



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2021 – 01:14 AM EDT

PDB ID : 3B8U  
Title : Crystal structure of Escherichia coli alaine racemase mutant E221A  
Authors : Wu, D.; Hu, T.; Zhang, L.; Jiang, H.; Shen, X.  
Deposited on : 2007-11-02  
Resolution : 3.00 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](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	:	2.23.2
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)	:	2.23.2



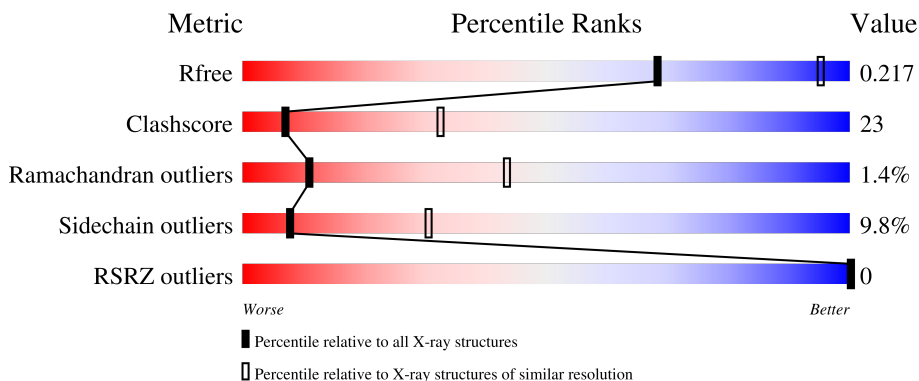
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	379	
1	B	379	
1	C	379	
1	D	379	

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
2	SO4	C	360	-	-	X	-
2	SO4	D	360	-	-	X	-
3	PLP	D	1001	-	X	-	-



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11327 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 Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2750	1732	498	505	15			
1	B	358	Total	C	N	O	S	0	0	0
			2742	1727	497	504	14			
1	C	350	Total	C	N	O	S	0	0	0
			2687	1696	488	490	13			
1	D	349	Total	C	N	O	S	0	0	0
			2674	1689	484	488	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P0A6B4
A	-18	GLY	-	expression tag	UNP P0A6B4
A	-17	SER	-	expression tag	UNP P0A6B4
A	-16	SER	-	expression tag	UNP P0A6B4
A	-15	HIS	-	expression tag	UNP P0A6B4
A	-14	HIS	-	expression tag	UNP P0A6B4
A	-13	HIS	-	expression tag	UNP P0A6B4
A	-12	HIS	-	expression tag	UNP P0A6B4
A	-11	HIS	-	expression tag	UNP P0A6B4
A	-10	HIS	-	expression tag	UNP P0A6B4
A	-9	SER	-	expression tag	UNP P0A6B4
A	-8	SER	-	expression tag	UNP P0A6B4
A	-7	GLY	-	expression tag	UNP P0A6B4
A	-6	LEU	-	expression tag	UNP P0A6B4
A	-5	VAL	-	expression tag	UNP P0A6B4
A	-4	PRO	-	expression tag	UNP P0A6B4
A	-3	ARG	-	expression tag	UNP P0A6B4
A	-2	GLY	-	expression tag	UNP P0A6B4
A	-1	SER	-	expression tag	UNP P0A6B4
A	0	HIS	-	expression tag	UNP P0A6B4
A	221	ALA	GLU	engineered mutation	UNP P0A6B4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P0A6B4
B	-18	GLY	-	expression tag	UNP P0A6B4
B	-17	SER	-	expression tag	UNP P0A6B4
B	-16	SER	-	expression tag	UNP P0A6B4
B	-15	HIS	-	expression tag	UNP P0A6B4
B	-14	HIS	-	expression tag	UNP P0A6B4
B	-13	HIS	-	expression tag	UNP P0A6B4
B	-12	HIS	-	expression tag	UNP P0A6B4
B	-11	HIS	-	expression tag	UNP P0A6B4
B	-10	HIS	-	expression tag	UNP P0A6B4
B	-9	SER	-	expression tag	UNP P0A6B4
B	-8	SER	-	expression tag	UNP P0A6B4
B	-7	GLY	-	expression tag	UNP P0A6B4
B	-6	LEU	-	expression tag	UNP P0A6B4
B	-5	VAL	-	expression tag	UNP P0A6B4
B	-4	PRO	-	expression tag	UNP P0A6B4
B	-3	ARG	-	expression tag	UNP P0A6B4
B	-2	GLY	-	expression tag	UNP P0A6B4
B	-1	SER	-	expression tag	UNP P0A6B4
B	0	HIS	-	expression tag	UNP P0A6B4
B	221	ALA	GLU	engineered mutation	UNP P0A6B4
C	-19	MET	-	expression tag	UNP P0A6B4
C	-18	GLY	-	expression tag	UNP P0A6B4
C	-17	SER	-	expression tag	UNP P0A6B4
C	-16	SER	-	expression tag	UNP P0A6B4
C	-15	HIS	-	expression tag	UNP P0A6B4
C	-14	HIS	-	expression tag	UNP P0A6B4
C	-13	HIS	-	expression tag	UNP P0A6B4
C	-12	HIS	-	expression tag	UNP P0A6B4
C	-11	HIS	-	expression tag	UNP P0A6B4
C	-10	HIS	-	expression tag	UNP P0A6B4
C	-9	SER	-	expression tag	UNP P0A6B4
C	-8	SER	-	expression tag	UNP P0A6B4
C	-7	GLY	-	expression tag	UNP P0A6B4
C	-6	LEU	-	expression tag	UNP P0A6B4
C	-5	VAL	-	expression tag	UNP P0A6B4
C	-4	PRO	-	expression tag	UNP P0A6B4
C	-3	ARG	-	expression tag	UNP P0A6B4
C	-2	GLY	-	expression tag	UNP P0A6B4
C	-1	SER	-	expression tag	UNP P0A6B4
C	0	HIS	-	expression tag	UNP P0A6B4
C	221	ALA	GLU	engineered mutation	UNP P0A6B4

