



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 05:00 PM BST

PDB ID : 3UXD
Title : Designed protein KE59 R1 7/10H with dichlorobenzotriazole (DBT)
Authors : Khersonsky, O.; Kiss, G.; Roethlisberger, D.; Dym, O.; Albeck, S.; Houk, K.N.; Baker, D.; Tawfik, D.S.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2011-12-05
Resolution : 1.80 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 ⓘ symbol.

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 : 2.13
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) : 2.13

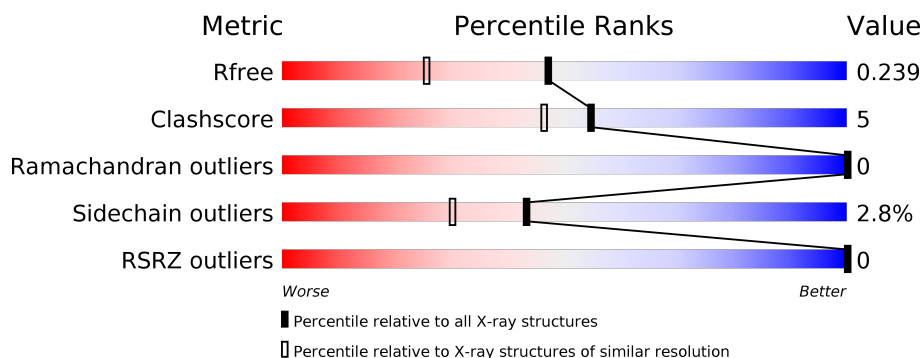
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 ≥ 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	252	 89% 7% ...
1	B	252	 81% 16% ..

2 Entry composition [i](#)

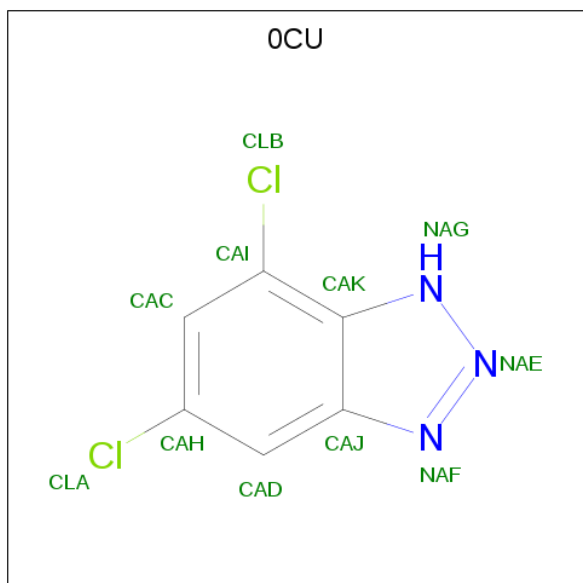
There are 4 unique types of molecules in this entry. The entry contains 4133 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kemp eliminase KE59 R1 7/10H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1944	1244	331	364	5			
1	B	247	Total	C	N	O	S	0	1	0
			1961	1249	339	368	5			

- Molecule 2 is 5,7-dichloro-1H-benzotriazole (three-letter code: 0CU) (formula: $C_6H_3Cl_2N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			11	6	2	3		
2	B	1	Total	C	Cl	N	0	0
			11	6	2	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

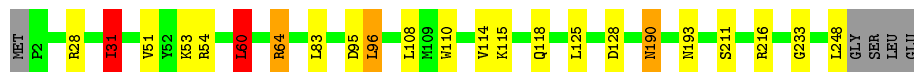
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total	O	0	0
			90	90		
4	B	76	Total	O	0	0
			76	76		

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.

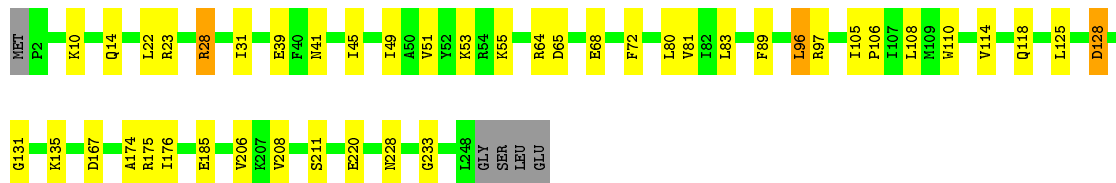
- Molecule 1: Kemp eliminase KE59 R1 7/10H

Chain A:  89% 7% ...



