



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:58 PM UTC

PDB ID : 1TYZ / pdb_00001tyz
Title : Crystal structure of 1-Aminocyclopropane-1-carboxylate Deaminase from Pseudomonas
Authors : Karthikeyan, S.; Zhou, Q.; Zhao, Z.; Kao, C.L.; Tao, Z.; Robinson, H.; Liu, H.W.; Zhang, H.
Deposited on : 2004-07-08
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

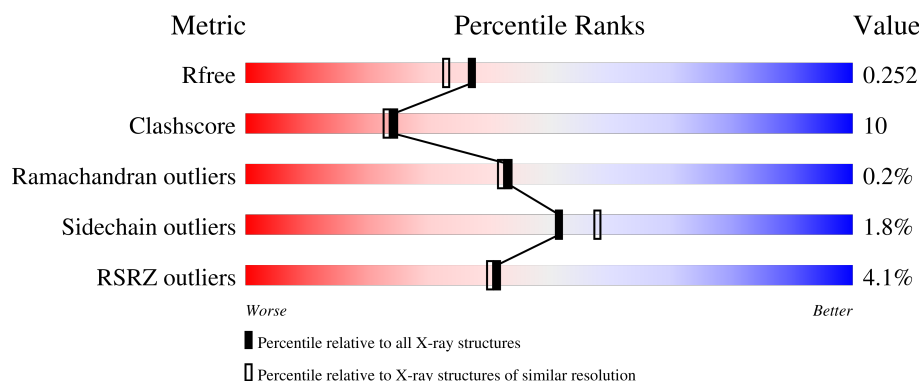
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 ≥ 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	338	4% 79% 17% ..
1	B	338	3% 76% 19% ..
1	C	338	6% 78% 20% .
1	D	338	4% 75% 21% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10486 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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2514	1576	451	472	15			
1	B	329	Total	C	N	O	S	0	0	0
			2499	1567	449	468	15			
1	C	338	Total	C	N	O	S	0	0	0
			2571	1614	461	481	15			
1	D	329	Total	C	N	O	S	0	0	0
			2499	1567	449	468	15			

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



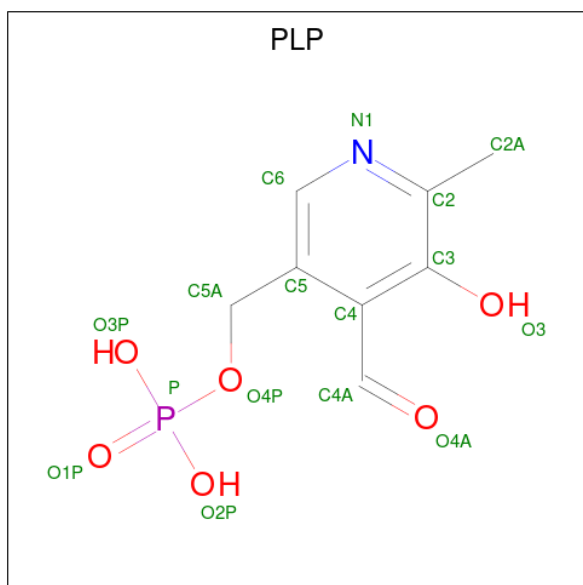
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	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	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	92	Total	O	0	0
			92	92		
4	B	85	Total	O	0	0
			85	85		
4	C	73	Total	O	0	0
			73	73		

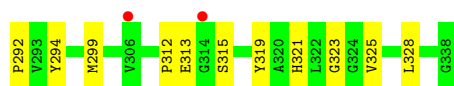
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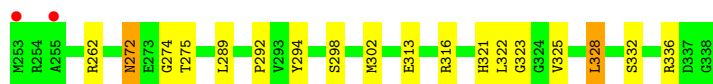
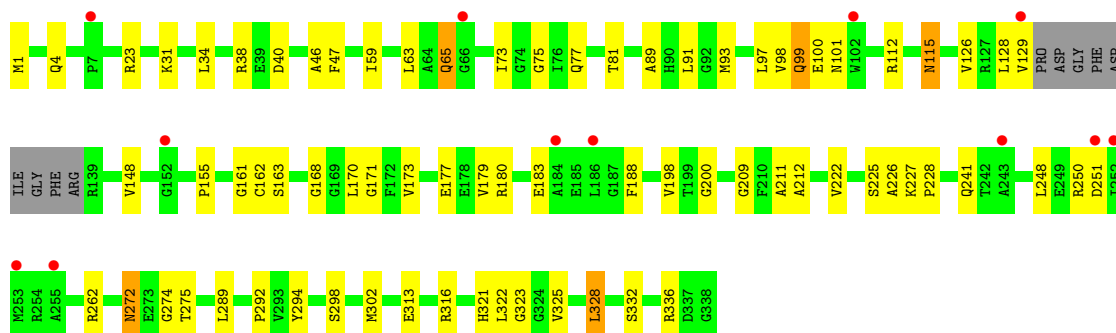
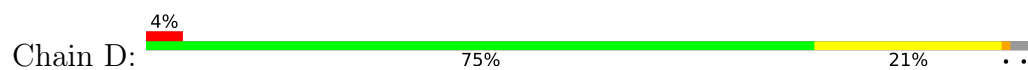
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	73	Total	O	0	0
			73	73		

- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.72Å 68.65Å 350.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 2.00 39.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.5 (39.73-2.00) 86.5 (39.73-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.251 0.215 , 0.252	Depositor DCC
R_{free} test set	4851 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10486	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: 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	0.66	1/2561 (0.0%)	1.09	12/3461 (0.3%)
1	B	0.61	0/2545	1.10	15/3438 (0.4%)
1	C	0.67	0/2621	1.13	13/3542 (0.4%)