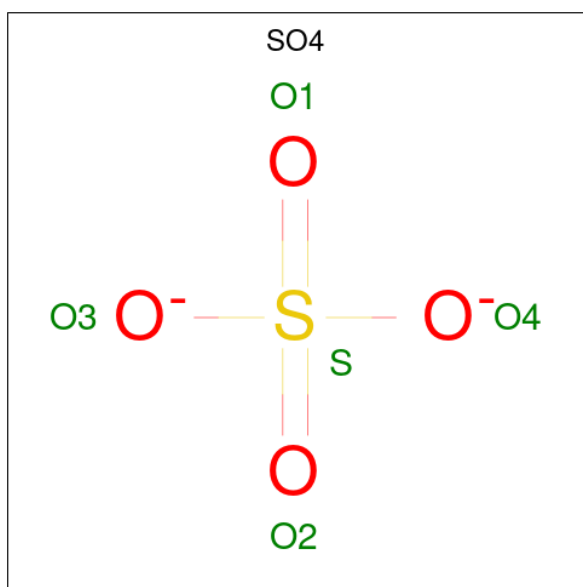
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P0A6B4
D	-18	GLY	-	expression tag	UNP P0A6B4
D	-17	SER	-	expression tag	UNP P0A6B4
D	-16	SER	-	expression tag	UNP P0A6B4
D	-15	HIS	-	expression tag	UNP P0A6B4
D	-14	HIS	-	expression tag	UNP P0A6B4
D	-13	HIS	-	expression tag	UNP P0A6B4
D	-12	HIS	-	expression tag	UNP P0A6B4
D	-11	HIS	-	expression tag	UNP P0A6B4
D	-10	HIS	-	expression tag	UNP P0A6B4
D	-9	SER	-	expression tag	UNP P0A6B4
D	-8	SER	-	expression tag	UNP P0A6B4
D	-7	GLY	-	expression tag	UNP P0A6B4
D	-6	LEU	-	expression tag	UNP P0A6B4
D	-5	VAL	-	expression tag	UNP P0A6B4
D	-4	PRO	-	expression tag	UNP P0A6B4
D	-3	ARG	-	expression tag	UNP P0A6B4
D	-2	GLY	-	expression tag	UNP P0A6B4
D	-1	SER	-	expression tag	UNP P0A6B4
D	0	HIS	-	expression tag	UNP P0A6B4
D	221	ALA	GLU	engineered mutation	UNP P0A6B4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

