wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:48 PM BST

PDB ID	:	3J4K
EMDB ID:	:	EMD-5751
Title	:	Cryo-EM structures of the actin:tropomyosin filament reveal the mechanism for the transition from C- to M-state
Authors	:	Sousa, D.R.; Stagg, S.M.; Stroupe, M.E.
Deposited on	:	2013-08-26
Resolution	:	8.00 Å(reported)
Based on PDB ID	:	4A7F

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

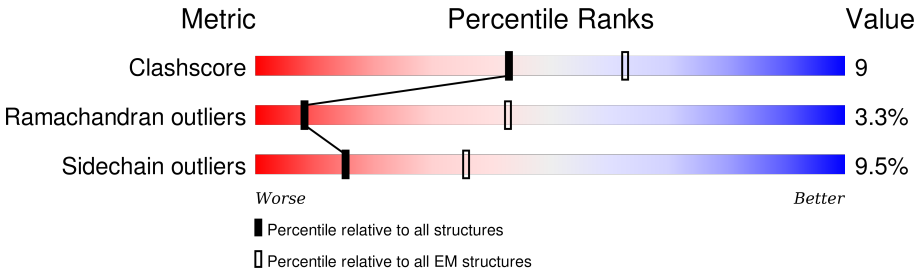
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 8.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	375	67% 25% 7% •
1	B	375	64% 29% 6% •
1	C	375	68% 24% 7% •
1	D	375	62% 27% 10% •
1	E	375	63% 29% 8% •
2	F	136	100%
2	G	136	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16160 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.

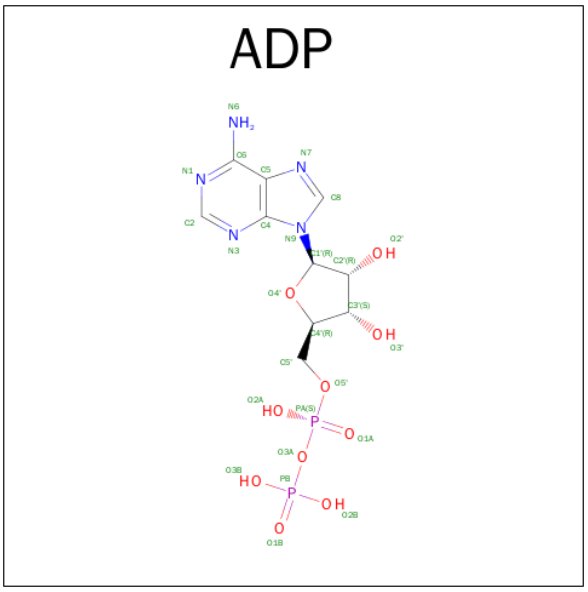
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

- Molecule 2 is a protein called tropomyosin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	136	Total	C	N	O	0	0
			680	408	136	136		
2	G	136	Total	C	N	O	0	0
			680	408	136	136		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



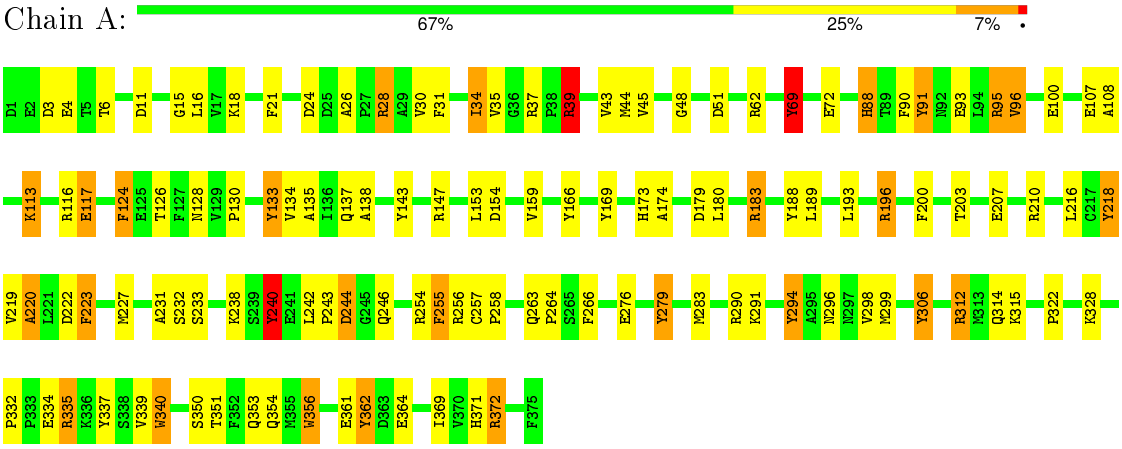
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

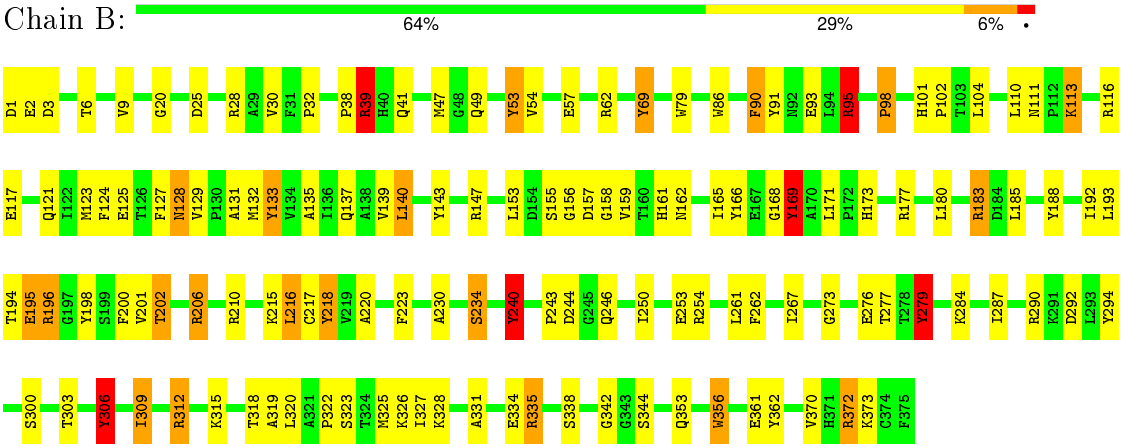
- Molecule 1: Actin, alpha skeletal muscle

Chain A:



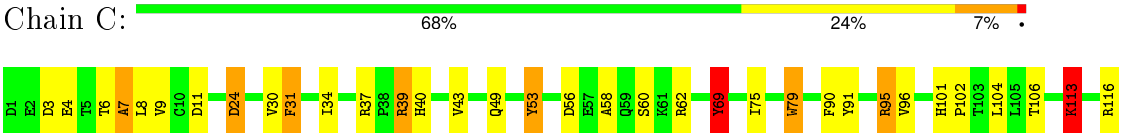
- Molecule 1: Actin, alpha skeletal muscle

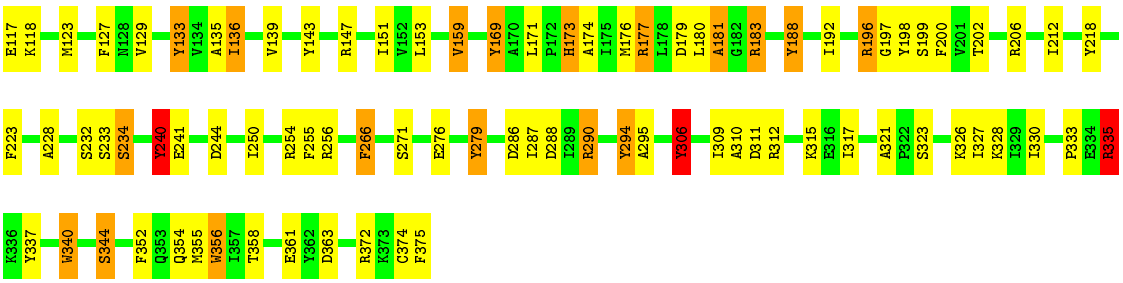
Chain B:



- Molecule 1: Actin, alpha skeletal muscle

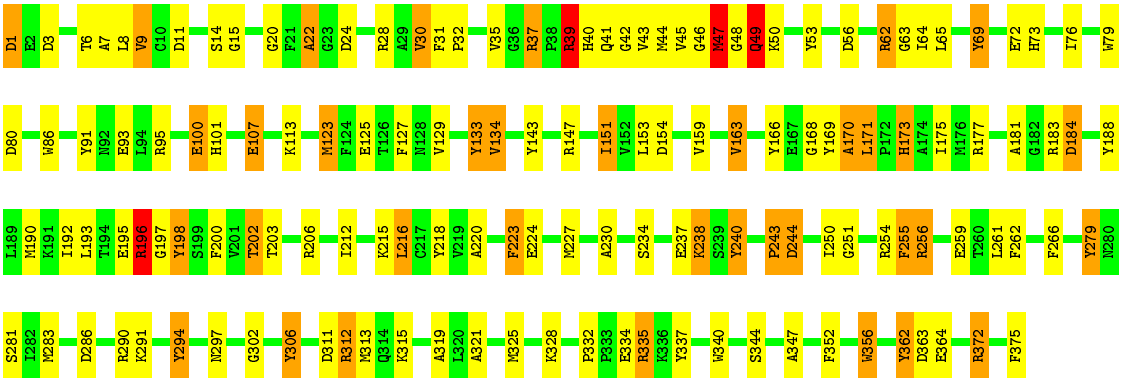
Chain C:





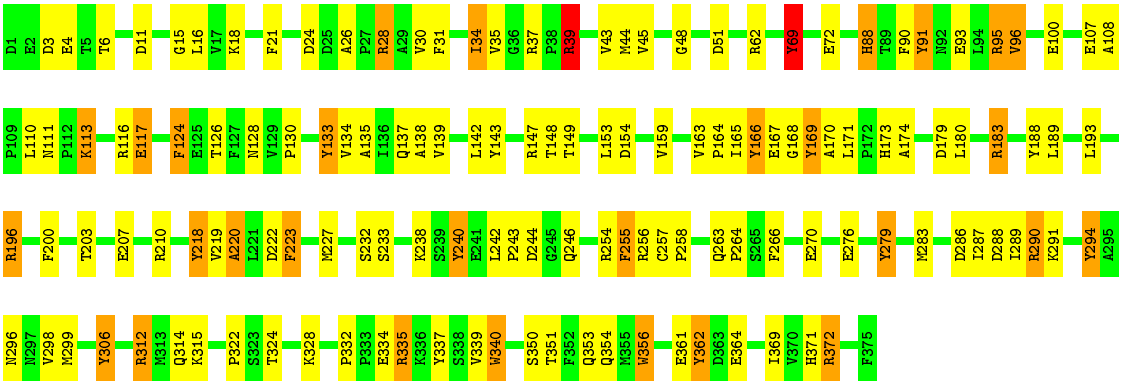
• Molecule 1: Actin, alpha skeletal muscle

Chain D:



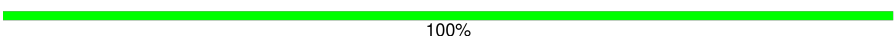
• Molecule 1: Actin, alpha skeletal muscle

Chain E:



• Molecule 2: tropomyosin

Chain F:



There are no outlier residues recorded for this chain.

• Molecule 2: tropomyosin

Chain G:

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	224337	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	individual images	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	Gatan Ultrascan 4000	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	1.74	25/2996 (0.8%)	1.97	78/4058 (1.9%)
1	B	1.75	35/2996 (1.2%)	2.00	80/4058 (2.0%)
1	C	1.71	21/2996 (0.7%)	1.99	86/4058 (2.1%)
1	D	1.73	29/2996 (1.0%)	2.11	108/4058 (2.7%)
1	E	1.74	26/2996 (0.9%)	1.97	77/4058 (1.9%)
All	All	1.73	136/14980 (0.9%)	2.01	429/20290 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	B	0	11
1	C	0	12
1	D	0	8
1	E	0	15
All	All	0	61