1	D	0.62	0/2545	1.12	13/3438 (0.4%)
All	All	0.64	1/10272 (0.0%)	1.11	53/13879 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	ILE	CA-CB	7.47	1.58	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	VAL	N-CA-C	-13.00	98.21	110.82
1	C	200	GLY	N-CA-C	12.93	130.47	115.08
1	D	200	GLY	N-CA-C	12.72	128.68	113.79
1	B	173	VAL	N-CA-C	-12.53	98.07	110.72
1	B	200	GLY	N-CA-C	12.34	129.76	115.08
1	A	200	GLY	N-CA-C	11.65	130.35	115.21
1	D	173	VAL	N-CA-C	-11.48	98.49	111.00
1	C	173	VAL	N-CA-C	-10.87	99.16	111.00
1	B	163	SER	N-CA-C	10.61	122.53	110.97
1	C	65	GLN	N-CA-C	-10.01	97.62	110.53
1	D	163	SER	N-CA-C	9.55	121.77	111.36
1	A	65	GLN	N-CA-C	-8.62	99.51	110.19
1	D	227	LYS	CA-C-N	8.29	127.86	119.24
1	D	227	LYS	C-N-CA	8.29	127.86	119.24
1	A	163	SER	N-CA-C	8.18	120.11	111.03
1	D	38	ARG	N-CA-C	7.67	121.58	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	ALA	N-CA-C	-7.67	102.93	111.82
1	C	38	ARG	N-CA-C	7.38	121.12	109.39
1	C	211	ALA	N-CA-C	-7.30	103.33	111.28
1	A	38	ARG	N-CA-C	7.22	120.87	109.39
1	D	65	GLN	N-CA-C	-6.54	101.72	110.55
1	B	43	SER	N-CA-C	6.50	118.95	109.07
1	C	248	LEU	N-CA-C	-6.48	101.36	110.50
1	B	65	GLN	N-CA-C	-6.31	102.20	110.53
1	A	272	ASN	N-CA-C	-6.18	101.05	109.95
1	B	64	ALA	N-CA-C	-6.17	103.50	111.02
1	A	211	ALA	N-CA-C	-6.10	104.70	111.71
1	B	272	ASN	N-CA-C	-6.04	101.26	109.95
1	B	53	ARG	N-CA-C	-5.82	105.07	111.82
1	B	211	ALA	N-CA-C	-5.79	105.05	111.71
1	B	168	GLY	N-CA-C	5.67	121.25	113.99
1	C	299	MET	N-CA-C	-5.63	104.76	111.69
1	B	38	ARG	N-CA-C	5.62	118.31	108.52
1	D	262	ARG	N-CA-C	5.57	119.69	113.01
1	A	262	ARG	N-CA-C	5.50	119.60	113.01
1	D	115	ASN	N-CA-C	5.47	116.92	111.07
1	A	42	ASN	N-CA-C	5.44	119.77	113.18
1	D	322	LEU	N-CA-C	5.40	119.71	113.18
1	C	76	ILE	N-CA-C	5.36	116.73	110.62
1	B	6	PHE	N-CA-C	5.32	117.34	109.62
1	A	227	LYS	CA-C-N	5.32	126.49	119.84
1	A	227	LYS	C-N-CA	5.32	126.49	119.84
1	A	265	GLY	N-CA-C	5.31	123.18	112.34
1	C	163	SER	N-CA-C	5.31	122.11	110.80
1	C	115	ASN	N-CA-C	5.30	116.75	111.07
1	D	332	SER	N-CA-C	5.23	117.06	111.36
1	B	262	ARG	N-CA-C	5.21	119.39	113.19
1	B	218	ARG	N-CA-C	-5.15	107.00	113.28
1	C	262	ARG	N-CA-C	5.15	119.28	112.89
1	C	144	ALA	N-CA-C	-5.09	105.62	111.07
1	D	168	GLY	N-CA-C	5.06	120.47	113.99
1	B	115	ASN	N-CA-C	5.04	116.58	111.14
