Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:48 pm GMT

PDB ID	:	2Y83
EMDB ID	:	EMD-1872
Title	:	Actin filament pointed end
Authors	:	Narita, A.; Oda, T.; Maeda, Y.
Deposited on	:	2011-02-02
Resolution	:	22.90 Å(reported)
Based on initial model	:	2ZWH

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

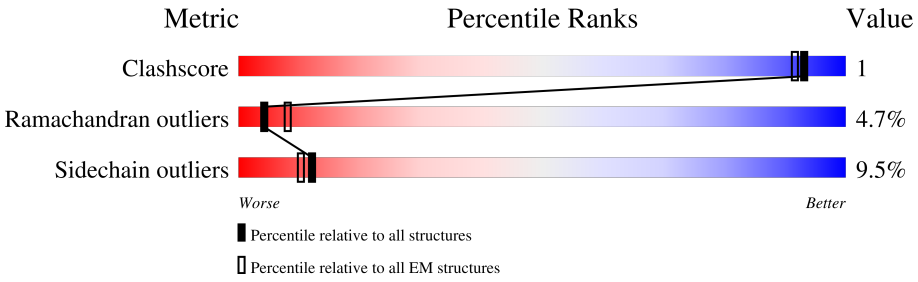
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 22.90 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	375	51% 79% 18%
1	P	375	12% 79% 18%
1	Q	375	6% 79% 16%
1	R	375	11% 82% 15%
1	S	375	11% 79% 17%
1	T	375	12% 82% 14%

2 Entry composition (i)

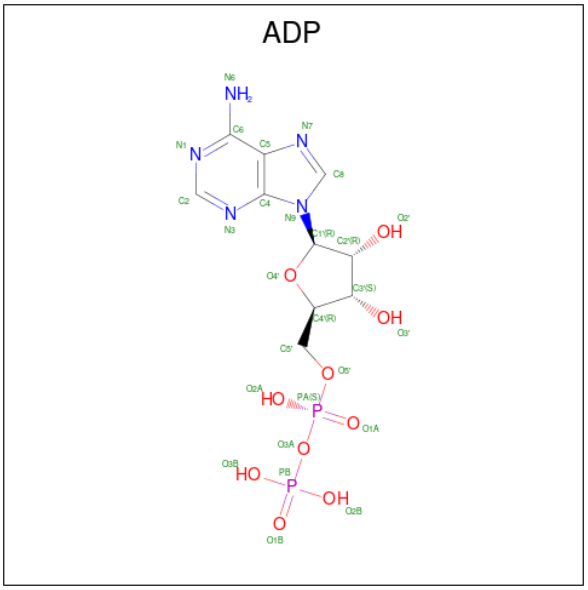
There are 3 unique types of molecules in this entry. The entry contains 33546 atoms, of which 15780 are hydrogens and 0 are deuteriums.

In the tables below, 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 ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	O	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	P	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	Q	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	R	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	S	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		
1	T	375	Total	C	H	N	O	S	0	0
			5551	1854	2618	493	565	21		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
2	O	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	P	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	Q	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	R	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	S	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
2	T	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

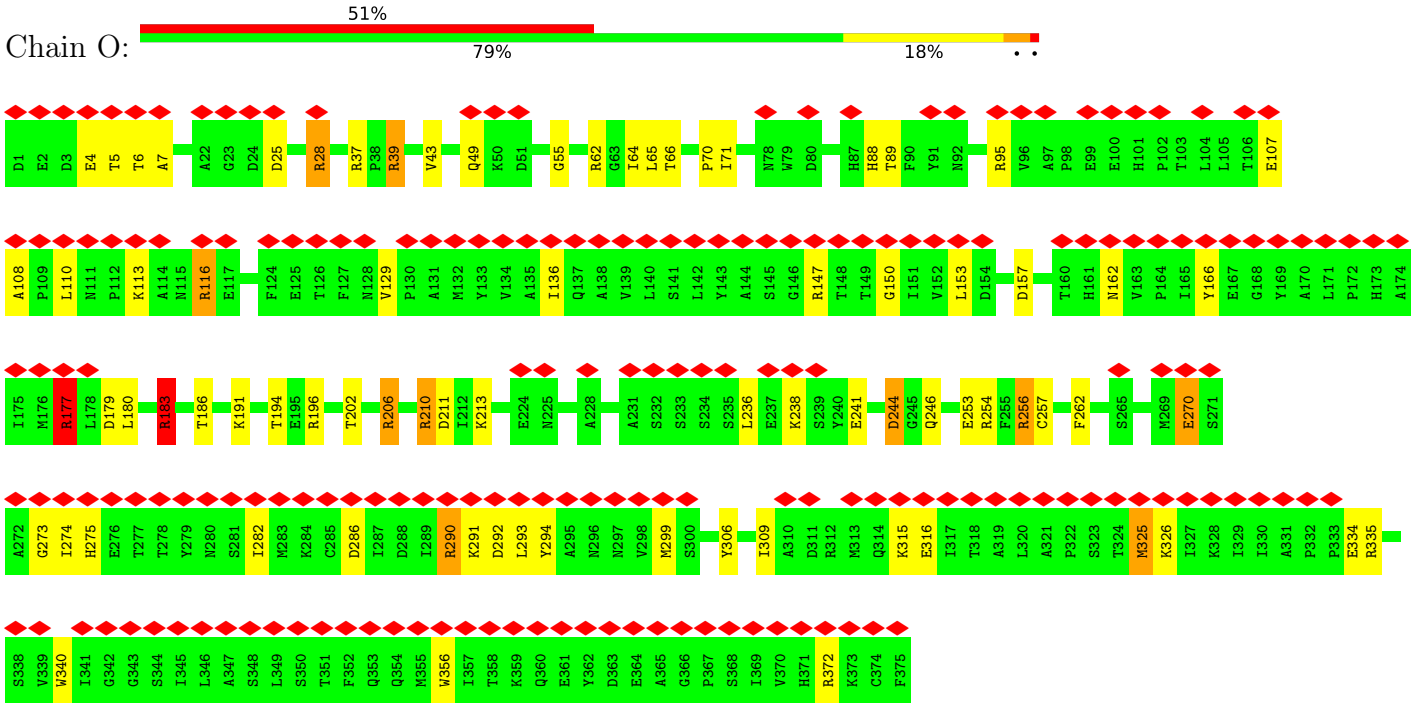
Mol	Chain	Residues	Atoms		AltConf
3	O	1	Total	Ca	0
			1	1	
3	P	1	Total	Ca	0
			1	1	
3	Q	1	Total	Ca	0
			1	1	
3	R	1	Total	Ca	0
			1	1	
3	S	1	Total	Ca	0
			1	1	
3	T	1	Total	Ca	0
			1	1	

3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

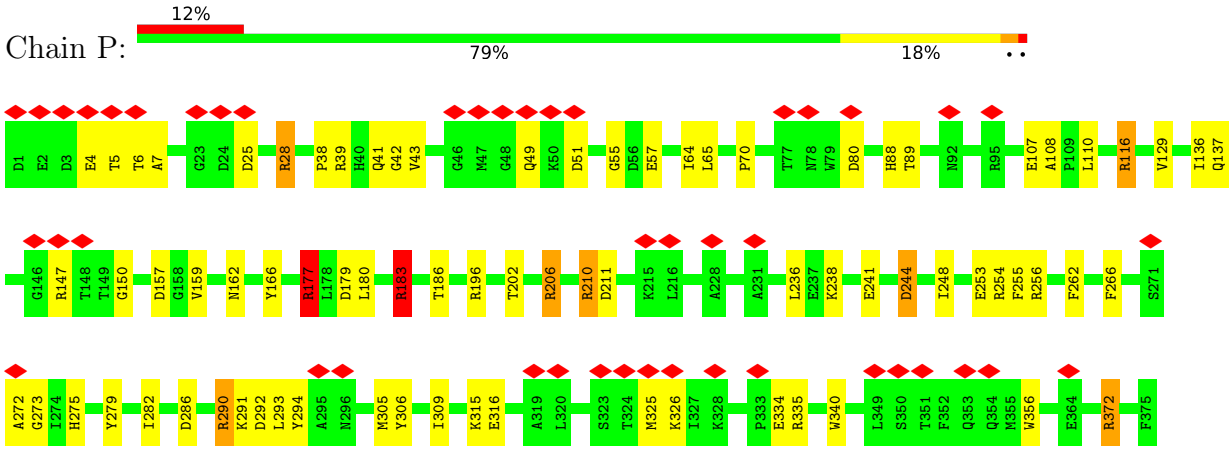
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain O:



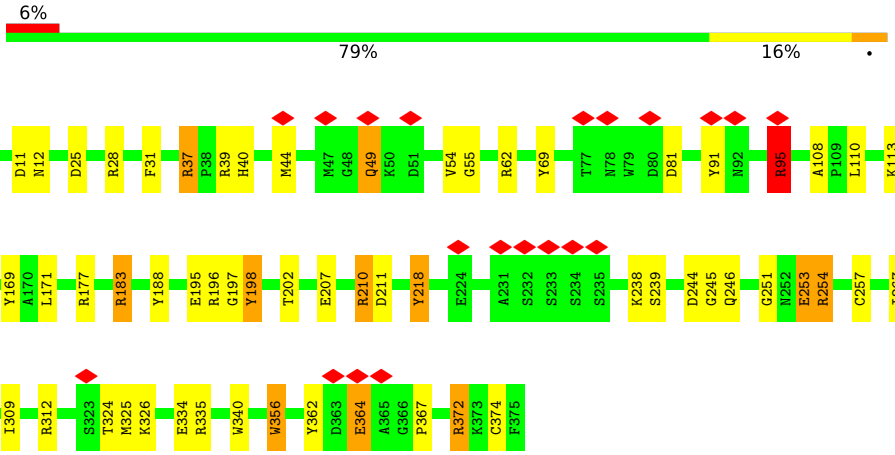
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain P:



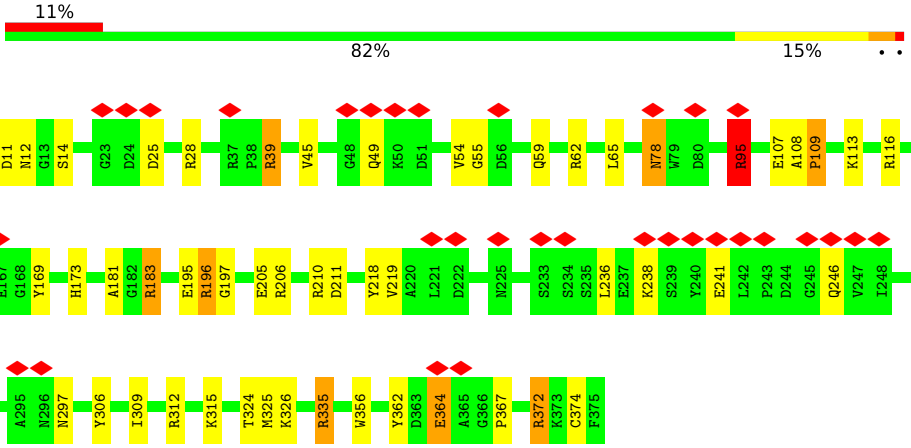
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain Q:



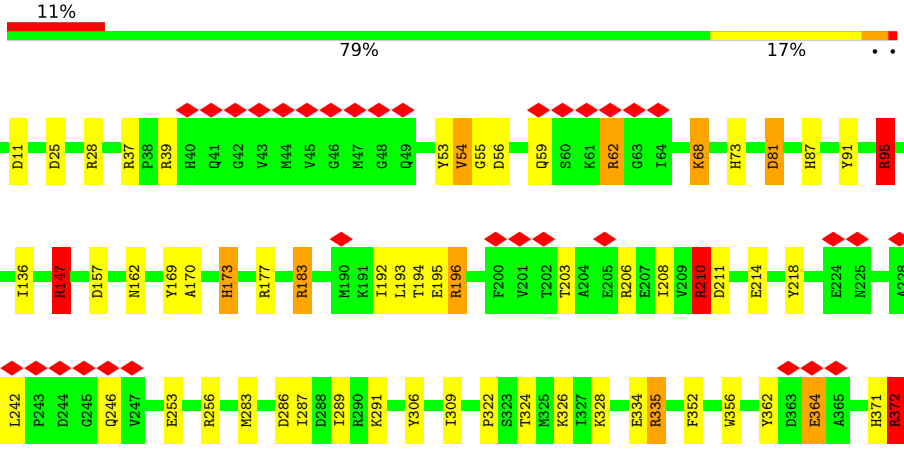
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain R:



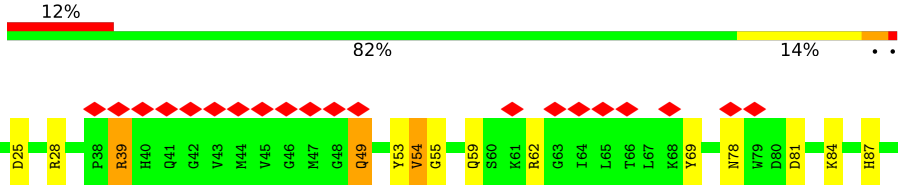
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

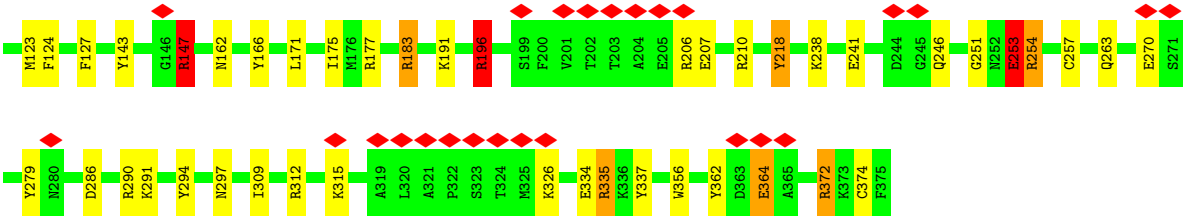
Chain S:



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain T:




M123
F124
F127
Y143
G146
R147
N162
Y166
L171
I175
M176
R177
R183
K191
R196
S199
F200
V201
T202
T203
A204
E205
R206
E207
R210
Y218
K238
E241
D244
G245
Q246
G251
N252
E253
R254
C257
Q263
E270
S271
Y279
N280
D286
R290
K291
Y294
N297
I309
R312
K315
A319
L320
A321
P322
S323
T324
M325
K326
E334
R335
K336
Y337
W356
Y362
D363
E364
A365
R372
K373
C374
F375

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	714	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE AND AMPLITUDE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	8000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	16.474	Depositor
Minimum map value	-11.913	Depositor
Average map value	0.224	Depositor
Map value standard deviation	3.230	Depositor
Recommended contour level	4.61	Depositor
Map size (Å)	136.5, 136.5, 197.925	wwPDB
Map dimensions	40, 40, 58	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	3.4125, 3.4125, 3.4125	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ADP

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	O	0.79	0/2996	1.26	17/4058 (0.4%)
1	P	0.79	0/2996	1.27	19/4058 (0.5%)
1	Q	0.69	0/2996	1.24	24/4058 (0.6%)
1	R	0.69	0/2996	1.18	17/4058 (0.4%)
1	S	0.68	0/2996	1.20	17/4058 (0.4%)
1	T	0.70	0/2996	1.23	28/4058 (0.7%)
All	All	0.72	0/17976	1.23	122/24348 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	14
1	P	0	13
1	Q	0	13
1	R	0	12
1	S	0	16
1	T	0	12
All	All	0	80

There are no bond length outliers.

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	183	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	S	183	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	Q	183	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	Q	91	TYR	CB-CG-CD2	-9.42	115.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	218	TYR	CB-CG-CD2	-9.40	115.36	121.00
1	Q	210	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	R	183	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	Q	218	TYR	CB-CG-CD1	9.12	126.47	121.00
1	O	290	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	P	290	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	Q	62	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	S	169	TYR	CB-CG-CD2	-8.46	115.92	121.00
1	O	206	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	Q	91	TYR	CB-CG-CD1	8.38	126.03	121.00
1	P	206	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	O	210	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	S	169	TYR	CB-CG-CD1	8.30	125.98	121.00
1	T	254	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	Q	254	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	P	39	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	T	116	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	T	206	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	P	166	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	O	62	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	O	166	TYR	CB-CG-CD1	-7.58	116.45	121.00
1	R	62	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	P	210	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	R	210	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	S	372	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	Q	124	PHE	CB-CG-CD2	-7.42	115.61	120.80
1	Q	124	PHE	CB-CG-CD1	7.29	125.90	120.80
1	T	143	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	R	124	PHE	CB-CG-CD1	7.23	125.86	120.80
1	R	124	PHE	CB-CG-CD2	-7.12	115.82	120.80
1	T	124	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	S	124	PHE	CB-CG-CD2	-7.05	115.87	120.80
1	T	143	TYR	CB-CG-CD1	7.03	125.22	121.00
1	S	62	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	T	290	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	R	372	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	Q	372	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	T	124	PHE	CB-CG-CD1	6.86	125.60	120.80
1	S	147	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	S	124	PHE	CB-CG-CD1	6.85	125.59	120.80
1	S	37	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	T	147	ARG	NE-CZ-NH1	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	11	ASP	CB-CG-OD1	6.74	124.36	118.30
1	O	177	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	T	210	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	R	147	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	T	279	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	S	95	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	T	372	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	S	210	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	T	337	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	O	116	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	O	62	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	Q	62	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	R	62	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	T	218	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	T	39	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	P	177	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	T	337	TYR	CB-CG-CD1	6.33	124.80	121.00
1	T	196	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	T	147	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	S	256	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	O	291	LYS	C-N-CA	6.09	136.93	121.70
1	P	166	TYR	CB-CG-CD2	6.06	124.64	121.00
1	P	266	PHE	CB-CG-CD1	6.05	125.04	120.80
1	T	294	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	S	335	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	T	218	TYR	CB-CG-CD1	6.04	124.62	121.00
1	Q	95	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	O	326	LYS	N-CA-CB	6.01	121.41	110.60
1	P	291	LYS	C-N-CA	5.99	136.67	121.70
1	O	166	TYR	CB-CG-CD2	5.96	124.58	121.00
1	Q	133	TYR	CB-CG-CD1	5.94	124.56	121.00
1	R	95	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	S	206	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	R	290	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	T	95	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	R	335	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	R	39	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	T	279	TYR	CB-CG-CD1	5.87	124.52	121.00
1	Q	183	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	T	335	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	Q	37	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	R	28	ARG	NE-CZ-NH2	-5.80	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	356	TRP	CA-CB-CG	5.80	124.72	113.70
1	P	254	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	T	6	THR	N-CA-CB	5.71	121.16	110.30
1	Q	147	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	P	196	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	Q	11	ASP	CB-CG-OD1	5.68	123.41	118.30
1	O	196	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	P	266	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	T	294	TYR	CB-CG-CD1	5.55	124.33	121.00
1	O	39	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	O	28	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	T	196	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	O	183	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	P	177	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	P	272	ALA	CB-CA-C	5.51	118.37	110.10
1	O	254	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	P	183	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	Q	279	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	R	11	ASP	CB-CG-OD1	5.31	123.08	118.30
1	R	6	THR	N-CA-CB	5.31	120.38	110.30
1	P	57	GLU	N-CA-CB	5.30	120.15	110.60
1	P	28	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	Q	28	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	S	147	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	S	28	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	Q	6	THR	N-CA-CB	5.19	120.17	110.30
1	R	254	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	P	326	LYS	N-CA-CB	5.11	119.80	110.60
1	R	78	ASN	N-CA-CB	5.08	119.75	110.60
1	Q	69	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	T	290	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	P	279	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	O	325	MET	N-CA-C	5.02	124.55	111.00
1	Q	133	TYR	CB-CG-CD2	-5.01	117.99	121.00

