



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 PM UTC

PDB ID : 1C3U / pdb_00001c3u
Title : T. MARITIMA ADENYLOSUCCINATE LYASE
Authors : Toth, E.A.; Yeates, T.O.
Deposited on : 1999-07-28
Resolution : 2.30 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

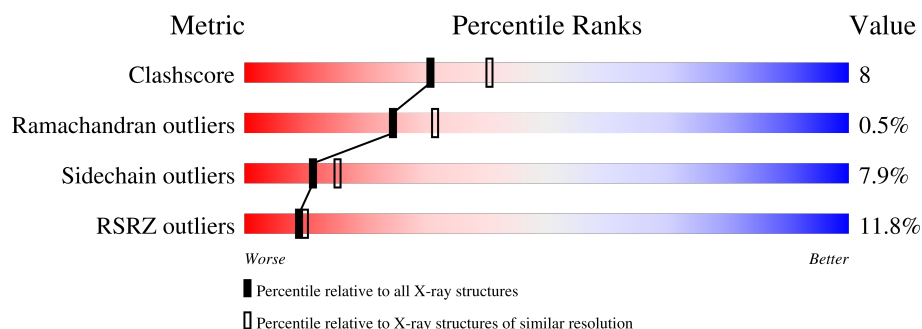
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	431	
1	B	431	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7128 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 ADENYLOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3358	2146	577	623	12			
1	B	423	Total	C	N	O	S	0	0	0
			3358	2146	577	623	12			

- 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	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

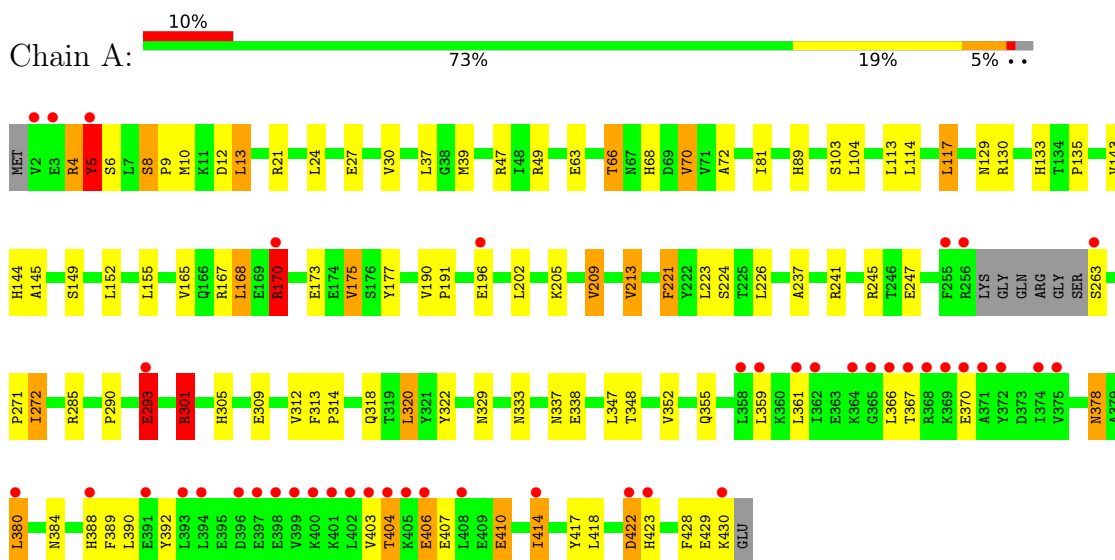
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	192	Total 192	O 192	0	0
3	B	200	Total 200	O 200	0	0