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ARG	NE-CZ	9.09	1.44	1.33
1	E	37	ARG	NE-CZ	9.08	1.44	1.33
1	B	95	ARG	CD-NE	8.06	1.60	1.46
1	C	169	TYR	CG-CD1	7.54	1.49	1.39
1	D	32	PRO	N-CD	-7.51	1.37	1.47
1	C	206	ARG	CZ-NH1	7.30	1.42	1.33
1	E	372	ARG	CZ-NH1	7.10	1.42	1.33
1	A	372	ARG	CZ-NH1	7.08	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	ARG	NE-CZ	7.02	1.42	1.33
1	C	234	SER	CA-CB	6.94	1.63	1.52
1	B	147	ARG	CD-NE	6.85	1.58	1.46
1	C	271	SER	CB-OG	6.82	1.51	1.42
1	C	323	SER	CA-CB	6.72	1.63	1.52
1	E	91	TYR	CB-CG	-6.72	1.41	1.51
1	A	91	TYR	CB-CG	-6.69	1.41	1.51
1	D	281	SER	CA-CB	6.60	1.62	1.52
1	B	290	ARG	CZ-NH1	6.55	1.41	1.33
1	D	147	ARG	CZ-NH1	6.52	1.41	1.33
1	D	250	ILE	C-N	6.52	1.44	1.33
1	B	168	GLY	CA-C	-6.47	1.41	1.51
1	D	259	GLU	CB-CG	6.46	1.64	1.52
1	B	273	GLY	CA-C	-6.39	1.41	1.51
1	E	196	ARG	CZ-NH1	6.39	1.41	1.33
1	D	169	TYR	CG-CD2	6.38	1.47	1.39
1	C	79	TRP	CB-CG	6.38	1.61	1.50
1	D	14	SER	CA-CB	6.37	1.62	1.52
1	E	223	PHE	CB-CG	6.37	1.62	1.51
1	D	107	GLU	CD-OE2	6.37	1.32	1.25
1	A	223	PHE	CB-CG	6.36	1.62	1.51
1	A	196	ARG	CZ-NH1	6.34	1.41	1.33
1	E	48	GLY	N-CA	-6.32	1.36	1.46
1	A	48	GLY	N-CA	-6.30	1.36	1.46
1	B	169	TYR	CG-CD2	6.30	1.47	1.39
1	C	116	ARG	NE-CZ	6.23	1.41	1.33
1	D	20	GLY	N-CA	-6.20	1.36	1.46
1	B	253	GLU	CD-OE2	6.20	1.32	1.25
1	C	135	ALA	CA-CB	6.17	1.65	1.52
1	B	206	ARG	CD-NE	6.13	1.56	1.46
1	C	147	ARG	CD-NE	6.12	1.56	1.46
1	E	256	ARG	NE-CZ	6.11	1.41	1.33
1	A	256	ARG	NE-CZ	6.09	1.41	1.33
1	B	198	TYR	CE2-CZ	6.08	1.46	1.38
1	B	276	GLU	CG-CD	6.06	1.61	1.51
1	B	206	ARG	CZ-NH2	6.05	1.41	1.33
1	D	312	ARG	CD-NE	6.05	1.56	1.46
1	B	39	ARG	CZ-NH2	6.01	1.40	1.33
1	C	233	SER	CA-CB	6.00	1.61	1.52
1	A	39	ARG	NE-CZ	5.99	1.40	1.33
1	E	39	ARG	NE-CZ	5.97	1.40	1.33
1	B	338	SER	CA-CB	5.96	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ARG	CZ-NH2	5.93	1.40	1.33
1	E	62	ARG	CZ-NH2	5.93	1.40	1.33
1	B	335	ARG	CZ-NH1	5.88	1.40	1.33
1	B	198	TYR	CD2-CE2	5.81	1.48	1.39
1	D	28	ARG	CZ-NH2	5.80	1.40	1.33
1	A	21	PHE	CG-CD2	5.79	1.47	1.38
1	D	251	GLY	CA-C	-5.79	1.42	1.51
1	E	21	PHE	CG-CD2	5.79	1.47	1.38
1	D	62	ARG	NE-CZ	5.78	1.40	1.33
1	A	179	ASP	N-CA	-5.77	1.34	1.46
1	E	179	ASP	N-CA	-5.75	1.34	1.46
1	C	256	ARG	NE-CZ	5.75	1.40	1.33
1	B	240	TYR	CZ-OH	5.71	1.47	1.37
1	A	183	ARG	NE-CZ	5.69	1.40	1.33
1	A	266	PHE	CG-CD1	5.69	1.47	1.38
1	A	28	ARG	NE-CZ	5.64	1.40	1.33
1	E	266	PHE	CG-CD1	5.64	1.47	1.38
1	E	183	ARG	NE-CZ	5.62	1.40	1.33
1	C	356	TRP	CD2-CE2	-5.61	1.34	1.41
1	D	100	GLU	CG-CD	5.61	1.60	1.51
1	D	188	TYR	CE2-CZ	5.60	1.45	1.38
1	E	28	ARG	NE-CZ	5.60	1.40	1.33
1	D	196	ARG	NE-CZ	5.57	1.40	1.33
1	B	20	GLY	CA-C	-5.54	1.43	1.51
1	B	188	TYR	CZ-OH	5.52	1.47	1.37
1	D	362	TYR	CE2-CZ	5.50	1.45	1.38
1	B	356	TRP	CB-CG	5.49	1.60	1.50
1	D	372	ARG	NE-CZ	5.48	1.40	1.33
1	E	314	GLN	CG-CD	5.47	1.63	1.51
1	A	314	GLN	CG-CD	5.46	1.63	1.51
1	B	372	ARG	CZ-NH2	5.46	1.40	1.33
1	C	375	PHE	CG-CD1	5.44	1.47	1.38
1	D	183	ARG	CZ-NH1	5.41	1.40	1.33
1	B	323	SER	CA-CB	5.41	1.61	1.52
1	D	133	TYR	CE2-CZ	5.41	1.45	1.38
1	B	217	CYS	CB-SG	5.39	1.91	1.82
1	E	364	GLU	CG-CD	5.39	1.60	1.51
1	A	364	GLU	CG-CD	5.38	1.60	1.51
1	D	335	ARG	CZ-NH1	5.38	1.40	1.33
1	B	69	TYR	CZ-OH	5.36	1.47	1.37
1	B	323	SER	CB-OG	-5.36	1.35	1.42
1	D	243	PRO	N-CD	5.34	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	364	GLU	CB-CG	5.34	1.62	1.52
1	B	206	ARG	CZ-NH1	5.33	1.40	1.33
1	D	39	ARG	CZ-NH1	5.33	1.40	1.33
1	D	254	ARG	CZ-NH1	5.32	1.40	1.33
1	B	312	ARG	CZ-NH1	5.32	1.40	1.33
1	A	296	ASN	CA-C	-5.30	1.39	1.52
1	C	133	TYR	CG-CD1	5.30	1.46	1.39
1	D	69	TYR	CZ-OH	5.30	1.46	1.37
1	B	361	GLU	CD-OE1	-5.30	1.19	1.25
1	B	254	ARG	NE-CZ	5.29	1.40	1.33
1	D	375	PHE	CE1-CZ	5.29	1.47	1.37
1	C	183	ARG	CZ-NH1	5.29	1.40	1.33
1	C	232	SER	N-CA	-5.29	1.35	1.46
1	E	296	ASN	CA-C	-5.28	1.39	1.52
1	D	125	GLU	CG-CD	5.27	1.59	1.51
1	B	86	TRP	CB-CG	5.21	1.59	1.50
1	E	290	ARG	CZ-NH1	5.20	1.39	1.33
1	B	69	TYR	CE2-CZ	5.20	1.45	1.38
1	E	69	TYR	CE1-CZ	5.20	1.45	1.38
1	A	166	TYR	CE1-CZ	5.19	1.45	1.38
1	B	327	ILE	N-CA	-5.19	1.35	1.46
1	C	327	ILE	N-CA	-5.19	1.35	1.46
1	A	290	ARG	CZ-NH1	5.16	1.39	1.33
1	C	60	SER	CA-CB	5.16	1.60	1.52
1	A	69	TYR	CE1-CZ	5.15	1.45	1.38
1	E	166	TYR	CE1-CZ	5.15	1.45	1.38
1	C	4	GLU	CG-CD	5.14	1.59	1.51
1	A	254	ARG	CZ-NH1	5.14	1.39	1.33
1	E	96	VAL	CB-CG1	5.14	1.63	1.52
1	C	312	ARG	CZ-NH2	5.13	1.39	1.33
1	A	96	VAL	CB-CG1	5.12	1.63	1.52
1	A	218	TYR	CA-CB	5.11	1.65	1.53
1	E	218	TYR	CA-CB	5.11	1.65	1.53
1	D	352	PHE	CG-CD2	5.10	1.46	1.38
1	E	254	ARG	CZ-NH1	5.10	1.39	1.33
1	C	69	TYR	CD1-CE1	5.09	1.47	1.39
1	A	188	TYR	CG-CD2	5.08	1.45	1.39
1	B	198	TYR	CG-CD1	-5.08	1.32	1.39
1	B	62	ARG	CD-NE	5.07	1.55	1.46
1	E	183	ARG	CZ-NH2	5.06	1.39	1.33
1	E	188	TYR	CG-CD2	5.05	1.45	1.39
1	A	183	ARG	CZ-NH2	5.04	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	356	TRP	CD2-CE2	-5.03	1.35	1.41
1	B	223	PHE	CA-CB	5.00	1.65	1.53

