



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 07:35 PM UTC

PDB ID : 2RJG / pdb_00002rjg
Title : Crystal structure of biosynthetic alaine racemase from Escherichia coli
Authors : Wu, D.; Hu, T.; Zhang, L.; Jiang, H.; Shen, X.
Deposited on : 2007-10-15
Resolution : 2.40 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

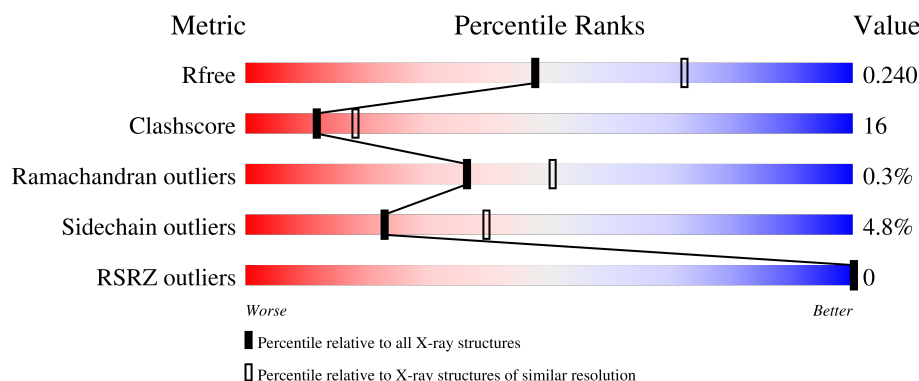
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	379	 67% 25% • 5%
1	B	379	 66% 26% • 5%
1	C	379	 61% 29% • 7%
1	D	379	 61% 28% • 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	C	1001	-	X	-	-
3	PLP	D	1001	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11538 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
			2754	1734	498	507	15			
1	B	359	Total	C	N	O	S	0	0	0
			2754	1734	498	507	15			
1	C	353	Total	C	N	O	S	0	0	0
			2708	1707	491	497	13			
1	D	353	Total	C	N	O	S	0	0	0
			2708	1707	491	497	13			

There are 80 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
B	-19	MET	-	expression tag	UNP P0A6B4

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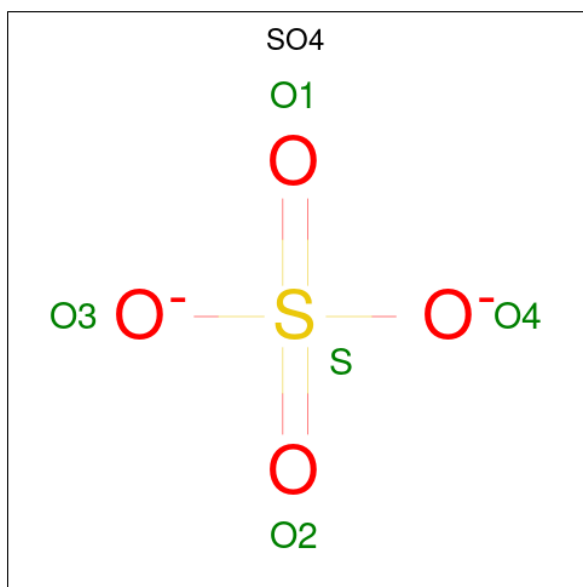
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P0A6B4
B	-17	SER	-	expression tag	UNP P0A6B4
B	-16	SER	-	expression tag	UNP P0A6B4
B	-15	HIS	-	expression tag	UNP P0A6B4
B	-14	HIS	-	expression tag	UNP P0A6B4
B	-13	HIS	-	expression tag	UNP P0A6B4
B	-12	HIS	-	expression tag	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
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
D	-19	MET	-	expression tag	UNP P0A6B4
D	-18	GLY	-	expression tag	UNP P0A6B4
D	-17	SER	-	expression tag	UNP P0A6B4

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



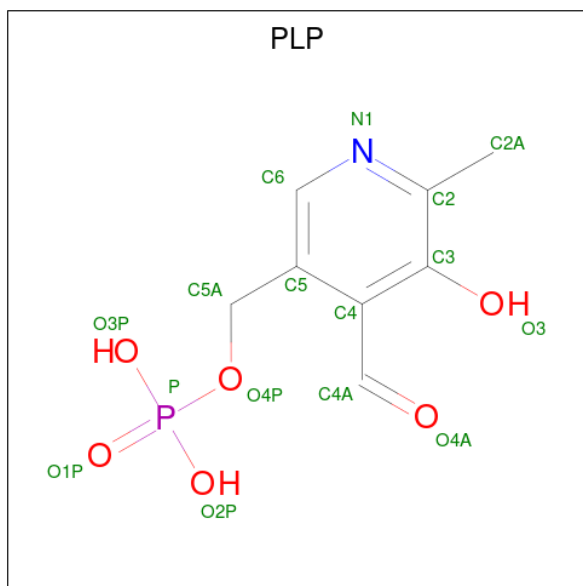
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: 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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	151	Total	O	0	0
			151	151		
4	B	173	Total	O	0	0
			173	173		
4	C	82	Total	O	0	0
			82	82		
4	D	88	Total	O	0	0
			88	88		

