



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:45 pm GMT

PDB ID : 3EXI  
Title : Crystal structure of the pyruvate dehydrogenase (E1p) component of human pyruvate dehydrogenase complex with the subunit-binding domain (SBD) of E2p, but SBD cannot be modeled into the electron density  
Authors : Kato, M.; Wynn, R.M.; Chuang, J.L.; Tso, S.-C.; Machius, M.; Li, J.; Chuang, D.T.  
Deposited on : 2008-10-16  
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](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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

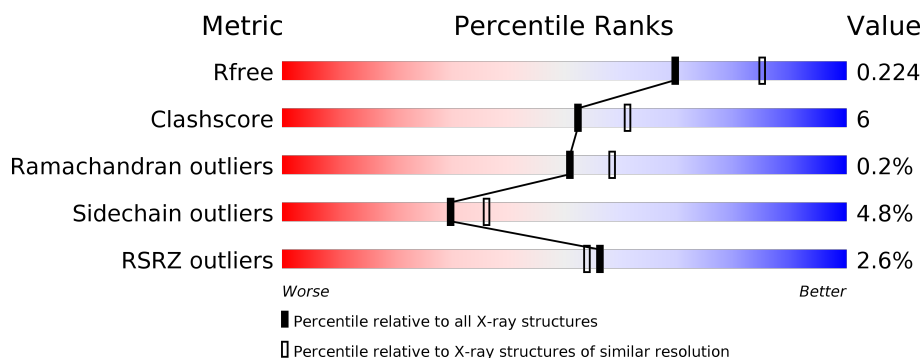
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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  $\geq 3$ , 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	382	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 4%, orange 15%, yellow 18%, green 70%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">70% 15% • 13%</div> </div> </div>
2	B	329	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">4%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 4%, orange 10%, yellow 10%, green 88%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">88% 10% •</div> </div> </div>

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
3	K	A	1001	-	-	-	X
3	K	B	1002	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5425 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 Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	1	0
			2588	1632	451	481	24			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P08559
A	-19	GLY	-	EXPRESSION TAG	UNP P08559
A	-18	SER	-	EXPRESSION TAG	UNP P08559
A	-17	SER	-	EXPRESSION TAG	UNP P08559
A	-16	HIS	-	EXPRESSION TAG	UNP P08559
A	-15	HIS	-	EXPRESSION TAG	UNP P08559
A	-14	HIS	-	EXPRESSION TAG	UNP P08559
A	-13	HIS	-	EXPRESSION TAG	UNP P08559
A	-12	HIS	-	EXPRESSION TAG	UNP P08559
A	-11	HIS	-	EXPRESSION TAG	UNP P08559
A	-10	SER	-	EXPRESSION TAG	UNP P08559
A	-9	SER	-	EXPRESSION TAG	UNP P08559
A	-8	GLY	-	EXPRESSION TAG	UNP P08559
A	-7	LEU	-	EXPRESSION TAG	UNP P08559
A	-6	VAL	-	EXPRESSION TAG	UNP P08559
A	-5	PRO	-	EXPRESSION TAG	UNP P08559
A	-4	ARG	-	EXPRESSION TAG	UNP P08559
A	-3	GLY	-	EXPRESSION TAG	UNP P08559
A	-2	SER	-	EXPRESSION TAG	UNP P08559
A	-1	HIS	-	EXPRESSION TAG	UNP P08559
A	0	MET	-	EXPRESSION TAG	UNP P08559
A	89	PHE	TYR	ENGINEERED	UNP P08559

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2516	1601	427	469	19			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

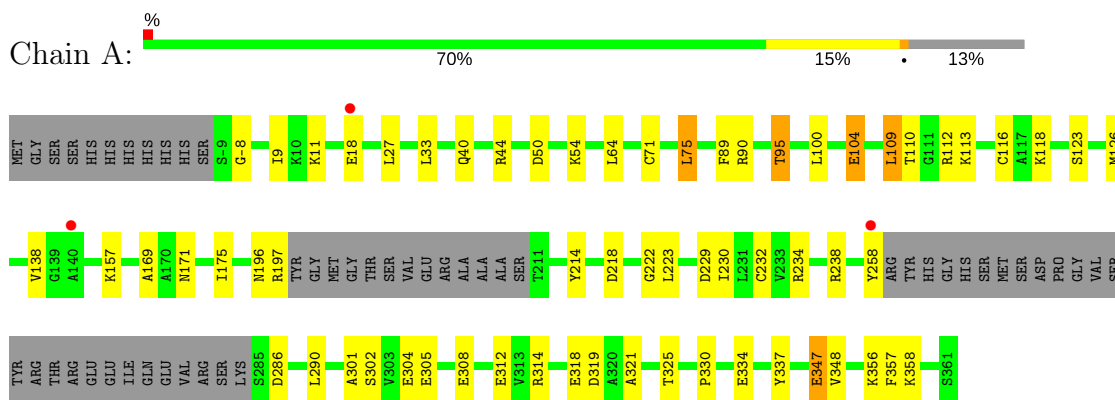
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	153	Total	O	0	0
			153	153		