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	196	ARG	NE-CZ-NH2	-18.93	110.83	120.30
1	D	62	ARG	NE-CZ-NH2	-16.66	111.97	120.30
1	A	39	ARG	NE-CZ-NH2	14.71	127.66	120.30
1	E	39	ARG	NE-CZ-NH2	14.65	127.62	120.30
1	B	127	PHE	CB-CG-CD1	-14.49	110.66	120.80
1	D	290	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	B	169	TYR	CB-CG-CD2	-13.24	113.06	121.00
1	E	335	ARG	NE-CZ-NH1	-13.13	113.73	120.30
1	A	335	ARG	NE-CZ-NH1	-13.06	113.77	120.30
1	D	279	TYR	CB-CG-CD2	-13.06	113.17	121.00
1	B	127	PHE	CB-CG-CD2	12.91	129.84	120.80
1	D	169	TYR	CB-CG-CD1	12.78	128.66	121.00
1	D	294	TYR	CB-CG-CD1	-12.77	113.34	121.00
1	A	39	ARG	NE-CZ-NH1	-12.31	114.14	120.30
1	C	306	TYR	CB-CG-CD2	-12.29	113.63	121.00
1	E	39	ARG	NE-CZ-NH1	-12.28	114.16	120.30
1	D	196	ARG	NE-CZ-NH1	12.17	126.38	120.30
1	B	279	TYR	CB-CG-CD2	-11.68	113.99	121.00
1	D	290	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	E	62	ARG	NE-CZ-NH2	-11.41	114.59	120.30
1	A	62	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	D	143	TYR	CB-CG-CD1	-11.30	114.22	121.00
1	A	143	TYR	CB-CG-CD2	-11.19	114.29	121.00
1	E	143	TYR	CB-CG-CD2	-11.15	114.31	121.00
1	C	37	ARG	NE-CZ-NH2	11.04	125.82	120.30
1	C	335	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	E	62	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	62	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	D	28	ARG	NE-CZ-NH2	-10.97	114.82	120.30
1	D	143	TYR	CB-CG-CD2	10.77	127.46	121.00
1	C	352	PHE	CB-CG-CD2	-10.75	113.27	120.80
1	B	188	TYR	CB-CG-CD2	-10.58	114.65	121.00
1	B	198	TYR	CB-CG-CD2	-10.46	114.72	121.00
1	B	290	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	C	177	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	C	127	PHE	CB-CG-CD1	10.22	127.95	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	196	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	D	28	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	D	372	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	C	127	PHE	CB-CG-CD2	-9.93	113.85	120.80
1	E	210	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	A	210	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	D	206	ARG	NE-CZ-NH1	-9.82	115.39	120.30
1	B	169	TYR	CG-CD2-CE2	-9.77	113.49	121.30
1	A	255	PHE	CB-CG-CD1	9.72	127.60	120.80
1	E	255	PHE	CB-CG-CD1	9.64	127.55	120.80
1	B	116	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	372	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	D	3	ASP	CB-CG-OD2	9.58	126.92	118.30
1	B	196	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	C	254	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	D	256	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	D	200	PHE	CB-CG-CD2	-9.23	114.34	120.80
1	A	166	TYR	CB-CG-CD1	9.22	126.53	121.00
1	E	166	TYR	CB-CG-CD1	9.16	126.50	121.00
1	A	210	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	E	210	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	B	206	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	E	312	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	312	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	D	169	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	C	306	TYR	CB-CG-CD1	8.96	126.38	121.00
1	D	362	TYR	CB-CG-CD1	-8.94	115.64	121.00
1	C	143	TYR	CB-CG-CD2	-8.88	115.67	121.00
1	B	79	TRP	CB-CG-CD1	8.87	138.54	127.00
1	D	183	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	B	79	TRP	CG-CD2-CE3	-8.83	125.95	133.90
1	B	169	TYR	CB-CG-CD1	8.82	126.29	121.00
1	E	218	TYR	CB-CG-CD1	-8.70	115.78	121.00
1	A	218	TYR	CB-CG-CD1	-8.67	115.80	121.00
1	B	279	TYR	CB-CG-CD1	8.62	126.17	121.00
1	B	262	PHE	CB-CG-CD1	-8.51	114.84	120.80
1	D	262	PHE	CB-CG-CD2	8.48	126.74	120.80
1	C	90	PHE	CB-CG-CD2	8.46	126.73	120.80
1	B	218	TYR	CB-CG-CD2	-8.43	115.94	121.00
1	D	3	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	C	375	PHE	CB-CG-CD2	8.27	126.59	120.80
1	D	362	TYR	CB-CG-CD2	8.25	125.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	124	PHE	CB-CG-CD2	-8.23	115.04	120.80
1	C	90	PHE	CB-CG-CD1	-8.21	115.06	120.80
1	A	290	ARG	NE-CZ-NH2	8.11	124.35	120.30
1	D	31	PHE	CB-CG-CD2	-8.09	115.14	120.80
1	E	266	PHE	CB-CG-CD2	-8.08	115.14	120.80
1	E	31	PHE	CB-CG-CD2	-8.07	115.15	120.80
1	E	290	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	A	31	PHE	CB-CG-CD2	-8.01	115.19	120.80
1	A	266	PHE	CB-CG-CD2	-8.00	115.20	120.80
1	D	11	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	A	147	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	E	147	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	177	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	D	127	PHE	CB-CG-CD2	-7.84	115.31	120.80