- Molecule 1: Alanine racemase

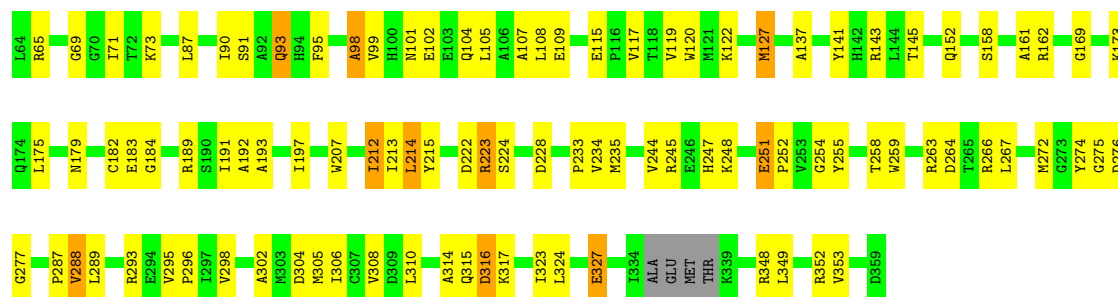
I323	L324	R333	M337	K338	K339	R348	L349	R352	V353	A354	M355	D359	T191	A192	A193	T197	L198	Q202	W207	T212	T213	L214	S218	P219	L220	R223	S224	D228	V234	M235	S240	P252	Y255	T258	W259	R263	D264	M272	G275	D276	G277	V288	L289	V298	M303	D304	M305	L306	C307	V308	A314	Q315	K73	P74	T89	Y90	Q93	H94	F95	A98	V99	H100	M101	Q104	L105	A106	A107	L108	E109	V119	W120	H121	K122	M127	H128	L129	A137	T145	G146	C147	R151	Q152	S158	D164	G169	K173	H174	L175	M179	C182	E183	G184	X185	P186	M189	S189	T191	A192	A193	T197	L198	Q202	W207	T212	T213	L214	S218	P219	L220	R223	S224	D228	V234	M235	S240	P252	Y255	T258	W259	R263	D264	M272	G275	D276	G277	V288	L289	V298	M303	D304	M305	L306	C307	V308	A314	Q315	K73	P74	T89	Y90	Q93	H94	F95	A98	V99	H100	M101	Q104	L105	A106	A107	L108	E109	V119	W120	H121	K122	M127	H128	L129	A137	T145	G146	C147	R151	Q152	S158	D164	G169	K173	H174	L175	M179	C182	E183	G184	X185	P186	M189	S189	T191	A192	A193	T197	L198	Q202	W207	T212	T213	L214	S218	P219	L220	R223	S224	D228	V234	M235	S240	P252	Y255	T258	W259	R263	D264	M272	G275	D276	G277	V288	L289	V298	M303	D304	M305	L306	C307	V308	A314	Q315	K73	P74	T89	Y90	Q93	H94	F95	A98	V99	H100	M101	Q104	L105	A106	A107	L108	E109	V119	W120	H121	K122	M127	H128	L129	A137	T145	G146	C147	R151	Q152	S158	D164	G169	K173	H174	L175	M179	C182	E183	G184	X185	P186	M189	S189	T191	A192	A193	T197	L198	Q202	W207	T212	T213	L214	S218	P219	L220	R223	S224	D228	V234	M235	S240	P252	Y255	T258	W259	R263	D264	M272	G275	D276	G277	V288	L289	V298	M303	D304	M305	L306	C307	V308	A314	Q315	K73	P74	T89	Y90	Q93	H94	F95	A98	V99	H100	M101	Q104	L105	A106	A107	L108	E109	V119	W120	H121	K122	M127	H128	L129	A137	T145	G146	C147	R151	Q152	S158	D164	G169	K173	H174	L175	M179	C182	E183	G184	X185	P186	M189	S189	T191	A192	A193	T197	L198	Q202	W207	T212	T213	L214	S218	P219	L220	R223	S224	D228	V234	M235	S240	P252	Y255	T258	W259	R263	D264	M272	G275	D276	G277	V288	L289	V298	M303	D304	M305	L306	C307	V308	A314	Q315	K73	P74	T89	Y90	Q93	H94	F95	A98	V99	H100	M101	Q104	L105	A106	A107	L108	E109	V119	W120	H121	K122	M127	H128	L129	A137	T145	G146	C147	R151	Q152	S158	D164	G169	K173	H174	L175	M179	C182	E183	G184	X185	P186	M189	S189	T191	A192	A193	T197	L198	Q202	W207	T212	T213	L214	S218	P219	L220	R223	S224	D228	V234	M235	S240	P252	Y255	T258	W259	R263	D264	M272	G275	D276	G277	V288	L289	V298	M303	D304	M305	L306	C307	V308	A314	Q315	K73	P74	T89	Y90	Q93	H94	F95	A98	V99	H100	M101	Q104	L105	A106	A107	L108	E109	V119	W120	H121	K122	M127	H128	L129	A137	T145	G146	C147	R151	Q152	S158	D164	G169	K173	H174	L175	M179	C182</
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- Molecule 1: Alanine racemase