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	108	ALA	Peptide
1	O	116	ARG	Sidechain
1	O	177	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	O	179	ASP	Peptide
1	O	183	ARG	Sidechain
1	O	206	ARG	Sidechain
1	O	256	ARG	Sidechain
1	O	28	ARG	Sidechain
1	O	306	TYR	Sidechain
1	O	335	ARG	Sidechain
1	O	37	ARG	Sidechain
1	O	372	ARG	Sidechain
1	O	65	LEU	Peptide
1	O	95	ARG	Sidechain
1	P	108	ALA	Peptide
1	P	116	ARG	Sidechain
1	P	177	ARG	Sidechain
1	P	179	ASP	Peptide
1	P	183	ARG	Sidechain
1	P	206	ARG	Sidechain
1	P	255	PHE	Sidechain
1	P	256	ARG	Sidechain
1	P	28	ARG	Sidechain
1	P	306	TYR	Sidechain
1	P	335	ARG	Sidechain
1	P	372	ARG	Sidechain
1	P	65	LEU	Peptide
1	Q	108	ALA	Peptide
1	Q	116	ARG	Sidechain
1	Q	177	ARG	Sidechain
1	Q	188	TYR	Sidechain
1	Q	196	ARG	Sidechain
1	Q	198	TYR	Sidechain
1	Q	239	SER	Peptide
1	Q	254	ARG	Sidechain
1	Q	306	TYR	Peptide
1	Q	312	ARG	Sidechain
1	Q	335	ARG	Sidechain
1	Q	39	ARG	Sidechain
1	Q	95	ARG	Sidechain
1	R	108	ALA	Peptide
1	R	116	ARG	Sidechain
1	R	147	ARG	Sidechain
1	R	196	ARG	Sidechain
1	R	206	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	R	266	PHE	Sidechain
1	R	306	TYR	Peptide
1	R	312	ARG	Sidechain
1	R	335	ARG	Sidechain
1	R	45	VAL	Peptide
1	R	65	LEU	Peptide
1	R	95	ARG	Sidechain
1	S	108	ALA	Peptide
1	S	116	ARG	Sidechain
1	S	133	TYR	Sidechain
1	S	147	ARG	Sidechain
1	S	173	HIS	Sidechain
1	S	177	ARG	Sidechain
1	S	193	LEU	Peptide
1	S	196	ARG	Sidechain
1	S	210	ARG	Sidechain
1	S	306	TYR	Peptide
1	S	335	ARG	Sidechain
1	S	372	ARG	Sidechain
1	S	39	ARG	Sidechain
1	S	53	TYR	Sidechain
1	S	7	ALA	Peptide
1	S	95	ARG	Sidechain
1	T	108	ALA	Peptide
1	T	147	ARG	Sidechain
1	T	177	ARG	Sidechain
1	T	196	ARG	Sidechain
1	T	254	ARG	Sidechain
1	T	28	ARG	Sidechain
1	T	312	ARG	Sidechain
1	T	335	ARG	Sidechain
1	T	39	ARG	Sidechain
1	T	53	TYR	Sidechain
1	T	69	TYR	Peptide
1	T	95	ARG	Sidechain

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	O	2933	2618	2894	10	0
1	P	2933	2618	2894	9	0
1	Q	2933	2618	2894	8	0
1	R	2933	2618	2894	3	0
1	S	2933	2618	2894	13	0
1	T	2933	2618	2894	6	0
2	O	27	12	12	0	0
2	P	27	12	12	0	0
2	Q	27	12	12	0	0
2	R	27	12	12	0	0
2	S	27	12	12	0	0
2	T	27	12	12	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
All	All	17766	15780	17436	47	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 1.

All (47) 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:Q:253:GLU:H	1:Q:253:GLU:CD	2.02	0.64
1:S:208:ILE:HD12	1:S:242:LEU:HD22	1.83	0.61
1:T:54:VAL:HG22	1:T:55:GLY:H	1.70	0.57
1:R:253:GLU:H	1:R:253:GLU:CD	2.08	0.56
1:T:253:GLU:H	1:T:253:GLU:CD	2.09	0.56
1:P:262:PHE:HA	1:P:273:GLY:HA3	1.88	0.56
1:O:262:PHE:HA	1:O:273:GLY:HA3	1.86	0.56
1:S:113:LYS:HZ2	1:S:371:HIS:CE1	2.24	0.54
1:P:150:GLY:HA2	1:P:293:LEU:HA	1.90	0.54
1:O:150:GLY:HA2	1:O:293:LEU:HA	1.90	0.54
1:Q:54:VAL:HG22	1:Q:55:GLY:H	1.75	0.51
1:S:54:VAL:HG22	1:S:55:GLY:H	1.76	0.51
1:O:186:THR:HG23	1:O:210:ARG:HA	1.92	0.50
1:S:136:ILE:H	1:S:136:ILE:HD12	1.77	0.50
1:O:153:LEU:HD11	1:O:274:ILE:HB	1.93	0.49
1:R:364:GLU:H	1:R:364:GLU:CD	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:364:GLU:H	1:Q:364:GLU:CD	2.15	0.49
1:S:286:ASP:CG	1:S:287:ILE:H	2.17	0.48
1:S:364:GLU:H	1:S:364:GLU:CD	2.17	0.48
1:P:4:GLU:CD	1:P:5:THR:H	2.18	0.47
1:O:270:GLU:H	1:O:270:GLU:CD	2.17	0.47
1:Q:287:ILE:HA	1:Q:290:ARG:HH12	1.79	0.47
1:O:4:GLU:CD	1:O:5:THR:H	2.18	0.46
1:Q:136:ILE:HD12	1:Q:136:ILE:H	1.80	0.46
1:S:195:GLU:CD	1:T:113:LYS:HZ3	2.19	0.46
1:S:253:GLU:H	1:S:253:GLU:CD	2.19	0.46
1:S:87:HIS:CE1	1:S:91:TYR:CE1	3.06	0.44
1:Q:40:HIS:CE1	1:S:170:ALA:HA	2.52	0.44
1:T:364:GLU:CD	1:T:364:GLU:H	2.20	0.44
1:O:282:ILE:HD13	1:O:294:TYR:CE2	2.53	0.44
1:P:186:THR:HG23	1:P:210:ARG:HA	1.99	0.44
1:O:253:GLU:H	1:O:253:GLU:CD	2.21	0.43
1:P:253:GLU:H	1:P:253:GLU:CD	2.22	0.43
1:P:136:ILE:HD12	1:P:136:ILE:H	1.84	0.43
1:S:68:LYS:HZ1	1:S:81:ASP:CG	2.22	0.43
1:Q:4:GLU:CD	1:Q:5:THR:H	2.22	0.42
1:P:282:ILE:HD13	1:P:294:TYR:CE2	2.54	0.42
1:Q:165:ILE:HD12	1:Q:169:TYR:CE1	2.55	0.41
1:S:210:ARG:HH21	1:S:214:GLU:CD	2.24	0.41
1:O:64:ILE:HD12	1:O:64:ILE:H	1.85	0.41
1:R:109:PRO:HB2	1:R:161:HIS:CG	2.56	0.41
1:T:84:LYS:HA	1:T:87:HIS:CD2	2.55	0.41
1:P:248:ILE:H	1:P:248:ILE:HD12	1.85	0.41
1:T:87:HIS:CD2	1:T:127:PHE:CZ	3.09	0.41
1:S:62:ARG:HH22	1:S:211:ASP:CG	2.24	0.41
1:O:136:ILE:HD12	1:O:136:ILE:H	1.87	0.40
1:P:107:GLU:CD	1:P:116:ARG:HH12	2.25	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	O	373/375 (100%)	301 (81%)	57 (15%)	15 (4%)	3	23
1	P	373/375 (100%)	306 (82%)	50 (13%)	17 (5%)	2	21
1	Q	373/375 (100%)	299 (80%)	55 (15%)	19 (5%)	2	19
1	R	373/375 (100%)	298 (80%)	53 (14%)	22 (6%)	1	17
1	S	373/375 (100%)	301 (81%)	54 (14%)	18 (5%)	2	21
1	T	373/375 (100%)	301 (81%)	57 (15%)	15 (4%)	3	23
All	All	2238/2250 (100%)	1806 (81%)	326 (15%)	106 (5%)	4	21

