wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2023 – 11:15 PM EDT

PDB ID	:	3B8W
Title	:	Crystal structure of Escherichia coli alaine racemase mutant E221P
Authors	:	Wu, D.; Hu, T.; Zhang, L.; Jiang, H.; Shen, X.
Deposited on	:	2007-11-02
Resolution	:	2.70 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:

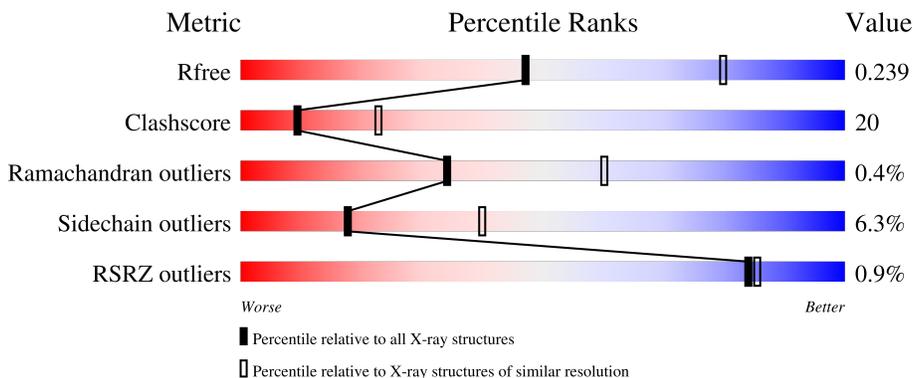|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		20
Ramachandran outliers		0.4%
Sidechain outliers		6.3%
RSRZ outliers		0.9%

Worse — *Better*

▮ Percentile relative to all X-ray structures
◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	67% 24% • 5%
1	B	379	68% 24% • 5%
1	C	379	% 59% 29% • 8%
1	D	379	3% 59% 30% • 7%

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	PLP	A	1001	-	-	X	-
3	PLP	D	1001	-	X	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11469 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 2752	C 1734	N 498	O 505	S 15	0	0	0
1	B	359	Total 2752	C 1734	N 498	O 505	S 15	0	0	0
1	C	347	Total 2659	C 1679	N 481	O 486	S 13	0	0	0
1	D	353	Total 2706	C 1707	N 491	O 495	S 13	0	0	0

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	PRO	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	PRO	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	PRO	GLU	engineered mutation	UNP P0A6B4

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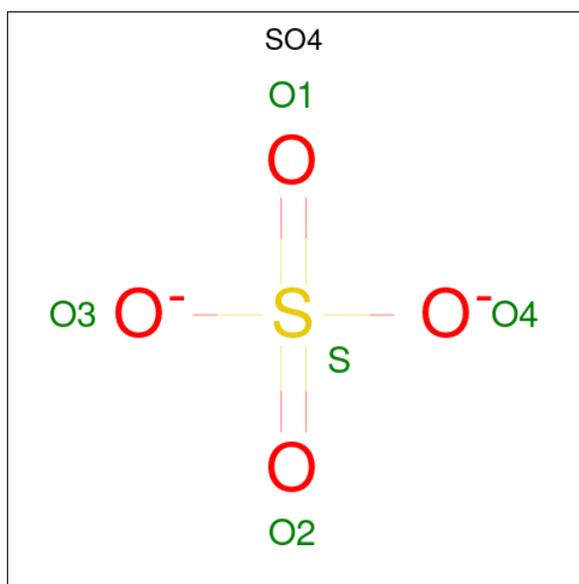
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P0A6B4
D	-18	GLY	-	expression tag	UNP P0A6B4
D	-17	SER	-	expression tag	UNP P0A6B4
D	-16	SER	-	expression tag	UNP P0A6B4
D	-15	HIS	-	expression tag	UNP P0A6B4
D	-14	HIS	-	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	PRO	GLU	engineered mutation	UNP P0A6B4