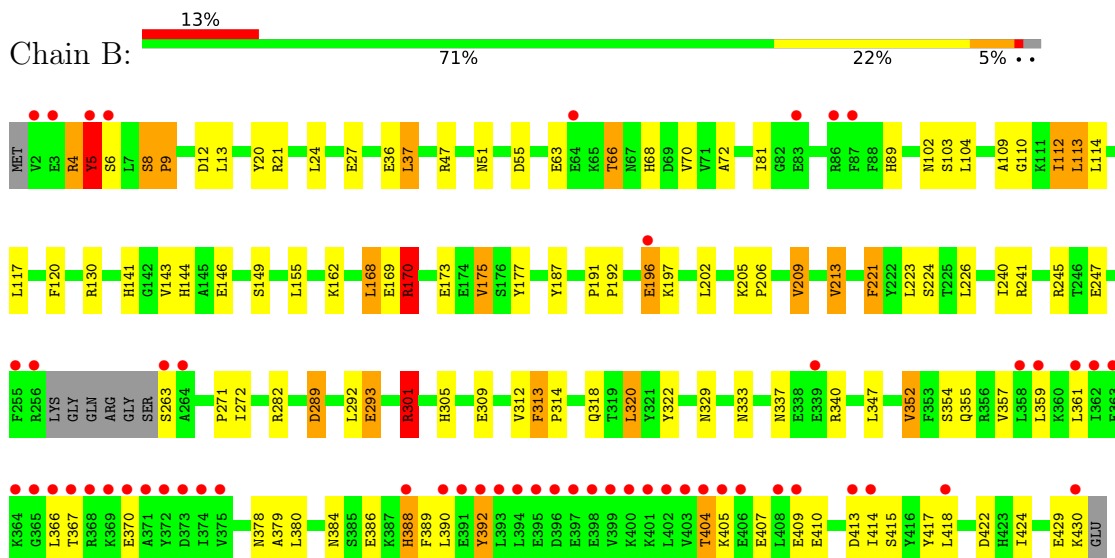
3 Residue-property plots

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: ADENYLOSUCCINATE LYASE



• Molecule 1: ADENYLOSUCCINATE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.50Å 126.21Å 169.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.30) 99.7 (50.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 2.29Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.199 , 0.230 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7128	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.79	3/3427 (0.1%)	1.66	50/4647 (1.1%)
1	B	0.82	3/3427 (0.1%)	1.80	75/4647 (1.6%)
All	All	0.81	6/6854 (0.1%)	1.73	125/9294 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	SER	CA-C	-15.12	1.34	1.53
1	A	9	PRO	N-CA	-9.65	1.30	1.47
1	B	9	PRO	N-CA	9.07	1.62	1.47
1	A	406	GLU	C-N	7.84	1.44	1.34
1	A	423	HIS	N-CA	5.78	1.53	1.46
1	B	418	LEU	N-CA	-5.73	1.37	1.46

