



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:48 PM BST

PDB ID : 3G37
EMDB ID: : EMD-1674
Title : Cryo-EM structure of actin filament in the presence of phosphate
Authors : Wakabayshi, T.; Murakami, K.; Yasunaga, T.; Noguchi, T.Q.; Uyeda, T.Q.
Deposited on : 2009-02-02
Resolution : 6.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

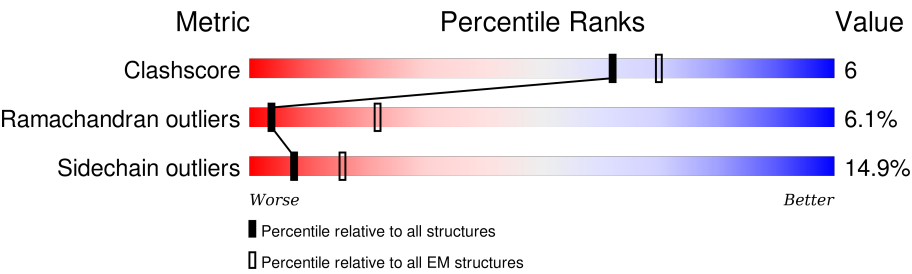
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	O	376	70% 25% . .
1	P	376	66% 27% 5% .
1	Q	376	65% 26% 8% .
1	R	376	69% 24% 6% .
1	S	376	65% 26% 7% .
1	T	376	67% 27% 6% .
1	U	376	66% 26% 7% .
1	V	376	65% 27% 7% .
1	W	376	66% 25% 8% .

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Mol	Chain	Length	Quality of chain
1	X	376	 68% 26% 6% •
1	Y	376	 70% 24% 5% •
1	Z	376	 68% 24% 6% •

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
3	PO4	Y	801	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35808 atoms, of which 0 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	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	P	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Q	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	R	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	S	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	T	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	U	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	V	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	W	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	X	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Y	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Z	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	ACE	-	ACETYLATION	UNP P68135
P	0	ACE	-	ACETYLATION	UNP P68135
Q	0	ACE	-	ACETYLATION	UNP P68135
R	0	ACE	-	ACETYLATION	UNP P68135
S	0	ACE	-	ACETYLATION	UNP P68135
T	0	ACE	-	ACETYLATION	UNP P68135

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Chain	Residue	Modelled	Actual	Comment	Reference
U	0	ACE	-	ACETYLATION	UNP P68135
V	0	ACE	-	ACETYLATION	UNP P68135
W	0	ACE	-	ACETYLATION	UNP P68135
X	0	ACE	-	ACETYLATION	UNP P68135
Y	0	ACE	-	ACETYLATION	UNP P68135
Z	0	ACE	-	ACETYLATION	UNP P68135

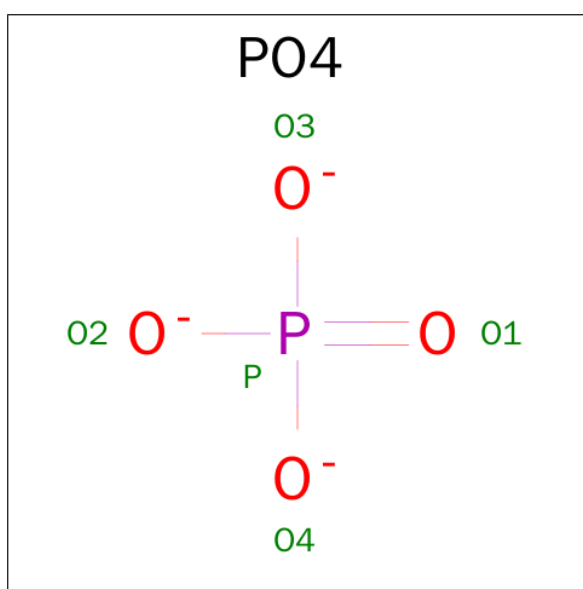
- # ADP
-

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Mol	Chain	Residues	Atoms					AltConf
2	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
3	P	1	Total	O	P	0
			15	12	3	
3	O	1	Total	O	P	0
			15	12	3	
3	O	1	Total	O	P	0
			15	12	3	
3	O	1	Total	O	P	0
			15	12	3	
3	P	1	Total	O	P	0
			15	12	3	
3	P	1	Total	O	P	0
			15	12	3	
3	R	1	Total	O	P	0
			15	12	3	

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Mol	Chain	Residues	Atoms			AltConf
3	Q	1	Total 15	O 12	P 3	0
3	Q	1	Total 15	O 12	P 3	0
3	Q	1	Total 15	O 12	P 3	0
3	R	1	Total 15	O 12	P 3	0
3	R	1	Total 15	O 12	P 3	0
3	T	1	Total 20	O 16	P 4	0
3	T	1	Total 20	O 16	P 4	0
3	S	1	Total 15	O 12	P 3	0
3	S	1	Total 15	O 12	P 3	0
3	S	1	Total 15	O 12	P 3	0
3	T	1	Total 20	O 16	P 4	0
3	T	1	Total 20	O 16	P 4	0
3	U	1	Total 15	O 12	P 3	0
3	U	1	Total 15	O 12	P 3	0
3	U	1	Total 15	O 12	P 3	0
3	V	1	Total 10	O 8	P 2	0
3	V	1	Total 10	O 8	P 2	0
3	X	1	Total 15	O 12	P 3	0
3	W	1	Total 15	O 12	P 3	0
3	W	1	Total 15	O 12	P 3	0
3	W	1	Total 15	O 12	P 3	0

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Mol	Chain	Residues	Atoms			AltConf
3	X	1	Total	O	P	0
			15	12	3	
3	X	1	Total	O	P	0
			15	12	3	
3	Z	1	Total	O	P	0
			15	12	3	
3	Y	1	Total	O	P	0
			15	12	3	
3	Y	1	Total	O	P	0
			15	12	3	
3	Y	1	Total	O	P	0
			15	12	3	
3	Z	1	Total	O	P	0
			15	12	3	
3	Z	1	Total	O	P	0
			15	12	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	P	5	Total	Mg	0
			5	5	
4	Q	7	Total	Mg	0
			7	7	
4	V	6	Total	Mg	0
			6	6	
4	W	6	Total	Mg	0
			6	6	
4	Z	6	Total	Mg	0
			6	6	
4	T	6	Total	Mg	0
			6	6	
4	U	6	Total	Mg	0
			6	6	
4	X	6	Total	Mg	0
			6	6	
4	O	6	Total	Mg	0
			6	6	
4	R	6	Total	Mg	0
			6	6	
4	Y	6	Total	Mg	0
			6	6	

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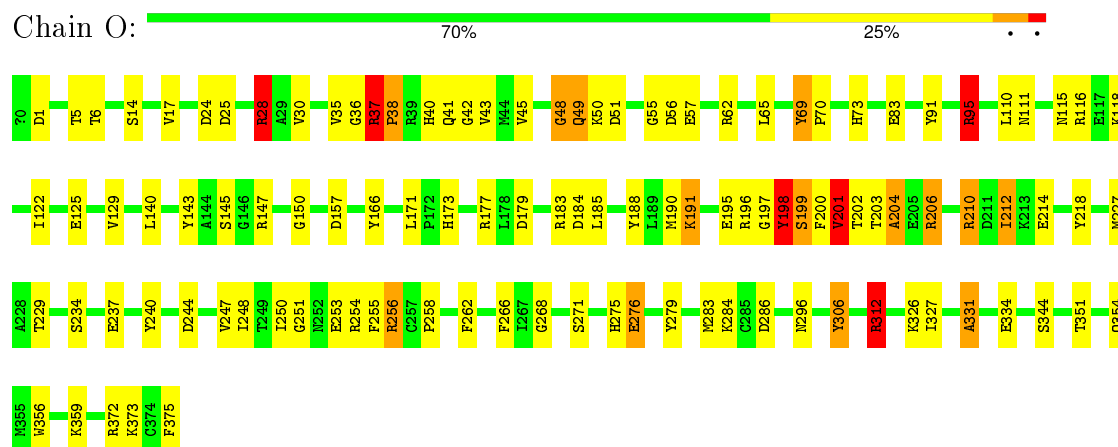
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	S	6	6	6	0

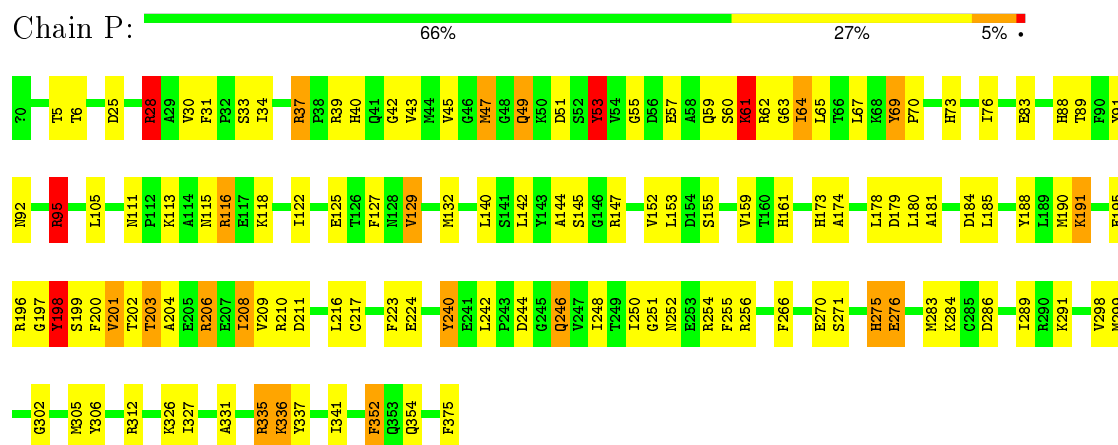
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

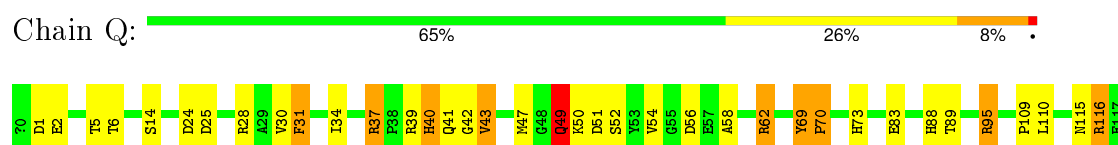
- Molecule 1: Actin, alpha skeletal muscle

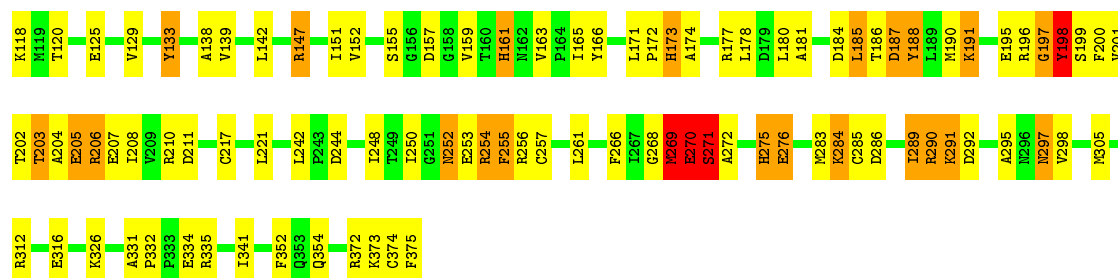


- Molecule 1: Actin, alpha skeletal muscle



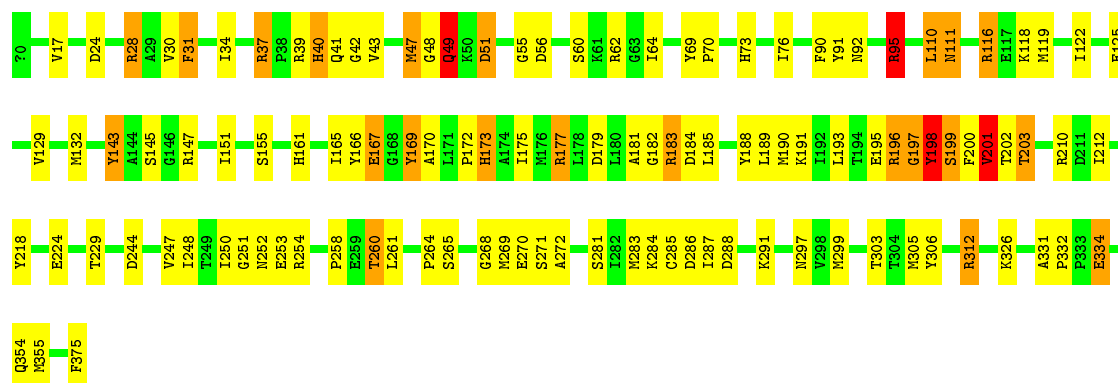
- Molecule 1: Actin, alpha skeletal muscle





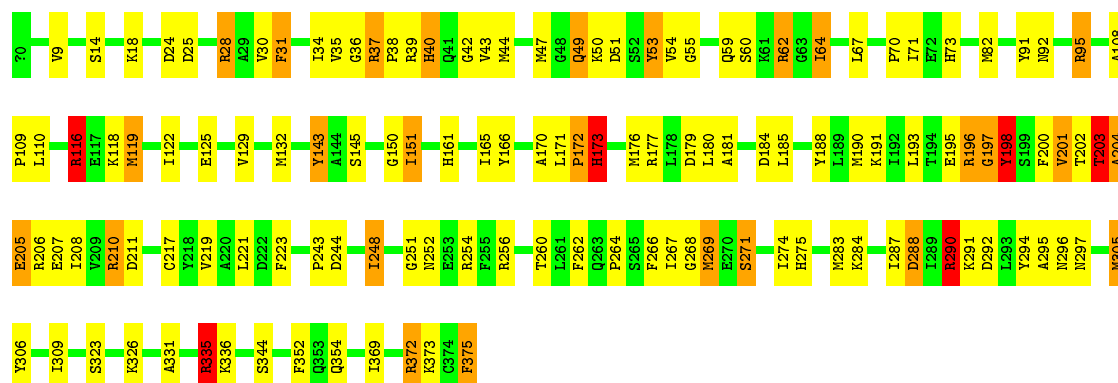
- Molecule 1: Actin, alpha skeletal muscle

Chain R: 69% 24% 6% •



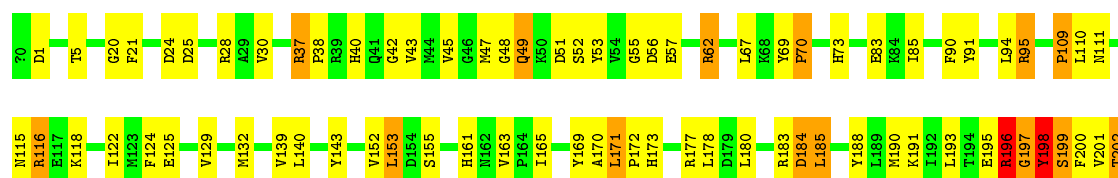
- Molecule 1: Actin, alpha skeletal muscle