1	C	254	ARG	N-CA-C	-5.03	105.93	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2485	43	0
1	B	2499	0	2475	52	0
1	C	2571	0	2539	58	0
1	D	2499	0	2474	50	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	7	0	0
4	A	92	0	0	0	0
4	B	85	0	0	2	0
4	C	73	0	0	3	0
4	D	73	0	0	2	0
All	All	10486	0	10001	200	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 10.

All (200) 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:1:MET:HE3	1:B:212:ALA:HB2	1.32	1.07
1:D:1:MET:HE3	1:D:212:ALA:HB2	1.42	1.00
1:C:1:MET:HE3	1:C:212:ALA:HB2	1.42	0.99
1:A:4:GLN:NE2	1:A:4:GLN:H	1.63	0.96
1:B:100:GLU:HG3	1:B:129:VAL:HG21	1.45	0.96
1:A:139:ARG:HG3	1:A:142:GLU:H	1.32	0.93
1:C:272:ASN:HD22	1:C:274:GLY:H	1.20	0.86
1:D:1:MET:CE	1:D:212:ALA:HB2	2.10	0.82
1:A:4:GLN:H	1:A:4:GLN:HE21	1.23	0.81
1:B:272:ASN:HD22	1:B:274:GLY:H	1.28	0.81
1:A:139:ARG:HD2	1:A:141:TRP:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HD2	1:B:141:TRP:HB3	1.63	0.79
1:A:272:ASN:HD22	1:A:274:GLY:H	1.30	0.79
1:B:1:MET:CE	1:B:212:ALA:HB2	2.11	0.78
1:B:77:GLN:HE22	1:B:115:ASN:H	1.32	0.77
1:C:272:ASN:HD22	1:C:274:GLY:N	1.84	0.74
1:B:100:GLU:HG3	1:B:129:VAL:CG2	2.17	0.73
1:A:99:GLN:HB2	1:A:128:LEU:HD23	1.71	0.73
1:C:4:GLN:H	1:C:4:GLN:CD	1.96	0.72
1:B:334:ILE:HG12	4:B:541:HOH:O	1.90	0.71
1:D:272:ASN:HD22	1:D:274:GLY:H	1.37	0.71
1:B:321:HIS:HD2	1:B:323:GLY:H	1.39	0.70
1:C:234:GLN:O	1:C:238:ILE:HG13	1.92	0.70
1:B:234:GLN:CD	1:B:237:ARG:HH21	1.99	0.69
1:A:4:GLN:NE2	1:A:4:GLN:N	2.38	0.69
1:D:289:LEU:O	1:D:321:HIS:HE1	1.76	0.67
1:B:91:LEU:HD13	1:B:93:MET:HE3	1.76	0.67
1:C:161:GLY:O	1:C:162:CYS:HB2	1.93	0.67
1:B:139:ARG:HD2	1:B:141:TRP:CB	2.24	0.67
1:D:179:VAL:O	1:D:183:GLU:HG3	1.95	0.67
1:C:21:LEU:HD11	1:C:36:ALA:HB2	1.77	0.66
1:D:99:GLN:HB2	1:D:128:LEU:HD23	1.77	0.66
1:A:100:GLU:HG3	1:A:102:TRP:NE1	2.11	0.66
1:A:161:GLY:O	1:A:162:CYS:HB2	1.96	0.66
1:C:191:ASP:O	1:C:218:ARG:HD2	1.96	0.66
1:D:228:PRO:HG3	4:D:522:HOH:O	1.95	0.66
1:C:77:GLN:HE22	1:C:115:ASN:H	1.42	0.65
1:A:1:MET:HE2	1:A:212:ALA:HB2	1.79	0.64
1:B:139:ARG:HG2	1:B:139:ARG:HH11	1.61	0.64
1:B:272:ASN:HD22	1:B:274:GLY:N	1.98	0.62
1:B:1:MET:HE3	1:B:212:ALA:CB	2.21	0.62
1:A:1:MET:CE	1:A:212:ALA:HB2	2.29	0.61
1:C:2:ASN:OD1	1:C:4:GLN:NE2	2.34	0.61