1	D	69	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	D	363	ASP	CB-CG-OD1	7.78	125.30	118.30
1	C	344	SER	N-CA-CB	7.77	122.15	110.50
1	E	133	TYR	CB-CG-CD1	-7.76	116.34	121.00
1	D	372	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	133	TYR	CB-CG-CD1	-7.74	116.35	121.00
1	D	9	VAL	N-CA-C	-7.73	90.12	111.00
1	D	279	TYR	CB-CG-CD1	7.69	125.61	121.00
1	A	21	PHE	CB-CG-CD1	7.63	126.14	120.80
1	E	21	PHE	CB-CG-CD1	7.60	126.12	120.80
1	D	266	PHE	CB-CG-CD1	-7.57	115.50	120.80
1	C	37	ARG	NH1-CZ-NH2	-7.50	111.15	119.40
1	C	196	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	D	203	THR	CA-CB-CG2	-7.46	101.96	112.40
1	C	255	PHE	CB-CG-CD1	-7.44	115.59	120.80
1	B	318	THR	CA-CB-CG2	-7.42	102.02	112.40
1	D	240	TYR	CB-CG-CD1	-7.38	116.57	121.00
1	D	240	TYR	CB-CG-CD2	7.37	125.42	121.00
1	D	193	LEU	CB-CG-CD1	7.37	123.53	111.00
1	B	98	PRO	N-CA-CB	7.37	112.14	103.30
1	A	279	TYR	CG-CD1-CE1	-7.36	115.41	121.30
1	E	279	TYR	CG-CD1-CE1	-7.35	115.42	121.30
1	A	254	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	B	147	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	E	254	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	E	283	MET	CG-SD-CE	-7.29	88.53	100.20
1	C	198	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	A	283	MET	CG-SD-CE	-7.29	88.54	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	372	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	D	170	ALA	N-CA-CB	7.27	120.28	110.10
1	D	218	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	E	266	PHE	CB-CG-CD1	7.12	125.78	120.80
1	A	266	PHE	CB-CG-CD1	7.09	125.76	120.80
1	D	24	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	D	134	VAL	CG1-CB-CG2	7.07	122.22	110.90
1	B	206	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	D	337	TYR	CB-CG-CD2	-7.01	116.79	121.00
1	D	188	TYR	CZ-CE2-CD2	-7.00	113.50	119.80
1	D	184	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	A	69	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	D	294	TYR	CG-CD2-CE2	-6.95	115.74	121.30
1	E	69	TYR	CB-CG-CD1	-6.92	116.85	121.00
1	B	362	TYR	CG-CD2-CE2	6.92	126.83	121.30
1	B	91	TYR	CD1-CE1-CZ	6.90	126.01	119.80
1	D	69	TYR	CB-CG-CD1	6.89	125.14	121.00
1	B	95	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	E	218	TYR	CZ-CE2-CD2	-6.84	113.64	119.80
1	E	95	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	79	TRP	CB-CG-CD2	-6.81	117.74	126.60
1	A	218	TYR	CZ-CE2-CD2	-6.81	113.67	119.80
1	A	95	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	292	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	A	108	ALA	N-CA-CB	6.74	119.53	110.10
1	E	108	ALA	N-CA-CB	6.73	119.53	110.10
1	B	183	ARG	NE-CZ-NH2	6.73	123.66	120.30
1	D	1	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	B	169	TYR	CZ-CE2-CD2	6.70	125.83	119.80
1	B	210	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	C	356	TRP	CG-CD2-CE3	-6.67	127.90	133.90
1	E	196	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	C	39	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	262	PHE	CB-CG-CD2	6.61	125.43	120.80
1	A	196	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	B	215	LYS	CB-CA-C	6.58	123.55	110.40
1	E	223	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	A	223	PHE	CB-CG-CD2	-6.55	116.21	120.80
1	A	233	SER	CB-CA-C	-6.55	97.66	110.10
1	D	31	PHE	CB-CG-CD1	6.54	125.38	120.80
1	E	233	SER	CB-CA-C	-6.54	97.68	110.10
1	D	188	TYR	CG-CD1-CE1	6.53	126.53	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	123	MET	CG-SD-CE	-6.50	89.81	100.20
1	D	91	TYR	CG-CD1-CE1	-6.49	116.11	121.30
1	C	240	TYR	N-CA-CB	6.48	122.26	110.60
1	B	132	MET	CG-SD-CE	-6.47	89.85	100.20
1	A	34	ILE	CA-CB-CG1	6.45	123.26	111.00
1	C	352	PHE	CB-CG-CD1	6.44	125.31	120.80
1	C	256	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	E	34	ILE	CA-CB-CG1	6.43	123.21	111.00
1	B	198	TYR	N-CA-CB	6.42	122.15	110.60
1	D	37	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	D	37	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	207	GLU	OE1-CD-OE2	6.37	130.94	123.30
1	C	91	TYR	CD1-CE1-CZ	6.36	125.53	119.80
1	D	163	VAL	CA-CB-CG2	-6.36	101.36	110.90
1	C	337	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	D	223	PHE	CB-CG-CD1	6.35	125.24	120.80
1	E	207	GLU	OE1-CD-OE2	6.34	130.91	123.30
1	B	254	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	C	223	PHE	CB-CG-CD2	6.33	125.23	120.80
1	C	53	TYR	CB-CG-CD1	6.30	124.78	121.00
1	C	188	TYR	CB-CG-CD2	6.28	124.77	121.00
1	D	91	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	A	35	VAL	N-CA-C	-6.26	94.09	111.00