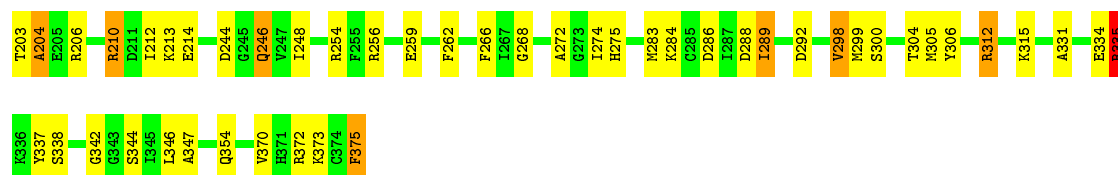
Chain S: 65% 26% 7% •



- Molecule 1: Actin, alpha skeletal muscle

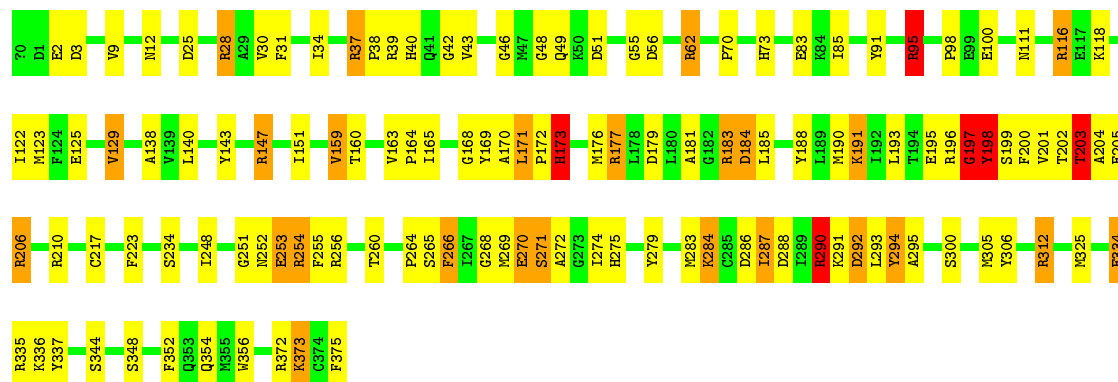
Chain T: 67% 27% 6% •





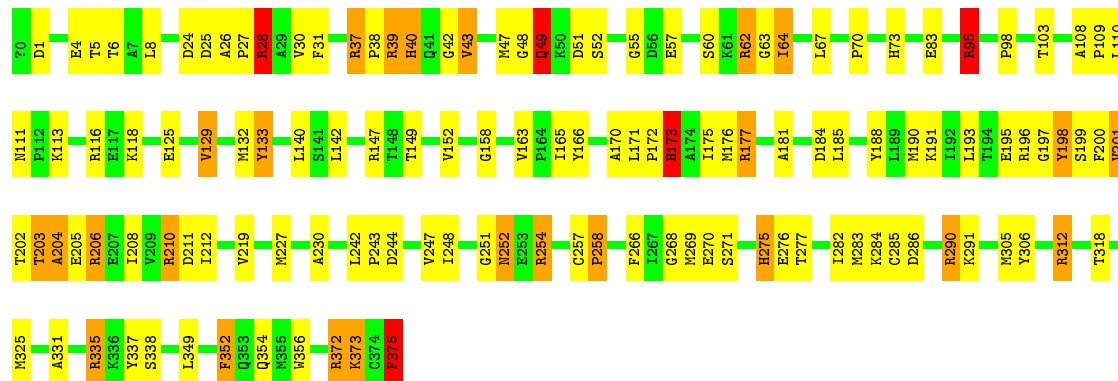
- Molecule 1: Actin, alpha skeletal muscle

Chain U: 66% 26% 7% •



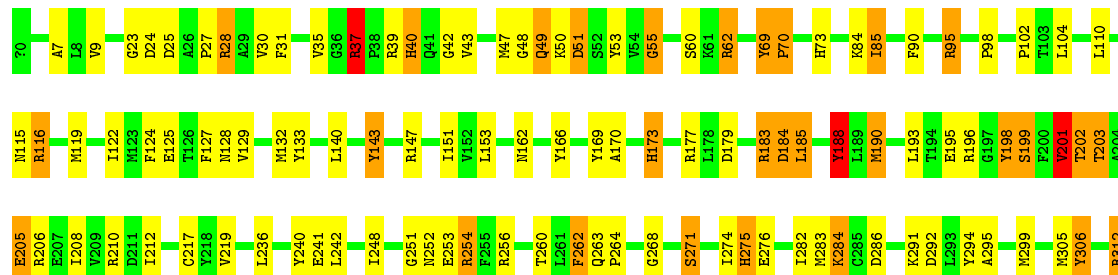
- Molecule 1: Actin, alpha skeletal muscle

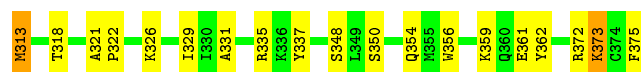
Chain V: 65% 27% 7% •



- Molecule 1: Actin, alpha skeletal muscle

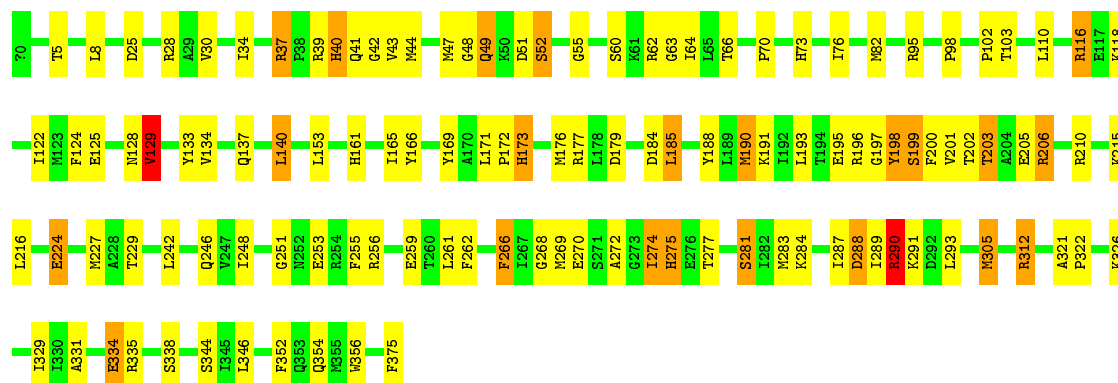
Chain W: 66% 25% 8% •





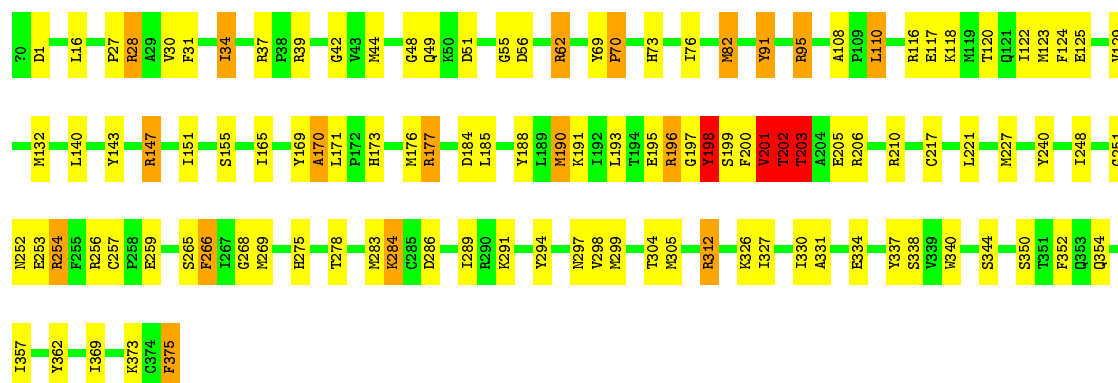
- Molecule 1: Actin, alpha skeletal muscle

Chain X: 68% 26% 6%



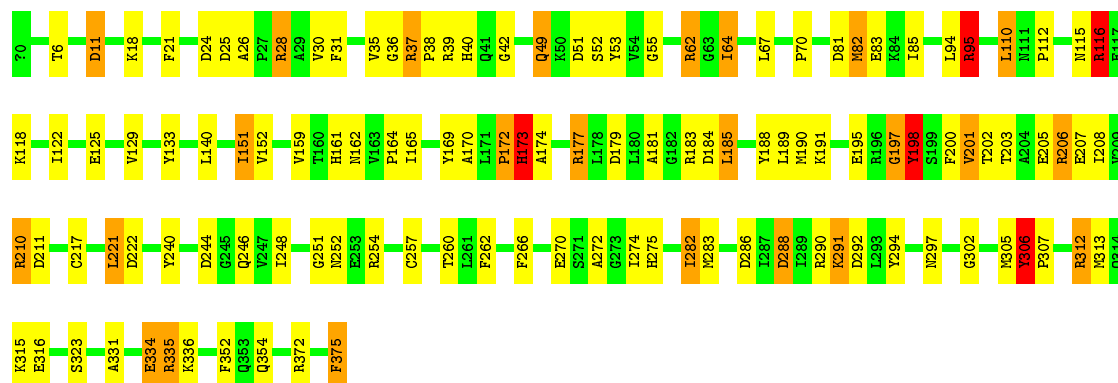
- Molecule 1: Actin, alpha skeletal muscle

Chain Y: 70% 24% 5%



- Molecule 1: Actin, alpha skeletal muscle

Chain Z: 68% 24% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FSC at 0.143 cut-off	Depositor
Microscope	HITACHI EF2000	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	100000	Depositor
Image detector	CCD	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, PO4, HIC, MG, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	O	0.73	0/2984	1.47	30/4042 (0.7%)
1	P	0.91	9/2984 (0.3%)	1.48	36/4042 (0.9%)
1	Q	0.80	4/2984 (0.1%)	1.52	31/4042 (0.8%)
1	R	0.87	3/2984 (0.1%)	1.48	27/4042 (0.7%)
1	S	0.74	1/2984 (0.0%)	1.49	30/4042 (0.7%)
1	T	0.74	0/2984	1.46	23/4042 (0.6%)
1	U	0.73	0/2984	1.44	29/4042 (0.7%)
1	V	0.71	0/2984	1.45	34/4042 (0.8%)
1	W	0.73	0/2984	1.48	34/4042 (0.8%)
1	X	0.72	0/2984	1.45	29/4042 (0.7%)
1	Y	0.72	0/2984	1.40	27/4042 (0.7%)
1	Z	0.72	0/2984	1.44	27/4042 (0.7%)
All	All	0.76	17/35808 (0.0%)	1.46	357/48504 (0.7%)

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	18
1	P	0	17
1	Q	0	25
1	R	0	16
1	S	0	21
1	T	0	19
1	U	0	25
1	V	0	19
1	W	0	24
1	X	0	14
1	Y	0	22

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Z	0	23
All	All	0	243

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	167	GLU	CD-OE1	-17.54	1.06	1.25
1	R	167	GLU	CD-OE2	12.87	1.39	1.25
1	P	62	ARG	C-N	12.41	1.55	1.33
1	P	61	LYS	CG-CD	10.97	1.89	1.52
1	Q	187	ASP	CG-OD2	-9.47	1.03	1.25
1	Q	187	ASP	CG-OD1	8.86	1.45	1.25
1	P	61	LYS	CD-CE	8.82	1.73	1.51
1	P	62	ARG	C-O	-8.17	1.07	1.23
1	P	62	ARG	CA-C	7.35	1.72	1.52
1	Q	276	GLU	CD-OE1	7.21	1.33	1.25
1	P	61	LYS	CB-CG	6.99	1.71	1.52
1	P	63	GLY	N-CA	-6.46	1.36	1.46
1	P	60	SER	CA-CB	6.32	1.62	1.52
1	P	61	LYS	CE-NZ	6.14	1.64	1.49
1	R	169	TYR	CB-CG	-6.07	1.42	1.51
1	Q	270	GLU	CG-CD	5.95	1.60	1.51
1	S	207	GLU	CB-CG	5.06	1.61	1.52