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	SER	O-C-N	-24.70	93.50	121.66
1	B	418	LEU	N-CA-C	21.86	138.35	113.21
1	A	170	ARG	CD-NE-CZ	19.48	151.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	SER	CA-C-O	-11.43	104.50	120.16
1	B	209	VAL	CB-CA-C	-10.28	96.54	110.42
1	A	209	VAL	CB-CA-C	-9.67	96.97	110.12
1	B	413	ASP	CA-CB-CG	9.61	122.21	112.60
1	B	5	TYR	CB-CA-C	-9.20	96.12	111.02
1	B	388	HIS	CA-CB-CG	-9.10	104.70	113.80
1	B	170	ARG	NE-CZ-NH2	9.01	127.31	119.20
1	A	5	TYR	CB-CA-C	-8.96	96.59	111.02
1	B	415	SER	CA-C-O	-8.94	110.00	120.10
1	B	170	ARG	CD-NE-CZ	8.65	136.51	124.40
1	B	213	VAL	N-CA-CB	-8.39	96.84	112.36
1	A	9	PRO	N-CA-CB	8.29	111.72	102.60
1	B	418	LEU	CB-CA-C	-8.02	96.52	110.72
1	A	21	ARG	CD-NE-CZ	7.88	135.43	124.40
1	B	271	PRO	CA-C-N	7.82	131.52	120.42
1	B	271	PRO	C-N-CA	7.82	131.52	120.42
1	A	8	SER	O-C-N	7.79	130.28	121.32
1	B	170	ARG	NH1-CZ-NH2	-7.63	109.38	119.30
1	A	213	VAL	N-CA-CB	-7.55	98.38	112.36
1	A	388	HIS	CA-CB-CG	-7.54	106.26	113.80
1	A	170	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	B	8	SER	CB-CA-C	7.46	122.88	109.61
1	A	175	VAL	N-CA-CB	-7.43	99.59	112.08
1	A	418	LEU	CA-C-O	-7.31	110.80	119.35
1	B	175	VAL	N-CA-CB	-7.30	99.81	112.08
1	B	173	GLU	CB-CG-CD	7.22	124.88	112.60
1	B	9	PRO	CA-N-CD	-7.11	101.55	111.50
1	B	12	ASP	CA-CB-CG	-7.04	105.56	112.60
1	B	417	TYR	N-CA-C	-7.00	103.72	112.90
1	B	318	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	6	SER	CB-CA-C	6.92	121.11	109.84
1	A	145	ALA	CA-C-O	-6.87	114.80	119.68
1	B	6	SER	CB-CA-C	6.85	121.01	109.84
1	B	241	ARG	NE-CZ-NH1	-6.80	114.70	121.50
1	A	12	ASP	CA-CB-CG	-6.79	105.81	112.60
1	B	209	VAL	N-CA-CB	6.75	121.00	111.82
1	A	170	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	B	103	SER	N-CA-CB	6.68	119.69	110.01
1	B	5	TYR	CA-C-N	-6.63	112.02	121.50
1	B	5	TYR	C-N-CA	-6.63	112.02	121.50
1	A	173	GLU	CB-CG-CD	6.51	123.67	112.60
1	B	21	ARG	CD-NE-CZ	6.47	133.46	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	HIS	N-CA-C	-6.40	104.23	111.14
1	B	392	TYR	CA-C-O	-6.36	113.81	120.55
1	B	47	ARG	CD-NE-CZ	6.31	133.23	124.40
1	B	120	PHE	CA-CB-CG	6.29	120.09	113.80
1	B	379	ALA	CA-C-O	6.22	127.35	120.82
1	B	9	PRO	CB-CA-C	-6.20	96.49	112.00
1	A	389	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	422	ASP	CB-CA-C	-6.17	100.55	110.79
1	B	352	VAL	N-CA-CB	-6.09	101.19	111.23
1	B	292	LEU	CA-C-O	-6.07	113.99	120.42
1	A	30	VAL	CA-C-O	-5.99	114.50	120.85
1	A	209	VAL	N-CA-CB	5.94	120.78	111.99
1	B	240	ILE	CA-C-O	-5.90	114.82	120.95
1	A	224	SER	CB-CA-C	-5.88	101.64	110.88
1	A	221	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	8	SER	CA-C-N	5.86	141.06	127.00
1	A	8	SER	C-N-CA	5.86	141.06	127.00
1	A	103	SER	CA-C-O	-5.84	114.68	120.82
