Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:58 pm BST

PDB ID	:	1C3C
Title	:	T. MARITIMA ADENYLOSUCCINATE LYASE
Authors	:	Toth, E.A.; Yeates, T.O.
Deposited on	:	1999-07-27
Resolution	:	1.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

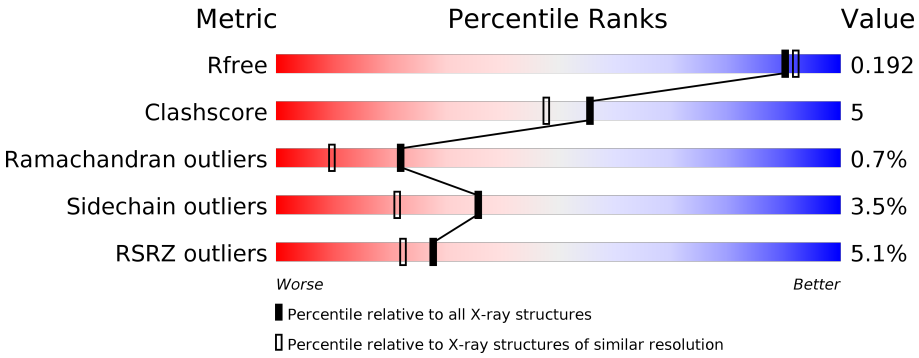
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	4% 83% 11%
1	B	429	6% 82% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7427 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 PROTEIN (ADENYLOSUCCINATE LYASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3367	2154	577	624	12			
1	B	424	Total	C	N	O	S	0	0	0
			3367	2154	577	624	12			

- Molecule 2 is water.

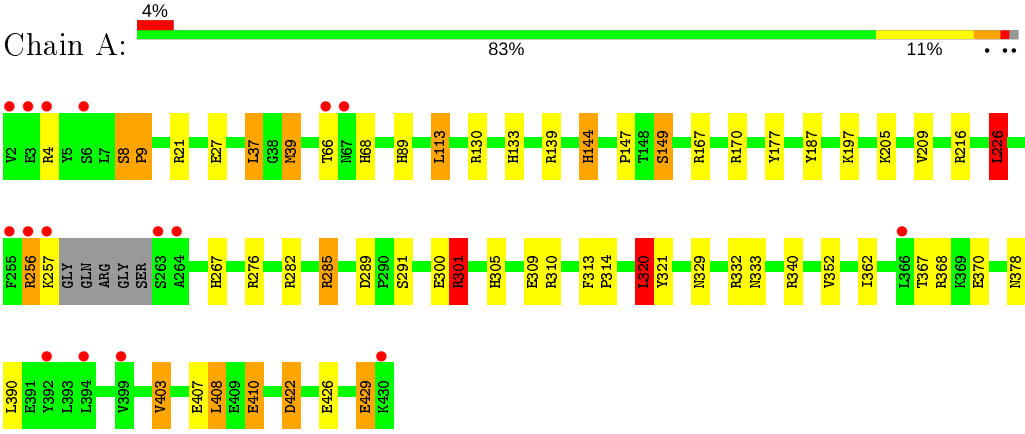
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	347	Total	O	0	0
			347	347		
2	B	346	Total	O	0	0
			346	346		

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.