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	269	MET	CG-SD-CE	-16.11	74.43	100.20
1	S	288	ASP	CB-CG-OD1	14.03	130.92	118.30
1	R	166	TYR	CB-CG-CD1	-13.80	112.72	121.00
1	Q	187	ASP	CB-CG-OD2	12.64	129.68	118.30
1	R	166	TYR	CB-CG-CD2	12.48	128.49	121.00
1	P	37	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	T	286	ASP	CB-CG-OD2	11.36	128.53	118.30
1	S	198	TYR	N-CA-CB	11.00	130.40	110.60
1	Q	286	ASP	CB-CG-OD2	10.85	128.06	118.30
1	P	204	ALA	N-CA-CB	-10.79	94.99	110.10
1	U	198	TYR	N-CA-CB	10.34	129.22	110.60
1	W	190	MET	CG-SD-CE	10.32	116.71	100.20
1	Q	198	TYR	N-CA-CB	10.28	129.11	110.60
1	T	198	TYR	N-CA-CB	10.18	128.93	110.60
1	S	196	ARG	NE-CZ-NH2	9.95	125.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	39	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	R	198	TYR	N-CA-CB	9.78	128.19	110.60
1	Z	198	TYR	N-CA-CB	9.73	128.11	110.60
1	Z	312	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	V	39	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	O	198	TYR	N-CA-CB	9.55	127.79	110.60
1	S	375	PHE	CB-CG-CD1	9.41	127.39	120.80
1	P	198	TYR	N-CA-CB	9.29	127.32	110.60
1	V	375	PHE	CB-CG-CD2	-9.29	114.30	120.80
1	O	196	ARG	NE-CZ-NH2	9.14	124.87	120.30
1	X	177	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	U	286	ASP	CB-CG-OD2	8.96	126.36	118.30
1	Q	177	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	V	375	PHE	CB-CG-CD1	8.89	127.02	120.80
1	U	294	TYR	CB-CG-CD2	-8.87	115.68	121.00
1	S	375	PHE	CB-CG-CD2	-8.83	114.62	120.80
1	X	290	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	U	290	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	P	62	ARG	CB-CA-C	-8.72	92.95	110.40
1	Y	196	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	X	37	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	P	37	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	O	37	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	S	206	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	W	375	PHE	CB-CG-CD2	-8.39	114.93	120.80
1	Y	198	TYR	N-CA-CB	8.37	125.67	110.60
1	Q	375	PHE	CB-CG-CD2	-8.35	114.96	120.80
1	X	375	PHE	CB-CG-CD2	-8.33	114.97	120.80
1	P	286	ASP	CB-CG-OD2	8.32	125.79	118.30
1	W	196	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	W	206	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	P	206	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	Q	147	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	O	372	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	X	375	PHE	CB-CG-CD1	8.02	126.41	120.80
1	Z	37	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	Q	271	SER	N-CA-CB	8.00	122.49	110.50
1	Z	177	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	U	95	ARG	NE-CZ-NH2	7.91	124.26	120.30
1	P	95	ARG	NE-CZ-NH2	7.87	124.24	120.30
1	Q	37	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	T	312	ARG	NE-CZ-NH2	-7.83	116.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	196	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	V	95	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	P	61	LYS	CB-CG-CD	7.74	131.71	111.60
1	Y	176	MET	CG-SD-CE	-7.71	87.87	100.20
1	X	82	MET	CG-SD-CE	-7.65	87.97	100.20
1	T	337	TYR	CB-CG-CD2	-7.61	116.44	121.00
1	R	201	VAL	CA-CB-CG1	7.59	122.28	110.90
1	Q	375	PHE	CB-CG-CD1	7.58	126.11	120.80
1	W	201	VAL	CA-CB-CG1	7.57	122.25	110.90
1	P	61	LYS	N-CA-CB	-7.56	96.99	110.60
1	R	177	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	W	375	PHE	CB-CG-CD1	7.53	126.07	120.80
1	S	116	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	V	28	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	V	210	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	R	375	PHE	CB-CG-CD2	-7.42	115.61	120.80
1	X	288	ASP	CB-CG-OD1	7.40	124.96	118.30
1	U	294	TYR	CB-CG-CD1	7.40	125.44	121.00
1	Q	31	PHE	CB-CG-CD1	7.38	125.97	120.80
1	Y	147	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	Z	133	TYR	CB-CG-CD1	-7.38	116.57	121.00
1	P	62	ARG	O-C-N	-7.37	110.67	123.20
1	W	37	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	W	90	PHE	CB-CG-CD1	7.36	125.95	120.80
1	T	37	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	Z	210	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	Z	177	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	Y	201	VAL	CA-CB-CG1	7.33	121.89	110.90
1	W	90	PHE	CB-CG-CD2	-7.31	115.69	120.80
1	Y	82	MET	CG-SD-CE	-7.30	88.52	100.20
1	O	206	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	P	201	VAL	CA-CB-CG1	7.26	121.80	110.90
1	W	69	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	Z	62	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	Q	31	PHE	CB-CG-CD2	-7.21	115.75	120.80
1	U	286	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	Z	288	ASP	CB-CG-OD1	7.16	124.74	118.30
1	T	37	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	O	95	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	Q	312	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	O	69	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	R	375	PHE	CB-CG-CD1	7.03	125.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	269	MET	CG-SD-CE	-7.01	88.99	100.20
1	U	335	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	P	91	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	W	53	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	X	177	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	W	198	TYR	N-CA-C	-6.94	92.26	111.00
1	V	198	TYR	N-CA-CB	6.93	123.08	110.60
1	W	143	TYR	CB-CG-CD2	6.92	125.15	121.00
1	X	269	MET	CG-SD-CE	-6.91	89.14	100.20
1	V	312	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	S	204	ALA	N-CA-CB	-6.89	100.45	110.10
1	T	337	TYR	CB-CG-CD1	6.88	125.13	121.00
1	Q	177	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	P	203	THR	N-CA-CB	6.84	123.29	110.30
1	V	37	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	Y	91	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	V	269	MET	CG-SD-CE	-6.78	89.35	100.20
1	V	206	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	P	61	LYS	N-CA-C	-6.77	92.72	111.00
1	Y	62	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	S	210	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	Y	95	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	V	62	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	P	69	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	O	206	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	O	256	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	T	204	ALA	N-CA-CB	6.64	119.39	110.10
1	V	177	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	U	37	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	V	62	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	S	37	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	V	286	ASP	CB-CG-OD2	6.59	124.23	118.30
1	V	28	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	S	95	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	P	51	ASP	C-N-CA	6.57	138.12	121.70
1	X	203	THR	N-CA-CB	6.55	122.75	110.30
1	T	143	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	O	286	ASP	CB-CG-OD2	6.50	124.15	118.30
1	P	91	TYR	CB-CG-CD1	6.50	124.90	121.00
1	P	53	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	Z	62	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	W	147	ARG	NE-CZ-NH1	6.47	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	39	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	Y	294	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	U	337	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	O	356	TRP	CA-CB-CG	6.40	125.87	113.70
1	V	37	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	V	201	VAL	CA-CB-CG1	6.38	120.47	110.90
1	U	375	PHE	CB-CG-CD2	-6.38	116.34	120.80
1	W	203	THR	N-CA-CB	6.37	122.40	110.30
1	O	201	VAL	CA-CB-CG1	6.35	120.43	110.90
1	Q	39	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	O	276	GLU	CB-CG-CD	6.33	131.29	114.20
1	Z	133	TYR	CB-CG-CD2	6.32	124.79	121.00
1	O	191	LYS	CA-CB-CG	6.32	127.29	113.40
1	O	375	PHE	CB-CG-CD1	6.32	125.22	120.80
1	U	116	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	T	143	TYR	CB-CG-CD2	6.27	124.76	121.00
1	X	116	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	W	177	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	V	47	MET	CG-SD-CE	-6.25	90.19	100.20
1	R	286	ASP	CB-CG-OD2	6.21	123.89	118.30
1	Q	206	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	X	39	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	P	147	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	T	183	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	W	143	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	Z	37	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	O	375	PHE	CB-CG-CD2	-6.15	116.50	120.80
1	V	312	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	R	312	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	W	205	GLU	CB-CA-C	6.11	122.62	110.40
1	X	206	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	R	161	HIS	CB-CA-C	-6.08	98.25	110.40
1	U	206	ARG	CB-CA-C	6.08	122.55	110.40
1	W	286	ASP	CB-CG-OD2	6.07	123.77	118.30
1	Y	312	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	O	28	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	R	147	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	Y	177	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	P	191	LYS	CA-CB-CG	6.04	126.70	113.40
1	R	312	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	S	288	ASP	OD1-CG-OD2	-6.04	111.83	123.30
1	U	203	THR	N-CA-CB	6.02	121.75	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	286	ASP	CB-CG-OD2	6.02	123.72	118.30
1	T	312	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	W	183	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	U	147	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	U	176	MET	CG-SD-CE	-5.98	90.64	100.20
1	U	62	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	X	196	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	U	204	ALA	N-CA-CB	-5.97	101.75	110.10
1	U	203	THR	O-C-N	-5.96	113.16	122.70
1	Q	69	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	U	39	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	P	375	PHE	CB-CG-CD1	5.96	124.97	120.80
1	W	39	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	T	375	PHE	CB-CG-CD1	5.93	124.95	120.80
1	U	177	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	Q	206	ARG	CB-CA-C	5.91	122.22	110.40
1	R	62	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	W	177	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	S	294	TYR	CB-CG-CD2	-5.89	117.46	121.00
1	R	183	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	V	210	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	Q	269	MET	CB-CG-SD	5.82	129.87	112.40
1	W	53	TYR	CB-CG-CD1	5.82	124.49	121.00
1	P	47	MET	CG-SD-CE	-5.82	90.89	100.20
1	Y	375	PHE	CB-CG-CD1	5.82	124.88	120.80
1	S	62	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	P	337	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	O	147	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	Q	49	GLN	N-CA-CB	5.79	121.02	110.60
1	R	166	TYR	C-N-CA	5.79	136.17	121.70
1	X	288	ASP	OD1-CG-OD2	-5.78	112.32	123.30
1	U	183	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	X	179	ASP	CB-CG-OD1	5.78	123.50	118.30
1	Z	82	MET	CG-SD-CE	-5.77	90.96	100.20
1	Z	11	ASP	CB-CG-OD1	5.77	123.49	118.30
1	S	116	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	X	190	MET	CA-CB-CG	5.76	123.10	113.30
1	X	62	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	X	39	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	S	176	MET	CG-SD-CE	-5.75	91.00	100.20
1	X	198	TYR	N-CA-CB	5.75	120.95	110.60
1	Y	312	ARG	NE-CZ-NH2	-5.75	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	299	MET	CG-SD-CE	-5.75	91.01	100.20
1	Y	198	TYR	N-CA-C	-5.74	95.50	111.00
1	Q	203	THR	N-CA-CB	5.74	121.20	110.30
1	O	203	THR	N-CA-CB	5.73	121.19	110.30
1	O	276	GLU	CG-CD-OE2	-5.73	106.84	118.30
1	R	355	MET	CG-SD-CE	-5.72	91.05	100.20
1	V	203	THR	N-CA-CB	5.72	121.17	110.30
1	O	183	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	V	352	PHE	CB-CG-CD1	-5.72	116.80	120.80
1	R	132	MET	CA-CB-CG	5.71	123.00	113.30
1	Q	297	ASN	CB-CA-C	-5.70	99.00	110.40
1	P	240	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	U	177	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	V	39	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	R	47	MET	CG-SD-CE	-5.67	91.13	100.20
1	X	52	SER	N-CA-CB	5.67	119.01	110.50
1	T	206	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	U	91	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	V	352	PHE	CB-CG-CD2	5.65	124.76	120.80
1	S	203	THR	N-CA-CB	5.65	121.03	110.30
1	R	69	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	Y	39	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	Q	47	MET	CG-SD-CE	-5.64	91.17	100.20
1	U	37	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	P	39	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	O	312	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	R	177	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	U	375	PHE	CB-CG-CD1	5.62	124.73	120.80
1	S	205	GLU	CB-CA-C	5.58	121.56	110.40
1	O	166	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	Z	53	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	V	133	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	W	198	TYR	N-CA-CB	5.53	120.56	110.60
1	Z	375	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	S	290	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	V	203	THR	O-C-N	-5.52	113.87	122.70
1	Y	123	MET	CG-SD-CE	-5.51	91.39	100.20
1	V	177	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Y	202	THR	CA-CB-CG2	5.49	120.09	112.40
1	O	37	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	Y	299	MET	CG-SD-CE	-5.48	91.43	100.20
1	Y	44	MET	CG-SD-CE	-5.47	91.44	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	375	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	P	69	TYR	CB-CG-CD1	5.46	124.27	121.00
1	S	143	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	T	196	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	S	166	TYR	CB-CG-CD1	5.44	124.26	121.00
1	Y	177	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	T	286	ASP	CB-CG-OD1	-5.43	113.42	118.30
1	T	210	ARG	CG-CD-NE	-5.42	100.41	111.80
1	P	352	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	V	204	ALA	N-CA-CB	-5.42	102.51	110.10
1	O	204	ALA	N-CA-CB	-5.42	102.52	110.10
1	P	28	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	Q	62	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	Q	161	HIS	CA-CB-CG	5.41	122.80	113.60
1	R	143	TYR	CB-CG-CD2	5.40	124.24	121.00
1	W	119	MET	CG-SD-CE	-5.39	91.57	100.20
1	S	53	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	S	82	MET	CG-SD-CE	-5.38	91.58	100.20
1	X	206	ARG	CB-CA-C	5.38	121.16	110.40
1	R	167	GLU	CA-CB-CG	5.38	125.23	113.40
1	Q	205	GLU	CB-CA-C	5.37	121.13	110.40
1	P	204	ALA	N-CA-C	5.37	125.49	111.00
1	S	37	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	Z	210	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	Z	152	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	W	62	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	X	281	SER	N-CA-CB	5.34	118.51	110.50
1	X	305	MET	CG-SD-CE	-5.33	91.67	100.20
1	S	166	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	W	127	PHE	CB-CG-CD1	5.32	124.52	120.80
1	Q	270	GLU	CA-CB-CG	5.31	125.09	113.40
1	T	90	PHE	CB-CG-CD1	5.31	124.52	120.80
1	O	95	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	R	51	ASP	C-N-CA	5.29	134.91	121.70
1	Q	203	THR	O-C-N	-5.28	114.25	122.70
1	U	312	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	W	337	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	Z	64	ILE	CA-CB-CG1	5.26	121.00	111.00
1	Y	62	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	Z	116	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	W	39	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	X	44	MET	CG-SD-CE	-5.23	91.83	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	372	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	P	127	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	X	66	THR	CA-CB-CG2	5.20	119.69	112.40
1	Z	95	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	V	206	ARG	N-CA-C	5.19	125.02	111.00
1	W	312	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	V	337	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	X	312	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	Y	337	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	Z	161	HIS	CB-CA-C	-5.16	100.09	110.40
1	T	202	THR	CA-CB-OG1	5.15	119.82	109.00
1	X	293	LEU	CB-CG-CD1	5.15	119.76	111.00
1	Y	190	MET	CA-CB-CG	5.15	122.06	113.30
1	T	335	ARG	N-CA-CB	-5.15	101.33	110.60
1	X	129	VAL	CA-CB-CG2	5.14	118.62	110.90
1	P	196	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	W	55	GLY	N-CA-C	5.14	125.94	113.10
1	O	210	ARG	CG-CD-NE	-5.13	101.02	111.80
1	O	227	MET	CG-SD-CE	-5.13	91.99	100.20
1	W	69	TYR	CB-CG-CD1	5.12	124.07	121.00
1	P	53	TYR	CB-CG-CD2	5.12	124.07	121.00
1	T	48	GLY	N-CA-C	5.11	125.88	113.10
1	Y	108	ALA	N-CA-CB	-5.11	102.94	110.10
1	P	335	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	Y	205	GLU	CB-CA-C	5.11	120.62	110.40
1	T	90	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	O	48	GLY	N-CA-C	5.10	125.85	113.10
1	S	31	PHE	CB-CG-CD1	5.10	124.37	120.80
1	T	132	MET	CA-CB-CG	5.10	121.97	113.30
1	R	39	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	Q	372	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	W	313	MET	CG-SD-CE	-5.08	92.06	100.20
1	P	28	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	Z	39	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	Z	375	PHE	CB-CG-CD1	5.04	124.33	120.80
1	Y	286	ASP	CB-CG-OD1	5.04	122.84	118.30
1	Z	306	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	W	166	TYR	CB-CG-CD2	5.04	124.02	121.00
1	S	248	ILE	CA-CB-CG1	5.03	120.56	111.00
1	V	372	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	S	44	MET	CG-SD-CE	-5.02	92.17	100.20
1	U	206	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	41	GLN	CB-CA-C	5.02	120.43	110.40
1	U	171	LEU	CB-CG-CD2	5.01	119.51	111.00
1	V	227	MET	CG-SD-CE	-5.00	92.19	100.20
1	R	281	SER	N-CA-CB	5.00	118.00	110.50
1	V	147	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	Z	161	HIS	CA-CB-CG	5.00	122.10	113.60

There are no chirality outliers.

All (243) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	177	ARG	Sidechain
1	O	197	GLY	Peptide
1	O	200	PHE	Peptide
1	O	210	ARG	Sidechain
1	O	218	TYR	Sidechain
1	O	240	TYR	Sidechain
1	O	253	GLU	Peptide
1	O	256	ARG	Sidechain
1	O	266	PHE	Peptide
1	O	279	TYR	Sidechain
1	O	28	ARG	Sidechain
1	O	312	ARG	Sidechain
1	O	331	ALA	Peptide
1	O	38	PRO	Peptide
1	O	50	LYS	Peptide
1	O	69	TYR	Sidechain
1	O	91	TYR	Sidechain
1	O	95	ARG	Sidechain
1	P	116	ARG	Sidechain
1	P	161	HIS	Sidechain
1	P	197	GLY	Peptide
1	P	200	PHE	Peptide
1	P	208	ILE	Peptide
1	P	210	ARG	Sidechain
1	P	240	TYR	Sidechain
1	P	256	ARG	Sidechain
1	P	266	PHE	Peptide
1	P	28	ARG	Sidechain
1	P	306	TYR	Sidechain
1	P	312	ARG	Sidechain
1	P	331	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	P	53	TYR	Sidechain
1	P	61	LYS	Mainchain
1	P	69	TYR	Sidechain
1	P	95	ARG	Sidechain
1	Q	116	ARG	Sidechain
1	Q	133	TYR	Sidechain
1	Q	147	ARG	Sidechain
1	Q	171	LEU	Peptide
1	Q	187	ASP	Mainchain
1	Q	188	TYR	Sidechain
1	Q	200	PHE	Sidechain,Peptide
1	Q	210	ARG	Sidechain
1	Q	250	ILE	Peptide
1	Q	253	GLU	Peptide
1	Q	256	ARG	Sidechain
1	Q	266	PHE	Peptide
1	Q	269	MET	Peptide
1	Q	270	GLU	Peptide
1	Q	271	SER	Peptide
1	Q	290	ARG	Sidechain
1	Q	316	GLU	Peptide
1	Q	331	ALA	Peptide
1	Q	334	GLU	Peptide
1	Q	34	ILE	Peptide
1	Q	50	LYS	Peptide
1	Q	58	ALA	Peptide
1	Q	69	TYR	Sidechain
1	Q	95	ARG	Sidechain
1	R	169	TYR	Sidechain
1	R	177	ARG	Sidechain
1	R	183	ARG	Sidechain
1	R	196	ARG	Sidechain
1	R	197	GLY	Peptide
1	R	200	PHE	Peptide
1	R	210	ARG	Sidechain
1	R	218	TYR	Sidechain
1	R	28	ARG	Sidechain
1	R	312	ARG	Sidechain
1	R	331	ALA	Peptide
1	R	334	GLU	Peptide
1	R	37	ARG	Sidechain
1	R	90	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	R	91	TYR	Sidechain
1	R	95	ARG	Sidechain
1	S	116	ARG	Sidechain
1	S	143	TYR	Sidechain
1	S	172	PRO	Peptide
1	S	177	ARG	Sidechain
1	S	197	GLY	Peptide
1	S	200	PHE	Sidechain,Peptide
1	S	210	ARG	Sidechain
1	S	223	PHE	Sidechain
1	S	256	ARG	Sidechain
1	S	266	PHE	Peptide
1	S	271	SER	Peptide
1	S	28	ARG	Sidechain
1	S	290	ARG	Sidechain
1	S	306	TYR	Sidechain
1	S	331	ALA	Peptide
1	S	335	ARG	Sidechain
1	S	372	ARG	Sidechain
1	S	50	LYS	Peptide
1	S	53	TYR	Sidechain
1	S	91	TYR	Sidechain
1	T	116	ARG	Sidechain
1	T	124	PHE	Sidechain
1	T	171	LEU	Peptide
1	T	177	ARG	Sidechain
1	T	196	ARG	Sidechain
1	T	197	GLY	Peptide
1	T	200	PHE	Peptide
1	T	210	ARG	Sidechain
1	T	266	PHE	Peptide
1	T	306	TYR	Sidechain
1	T	312	ARG	Sidechain
1	T	331	ALA	Peptide
1	T	334	GLU	Peptide
1	T	335	ARG	Sidechain
1	T	38	PRO	Peptide
1	T	53	TYR	Sidechain
1	T	62	ARG	Sidechain
1	T	69	TYR	Sidechain
1	T	91	TYR	Sidechain
1	U	100	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	U	12	ASN	Peptide
1	U	143	TYR	Sidechain
1	U	147	ARG	Sidechain
1	U	168	GLY	Peptide
1	U	169	TYR	Sidechain
1	U	177	ARG	Sidechain
1	U	197	GLY	Peptide
1	U	200	PHE	Peptide
1	U	210	ARG	Sidechain
1	U	253	GLU	Peptide
1	U	256	ARG	Sidechain
1	U	266	PHE	Peptide
1	U	271	SER	Peptide
1	U	28	ARG	Sidechain
1	U	290	ARG	Sidechain
1	U	294	TYR	Sidechain
1	U	312	ARG	Sidechain
1	U	334	GLU	Peptide
1	U	372	ARG	Sidechain
1	U	373	LYS	Peptide
1	U	38	PRO	Peptide
1	U	40	HIS	Sidechain
1	U	62	ARG	Sidechain
1	U	95	ARG	Sidechain
1	V	133	TYR	Sidechain
1	V	177	ARG	Sidechain
1	V	197	GLY	Peptide
1	V	200	PHE	Peptide
1	V	210	ARG	Sidechain
1	V	254	ARG	Sidechain
1	V	258	PRO	Peptide
1	V	266	PHE	Peptide
1	V	28	ARG	Sidechain
1	V	290	ARG	Sidechain
1	V	306	TYR	Sidechain
1	V	312	ARG	Sidechain
1	V	331	ALA	Peptide
1	V	335	ARG	Sidechain
1	V	372	ARG	Sidechain
1	V	373	LYS	Peptide
1	V	38	PRO	Peptide
1	V	62	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	V	95	ARG	Sidechain
1	W	116	ARG	Sidechain
1	W	133	TYR	Sidechain
1	W	169	TYR	Sidechain
1	W	170	ALA	Peptide
1	W	183	ARG	Sidechain
1	W	188	TYR	Sidechain
1	W	210	ARG	Sidechain
1	W	23	GLY	Peptide
1	W	256	ARG	Sidechain
1	W	262	PHE	Sidechain
1	W	271	SER	Peptide
1	W	28	ARG	Sidechain
1	W	306	TYR	Sidechain
1	W	312	ARG	Sidechain
1	W	331	ALA	Peptide
1	W	362	TYR	Sidechain
1	W	37	ARG	Sidechain
1	W	372	ARG	Sidechain
1	W	373	LYS	Peptide
1	W	50	LYS	Peptide
1	W	51	ASP	Peptide
1	W	62	ARG	Sidechain
1	W	69	TYR	Sidechain
1	W	95	ARG	Sidechain
1	X	124	PHE	Sidechain
1	X	133	TYR	Sidechain
1	X	169	TYR	Sidechain
1	X	197	GLY	Peptide
1	X	200	PHE	Peptide
1	X	210	ARG	Sidechain
1	X	215	LYS	Peptide
1	X	256	ARG	Sidechain
1	X	266	PHE	Peptide
1	X	28	ARG	Sidechain
1	X	290	ARG	Sidechain
1	X	312	ARG	Sidechain
1	X	331	ALA	Peptide
1	X	334	GLU	Peptide
1	Y	124	PHE	Sidechain
1	Y	143	TYR	Sidechain
1	Y	147	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	Y	169	TYR	Sidechain
1	Y	170	ALA	Peptide
1	Y	171	LEU	Peptide
1	Y	177	ARG	Sidechain
1	Y	197	GLY	Peptide
1	Y	200	PHE	Peptide
1	Y	206	ARG	Sidechain
1	Y	210	ARG	Sidechain
1	Y	240	TYR	Sidechain
1	Y	256	ARG	Sidechain
1	Y	266	PHE	Peptide
1	Y	28	ARG	Sidechain
1	Y	31	PHE	Sidechain
1	Y	312	ARG	Sidechain
1	Y	331	ALA	Peptide
1	Y	334	GLU	Peptide
1	Y	362	TYR	Sidechain
1	Y	62	ARG	Sidechain
1	Y	91	TYR	Sidechain
1	Z	116	ARG	Sidechain,Peptide
1	Z	177	ARG	Sidechain
1	Z	197	GLY	Peptide
1	Z	200	PHE	Peptide
1	Z	206	ARG	Sidechain
1	Z	210	ARG	Sidechain
1	Z	221	LEU	Peptide
1	Z	240	TYR	Sidechain
1	Z	26	ALA	Peptide
1	Z	266	PHE	Sidechain
1	Z	28	ARG	Sidechain
1	Z	290	ARG	Sidechain
1	Z	294	TYR	Sidechain
1	Z	312	ARG	Sidechain
1	Z	316	GLU	Peptide
1	Z	331	ALA	Peptide
1	Z	334	GLU	Peptide
1	Z	335	ARG	Sidechain
1	Z	372	ARG	Sidechain
1	Z	38	PRO	Peptide
1	Z	62	ARG	Sidechain
1	Z	95	ARG	Sidechain

