	0.50
1:B:220:LEU:HD21	1:B:226:ILE:CD1	2.40	0.50
1:B:123:TYR:CZ	1:B:127:MET:HE3	2.45	0.50
1:B:113:ARG:NH2	1:B:155:GLU:CD	2.66	0.50
1:A:134:ILE:HB	1:A:137:THR:HG21	1.93	0.49
1:B:282:PHE:CD1	1:B:285:MET:HE3	2.47	0.49
1:A:137:THR:OG1	1:A:139:ILE:HD12	2.12	0.49
1:A:127:MET:HE1	1:A:167:ALA:CA	2.41	0.49
1:A:46:GLU:OE1	1:A:46:GLU:HA	2.12	0.49
1:A:63:ILE:HD11	1:A:295:PHE:CZ	2.48	0.49
1:A:123:TYR:CE1	1:A:127:MET:HE3	2.47	0.49
1:B:43:ARG:HH12	1:B:46:GLU:HB3	1.78	0.49
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.65	0.48
1:B:174:VAL:HG13	1:B:323:LEU:HD11	1.94	0.48
1:A:55:ALA:CB	1:A:90:LEU:HD22	2.41	0.48
1:A:3:GLU:HG2	1:A:4:MET:HG2	1.97	0.47
1:B:143:VAL:HG11	1:B:176:ILE:HD13	1.97	0.47
1:B:276:PHE:HE2	1:B:278:LEU:HD21	1.80	0.47
1:A:87:GLU:HG3	1:A:87:GLU:O	2.15	0.47
1:B:43:ARG:NH1	1:B:46:GLU:HB3	2.30	0.47
1:B:23:HIS:CD2	1:B:69:PRO:HG3	2.50	0.46
1:A:228:PHE:HB2	1:A:263:LEU:HD23	1.98	0.46
1:A:236:MET:O	1:A:237:VAL:HG12	2.16	0.46
1:A:237:VAL:HG13	1:A:237:VAL:O	2.15	0.45
1:A:39:ARG:HE	1:B:124:ASP:CG	2.20	0.45
1:B:207:MET:O	1:B:216:HIS:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:O	1:A:82:ARG:HG3	2.17	0.45
1:A:234:GLN:C	1:A:285:MET:HE3	2.34	0.44
1:B:206:HIS:CG	1:B:230:ARG:HE	2.35	0.44
1:B:8:VAL:HG13	1:B:92:ILE:O	2.18	0.44
1:A:44:GLU:HG2	1:A:83:ARG:HH21	1.83	0.44
1:A:93:ILE:HG23	1:A:142:GLY:HA3	2.00	0.43
1:B:75:GLY:O	1:B:76:ARG:C	2.56	0.43
1:B:113:ARG:NE	1:B:155:GLU:OE2	2.51	0.43
1:A:280:GLU:CA	1:A:280:GLU:OE2	2.66	0.43
1:B:207:MET:HG3	1:B:226:ILE:HB	2.01	0.42
1:B:312:LEU:O	1:B:316:PHE:HD1	2.02	0.42
1:A:154:THR:O	1:A:158:LYS:HG3	2.19	0.42
1:B:211:THR:O	1:B:213:PRO:HD3	2.20	0.42
1:A:27:LEU:HD21	1:A:80:PHE:CE2	2.55	0.42
1:B:24:GLU:OE2	1:B:264:SER:OG	2.31	0.42
1:B:236:MET:HE1	1:B:282:PHE:HE2	1.77	0.41
1:A:216:HIS:CE1	1:A:248:THR:HG21	2.55	0.41
1:A:278:LEU:HA	1:A:279:PRO:HD2	1.81	0.41
1:B:32:GLY:N	1:B:34:GLN:HE21	2.10	0.41
1:B:31:PRO:HB3	1:B:105:ALA:HB2	2.01	0.41
1:A:298:ILE:HD13	1:A:298:ILE:HA	1.87	0.41
1:B:3:GLU:O	1:B:14:VAL:HG23	2.21	0.41
1:B:23:HIS:CD2	1:B:69:PRO:CG	3.04	0.41
1:A:23:HIS:CD2	1:A:266:ASP:OD1	2.73	0.41
1:B:53:GLU:OE1	1:B:57:LYS:HE3	2.20	0.41
1:B:259:LYS:HZ3	1:B:259:LYS:HG3	1.67	0.41
1:B:99:TYR:HA	1:B:99:TYR:HD1	1.80	0.41
1:B:20:THR:HB	1:B:320:PRO:HG2	2.02	0.41
1:B:5:VAL:O	1:B:11:PRO:HA	2.21	0.40
1:B:147:ALA:HA	1:B:178:HIS:HB3	2.04	0.40
1:B:64:GLN:O	1:B:90:LEU:HD12	2.21	0.40
1:B:212:ASP:C	1:B:212:ASP:OD1	2.60	0.40
1:B:200:LYS:C	1:B:201:LYS:HG2	2.40	0.40
1:B:191:TYR:O	1:B:195:HIS:CD2	2.72	0.40
1:A:12:VAL:HG13	1:A:13:PRO:HD2	2.03	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	321/326 (98%)	302 (94%)	15 (5%)	4 (1%)	16	23
1	B	321/326 (98%)	301 (94%)	16 (5%)	4 (1%)	16	23
All	All	642/652 (98%)	603 (94%)	31 (5%)	8 (1%)	16	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	PRO
1	B	237	VAL
1	B	279	PRO
1	A	287	LYS
1	B	238	GLY
1	B	289	TRP
1	A	23	HIS
1	A	280	GLU