1:A:289:LEU:O	1:A:321:HIS:HE1	1.84	0.60
1:D:272:ASN:HD22	1:D:274:GLY:N	1.98	0.60
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.64	0.60
1:C:312:PRO:HG2	1:C:315:SER:OG	2.02	0.60
1:D:77:GLN:HE22	1:D:115:ASN:H	1.48	0.60
1:D:180:ARG:NH2	1:D:209:GLY:O	2.33	0.60
1:D:1:MET:HE3	1:D:212:ALA:CB	2.26	0.60
1:B:289:LEU:O	1:B:321:HIS:HE1	1.84	0.59
1:A:77:GLN:HE22	1:A:115:ASN:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:PRO:HG3	4:B:558:HOH:O	2.02	0.59
1:D:321:HIS:HD2	1:D:323:GLY:H	1.51	0.59
1:A:272:ASN:HD22	1:A:274:GLY:N	1.98	0.59
1:C:4:GLN:H	1:C:4:GLN:NE2	2.01	0.59
1:B:99:GLN:HG3	1:B:126:VAL:HG13	1.85	0.59
1:B:139:ARG:HG2	1:B:139:ARG:NH1	2.17	0.58
1:C:321:HIS:HD2	1:C:323:GLY:H	1.51	0.58
1:A:100:GLU:HG3	1:A:102:TRP:CE2	2.39	0.58
1:C:312:PRO:O	1:C:315:SER:OG	2.21	0.58
1:D:272:ASN:ND2	1:D:275:THR:H	2.02	0.57
1:C:272:ASN:ND2	1:C:275:THR:H	2.01	0.57
1:C:1:MET:HE3	1:C:212:ALA:CB	2.27	0.56
1:B:99:GLN:HB2	1:B:128:LEU:HD23	1.86	0.56
1:D:161:GLY:O	1:D:162:CYS:HB2	2.06	0.55
1:C:179:VAL:O	1:C:183:GLU:HG3	2.06	0.55
1:D:222:VAL:HG11	1:D:298:SER:HA	1.88	0.55
1:B:91:LEU:CD1	1:B:93:MET:HE3	2.36	0.55
1:D:31:LYS:HB3	1:D:313:GLU:HG3	1.89	0.55
1:A:321:HIS:HD2	1:A:323:GLY:H	1.55	0.54
1:D:250:ARG:HD3	1:D:251:ASP:O	2.07	0.54
1:C:1:MET:CE	1:C:212:ALA:HB2	2.26	0.54
1:A:215:ARG:O	1:A:218:ARG:HB2	2.08	0.54
1:A:163:SER:HA	1:A:201:SER:HB3	1.90	0.54
1:D:99:GLN:HG3	1:D:126:VAL:HG13	1.88	0.54
1:B:179:VAL:O	1:B:183:GLU:HG3	2.08	0.54
1:C:213:ASP:OD1	1:C:215:ARG:HG3	2.08	0.53
1:B:164:ASP:CG	1:B:237:ARG:HH22	2.17	0.53
1:B:321:HIS:CD2	1:B:323:GLY:H	2.24	0.53
1:C:61:GLU:O	1:C:65:GLN:HG3	2.10	0.52
1:D:198:VAL:HG21	1:D:294:TYR:CE1	2.44	0.52
1:B:161:GLY:O	1:B:162:CYS:HB2	2.09	0.52
1:C:91:LEU:CD1	1:C:93:MET:HE2	2.39	0.52
1:A:63:LEU:O	1:A:65:GLN:O	2.27	0.52
1:C:63:LEU:O	1:C:65:GLN:O	2.27	0.52
1:C:289:LEU:O	1:C:321:HIS:HE1	1.93	0.52
1:C:133:PHE:CE1	1:C:138:ARG:HD3	2.45	0.52
1:C:237:ARG:HH11	1:C:241:GLN:HE22	1.57	0.52
1:A:139:ARG:CG	1:A:142:GLU:H	2.14	0.51
1:A:81:THR:HB	1:A:97:LEU:HD13	1.91	0.51
1:A:99:GLN:HB2	1:A:128:LEU:CD2	2.39	0.51
1:B:63:LEU:O	1:B:65:GLN:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG11	1:B:155:PRO:HB3	1.93	0.50
1:C:23:ARG:NH1	1:D:89:ALA:O	2.44	0.50
1:B:291:ASP:HB2	1:B:292:PRO:HD2	1.94	0.50