1	E	35	VAL	N-CA-C	-6.25	94.11	111.00
1	C	53	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	D	65	LEU	CB-CG-CD1	6.25	121.63	111.00
1	C	340	TRP	CD1-NE1-CE2	-6.22	103.40	109.00
1	B	306	TYR	CD1-CE1-CZ	6.21	125.39	119.80
1	D	306	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	C	335	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	11	ASP	CB-CG-OD1	6.18	123.86	118.30
1	D	35	VAL	N-CA-C	-6.16	94.37	111.00
1	A	332	PRO	N-CA-CB	6.15	110.68	103.30
1	E	332	PRO	N-CA-CB	6.14	110.67	103.30
1	C	256	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	B	188	TYR	CG-CD2-CE2	-6.13	116.39	121.30
1	D	168	GLY	N-CA-C	-6.12	97.81	113.10
1	A	37	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	199	SER	N-CA-CB	6.11	119.66	110.50
1	C	91	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	B	356	TRP	CB-CG-CD2	-6.08	118.69	126.60
1	C	95	ARG	NE-CZ-NH1	6.08	123.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	MET	CA-CB-CG	6.08	123.64	113.30
1	E	227	MET	CA-CB-CG	6.06	123.61	113.30
1	D	340	TRP	CG-CD2-CE3	-6.05	128.46	133.90
1	B	28	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	E	37	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	E	133	TYR	CB-CG-CD2	6.02	124.61	121.00
1	D	37	ARG	NH1-CZ-NH2	-5.99	112.81	119.40
1	D	62	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	E	24	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	C	279	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	C	179	ASP	CA-CB-CG	-5.97	100.27	113.40
1	A	133	TYR	CB-CG-CD2	5.96	124.58	121.00
1	A	88	HIS	CA-CB-CG	5.95	123.72	113.60
1	E	200	PHE	CB-CG-CD1	5.94	124.96	120.80
1	E	294	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	A	340	TRP	CG-CD2-CE3	-5.93	128.56	133.90
1	E	88	HIS	CA-CB-CG	5.93	123.68	113.60
1	B	306	TYR	CG-CD2-CE2	5.93	126.04	121.30
1	A	24	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	240	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	E	130	PRO	N-CD-CG	5.92	112.08	103.20
1	A	130	PRO	N-CD-CG	5.92	112.08	103.20
1	D	313	MET	CG-SD-CE	-5.91	90.74	100.20
1	E	240	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	E	340	TRP	CG-CD2-CE3	-5.91	128.58	133.90
1	D	237	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	B	243	PRO	O-C-N	5.90	132.14	122.70
1	A	200	PHE	CB-CG-CD1	5.89	124.92	120.80
1	D	198	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	A	294	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	C	113	LYS	CB-CG-CD	5.88	126.89	111.60
1	D	286	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	155	SER	N-CA-C	-5.86	95.19	111.00
1	B	131	ALA	CB-CA-C	-5.85	101.33	110.10
1	C	136	ILE	C-N-CA	5.84	136.30	121.70
1	C	276	GLU	N-CA-CB	5.83	121.10	110.60
1	C	344	SER	CB-CA-C	-5.82	99.04	110.10
1	D	188	TYR	CB-CG-CD2	5.82	124.49	121.00
1	E	238	LYS	N-CA-CB	5.81	121.06	110.60
1	C	11	ASP	N-CA-CB	5.81	121.05	110.60
1	A	220	ALA	N-CA-CB	5.80	118.22	110.10
1	B	53	TYR	CB-CG-CD2	5.80	124.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	LYS	N-CA-CB	5.79	121.03	110.60
1	D	39	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	C	31	PHE	N-CA-CB	5.79	121.02	110.60
1	E	220	ALA	N-CA-CB	5.79	118.20	110.10
1	A	16	LEU	N-CA-CB	5.79	121.97	110.40
1	E	299	MET	CG-SD-CE	-5.78	90.95	100.20
1	C	361	GLU	N-CA-CB	5.78	121.01	110.60
1	E	279	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	335	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	C	240	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	279	TYR	CB-CG-CD2	-5.77	117.53	121.00
1	A	124	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	299	MET	CG-SD-CE	-5.77	90.96	100.20
1	D	238	LYS	N-CA-CB	5.77	120.99	110.60
1	C	266	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	E	16	LEU	N-CA-CB	5.77	121.94	110.40
1	E	124	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	D	319	ALA	N-CA-CB	5.76	118.16	110.10
1	C	8	LEU	CB-CG-CD2	5.75	120.78	111.00
1	E	335	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	A	138	ALA	CB-CA-C	-5.74	101.49	110.10
1	D	177	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	138	ALA	CB-CA-C	-5.73	101.50	110.10
1	B	325	MET	N-CA-CB	5.71	120.87	110.60
1	D	80	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	322	PRO	N-CD-CG	5.70	111.75	103.20
1	C	254	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	283	MET	N-CA-CB	5.70	120.85	110.60
1	C	43	VAL	CA-CB-CG2	5.69	119.43	110.90
1	D	230	ALA	N-CA-CB	5.69	118.06	110.10
1	D	202	THR	N-CA-CB	5.68	121.09	110.30
1	C	363	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	B	140	LEU	CB-CG-CD1	5.66	120.61	111.00