1	A	5	TYR	CB-CG-CD1	-5.83	112.05	120.80
1	B	313	PHE	CA-C-O	5.83	124.44	118.73
1	B	20	TYR	CA-C-O	-5.82	114.38	120.55
1	A	378	ASN	CA-CB-CG	-5.79	106.81	112.60
1	A	417	TYR	CA-C-O	5.79	126.48	119.31
1	B	55	ASP	CA-C-N	5.78	127.84	120.56
1	B	55	ASP	C-N-CA	5.78	127.84	120.56
1	B	301	ARG	N-CA-CB	5.74	120.18	110.49
1	A	293	GLU	CB-CG-CD	-5.71	102.89	112.60
1	B	162	LYS	CB-CA-C	-5.71	101.14	110.85
1	B	112	ILE	CA-C-O	5.69	126.87	120.95
1	B	110	GLY	N-CA-C	-5.69	105.90	112.73
1	A	338	GLU	N-CA-C	5.68	117.47	111.28
1	B	209	VAL	CA-CB-CG2	5.68	120.05	110.40
1	B	417	TYR	CA-CB-CG	-5.66	103.71	113.90
1	B	221	PHE	CA-CB-CG	-5.59	108.20	113.80
1	A	130	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	A	241	ARG	NE-CZ-NH1	-5.50	116.00	121.50
1	B	340	ARG	NH1-CZ-NH2	5.47	126.42	119.30
1	A	271	PRO	CA-C-N	5.47	128.19	120.42
1	A	271	PRO	C-N-CA	5.47	128.19	120.42
1	B	384	ASN	CA-CB-CG	-5.47	107.13	112.60
1	B	146	GLU	O-C-N	5.45	125.80	121.55
1	B	224	SER	CA-C-O	-5.45	114.77	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	ASP	O-C-N	5.45	128.97	122.27
1	B	191	PRO	CA-C-N	5.43	125.05	119.56
1	B	191	PRO	C-N-CA	5.43	125.05	119.56
1	B	357	VAL	N-CA-C	5.43	116.06	110.36
1	B	130	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	A	237	ALA	CA-C-O	-5.40	114.70	120.42
1	B	196	GLU	CB-CG-CD	5.38	121.74	112.60
1	A	129	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	422	ASP	CA-C-N	5.37	127.74	120.44
1	A	422	ASP	C-N-CA	5.37	127.74	120.44
1	B	5	TYR	CB-CG-CD1	-5.36	112.76	120.80
1	A	70	VAL	N-CA-CB	5.35	121.06	110.95
1	A	428	PHE	CA-CB-CG	-5.35	108.45	113.80
1	B	354	SER	CA-C-O	-5.34	113.83	119.97
1	B	169	GLU	CA-C-O	-5.34	114.89	120.55
1	A	81	ILE	N-CA-C	-5.33	107.53	112.43
1	B	282	ARG	CD-NE-CZ	5.33	131.85	124.40
1	A	301	ARG	N-CA-CB	5.28	119.41	110.49
1	B	422	ASP	O-C-N	5.28	127.71	122.12
1	B	102	ASN	CA-C-O	-5.25	113.93	119.97
1	B	422	ASP	N-CA-C	5.25	117.00	111.28
1	B	386	GLU	CA-C-O	-5.24	113.08	119.32
1	B	5	TYR	CA-CB-CG	-5.24	104.48	113.90
1	A	49	ARG	CA-C-O	-5.23	115.33	120.82
1	B	424	ILE	N-CA-C	5.22	115.95	110.62
1	B	51	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	81	ILE	CA-C-O	5.19	123.90	119.38
1	B	5	TYR	O-C-N	5.16	128.93	122.22
1	A	13	LEU	N-CA-C	5.15	117.64	111.71
1	A	152	LEU	CA-C-O	-5.14	115.42	120.82
1	A	406	GLU	CA-C-N	5.09	127.61	120.28
1	A	406	GLU	C-N-CA	5.09	127.61	120.28
1	A	285	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	B	289	ASP	CA-CB-CG	-5.06	107.54	112.60
1	B	389	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	175	VAL	CB-CA-C	5.03	119.82	111.37
1	B	5	TYR	CA-C-O	-5.01	113.88	119.95
1	B	6	SER	N-CA-C	-5.01	101.80	109.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Mainchain
1	B	8	SER	Mainchain