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	70	PRO
1	O	180	LEU
1	P	70	PRO
1	P	180	LEU
1	Q	6	THR
1	Q	49	GLN
1	Q	81	ASP
1	Q	324	THR
1	R	6	THR
1	R	78	ASN
1	R	137	GLN
1	R	173	HIS
1	S	2	GLU
1	S	81	ASP
1	S	95	ARG
1	S	236	LEU
1	T	49	GLN
1	O	129	VAL
1	O	246	GLN
1	O	290	ARG
1	O	309	ILE
1	P	43	VAL
1	P	129	VAL
1	P	236	LEU
1	P	290	ARG
1	P	309	ILE
1	Q	95	ARG

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Mol	Chain	Res	Type
1	Q	146	GLY
1	Q	244	ASP
1	Q	267	ILE
1	R	2	GLU
1	R	55	GLY
1	R	236	LEU
1	R	272	ALA
1	R	324	THR
1	S	194	THR
1	S	289	ILE
1	T	6	THR
1	O	43	VAL
1	O	236	LEU
1	O	244	ASP
1	P	110	LEU
1	Q	2	GLU
1	Q	251	GLY
1	R	95	ARG
1	R	253	GLU
1	R	315	LYS
1	R	374	CYS
1	S	25	ASP
1	S	203	THR
1	S	324	THR
1	T	2	GLU
1	T	110	LEU
1	O	25	ASP
1	O	89	THR
1	O	110	LEU
1	P	25	ASP
1	P	51	ASP
1	Q	25	ASP
1	Q	110	LEU
1	Q	309	ILE
1	Q	362	TYR
1	Q	374	CYS
1	R	25	ASP
1	R	362	TYR
1	S	5	THR
1	S	128	ASN
1	S	309	ILE
1	S	362	TYR

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Mol	Chain	Res	Type
1	T	25	ASP
1	T	62	ARG
1	T	253	GLU
1	T	315	LYS
1	O	7	ALA
1	P	7	ALA
1	P	244	ASP
1	Q	245	GLY
1	Q	257	CYS
1	R	181	ALA
1	R	197	GLY
1	R	251	GLY
1	R	309	ILE
1	T	257	CYS
1	T	309	ILE
1	T	374	CYS
1	P	89	THR
1	P	137	GLN
1	S	73	HIS
1	S	230	ALA
1	S	322	PRO
1	S	374	CYS
1	T	54	VAL
1	T	362	TYR
1	P	42	GLY
1	Q	197	GLY
1	Q	289	ILE
1	S	54	VAL
1	O	55	GLY
1	P	55	GLY
1	R	289	ILE
1	O	71	ILE
1	P	38	PRO
1	R	158	GLY
1	T	251	GLY
1	T	175	ILE
1	R	54	VAL

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 PDB entries followed by that with respect to all EM

entries.

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	O	318/318 (100%)	285 (90%)	33 (10%)	7 24
1	P	318/318 (100%)	290 (91%)	28 (9%)	10 31
1	Q	318/318 (100%)	286 (90%)	32 (10%)	7 25
1	R	318/318 (100%)	287 (90%)	31 (10%)	8 27
1	S	318/318 (100%)	291 (92%)	27 (8%)	10 33
1	T	318/318 (100%)	288 (91%)	30 (9%)	8 28
All	All	1908/1908 (100%)	1727 (90%)	181 (10%)	12 27

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	6	THR
1	O	39	ARG
1	O	49	GLN
1	O	66	THR
1	O	88	HIS
1	O	107	GLU
1	O	113	LYS
1	O	147	ARG
1	O	157	ASP
1	O	162	ASN
1	O	177	ARG
1	O	183	ARG
1	O	191	LYS
1	O	194	THR
1	O	202	THR
1	O	211	ASP
1	O	213	LYS
1	O	238	LYS
1	O	241	GLU
1	O	244	ASP
1	O	256	ARG
1	O	257	CYS
1	O	270	GLU
1	O	275	HIS
1	O	286	ASP
1	O	292	ASP

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Mol	Chain	Res	Type
1	O	299	MET
1	O	315	LYS
1	O	316	GLU
1	O	325	MET
1	O	334	GLU
1	O	340	TRP
1	O	356	TRP
1	P	6	THR
1	P	41	GLN
1	P	49	GLN
1	P	64	ILE
1	P	80	ASP
1	P	88	HIS
1	P	147	ARG
1	P	157	ASP
1	P	159	VAL
1	P	162	ASN
1	P	177	ARG
1	P	183	ARG
1	P	202	THR
1	P	211	ASP
1	P	238	LYS
1	P	241	GLU
1	P	244	ASP
1	P	275	HIS
1	P	286	ASP
1	P	292	ASP
1	P	305	MET
1	P	315	LYS
1	P	316	GLU
1	P	325	MET
1	P	334	GLU
1	P	340	TRP
1	P	356	TRP
1	P	372	ARG
1	Q	4	GLU
1	Q	12	ASN
1	Q	31	PHE
1	Q	37	ARG
1	Q	44	MET
1	Q	49	GLN
1	Q	113	LYS

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Mol	Chain	Res	Type
1	Q	123	MET
1	Q	133	TYR
1	Q	147	ARG
1	Q	171	LEU
1	Q	183	ARG
1	Q	195	GLU
1	Q	198	TYR
1	Q	202	THR
1	Q	207	GLU
1	Q	210	ARG
1	Q	211	ASP
1	Q	218	TYR
1	Q	238	LYS
1	Q	246	GLN
1	Q	253	GLU
1	Q	270	GLU
1	Q	291	LYS
1	Q	325	MET
1	Q	326	LYS
1	Q	334	GLU
1	Q	340	TRP
1	Q	356	TRP
1	Q	364	GLU
1	Q	367	PRO
1	Q	372	ARG
1	R	12	ASN
1	R	14	SER
1	R	39	ARG
1	R	49	GLN
1	R	59	GLN
1	R	107	GLU
1	R	109	PRO
1	R	113	LYS
1	R	123	MET
1	R	137	GLN
1	R	147	ARG
1	R	169	TYR
1	R	183	ARG
1	R	195	GLU
1	R	196	ARG
1	R	205	GLU
1	R	211	ASP

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Mol	Chain	Res	Type
1	R	218	TYR
1	R	219	VAL
1	R	238	LYS
1	R	241	GLU
1	R	246	GLN
1	R	270	GLU
1	R	291	LYS
1	R	297	ASN
1	R	325	MET
1	R	326	LYS
1	R	356	TRP
1	R	364	GLU
1	R	367	PRO
1	R	372	ARG
1	S	56	ASP
1	S	59	GLN
1	S	68	LYS
1	S	111	ASN
1	S	113	LYS
1	S	123	MET
1	S	147	ARG
1	S	157	ASP
1	S	162	ASN
1	S	173	HIS
1	S	183	ARG
1	S	192	ILE
1	S	196	ARG
1	S	210	ARG
1	S	218	TYR
1	S	238	LYS
1	S	241	GLU
1	S	246	GLN
1	S	283	MET
1	S	291	LYS
1	S	326	LYS
1	S	328	LYS
1	S	334	GLU
1	S	352	PHE
1	S	356	TRP
1	S	364	GLU
1	S	372	ARG
1	T	4	GLU

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Mol	Chain	Res	Type
1	T	49	GLN
1	T	59	GLN
1	T	78	ASN
1	T	81	ASP
1	T	101	HIS
1	T	123	MET
1	T	147	ARG
1	T	162	ASN
1	T	166	TYR
1	T	171	LEU
1	T	183	ARG
1	T	191	LYS
1	T	196	ARG
1	T	207	GLU
1	T	218	TYR
1	T	238	LYS
1	T	241	GLU
1	T	246	GLN
1	T	253	GLU
1	T	263	GLN
1	T	270	GLU
1	T	286	ASP
1	T	291	LYS
1	T	297	ASN
1	T	326	LYS
1	T	334	GLU
1	T	356	TRP
1	T	364	GLU
1	T	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	88	HIS
1	O	173	HIS
1	O	246	GLN
1	P	88	HIS
1	Q	40	HIS
1	R	73	HIS
1	R	87	HIS
1	R	92	ASN
1	S	246	GLN

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Mol	Chain	Res	Type
1	T	87	HIS
1	T	297	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	ADP	R	400	3	24,29,29	0.81	0	29,45,45	1.87	3 (10%)
2	ADP	S	400	3	24,29,29	0.72	0	29,45,45	1.59	4 (13%)
2	ADP	Q	400	3	24,29,29	0.84	0	29,45,45	1.56	6 (20%)
2	ADP	P	400	3	24,29,29	0.92	0	29,45,45	1.60	4 (13%)
2	ADP	T	400	3	24,29,29	0.76	0	29,45,45	1.40	4 (13%)
2	ADP	O	400	3	24,29,29	0.92	0	29,45,45	1.62	4 (13%)