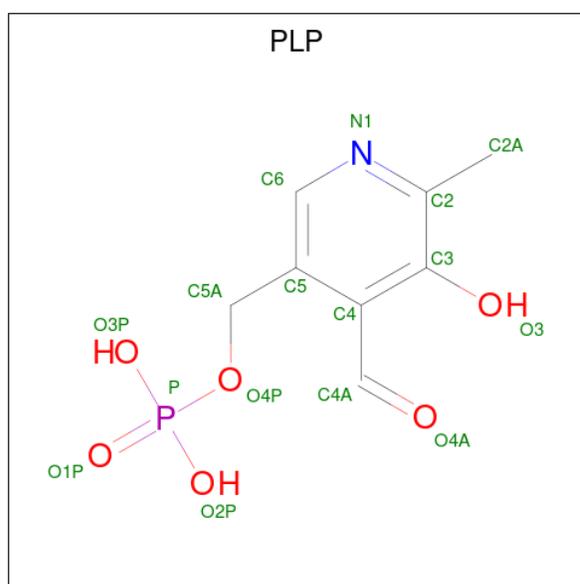- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

- 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 15	C 8	N 1	O 5	P 1	0	0
3	B	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	C	1	Total 15	C 8	N 1	O 5	P 1	0	0
3	D	1	Total 15	C 8	N 1	O 5	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total 134	O 134	0	0
4	B	182	Total 182	O 182	0	0
4	C	91	Total 91	O 91	0	0
4	D	93	Total 93	O 93	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.
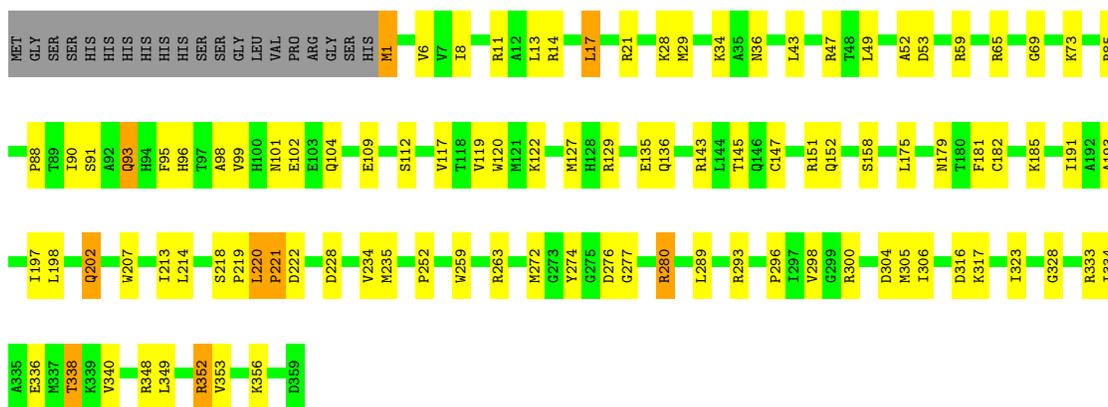
- Molecule 1: Alanine racemase