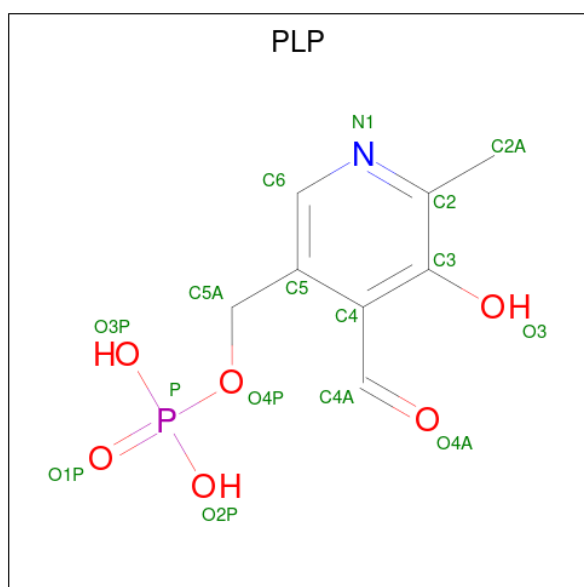
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

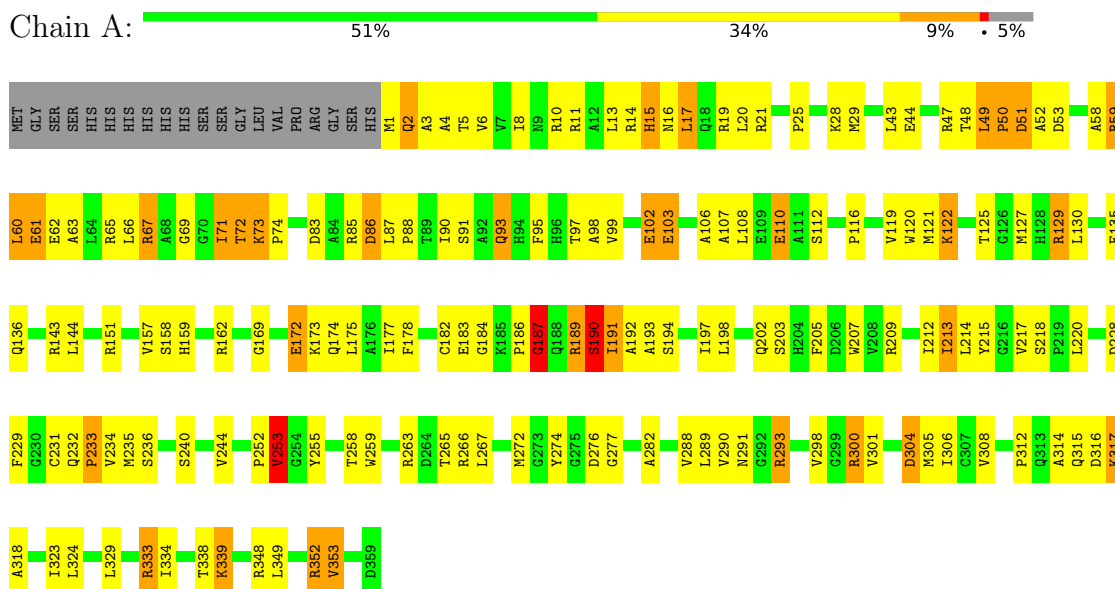
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	134	Total	O	0	0
			134	134		
4	C	60	Total	O	0	0
			60	60		
4	D	62	Total	O	0	0
			62	62		