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	O	2936	0	2896	30	0
1	P	2936	0	2895	38	0
1	Q	2936	0	2896	52	0
1	R	2936	0	2896	35	0
1	S	2936	0	2896	40	0
1	T	2936	0	2896	42	0
1	U	2936	0	2896	37	0
1	V	2936	0	2896	48	0
1	W	2936	0	2896	41	0
1	X	2936	0	2896	37	0
1	Y	2936	0	2896	33	0
1	Z	2936	0	2896	23	0
2	O	27	0	12	1	0
2	P	27	0	12	0	0
2	Q	27	0	12	0	0
2	R	27	0	12	0	0
2	S	27	0	12	0	0
2	T	27	0	12	0	0
2	U	27	0	12	1	0
2	V	27	0	12	0	0
2	W	27	0	12	0	0
2	X	27	0	12	0	0
2	Y	27	0	12	0	0
2	Z	27	0	12	0	0
3	O	15	0	0	0	0
3	P	15	0	0	1	0
3	Q	15	0	0	0	0
3	R	15	0	0	1	0
3	S	15	0	0	0	0
3	T	20	0	0	1	0
3	U	15	0	0	0	0
3	V	10	0	0	0	0
3	W	15	0	0	0	0
3	X	15	0	0	0	0
3	Y	15	0	0	2	0
3	Z	15	0	0	0	0
4	O	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	5	0	0	0	0
4	Q	7	0	0	0	0
4	R	6	0	0	0	0
4	S	6	0	0	0	0
4	T	6	0	0	0	0
4	U	6	0	0	0	0
4	V	6	0	0	0	0
4	W	6	0	0	0	0
4	X	6	0	0	0	0
4	Y	6	0	0	0	0
4	Z	6	0	0	0	0
All	All	35808	0	34895	391	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 6.