1:C:2:ASN:HA	1:C:4:GLN:HE22	1.75	0.50
1:D:188:PHE:HB2	1:D:316:ARG:NH1	2.26	0.50
1:C:1:MET:HE2	1:C:248:LEU:HD13	1.92	0.50
1:D:198:VAL:HG21	1:D:294:TYR:HE1	1.76	0.50
1:D:250:ARG:CD	1:D:251:ASP:O	2.60	0.50
1:B:91:LEU:HD13	1:B:93:MET:CE	2.42	0.49
1:C:325:VAL:HG23	4:C:515:HOH:O	2.10	0.49
1:B:61:GLU:HG2	1:B:65:GLN:NE2	2.27	0.49
1:B:71:VAL:HG22	1:B:96:VAL:HB	1.94	0.49
1:D:59:ILE:HD12	1:D:91:LEU:CD1	2.43	0.49
1:C:92:GLY:HA2	1:D:23:ARG:CZ	2.43	0.49
1:C:312:PRO:O	1:C:313:GLU:C	2.55	0.49
1:C:294:TYR:OH	2:C:503:SO4:O1	2.30	0.48
1:C:228:PRO:HG3	4:C:550:HOH:O	2.13	0.48
1:D:40:ASP:HB3	1:D:323:GLY:HA2	1.94	0.48
1:B:292:PRO:HD3	1:B:328:LEU:CD1	2.44	0.48
1:C:91:LEU:HD12	1:C:93:MET:HE2	1.94	0.48
1:D:23:ARG:HG2	1:D:23:ARG:HH11	1.78	0.48
1:D:148:VAL:HG11	1:D:155:PRO:HB3	1.94	0.48
1:C:251:ASP:O	1:C:253:MET:HE2	2.13	0.48
1:D:91:LEU:HD13	1:D:93:MET:HE2	1.95	0.48
1:C:100:GLU:OE1	1:C:135:ILE:HG12	2.15	0.47
1:A:36:ALA:HA	1:A:319:TYR:O	2.14	0.47
1:C:138:ARG:O	1:C:139:ARG:HB2	2.14	0.47
1:B:23:ARG:NH1	1:B:285:THR:HA	2.30	0.47
1:A:74:GLY:HA2	1:A:102:TRP:CZ3	2.51	0.46
1:B:292:PRO:HD3	1:B:328:LEU:HD13	1.97	0.46
1:D:289:LEU:O	1:D:321:HIS:CE1	2.64	0.46
1:C:175:PHE:O	1:C:179:VAL:HG23	2.14	0.46
1:B:6:PHE:HA	1:B:7:PRO:HD3	1.79	0.46
1:C:272:ASN:ND2	1:C:274:GLY:N	2.61	0.46
1:C:225:SER:O	1:C:226:ALA:HB3	2.14	0.46
1:A:226:ALA:C	1:A:228:PRO:HD3	2.41	0.46
1:A:225:SER:O	1:A:226:ALA:HB3	2.15	0.45
1:B:250:ARG:HG2	1:B:251:ASP:N	2.31	0.45
1:C:6:PHE:HA	1:C:7:PRO:HD3	1.86	0.45
1:D:225:SER:O	1:D:226:ALA:HB3	2.16	0.45
1:A:188:PHE:C	1:A:188:PHE:CD1	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:O	1:A:321:HIS:CE1	2.69	0.45
1:D:101:ASN:HB2	4:D:552:HOH:O	2.16	0.45
1:A:223:ASP:O	1:A:264:ALA:HB2	2.17	0.44
1:B:1:MET:HB2	1:B:246:VAL:O	2.18	0.44
1:B:2:ASN:HD22	1:B:2:ASN:H	1.65	0.44
1:C:91:LEU:HD12	1:C:93:MET:CE	2.47	0.44
1:C:321:HIS:CD2	1:C:323:GLY:H	2.33	0.44
1:C:191:ASP:OD2	1:C:315:SER:HA	2.17	0.44
1:A:64:ALA:C	1:A:65:GLN:O	2.58	0.44
1:B:242:THR:O	1:B:246:VAL:HG22	2.17	0.44
1:C:36:ALA:HA	1:C:319:TYR:O	2.17	0.44
1:C:188:PHE:CD1	1:C:188:PHE:C	2.96	0.44
1:D:325:VAL:O	1:D:328:LEU:HB2	2.18	0.44
1:D:73:ILE:HG13	1:D:98:VAL:O	2.17	0.44
1:A:101:ASN:HD21	1:D:336:ARG:NH2	2.16	0.44
1:D:34:LEU:HD13	1:D:302:MET:HE3	1.99	0.44