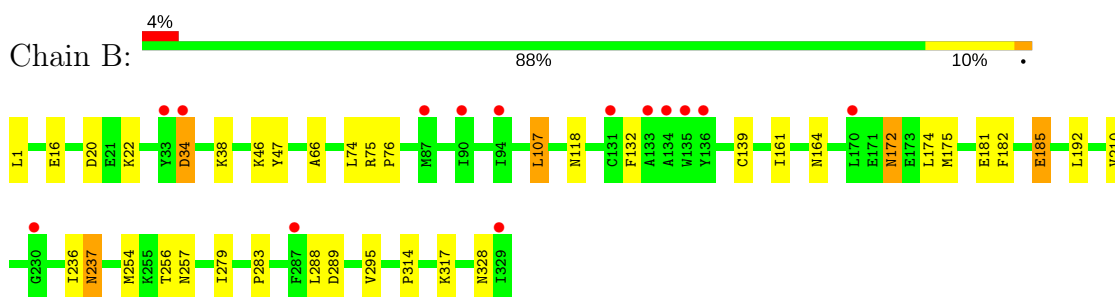
### 3 Residue-property plots

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: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.38Å 154.38Å 82.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.20 39.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.20) 97.8 (39.26-2.20)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.4	Depositor
R, $R_{free}$	0.187 , 0.226 0.188 , 0.224	Depositor DCC
$R_{free}$ test set	1511 reflections (2.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: K, CL

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	0.92	1/2638 (0.0%)	0.85	1/3550 (0.0%)
2	B	0.95	0/2571	0.85	1/3484 (0.0%)
All	All	0.93	1/5209 (0.0%)	0.85	2/7034 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CB-CG	-5.71	1.41	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASP	CB-CG-OD1	5.86	123.57	118.30
2	B	107	LEU	CA-CB-CG	5.52	128.00	115.30

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	2588	0	2560	35	0
2	B	2516	0	2508	29	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
4	A	1	0	0	1	0
5	A	165	0	0	2	0
5	B	153	0	0	3	0
All	All	5425	0	5068	64	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 (64) 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)
2:B:139:CYS:HB3	5:B:2249:HOH:O	1.56	1.06
1:A:95:THR:HG22	1:A:100:LEU:HD22	1.43	0.98
2:B:118:ASN:HD21	2:B:132:PHE:H	1.17	0.86
2:B:172:ASN:HD22	2:B:175:MET:H	1.28	0.81
2:B:34:ASP:HB3	2:B:38:LYS:HE3	1.66	0.78
1:A:348:VAL:HG23	1:A:357:PHE:HB2	1.66	0.77
2:B:1:LEU:N	2:B:181:GLU:OE2	2.19	0.74
1:A:314:ARG:O	1:A:318:GLU:HG2	1.87	0.74
1:A:95:THR:CG2	1:A:100:LEU:HD22	2.21	0.69
1:A:347:GLU:HG2	1:A:356:LYS:HB3	1.75	0.68
2:B:34:ASP:CB	2:B:38:LYS:HE3	2.32	0.59
1:A:9:ILE:HB	1:A:232[A]:CYS:SG	2.42	0.58
1:A:348:VAL:CG2	1:A:357:PHE:HB2	2.35	0.56
2:B:46:LYS:HG2	2:B:47:TYR:CE2	2.40	0.56
1:A:302:SER:OG	1:A:305:GLU:HG3	2.06	0.56
2:B:118:ASN:HD21	2:B:132:PHE:N	1.97	0.55
1:A:334:GLU:HG2	1:A:337:TYR:CE2	2.42	0.55
2:B:254:MET:CE	2:B:283:PRO:HB2	2.38	0.53
2:B:75:ARG:HH12	2:B:164:ASN:ND2	2.07	0.53
2:B:66:ALA:O	2:B:76:PRO:HG3	2.10	0.51
1:A:301:ALA:HA	1:A:305:GLU:OE1	2.11	0.50
1:A:286:ASP:O	1:A:290:LEU:HG	2.13	0.49
1:A:234:ARG:O	1:A:238:ARG:HG3	2.11	0.49
2:B:75:ARG:HH22	2:B:164:ASN:ND2	2.10	0.49
2:B:237:ASN:HD22	2:B:237:ASN:C	2.16	0.48
2:B:34:ASP:HB3	2:B:38:LYS:CE	2.41	0.48
2:B:210:VAL:HG22	2:B:236:ILE:HB	1.96	0.48
1:A:109:LEU:HD13	1:A:126:MET:CE	2.44	0.47
1:A:304:GLU:H	1:A:304:GLU:CD	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ASP:CA	2:B:38:LYS:HE3	2.45	0.47
1:A:302:SER:HB2	1:A:304:GLU:OE1	2.15	0.47
1:A:-8:GLY:HA2	5:A:2113:HOH:O	2.16	0.46
1:A:196:ASN:O	1:A:197:ARG:HB2	2.15	0.46
1:A:64:LEU:O	1:A:90:ARG:HD3	2.16	0.46
1:A:169:ALA:O	1:A:175:ILE:HD12	2.15	0.46
1:A:40:GLN:O	1:A:44:ARG:HG2	2.15	0.45
2:B:256:THR:O	2:B:257:ASN:HB2	2.16	0.45
1:A:138:VAL:HG13	1:A:169:ALA:HB2	1.98	0.45
1:A:197:ARG:HG3	1:A:258:TYR:HA	2.00	0.44
2:B:185:GLU:HB3	5:B:2318:HOH:O	2.16	0.44
2:B:172:ASN:ND2	2:B:175:MET:H	2.05	0.44
2:B:172:ASN:HD21	2:B:174:LEU:HB2	1.83	0.44
2:B:254:MET:HE1	2:B:283:PRO:HB2	1.99	0.44
1:A:314:ARG:HG3	4:A:1003:CL:CL	2.56	0.43
2:B:172:ASN:HD22	2:B:175:MET:N	2.07	0.43
1:A:321:ALA:O	1:A:325:THR:HG23	2.19	0.43
1:A:110:THR:OG1	1:A:112:ARG:HG2	2.19	0.42
1:A:171:ASN:HB2	5:A:2167:HOH:O	2.19	0.42
2:B:16:GLU:HB3	2:B:161:ILE:HG21	2.01	0.42
1:A:318:GLU:HG2	1:A:318:GLU:H	1.68	0.42
1:A:50:ASP:O	1:A:54:LYS:HG3	2.20	0.42
1:A:113:LYS:O	1:A:118:LYS:HG2	2.20	0.41
1:A:113:LYS:HB3	1:A:330:PRO:HA	2.03	0.41
1:A:71:CYS:O	1:A:75:LEU:HD22	2.20	0.41
1:A:214:TYR:O	1:A:222:GLY:HA3	2.20	0.41
2:B:295:VAL:HG12	2:B:314:PRO:HB3	2.02	0.41
2:B:34:ASP:HA	2:B:38:LYS:HE3	2.02	0.41
1:A:109:LEU:CD1	1:A:123:SER:HA	2.50	0.41
2:B:20:ASP:OD1	2:B:20:ASP:C	2.59	0.41
1:A:308:GLU:O	1:A:312:GLU:HG3	2.20	0.41
2:B:22:LYS:NZ	5:B:2293:HOH:O	2.35	0.41
2:B:279:ILE:HD13	2:B:279:ILE:HA	1.96	0.41
1:A:104:GLU:HB3	1:A:116:CYS:HB3	2.02	0.40
2:B:118:ASN:ND2	2:B:132:PHE:H	1.99	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	327/382 (86%)	321 (98%)	5 (2%)	1 (0%)	44	49
2	B	327/329 (99%)	314 (96%)	13 (4%)	0	100	100
All	All	654/711 (92%)	635 (97%)	18 (3%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ASP