All (391) 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:P:61:LYS:CD	1:P:61:LYS:CG	1.89	1.50
1:Q:202:THR:HG23	1:Q:203:THR:H	1.48	0.78
1:P:202:THR:HG23	1:P:203:THR:H	1.50	0.76
1:O:201:VAL:HG13	1:O:202:THR:HG22	1.68	0.74
1:V:275:HIS:CD2	1:V:276:GLU:H	2.05	0.74
1:O:201:VAL:HG13	1:O:202:THR:H	1.53	0.72
1:S:204:ALA:HB1	1:U:290:ARG:HH21	1.55	0.71
1:V:202:THR:HG23	1:V:203:THR:H	1.57	0.70
1:R:201:VAL:HG13	1:R:202:THR:HG22	1.73	0.69
1:R:193:LEU:HD23	1:R:196:ARG:HE	1.56	0.69
1:W:201:VAL:HG13	1:W:202:THR:H	1.56	0.69
1:T:193:LEU:HD23	1:T:196:ARG:HE	1.59	0.67
1:S:204:ALA:HB1	1:U:290:ARG:NH2	2.10	0.66
1:Y:202:THR:HG23	1:Y:203:THR:H	1.60	0.66
1:V:40:HIS:CD2	1:V:43:VAL:H	2.14	0.65
1:S:201:VAL:HG13	1:S:202:THR:H	1.62	0.65
1:O:43:VAL:HG22	1:Q:110:LEU:HD13	1.78	0.64
1:O:276:GLU:O	1:O:276:GLU:HG3	1.96	0.64
1:R:40:HIS:CD2	1:R:43:VAL:H	2.16	0.63
1:Q:185:LEU:HD12	1:Q:257:CYS:SG	2.38	0.63
1:V:204:ALA:HB1	1:X:290:ARG:NH2	2.14	0.63
1:X:262:PHE:HA	1:X:274:ILE:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:34:ILE:HB	1:P:67:LEU:HD11	1.81	0.62
1:Q:40:HIS:CD2	1:Q:43:VAL:H	2.17	0.62
1:T:262:PHE:HA	1:T:274:ILE:HG22	1.82	0.62
1:R:47:MET:SD	1:T:170:ALA:HB3	2.41	0.60
1:P:202:THR:HG23	1:P:203:THR:N	2.15	0.60
1:U:198:TYR:HD2	1:U:198:TYR:N	1.99	0.60
1:Q:198:TYR:HD2	1:Q:198:TYR:N	2.00	0.59
1:Z:198:TYR:HD2	1:Z:198:TYR:N	2.00	0.59
1:U:217:CYS:HA	1:U:254:ARG:HA	1.85	0.59
1:U:198:TYR:CD2	1:U:198:TYR:N	2.70	0.59
1:S:198:TYR:HD2	1:S:198:TYR:N	2.01	0.59
1:X:202:THR:HG23	1:X:203:THR:H	1.67	0.59
1:R:287:ILE:HG23	1:R:288:ASP:OD2	2.03	0.58
1:P:88:HIS:CE1	1:P:92:ASN:HD21	2.21	0.58
1:U:201:VAL:HG13	1:U:202:THR:H	1.67	0.58
1:W:202:THR:HG23	1:W:203:THR:H	1.67	0.58
1:T:21:PHE:CZ	1:T:94:LEU:HD22	2.39	0.58
1:R:198:TYR:HD2	1:R:198:TYR:N	2.01	0.58
1:W:47:MET:SD	1:Y:170:ALA:HB3	2.44	0.58
1:S:305:MET:HA	1:S:335:ARG:HH21	1.69	0.57
1:Y:201:VAL:HG13	1:Y:202:THR:H	1.67	0.57
1:Z:198:TYR:CD2	1:Z:198:TYR:N	2.72	0.57
1:X:199:SER:HB3	1:X:201:VAL:HB	1.85	0.57
1:S:73:HIC:HD2	1:S:73:HIC:O	2.04	0.57
1:S:198:TYR:CD2	1:S:198:TYR:N	2.72	0.57
1:P:40:HIS:CD2	1:P:43:VAL:H	2.22	0.57
1:R:198:TYR:N	1:R:198:TYR:CD2	2.73	0.57
1:V:165:ILE:HG12	1:V:170:ALA:HB2	1.85	0.57
1:Z:21:PHE:CZ	1:Z:94:LEU:HD22	2.39	0.57
1:P:284:LYS:C	1:P:284:LYS:HD2	2.26	0.57
1:Y:198:TYR:N	1:Y:198:TYR:HD2	2.01	0.57
1:Q:198:TYR:CD2	1:Q:198:TYR:N	2.72	0.56
1:Q:275:HIS:CD2	1:Q:276:GLU:H	2.23	0.56
1:S:35:VAL:HG12	1:S:36:GLY:H	1.69	0.56
1:O:38:PRO:HB3	1:O:65:LEU:HD23	1.87	0.56
1:V:204:ALA:HB1	1:X:290:ARG:HH21	1.70	0.56
1:Y:298:VAL:HG12	1:Y:330:ILE:HB	1.88	0.56
1:R:261:LEU:HD11	1:R:303:THR:CG2	2.36	0.56
1:Y:198:TYR:N	1:Y:198:TYR:CD2	2.74	0.56
1:U:159:VAL:HG12	1:U:179:ASP:HA	1.88	0.56
1:T:198:TYR:HD2	1:T:198:TYR:N	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:198:TYR:HD2	1:O:198:TYR:N	2.04	0.56
1:V:198:TYR:N	1:V:198:TYR:HD2	2.02	0.56
1:P:246:GLN:HA	1:P:246:GLN:HE21	1.71	0.56
1:V:172:PRO:HG2	1:V:173:HIS:CE1	2.41	0.55
1:O:73:HIC:O	1:O:73:HIC:HD2	2.06	0.55
1:T:198:TYR:CD2	1:T:198:TYR:N	2.74	0.55
1:Y:284:LYS:C	1:Y:284:LYS:HD2	2.27	0.55
1:P:202:THR:HG21	3:R:801:PO4:O2	2.07	0.55
1:X:47:MET:SD	1:Z:170:ALA:HB3	2.46	0.55
1:Z:185:LEU:HD22	1:Z:185:LEU:H	1.72	0.55
1:P:198:TYR:N	1:P:198:TYR:HD2	2.04	0.55
1:U:193:LEU:HD23	1:U:196:ARG:HE	1.72	0.55
1:S:193:LEU:HD22	1:S:196:ARG:HH11	1.72	0.54
1:Q:201:VAL:HG21	1:R:179:ASP:HB2	1.88	0.54
1:O:262:PHE:CZ	1:O:312:ARG:HG2	2.42	0.54
1:S:40:HIS:CD2	1:S:43:VAL:H	2.25	0.54
1:V:198:TYR:CD2	1:V:198:TYR:N	2.76	0.54
1:W:217:CYS:HA	1:W:254:ARG:HA	1.90	0.54
1:T:204:ALA:HB1	1:V:290:ARG:CZ	2.38	0.54
1:S:203:THR:HG21	1:U:173:HIS:CE1	2.42	0.54
1:T:139:VAL:HG22	1:T:165:ILE:HD13	1.90	0.54
1:Y:202:THR:HG23	1:Y:203:THR:N	2.22	0.54
1:P:198:TYR:CD2	1:P:198:TYR:N	2.76	0.54
1:P:202:THR:O	1:Q:269:MET:HE1	2.08	0.53
1:T:204:ALA:HB2	1:V:285:CYS:O	2.08	0.53
1:X:185:LEU:HD21	1:X:261:LEU:HD23	1.89	0.53
1:S:262:PHE:HA	1:S:274:ILE:HG22	1.89	0.53
1:O:35:VAL:HG12	1:O:36:GLY:H	1.74	0.53
1:T:140:LEU:HB3	1:T:342:GLY:HA3	1.90	0.53
1:O:201:VAL:HG13	1:O:202:THR:N	2.24	0.53
1:X:199:SER:OG	1:Y:73:HIC:HD2	2.08	0.53
1:Y:34:ILE:HG23	1:Y:69:TYR:CD2	2.43	0.53
1:W:282:ILE:HD12	1:W:294:TYR:CD1	2.44	0.53
1:P:275:HIS:CD2	1:P:276:GLU:H	2.27	0.53
1:W:153:LEU:HB2	1:W:299:MET:HG2	1.89	0.53
1:X:198:TYR:N	1:X:198:TYR:HD2	2.04	0.53
1:Q:151:ILE:HG23	1:Q:297:ASN:HA	1.91	0.52
1:Q:185:LEU:HD21	1:Q:261:LEU:HD23	1.90	0.52
1:U:265:SER:HA	1:U:269:MET:H	1.73	0.52
1:S:108:ALA:HB1	1:S:109:PRO:HD2	1.92	0.52
1:U:160:THR:HG21	1:U:274:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:73:HIC:HD2	1:T:73:HIC:O	2.10	0.52
1:Y:199:SER:HB2	1:Y:201:VAL:HB	1.91	0.52
1:O:201:VAL:CG1	1:O:202:THR:H	2.21	0.52
1:V:219:VAL:HG22	1:V:258:PRO:HB2	1.91	0.52
1:Z:35:VAL:HG12	1:Z:36:GLY:H	1.75	0.52
1:Y:132:MET:SD	1:Y:357:ILE:HD12	2.50	0.52
1:Q:208:ILE:HD12	1:Q:211:ASP:HB3	1.91	0.52
1:P:47:MET:SD	1:R:170:ALA:HB3	2.50	0.52
1:V:275:HIS:CG	1:V:276:GLU:H	2.28	0.52
1:P:53:TYR:HD1	1:P:65:LEU:HD11	1.75	0.52
1:X:198:TYR:N	1:X:198:TYR:CD2	2.78	0.51
1:Q:204:ALA:HB1	1:S:290:ARG:NH2	2.25	0.51
1:V:142:LEU:HD13	1:V:152:VAL:HG23	1.92	0.51
1:Y:76:ILE:H	1:Y:76:ILE:HD12	1.75	0.51
1:T:109:PRO:HG3	1:T:163:VAL:HG21	1.92	0.51
1:S:47:MET:SD	1:U:170:ALA:HB3	2.50	0.51
1:O:198:TYR:CD2	1:O:198:TYR:N	2.77	0.51
1:V:199:SER:OG	1:W:73:HIC:HD2	2.11	0.51
1:U:306:TYR:CE2	2:U:800:ADP:H2	2.28	0.51
1:Z:11:ASP:HB3	1:Z:18:LYS:HB2	1.91	0.51
1:Q:202:THR:HG23	1:Q:203:THR:N	2.23	0.51
1:W:198:TYR:HD2	1:W:198:TYR:N	2.06	0.51
1:Q:166:TYR:CE1	1:Q:289:ILE:HG22	2.46	0.51
1:Y:120:THR:HG23	1:Y:132:MET:SD	2.51	0.51
1:Y:217:CYS:HA	1:Y:254:ARG:HA	1.93	0.50
1:O:40:HIS:NE2	1:O:43:VAL:HG23	2.26	0.50
1:P:43:VAL:HG22	1:R:110:LEU:HD22	1.93	0.50
1:Z:201:VAL:HG13	1:Z:202:THR:H	1.75	0.50
1:V:203:THR:HG21	1:X:173:HIS:CE1	2.47	0.50
1:O:43:VAL:HG22	1:Q:110:LEU:CD1	2.41	0.50
1:T:20:GLY:HA2	1:T:94:LEU:HD21	1.93	0.50
1:W:40:HIS:CD2	1:W:43:VAL:H	2.29	0.50
1:Q:178:LEU:HD11	1:Q:180:LEU:HG	1.93	0.50
1:W:262:PHE:HA	1:W:274:ILE:HG22	1.94	0.49
1:Q:199:SER:OG	1:R:73:HIC:HD2	2.12	0.49
1:W:35:VAL:HG11	1:W:84:LYS:HD2	1.94	0.49
1:W:198:TYR:CD2	1:W:198:TYR:N	2.80	0.49
1:O:40:HIS:CD2	1:O:43:VAL:H	2.31	0.49
1:T:199:SER:OG	1:U:73:HIC:HD2	2.12	0.49
1:P:76:ILE:H	1:P:76:ILE:HD12	1.76	0.49
1:W:202:THR:HG23	1:W:203:THR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:282:ILE:HB	1:W:294:TYR:CE1	2.48	0.49
1:S:165:ILE:HG12	1:S:170:ALA:HB2	1.94	0.49
1:U:287:ILE:HA	1:U:290:ARG:HD2	1.94	0.49
1:V:64:ILE:HG22	1:X:172:PRO:HG3	1.93	0.49
1:Z:262:PHE:HA	1:Z:274:ILE:HG22	1.95	0.49
1:V:252:ASN:C	1:V:254:ARG:H	2.16	0.49
1:Z:217:CYS:HA	1:Z:254:ARG:HA	1.95	0.49
1:T:152:VAL:O	1:T:152:VAL:HG12	2.13	0.48
1:O:204:ALA:HB1	1:Q:290:ARG:NH2	2.27	0.48
1:U:193:LEU:CD2	1:U:196:ARG:HE	2.27	0.48
1:O:204:ALA:HB1	1:Q:290:ARG:CZ	2.44	0.48
1:W:208:ILE:HG12	1:W:242:LEU:HD22	1.94	0.48
1:W:321:ALA:HB1	1:W:322:PRO:HD2	1.93	0.48
1:P:201:VAL:HG13	1:P:202:THR:H	1.78	0.48
1:Y:193:LEU:HD21	1:Y:253:GLU:HG2	1.94	0.48
1:X:64:ILE:HG22	1:Z:172:PRO:HG3	1.95	0.48
1:Q:43:VAL:HG11	1:S:172:PRO:HA	1.96	0.48
1:Q:217:CYS:HA	1:Q:254:ARG:HA	1.95	0.48
1:U:260:THR:HG23	1:U:264:PRO:HA	1.95	0.48
1:S:217:CYS:HA	1:S:254:ARG:HA	1.95	0.48
1:X:40:HIS:CD2	1:X:43:VAL:H	2.31	0.48
1:V:282:ILE:HA	1:V:285:CYS:HB2	1.94	0.48
1:T:246:GLN:HA	1:T:246:GLN:HE21	1.78	0.48
1:P:217:CYS:HA	1:P:254:ARG:HA	1.96	0.47
1:U:191:LYS:HD2	1:V:175:ILE:HD13	1.95	0.47
1:T:40:HIS:CD2	1:T:43:VAL:H	2.32	0.47
1:O:199:SER:OG	1:P:73:HIC:HD2	2.14	0.47
1:S:201:VAL:HG13	1:S:202:THR:N	2.26	0.47
1:R:151:ILE:HG23	1:R:297:ASN:HA	1.96	0.47
1:Q:54:VAL:HG11	1:Q:88:HIS:CG	2.49	0.47
1:Q:208:ILE:HG12	1:Q:242:LEU:HD13	1.95	0.47
1:P:64:ILE:HG22	1:R:172:PRO:HG3	1.97	0.47
1:V:199:SER:OG	1:W:73:HIC:CD2	2.63	0.47
1:Z:202:THR:HG23	1:Z:203:THR:H	1.79	0.47
1:X:40:HIS:CG	1:X:41:GLN:H	2.32	0.47
1:O:237:GLU:HA	1:O:251:GLY:HA2	1.97	0.47
1:Q:43:VAL:HG22	1:S:110:LEU:CD2	2.45	0.46
1:W:193:LEU:HD11	1:W:253:GLU:HG2	1.96	0.46
1:Q:152:VAL:HG22	1:Q:298:VAL:HG23	1.95	0.46
1:S:109:PRO:CD	1:S:161:HIS:CD2	2.99	0.46
1:V:8:LEU:HB2	1:V:103:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:208:ILE:HD12	1:S:211:ASP:HB3	1.98	0.46
1:X:137:GLN:OE1	1:X:161:HIS:CE1	2.68	0.46
1:R:265:SER:HA	1:R:269:MET:H	1.80	0.46
1:O:199:SER:HB3	1:O:201:VAL:HB	1.97	0.46
1:X:202:THR:HG23	1:X:203:THR:N	2.29	0.46
1:V:109:PRO:HG3	1:V:163:VAL:HG21	1.97	0.46
1:R:43:VAL:HG11	1:T:172:PRO:HA	1.98	0.46
1:U:165:ILE:HG12	1:U:170:ALA:HB2	1.98	0.46
1:O:212:ILE:HG12	1:O:250:ILE:HD13	1.97	0.46
1:V:208:ILE:HD12	1:V:211:ASP:HB3	1.97	0.46
1:O:43:VAL:HG22	1:Q:110:LEU:HD22	1.97	0.46
1:T:298:VAL:O	1:T:299:MET:HG3	2.16	0.46
1:Z:151:ILE:CD1	1:Z:282:ILE:HD11	2.45	0.46
1:Y:202:THR:HG22	3:Y:801:PO4:O2	2.16	0.46
1:P:67:LEU:HD12	1:P:67:LEU:HA	1.72	0.46
1:P:203:THR:HG21	1:R:173:HIS:CE1	2.51	0.46
1:Q:161:HIS:HB3	1:Q:163:VAL:HG23	1.97	0.46
1:P:201:VAL:HG13	1:P:202:THR:HG22	1.97	0.45
1:R:202:THR:HG23	1:R:203:THR:H	1.80	0.45
1:X:185:LEU:HD21	1:X:261:LEU:CD2	2.46	0.45
1:W:27:PRO:HG2	1:W:30:VAL:HG11	1.98	0.45
1:P:208:ILE:HD12	1:P:211:ASP:HB3	1.98	0.45
1:Q:40:HIS:CD2	1:Q:43:VAL:HG23	2.52	0.45
1:Q:109:PRO:HG3	1:Q:163:VAL:HG21	1.98	0.45
1:V:39:ARG:HH22	1:W:263:GLN:HG2	1.81	0.45
1:Q:201:VAL:HG13	1:Q:202:THR:H	1.80	0.45
1:U:98:PRO:HB2	1:U:129:VAL:HG22	1.99	0.45
1:U:193:LEU:HD21	1:U:253:GLU:HG2	1.99	0.45
1:P:216:LEU:HG	1:P:250:ILE:HG21	1.98	0.45
1:S:219:VAL:HG21	1:S:309:ILE:HB	1.99	0.45
1:X:73:HIC:CD2	1:X:73:HIC:O	2.64	0.45
1:T:47:MET:CE	1:V:170:ALA:HB3	2.47	0.45
1:T:47:MET:HE3	1:V:170:ALA:HB3	1.99	0.45
1:X:275:HIS:H	1:X:275:HIS:CD2	2.34	0.45
1:Y:27:PRO:HA	1:Y:340:TRP:CH2	2.52	0.45
1:Q:199:SER:OG	1:R:73:HIC:CD2	2.65	0.45
1:T:73:HIC:CD2	1:T:73:HIC:O	2.65	0.45
1:W:35:VAL:HG11	1:W:84:LYS:CD	2.46	0.45
1:T:184:ASP:OD2	1:T:185:LEU:HD22	2.17	0.45
1:S:292:ASP:HA	1:S:295:ALA:HB3	1.99	0.45
1:P:153:LEU:HB2	1:P:299:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:208:ILE:O	1:W:212:ILE:HG22	2.17	0.44
1:R:212:ILE:HG12	1:R:250:ILE:HD13	1.99	0.44
1:V:26:ALA:HB1	1:V:27:PRO:HD2	1.98	0.44
1:Y:193:LEU:HD22	1:Y:196:ARG:HE	1.81	0.44
1:Z:151:ILE:HA	1:Z:164:PRO:HA	1.99	0.44
1:W:284:LYS:HD2	1:W:284:LYS:C	2.36	0.44
1:W:43:VAL:HG22	1:Y:110:LEU:HD22	1.99	0.44
1:V:193:LEU:HD23	1:V:196:ARG:HE	1.83	0.44
1:R:76:ILE:HD12	1:R:76:ILE:H	1.83	0.44
1:V:48:GLY:O	1:V:49:GLN:HB2	2.18	0.44
1:Q:172:PRO:HG2	1:Q:173:HIS:CE1	2.53	0.44
1:Y:201:VAL:HG13	1:Y:202:THR:N	2.32	0.44
1:U:164:PRO:HB3	1:U:293:LEU:HD22	1.99	0.44
1:U:199:SER:OG	1:V:73:HIC:HD2	2.18	0.44
1:T:203:THR:HG21	1:V:173:HIS:CE1	2.53	0.44
1:W:43:VAL:HG22	1:Y:110:LEU:HD13	1.98	0.44
1:W:35:VAL:HG21	1:W:84:LYS:HG3	2.00	0.44
1:X:102:PRO:HB2	1:X:356:TRP:CZ2	2.53	0.44
1:P:144:ALA:HB1	1:P:341:ILE:HG22	1.99	0.44
1:Q:133:TYR:CE1	1:Q:374:CYS:HA	2.52	0.44
1:X:176:MET:HG2	1:X:277:THR:HG23	2.00	0.44
1:O:204:ALA:HB2	1:Q:285:CYS:H	1.83	0.44
1:R:258:PRO:HB3	1:R:306:TYR:CE1	2.52	0.44
1:X:321:ALA:HB1	1:X:322:PRO:HD2	1.99	0.44
1:O:326:LYS:HD3	1:O:327:ILE:H	1.82	0.44
1:T:254:ARG:NH1	3:T:803:PO4:O3	2.51	0.43
1:O:150:GLY:HA2	1:O:296:ASN:HB3	2.00	0.43
1:U:184:ASP:OD2	1:U:185:LEU:HD22	2.18	0.43
1:R:165:ILE:HA	1:R:170:ALA:HA	2.00	0.43
1:P:129:VAL:HG11	1:P:132:MET:HB3	2.00	0.43
1:P:199:SER:OG	1:Q:73:HIC:HD2	2.19	0.43
1:W:184:ASP:O	1:W:188:TYR:HB3	2.18	0.43
1:P:142:LEU:HD13	1:P:152:VAL:HG23	2.00	0.43
1:P:178:LEU:HG	1:P:180:LEU:H	1.83	0.43
1:W:9:VAL:HG13	1:W:104:LEU:HD23	2.01	0.43
1:T:47:MET:SD	1:V:170:ALA:HB3	2.58	0.43
1:V:108:ALA:HB1	1:V:109:PRO:HD2	2.00	0.43
1:R:48:GLY:HA2	1:T:169:TYR:CD2	2.53	0.43
1:W:73:HIC:HD2	1:W:73:HIC:O	2.18	0.43
1:R:173:HIS:CD2	1:R:173:HIS:N	2.86	0.43
1:V:73:HIC:CD2	1:V:73:HIC:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:165:ILE:HG12	1:Y:170:ALA:HB2	2.00	0.43
1:U:73:HIC:O	1:U:73:HIC:HD2	2.19	0.43
1:Y:193:LEU:CD2	1:Y:196:ARG:HE	2.32	0.43
1:S:260:THR:HG21	1:S:267:ILE:HG13	1.99	0.43
1:T:49:GLN:HG3	1:V:375:PHE:CE2	2.54	0.43
1:S:269:MET:HB2	1:S:269:MET:HE2	1.98	0.43
1:S:73:HIC:O	1:S:73:HIC:CD2	2.67	0.43
1:Y:202:THR:HG22	3:Y:801:PO4:P	2.59	0.43
1:T:43:VAL:HG11	1:V:172:PRO:HA	2.01	0.43
1:W:124:PHE:CE1	1:W:359:LYS:HG2	2.53	0.43
1:Y:151:ILE:HG23	1:Y:297:ASN:HA	1.99	0.43
1:R:73:HIC:HD2	1:R:73:HIC:O	2.17	0.43
1:X:8:LEU:HB2	1:X:103:THR:HG23	2.00	0.43
1:U:223:PHE:CE2	1:U:266:PHE:CE2	3.07	0.43
1:Q:199:SER:HB3	1:Q:201:VAL:HB	2.00	0.43
1:Q:269:MET:HG3	1:Q:270:GLU:H	1.83	0.43
1:V:149:THR:HG23	1:V:166:TYR:HA	2.01	0.43
1:U:203:THR:HG21	1:W:173:HIS:CE1	2.54	0.43
1:X:48:GLY:HA2	1:Z:169:TYR:CD2	2.53	0.43
1:W:260:THR:HG23	1:W:264:PRO:HA	2.00	0.42
1:Y:253:GLU:O	1:Y:257:CYS:HB3	2.19	0.42
1:U:203:THR:HG22	1:U:203:THR:O	2.19	0.42
1:U:9:VAL:HG21	1:U:344:SER:HA	2.01	0.42
1:U:284:LYS:HD2	1:U:284:LYS:C	2.40	0.42
1:X:63:GLY:O	1:Z:173:HIS:CE1	2.72	0.42
1:X:259:GLU:HG3	1:X:266:PHE:CD1	2.55	0.42
1:X:73:HIC:HD2	1:X:73:HIC:O	2.19	0.42
1:T:300:SER:HA	1:T:335:ARG:HB2	2.00	0.42
1:X:76:ILE:HD12	1:X:76:ILE:H	1.84	0.42
1:Q:174:ALA:HB2	1:Q:284:LYS:O	2.19	0.42
1:W:153:LEU:HG	1:W:162:ASN:HD22	1.85	0.42
1:S:151:ILE:HG23	1:S:297:ASN:HA	2.02	0.42
1:R:17:VAL:HB	1:R:31:PHE:CD1	2.54	0.42
1:Q:252:ASN:HA	1:Q:255:PHE:CZ	2.54	0.42
1:U:292:ASP:HA	1:U:295:ALA:HB3	2.01	0.42
1:T:288:ASP:O	1:T:289:ILE:HG23	2.19	0.42
1:V:199:SER:CB	1:V:201:VAL:HB	2.50	0.42
1:Q:73:HIC:HD2	1:Q:73:HIC:O	2.20	0.42
1:Q:73:HIC:O	1:Q:73:HIC:CD2	2.68	0.42
1:S:9:VAL:HG21	1:S:344:SER:HA	2.01	0.42
1:R:189:LEU:HD11	1:R:253:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:VAL:HG12	1:O:36:GLY:N	2.34	0.42
1:Q:173:HIS:N	1:Q:173:HIS:CD2	2.87	0.42
1:T:165:ILE:HA	1:T:170:ALA:HA	2.02	0.42
1:U:199:SER:CB	1:U:201:VAL:HB	2.50	0.42
1:R:49:GLN:HG2	1:T:375:PHE:CE2	2.55	0.42
1:R:260:THR:HG22	1:R:264:PRO:HA	2.02	0.42
1:V:202:THR:HG23	1:V:203:THR:N	2.30	0.41
1:Y:202:THR:CG2	1:Y:203:THR:N	2.81	0.41
1:T:171:LEU:HA	1:T:172:PRO:HD3	1.95	0.41
1:Q:284:LYS:C	1:Q:284:LYS:HD2	2.40	0.41
1:Y:259:GLU:HG3	1:Y:266:PHE:CD1	2.55	0.41
1:P:203:THR:HA	1:Q:269:MET:SD	2.61	0.41
1:Z:165:ILE:HA	1:Z:170:ALA:HA	2.01	0.41
1:Q:191:LYS:HD2	1:R:175:ILE:HG21	2.02	0.41
1:T:201:VAL:HG13	1:T:202:THR:H	1.85	0.41
1:T:139:VAL:HG22	1:T:165:ILE:CD1	2.50	0.41
1:X:199:SER:OG	1:Y:73:HIC:CD2	2.68	0.41
1:T:178:LEU:HG	1:T:180:LEU:H	1.85	0.41
1:Y:155:SER:HB3	1:Y:304:THR:HG23	2.02	0.41
1:Q:292:ASP:HA	1:Q:295:ALA:HB3	2.02	0.41
1:Q:197:GLY:C	1:Q:198:TYR:CD2	2.94	0.41
1:O:73:HIC:CD2	1:O:73:HIC:O	2.68	0.41
1:R:111:ASN:HB3	1:R:116:ARG:HG3	2.03	0.41
1:O:214:GLU:HG3	2:O:800:ADP:C6	2.56	0.41
1:Z:185:LEU:CD2	1:Z:185:LEU:H	2.34	0.41
1:S:109:PRO:HD3	1:S:161:HIS:CD2	2.55	0.41
1:Z:151:ILE:HG12	1:Z:151:ILE:O	2.20	0.41
1:U:163:VAL:HA	1:U:164:PRO:HD2	1.86	0.41
1:W:201:VAL:HG13	1:W:202:THR:N	2.27	0.41
1:Q:185:LEU:HD11	1:Q:261:LEU:CD2	2.51	0.41
1:V:142:LEU:HD22	1:V:165:ILE:HD12	2.01	0.41
1:Z:291:LYS:HB2	1:Z:292:ASP:H	1.64	0.41
1:X:193:LEU:HD21	1:X:253:GLU:HG2	2.02	0.41
1:U:197:GLY:C	1:U:198:TYR:CD2	2.94	0.41
1:P:76:ILE:CD1	1:P:76:ILE:H	2.33	0.41
1:Q:291:LYS:HB2	1:Q:292:ASP:H	1.67	0.41
1:T:155:SER:HB3	1:T:304:THR:HG23	2.03	0.41
1:R:199:SER:HB3	1:R:201:VAL:CG2	2.51	0.41
1:S:172:PRO:HG2	1:S:173:HIS:CG	2.56	0.41
1:V:171:LEU:HG	1:V:285:CYS:SG	2.61	0.41
1:X:43:VAL:HG22	1:Z:110:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:256:ARG:HA	1:T:259:GLU:HB3	2.01	0.41
1:P:302:GLY:HA2	1:P:336:LYS:HG3	2.02	0.41
1:S:119:MET:HA	1:S:122:ILE:HG22	2.03	0.41
1:V:43:VAL:HG11	1:X:172:PRO:HA	2.03	0.41
1:T:165:ILE:HG12	1:T:170:ALA:HB2	2.03	0.41
1:T:161:HIS:HB3	1:T:163:VAL:HG23	2.01	0.41
1:Z:306:TYR:HA	1:Z:307:PRO:HD2	1.97	0.41
1:V:176:MET:HG3	1:V:277:THR:HG21	2.03	0.41
1:X:140:LEU:HD22	1:X:346:LEU:HD22	2.03	0.41
1:S:150:GLY:HA2	1:S:296:ASN:HB3	2.03	0.41
1:O:37:ARG:HH11	1:O:37:ARG:HG3	1.86	0.41
1:O:258:PRO:HB3	1:O:306:TYR:CE1	2.56	0.41
1:Y:265:SER:HA	1:Y:269:MET:H	1.86	0.41
1:W:199:SER:OG	1:X:73:HIC:HD2	2.21	0.40
1:S:64:ILE:HG22	1:U:172:PRO:HG3	2.02	0.40
1:R:201:VAL:CG1	1:R:202:THR:HG22	2.47	0.40
1:Q:43:VAL:CG1	1:S:172:PRO:HA	2.51	0.40
1:V:73:HIC:O	1:V:73:HIC:HD2	2.21	0.40
1:U:138:ALA:HB1	1:U:165:ILE:HD11	2.02	0.40
1:W:70:PRO:HG3	1:W:85:ILE:HD12	2.02	0.40
1:T:62:ARG:HH21	1:U:270:GLU:HG3	1.87	0.40
1:W:292:ASP:HA	1:W:295:ALA:HB3	2.02	0.40
1:V:205:GLU:HG3	1:X:290:ARG:HH22	1.86	0.40
1:S:260:THR:HG23	1:S:264:PRO:HA	2.02	0.40
1:W:313:MET:HB2	1:W:329:ILE:HG21	2.04	0.40
1:Q:142:LEU:HD22	1:Q:165:ILE:HD12	2.03	0.40
1:X:224:GLU:HA	1:X:227:MET:HB2	2.04	0.40
1:W:275:HIS:CD2	1:W:276:GLU:H	2.38	0.40
1:Z:302:GLY:HA2	1:Z:336:LYS:HG3	2.04	0.40
1:R:199:SER:OG	1:S:73:HIC:CD2	2.70	0.40
1:P:254:ARG:NH1	3:P:803:PO4:O2	2.51	0.40
1:S:180:LEU:HD11	1:S:264:PRO:HG3	2.03	0.40
1:P:105:LEU:HA	1:P:105:LEU:HD23	1.97	0.40
1:Y:326:LYS:HD3	1:Y:327:ILE:H	1.85	0.40
1:W:102:PRO:HB2	1:W:356:TRP:CZ2	2.57	0.40
1:S:35:VAL:HG13	1:S:54:VAL:HG22	2.04	0.40
1:P:152:VAL:HG22	1:P:298:VAL:HG23	2.04	0.40
1:V:98:PRO:HB2	1:V:129:VAL:HG22	2.03	0.40
1:V:242:LEU:HB3	1:V:243:PRO:HD2	2.03	0.40
1:W:240:TYR:CG	1:W:241:GLU:N	2.89	0.40
1:S:14:SER:HA	1:S:71:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	373/376 (99%)	283 (76%)	66 (18%)	24 (6%)	2	25
1	P	373/376 (99%)	298 (80%)	54 (14%)	21 (6%)	2	28
1	Q	373/376 (99%)	281 (75%)	66 (18%)	26 (7%)	1	22
1	R	373/376 (99%)	295 (79%)	52 (14%)	26 (7%)	1	22
1	S	373/376 (99%)	286 (77%)	67 (18%)	20 (5%)	2	29
1	T	373/376 (99%)	275 (74%)	73 (20%)	25 (7%)	1	23
1	U	373/376 (99%)	284 (76%)	66 (18%)	23 (6%)	2	25
1	V	373/376 (99%)	293 (79%)	56 (15%)	24 (6%)	2	25
1	W	373/376 (99%)	288 (77%)	60 (16%)	25 (7%)	1	23
1	X	373/376 (99%)	292 (78%)	63 (17%)	18 (5%)	3	31
1	Y	373/376 (99%)	292 (78%)	64 (17%)	17 (5%)	3	32
1	Z	373/376 (99%)	289 (78%)	59 (16%)	25 (7%)	1	23
All	All	4476/4512 (99%)	3456 (77%)	746 (17%)	274 (6%)	4	25