1:A:188:PHE:CE1	1:A:316:ARG:HD3	2.53	0.44
1:B:188:PHE:C	1:B:188:PHE:CD1	2.96	0.43
1:A:325:VAL:HG13	1:A:328:LEU:HD12	2.00	0.43
1:C:70:LEU:O	1:C:95:CYS:HA	2.18	0.43
1:C:163:SER:HA	1:C:201:SER:HB3	1.99	0.43
1:A:62:ALA:HA	1:A:156:TYR:CD1	2.53	0.43
1:A:112:ARG:HD3	4:C:539:HOH:O	2.17	0.43
1:B:2:ASN:O	1:B:2:ASN:ND2	2.51	0.43
1:D:63:LEU:O	1:D:65:GLN:O	2.36	0.43
1:C:139:ARG:HD3	1:C:139:ARG:HA	1.73	0.43
1:A:321:HIS:CD2	1:A:323:GLY:H	2.35	0.43
1:C:37:LYS:HD3	1:C:175:PHE:CE2	2.53	0.43
1:B:144:ALA:O	1:B:148:VAL:HG23	2.19	0.43
1:B:295:GLU:OE2	3:B:401:PLP:N1	2.52	0.43
1:B:193:VAL:HA	1:B:318:LEU:O	2.19	0.43
1:D:81:THR:HB	1:D:97:LEU:HD13	2.00	0.43
1:D:250:ARG:HD2	1:D:251:ASP:C	2.44	0.43
1:A:109:VAL:O	1:A:113:VAL:HG22	2.19	0.42
1:B:82:ARG:HA	1:B:119:SER:OG	2.19	0.42
1:B:325:VAL:O	1:B:328:LEU:HB2	2.19	0.42
1:C:133:PHE:CE2	1:C:138:ARG:NH1	2.87	0.42
1:D:183:GLU:HB3	1:D:188:PHE:O	2.19	0.42
1:C:180:ARG:HD3	1:C:213:ASP:OD2	2.19	0.42
1:B:250:ARG:NH2	1:B:256:ASP:CG	2.78	0.42
1:C:161:GLY:C	1:C:163:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLN:HB2	1:D:128:LEU:CD2	2.46	0.42
1:D:250:ARG:HH11	1:D:250:ARG:HG3	1.83	0.42
1:A:196:CYS:HB2	1:A:298:SER:HB3	2.01	0.42
1:A:39:GLU:HB2	1:A:321:HIS:O	2.19	0.42
1:A:272:ASN:ND2	1:A:275:THR:H	2.17	0.42
1:D:248:LEU:HG	1:D:250:ARG:H	1.84	0.42
1:B:228:PRO:HB3	1:B:261:GLU:HG2	2.00	0.42
1:B:80:GLN:HB3	2:B:502:SO4:O3	2.20	0.41
1:D:46:ALA:O	1:D:47:PHE:HB2	2.18	0.41
1:D:170:LEU:O	1:D:171:GLY:C	2.61	0.41
1:B:336:ARG:HH11	1:B:336:ARG:HG2	1.85	0.41
1:A:250:ARG:HG3	1:A:250:ARG:NH1	2.34	0.41
1:C:133:PHE:CD2	1:C:138:ARG:NH1	2.89	0.41
1:D:292:PRO:HD3	1:D:328:LEU:CD1	2.50	0.41
1:D:59:ILE:HD12	1:D:91:LEU:HD11	2.02	0.41
1:A:130:PRO:O	1:A:131:ASP:C	2.63	0.41
1:B:63:LEU:O	1:B:64:ALA:C	2.64	0.41
1:B:272:ASN:ND2	1:B:275:THR:H	2.19	0.41
1:C:31:LYS:HB3	1:C:313:GLU:HG3	2.03	0.41
1:D:100:GLU:HG3	1:D:129:VAL:CG2	2.51	0.41
1:D:177:GLU:HA	1:D:180:ARG:NH1	2.36	0.41
1:D:75:GLY:HA2	1:D:100:GLU:O	2.21	0.41
1:C:292:PRO:HD3	1:C:328:LEU:HD23	2.03	0.40
1:C:199:THR:OG1	3:C:401:PLP:O3P	2.36	0.40
1:C:237:ARG:NH1	1:C:241:GLN:HE22	2.20	0.40

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	327/338 (97%)	314 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	325/338 (96%)	316 (97%)	9 (3%)	0	100	100
