



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 02:02 AM EDT

PDB ID : 1C3U
Title : T. MARITIMA ADENYLOSUCCINATE LYASE
Authors : Toth, E.A.; Yeates, T.O.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

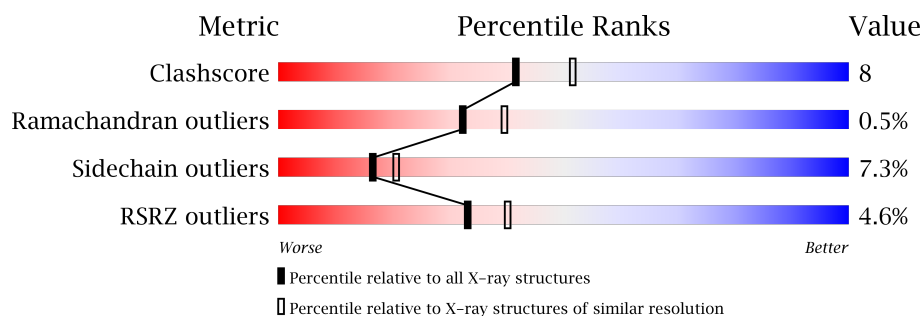
1 Overall quality at a glance

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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	433	-	-	-	X
2	SO4	B	433	-	-	-	X

2 Entry composition [i](#)

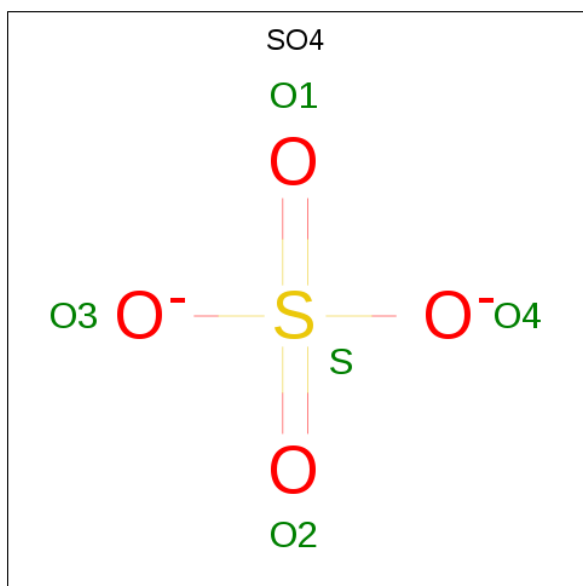
There are 3 unique types of molecules in this entry. The entry contains 7128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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		

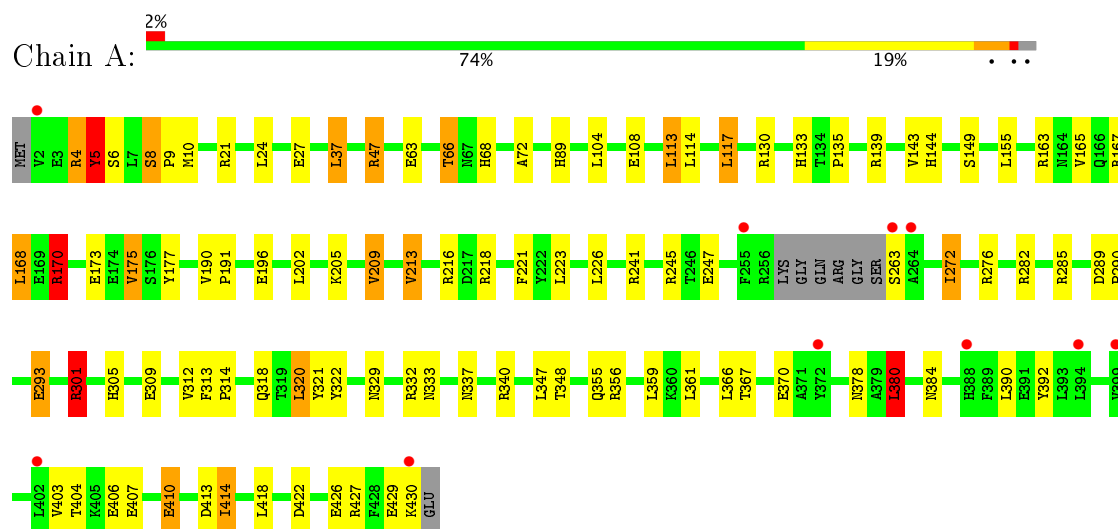
- Molecule 3 is water.

