



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:26 AM UTC

PDB ID : 3TW7 / pdb_00003tw7
Title : Structure of Rhizobium etli pyruvate carboxylase T882A crystallized without acetyl coenzyme-A
Authors : St Maurice, M.; Kumar, S.; Lietzan, A.D.
Deposited on : 2011-09-21
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

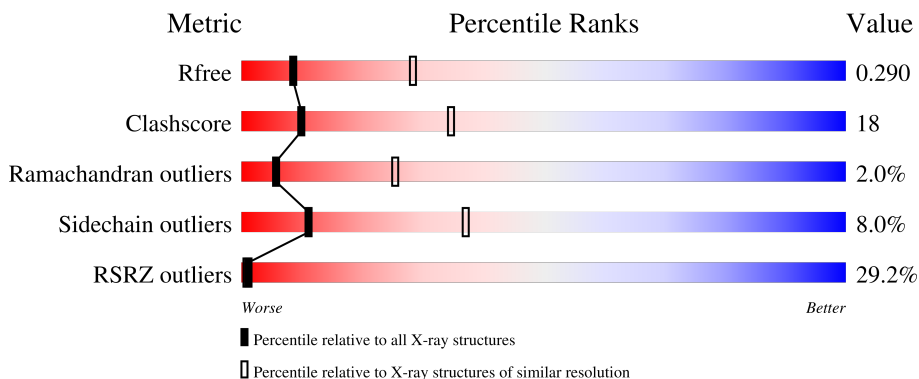
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	1165	
1	B	1165	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15185 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 carboxylase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1004	Total	C	N	O	S	0	15	0
			7544	4804	1275	1434	31			
1	B	1002	Total	C	N	O	S	0	16	0
			7623	4853	1290	1449	31			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q2K340
A	-9	HIS	-	expression tag	UNP Q2K340
A	-8	HIS	-	expression tag	UNP Q2K340
A	-7	HIS	-	expression tag	UNP Q2K340
A	-6	HIS	-	expression tag	UNP Q2K340
A	-5	HIS	-	expression tag	UNP Q2K340
A	-4	HIS	-	expression tag	UNP Q2K340
A	-3	HIS	-	expression tag	UNP Q2K340
A	-2	HIS	-	expression tag	UNP Q2K340
A	-1	HIS	-	expression tag	UNP Q2K340
A	0	GLY	-	expression tag	UNP Q2K340
A	1	GLY	-	expression tag	UNP Q2K340
A	882	ALA	THR	engineered mutation	UNP Q2K340
B	-10	MET	-	expression tag	UNP Q2K340
B	-9	HIS	-	expression tag	UNP Q2K340
B	-8	HIS	-	expression tag	UNP Q2K340
B	-7	HIS	-	expression tag	UNP Q2K340
B	-6	HIS	-	expression tag	UNP Q2K340
B	-5	HIS	-	expression tag	UNP Q2K340
B	-4	HIS	-	expression tag	UNP Q2K340
B	-3	HIS	-	expression tag	UNP Q2K340
B	-2	HIS	-	expression tag	UNP Q2K340
B	-1	HIS	-	expression tag	UNP Q2K340
B	0	GLY	-	expression tag	UNP Q2K340
B	1	GLY	-	expression tag	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
B	882	ALA	THR	engineered mutation	UNP Q2K340