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	3358	0	3302	60	1
1	B	3358	0	3302	54	4
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	192	0	0	7	5
3	B	200	0	0	8	3
All	All	7128	0	6604	111	8

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 8.

All (111) 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:378:ASN:HD22	1:B:392:TYR:HB3	1.26	0.98
1:A:290:PRO:HA	1:A:293:GLU:OE1	1.67	0.94
1:B:378:ASN:ND2	1:B:392:TYR:HB3	1.83	0.93
1:A:63:GLU:HA	1:A:66:THR:HG22	1.53	0.90
1:B:63:GLU:HA	1:B:66:THR:HG22	1.51	0.90
1:A:5:TYR:HB3	1:A:322:TYR:CG	2.17	0.79
1:A:170:ARG:HH12	1:A:221:PHE:HZ	1.31	0.79
1:B:5:TYR:HB3	1:B:322:TYR:CG	2.19	0.78
1:B:66:THR:HG23	1:B:68:HIS:H	1.49	0.78
1:A:66:THR:HG23	1:A:68:HIS:H	1.54	0.72
1:B:66:THR:HG21	1:B:72:ALA:HB2	1.72	0.71
1:B:5:TYR:HB3	1:B:322:TYR:CD1	2.27	0.69
1:B:170:ARG:HH12	1:B:221:PHE:HZ	1.41	0.67
1:A:5:TYR:HB3	1:A:322:TYR:CD1	2.30	0.65
1:A:313:PHE:HB2	1:A:314:PRO:HD3	1.80	0.64
1:A:329:ASN:ND2	1:A:333:ASN:HD22	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:THR:HG21	1:A:72:ALA:HB2	1.80	0.63
1:A:367:THR:HG22	1:A:370:GLU:HG3	1.79	0.63
1:B:355:GLN:HE21	1:B:359:LEU:HD11	1.62	0.63
1:B:27:GLU:OE2	1:B:89:HIS:HD2	1.81	0.62
1:A:133:HIS:HE1	1:A:422:ASP:OD1	1.81	0.62
1:B:329:ASN:ND2	1:B:333:ASN:HD22	1.98	0.62
1:B:66:THR:HG23	1:B:68:HIS:N	2.14	0.61
1:A:27:GLU:OE2	1:A:89:HIS:HD2	1.83	0.61
1:B:226:LEU:HG	1:B:320:LEU:HD12	1.83	0.61
1:A:247:GLU:OE1	1:B:144:HIS:HE1	1.84	0.61
1:A:301:ARG:HH21	1:A:305:HIS:CE1	2.19	0.60
1:A:301:ARG:HH21	1:A:305:HIS:HE1	1.50	0.59
1:B:301:ARG:HH21	1:B:305:HIS:CE1	2.20	0.59
1:B:367:THR:HG22	1:B:370:GLU:HG3	1.85	0.58
1:B:293:GLU:HA	3:B:2011:HOH:O	2.03	0.58
1:B:313:PHE:HB2	1:B:314:PRO:HD3	1.85	0.58
1:A:422:ASP:O	3:A:1015:HOH:O	2.17	0.58
1:A:144:HIS:HD2	3:A:1042:HOH:O	1.87	0.57
1:A:66:THR:HG23	1:A:68:HIS:N	2.19	0.56
1:A:177:TYR:HA	1:A:205:LYS:O	2.04	0.56
1:A:226:LEU:HG	1:A:320:LEU:HD12	1.86	0.56
1:A:329:ASN:HD21	1:A:333:ASN:HD22	1.53	0.55
1:A:337:ASN:HB3	3:A:1119:HOH:O	2.06	0.55
1:A:378:ASN:HD22	1:A:392:TYR:HB3	1.71	0.55
1:A:144:HIS:HE1	1:B:247:GLU:OE1	1.91	0.54
1:B:405:LYS:O	1:B:409:GLU:HG3	2.08	0.54
1:A:355:GLN:HE21	1:A:359:LEU:HD11	1.73	0.54
1:B:329:ASN:HD21	1:B:333:ASN:HD22	1.54	0.53
1:A:245:ARG:HD2	3:A:1106:HOH:O	2.09	0.53
1:B:355:GLN:NE2	1:B:359:LEU:HD11	2.23	0.53
1:B:361:LEU:HB3	1:B:366:LEU:HD12	1.91	0.53
1:A:39:MET:HE1	1:A:191:PRO:HG2	1.91	0.52
1:A:47:ARG:HD3	3:A:1181:HOH:O	2.09	0.51
1:A:329:ASN:ND2	1:A:333:ASN:ND2	2.59	0.51
1:A:361:LEU:HB3	1:A:366:LEU:HD12	1.92	0.50
1:B:66:THR:CG2	1:B:68:HIS:H	2.22	0.50