1	D	22	ALA	N-CA-CB	5.65	118.02	110.10
1	B	220	ALA	CB-CA-C	-5.65	101.63	110.10
1	E	4	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	E	298	VAL	CG1-CB-CG2	-5.63	101.88	110.90
1	E	16	LEU	CB-CA-C	-5.63	99.51	110.20
1	A	4	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	B	277	THR	CA-CB-CG2	-5.62	104.54	112.40
1	A	298	VAL	CG1-CB-CG2	-5.61	101.92	110.90
1	A	16	LEU	CB-CA-C	-5.61	99.54	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	373	LYS	N-CA-CB	5.60	120.68	110.60
1	B	133	TYR	CG-CD1-CE1	-5.60	116.82	121.30
1	C	133	TYR	CG-CD1-CE1	-5.58	116.84	121.30
1	D	311	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	D	30	VAL	CA-CB-CG1	-5.56	102.56	110.90
1	C	290	ARG	CB-CA-C	-5.56	99.29	110.40
1	A	372	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	244	ASP	N-CA-CB	5.54	120.58	110.60
1	D	91	TYR	CD1-CE1-CZ	5.54	124.79	119.80
1	D	95	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	262	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	C	355	MET	CG-SD-CE	5.50	109.00	100.20
1	E	189	LEU	CB-CG-CD1	5.50	120.35	111.00
1	A	189	LEU	CB-CG-CD1	5.50	120.34	111.00
1	D	255	PHE	CB-CG-CD2	5.47	124.63	120.80
1	E	372	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	49	GLN	O-C-N	-5.46	113.96	122.70
1	D	166	TYR	CB-CG-CD2	5.46	124.27	121.00
1	B	230	ALA	N-CA-CB	5.45	117.73	110.10
1	C	181	ALA	CB-CA-C	5.45	118.28	110.10
1	C	256	ARG	CD-NE-CZ	-5.45	115.97	123.60
1	B	32	PRO	O-C-N	5.45	131.42	122.70
1	B	123	MET	CG-SD-CE	-5.45	91.48	100.20
1	C	223	PHE	CG-CD2-CE2	5.44	126.78	120.80
1	E	222	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	222	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	135	ALA	N-CA-CB	5.41	117.67	110.10
1	B	200	PHE	N-CA-CB	5.40	120.32	110.60
1	C	310	ALA	N-CA-CB	5.39	117.65	110.10
1	D	237	GLU	CA-CB-CG	-5.39	101.54	113.40
1	C	37	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	D	321	ALA	O-C-N	-5.38	110.87	121.10
1	E	169	TYR	CD1-CE1-CZ	5.37	124.63	119.80
1	A	306	TYR	CD1-CE1-CZ	-5.36	114.97	119.80
1	E	240	TYR	N-CA-C	-5.36	96.53	111.00
1	C	139	VAL	CA-CB-CG2	-5.36	102.86	110.90
1	B	202	THR	N-CA-CB	5.35	120.47	110.30
1	C	96	VAL	CA-CB-CG1	5.35	118.93	110.90
1	A	240	TYR	N-CA-C	-5.35	96.56	111.00
1	A	169	TYR	CD1-CE1-CZ	5.35	124.61	119.80
1	B	267	ILE	CB-CA-C	-5.34	100.91	111.60
1	B	325	MET	CA-CB-CG	5.34	122.38	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	157	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	330	ILE	N-CA-C	-5.34	96.58	111.00
1	E	362	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	E	306	TYR	CD1-CE1-CZ	-5.34	115.00	119.80
1	B	306	TYR	CG-CD1-CE1	-5.32	117.04	121.30
1	B	331	ALA	N-CA-CB	5.31	117.54	110.10
1	C	147	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	116	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	86	TRP	CG-CD2-CE3	-5.29	129.14	133.90
1	C	295	ALA	CB-CA-C	-5.29	102.17	110.10
1	A	356	TRP	CA-CB-CG	5.29	123.74	113.70
1	C	196	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	C	340	TRP	CB-CG-CD2	-5.29	119.73	126.60
1	E	356	TRP	CA-CB-CG	5.29	123.74	113.70
1	A	362	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	B	290	ARG	CB-CA-C	-5.28	99.85	110.40
1	A	143	TYR	CB-CG-CD1	5.28	124.17	121.00
1	C	75	ILE	N-CA-C	-5.28	96.75	111.00
1	D	294	TYR	CD1-CG-CD2	5.28	123.70	117.90
1	E	143	TYR	CG-CD1-CE1	-5.27	117.08	121.30
1	D	302	GLY	O-C-N	5.26	131.11	122.70
1	D	127	PHE	CB-CG-CD1	5.25	124.47	120.80
1	C	290	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	143	TYR	CB-CG-CD1	5.24	124.14	121.00
1	A	143	TYR	CG-CD1-CE1	-5.23	117.11	121.30
1	C	279	TYR	N-CA-CB	5.23	120.02	110.60
1	B	162	ASN	N-CA-CB	5.23	120.02	110.60
1	C	9	VAL	N-CA-C	-5.22	96.90	111.00
1	B	216	LEU	O-C-N	-5.22	114.34	122.70
1	A	154	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	200	PHE	CB-CG-CD2	5.22	124.45	120.80
1	B	319	ALA	N-CA-CB	5.22	117.40	110.10
1	D	147	ARG	N-CA-CB	5.21	119.98	110.60
1	C	199	SER	CB-CA-C	-5.21	100.20	110.10
1	D	240	TYR	CZ-CE2-CD2	-5.21	115.11	119.80
1	C	240	TYR	CD1-CE1-CZ	5.20	124.48	119.80
1	E	154	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	54	VAL	CB-CA-C	5.20	121.28	111.40
1	C	375	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	B	331	ALA	CB-CA-C	-5.20	102.30	110.10
1	A	21	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	C	24	ASP	CA-CB-CG	-5.19	101.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	200	PHE	CB-CG-CD1	5.19	124.43	120.80
1	B	91	TYR	CG-CD2-CE2	5.19	125.45	121.30
1	C	202	THR	O-C-N	-5.19	114.40	122.70
1	D	356	TRP	CA-CB-CG	5.18	123.55	113.70
1	B	157	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	176	MET	CB-CA-C	-5.18	100.04	110.40