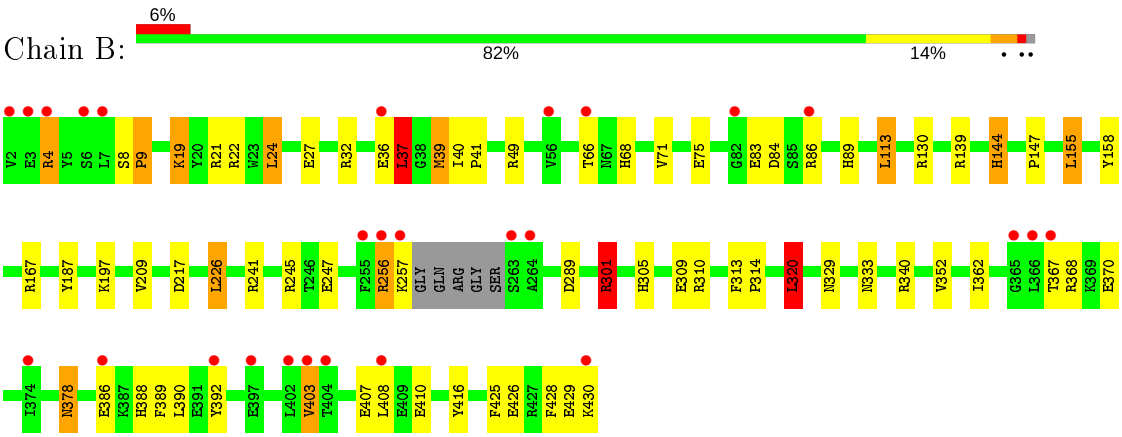
- Molecule 1: PROTEIN (ADENYLOSUCCINATE LYASE)

Chain A:



- Molecule 1: PROTEIN (ADENYLOSUCCINATE LYASE)

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	120.81Å 126.75Å 169.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 47.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-1.80) 97.9 (47.36-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.207 0.167 , 0.192	Depositor DCC
R_{free} test set	5858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7427	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.72	2/3436 (0.1%)	1.46	51/4659 (1.1%)
1	B	0.75	0/3436	1.46	46/4659 (1.0%)
All	All	0.73	2/6872 (0.0%)	1.46	97/9318 (1.0%)

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	3
1	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	SER	CB-OG	-5.65	1.34	1.42
1	A	291	SER	CB-OG	5.56	1.49	1.42