1:B:388:HIS:HB3	3:B:2071:HOH:O	2.10	0.49
1:B:404:THR:HB	1:B:407:GLU:OE1	2.12	0.49
1:B:329:ASN:ND2	1:B:333:ASN:ND2	2.61	0.49
1:B:187:TYR:HB3	1:B:192:PRO:HD3	1.94	0.49
1:B:301:ARG:HH21	1:B:305:HIS:HE1	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLN:NE2	1:A:359:LEU:HD11	2.28	0.49
1:B:170:ARG:HB2	1:B:170:ARG:CZ	2.43	0.49
1:A:404:THR:HG22	1:A:406:GLU:H	1.78	0.49
1:B:104:LEU:HD21	1:B:202:LEU:HB3	1.95	0.48
1:B:329:ASN:HD21	1:B:333:ASN:ND2	2.12	0.48
1:A:167:ARG:HG2	1:A:170:ARG:HH21	1.78	0.48
1:B:170:ARG:HB2	1:B:170:ARG:NH1	2.29	0.48
1:A:429:GLU:O	1:A:430:LYS:HB3	2.14	0.47
1:A:305:HIS:HD2	1:A:309:GLU:OE1	1.97	0.47
1:B:245:ARG:HD2	3:B:2106:HOH:O	2.14	0.47
1:B:37:LEU:HD13	1:B:197:LYS:HE3	1.96	0.47
1:B:305:HIS:HD2	1:B:309:GLU:OE1	1.97	0.46
1:A:66:THR:CG2	1:A:68:HIS:H	2.22	0.46
1:A:293:GLU:HA	3:A:1011:HOH:O	2.15	0.46
1:A:104:LEU:HD21	1:A:202:LEU:HB3	1.98	0.46
1:A:114:LEU:HA	1:A:168:LEU:HD13	1.97	0.46
1:B:223:LEU:HD13	1:B:312:VAL:HG11	1.97	0.46
1:A:117:LEU:HD13	1:A:165:VAL:CG2	2.46	0.46
1:A:404:THR:HG22	1:A:406:GLU:N	2.30	0.46
1:B:177:TYR:HA	1:B:205:LYS:O	2.16	0.45
1:A:329:ASN:HD21	1:A:333:ASN:ND2	2.13	0.45
1:B:114:LEU:HA	1:B:168:LEU:HD13	1.99	0.45
1:B:337:ASN:HB3	3:B:2119:HOH:O	2.16	0.45
1:A:143:VAL:HA	3:B:2082:HOH:O	2.17	0.45
1:A:170:ARG:CZ	1:A:170:ARG:HB2	2.47	0.45
1:B:144:HIS:HD2	3:B:2042:HOH:O	2.00	0.45
1:B:378:ASN:HD22	1:B:392:TYR:CB	2.13	0.45
1:B:404:THR:HG22	1:B:407:GLU:H	1.83	0.44
1:A:223:LEU:HD13	1:A:312:VAL:HG11	1.98	0.44
1:A:5:TYR:HB3	1:A:322:TYR:CB	2.47	0.44
1:A:290:PRO:HA	1:A:293:GLU:CD	2.38	0.43
1:A:117:LEU:HD13	1:A:165:VAL:HG23	1.99	0.43
1:A:348:THR:HG21	3:B:2129:HOH:O	2.17	0.43
1:A:135:PRO:HB3	1:A:414:ILE:HD11	2.01	0.43
1:A:190:VAL:HA	1:A:191:PRO:HD3	1.90	0.43
1:A:63:GLU:HA	1:A:66:THR:CG2	2.38	0.43
1:B:143:VAL:O	1:B:144:HIS:C	2.62	0.43
1:A:272:ILE:HD11	1:B:141:HIS:CE1	2.54	0.42
1:B:9:PRO:HB2	1:B:112:ILE:HD13	2.01	0.42
1:A:367:THR:HG22	1:A:370:GLU:CG	2.47	0.42
1:B:429:GLU:O	1:B:430:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LYS:O	1:B:405:LYS:HG3	2.18	0.42
1:B:289:ASP:HB3	3:B:2051:HOH:O	2.19	0.42
1:A:380:LEU:HD12	1:A:384:ASN:ND2	2.35	0.42
1:A:403:VAL:HG12	1:A:407:GLU:HB2	2.01	0.42
1:B:5:TYR:HB3	1:B:322:TYR:CB	2.50	0.41
1:A:170:ARG:NH2	3:A:1067:HOH:O	2.54	0.41
1:B:187:TYR:CB	1:B:192:PRO:HD3	2.50	0.41
1:B:205:LYS:HB3	1:B:206:PRO:HD2	2.02	0.41
1:B:367:THR:HG22	1:B:370:GLU:CG	2.50	0.41
1:B:109:ALA:O	1:B:113:LEU:HB2	2.21	0.41
1:A:430:LYS:O	1:A:430:LYS:HG3	2.20	0.40
1:A:293:GLU:OE2	1:A:293:GLU:C	2.64	0.40
1:A:10:MET:HG3	1:A:318:GLN:HG2	2.03	0.40