K317	S190	T72	R85	P88	T89	S91	A92	G93	H94	P95	A98	V99	H100	N101	E102	E103	Q104	V117	T118	V119	M120	M121	K122	M127	E135	Q136	A137	R143	L144	T145	R151	Q152	S158	F160	A161	R162	G169	K173	O174	L175	M179	E183	P189					
I323	A191	K337	A335	E336	V340	R348	L349	R352	V353	K356	E359	V234	M235	P252	Y255	W259	R263	D264	M272	G275	D276	G277	P287	V288	L289	E294	V295	P296	T297	V298	G299	R300	M303	D304	M305	I306	A314	Q315	R316									
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	M1	Q2	V6	V7	I8	R11	A12	L13	R14	L17	L20	R21	K28	M29	K34	A35	N36	A37	Y38	L43	R47	T48	L49	P50	D51	A52	D53	R59	L60	P65

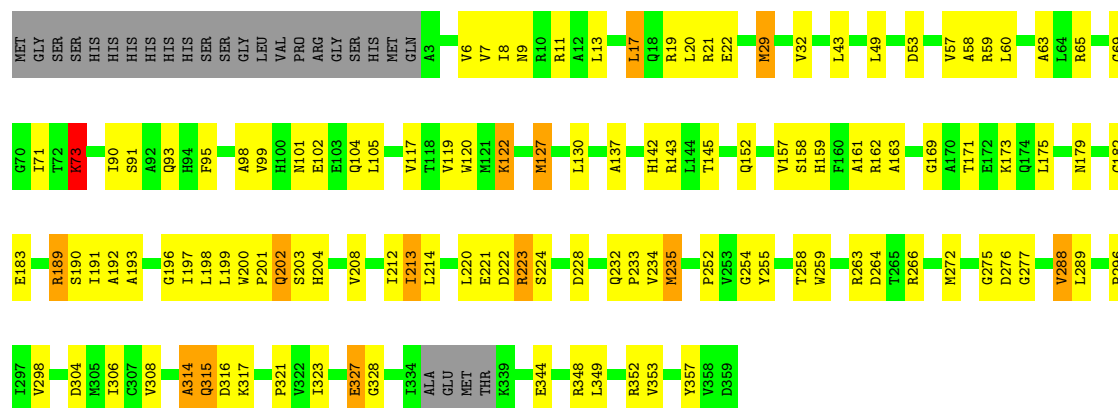
- Molecule 1: Alanine racemase

MET	GLY	SER	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	GLN	A3	A3	V6	V7	I8	N9	R10	R11	A12	L13	L17	R21	A24	P25	A26	S27	K28	M29	K34	L43	L49	P50	D53	V57	A58	R59	L60	E61	F62	F62
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• Molecule 1: Alanine racemase

Chain D: 61% 28% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	147.98Å 147.98Å 163.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.40) 99.5 (15.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.247 0.210 , 0.240	Depositor DCC
R_{free} test set	7554 reflections (9.59%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 10.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11538	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 3.83% 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: KCX, PLP, SO4

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	0.75	2/2799 (0.1%)	1.15	15/3800 (0.4%)
1	B	0.69	3/2799 (0.1%)	1.20	24/3800 (0.6%)
1	C	0.65	0/2752	1.13	22/3736 (0.6%)
1	D	0.64	0/2752	1.19	18/3736 (0.5%)
All	All	0.69	5/11102 (0.0%)	1.17	79/15072 (0.5%)