1	C	336/338 (99%)	322 (96%)	13 (4%)	1 (0%)	36	35
1	D	325/338 (96%)	315 (97%)	9 (3%)	1 (0%)	36	35
All	All	1313/1352 (97%)	1267 (96%)	44 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	212	ALA
1	D	4	GLN

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	258/264 (98%)	252 (98%)	6 (2%)	44	49
1	B	256/264 (97%)	251 (98%)	5 (2%)	48	54
1	C	263/264 (100%)	260 (99%)	3 (1%)	65	73
1	D	256/264 (97%)	251 (98%)	5 (2%)	48	54
All	All	1033/1056 (98%)	1014 (98%)	19 (2%)	51	58

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	99	GLN
1	A	100	GLU
1	A	142	GLU
1	A	146	GLU
1	A	304	GLU
1	B	2	ASN
1	B	99	GLN
1	B	281	LEU

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Mol	Chain	Res	Type
1	B	304	GLU
1	B	328	LEU
1	C	4	GLN
1	C	128	LEU
1	C	177	GLU
1	D	99	GLN
1	D	112	ARG
1	D	241	GLN
1	D	272	ASN
1	D	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	77	GLN
1	A	99	GLN
1	A	272	ASN
1	A	321	HIS
1	B	2	ASN
1	B	65	GLN
1	B	77	GLN
1	B	99	GLN
1	B	272	ASN
1	B	321	HIS
1	C	2	ASN
1	C	4	GLN
1	C	65	GLN
1	C	77	GLN
1	C	99	GLN
1	C	230	GLN
1	C	241	GLN
1	C	272	ASN
1	C	308	ASN
1	C	321	HIS
1	D	2	ASN
1	D	77	GLN
1	D	99	GLN
1	D	230	GLN
1	D	241	GLN
1	D	272	ASN
1	D	308	ASN

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Mol	Chain	Res	Type
1	D	321	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	502	-	4,4,4	0.43	0	6,6,6	0.16	0
3	PLP	D	401	1	15,15,16	1.60	5 (33%)	21,22,23	0.87	0
2	SO4	A	501	-	4,4,4	0.40	0	6,6,6	0.28	0
2	SO4	C	503	-	4,4,4	0.43	0	6,6,6	0.32	0
2	SO4	D	504	-	4,4,4	0.40	0	6,6,6	0.24	0
3	PLP	C	401	1	15,15,16	1.66	5 (33%)	21,22,23	1.02	0
3	PLP	B	401	1	15,15,16	1.91	4 (26%)	21,22,23	1.05	1 (4%)
3	PLP	A	401	1	15,15,16	1.97	4 (26%)	21,22,23	0.90	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	B	401	1	-	0/6/6/8	0/1/1/1
3	PLP	C	401	1	-	0/6/6/8	0/1/1/1
3	PLP	D	401	1	-	0/6/6/8	0/1/1/1
3	PLP	A	401	1	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PLP	C5-C4	5.01	1.46	1.40
3	B	401	PLP	C5-C4	3.96	1.45	1.40
3	B	401	PLP	C3-C2	3.51	1.44	1.41
3	B	401	PLP	C2A-C2	3.51	1.55	1.50
3	C	401	PLP	C2A-C2	3.31	1.55	1.50
3	C	401	PLP	C5-C4	3.29	1.44	1.40
3	D	401	PLP	C2A-C2	3.07	1.55	1.50
3	A	401	PLP	C6-C5	2.73	1.43	1.37
3	A	401	PLP	C2A-C2	2.60	1.54	1.50
3	D	401	PLP	C5-C4	2.58	1.43	1.40
3	D	401	PLP	C3-C2	2.54	1.43	1.41