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	ADP	R	400	3	-	2/12/32/32	0/3/3/3
2	ADP	S	400	3	-	1/12/32/32	0/3/3/3
2	ADP	Q	400	3	-	5/12/32/32	0/3/3/3
2	ADP	P	400	3	-	4/12/32/32	0/3/3/3
2	ADP	T	400	3	-	0/12/32/32	0/3/3/3
2	ADP	O	400	3	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	400	ADP	PA-O3A-PB	-7.91	105.67	132.83
2	O	400	ADP	PA-O3A-PB	-5.81	112.89	132.83
2	S	400	ADP	PA-O3A-PB	-5.71	113.24	132.83
2	P	400	ADP	PA-O3A-PB	-5.63	113.51	132.83
2	Q	400	ADP	PA-O3A-PB	-5.06	115.45	132.83
2	T	400	ADP	PA-O3A-PB	-4.87	116.13	132.83
2	O	400	ADP	O3B-PB-O1B	-3.90	95.43	110.68
2	P	400	ADP	O3B-PB-O1B	-3.86	95.57	110.68
2	R	400	ADP	O3B-PB-O1B	-3.74	96.04	110.68
2	S	400	ADP	C5-C6-N6	3.38	125.48	120.35
2	T	400	ADP	C5-C6-N6	3.29	125.35	120.35
2	Q	400	ADP	C5-C6-N6	3.19	125.20	120.35
2	S	400	ADP	O3B-PB-O1B	-2.86	99.47	110.68
2	P	400	ADP	C5-C6-N6	2.71	124.47	120.35
2	Q	400	ADP	O3B-PB-O1B	-2.65	100.30	110.68
2	S	400	ADP	O3B-PB-O2B	2.61	117.61	107.64
2	O	400	ADP	C5-C6-N6	2.54	124.22	120.35
2	T	400	ADP	O3B-PB-O1B	-2.43	101.17	110.68
2	T	400	ADP	O3B-PB-O2B	2.38	116.74	107.64
2	Q	400	ADP	O3B-PB-O2B	2.21	116.07	107.64
2	O	400	ADP	O5'-PA-O1A	-2.19	100.50	109.07
2	Q	400	ADP	O4'-C1'-C2'	-2.19	103.73	106.93
2	P	400	ADP	O5'-PA-O1A	-2.18	100.54	109.07
2	R	400	ADP	C5-C6-N6	2.18	123.66	120.35
2	Q	400	ADP	C3'-C2'-C1'	-2.09	97.83	100.98

There are no chirality outliers.

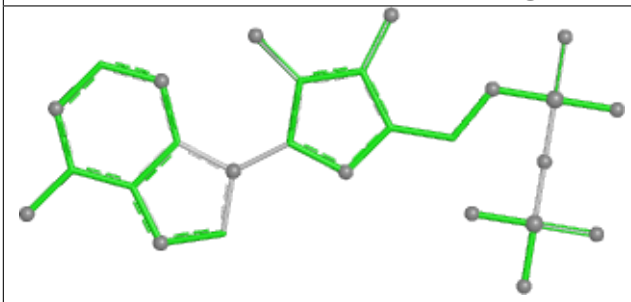
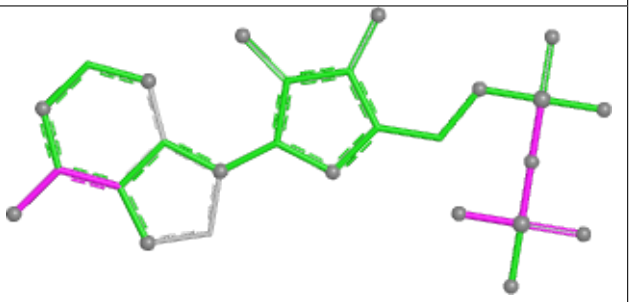
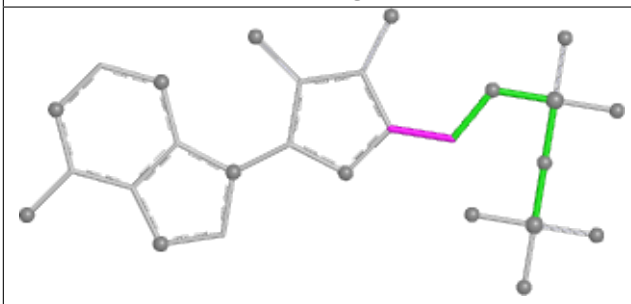
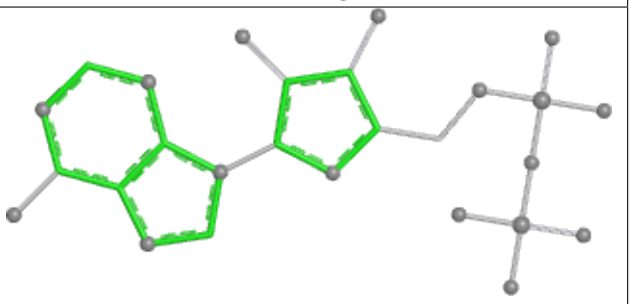
All (16) torsion outliers are listed below:

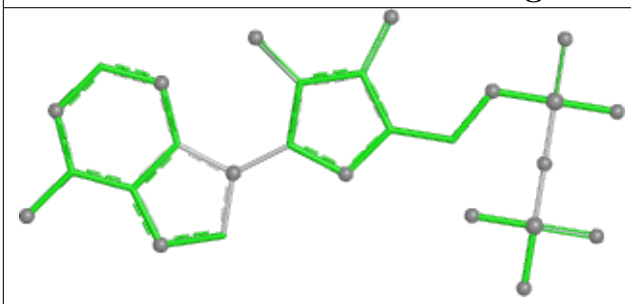
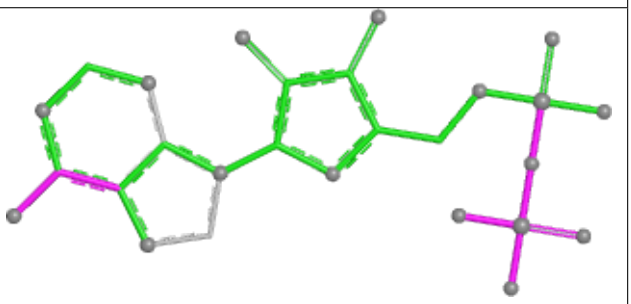
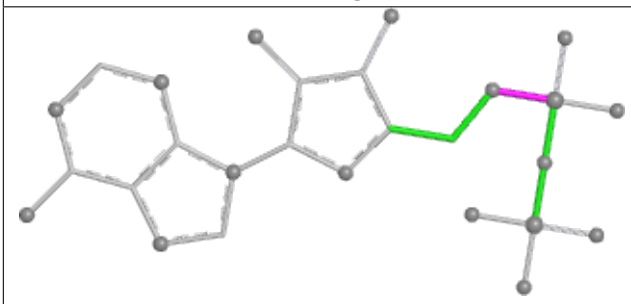
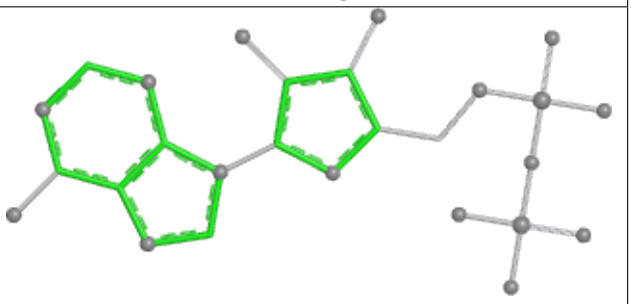
Mol	Chain	Res	Type	Atoms
2	O	400	ADP	C5'-O5'-PA-O3A
2	P	400	ADP	C5'-O5'-PA-O3A
2	Q	400	ADP	C5'-O5'-PA-O1A
2	Q	400	ADP	C5'-O5'-PA-O2A
2	Q	400	ADP	C3'-C4'-C5'-O5'
2	O	400	ADP	C3'-C4'-C5'-O5'
2	P	400	ADP	C3'-C4'-C5'-O5'
2	R	400	ADP	O4'-C4'-C5'-O5'
2	R	400	ADP	C3'-C4'-C5'-O5'
2	Q	400	ADP	O4'-C4'-C5'-O5'
2	Q	400	ADP	C5'-O5'-PA-O3A
2	O	400	ADP	C5'-O5'-PA-O1A
2	P	400	ADP	C5'-O5'-PA-O1A
2	P	400	ADP	O4'-C4'-C5'-O5'
2	O	400	ADP	O4'-C4'-C5'-O5'
2	S	400	ADP	C5'-O5'-PA-O1A

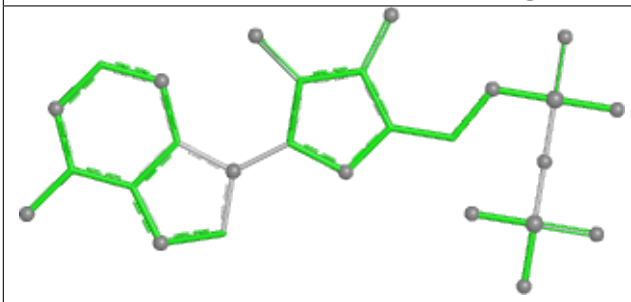
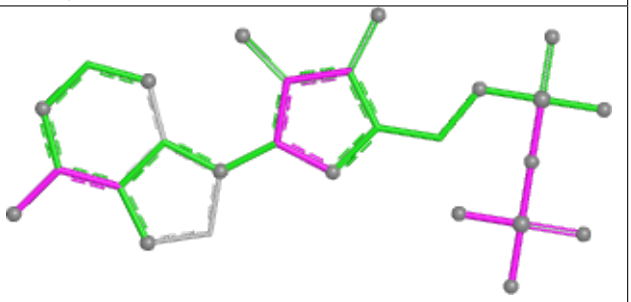
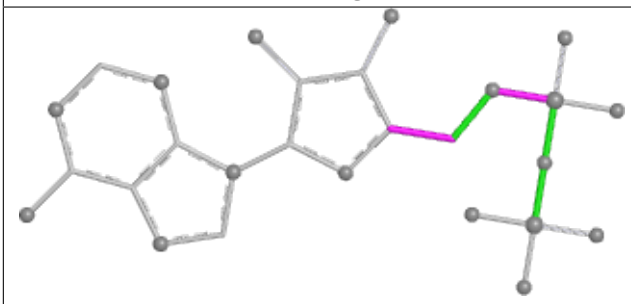
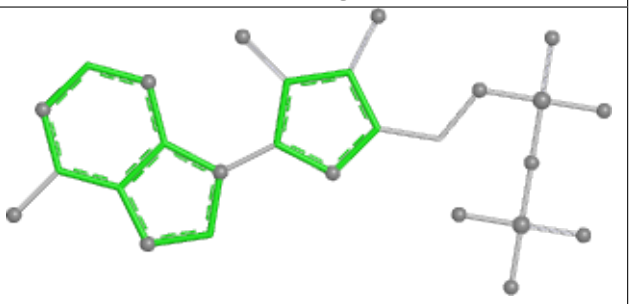
There are no ring outliers.