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	ARG	CD-NE-CZ	19.74	151.24	123.60
1	A	422	ASP	CB-CG-OD2	19.02	135.42	118.30
1	B	310	ARG	CD-NE-CZ	16.67	146.93	123.60
1	B	21	ARG	CD-NE-CZ	16.55	146.77	123.60
1	A	310	ARG	CD-NE-CZ	14.90	144.47	123.60
1	A	429	GLU	C-N-CA	13.91	156.46	121.70
1	A	310	ARG	NE-CZ-NH2	-13.87	113.37	120.30
1	B	310	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	B	310	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	B	241	ARG	NE-CZ-NH1	-12.64	113.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	386	GLU	OE1-CD-OE2	12.51	138.31	123.30
1	B	21	ARG	NE-CZ-NH1	-11.99	114.31	120.30
1	A	167	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	A	130	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	A	426	GLU	OE1-CD-OE2	-10.58	110.60	123.30
1	A	310	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	B	340	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	429	GLU	O-C-N	-10.14	106.47	122.70
1	A	422	ASP	CB-CG-OD1	-9.86	109.43	118.30
1	B	130	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	241	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	A	410	GLU	OE1-CD-OE2	-9.60	111.78	123.30
1	A	285	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	B	21	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	B	39	MET	CG-SD-CE	9.03	114.65	100.20
1	B	429	GLU	C-N-CA	9.03	144.27	121.70
1	A	216	ARG	NE-CZ-NH1	-8.85	115.88	120.30
1	A	9	PRO	CA-N-CD	-8.61	99.45	111.50
1	B	24	LEU	CB-CG-CD2	8.40	125.28	111.00
1	A	21	ARG	NE-CZ-NH2	8.34	124.47	120.30
1	A	301	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	139	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	209	VAL	CB-CA-C	-8.22	95.79	111.40
1	A	300	GLU	OE1-CD-OE2	-8.15	113.52	123.30
1	B	9	PRO	CA-N-CD	-8.14	100.10	111.50
1	B	426	GLU	OE1-CD-OE2	-8.12	113.56	123.30
1	B	241	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	B	245	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	320	LEU	CB-CG-CD2	7.75	124.18	111.00
1	A	340	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	21	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	B	416	TYR	CB-CG-CD2	-7.43	116.54	121.00
1	A	282	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	B	167	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	320	LEU	CB-CG-CD2	7.14	123.14	111.00
1	B	209	VAL	CB-CA-C	-7.03	98.04	111.40
1	A	187	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	B	113	LEU	CB-CG-CD1	6.88	122.69	111.00
1	A	113	LEU	CB-CG-CD1	6.86	122.66	111.00
1	B	386	GLU	CG-CD-OE2	-6.70	104.90	118.30
1	A	429	GLU	CA-C-N	6.67	131.88	117.20
1	B	155	LEU	CB-CG-CD2	6.66	122.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	285	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	84	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	139	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	386	GLU	CA-CB-CG	-6.33	99.47	113.40
1	B	9	PRO	N-CA-CB	6.31	110.88	103.30
1	B	155	LEU	CB-CG-CD1	6.30	121.70	111.00
1	B	22	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	A	9	PRO	N-CA-C	6.22	128.27	112.10
1	A	321	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	170	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	39	MET	CG-SD-CE	6.14	110.02	100.20
1	B	139	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	37	LEU	CB-CG-CD1	6.03	121.25	111.00
1	A	9	PRO	N-CA-CB	6.02	110.52	103.30
1	B	289	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	378	ASN	OD1-CG-ND2	-5.92	108.29	121.90
1	A	209	VAL	CA-CB-CG2	5.91	119.76	110.90
1	A	8	SER	CA-C-O	-5.90	107.71	120.10
1	A	8	SER	O-C-N	5.79	132.11	121.10
1	B	19	LYS	CD-CE-NZ	5.77	124.97	111.70
1	B	158	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	332	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	B	389	PHE	CB-CG-CD2	5.62	124.73	120.80
1	B	340	ARG	NH1-CZ-NH2	5.61	125.57	119.40
1	B	187	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	B	217	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	4	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	378	ASN	OD1-CG-ND2	-5.43	109.41	121.90
1	A	426	GLU	N-CA-CB	-5.39	100.89	110.60
1	B	416	TYR	CB-CG-CD1	5.39	124.23	121.00
1	A	426	GLU	CG-CD-OE1	5.33	128.96	118.30
1	A	408	LEU	CB-CG-CD2	5.31	120.03	111.00
1	B	425	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	226	LEU	CB-CG-CD2	5.28	119.97	111.00
1	A	408	LEU	CD1-CG-CD2	-5.28	94.67	110.50
1	A	289	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	37	LEU	CB-CG-CD1	5.22	119.87	111.00
1	A	113	LEU	CA-CB-CG	5.21	127.30	115.30
1	B	301	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	276	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	167	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	378	ASN	CB-CG-OD1	5.12	131.85	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	408	LEU	CD1-CG-CD2	-5.11	95.16	110.50
1	A	8	SER	CB-CA-C	5.05	119.69	110.10
1	A	241	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	GLU	Peptide
1	A	8	SER	Mainchain,Peptide
1	B	8	SER	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	3367	0	3311	33	2
1	B	3367	0	3311	37	2
2	A	347	0	0	8	0
2	B	346	0	0	6	0
All	All	7427	0	6622	68	2