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

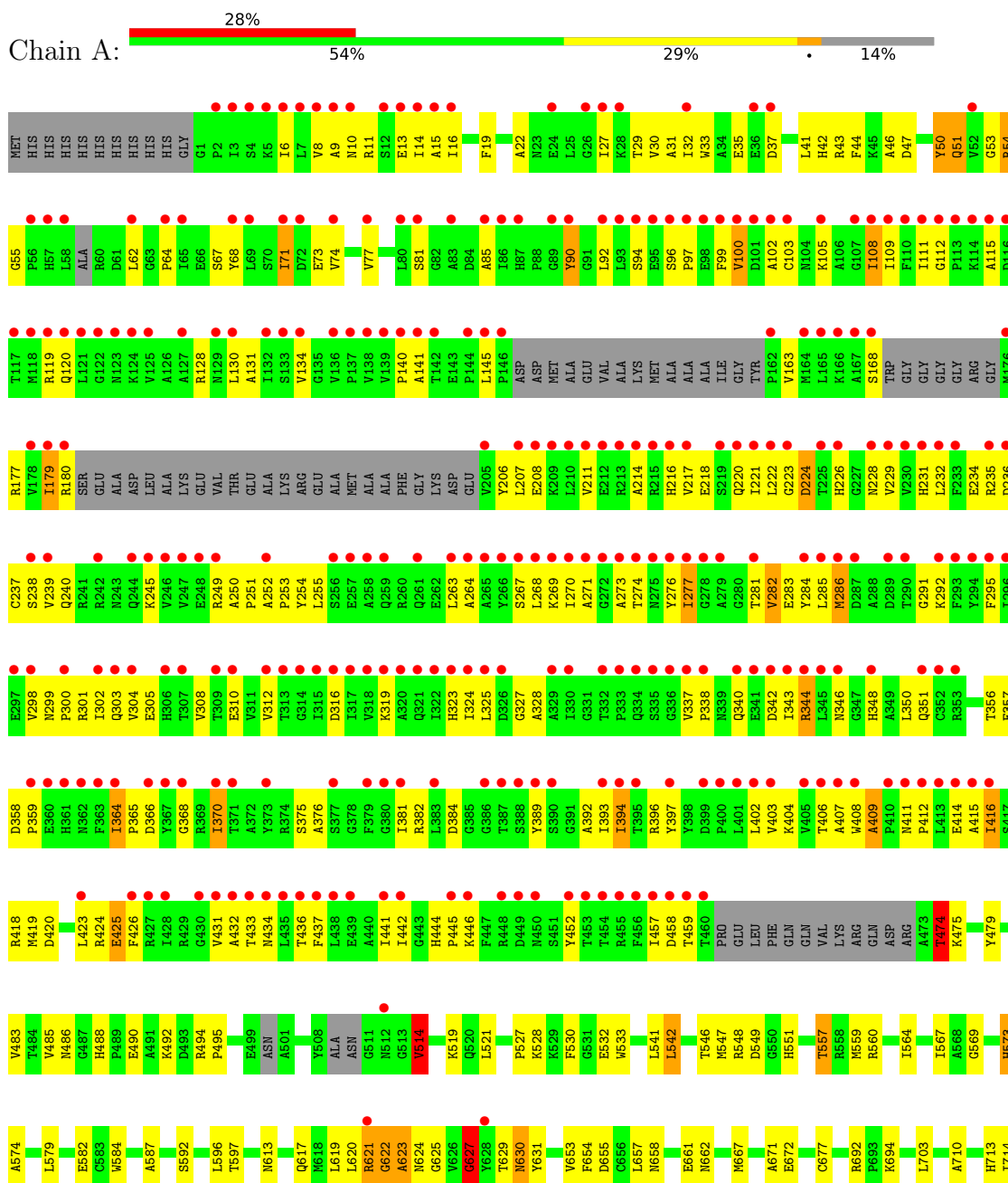
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	5	Total O 5 5	0	0

3 Residue-property plots

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: Pyruvate carboxylase protein



GLU	I1061	L926	W814	G627	ALA
THR	K1062	G927	R818	Y628	ASN
ALA	V1063	Q928	K829	Y631	GLY
ILE	P1064	P929	K829	Y631	ASN
HIS	D1065	P930	K829	Y631	G513
ALA	R1066	P931	K829	Y631	V514
GLU	ALA	S931	E834	N634	K519
LYS	HIS	Q938	E834	L650	Q520
ASP	GLY	Q938	H838	L650	L521
GLY	ALA	A941	E839	C656	T524
THR	ALA	A941	M840	L657	G831
THR	THR	V950	M840	M658	M534
ILE	GLY	V950	G843	W658	L542
ALA	ALA	L955	Q844	W659	L542
ALA	ALA	L955	Q844	V660	M547
GLU	VAL	E958	F845	E661	R548
VAL	VAL	E958	F845	E661	H551
LEU	ARG	Y987	Q851	R664	L555
VAL	ARG	Y987	Q851	V665	A556
LYS	LYS	Y987	A852	V665	T557
ALA	ALA	V990	R853	S666	R558
GLY	GLU	V990	R853	S666	M559
ASP	PRO	S998	L857	M667	R560
GLN	GLY	S998	L857	M667	T561
ILE	ASN	Y1001	E858	L676	Y662
ASP	ALA	Y1001	T859	C677	D663
LYS	ALA	G1002	R860	C677	I664
ASP	VAL	P1003	W861	E678	A665
LEU	VAL	P1003	W861	E678	R566
LEU	GLY	T1009	H862	H713	A574
ALA	ALA	T1009	H862	I714	L579
ALA	ALA	E1021	Q863	I714	E582
VAL	MET	E1021	Q863	I714	C583
TYR	PRO	D1025	L881	M720	W584
GLY	GLY	I1026	V881	M720	D590
GLY	ILE	E1027	A862	M720	T597
ILE	VAL	K1028	A862	M720	E588
SER	VAL	G1029	P883	K725	C583
ARG	SER	G1029	P883	K725	W584
VAL	ARG	K1030	S884	L724	D590
PHE	VAL	T1031	S884	L724	T597
VAL	VAL	T1031	S884	L724	E588
SER	SER	V1032	K886	K725	D599
SER	GLY	V1032	V887	K725	P600
GLY	GLN	N1036	A892	L754	R603
GLN	ALA	Q1037	A892	L754	P804
ALA	VAL	T1042	L893	I754	L604
VAL	VAL	D1043	L893	I754	L615
ASN	ASN	S1044	M894	D771	M624
ALA	ALA	Q1045	M894	D771	G625
GLY	GLY	G1046	M895	D771	Y813
ASP	ASP	W1047	V896	M774	
VAL	VAL	V1048	V896	D775	
LEU	LEU	F1051	L900	D775	
VAL	VAL	F1051	L900	D775	
SER	SER	F1052	T901	P784	
ILE	ILE	E1053	V902	P784	
GLU	GLU	L1054	A903	I789	
ALA	ALA	L1054	A903	I789	
MET	MET	P1058	D904	I789	
LYS	LYS	R1059	S907	D803	
MET	MET	R1060	S907	D803	