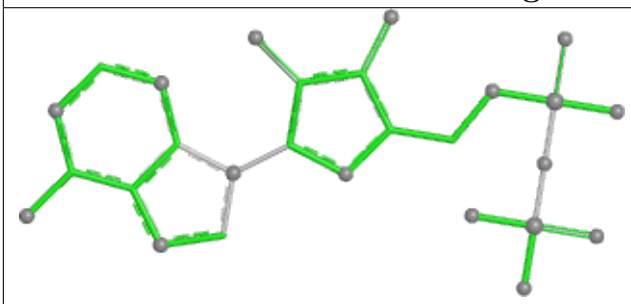
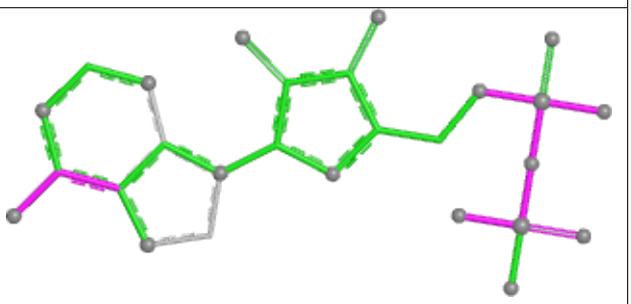
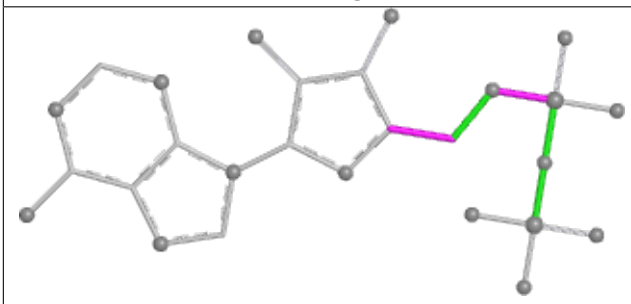
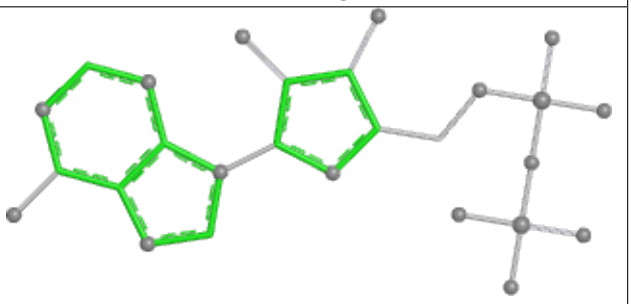
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

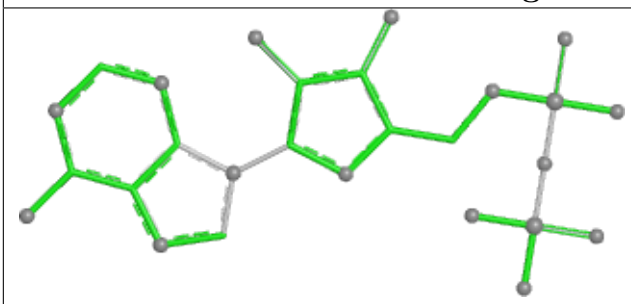
Ligand ADP R 400	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP S 400	
 Bond lengths	 Bond angles
 Torsions	 Rings

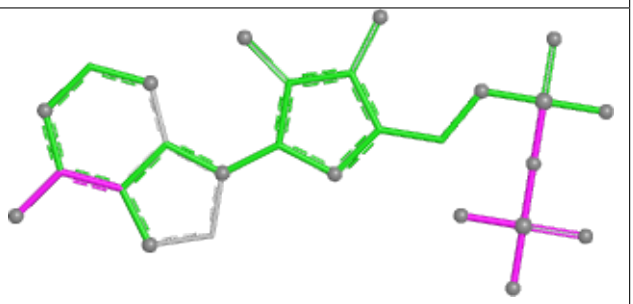
Ligand ADP Q 400	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP P 400	
 Bond lengths	 Bond angles
 Torsions	 Rings

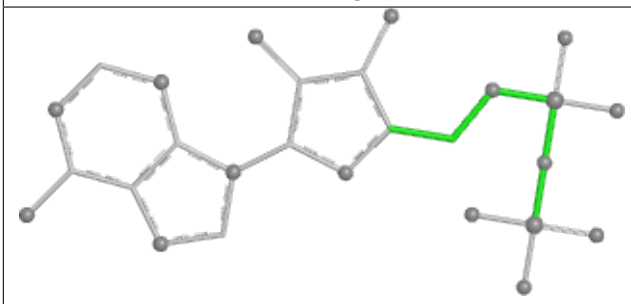
Ligand ADP T 400



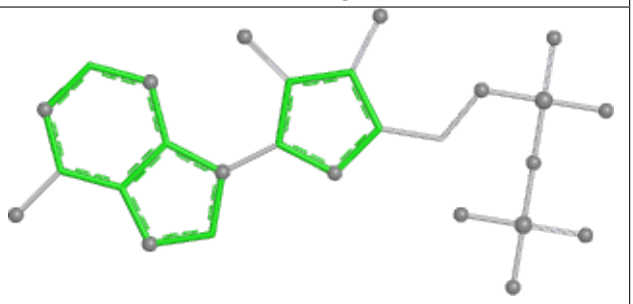
Bond lengths



Bond angles

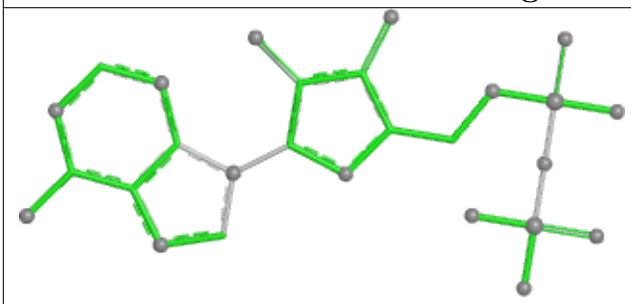


Torsions

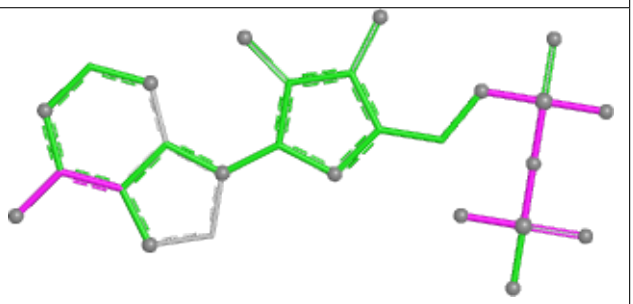


Rings

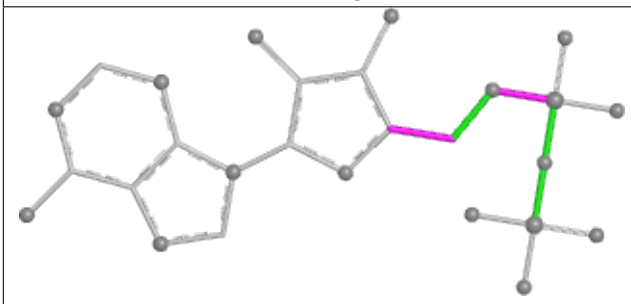
Ligand ADP O 400



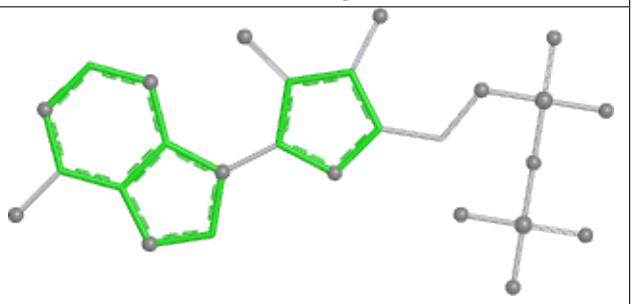
Bond lengths



Bond angles



Torsions



Rings

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 Map visualisation

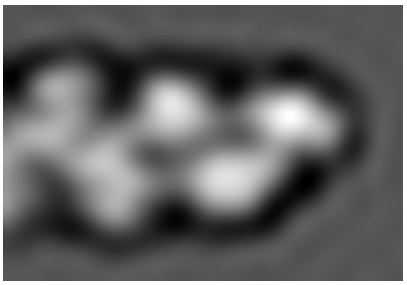
This section contains visualisations of the EMDB entry EMD-1872. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

X



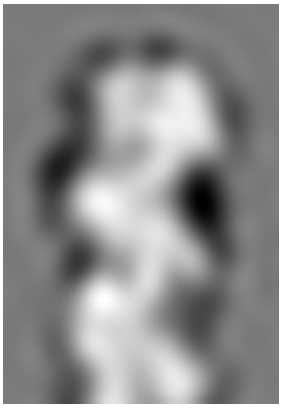
Y

Z

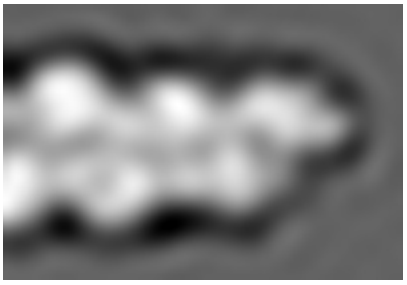
The images above show the map projected in three orthogonal directions.