All (274) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	42	GLY
1	O	51	ASP
1	O	129	VAL
1	O	254	ARG
1	P	42	GLY
1	P	55	GLY
1	P	129	VAL
1	P	185	LEU
1	Q	6	THR

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Mol	Chain	Res	Type
1	Q	49	GLN
1	Q	51	ASP
1	Q	52	SER
1	Q	70	PRO
1	Q	129	VAL
1	Q	185	LEU
1	Q	254	ARG
1	Q	271	SER
1	Q	272	ALA
1	Q	291	LYS
1	R	51	ASP
1	R	60	SER
1	R	125	GLU
1	R	167	GLU
1	R	291	LYS
1	S	49	GLN
1	S	51	ASP
1	S	55	GLY
1	S	125	GLU
1	S	129	VAL
1	S	291	LYS
1	S	335	ARG
1	T	42	GLY
1	T	51	ASP
1	T	52	SER
1	T	70	PRO
1	T	214	GLU
1	U	55	GLY
1	U	129	VAL
1	U	203	THR
1	U	254	ARG
1	U	287	ILE
1	V	6	THR
1	V	49	GLN
1	V	52	SER
1	V	60	SER
1	V	113	LYS
1	V	125	GLU
1	V	129	VAL
1	W	49	GLN
1	W	51	ASP
1	W	202	THR

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Mol	Chain	Res	Type
1	W	291	LYS
1	W	350	SER
1	X	49	GLN
1	X	51	ASP
1	X	52	SER
1	X	129	VAL
1	X	272	ALA
1	Y	42	GLY
1	Y	70	PRO
1	Y	125	GLU
1	Y	203	THR
1	Z	6	THR
1	Z	51	ASP
1	Z	70	PRO
1	Z	129	VAL
1	Z	291	LYS
1	Z	297	ASN
1	O	55	GLY
1	O	125	GLU
1	O	185	LEU
1	O	199	SER
1	O	247	VAL
1	O	268	GLY
1	O	271	SER
1	P	5	THR
1	P	45	VAL
1	P	49	GLN
1	P	125	GLU
1	P	251	GLY
1	Q	42	GLY
1	R	42	GLY
1	R	49	GLN
1	R	55	GLY
1	R	95	ARG
1	R	185	LEU
1	S	42	GLY
1	S	173	HIS
1	S	185	LEU
1	S	251	GLY
1	S	268	GLY
1	T	55	GLY
1	T	56	ASP

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Mol	Chain	Res	Type
1	T	125	GLU
1	T	272	ALA
1	U	42	GLY
1	U	51	ASP
1	U	56	ASP
1	U	70	PRO
1	U	95	ARG
1	U	125	GLU
1	U	251	GLY
1	U	279	TYR
1	V	42	GLY
1	V	51	ASP
1	V	55	GLY
1	V	173	HIS
1	V	268	GLY
1	V	291	LYS
1	W	55	GLY
1	W	125	GLU
1	W	185	LEU
1	W	199	SER
1	W	335	ARG
1	X	42	GLY
1	X	55	GLY
1	X	70	PRO
1	X	251	GLY
1	Y	51	ASP
1	Y	55	GLY
1	Y	185	LEU
1	Y	201	VAL
1	Y	251	GLY
1	Y	268	GLY
1	Y	291	LYS
1	Z	49	GLN
1	Z	52	SER
1	Z	55	GLY
1	Z	125	GLU
1	Z	174	ALA
1	Z	201	VAL
1	Z	272	ALA
1	O	5	THR
1	O	56	ASP
1	O	62	ARG

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Mol	Chain	Res	Type
1	O	70	PRO
1	P	70	PRO
1	P	209	VAL
1	P	271	SER
1	Q	125	GLU
1	Q	181	ALA
1	Q	268	GLY
1	R	70	PRO
1	R	129	VAL
1	R	181	ALA
1	R	199	SER
1	R	251	GLY
1	R	271	SER
1	S	60	SER
1	S	181	ALA
1	S	271	SER
1	T	95	ARG
1	T	199	SER
1	T	213	LYS
1	T	347	ALA
1	U	173	HIS
1	U	206	ARG
1	V	70	PRO
1	W	48	GLY
1	W	60	SER
1	W	128	ASN
1	W	129	VAL
1	W	254	ARG
1	W	271	SER
1	X	125	GLU
1	X	128	ASN
1	X	199	SER
1	Y	48	GLY
1	Y	129	VAL
1	Z	42	GLY
1	Z	306	TYR
1	O	6	THR
1	O	351	THR
1	P	6	THR
1	P	174	ALA
1	P	181	ALA
1	Q	41	GLN

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Mol	Chain	Res	Type
1	Q	138	ALA
1	Q	206	ARG
1	Q	335	ARG
1	S	62	ARG
1	S	70	PRO
1	T	129	VAL
1	T	153	LEU
1	T	185	LEU
1	T	315	LYS
1	T	372	ARG
1	U	181	ALA
1	U	348	SER
1	V	185	LEU
1	V	230	ALA
1	V	271	SER
1	W	42	GLY
1	W	236	LEU
1	X	60	SER
1	X	185	LEU
1	X	268	GLY
1	Y	56	ASP
1	Y	254	ARG
1	Z	110	LEU
1	Z	112	PRO
1	Z	173	HIS
1	Z	181	ALA
1	Z	185	LEU
1	O	49	GLN
1	O	110	LEU
1	O	201	VAL
1	O	306	TYR
1	P	113	LYS
1	P	155	SER
1	P	291	LYS
1	P	335	ARG
1	Q	5	THR
1	Q	56	ASP
1	Q	62	ARG
1	Q	332	PRO
1	R	56	ASP
1	R	110	LEU
1	R	254	ARG

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Mol	Chain	Res	Type
1	T	110	LEU
1	T	298	VAL
1	U	197	GLY
1	U	268	GLY
1	U	271	SER
1	U	272	ALA
1	V	110	LEU
1	V	181	ALA
1	V	251	GLY
1	V	335	ARG
1	W	110	LEU
1	X	110	LEU
1	X	242	LEU
1	Y	350	SER
1	Z	315	LYS
1	Z	335	ARG
1	P	223	PHE
1	Q	197	GLY
1	Q	207	GLU
1	R	155	SER
1	R	197	GLY
1	R	272	ALA
1	T	197	GLY
1	T	268	GLY
1	T	289	ILE
1	W	7	ALA
1	Y	110	LEU
1	O	45	VAL
1	R	247	VAL
1	R	268	GLY
1	U	46	GLY
1	V	63	GLY
1	V	158	GLY
1	W	98	PRO
1	W	251	GLY
1	X	98	PRO
1	Z	172	PRO
1	O	48	GLY
1	O	331	ALA
1	R	332	PRO
1	W	70	PRO
1	W	268	GLY

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Mol	Chain	Res	Type
1	W	306	TYR
1	V	247	VAL
1	Z	251	GLY
1	P	242	LEU
1	Q	341	ILE
1	R	182	GLY
1	S	197	GLY
1	Z	197	GLY
1	S	201	VAL
1	S	243	PRO
1	T	45	VAL
1	T	109	PRO
1	U	48	GLY

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 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	317/317 (100%)	272 (86%)	45 (14%)	4	26
1	P	317/317 (100%)	269 (85%)	48 (15%)	3	23
1	Q	317/317 (100%)	269 (85%)	48 (15%)	3	23
1	R	317/317 (100%)	275 (87%)	42 (13%)	5	28
1	S	317/317 (100%)	265 (84%)	52 (16%)	3	20
1	T	317/317 (100%)	275 (87%)	42 (13%)	5	28
1	U	317/317 (100%)	265 (84%)	52 (16%)	3	20
1	V	317/317 (100%)	269 (85%)	48 (15%)	3	23
1	W	317/317 (100%)	279 (88%)	38 (12%)	6	31
1	X	317/317 (100%)	266 (84%)	51 (16%)	3	20
1	Y	317/317 (100%)	276 (87%)	41 (13%)	5	29
1	Z	317/317 (100%)	259 (82%)	58 (18%)	2	15
All	All	3804/3804 (100%)	3239 (85%)	565 (15%)	7	24

All (565) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	1	ASP
1	O	14	SER
1	O	17	VAL
1	O	24	ASP
1	O	25	ASP
1	O	28	ARG
1	O	30	VAL
1	O	37	ARG
1	O	49	GLN
1	O	57	GLU
1	O	83	GLU
1	O	95	ARG
1	O	111	ASN
1	O	115	ASN
1	O	116	ARG
1	O	118	LYS
1	O	122	ILE
1	O	140	LEU
1	O	143	TYR
1	O	145	SER
1	O	157	ASP
1	O	171	LEU
1	O	173	HIS
1	O	179	ASP
1	O	184	ASP
1	O	188	TYR
1	O	190	MET
1	O	191	LYS
1	O	195	GLU
1	O	198	TYR
1	O	206	ARG
1	O	212	ILE
1	O	229	THR
1	O	234	SER
1	O	244	ASP
1	O	248	ILE
1	O	255	PHE
1	O	275	HIS
1	O	283	MET
1	O	284	LYS
1	O	334	GLU
1	O	344	SER

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Mol	Chain	Res	Type
1	O	354	GLN
1	O	359	LYS
1	O	373	LYS
1	P	25	ASP
1	P	28	ARG
1	P	30	VAL
1	P	31	PHE
1	P	33	SER
1	P	37	ARG
1	P	49	GLN
1	P	57	GLU
1	P	59	GLN
1	P	61	LYS
1	P	64	ILE
1	P	83	GLU
1	P	89	THR
1	P	95	ARG
1	P	111	ASN
1	P	115	ASN
1	P	116	ARG
1	P	118	LYS
1	P	122	ILE
1	P	140	LEU
1	P	145	SER
1	P	159	VAL
1	P	173	HIS
1	P	179	ASP
1	P	184	ASP
1	P	188	TYR
1	P	190	MET
1	P	191	LYS
1	P	195	GLU
1	P	198	TYR
1	P	206	ARG
1	P	224	GLU
1	P	244	ASP
1	P	246	GLN
1	P	248	ILE
1	P	252	ASN
1	P	255	PHE
1	P	270	GLU
1	P	275	HIS

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Mol	Chain	Res	Type
1	P	276	GLU
1	P	283	MET
1	P	289	ILE
1	P	305	MET
1	P	326	LYS
1	P	327	ILE
1	P	336	LYS
1	P	352	PHE
1	P	354	GLN
1	Q	1	ASP
1	Q	2	GLU
1	Q	14	SER
1	Q	24	ASP
1	Q	25	ASP
1	Q	28	ARG
1	Q	30	VAL
1	Q	31	PHE
1	Q	37	ARG
1	Q	40	HIS
1	Q	43	VAL
1	Q	49	GLN
1	Q	70	PRO
1	Q	83	GLU
1	Q	89	THR
1	Q	95	ARG
1	Q	115	ASN
1	Q	116	ARG
1	Q	118	LYS
1	Q	120	THR
1	Q	139	VAL
1	Q	155	SER
1	Q	157	ASP
1	Q	159	VAL
1	Q	173	HIS
1	Q	184	ASP
1	Q	186	THR
1	Q	188	TYR
1	Q	190	MET
1	Q	191	LYS
1	Q	195	GLU
1	Q	198	TYR
1	Q	205	GLU