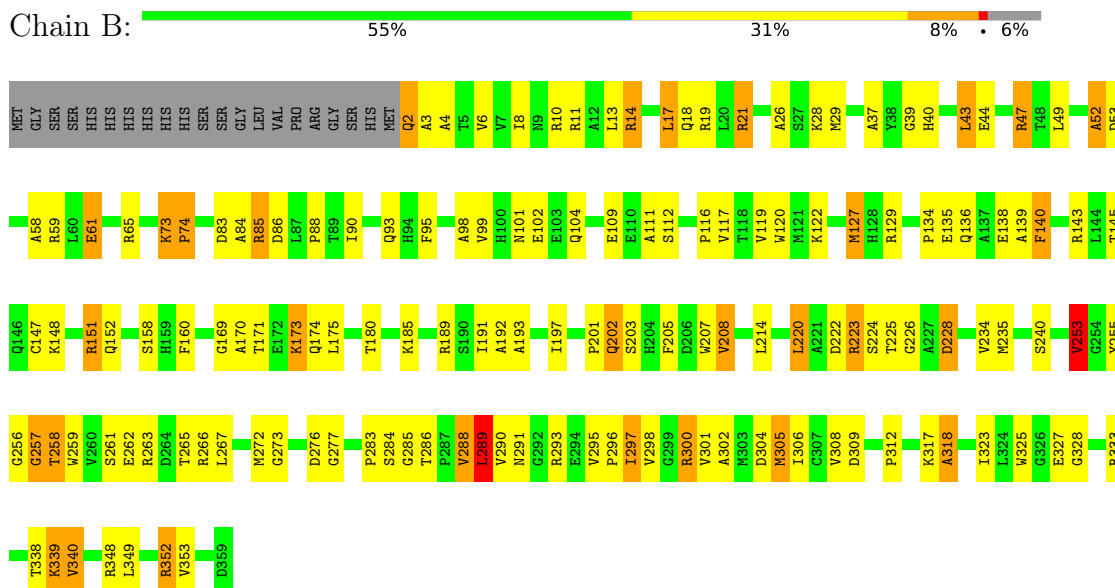
### 3 Residue-property plots

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: Alanine racemase



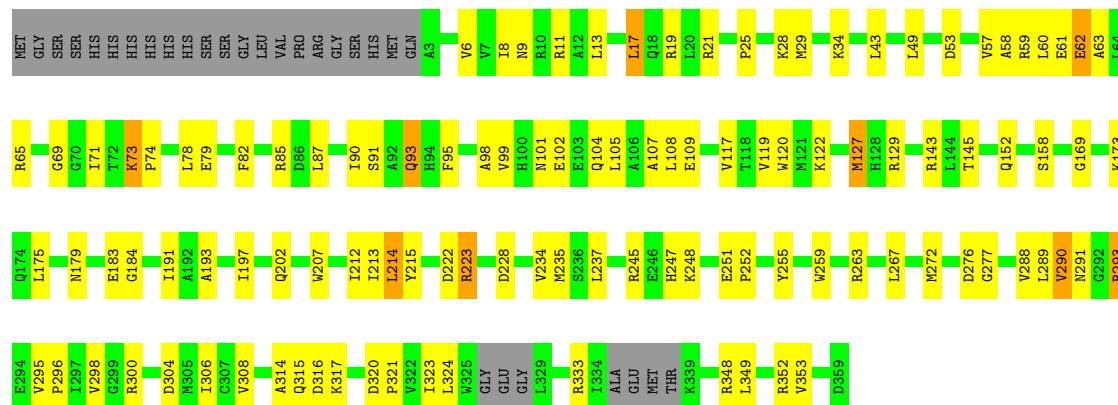
#### • Molecule 1: Alanine racemase





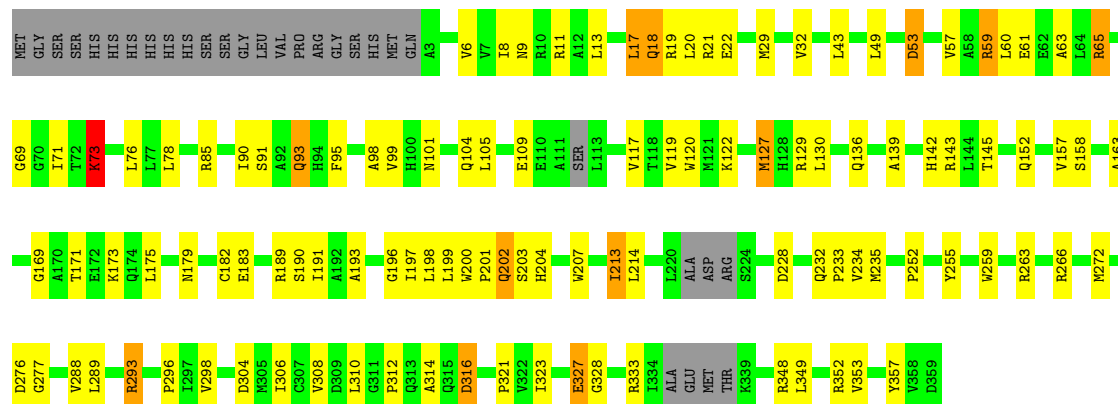
- Molecule 1: Alanine racemase

Chain C:  63% 27% 8%



- Molecule 1: Alanine racemase

Chain D:  63% 26% 8%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.95Å 147.95Å 163.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 35.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (15.00-3.00) 97.4 (35.54-3.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.224 0.208 , 0.217	Depositor DCC
$R_{free}$ test set	3765 reflections (9.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 3.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.459 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: SO4, PLP, 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	0.94	1/2795 (0.0%)	0.95	6/3795 (0.2%)
1	B	0.92	2/2787 (0.1%)	0.94	10/3785 (0.3%)
1	C	0.55	0/2730	0.90	11/3706 (0.3%)
1	D	0.49	0/2716	0.79	8/3685 (0.2%)