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 5.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:MET:SD	2:A:775:HOH:O	2.27	0.93
1:A:301:ARG:HH21	1:A:305:HIS:CE1	2.06	0.73
1:A:39:MET:CG	2:A:775:HOH:O	2.36	0.73
1:B:301:ARG:HH21	1:B:305:HIS:CE1	2.08	0.72
1:A:301:ARG:HH21	1:A:305:HIS:HE1	1.38	0.70
1:B:301:ARG:HH21	1:B:305:HIS:HE1	1.39	0.70
1:A:329:ASN:ND2	1:A:333:ASN:HD22	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASN:ND2	1:B:333:ASN:HD22	1.94	0.66
1:A:27:GLU:OE2	1:A:89:HIS:HD2	1.80	0.64
1:B:27:GLU:OE2	1:B:89:HIS:HD2	1.81	0.62
1:B:37:LEU:HD22	1:B:197:LYS:HD2	1.81	0.62
1:A:247:GLU:OE1	1:B:144:HIS:HE1	1.84	0.60
1:A:329:ASN:HD21	1:A:333:ASN:HD22	1.50	0.60
1:B:226:LEU:HG	1:B:320:LEU:HD12	1.83	0.59
1:B:144:HIS:HD2	2:B:457:HOH:O	1.86	0.57
1:A:144:HIS:HD2	2:A:448:HOH:O	1.87	0.57
1:A:144:HIS:HE1	1:B:247:GLU:OE1	1.89	0.56
1:B:428:PHE:HA	1:B:430:LYS:HE3	1.87	0.56
1:A:329:ASN:ND2	1:A:333:ASN:ND2	2.53	0.55
1:A:66:THR:HG22	1:A:68:HIS:N	2.21	0.55
1:A:226:LEU:HG	1:A:320:LEU:HD12	1.88	0.55
1:B:367:THR:HG22	1:B:370:GLU:OE2	2.07	0.55
1:B:362:ILE:HD11	1:B:368:ARG:HA	1.89	0.54
1:A:367:THR:HG22	1:A:370:GLU:OE2	2.06	0.54
1:A:39:MET:HG2	2:A:775:HOH:O	2.06	0.53
1:A:66:THR:HG22	1:A:68:HIS:H	1.73	0.53
1:B:388:HIS:HD2	2:B:520:HOH:O	1.91	0.53
1:A:256:ARG:O	1:A:257:LYS:CB	2.56	0.53
1:B:256:ARG:O	1:B:257:LYS:CB	2.56	0.53
1:B:83:GLU:O	1:B:86:ARG:HG3	2.09	0.52
1:B:32:ARG:O	1:B:36:GLU:HG3	2.10	0.52
1:A:329:ASN:HD21	1:A:333:ASN:ND2	2.06	0.52
1:B:27:GLU:OE2	1:B:89:HIS:CD2	2.61	0.52
1:A:388:HIS:HD2	2:A:509:HOH:O	1.93	0.51
1:B:378:ASN:HD22	1:B:392:TYR:HB3	1.76	0.50
1:B:329:ASN:ND2	1:B:333:ASN:ND2	2.57	0.50
1:B:329:ASN:HD21	1:B:333:ASN:HD22	1.59	0.50
1:A:410:GLU:OE2	2:A:585:HOH:O	2.20	0.48
1:A:267:HIS:H	1:A:267:HIS:HD1	1.62	0.47
1:A:27:GLU:OE2	1:A:89:HIS:CD2	2.65	0.47
1:A:403:VAL:HG23	1:A:407:GLU:HB2	1.96	0.47
1:B:197:LYS:HG3	2:B:774:HOH:O	2.13	0.47
1:B:313:PHE:HB2	1:B:314:PRO:HD3	1.96	0.47
1:B:403:VAL:HG23	1:B:407:GLU:HB2	1.96	0.47
1:B:147:PRO:HD3	1:B:352:VAL:CG1	2.44	0.47
1:A:407:GLU:O	1:A:410:GLU:HG2	2.15	0.47
1:B:71:VAL:O	1:B:75:GLU:HG3	2.15	0.47
1:B:89:HIS:HE1	2:B:573:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:MET:HE1	2:B:652:HOH:O	2.14	0.47
1:A:89:HIS:HE1	2:A:562:HOH:O	1.98	0.47
1:A:147:PRO:HD3	1:A:352:VAL:CG1	2.44	0.47
1:B:37:LEU:HD13	1:B:197:LYS:HE2	1.97	0.46
1:A:362:ILE:HD11	1:A:368:ARG:HA	1.97	0.46
1:B:49:ARG:HH11	1:B:49:ARG:HD2	1.57	0.45
1:B:40:ILE:HB	1:B:41:PRO:HD2	1.99	0.45
1:B:40:ILE:HB	1:B:41:PRO:CD	2.46	0.45
1:A:305:HIS:HD2	1:A:309:GLU:OE1	1.99	0.44
1:B:66:THR:HG22	1:B:68:HIS:H	1.82	0.44
1:B:305:HIS:HD2	1:B:309:GLU:OE1	2.00	0.44
1:A:313:PHE:HB2	1:A:314:PRO:HD3	1.99	0.44
1:B:66:THR:HG22	1:B:68:HIS:N	2.32	0.44
1:B:19:LYS:HB3	1:B:19:LYS:HE3	1.80	0.42
1:A:133:HIS:HE1	1:A:422:ASP:OD1	2.01	0.42
1:A:197:LYS:HG3	2:A:766:HOH:O	2.19	0.41
1:B:407:GLU:O	1:B:410:GLU:HG2	2.20	0.41
1:B:86:ARG:NH2	2:B:534:HOH:O	2.53	0.41
1:A:367:THR:HG22	1:A:370:GLU:HG3	2.03	0.41
1:A:177:TYR:CZ	1:A:205:LYS:HE2	2.56	0.40