All (8) 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)
3:B:2018:HOH:O	3:B:2076:HOH:O[4_555]	0.20	2.00
3:B:2078:HOH:O	3:B:2144:HOH:O[4_555]	0.32	1.88
3:A:1142:HOH:O	3:B:2081:HOH:O[8_455]	0.51	1.69
1:B:293:GLU:OE1	3:A:1047:HOH:O[4_555]	0.82	1.38
3:A:1078:HOH:O	3:A:1144:HOH:O[4_555]	0.82	1.38
1:B:293:GLU:CD	3:A:1047:HOH:O[4_555]	0.86	1.34
1:B:293:GLU:OE2	3:A:1047:HOH:O[4_555]	1.45	0.75
1:A:410:GLU:OE1	1:B:36:GLU:OE2[5_455]	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	419/431 (97%)	408 (97%)	9 (2%)	2 (0%)	24 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	419/431 (97%)	408 (97%)	9 (2%)	2 (0%)	24	31
All	All	838/862 (97%)	816 (97%)	18 (2%)	4 (0%)	24	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	ARG
1	B	4	ARG
1	B	301	ARG
1	A	4	ARG

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	355/384 (92%)	327 (92%)	28 (8%)	11	15
1	B	355/384 (92%)	327 (92%)	28 (8%)	11	15
All	All	710/768 (92%)	654 (92%)	56 (8%)	11	15

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	TYR
1	A	13	LEU
1	A	24	LEU
1	A	37	LEU
1	A	66	THR
1	A	70	VAL
1	A	113	LEU
1	A	117	LEU
1	A	149	SER
1	A	155	LEU
1	A	168	LEU

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Mol	Chain	Res	Type
1	A	170	ARG
1	A	175	VAL
1	A	196	GLU
1	A	209	VAL
1	A	213	VAL
1	A	263	SER
1	A	272	ILE
1	A	293	GLU
1	A	320	LEU
1	A	347	LEU
1	A	352	VAL
1	A	380	LEU
1	A	390	LEU
1	A	404	THR
1	A	410	GLU
1	A	414	ILE
1	B	4	ARG
1	B	5	TYR
1	B	13	LEU
1	B	24	LEU
1	B	37	LEU
1	B	66	THR
1	B	70	VAL
1	B	113	LEU
1	B	117	LEU
1	B	149	SER
1	B	155	LEU
1	B	168	LEU
1	B	170	ARG
1	B	175	VAL
1	B	196	GLU
1	B	209	VAL
1	B	213	VAL
1	B	263	SER
1	B	272	ILE
1	B	293	GLU
1	B	320	LEU
1	B	347	LEU
1	B	352	VAL
1	B	380	LEU
1	B	390	LEU
1	B	404	THR