- Molecule 1: Kemp eliminase KE59 R1 7/10H

Chain B:  81% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	62.13Å 62.13Å 120.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.08 – 1.80 40.08 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.08-1.80) 99.7 (40.08-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.175 , 0.233 0.181 , 0.239	Depositor DCC
R_{free} test set	2421 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	1.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.467 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4133	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, OCU

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	1.10	1/1968 (0.1%)	0.96	5/2653 (0.2%)
1	B	1.11	5/1988 (0.3%)	0.97	6/2679 (0.2%)
All	All	1.11	6/3956 (0.2%)	0.97	11/5332 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	ALA	C-O	8.57	1.39	1.23
1	B	174	ALA	CA-C	6.51	1.69	1.52
1	B	39	GLU	CG-CD	5.82	1.60	1.51
1	A	110	TRP	CB-CG	5.72	1.60	1.50
1	B	220	GLU	CB-CG	5.46	1.62	1.52
1	B	72	PHE	CE1-CZ	5.18	1.47	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH1	-10.62	114.99	120.30
1	B	28	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	B	174	ALA	N-CA-C	8.07	132.79	111.00
1	B	175	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	23	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	60	LEU	CB-CG-CD1	6.45	121.96	111.00
1	B	28	ARG	NE-CZ-NH2	5.37	122.99	120.30
1	B	128	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	28	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	64	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	31	ILE	CG1-CB-CG2	-5.09	100.19	111.40

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	1944	0	2017	15	0
1	B	1961	0	2036	28	0
2	A	11	0	3	1	0
2	B	11	0	3	1	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
4	A	90	0	0	1	0
4	B	76	0	0	1	0
All	All	4133	0	4059	42	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 5.

All (42) 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:114:VAL:H	1:B:118:GLN:HE22	1.22	0.85
1:A:114:VAL:H	1:A:118:GLN:HE22	1.27	0.82
1:B:114:VAL:H	1:B:118:GLN:NE2	1.86	0.74
1:B:135:LYS:HE2	1:B:185:GLU:HG3	1.69	0.74
1:A:216:ARG:CD	4:A:321:HOH:O	2.37	0.71
1:A:114:VAL:H	1:A:118:GLN:NE2	1.89	0.70
1:B:65:ASP:OD2	1:B:68:GLU:HG3	1.98	0.64
1:B:131:GLY:HA3	2:B:291:OCU:CLA	2.39	0.59
1:A:108:LEU:HD21	2:A:291:OCU:CLA	2.39	0.59
1:B:176:ILE:HD12	1:B:206:VAL:O	2.04	0.58
1:A:190:ASN:C	1:A:190:ASN:HD22	2.08	0.57
1:A:190:ASN:ND2	1:A:193:ASN:H	2.03	0.56
1:B:176:ILE:HD13	1:B:206:VAL:CG1	2.36	0.55
1:A:53:LYS:HB3	1:A:83:LEU:HD23	1.89	0.55
1:B:31:ILE:HG22	1:B:128:ASP:OD1	2.08	0.53
1:B:110:TRP:C	1:B:110:TRP:CD1	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ILE:CG2	1:B:81:VAL:HG23	2.42	0.48
1:A:96:LEU:HD13	1:A:125:LEU:CB	2.43	0.48
1:B:51:VAL:HB	1:B:233:GLY:HA2	1.95	0.47
1:B:53:LYS:HB3	1:B:83:LEU:HD23	1.96	0.47
1:A:96:LEU:HD13	1:A:125:LEU:HB3	1.97	0.47
1:A:51:VAL:HB	1:A:233:GLY:HA2	1.98	0.46
1:B:96:LEU:HD13	1:B:125:LEU:CB	2.47	0.45
1:A:115:LYS:H	1:A:118:GLN:HE21	1.64	0.45
1:B:176:ILE:CD1	1:B:206:VAL:HG12	2.46	0.44
1:A:31:ILE:HG21	1:A:31:ILE:HD13	1.40	0.44
1:B:176:ILE:HD11	1:B:208:VAL:HG23	2.01	0.43
1:B:97:ARG:HG2	1:B:97:ARG:HH11	1.84	0.43
1:B:108:LEU:HD23	1:B:108:LEU:C	2.40	0.43
1:B:41:ASN:HD21	1:B:228:ASN:HB3	1.84	0.42
1:B:10:LYS:O	1:B:14:GLN:HG3	2.19	0.42
1:B:80:LEU:HG	1:B:105:ILE:HD11	2.02	0.42
1:B:31:ILE:HG12	1:B:106:PRO:HG3	2.02	0.42
1:B:41:ASN:ND2	1:B:228:ASN:HD22	2.18	0.42
1:B:55:LYS:O	1:B:89:PHE:HA	2.19	0.41
1:A:31:ILE:HG22	1:A:128:ASP:OD1	2.20	0.40
1:A:60:LEU:HD22	1:B:167:ASP:HB2	2.03	0.40
1:B:176:ILE:HD13	1:B:206:VAL:HG12	2.04	0.40
1:B:96:LEU:HD13	1:B:125:LEU:HB2	2.02	0.40
1:A:54:ARG:NH2	1:A:95:ASP:OD2	2.46	0.40
1:B:28:ARG:HD2	1:B:28:ARG:HH11	1.68	0.40
1:B:31:ILE:HD11	4:B:316:HOH:O	2.20	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	245/252 (97%)	238 (97%)	7 (3%)	0	100	100
1	B	246/252 (98%)	238 (97%)	8 (3%)	0	100	100
All	All	491/504 (97%)	476 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	209/224 (93%)	202 (97%)	7 (3%)	38	23
1	B	214/224 (96%)	209 (98%)	5 (2%)	50	37
All	All	423/448 (94%)	411 (97%)	12 (3%)	43	30