All (2) 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)
1:A:410:GLU:OE1	1:B:36:GLU:OE2[5_455]	1.90	0.30
1:A:410:GLU:OE2	1:B:36:GLU:OE2[5_455]	2.19	0.01

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	420/429 (98%)	410 (98%)	7 (2%)	3 (1%)	22 10
1	B	420/429 (98%)	409 (97%)	8 (2%)	3 (1%)	22 10
All	All	840/858 (98%)	819 (98%)	15 (2%)	6 (1%)	22 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	256	ARG
1	A	301	ARG
1	B	9	PRO
1	B	256	ARG
1	B	301	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	355/382 (93%)	341 (96%)	14 (4%)	32 17
1	B	355/382 (93%)	344 (97%)	11 (3%)	40 25
All	All	710/764 (93%)	685 (96%)	25 (4%)	36 21

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	37	LEU
1	A	113	LEU
1	A	144	HIS
1	A	149	SER
1	A	226	LEU
1	A	254	PRO
1	A	285	ARG
1	A	301	ARG
1	A	320	LEU

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Mol	Chain	Res	Type
1	A	386	GLU
1	A	390	LEU
1	A	403	VAL
1	A	408	LEU
1	B	4	ARG
1	B	24	LEU
1	B	37	LEU
1	B	113	LEU
1	B	144	HIS
1	B	155	LEU
1	B	226	LEU
1	B	301	ARG
1	B	320	LEU
1	B	390	LEU
1	B	403	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	388	HIS
1	B	89	HIS
1	B	144	HIS
1	B	305	HIS
1	B	329	ASN
1	B	378	ASN
1	B	388	HIS

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

There are no ligands in this entry.

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, 95^{th} 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	424/429 (98%)	-0.15	16 (3%)	40	35	8, 15, 45, 57	0
1	B	424/429 (98%)	0.00	27 (6%)	19	15	8, 15, 45, 57	0
All	All	848/858 (98%)	-0.07	43 (5%)	28	22	8, 15, 45, 57	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	ARG	7.5
1	B	430	LYS	5.8
1	B	257	LYS	5.8
1	B	263	SER	5.5
1	A	256	ARG	4.3
1	A	257	LYS	4.2
1	B	367	THR	4.2
1	A	263	SER	4.1
1	B	66	THR	3.9
1	A	4	ARG	3.6
1	B	6	SER	3.5
1	B	255	PHE	3.5
1	B	4	ARG	3.4
1	B	386	GLU	3.4
1	A	399	VAL	3.3
1	A	3	GLU	3.3
1	A	264	ALA	3.2
1	B	7	LEU	3.2
1	B	3	GLU	3.2
1	B	402	LEU	3.1
1	A	392	TYR	3.1
1	B	365	GLY	3.0
1	B	403	VAL	2.9
1	B	408	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	264	ALA	2.9
1	B	86	ARG	2.8
1	A	66	THR	2.7
1	B	374	ILE	2.7
1	B	404	THR	2.6
1	A	430	LYS	2.6
1	B	366	LEU	2.5
1	A	255	PHE	2.5
1	B	392	TYR	2.5
1	A	6	SER	2.4
1	A	2	VAL	2.4
1	B	56	VAL	2.3
1	B	82	GLY	2.2
1	B	2	VAL	2.2
1	A	394	LEU	2.1
1	B	397	GLU	2.1
1	B	36	GLU	2.1
1	A	67	ASN	2.0
1	A	366	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.