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	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	SD-CE	6.38	1.95	1.79
1	A	89	THR	C-O	-5.79	1.17	1.24
1	B	89	THR	C-O	-5.55	1.17	1.24
1	B	151	ARG	C-O	-5.32	1.17	1.24
1	A	107	ALA	C-O	-5.20	1.18	1.24

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	315	GLN	N-CA-CB	-22.78	75.86	111.39
1	D	314	ALA	N-CA-C	-13.30	91.75	110.50
1	C	315	GLN	N-CA-CB	-12.45	90.99	110.92
1	B	315	GLN	N-CA-CB	-11.97	91.77	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ARG	NE-CZ-NH2	11.68	129.71	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	60	LEU	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	2754	0	2758	82	1
1	B	2754	0	2758	76	1
1	C	2708	0	2710	104	1
1	D	2708	0	2710	113	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	1	0
2	D	15	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
3	C	15	0	7	0	0
3	D	15	0	7	2	0
4	A	151	0	0	11	1
4	B	173	0	0	6	0
4	C	82	0	0	19	0
4	D	88	0	0	30	1
All	All	11538	0	10964	349	3

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 16.

The worst 5 of 349 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:C:233:PRO:HD3	4:C:1016:HOH:O	1.48	1.09
1:A:52:ALA:O	1:A:73:LYS:HE2	1.52	1.06
1:C:267:LEU:HD12	4:D:1032:HOH:O	1.57	1.02
1:D:8:ILE:HD13	4:D:1050:HOH:O	1.63	0.96
1:C:215:TYR:HE1	4:C:1041:HOH:O	1.48	0.96

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1037:HOH:O	4:A:1082:HOH:O[4_655]	1.92	0.28
1:A:333:ARG:NH1	1:B:294:GLU:OE2[6_555]	2.11	0.09
1:C:293:ARG:NH1	4:D:1004:HOH:O[5_555]	2.13	0.07

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%)	339 (95%)	17 (5%)	0	100	100
1	B	356/379 (94%)	342 (96%)	14 (4%)	0	100	100
1	C	348/379 (92%)	334 (96%)	12 (3%)	2 (1%)	21	32
1	D	348/379 (92%)	333 (96%)	13 (4%)	2 (1%)	21	32
All	All	1408/1516 (93%)	1348 (96%)	56 (4%)	4 (0%)	36	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	61	GLU
1	C	327	GLU
1	D	73	LYS
1	D	327	GLU

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	286/303 (94%)	271 (95%)	15 (5%)	21	36
1	B	286/303 (94%)	272 (95%)	14 (5%)	22	39
1	C	281/303 (93%)	270 (96%)	11 (4%)	28	48
1	D	281/303 (93%)	267 (95%)	14 (5%)	22	38
All	All	1134/1212 (94%)	1080 (95%)	54 (5%)	23	40

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	296	PRO
1	C	214	LEU
1	D	228	ASP
1	C	17	LEU
1	C	93	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	202	GLN
1	D	96	HIS
1	D	94	HIS
1	D	152	GLN
1	B	94	HIS

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	10,11,12	1.65	2 (20%)	6,12,14	2.83	2 (33%)
1	KCX	B	122	1	10,11,12	1.57	1 (10%)	6,12,14	2.83	2 (33%)
1	KCX	C	122	1	10,11,12	1.57	2 (20%)	6,12,14	2.68	2 (33%)
1	KCX	D	122	1	10,11,12	1.73	2 (20%)	6,12,14	2.98	2 (33%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	122	KCX	CE-NZ	4.58	1.56	1.46
1	A	122	KCX	CE-NZ	4.34	1.55	1.46
1	B	122	KCX	CE-NZ	4.02	1.55	1.46
1	C	122	KCX	CE-NZ	3.91	1.55	1.46
1	C	122	KCX	OQ1-CX	2.08	1.25	1.21