6.2 Central slices

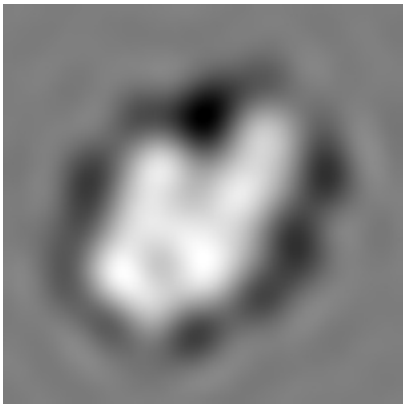
6.2.1 Primary map



X Index: 20



Y Index: 20



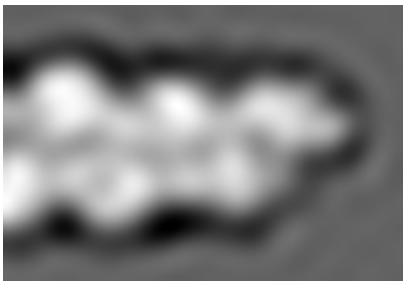
Z Index: 29

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 15



Y Index: 20

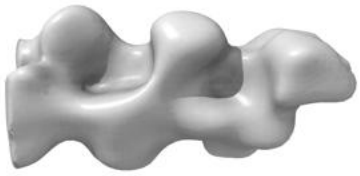
Z Index: 15

The images above show the largest variance slices of the map in three orthogonal directions.

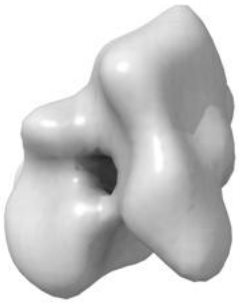
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.61. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

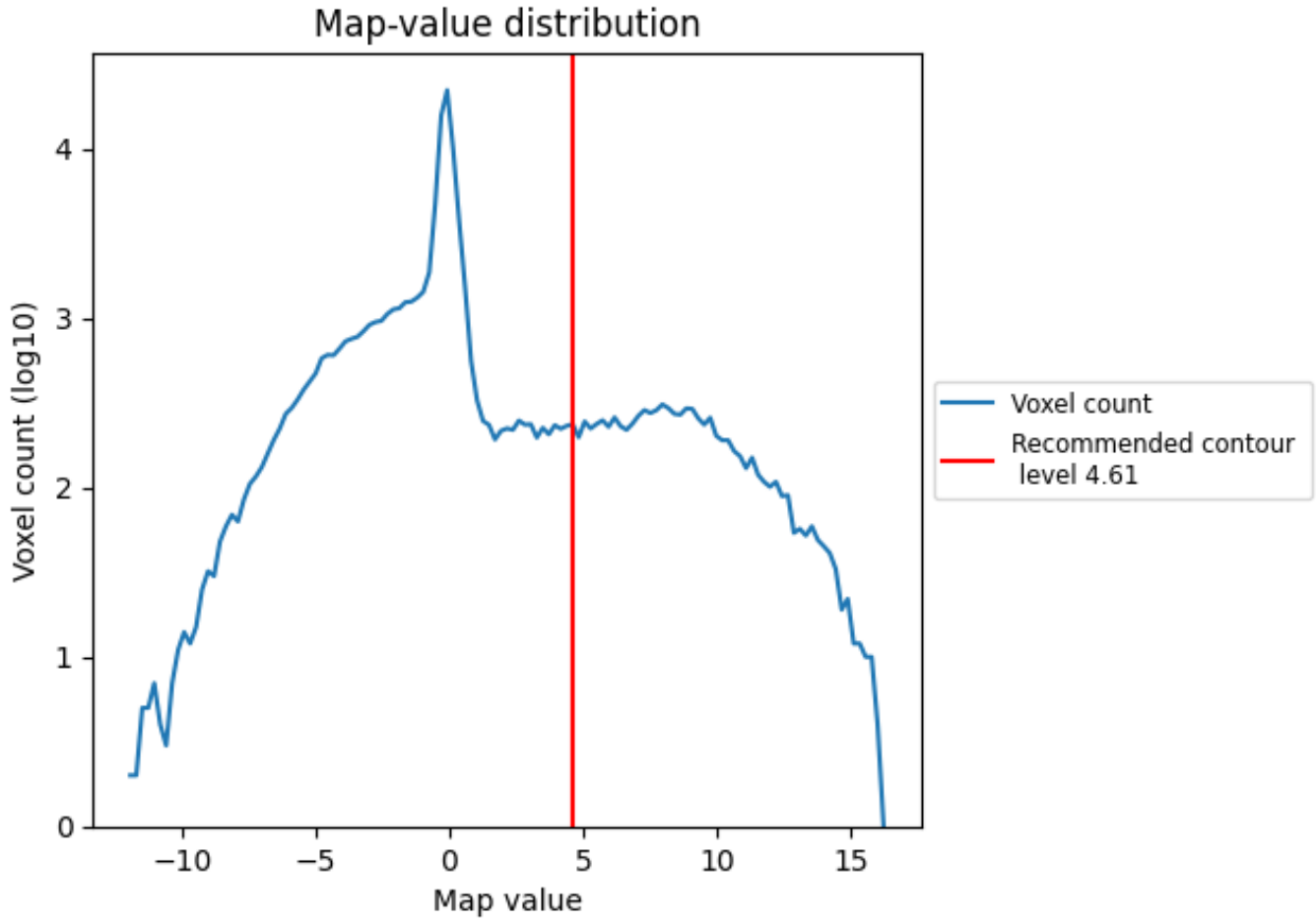
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

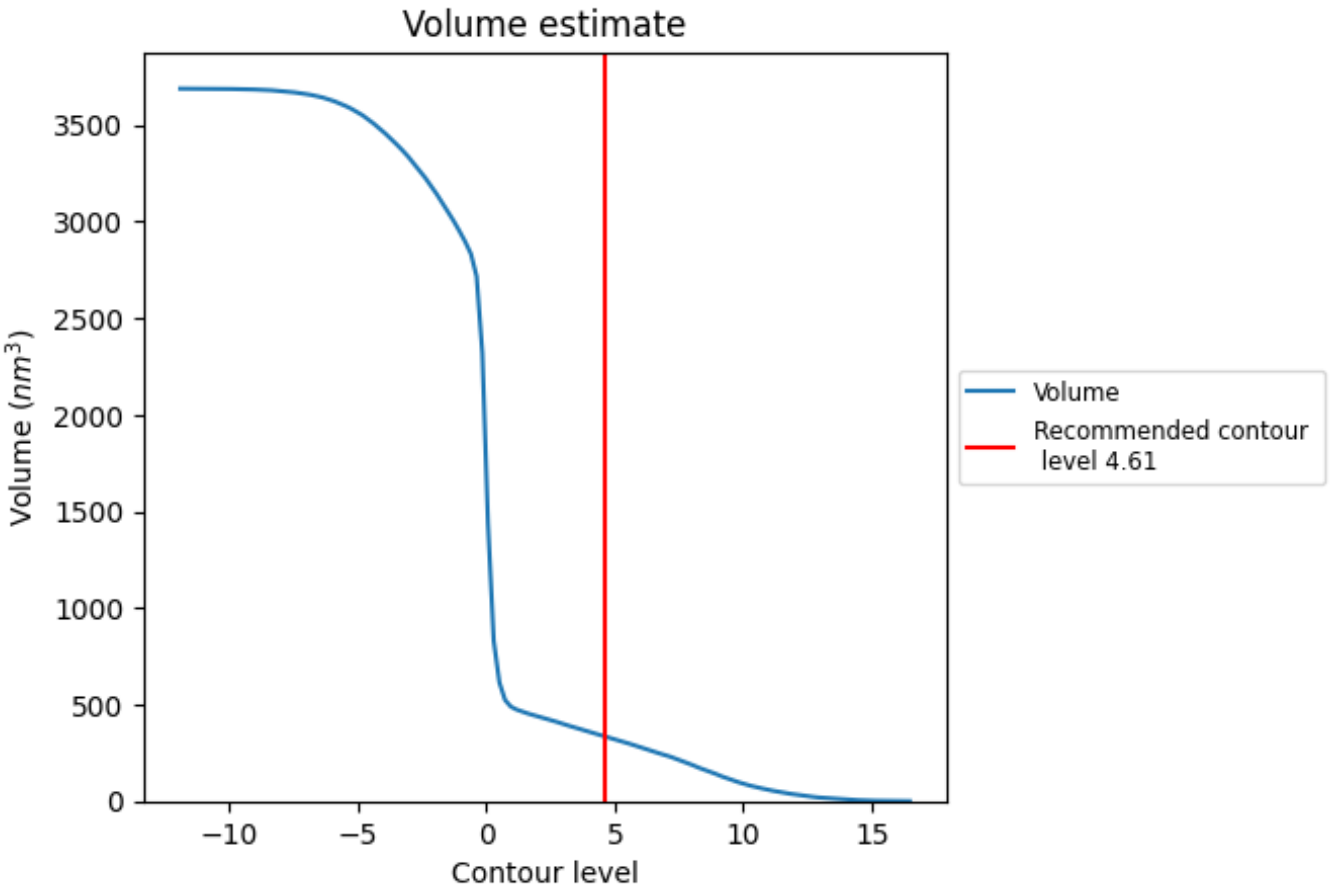
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 335 nm^3; this corresponds to an approximate mass of 303 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