4 Data and refinement statistics i

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	264.16Å 264.16Å 91.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.10) 99.9 (50.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.13 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.250 , 0.292 0.248 , 0.290	Depositor DCC
R_{free} test set	2964 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15185	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, ZN, KCX, MG

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	0.94	6/7719 (0.1%)	1.12	28/10500 (0.3%)
1	B	0.96	2/7799 (0.0%)	1.18	42/10603 (0.4%)
All	All	0.95	8/15518 (0.1%)	1.15	70/21103 (0.3%)

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	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1045	GLN	CD-NE2	7.97	1.50	1.33
1	A	749	HIS	CA-C	-6.75	1.44	1.52
1	A	1043	ASP	CA-C	6.33	1.56	1.53
1	A	573	HIS	CG-CD2	5.89	1.42	1.35
1	A	1045	GLN	CG-CD	5.88	1.66	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	GLU	N-CA-C	9.06	121.98	111.11
1	B	626	VAL	N-CA-C	-8.20	105.33	113.20
1	B	125	VAL	N-CA-C	-8.18	105.05	112.90
1	B	851	GLN	N-CA-C	-8.15	103.28	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	ASP	N-CA-C	7.84	116.28	108.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1046	GLY	Peptide
1	B	1065	ASP	Peptide

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	7544	0	7261	257	0
1	B	7623	0	7393	269	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	7	0	0	0	0
5	B	5	0	0	0	0
All	All	15185	0	14654	522	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 18.

The worst 5 of 522 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:4:SER:O	1:B:28:LYS:HG3	1.53	1.08
1:A:359:PRO:HD3	1:A:433:THR:O	1.55	1.06
1:A:90:TYR:HB2	1:A:301:ARG:HH11	1.21	1.05
1:A:1029:GLY:HA3	1:A:1030:LYS:HB2	1.39	1.04
1:B:1029:GLY:CA	1:B:1030:LYS:HB2	1.88	1.04

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	1001/1165 (86%)	875 (87%)	107 (11%)	19 (2%)	6	27
1	B	1002/1165 (86%)	899 (90%)	82 (8%)	21 (2%)	5	25
All	All	2003/2330 (86%)	1774 (89%)	189 (9%)	40 (2%)	6	25

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	622	GLY
1	A	623	ALA
1	A	1030	LYS
1	B	92	LEU

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	749/933 (80%)	695 (93%)	54 (7%)	13	40
1	B	769/933 (82%)	701 (91%)	68 (9%)	9	33
All	All	1518/1866 (81%)	1396 (92%)	122 (8%)	11	37

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	69	LEU
1	B	885	SER
1	B	263[A]	LEU
1	B	884	SER
1	B	1042	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	486	ASN
1	B	1057	GLN
1	B	536	ASN
1	B	847	ASN
1	A	820	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	B	718[A]	3,1	10,11,12	0.94	0	6,12,14	0.92	0
1	KCX	A	718[A]	3,1	10,11,12	0.72	0	6,12,14	1.02	1 (16%)

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	B	718[A]	3,1	-	3/9/10/12	-
1	KCX	A	718[A]	3,1	-	1/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718[A]	KCX	CD-CG-CB	-2.22	105.24	113.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718[A]	KCX	O-C-CA-CB
1	B	718[A]	KCX	O-C-CA-CB
1	B	718[A]	KCX	CG-CD-CE-NZ
1	B	718[A]	KCX	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1003/1165 (86%)	1.17	330 (32%) 1 0	16, 71, 162, 191	22 (2%)
1	B	1001/1165 (85%)	0.93	255 (25%) 1 1	17, 56, 139, 190	22 (2%)
All	All	2004/2330 (86%)	1.05	585 (29%) 1 1	16, 64, 156, 191	44 (2%)

The worst 5 of 585 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	LEU	10.9
1	B	335	SER	9.3
1	A	285	LEU	8.8
1	B	167	ALA	8.2
1	A	367	TYR	7.1

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, 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
1	KCX	A	718[A]	12/13	0.97	0.07	20,21,22,22	0
1	KCX	B	718[A]	12/13	0.97	0.07	19,21,22,22	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(\AA^2)	Q<0.9
2	MG	A	1200	1/1	0.88	0.14	25,25,25,25	0
2	MG	B	1200	1/1	0.92	0.15	40,40,40,40	0
4	CL	A	1202	1/1	0.96	0.10	24,24,24,24	0
3	ZN	A	1201	1/1	0.98	0.04	56,56,56,56	0
3	ZN	B	1201	1/1	0.99	0.05	59,59,59,59	0
4	CL	B	1202	1/1	0.99	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.