Chain A:
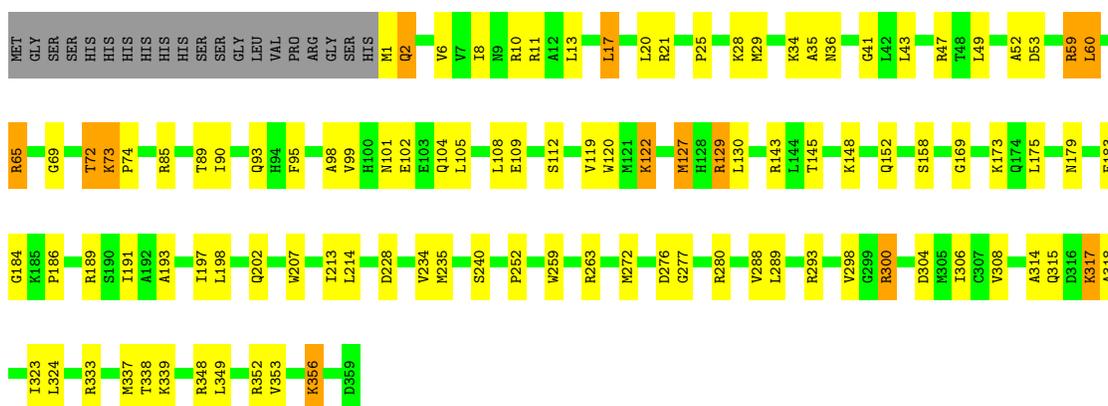
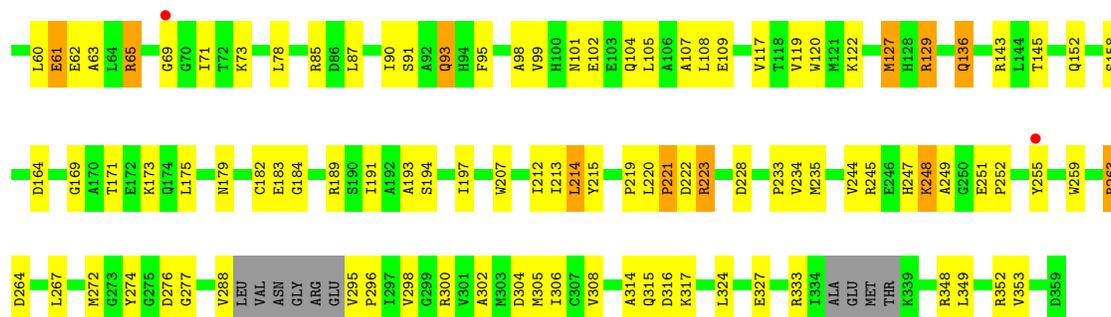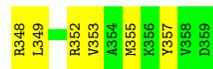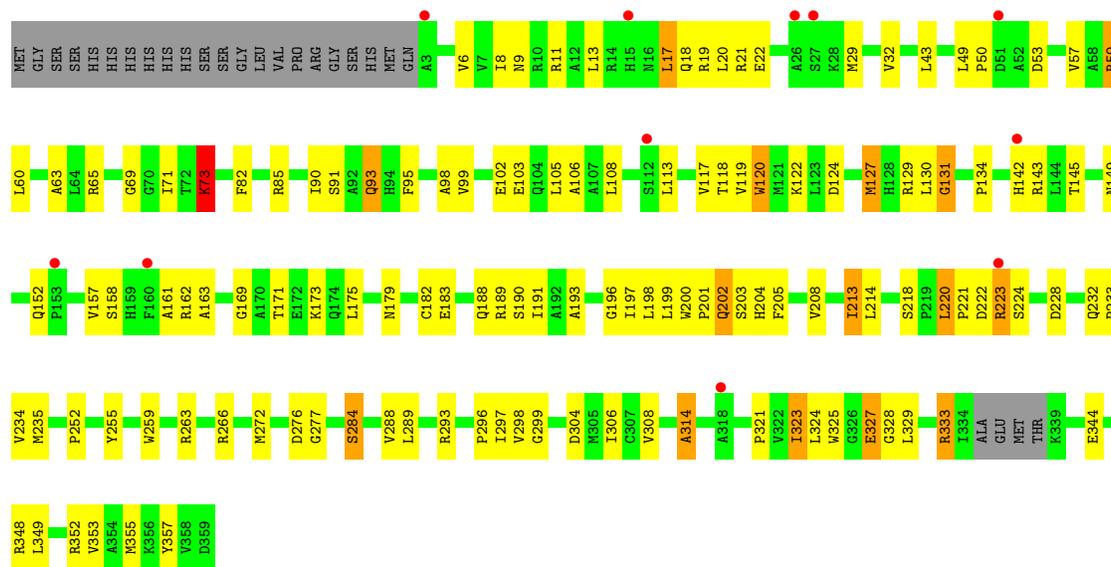
- Molecule 1: Alanine racemase

Chain B:

- Molecule 1: Alanine racemase

Chain C:

• Molecule 1: Alanine racemase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	148.21Å 148.21Å 163.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.70 40.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-2.70) 99.3 (40.91-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.243 0.225 , 0.239	Depositor DCC
R_{free} test set	5277 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 14.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	11469	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 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: KCX, SO4, PLP

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	0.71	0/2798	0.96	12/3800 (0.3%)
1	B	0.72	3/2798 (0.1%)	0.98	11/3800 (0.3%)
1	C	0.53	0/2703	0.95	14/3670 (0.4%)
1	D	0.52	0/2751	0.89	13/3736 (0.3%)
All	All	0.63	3/11050 (0.0%)	0.95	50/15006 (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	C	0	2
1	D	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	CYS	CB-SG	-8.42	1.68	1.82
1	B	182	CYS	CB-SG	-6.12	1.71	1.82
1	B	109	GLU	CD-OE2	-5.69	1.19	1.25

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH1	-19.71	110.44	120.30
1	B	85	ARG	NE-CZ-NH1	-19.42	110.59	120.30
1	B	85	ARG	NE-CZ-NH2	18.83	129.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH2	15.29	127.94	120.30
1	D	65	ARG	NE-CZ-NH2	-14.85	112.87	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	GLY	Peptide
1	C	221	PRO	Peptide
1	C	61	GLU	Peptide
1	D	131	GLY	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	2752	0	2761	91	0
1	B	2752	0	2759	90	0
1	C	2659	0	2662	108	0
1	D	2706	0	2711	159	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
3	A	15	0	7	9	0
3	B	15	0	7	0	0
3	C	15	0	7	1	0
3	D	15	0	7	2	0
4	A	134	0	0	11	0
4	B	182	0	0	7	0
4	C	91	0	0	15	0
4	D	93	0	0	60	0
All	All	11469	0	10921	430	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 20.

The worst 5 of 430 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:34:LYS:CE	3:A:1001:PLP:C4A	2.03	1.34
1:A:34:LYS:NZ	3:A:1001:PLP:C4	1.95	1.30
1:C:263:ARG:HD2	4:C:1080:HOH:O	1.39	1.21
1:C:22:GLU:HB3	4:C:1074:HOH:O	1.45	1.11
1:C:233:PRO:HD3	4:C:1016:HOH:O	1.48	1.10

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	336 (94%)	20 (6%)	0	100	100
1	B	356/379 (94%)	337 (95%)	18 (5%)	1 (0%)	41	66
1	C	340/379 (90%)	327 (96%)	12 (4%)	1 (0%)	41	66
1	D	348/379 (92%)	328 (94%)	17 (5%)	3 (1%)	17	40
All	All	1400/1516 (92%)	1328 (95%)	67 (5%)	5 (0%)	34	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	223	ARG
1	C	327	GLU
1	D	73	LYS
1	D	327	GLU
1	B	221	PRO

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	286/303 (94%)	267 (93%)	19 (7%)	16	38
1	B	286/303 (94%)	267 (93%)	19 (7%)	16	38
1	C	276/303 (91%)	261 (95%)	15 (5%)	22	47
1	D	281/303 (93%)	263 (94%)	18 (6%)	17	39
All	All	1129/1212 (93%)	1058 (94%)	71 (6%)	18	40

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	93	GLN
1	D	127	MET
1	D	228	ASP
1	B	127	MET
1	B	112	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	93	GLN
1	D	202	GLN
1	D	313	GLN
1	D	179	ASN
1	C	96	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	122	1	9,11,12	1.76	2 (22%)	5,12,14	2.99	2 (40%)
1	KCX	A	122	1	9,11,12	1.08	1 (11%)	5,12,14	3.49	2 (40%)
1	KCX	B	122	1	9,11,12	1.62	2 (22%)	5,12,14	2.88	2 (40%)
1	KCX	C	122	1	9,11,12	0.91	0	5,12,14	1.19	1 (20%)