All	All	0.75	3/11028 (0.0%)	0.90	35/14971 (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	A	0	6
1	B	0	6
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	CYS	CB-SG	-7.99	1.68	1.82
1	A	182	CYS	CB-SG	-5.78	1.72	1.81
1	B	109	GLU	CD-OE2	-5.69	1.19	1.25

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH1	-19.71	110.44	120.30
1	A	129	ARG	NE-CZ-NH2	15.29	127.94	120.30
1	B	65	ARG	NE-CZ-NH1	-14.65	112.97	120.30
1	C	65	ARG	NE-CZ-NH2	-14.47	113.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ARG	NE-CZ-NH2	13.88	127.24	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	GLY	Peptide
1	A	190	SER	Peptide
1	A	2	GLN	Peptide
1	A	3	ALA	Peptide
1	A	71	ILE	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	2750	0	2757	158	0
1	B	2742	0	2745	131	0
1	C	2687	0	2696	109	0
1	D	2674	0	2680	119	0
2	A	15	0	0	2	0
2	B	15	0	0	1	0
2	C	15	0	0	6	0
2	D	15	0	0	3	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
3	C	15	0	7	1	0
3	D	15	0	7	2	0
4	A	98	0	0	6	0
4	B	134	0	0	7	0
4	C	60	0	0	8	0
4	D	62	0	0	20	0
All	All	11327	0	10906	499	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 23.