### 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	271/312 (87%)	257 (95%)	14 (5%)	27	32
2	B	267/268 (100%)	255 (96%)	12 (4%)	32	39
All	All	538/580 (93%)	512 (95%)	26 (5%)	30	36

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	18	GLU
1	A	27	LEU
1	A	33	LEU
1	A	75	LEU

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Mol	Chain	Res	Type
1	A	89	PHE
1	A	95	THR
1	A	109	LEU
1	A	157	LYS
1	A	223	LEU
1	A	230	ILE
1	A	319	ASP
1	A	347	GLU
1	A	358	LYS
2	B	34	ASP
2	B	74	LEU
2	B	107	LEU
2	B	172	ASN
2	B	182	PHE
2	B	185	GLU
2	B	192	LEU
2	B	237	ASN
2	B	288	LEU
2	B	289	ASP
2	B	317	LYS
2	B	328	ASN

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	55	GLN
1	A	63	HIS
1	A	80	ASN
1	A	130	ASN
1	A	297	ASN
2	B	118	ASN
2	B	164	ASN
2	B	172	ASN
2	B	237	ASN
2	B	328	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 ⓘ

### 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	332/382 (86%)	-0.31	3 (0%) 84 83	41, 48, 59, 79	0
2	B	329/329 (100%)	-0.04	14 (4%) 36 34	41, 48, 56, 74	0
All	All	661/711 (92%)	-0.18	17 (2%) 56 54	41, 48, 58, 79	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	TYR	4.6
1	A	258	TYR	4.0
2	B	90	ILE	3.4
2	B	287	PHE	2.7
2	B	87	MET	2.7
2	B	34	ASP	2.7
1	A	18	GLU	2.4
2	B	94	ILE	2.4
2	B	329	ILE	2.4
2	B	135	TRP	2.3
2	B	134	ALA	2.2
2	B	230	GLY	2.2
2	B	136	TYR	2.2
2	B	131	CYS	2.2
2	B	170	LEU	2.1
1	A	140	ALA	2.1
2	B	133	ALA	2.0

### 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 [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
3	K	B	1002	1/1	0.96	0.16	2.38	75,75,75,75	0
3	K	A	1001	1/1	0.97	0.15	2.24	59,59,59,59	0
4	CL	A	1003	1/1	0.98	0.25	-	62,62,62,62	0

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

There are no such residues in this entry.