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Mol	Chain	Res	Type
1	Q	221	LEU
1	Q	244	ASP
1	Q	248	ILE
1	Q	252	ASN
1	Q	255	PHE
1	Q	270	GLU
1	Q	275	HIS
1	Q	283	MET
1	Q	284	LYS
1	Q	289	ILE
1	Q	305	MET
1	Q	326	LYS
1	Q	352	PHE
1	Q	354	GLN
1	Q	373	LYS
1	R	24	ASP
1	R	28	ARG
1	R	30	VAL
1	R	31	PHE
1	R	34	ILE
1	R	37	ARG
1	R	40	HIS
1	R	41	GLN
1	R	49	GLN
1	R	64	ILE
1	R	92	ASN
1	R	95	ARG
1	R	111	ASN
1	R	116	ARG
1	R	118	LYS
1	R	119	MET
1	R	122	ILE
1	R	143	TYR
1	R	145	SER
1	R	173	HIS
1	R	184	ASP
1	R	188	TYR
1	R	190	MET
1	R	191	LYS
1	R	195	GLU
1	R	198	TYR
1	R	201	VAL

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Mol	Chain	Res	Type
1	R	203	THR
1	R	224	GLU
1	R	229	THR
1	R	244	ASP
1	R	248	ILE
1	R	252	ASN
1	R	260	THR
1	R	270	GLU
1	R	283	MET
1	R	284	LYS
1	R	285	CYS
1	R	305	MET
1	R	326	LYS
1	R	334	GLU
1	R	354	GLN
1	S	18	LYS
1	S	24	ASP
1	S	25	ASP
1	S	28	ARG
1	S	30	VAL
1	S	31	PHE
1	S	34	ILE
1	S	37	ARG
1	S	38	PRO
1	S	40	HIS
1	S	49	GLN
1	S	59	GLN
1	S	64	ILE
1	S	67	LEU
1	S	92	ASN
1	S	95	ARG
1	S	116	ARG
1	S	118	LYS
1	S	119	MET
1	S	132	MET
1	S	145	SER
1	S	151	ILE
1	S	171	LEU
1	S	173	HIS
1	S	179	ASP
1	S	184	ASP
1	S	188	TYR

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Mol	Chain	Res	Type
1	S	190	MET
1	S	191	LYS
1	S	195	GLU
1	S	198	TYR
1	S	203	THR
1	S	205	GLU
1	S	221	LEU
1	S	244	ASP
1	S	248	ILE
1	S	252	ASN
1	S	275	HIS
1	S	283	MET
1	S	284	LYS
1	S	287	ILE
1	S	288	ASP
1	S	305	MET
1	S	323	SER
1	S	326	LYS
1	S	336	LYS
1	S	352	PHE
1	S	354	GLN
1	S	369	ILE
1	S	372	ARG
1	S	373	LYS
1	S	375	PHE
1	T	1	ASP
1	T	5	THR
1	T	24	ASP
1	T	25	ASP
1	T	28	ARG
1	T	30	VAL
1	T	37	ARG
1	T	49	GLN
1	T	57	GLU
1	T	67	LEU
1	T	70	PRO
1	T	83	GLU
1	T	85	ILE
1	T	95	ARG
1	T	111	ASN
1	T	115	ASN
1	T	116	ARG

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Mol	Chain	Res	Type
1	T	118	LYS
1	T	122	ILE
1	T	153	LEU
1	T	173	HIS
1	T	184	ASP
1	T	188	TYR
1	T	190	MET
1	T	191	LYS
1	T	195	GLU
1	T	198	TYR
1	T	212	ILE
1	T	244	ASP
1	T	246	GLN
1	T	248	ILE
1	T	275	HIS
1	T	283	MET
1	T	284	LYS
1	T	292	ASP
1	T	305	MET
1	T	338	SER
1	T	344	SER
1	T	346	LEU
1	T	354	GLN
1	T	370	VAL
1	T	373	LYS
1	U	2	GLU
1	U	3	ASP
1	U	25	ASP
1	U	28	ARG
1	U	30	VAL
1	U	31	PHE
1	U	34	ILE
1	U	37	ARG
1	U	43	VAL
1	U	49	GLN
1	U	83	GLU
1	U	85	ILE
1	U	95	ARG
1	U	111	ASN
1	U	116	ARG
1	U	118	LYS
1	U	122	ILE

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Mol	Chain	Res	Type
1	U	123	MET
1	U	140	LEU
1	U	151	ILE
1	U	159	VAL
1	U	171	LEU
1	U	173	HIS
1	U	183	ARG
1	U	184	ASP
1	U	188	TYR
1	U	190	MET
1	U	191	LYS
1	U	195	GLU
1	U	198	TYR
1	U	203	THR
1	U	205	GLU
1	U	234	SER
1	U	248	ILE
1	U	252	ASN
1	U	255	PHE
1	U	270	GLU
1	U	275	HIS
1	U	283	MET
1	U	284	LYS
1	U	288	ASP
1	U	291	LYS
1	U	292	ASP
1	U	300	SER
1	U	305	MET
1	U	325	MET
1	U	334	GLU
1	U	336	LYS
1	U	352	PHE
1	U	354	GLN
1	U	356	TRP
1	U	373	LYS
1	V	1	ASP
1	V	4	GLU
1	V	5	THR
1	V	24	ASP
1	V	25	ASP
1	V	28	ARG
1	V	30	VAL

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Mol	Chain	Res	Type
1	V	31	PHE
1	V	37	ARG
1	V	40	HIS
1	V	43	VAL
1	V	49	GLN
1	V	57	GLU
1	V	64	ILE
1	V	67	LEU
1	V	83	GLU
1	V	95	ARG
1	V	111	ASN
1	V	116	ARG
1	V	118	LYS
1	V	132	MET
1	V	140	LEU
1	V	173	HIS
1	V	184	ASP
1	V	188	TYR
1	V	190	MET
1	V	191	LYS
1	V	195	GLU
1	V	206	ARG
1	V	212	ILE
1	V	244	ASP
1	V	248	ILE
1	V	252	ASN
1	V	257	CYS
1	V	270	GLU
1	V	275	HIS
1	V	283	MET
1	V	284	LYS
1	V	305	MET
1	V	318	THR
1	V	325	MET
1	V	338	SER
1	V	349	LEU
1	V	352	PHE
1	V	354	GLN
1	V	356	TRP
1	V	373	LYS
1	V	375	PHE
1	W	24	ASP

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Mol	Chain	Res	Type
1	W	25	ASP
1	W	28	ARG
1	W	31	PHE
1	W	37	ARG
1	W	40	HIS
1	W	49	GLN
1	W	85	ILE
1	W	95	ARG
1	W	115	ASN
1	W	116	ARG
1	W	122	ILE
1	W	132	MET
1	W	140	LEU
1	W	143	TYR
1	W	151	ILE
1	W	173	HIS
1	W	179	ASP
1	W	184	ASP
1	W	185	LEU
1	W	188	TYR
1	W	190	MET
1	W	195	GLU
1	W	201	VAL
1	W	205	GLU
1	W	219	VAL
1	W	248	ILE
1	W	252	ASN
1	W	275	HIS
1	W	283	MET
1	W	284	LYS
1	W	305	MET
1	W	318	THR
1	W	326	LYS
1	W	348	SER
1	W	354	GLN
1	W	361	GLU
1	W	373	LYS
1	X	5	THR
1	X	25	ASP
1	X	30	VAL
1	X	34	ILE
1	X	37	ARG

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Mol	Chain	Res	Type
1	X	40	HIS
1	X	49	GLN
1	X	95	ARG
1	X	116	ARG
1	X	118	LYS
1	X	122	ILE
1	X	129	VAL
1	X	134	VAL
1	X	140	LEU
1	X	153	LEU
1	X	165	ILE
1	X	166	TYR
1	X	171	LEU
1	X	173	HIS
1	X	184	ASP
1	X	188	TYR
1	X	190	MET
1	X	191	LYS
1	X	195	GLU
1	X	205	GLU
1	X	206	ARG
1	X	216	LEU
1	X	224	GLU
1	X	229	THR
1	X	246	GLN
1	X	248	ILE
1	X	255	PHE
1	X	270	GLU
1	X	274	ILE
1	X	275	HIS
1	X	281	SER
1	X	283	MET
1	X	284	LYS
1	X	287	ILE
1	X	288	ASP
1	X	289	ILE
1	X	291	LYS
1	X	305	MET
1	X	326	LYS
1	X	329	ILE
1	X	334	GLU
1	X	335	ARG

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Mol	Chain	Res	Type
1	X	338	SER
1	X	344	SER
1	X	352	PHE
1	X	354	GLN
1	Y	1	ASP
1	Y	16	LEU
1	Y	28	ARG
1	Y	30	VAL
1	Y	34	ILE
1	Y	37	ARG
1	Y	49	GLN
1	Y	70	PRO
1	Y	82	MET
1	Y	95	ARG
1	Y	116	ARG
1	Y	117	GLU
1	Y	118	LYS
1	Y	122	ILE
1	Y	140	LEU
1	Y	173	HIS
1	Y	184	ASP
1	Y	188	TYR
1	Y	190	MET
1	Y	191	LYS
1	Y	195	GLU
1	Y	198	TYR
1	Y	202	THR
1	Y	203	THR
1	Y	221	LEU
1	Y	227	MET
1	Y	248	ILE
1	Y	252	ASN
1	Y	275	HIS
1	Y	278	THR
1	Y	283	MET
1	Y	284	LYS
1	Y	289	ILE
1	Y	305	MET
1	Y	338	SER
1	Y	344	SER
1	Y	352	PHE
1	Y	354	GLN

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Mol	Chain	Res	Type
1	Y	369	ILE
1	Y	373	LYS
1	Y	375	PHE
1	Z	24	ASP
1	Z	25	ASP
1	Z	28	ARG
1	Z	30	VAL
1	Z	31	PHE
1	Z	37	ARG
1	Z	40	HIS
1	Z	49	GLN
1	Z	64	ILE
1	Z	67	LEU
1	Z	81	ASP
1	Z	82	MET
1	Z	83	GLU
1	Z	85	ILE
1	Z	95	ARG
1	Z	115	ASN
1	Z	116	ARG
1	Z	118	LYS
1	Z	122	ILE
1	Z	140	LEU
1	Z	151	ILE
1	Z	159	VAL
1	Z	162	ASN
1	Z	173	HIS
1	Z	179	ASP
1	Z	183	ARG
1	Z	184	ASP
1	Z	188	TYR
1	Z	189	LEU
1	Z	190	MET
1	Z	191	LYS
1	Z	195	GLU
1	Z	198	TYR
1	Z	205	GLU
1	Z	206	ARG
1	Z	207	GLU
1	Z	208	ILE
1	Z	211	ASP
1	Z	221	LEU

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Mol	Chain	Res	Type
1	Z	222	ASP
1	Z	244	ASP
1	Z	246	GLN
1	Z	248	ILE
1	Z	252	ASN
1	Z	257	CYS
1	Z	260	THR
1	Z	270	GLU
1	Z	275	HIS
1	Z	282	ILE
1	Z	283	MET
1	Z	288	ASP
1	Z	305	MET
1	Z	313	MET
1	Z	323	SER
1	Z	334	GLU
1	Z	352	PHE
1	Z	354	GLN
1	Z	375	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	246	GLN
1	O	275	HIS
1	P	92	ASN
1	P	246	GLN
1	P	275	HIS
1	Q	49	GLN
1	Q	162	ASN
1	Q	275	HIS
1	S	40	HIS
1	S	246	GLN
1	T	246	GLN
1	U	162	ASN
1	V	101	HIS
1	V	162	ASN
1	V	173	HIS
1	V	275	HIS
1	W	87	HIS
1	W	111	ASN
1	W	173	HIS

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Mol	Chain	Res	Type
1	W	275	HIS
1	X	88	HIS
1	X	121	GLN
1	X	161	HIS
1	X	275	HIS
1	Y	92	ASN
1	Y	111	ASN
1	Y	162	ASN
1	Y	275	HIS
1	Z	111	ASN
1	Z	246	GLN
1	Z	252	ASN
1	Z	275	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	HIC	O	73	1	6,11,12	1.68	1 (16%)	6,14,16	0.59	0
1	HIC	P	73	1	6,11,12	2.86	1 (16%)	6,14,16	2.29	2 (33%)
1	HIC	Q	73	1	6,11,12	2.95	1 (16%)	6,14,16	2.32	3 (50%)
1	HIC	R	73	1	6,11,12	2.98	1 (16%)	6,14,16	2.51	3 (50%)
1	HIC	S	73	1	6,11,12	3.38	1 (16%)	6,14,16	2.77	2 (33%)
1	HIC	T	73	1	6,11,12	2.79	1 (16%)	6,14,16	1.98	2 (33%)
1	HIC	U	73	1	6,11,12	2.91	1 (16%)	6,14,16	1.45	1 (16%)
1	HIC	V	73	1	6,11,12	3.17	1 (16%)	6,14,16	2.29	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	W	73	1	6,11,12	3.28	1 (16%)	6,14,16	3.44	2 (33%)
1	HIC	X	73	1	6,11,12	3.27	1 (16%)	6,14,16	1.74	2 (33%)
1	HIC	Y	73	1	6,11,12	3.10	1 (16%)	6,14,16	2.52	2 (33%)
1	HIC	Z	73	1	6,11,12	3.32	1 (16%)	6,14,16	3.18	2 (33%)

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
1	HIC	O	73	1	-	0/4/6/8	0/1/1/1
1	HIC	P	73	1	-	0/4/6/8	0/1/1/1
1	HIC	Q	73	1	-	0/4/6/8	0/1/1/1
1	HIC	R	73	1	-	0/4/6/8	0/1/1/1
1	HIC	S	73	1	-	0/4/6/8	0/1/1/1
1	HIC	T	73	1	-	0/4/6/8	0/1/1/1
1	HIC	U	73	1	-	0/4/6/8	0/1/1/1
1	HIC	V	73	1	-	0/4/6/8	0/1/1/1
1	HIC	W	73	1	-	0/4/6/8	0/1/1/1
1	HIC	X	73	1	-	0/4/6/8	0/1/1/1
1	HIC	Y	73	1	-	0/4/6/8	0/1/1/1
1	HIC	Z	73	1	-	0/4/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	73	HIC	CZ-NE2	-7.97	1.26	1.48
1	Z	73	HIC	CZ-NE2	-7.96	1.27	1.48
1	W	73	HIC	CZ-NE2	-7.89	1.27	1.48
1	X	73	HIC	CZ-NE2	-7.81	1.27	1.48
1	V	73	HIC	CZ-NE2	-7.65	1.27	1.48
1	Y	73	HIC	CZ-NE2	-7.47	1.28	1.48
1	R	73	HIC	CZ-NE2	-7.21	1.29	1.48
1	Q	73	HIC	CZ-NE2	-7.15	1.29	1.48
1	P	73	HIC	CZ-NE2	-6.90	1.29	1.48
1	U	73	HIC	CZ-NE2	-6.89	1.29	1.48
1	T	73	HIC	CZ-NE2	-6.64	1.30	1.48
1	O	73	HIC	CZ-NE2	-3.96	1.37	1.48