The worst 5 of 499 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:122:KCX:HE3	4:A:1084:HOH:O	1.26	1.27
1:A:198:LEU:HD21	1:A:213:ILE:CD1	1.73	1.19
1:D:105:LEU:HD23	1:D:143:ARG:NH2	1.59	1.17
1:D:321:PRO:HA	4:D:1031:HOH:O	1.51	1.11
1:A:102:GLU:O	1:A:102:GLU:HG3	1.47	1.09

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	356/379 (94%)	323 (91%)	26 (7%)	7 (2%)	7	34
1	B	355/379 (94%)	317 (89%)	29 (8%)	9 (2%)	5	28
1	C	343/379 (90%)	330 (96%)	13 (4%)	0	100	100
1	D	340/379 (90%)	324 (95%)	13 (4%)	3 (1%)	17	55
All	All	1394/1516 (92%)	1294 (93%)	81 (6%)	19 (1%)	11	43

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	61	GLU
1	A	233	PRO
1	B	61	GLU
1	B	85	ARG



### 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	285/302 (94%)	244 (86%)	41 (14%)	3	15
1	B	284/302 (94%)	245 (86%)	39 (14%)	3	17
1	C	279/302 (92%)	265 (95%)	14 (5%)	24	60
1	D	277/302 (92%)	261 (94%)	16 (6%)	20	55
All	All	1125/1208 (93%)	1015 (90%)	110 (10%)	8	30

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	202	GLN
1	B	296	PRO
1	D	296	PRO
1	D	73	LYS
1	B	208	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	202	GLN
1	D	93	GLN
1	D	202	GLN
1	D	152	GLN
1	C	93	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](#)

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	A	122	1	7,11,12	2.05	1 (14%)	4,12,14	1.67	1 (25%)
1	KCX	B	122	1	7,11,12	1.82	1 (14%)	4,12,14	2.77	1 (25%)
1	KCX	D	122	1	7,11,12	2.03	1 (14%)	4,12,14	2.94	1 (25%)
1	KCX	C	122	1	7,11,12	1.80	1 (14%)	4,12,14	2.70	1 (25%)

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	122	1	-	2/7/10/12	-
1	KCX	B	122	1	-	0/7/10/12	-
1	KCX	D	122	1	-	0/7/10/12	-
1	KCX	C	122	1	-	0/7/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	KCX	CE-NZ	5.12	1.56	1.45
1	A	122	KCX	CE-NZ	5.09	1.56	1.45
1	B	122	KCX	CE-NZ	4.50	1.55	1.45
1	C	122	KCX	CE-NZ	4.39	1.55	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	KCX	CD-CE-NZ	5.67	126.74	111.49
1	B	122	KCX	CD-CE-NZ	5.34	125.84	111.49
1	C	122	KCX	CD-CE-NZ	5.24	125.58	111.49
1	A	122	KCX	CD-CE-NZ	2.48	118.16	111.49

There are no chirality outliers.



All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	122	KCX	N-CA-CB-CG
1	A	122	KCX	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	122	KCX	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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	PLP	A	1001	1	15,15,16	2.11	5 (33%)	20,22,23	2.85	11 (55%)
2	SO4	D	361	-	4,4,4	0.16	0	6,6,6	0.09	0
3	PLP	B	1001	1	15,15,16	2.78	6 (40%)	20,22,23	2.36	10 (50%)
3	PLP	C	1001	1	15,15,16	2.16	7 (46%)	20,22,23	2.50	10 (50%)
2	SO4	A	360	-	4,4,4	0.39	0	6,6,6	0.70	0
2	SO4	C	360	-	4,4,4	0.39	0	6,6,6	0.45	0
2	SO4	C	361	-	4,4,4	0.65	0	6,6,6	0.72	0
2	SO4	B	360	-	4,4,4	0.59	0	6,6,6	0.99	0
2	SO4	A	361	-	4,4,4	0.69	0	6,6,6	0.54	0
2	SO4	D	362	-	4,4,4	0.27	0	6,6,6	0.43	0
2	SO4	D	360	-	4,4,4	0.40	0	6,6,6	0.92	0
3	PLP	D	1001	1	15,15,16	2.68	7 (46%)	20,22,23	3.17	11 (55%)
2	SO4	C	362	-	4,4,4	0.32	0	6,6,6	0.53	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	362	-	4,4,4	0.37	0	6,6,6	0.26	0
2	SO4	B	362	-	4,4,4	0.54	0	6,6,6	0.28	0
2	SO4	B	361	-	4,4,4	0.63	0	6,6,6	0.22	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
3	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	D	1001	1	-	3/6/6/8	0/1/1/1
3	PLP	C	1001	1	-	0/6/6/8	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	PLP	C3-C2	7.12	1.48	1.40
3	D	1001	PLP	P-O1P	4.80	1.66	1.50
3	A	1001	PLP	P-O4P	-4.72	1.45	1.60
3	D	1001	PLP	C2-N1	4.39	1.42	1.33
3	C	1001	PLP	P-O1P	4.13	1.63	1.50