3	D	401	PLP	C6-C5	2.35	1.42	1.37
3	B	401	PLP	C4A-C4	2.31	1.56	1.51
3	C	401	PLP	C6-C5	2.27	1.42	1.37
3	C	401	PLP	C3-C4	2.17	1.44	1.40
3	C	401	PLP	C3-C2	2.13	1.43	1.41
3	A	401	PLP	C3-C4	2.06	1.44	1.40
3	D	401	PLP	C3-C4	2.02	1.44	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	PLP	C6-N1-C2	2.03	122.88	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	SO4	1	0
2	C	503	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	PLP	1	0
3	B	401	PLP	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

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	331/338 (97%)	0.20	13 (3%) 43 42	19, 33, 49, 70	0
1	B	329/338 (97%)	0.18	9 (2%) 56 55	21, 33, 55, 69	0
1	C	338/338 (100%)	0.52	20 (5%) 28 27	20, 36, 53, 63	0
1	D	329/338 (97%)	0.48	12 (3%) 46 45	22, 37, 57, 74	0
All	All	1327/1352 (98%)	0.34	54 (4%) 41 40	19, 34, 55, 74	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	VAL	5.7
1	C	188	PHE	3.9
1	D	66	GLY	3.7
1	B	253	MET	3.5
1	A	130	PRO	3.5
1	C	187	GLY	3.4
1	C	212	ALA	3.3
1	B	150	ALA	3.1
1	C	137	PHE	3.0
1	A	131	ASP	2.9
1	A	244	GLU	2.9
1	C	181	ALA	2.9
1	C	136	GLY	2.9
1	D	184	ALA	2.8
1	C	66	GLY	2.8
1	B	101	ASN	2.8
1	C	306	VAL	2.8
1	D	129	VAL	2.8
1	A	66	GLY	2.7
1	C	192	TYR	2.7
1	D	186	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	233	GLU	2.6
1	C	249	GLU	2.6
1	A	254	ARG	2.6
1	D	255	ALA	2.5
1	D	102	TRP	2.5
1	C	218	ARG	2.4
1	C	211	ALA	2.4
1	C	151	ALA	2.4
1	D	252	ILE	2.4
1	B	102	TRP	2.4
1	D	7	PRO	2.4
1	D	243	ALA	2.3
1	B	66	GLY	2.3
1	B	254	ARG	2.3
1	B	129	VAL	2.3
1	D	251	ASP	2.3
1	C	30	GLY	2.3
1	C	250	ARG	2.3
1	A	102	TRP	2.3
1	C	314	GLY	2.2
1	C	150	ALA	2.2
1	A	101	ASN	2.2
1	D	152	GLY	2.1
1	A	23	ARG	2.1
1	D	253	MET	2.1
1	A	243	ALA	2.1
1	C	186	LEU	2.1
1	A	1	MET	2.1
1	C	253	MET	2.1
1	B	188	PHE	2.1
1	A	65	GLN	2.0
1	C	64	ALA	2.0
1	B	338	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
2	SO4	B	502	5/5	0.82	0.17	75,75,76,76	0
2	SO4	C	503	5/5	0.83	0.15	59,60,63,64	0
2	SO4	A	501	5/5	0.85	0.14	68,68,69,70	0
2	SO4	D	504	5/5	0.87	0.15	65,66,67,67	0
3	PLP	A	401	15/16	0.96	0.06	24,26,28,30	0
3	PLP	B	401	15/16	0.97	0.07	23,26,28,28	0
3	PLP	C	401	15/16	0.97	0.07	22,27,29,29	0
3	PLP	D	401	15/16	0.97	0.06	26,29,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.