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	73	HIC	CZ-NE2-CE1	-4.63	100.52	125.34
1	Z	73	HIC	CZ-NE2-CE1	-4.39	101.79	125.34
1	S	73	HIC	CZ-NE2-CE1	-3.81	104.92	125.34
1	Y	73	HIC	CZ-NE2-CE1	-3.40	107.13	125.34
1	R	73	HIC	CZ-NE2-CE1	-3.34	107.45	125.34
1	V	73	HIC	CZ-NE2-CE1	-3.18	108.28	125.34
1	Q	73	HIC	CZ-NE2-CE1	-3.09	108.80	125.34
1	P	73	HIC	CZ-NE2-CE1	-3.05	109.01	125.34
1	T	73	HIC	CZ-NE2-CE1	-2.73	110.68	125.34
1	X	73	HIC	CZ-NE2-CE1	-2.35	112.76	125.34
1	R	73	HIC	O-C-CA	-2.17	119.89	125.72
1	Q	73	HIC	O-C-CA	-2.14	119.98	125.72
1	U	73	HIC	CZ-NE2-CD2	2.52	135.88	126.35
1	X	73	HIC	CZ-NE2-CD2	3.23	138.59	126.35
1	T	73	HIC	CZ-NE2-CD2	3.79	140.71	126.35
1	Q	73	HIC	CZ-NE2-CD2	4.25	142.47	126.35
1	P	73	HIC	CZ-NE2-CD2	4.30	142.64	126.35
1	V	73	HIC	CZ-NE2-CD2	4.43	143.12	126.35
1	R	73	HIC	CZ-NE2-CD2	4.64	143.93	126.35
1	Y	73	HIC	CZ-NE2-CD2	4.85	144.73	126.35
1	S	73	HIC	CZ-NE2-CD2	5.46	147.05	126.35
1	Z	73	HIC	CZ-NE2-CD2	6.35	150.43	126.35
1	W	73	HIC	CZ-NE2-CD2	6.74	151.91	126.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	O	73	HIC	2	0
1	P	73	HIC	1	0
1	Q	73	HIC	3	0
1	R	73	HIC	3	0
1	S	73	HIC	3	0
1	T	73	HIC	2	0
1	U	73	HIC	2	0
1	V	73	HIC	3	0
1	W	73	HIC	3	0
1	X	73	HIC	3	0
1	Y	73	HIC	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 120 ligands modelled in this entry, 72 are monoatomic - leaving 48 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	O	800	4	24,29,29	0.99	2 (8%)	23,45,45	1.38	3 (13%)
3	PO4	O	801	-	4,4,4	1.68	1 (25%)	6,6,6	0.55	0
3	PO4	O	802	-	4,4,4	1.74	1 (25%)	6,6,6	0.42	0
3	PO4	O	803	-	4,4,4	1.99	1 (25%)	6,6,6	0.52	0
2	ADP	P	800	4	24,29,29	0.95	2 (8%)	23,45,45	1.31	3 (13%)
3	PO4	P	801	-	4,4,4	1.92	1 (25%)	6,6,6	0.54	0
3	PO4	P	802	-	4,4,4	1.49	1 (25%)	6,6,6	0.35	0
3	PO4	P	803	-	4,4,4	1.78	1 (25%)	6,6,6	1.21	1 (16%)
2	ADP	Q	800	4	24,29,29	0.95	1 (4%)	23,45,45	1.33	3 (13%)
3	PO4	Q	801	4	4,4,4	1.74	1 (25%)	6,6,6	0.72	0
3	PO4	Q	802	-	4,4,4	1.80	1 (25%)	6,6,6	0.38	0
3	PO4	Q	803	-	4,4,4	1.72	1 (25%)	6,6,6	0.51	0
2	ADP	R	800	4	24,29,29	0.99	2 (8%)	23,45,45	1.53	4 (17%)
3	PO4	R	801	-	4,4,4	1.82	1 (25%)	6,6,6	0.49	0
3	PO4	R	802	-	4,4,4	1.43	1 (25%)	6,6,6	0.41	0
3	PO4	R	803	-	4,4,4	1.94	1 (25%)	6,6,6	0.96	0
2	ADP	S	800	4	24,29,29	0.91	1 (4%)	23,45,45	1.29	3 (13%)
3	PO4	S	801	-	4,4,4	1.35	1 (25%)	6,6,6	0.42	0
3	PO4	S	802	-	4,4,4	1.82	1 (25%)	6,6,6	0.34	0
3	PO4	S	803	-	4,4,4	1.86	1 (25%)	6,6,6	0.54	0
3	PO4	T	376	-	4,4,4	1.65	1 (25%)	6,6,6	0.57	0
2	ADP	T	800	4	24,29,29	0.84	1 (4%)	23,45,45	1.46	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	T	801	4	4,4,4	1.70	1 (25%)	6,6,6	0.56	0
3	PO4	T	802	-	4,4,4	1.83	1 (25%)	6,6,6	0.37	0
3	PO4	T	803	-	4,4,4	1.79	1 (25%)	6,6,6	0.67	0
2	ADP	U	800	4	24,29,29	0.83	1 (4%)	23,45,45	1.53	4 (17%)
3	PO4	U	801	-	4,4,4	1.82	1 (25%)	6,6,6	0.96	1 (16%)
3	PO4	U	802	-	4,4,4	1.39	1 (25%)	6,6,6	0.43	0
3	PO4	U	803	-	4,4,4	1.67	1 (25%)	6,6,6	0.40	0
2	ADP	V	800	4	24,29,29	0.92	2 (8%)	23,45,45	1.31	3 (13%)
3	PO4	V	802	-	4,4,4	1.80	1 (25%)	6,6,6	0.45	0
3	PO4	V	803	-	4,4,4	1.73	1 (25%)	6,6,6	0.55	0
2	ADP	W	800	4	24,29,29	0.91	2 (8%)	23,45,45	1.30	4 (17%)
3	PO4	W	801	-	4,4,4	1.69	1 (25%)	6,6,6	0.56	0
3	PO4	W	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.38	0
3	PO4	W	803	-	4,4,4	1.71	1 (25%)	6,6,6	0.58	0
2	ADP	X	800	4	24,29,29	0.91	2 (8%)	23,45,45	1.46	5 (21%)
3	PO4	X	801	-	4,4,4	1.50	1 (25%)	6,6,6	0.39	0
3	PO4	X	802	-	4,4,4	1.71	1 (25%)	6,6,6	0.43	0
3	PO4	X	803	-	4,4,4	1.73	1 (25%)	6,6,6	0.73	0
2	ADP	Y	800	4	24,29,29	0.87	1 (4%)	23,45,45	1.29	3 (13%)
3	PO4	Y	801	4	4,4,4	2.01	1 (25%)	6,6,6	0.36	0
3	PO4	Y	802	-	4,4,4	1.87	1 (25%)	6,6,6	0.34	0
3	PO4	Y	803	-	4,4,4	1.82	1 (25%)	6,6,6	0.66	0
2	ADP	Z	800	4	24,29,29	0.88	1 (4%)	23,45,45	1.33	2 (8%)
3	PO4	Z	801	-	4,4,4	1.77	1 (25%)	6,6,6	0.59	0
3	PO4	Z	802	-	4,4,4	1.91	1 (25%)	6,6,6	0.54	0
3	PO4	Z	803	-	4,4,4	1.62	1 (25%)	6,6,6	0.48	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	ADP	O	800	4	-	0/12/32/32	0/3/3/3
3	PO4	O	801	-	-	0/0/0/0	0/0/0/0
3	PO4	O	802	-	-	0/0/0/0	0/0/0/0
3	PO4	O	803	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	P	800	4	-	0/12/32/32	0/3/3/3
3	PO4	P	801	-	-	0/0/0/0	0/0/0/0
3	PO4	P	802	-	-	0/0/0/0	0/0/0/0
3	PO4	P	803	-	-	0/0/0/0	0/0/0/0
2	ADP	Q	800	4	-	0/12/32/32	0/3/3/3
3	PO4	Q	801	4	-	0/0/0/0	0/0/0/0
3	PO4	Q	802	-	-	0/0/0/0	0/0/0/0
3	PO4	Q	803	-	-	0/0/0/0	0/0/0/0
2	ADP	R	800	4	-	0/12/32/32	0/3/3/3
3	PO4	R	801	-	-	0/0/0/0	0/0/0/0
3	PO4	R	802	-	-	0/0/0/0	0/0/0/0
3	PO4	R	803	-	-	0/0/0/0	0/0/0/0
2	ADP	S	800	4	-	0/12/32/32	0/3/3/3
3	PO4	S	801	-	-	0/0/0/0	0/0/0/0
3	PO4	S	802	-	-	0/0/0/0	0/0/0/0
3	PO4	S	803	-	-	0/0/0/0	0/0/0/0
3	PO4	T	376	-	-	0/0/0/0	0/0/0/0
2	ADP	T	800	4	-	0/12/32/32	0/3/3/3
3	PO4	T	801	4	-	0/0/0/0	0/0/0/0
3	PO4	T	802	-	-	0/0/0/0	0/0/0/0
3	PO4	T	803	-	-	0/0/0/0	0/0/0/0
2	ADP	U	800	4	-	0/12/32/32	0/3/3/3
3	PO4	U	801	-	-	0/0/0/0	0/0/0/0
3	PO4	U	802	-	-	0/0/0/0	0/0/0/0
3	PO4	U	803	-	-	0/0/0/0	0/0/0/0
2	ADP	V	800	4	-	0/12/32/32	0/3/3/3
3	PO4	V	802	-	-	0/0/0/0	0/0/0/0
3	PO4	V	803	-	-	0/0/0/0	0/0/0/0
2	ADP	W	800	4	-	0/12/32/32	0/3/3/3
3	PO4	W	801	-	-	0/0/0/0	0/0/0/0
3	PO4	W	802	-	-	0/0/0/0	0/0/0/0
3	PO4	W	803	-	-	0/0/0/0	0/0/0/0
2	ADP	X	800	4	-	0/12/32/32	0/3/3/3
3	PO4	X	801	-	-	0/0/0/0	0/0/0/0
3	PO4	X	802	-	-	0/0/0/0	0/0/0/0
3	PO4	X	803	-	-	0/0/0/0	0/0/0/0
2	ADP	Y	800	4	-	0/12/32/32	0/3/3/3
3	PO4	Y	801	4	-	0/0/0/0	0/0/0/0
3	PO4	Y	802	-	-	0/0/0/0	0/0/0/0
3	PO4	Y	803	-	-	0/0/0/0	0/0/0/0
2	ADP	Z	800	4	-	0/12/32/32	0/3/3/3
3	PO4	Z	801	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	Z	802	-	-	0/0/0/0	0/0/0/0
3	PO4	Z	803	-	-	0/0/0/0	0/0/0/0

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	800	ADP	C2'-C1'	-2.63	1.49	1.53
2	P	800	ADP	C2'-C1'	-2.39	1.49	1.53
2	W	800	ADP	C2'-C1'	-2.30	1.50	1.53
2	O	800	ADP	C2'-C1'	-2.22	1.50	1.53
2	W	800	ADP	PB-O2B	-2.20	1.47	1.54
2	Y	800	ADP	PB-O2B	-2.20	1.47	1.54
2	S	800	ADP	PB-O2B	-2.19	1.47	1.54
2	Q	800	ADP	PB-O2B	-2.18	1.47	1.54
2	O	800	ADP	PB-O2B	-2.18	1.47	1.54
2	R	800	ADP	PB-O2B	-2.18	1.47	1.54
2	U	800	ADP	PB-O2B	-2.18	1.47	1.54
2	T	800	ADP	PB-O2B	-2.18	1.47	1.54
2	X	800	ADP	C2'-C1'	-2.18	1.50	1.53
2	P	800	ADP	PB-O2B	-2.18	1.47	1.54
2	V	800	ADP	PB-O2B	-2.17	1.47	1.54
2	Z	800	ADP	PB-O2B	-2.17	1.47	1.54
2	X	800	ADP	PB-O2B	-2.16	1.47	1.54
2	V	800	ADP	C2'-C1'	-2.01	1.50	1.53
3	S	801	PO4	P-O4	2.26	1.60	1.53
3	U	802	PO4	P-O4	2.26	1.60	1.53
3	R	802	PO4	P-O4	2.53	1.61	1.53
3	X	801	PO4	P-O4	2.64	1.61	1.53
3	P	802	PO4	P-O4	2.65	1.62	1.53
3	Z	803	PO4	P-O4	2.74	1.62	1.53
3	O	801	PO4	P-O4	2.75	1.62	1.53
3	W	802	PO4	P-O4	2.82	1.62	1.53
3	P	803	PO4	P-O1	2.83	1.63	1.53
3	U	801	PO4	P-O1	2.93	1.64	1.53
3	U	803	PO4	P-O4	2.93	1.62	1.53
3	V	803	PO4	P-O4	2.95	1.62	1.53
3	W	803	PO4	P-O4	2.95	1.62	1.53
3	Q	802	PO4	P-O4	2.97	1.63	1.53
3	Q	801	PO4	P-O4	2.99	1.63	1.53
3	X	802	PO4	P-O4	3.00	1.63	1.53
3	T	376	PO4	P-O4	3.04	1.63	1.53
3	O	802	PO4	P-O4	3.05	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	802	PO4	P-O4	3.06	1.63	1.53
3	W	801	PO4	P-O4	3.06	1.63	1.53
3	T	803	PO4	P-O4	3.07	1.63	1.53
3	T	801	PO4	P-O4	3.11	1.63	1.53
3	Q	803	PO4	P-O4	3.11	1.63	1.53
3	T	802	PO4	P-O4	3.14	1.63	1.53
3	X	803	PO4	P-O4	3.17	1.63	1.53
3	Y	803	PO4	P-O4	3.21	1.63	1.53
3	Y	802	PO4	P-O4	3.26	1.63	1.53
3	Z	801	PO4	P-O4	3.28	1.63	1.53
3	V	802	PO4	P-O4	3.31	1.64	1.53
3	R	801	PO4	P-O4	3.36	1.64	1.53
3	S	803	PO4	P-O4	3.37	1.64	1.53
3	R	803	PO4	P-O4	3.52	1.64	1.53
3	Y	801	PO4	P-O4	3.62	1.65	1.53
3	P	801	PO4	P-O4	3.64	1.65	1.53
3	Z	802	PO4	P-O4	3.66	1.65	1.53
3	O	803	PO4	P-O4	3.67	1.65	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	800	ADP	O3B-PB-O1B	-3.26	99.99	110.63
2	U	800	ADP	O3B-PB-O1B	-3.26	100.00	110.63
2	R	800	ADP	O3B-PB-O1B	-3.25	100.01	110.63
2	W	800	ADP	O3B-PB-O1B	-3.25	100.02	110.63
2	Z	800	ADP	O3B-PB-O1B	-3.25	100.02	110.63
2	Y	800	ADP	O3B-PB-O1B	-3.25	100.02	110.63
2	S	800	ADP	O3B-PB-O1B	-3.25	100.03	110.63
2	T	800	ADP	O3B-PB-O1B	-3.25	100.03	110.63
2	X	800	ADP	O3B-PB-O1B	-3.24	100.05	110.63
2	V	800	ADP	O3B-PB-O1B	-3.24	100.05	110.63
2	P	800	ADP	O3B-PB-O1B	-3.24	100.06	110.63
2	Q	800	ADP	O3B-PB-O1B	-3.23	100.07	110.63
2	U	800	ADP	N6-C6-N1	-3.13	113.26	118.52
2	T	800	ADP	N6-C6-N1	-2.82	113.79	118.52
3	P	803	PO4	O4-P-O1	-2.38	63.84	116.39
2	R	800	ADP	N6-C6-N1	-2.33	114.60	118.52
2	X	800	ADP	C4'-O4'-C1'	-2.30	107.21	109.64
2	Y	800	ADP	C1'-N9-C4	-2.20	124.35	126.81
2	W	800	ADP	C1'-N9-C4	-2.19	124.37	126.81
3	U	801	PO4	O4-P-O1	-2.12	69.57	116.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	800	ADP	O2A-PA-O3A	2.11	114.31	105.27
2	V	800	ADP	O2A-PA-O3A	2.17	114.55	105.27
2	X	800	ADP	O4'-C1'-N9	2.19	112.25	108.11
2	P	800	ADP	O2A-PA-O3A	2.21	114.75	105.27
2	S	800	ADP	O2A-PA-O3A	2.23	114.83	105.27
2	O	800	ADP	O2A-PA-O3A	2.30	115.12	105.27
2	X	800	ADP	O2A-PA-O3A	2.35	115.33	105.27
2	Q	800	ADP	O2A-PA-O3A	2.38	115.49	105.27
2	T	800	ADP	O2A-PA-O3A	2.56	116.23	105.27
2	R	800	ADP	O2A-PA-O3A	2.57	116.28	105.27
2	U	800	ADP	N3-C2-N1	2.96	131.20	128.87
2	R	800	ADP	O3B-PB-O2B	3.38	119.85	107.44
2	V	800	ADP	O3B-PB-O2B	3.38	119.85	107.44
2	Z	800	ADP	O3B-PB-O2B	3.38	119.85	107.44
2	Y	800	ADP	O3B-PB-O2B	3.38	119.86	107.44
2	P	800	ADP	O3B-PB-O2B	3.38	119.86	107.44
2	Q	800	ADP	O3B-PB-O2B	3.39	119.87	107.44
2	T	800	ADP	O3B-PB-O2B	3.39	119.88	107.44
2	S	800	ADP	O3B-PB-O2B	3.39	119.89	107.44
2	X	800	ADP	O3B-PB-O2B	3.39	119.89	107.44
2	O	800	ADP	O3B-PB-O2B	3.39	119.89	107.44
2	U	800	ADP	O3B-PB-O2B	3.39	119.89	107.44
2	W	800	ADP	O3B-PB-O2B	3.40	119.92	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	800	ADP	1	0
3	P	803	PO4	1	0
3	R	801	PO4	1	0
3	T	803	PO4	1	0
2	U	800	ADP	1	0
3	Y	801	PO4	2	0

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.