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

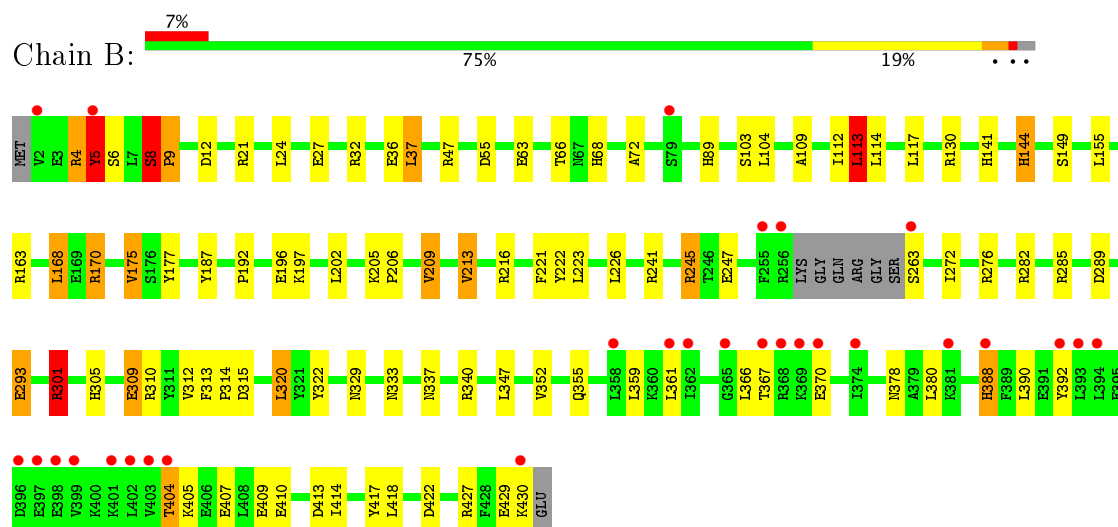
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 49.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.30) 99.7 (49.06-2.30)	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.	DCC
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 , 53.3	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	0.63	1/3427 (0.0%)	1.41	45/4647 (1.0%)
1	B	0.65	2/3427 (0.1%)	1.52	62/4647 (1.3%)
All	All	0.64	3/6854 (0.0%)	1.47	107/9294 (1.2%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	B	8	SER	CA-C	-7.18	1.34	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ARG	CD-NE-CZ	20.05	151.66	123.60
1	A	5	TYR	CB-CG-CD1	-14.91	112.05	121.00
1	B	8	SER	O-C-N	-14.53	93.50	121.10
1	B	170	ARG	NE-CZ-NH2	14.02	127.31	120.30
1	B	5	TYR	CB-CG-CD1	-13.73	112.76	121.00
1	A	21	ARG	NE-CZ-NH1	11.74	126.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	A	170	ARG	NE-CZ-NH2	11.34	125.97	120.30
1	B	241	ARG	NE-CZ-NH1	-11.20	114.70	120.30
1	A	170	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	B	422	ASP	CB-CG-OD2	-10.59	108.77	118.30
1	B	21	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	B	245	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	B	418	LEU	N-CA-C	10.13	138.35	111.00
1	B	21	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	B	427	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	B	422	ASP	CB-CG-OD1	9.44	126.79	118.30
1	B	163	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	8	SER	CA-C-N	9.33	143.23	117.10
1	B	276	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	170	ARG	CD-NE-CZ	9.22	136.51	123.60
1	B	170	ARG	NH1-CZ-NH2	-9.11	109.38	119.40
1	A	427	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	276	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	A	241	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	B	340	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	289	ASP	CB-CG-OD2	-8.53	110.63	118.30
1	A	21	ARG	CD-NE-CZ	8.45	135.43	123.60
1	B	130	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	A	21	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	B	113	LEU	CA-CB-CG	8.00	133.70	115.30
1	B	12	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	130	ARG	NE-CZ-NH2	7.83	124.21	120.30
1	B	209	VAL	CB-CA-C	-7.82	96.54	111.40
1	B	5	TYR	CG-CD2-CE2	-7.67	115.16	121.30
1	A	209	VAL	CB-CA-C	-7.59	96.97	111.40
1	A	8	SER	CA-C-O	-7.43	104.50	120.10
1	B	418	LEU	CB-CA-C	-7.20	96.52	110.20
1	A	418	LEU	CA-C-N	7.19	133.03	117.20
1	B	315	ASP	CB-CG-OD2	7.18	124.76	118.30
1	B	5	TYR	CB-CA-C	-7.14	96.12	110.40
1	B	9	PRO	CA-N-CD	-7.11	101.55	111.50
1	B	21	ARG	CD-NE-CZ	7.04	133.46	123.60
1	A	9	PRO	N-CA-CB	7.01	111.72	103.30
1	A	285	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	A	5	TYR	CB-CA-C	-6.90	96.59	110.40
1	B	47	ARG	CD-NE-CZ	6.88	133.23	123.60
1	B	8	SER	CB-CA-C	6.73	122.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ASP	CB-CG-OD1	6.71	124.33	118.30