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Mol	Chain	Res	Type
1	B	410	GLU
1	B	414	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	133	HIS
1	A	144	HIS
1	A	270	ASN
1	A	299	HIS
1	A	305	HIS
1	A	318	GLN
1	A	329	ASN
1	A	337	ASN
1	A	355	GLN
1	A	378	ASN
1	B	89	HIS
1	B	144	HIS
1	B	270	ASN
1	B	299	HIS
1	B	305	HIS
1	B	329	ASN
1	B	333	ASN
1	B	355	GLN
1	B	378	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	432	-	4,4,4	0.58	0	6,6,6	0.64	0
2	SO4	A	433	-	4,4,4	0.75	0	6,6,6	0.25	0
2	SO4	A	432	-	4,4,4	0.68	0	6,6,6	0.40	0
2	SO4	B	433	-	4,4,4	0.76	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	423/431 (98%)	0.19	45 (10%)	11 12	8, 16, 60, 78	0
1	B	423/431 (98%)	0.26	55 (13%)	7 8	8, 17, 60, 78	0
All	All	846/862 (98%)	0.22	100 (11%)	9 10	8, 17, 60, 78	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	THR	6.8
1	B	256	ARG	6.5
1	A	430	LYS	6.2
1	B	402	LEU	6.1
1	A	398	GLU	5.7
1	A	369	LYS	5.6
1	B	366	LEU	5.5
1	A	366	LEU	5.5
1	A	2	VAL	5.5
1	B	399	VAL	5.2
1	B	2	VAL	5.1
1	A	402	LEU	5.1
1	B	371	ALA	5.1
1	B	368	ARG	5.0
1	B	361	LEU	4.9
1	B	369	LYS	4.9
1	A	367	THR	4.8
1	B	370	GLU	4.8
1	B	362	ILE	4.7
1	B	372	TYR	4.5
1	A	368	ARG	4.5
1	A	293	GLU	4.5
1	B	358	LEU	4.4
1	B	413	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	403	VAL	4.3
1	A	5	TYR	4.3
1	A	256	ARG	4.3
1	A	399	VAL	4.2
1	B	5	TYR	4.2
1	B	263	SER	4.2
1	B	374	ILE	4.2
1	B	400	LYS	4.2
1	B	404	THR	4.2
1	A	255	PHE	4.1
1	A	362	ILE	4.1
1	B	398	GLU	4.1
1	B	430	LYS	4.0
1	A	396	ASP	4.0
1	B	396	ASP	4.0
1	B	394	LEU	3.9
1	A	263	SER	3.9
1	A	404	THR	3.9
1	A	364	LYS	3.8
1	B	418	LEU	3.8
1	B	406	GLU	3.6
1	B	365	GLY	3.6
1	A	359	LEU	3.6
1	B	359	LEU	3.6
1	B	255	PHE	3.6
1	A	371	ALA	3.6
1	A	370	GLU	3.5
1	A	388	HIS	3.5
1	B	86	ARG	3.5
1	A	361	LEU	3.5
1	A	397	GLU	3.5
1	B	408	LEU	3.5
1	B	364	LYS	3.4
1	A	403	VAL	3.4
1	B	363	GLU	3.3
1	B	393	LEU	3.3
1	B	401	LYS	3.3
1	A	400	LYS	3.2
1	B	64	GLU	3.2
1	A	365	GLY	3.1
1	B	414	ILE	3.0
1	A	372	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	392	TYR	2.8
1	B	373	ASP	2.8
1	B	375	VAL	2.8
1	A	401	LYS	2.8
1	A	3	GLU	2.8
1	B	397	GLU	2.7
1	A	406	GLU	2.6
1	B	196	GLU	2.6
1	B	395	GLU	2.6
1	B	405	LYS	2.6
1	A	405	LYS	2.6
1	B	409	GLU	2.5
1	A	408	LEU	2.5
1	A	423	HIS	2.5
1	A	196	GLU	2.4
1	B	6	SER	2.4
1	A	422	ASP	2.4
1	B	3	GLU	2.4
1	A	358	LEU	2.4
1	B	388	HIS	2.4
1	A	170	ARG	2.3
1	A	393	LEU	2.3
1	A	374	ILE	2.3
1	A	414	ILE	2.3
1	A	391	GLU	2.2
1	B	339	GLU	2.2
1	B	391	GLU	2.2
1	B	87	PHE	2.1
1	A	380	LEU	2.1
1	B	83	GLU	2.1
1	A	375	VAL	2.1
1	B	264	ALA	2.0
1	A	394	LEU	2.0
1	B	390	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	433	5/5	0.89	0.14	38,39,40,42	0
2	SO4	B	433	5/5	0.89	0.14	39,39,40,42	0
2	SO4	B	432	5/5	0.99	0.04	19,20,22,22	0
2	SO4	A	432	5/5	0.99	0.05	19,20,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.