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	60	LEU
1	A	64	ARG
1	A	96	LEU
1	A	190	ASN
1	A	211	SER
1	A	248	LEU
1	B	22	LEU
1	B	45	ILE
1	B	64	ARG
1	B	96	LEU
1	B	211	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN

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Mol	Chain	Res	Type
1	A	118	GLN
1	A	124	ASN
1	A	161	ASN
1	A	190	ASN
1	B	41	ASN
1	B	118	GLN
1	B	124	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	$\# Z > 2$
3	PO4	A	253	-	4,4,4	1.36	0	6,6,6	1.33	1 (16%)
3	PO4	B	256	-	4,4,4	1.59	1 (25%)	6,6,6	1.03	0
2	0CU	A	291	-	9,12,12	1.80	4 (44%)	10,17,17	2.35	5 (50%)
3	PO4	A	254	-	4,4,4	1.21	0	6,6,6	0.70	0
3	PO4	B	255	-	4,4,4	0.53	0	6,6,6	0.87	0
3	PO4	A	255	-	4,4,4	0.99	0	6,6,6	1.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	256	-	4,4,4	0.89	0	6,6,6	0.70	0
3	PO4	B	253	-	4,4,4	1.51	0	6,6,6	1.56	1 (16%)
3	PO4	B	254	-	4,4,4	1.02	0	6,6,6	0.93	0
2	0CU	B	291	-	9,12,12	1.37	1 (11%)	10,17,17	3.29	7 (70%)

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
2	0CU	A	291	-	-	-	0/2/2/2
2	0CU	B	291	-	-	-	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	291	0CU	CAI-CAK	-2.84	1.38	1.42
2	A	291	0CU	CAH-CLA	-2.66	1.68	1.74
2	B	291	0CU	CAH-CLA	-2.59	1.68	1.74
3	B	256	PO4	P-O1	2.54	1.56	1.50
2	A	291	0CU	CAD-CAJ	-2.51	1.37	1.41
2	A	291	0CU	CAK-NAG	-2.26	1.31	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	291	0CU	CAH-CAD-CAJ	-5.17	115.13	119.50
2	B	291	0CU	CAC-CAH-CLA	-5.03	112.86	119.15
2	B	291	0CU	CAK-CAI-CLB	4.42	123.02	118.97
2	A	291	0CU	CAH-CAD-CAJ	-4.14	116.01	119.50
2	B	291	0CU	CAC-CAI-CAK	-4.12	118.10	120.98
2	A	291	0CU	CAC-CAI-CAK	-3.60	118.47	120.98
2	A	291	0CU	CAK-CAI-CLB	2.81	121.54	118.97
2	B	291	0CU	CAD-CAH-CAC	2.57	124.87	121.66
2	A	291	0CU	CAD-CAH-CAC	2.52	124.81	121.66
3	A	253	PO4	O4-P-O1	-2.46	101.90	110.89
2	B	291	0CU	CAD-CAJ-NAF	2.42	134.43	130.51
3	B	253	PO4	O3-P-O1	-2.21	102.81	110.89
2	A	291	0CU	CAD-CAJ-NAF	2.13	133.97	130.51
2	B	291	0CU	CAD-CAH-CLA	2.09	122.26	119.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	291	0CU	1	0
2	B	291	0CU	1	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	247/252 (98%)	-0.71	0 100 100	14, 21, 30, 35	0
1	B	247/252 (98%)	-0.71	0 100 100	14, 21, 29, 37	0
All	All	494/504 (98%)	-0.71	0 100 100	14, 21, 30, 37	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	0CU	A	291	11/11	0.78	0.17	43,44,47,55	11
2	0CU	B	291	11/11	0.82	0.15	43,45,46,53	11
3	PO4	A	255	5/5	0.93	0.15	52,53,55,57	0
3	PO4	B	256	5/5	0.95	0.14	46,49,51,52	0
3	PO4	B	255	5/5	0.96	0.15	52,53,55,56	0
3	PO4	A	256	5/5	0.97	0.16	49,49,51,52	0
3	PO4	B	254	5/5	0.98	0.06	45,45,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	B	253	5/5	0.99	0.07	23,24,27,27	0
3	PO4	A	254	5/5	0.99	0.08	44,45,47,48	0
3	PO4	A	253	5/5	0.99	0.07	23,23,25,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.