1	B	213	VAL	N-CA-CB	-6.67	96.84	111.50
1	A	139	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	285	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	426	GLU	OE1-CD-OE2	6.46	131.05	123.30
1	A	282	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	108	GLU	OE1-CD-OE2	-6.44	115.58	123.30
1	B	413	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	310	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	340	ARG	NH1-CZ-NH2	6.38	126.42	119.40
1	A	340	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	5	TYR	CD1-CG-CD2	6.36	124.90	117.90
1	B	216	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	9	PRO	CB-CA-C	-6.20	96.49	112.00
1	B	222	TYR	CB-CG-CD1	-6.16	117.31	121.00
1	B	103	SER	N-CA-CB	6.13	119.69	110.50
1	B	209	VAL	CA-CB-CG2	6.10	120.05	110.90
1	B	170	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	245	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	282	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	213	VAL	N-CA-CB	-5.96	98.38	111.50
1	A	216	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	282	ARG	CD-NE-CZ	5.90	131.85	123.60
1	A	113	LEU	CA-CB-CG	5.87	128.80	115.30
1	B	213	VAL	CG1-CB-CG2	5.86	120.28	110.90
1	A	218	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	6	SER	CB-CA-C	5.80	121.11	110.10
1	B	32	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	B	6	SER	CB-CA-C	5.74	121.01	110.10
1	A	332	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	A	321	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	A	276	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	413	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	163	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	427	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	340	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	173	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	B	47	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	A	175	VAL	N-CA-CB	-5.41	99.59	111.50
1	A	213	VAL	CG1-CB-CG2	5.37	119.49	110.90
1	A	47	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	B	301	ARG	N-CA-CB	5.32	120.18	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	VAL	N-CA-CB	-5.32	99.81	111.50
1	B	309	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	B	222	TYR	CB-CG-CD2	5.28	124.17	121.00
1	A	5	TYR	CD1-CG-CD2	5.27	123.70	117.90
1	B	388	HIS	CA-CB-CG	-5.24	104.70	113.60
1	A	37	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	356	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	380	LEU	CA-CB-CG	5.12	127.09	115.30
1	B	427	ARG	CD-NE-CZ	5.11	130.76	123.60
1	B	427	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	B	417	TYR	CA-CB-CG	-5.10	103.71	113.40
1	A	5	TYR	CG-CD2-CE2	-5.10	117.22	121.30
1	A	427	ARG	CD-NE-CZ	5.08	130.71	123.60
1	A	5	TYR	CB-CG-CD2	5.04	124.02	121.00
1	B	130	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	A	340	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	B	315	ASP	OD1-CG-OD2	-5.02	113.77	123.30