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	D	122	1	-	0/9/10/12	-
1	KCX	A	122	1	-	2/9/10/12	-
1	KCX	B	122	1	-	0/9/10/12	-
1	KCX	C	122	1	-	3/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	KCX	CE-NZ	4.51	1.56	1.46
1	B	122	KCX	CE-NZ	3.96	1.55	1.46
1	B	122	KCX	OQ1-CX	2.03	1.25	1.21
1	D	122	KCX	OQ1-CX	2.01	1.25	1.21
1	A	122	KCX	CE-NZ	2.01	1.50	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	KCX	CE-NZ-CX	7.51	133.95	121.89
1	D	122	KCX	CD-CE-NZ	5.08	126.74	112.21
1	B	122	KCX	CD-CE-NZ	4.77	125.84	112.21
1	D	122	KCX	OQ1-CX-NZ	-4.17	118.50	124.96
1	B	122	KCX	OQ1-CX-NZ	-4.16	118.52	124.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	122	KCX	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\#|Z| > 2$
2	SO4	B	360	-	4,4,4	0.47	0	6,6,6	1.19	1 (16%)
3	PLP	B	1001	1	15,15,16	2.78	6 (40%)	20,22,23	2.36	10 (50%)
2	SO4	A	361	-	4,4,4	0.60	0	6,6,6	0.54	0
2	SO4	D	360	-	4,4,4	0.25	0	6,6,6	0.40	0
2	SO4	B	362	-	4,4,4	0.58	0	6,6,6	0.41	0
2	SO4	C	361	-	4,4,4	0.42	0	6,6,6	0.38	0
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	0.52	0	6,6,6	0.36	0
2	SO4	B	361	-	4,4,4	0.68	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PLP	D	1001	1	15,15,16	2.68	7 (46%)	20,22,23	3.17	11 (55%)
3	PLP	A	1001	1	15,15,16	2.11	5 (33%)	20,22,23	2.85	11 (55%)
2	SO4	C	360	-	4,4,4	0.36	0	6,6,6	0.15	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 43 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.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	PLP	1	0
3	D	1001	PLP	2	0
3	A	1001	PLP	9	0

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 ⓘ

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, 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	358/379 (94%)	-0.44	0	100	100	3, 11, 23, 40	0
1	B	358/379 (94%)	-0.40	0	100	100	2, 12, 24, 43	0
1	C	346/379 (91%)	0.17	2 (0%)	89	91	12, 30, 40, 48	0
1	D	352/379 (92%)	0.35	11 (3%)	49	49	15, 33, 45, 55	0
All	All	1414/1516 (93%)	-0.09	13 (0%)	84	85	2, 22, 40, 55	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	223	ARG	5.1
1	D	318	ALA	4.4
1	D	27	SER	3.4
1	D	26	ALA	3.1
1	D	51	ASP	2.7

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

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	D	122	12/13	0.79	0.23	33,37,45,46	0
1	KCX	C	122	12/13	0.91	0.16	23,25,29,34	0
1	KCX	A	122	12/13	0.91	0.16	12,17,23,26	0
1	KCX	B	122	12/13	0.92	0.16	8,11,18,19	0

6.3 Carbohydrates ⓘ

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, 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	SO4	B	360	5/5	0.91	0.27	64,64,65,65	0
2	SO4	D	360	5/5	0.91	0.27	88,88,89,89	0
2	SO4	A	361	5/5	0.92	0.26	86,86,87,87	0
2	SO4	A	360	5/5	0.93	0.15	51,52,53,53	0
3	PLP	D	1001	15/16	0.93	0.19	36,40,41,42	0
3	PLP	C	1001	15/16	0.94	0.16	30,32,39,40	0
2	SO4	C	360	5/5	0.95	0.16	46,47,47,48	0
2	SO4	B	362	5/5	0.96	0.12	67,67,67,68	0
3	PLP	A	1001	15/16	0.98	0.14	11,13,16,16	0
3	PLP	B	1001	15/16	0.98	0.12	1,2,4,5	0
2	SO4	C	361	5/5	0.98	0.14	77,77,77,77	0
2	SO4	B	361	5/5	0.98	0.12	36,36,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.