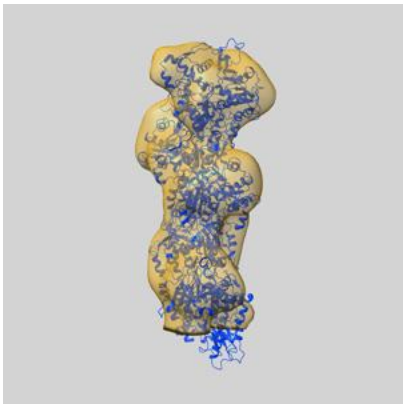
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

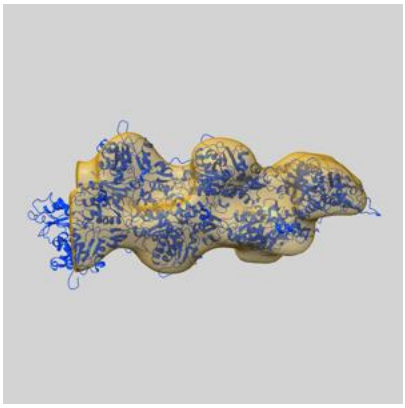
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1872 and PDB model 2Y83. Per-residue inclusion information can be found in section 3 on page 5.

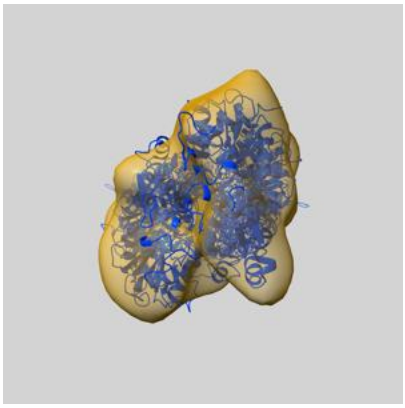
9.1 Map-model overlay



X



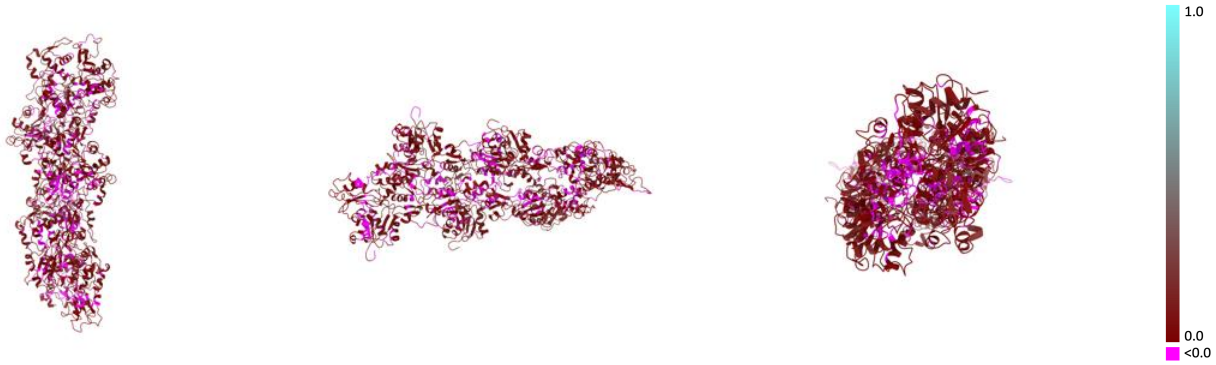
Y



Z

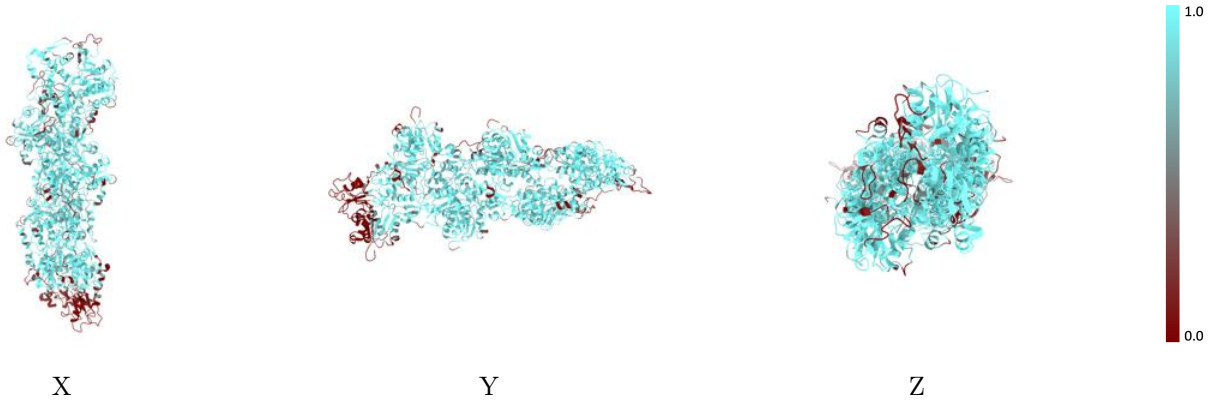
The images above show the 3D surface view of the map at the recommended contour level 4.61 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



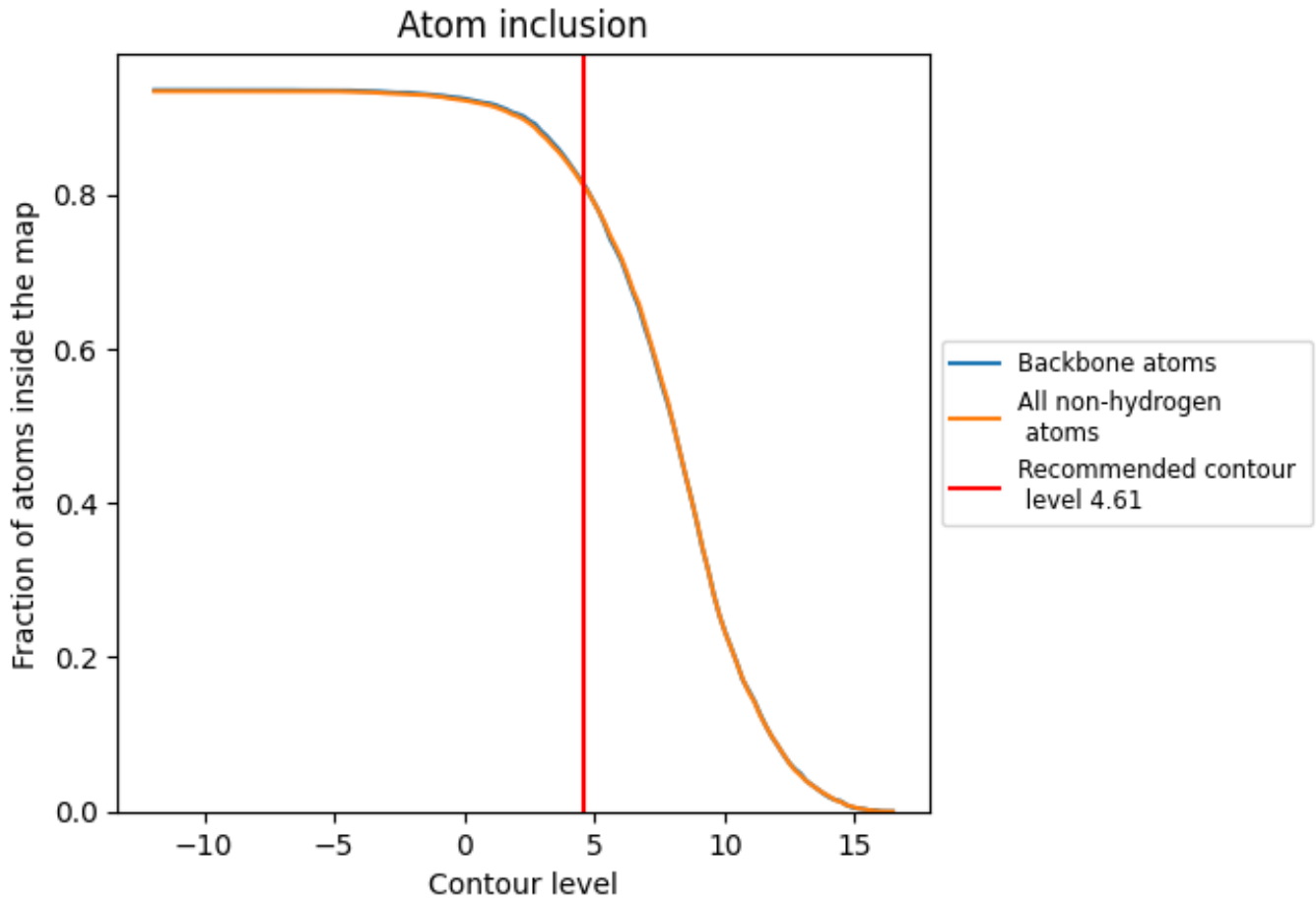
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.61).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.61) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8105	0.0520
O	0.4754	0.0280
P	0.8596	0.0540
Q	0.9129	0.0510
R	0.8764	0.0550
S	0.8781	0.0570
T	0.8623	0.0650