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1001	PLP	O3P-P-O4P	6.82	124.87	106.73
3	D	1001	PLP	O2P-P-O4P	-6.17	90.33	106.73
3	A	1001	PLP	O4P-C5A-C5	5.52	119.87	109.35
3	A	1001	PLP	C3-C4-C5	4.88	124.01	118.74
3	A	1001	PLP	C4A-C4-C5	-4.73	116.06	120.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1001	PLP	C5A-O4P-P-O2P
3	D	1001	PLP	C5A-O4P-P-O1P
3	D	1001	PLP	C5A-O4P-P-O3P



There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	361	SO4	1	0
3	C	1001	PLP	1	0
2	A	360	SO4	1	0
2	C	360	SO4	5	0
2	C	361	SO4	1	0
2	B	360	SO4	1	0
2	D	360	SO4	2	0
3	D	1001	PLP	2	0
2	A	362	SO4	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, 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	358/379 (94%)	-0.69	0 100 100	1, 11, 22, 37	0
1	B	357/379 (94%)	-0.68	0 100 100	1, 11, 23, 34	0
1	C	349/379 (92%)	-0.28	0 100 100	15, 28, 39, 44	0
1	D	348/379 (91%)	-0.16	0 100 100	13, 30, 42, 48	0
All	All	1412/1516 (93%)	-0.46	0 100 100	1, 20, 38, 48	0

There are no RSRZ outliers to report.

### 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	122	12/13	0.89	0.18	33,34,37,38	0
1	KCX	B	122	12/13	0.94	0.18	7,12,17,18	0
1	KCX	C	122	12/13	0.96	0.17	20,22,23,24	0
1	KCX	A	122	12/13	0.96	0.17	1,12,14,14	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands

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
2	SO4	A	362	5/5	0.87	0.21	82,82,83,83	0
2	SO4	D	360	5/5	0.87	0.51	82,83,83,84	0
2	SO4	D	361	5/5	0.88	0.21	80,81,81,81	0
2	SO4	B	360	5/5	0.90	0.39	65,65,67,67	0
2	SO4	C	360	5/5	0.90	0.43	76,76,76,76	0
2	SO4	D	362	5/5	0.90	0.26	79,79,79,79	0
3	PLP	D	1001	15/16	0.92	0.25	29,34,35,36	0
2	SO4	B	362	5/5	0.93	0.20	66,66,67,67	0
2	SO4	A	360	5/5	0.93	0.31	54,54,54,55	0
2	SO4	C	362	5/5	0.94	0.16	75,75,76,76	0
2	SO4	A	361	5/5	0.95	0.16	41,41,43,43	0
2	SO4	C	361	5/5	0.97	0.17	38,39,40,40	0
3	PLP	B	1001	15/16	0.97	0.16	2,5,7,7	0
2	SO4	B	361	5/5	0.97	0.11	31,32,35,35	0
3	PLP	C	1001	15/16	0.98	0.20	25,25,27,28	0
3	PLP	A	1001	15/16	0.98	0.16	1,8,10,11	0

## 6.5 Other polymers

There are no such residues in this entry.