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

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	57	1
1	B	3358	0	3302	53	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	107	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 (107) 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:170:ARG:HH12	1:A:221:PHE:HZ	1.31	0.79
1:A:5:TYR:HB3	1:A:322:TYR:CG	2.17	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
1:A:367:THR:HG22	1:A:370:GLU:HG3	1.79	0.63
1:A:66:THR:HG21	1:A:72:ALA:HB2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:429:GLU:O	1:B:430:LYS:HB3	2.19	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	32	39
1	B	419/431 (97%)	408 (97%)	9 (2%)	2 (0%)	32	39
All	All	838/862 (97%)	816 (97%)	18 (2%)	4 (0%)	32	39

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 [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	355/384 (92%)	330 (93%)	25 (7%)	18	22
1	B	355/384 (92%)	328 (92%)	27 (8%)	15	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	710/768 (92%)	658 (93%)	52 (7%)	16	21

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	TYR
1	A	24	LEU
1	A	37	LEU
1	A	66	THR
1	A	113	LEU
1	A	117	LEU
1	A	149	SER
1	A	155	LEU
1	A	168	LEU
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	301	ARG
1	A	320	LEU
1	A	347	LEU
1	A	380	LEU
1	A	390	LEU
1	A	410	GLU
1	A	414	ILE
1	B	4	ARG
1	B	5	TYR
1	B	8	SER
1	B	24	LEU
1	B	37	LEU
1	B	113	LEU
1	B	117	LEU
1	B	144	HIS
1	B	149	SER
1	B	155	LEU
1	B	168	LEU
1	B	175	VAL

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Mol	Chain	Res	Type
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	301	ARG
1	B	320	LEU
1	B	347	LEU
1	B	352	VAL
1	B	380	LEU
1	B	390	LEU
1	B	404	THR
1	B	410	GLU
1	B	414	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	133	HIS
1	A	144	HIS
1	A	305	HIS
1	A	329	ASN
1	A	355	GLN
1	A	378	ASN
1	B	89	HIS
1	B	144	HIS
1	B	305	HIS
1	B	329	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 carbohydrates in this entry.

5.6 Ligand geometry

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	A	432	-	4,4,4	0.67	0	6,6,6	0.38	0
2	SO4	A	433	-	4,4,4	0.75	0	6,6,6	0.28	0
2	SO4	B	432	-	4,4,4	0.58	0	6,6,6	0.61	0
2	SO4	B	433	-	4,4,4	0.77	0	6,6,6	0.56	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
2	SO4	A	432	-	-	0/0/0/0	0/0/0/0
2	SO4	A	433	-	-	0/0/0/0	0/0/0/0
2	SO4	B	432	-	-	0/0/0/0	0/0/0/0
2	SO4	B	433	-	-	0/0/0/0	0/0/0/0

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

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	423/431 (98%)	-0.35	10 (2%) 59 66	8, 16, 60, 78	0
1	B	423/431 (98%)	-0.22	29 (6%) 18 23	8, 17, 60, 78	0
All	All	846/862 (98%)	-0.29	39 (4%) 33 40	8, 17, 60, 78	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	LEU	6.0
1	B	367	THR	4.8
1	B	399	VAL	4.6
1	B	362	ILE	4.5
1	B	256	ARG	4.1
1	B	365	GLY	4.1
1	A	2	VAL	3.9
1	B	392	TYR	3.8
1	B	430	LYS	3.8
1	B	2	VAL	3.7
1	A	263	SER	3.7
1	B	263	SER	3.6
1	B	370	GLU	3.3
1	A	264	ALA	3.1
1	B	374	ILE	3.1
1	B	255	PHE	3.1
1	A	399	VAL	2.9
1	B	5	TYR	2.9
1	B	398	GLU	2.9
1	A	430	LYS	2.8
1	B	403	VAL	2.6
1	B	397	GLU	2.6
1	B	394	LEU	2.5
1	B	358	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	388	HIS	2.5
1	A	388	HIS	2.4
1	B	381	LYS	2.4
1	B	368	ARG	2.3
1	B	393	LEU	2.3
1	B	361	LEU	2.3
1	A	402	LEU	2.2
1	B	401	LYS	2.2
1	A	394	LEU	2.2
1	A	372	TYR	2.1
1	B	369	LYS	2.1
1	A	255	PHE	2.1
1	B	79	SER	2.1
1	B	404	THR	2.1
1	B	396	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	433	5/5	0.94	0.14	3.17	38,39,40,42	0
2	SO4	B	433	5/5	0.94	0.14	2.22	39,39,40,42	0
2	SO4	A	432	5/5	0.99	0.06	-1.06	19,20,21,22	0
2	SO4	B	432	5/5	0.99	0.07	-1.37	19,20,22,22	0

6.5 Other polymers

There are no such residues in this entry.