### 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	263/264 (100%)	248 (94%)	15 (6%)	25	40
1	B	263/264 (100%)	237 (90%)	26 (10%)	10	14
All	All	526/528 (100%)	485 (92%)	41 (8%)	16	24

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	41	THR
1	A	53	GLU
1	A	99	TYR
1	A	194	GLU
1	A	201	LYS
1	A	211	THR
1	A	254	ARG
1	A	264	SER
1	A	277	THR
1	A	285	MET
1	A	287	LYS
1	A	300	PRO
1	A	308	ARG
1	A	309	ASP
1	B	27	LEU
1	B	34	GLN
1	B	43	ARG
1	B	44	GLU
1	B	49	ARG
1	B	52	VAL
1	B	82	ARG
1	B	99	TYR
1	B	106	PRO
1	B	110	GLN
1	B	113	ARG
1	B	140	LYS
1	B	152	ARG
1	B	168	GLN
1	B	176	ILE
1	B	193	LEU
1	B	201	LYS
1	B	236	MET
1	B	249	LEU
1	B	255	ASP
1	B	264	SER
1	B	278	LEU
1	B	282	PHE
1	B	284	GLU
1	B	294	LEU
1	B	310	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	195	HIS
1	A	216	HIS
1	B	16	GLN
1	B	34	GLN
1	B	110	GLN
1	B	168	GLN
1	B	195	HIS
1	B	216	HIS
1	B	290	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	A	145	1,2	7,11,12	1.60	1 (14%)	7,12,14	1.81	1 (14%)
1	KCX	B	145	1,2	7,11,12	1.76	1 (14%)	7,12,14	2.30	2 (28%)

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	A	145	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	145	1,2	-	0/6/10/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	KCX	O-C	3.99	1.38	1.19
1	B	145	KCX	O-C	4.11	1.38	1.19

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	KCX	O-C-CA	-5.07	112.29	125.49
1	A	145	KCX	O-C-CA	-4.48	113.83	125.49
1	B	145	KCX	CE-NZ-CX	-2.04	121.18	123.49

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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, 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	323/326 (99%)	-0.32	0 100 100	25, 38, 55, 68	0
1	B	323/326 (99%)	-0.20	8 (2%) 61 60	26, 40, 59, 82	0
All	All	646/652 (99%)	-0.26	8 (1%) 81 81	25, 39, 57, 82	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	GLY	7.2
1	B	238	GLY	6.6
1	B	239	ALA	5.3
1	B	237	VAL	5.1
1	B	236	MET	4.9
1	B	282	PHE	3.3
1	B	213	PRO	2.2
1	B	250	LEU	2.2

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	B	145	12/13	0.96	0.13	-	28,29,40,41	0
1	KCX	A	145	12/13	0.97	0.11	-	29,32,35,37	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO	B	328	1/1	0.98	0.13	-0.03	54,54,54,54	0
2	CO	A	328	1/1	0.98	0.11	-0.69	43,43,43,43	0
2	CO	A	327	1/1	0.99	0.11	-	39,39,39,39	0
2	CO	B	327	1/1	1.00	0.15	-	48,48,48,48	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.