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	KCX	CD-CE-NZ	5.19	126.74	112.20
1	D	122	KCX	OQ1-CX-NZ	-4.98	117.35	124.92
1	A	122	KCX	OQ1-CX-NZ	-4.94	117.41	124.92
1	B	122	KCX	CD-CE-NZ	4.87	125.84	112.20
1	B	122	KCX	OQ1-CX-NZ	-4.79	117.64	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	122	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
2	SO4	C	361	-	4,4,4	0.46	0	6,6,6	0.15	0
2	SO4	A	362	-	4,4,4	0.50	0	6,6,6	0.47	0
2	SO4	B	362	-	4,4,4	0.57	0	6,6,6	0.44	0
2	SO4	C	360	-	4,4,4	0.60	0	6,6,6	0.44	0
2	SO4	C	362	-	4,4,4	0.34	0	6,6,6	0.37	0
2	SO4	B	360	-	4,4,4	0.56	0	6,6,6	0.38	0
2	SO4	D	360	-	4,4,4	0.60	0	6,6,6	0.43	0
2	SO4	D	361	-	4,4,4	0.66	0	6,6,6	0.31	0
3	PLP	A	1001	1	15,15,16	2.17	5 (33%)	21,22,23	2.82	11 (52%)
3	PLP	D	1001	1	15,15,16	2.77	7 (46%)	21,22,23	3.21	12 (57%)
2	SO4	A	361	-	4,4,4	0.60	0	6,6,6	0.37	0
2	SO4	D	362	-	4,4,4	0.28	0	6,6,6	0.32	0
3	PLP	C	1001	1	15,15,16	2.22	8 (53%)	21,22,23	2.59	11 (52%)
2	SO4	A	360	-	4,4,4	0.52	0	6,6,6	0.27	0
3	PLP	B	1001	1	15,15,16	2.78	6 (40%)	21,22,23	2.44	11 (52%)
2	SO4	B	361	-	4,4,4	0.38	0	6,6,6	0.45	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	D	1001	1	-	3/6/6/8	0/1/1/1
3	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	C	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	B	1001	1	-	0/6/6/8	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	PLP	C3-C2	6.80	1.48	1.41
3	D	1001	PLP	P-O1P	5.00	1.66	1.50
3	A	1001	PLP	P-O4P	-4.84	1.45	1.60
3	D	1001	PLP	C2-N1	4.66	1.42	1.33
3	C	1001	PLP	P-O1P	4.30	1.63	1.50

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1001	PLP	O3P-P-O4P	6.98	124.87	106.67
3	D	1001	PLP	O2P-P-O4P	-6.27	90.33	106.67
3	A	1001	PLP	O4P-C5A-C5	5.61	119.87	109.36
3	A	1001	PLP	C4A-C4-C5	-4.74	116.06	120.94
3	B	1001	PLP	C5A-C5-C6	-4.69	111.72	119.36

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	360	SO4	1	0
3	D	1001	PLP	2	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	358/379 (94%)	-1.64	0 100 100	6, 14, 25, 41	0
1	B	358/379 (94%)	-1.63	0 100 100	6, 14, 25, 43	0
1	C	352/379 (92%)	-1.43	0 100 100	15, 28, 40, 48	0
1	D	352/379 (92%)	-1.36	0 100 100	15, 30, 43, 51	0
All	All	1420/1516 (93%)	-1.52	0 100 100	6, 22, 39, 51	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, 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	122	12/13	0.99	0.03	13,16,24,25	0
1	KCX	B	122	12/13	0.99	0.04	14,15,21,22	0
1	KCX	C	122	12/13	0.99	0.04	22,27,30,30	0
1	KCX	D	122	12/13	0.99	0.04	30,34,39,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	D	362	5/5	0.97	0.09	69,69,70,70	0
2	SO4	D	361	5/5	0.98	0.06	70,71,72,72	0
2	SO4	A	362	5/5	0.98	0.08	74,74,75,76	0
2	SO4	B	362	5/5	0.99	0.05	64,65,66,66	0
2	SO4	C	360	5/5	0.99	0.07	68,68,69,69	0
2	SO4	C	361	5/5	0.99	0.04	28,29,31,31	0
2	SO4	C	362	5/5	0.99	0.05	65,65,65,65	0
2	SO4	D	360	5/5	0.99	0.09	69,69,69,70	0
2	SO4	A	361	5/5	0.99	0.03	37,38,39,40	0
2	SO4	B	360	5/5	0.99	0.05	44,44,45,46	0
3	PLP	C	1001	15/16	0.99	0.03	25,27,33,33	0
3	PLP	D	1001	15/16	0.99	0.03	28,34,35,36	0
3	PLP	A	1001	15/16	1.00	0.02	8,11,14,14	0
3	PLP	B	1001	15/16	1.00	0.02	7,9,12,13	0
2	SO4	B	361	5/5	1.00	0.02	20,21,21,23	0
2	SO4	A	360	5/5	1.00	0.04	29,29,31,31	0

6.5 Other polymers

There are no such residues in this entry.