1	E	21	PHE	CB-CG-CD2	-5.18	117.18	120.80
1	B	185	LEU	CB-CA-C	-5.17	100.37	110.20
1	B	104	LEU	CB-CG-CD1	5.17	119.79	111.00
1	D	312	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	62	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	227	MET	CG-SD-CE	5.14	108.43	100.20
1	C	228	ALA	CB-CA-C	-5.14	102.40	110.10
1	D	340	TRP	NE1-CE2-CZ2	5.13	136.05	130.40
1	C	196	ARG	NH1-CZ-NH2	5.13	125.05	119.40
1	D	123	MET	N-CA-CB	5.13	119.84	110.60
1	A	263	GLN	CB-CG-CD	5.12	124.91	111.60
1	B	279	TYR	CG-CD2-CE2	-5.12	117.20	121.30
1	C	288	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	11	ASP	N-CA-CB	5.12	119.81	110.60
1	E	11	ASP	N-CA-CB	5.12	119.81	110.60
1	E	340	TRP	CE2-CD2-CE3	5.12	124.84	118.70
1	E	263	GLN	CB-CG-CD	5.10	124.87	111.60
1	C	173	HIS	CA-CB-CG	5.10	122.27	113.60
1	E	340	TRP	CB-CG-CD2	-5.09	119.98	126.60
1	A	340	TRP	CE2-CD2-CE3	5.09	124.80	118.70
1	D	332	PRO	CA-C-O	-5.08	108.01	120.20
1	E	100	GLU	OE1-CD-OE2	5.07	129.39	123.30
1	C	333	PRO	O-C-N	5.07	130.82	122.70
1	D	47	MET	N-CA-CB	5.07	119.72	110.60
1	D	319	ALA	CB-CA-C	-5.07	102.50	110.10
1	D	73	HIS	N-CA-CB	5.06	119.71	110.60
1	E	26	ALA	CA-C-O	-5.06	109.48	120.10
1	C	101	HIS	CB-CA-C	-5.05	100.29	110.40
1	E	72	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	A	72	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	A	100	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	A	340	TRP	CB-CG-CD2	-5.05	120.04	126.60
1	C	286	ASP	C-N-CA	5.05	134.32	121.70
1	A	26	ALA	CA-C-O	-5.04	109.51	120.10
1	A	240	TYR	N-CA-CB	5.04	119.68	110.60
1	A	356	TRP	CE3-CZ3-CH2	-5.04	115.66	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	356	TRP	CB-CG-CD1	5.04	133.55	127.00
1	E	240	TYR	N-CA-CB	5.04	119.66	110.60
1	D	133	TYR	N-CA-CB	5.03	119.65	110.60
1	C	34	ILE	CA-CB-CG2	-5.02	100.85	110.90
1	A	232	SER	N-CA-C	-5.02	97.45	111.00
1	B	218	TYR	CB-CG-CD1	5.02	124.01	121.00
1	D	154	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	361	GLU	CB-CA-C	-5.02	100.37	110.40
1	D	190	MET	CG-SD-CE	-5.01	92.18	100.20
1	E	232	SER	N-CA-C	-5.01	97.47	111.00
1	E	356	TRP	CE3-CZ3-CH2	-5.01	115.69	121.20
1	A	231	ALA	N-CA-CB	5.01	117.11	110.10
1	A	312	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	D	216	LEU	CB-CA-C	-5.00	100.70	110.20
1	E	312	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	PHE	Sidechain
1	A	218	TYR	Sidechain
1	A	223	PHE	Sidechain
1	A	240	TYR	Sidechain
1	A	279	TYR	Sidechain
1	A	28	ARG	Sidechain
1	A	294	TYR	Sidechain
1	A	306	TYR	Sidechain
1	A	335	ARG	Sidechain
1	A	337	TYR	Sidechain
1	A	362	TYR	Sidechain
1	A	69	TYR	Sidechain
1	A	88	HIS	Sidechain
1	A	91	TYR	Sidechain
1	A	95	ARG	Sidechain
1	B	133	TYR	Sidechain
1	B	143	TYR	Sidechain
1	B	169	TYR	Sidechain
1	B	206	ARG	Sidechain
1	B	240	TYR	Sidechain
1	B	279	TYR	Sidechain
1	B	294	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	306	TYR	Sidechain
1	B	53	TYR	Sidechain
1	B	90	PHE	Sidechain
1	B	95	ARG	Sidechain
1	C	169	TYR	Sidechain
1	C	188	TYR	Sidechain
1	C	218	TYR	Sidechain
1	C	240	TYR	Sidechain
1	C	266	PHE	Sidechain
1	C	279	TYR	Sidechain
1	C	290	ARG	Sidechain
1	C	294	TYR	Sidechain
1	C	306	TYR	Sidechain
1	C	335	ARG	Sidechain
1	C	69	TYR	Sidechain
1	C	95	ARG	Sidechain
1	D	133	TYR	Sidechain
1	D	198	TYR	Sidechain
1	D	256	ARG	Sidechain
1	D	279	TYR	Sidechain
1	D	294	TYR	Sidechain
1	D	362	TYR	Sidechain
1	D	372	ARG	Sidechain
1	D	69	TYR	Sidechain
1	E	124	PHE	Sidechain
1	E	218	TYR	Sidechain
1	E	223	PHE	Sidechain
1	E	240	TYR	Sidechain
1	E	279	TYR	Sidechain
1	E	28	ARG	Sidechain
1	E	294	TYR	Sidechain
1	E	306	TYR	Sidechain
1	E	335	ARG	Sidechain
1	E	337	TYR	Sidechain
1	E	362	TYR	Sidechain
1	E	69	TYR	Sidechain
1	E	88	HIS	Sidechain
1	E	91	TYR	Sidechain
1	E	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	A	2933	0	2894	18	0
1	B	2933	0	2894	26	0
1	C	2933	0	2894	14	0
1	D	2933	0	2893	195	0
1	E	2933	0	2893	202	0
2	F	680	0	138	0	0
2	G	680	0	138	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	2	0
3	E	27	0	12	0	0
All	All	16160	0	14804	266	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 9.

All (266) 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:D:40:HIS:CD2	1:E:166:TYR:CD1	1.88	1.62
1:D:43:VAL:CG1	1:E:139:VAL:HG22	1.35	1.54
1:D:40:HIS:CD2	1:E:166:TYR:HD1	1.17	1.53
1:D:64:ILE:HD11	1:E:289:ILE:CG2	1.38	1.51
1:D:243:PRO:C	1:E:324:THR:HG21	1.36	1.46
1:D:64:ILE:CD1	1:E:289:ILE:HG21	1.43	1.43
1:D:243:PRO:CA	1:E:324:THR:CG2	2.00	1.39
1:D:64:ILE:CD1	1:E:289:ILE:CG2	1.97	1.39
1:B:195:GLU:HG2	1:E:110:LEU:CB	1.57	1.33
1:D:243:PRO:HA	1:E:324:THR:CG2	1.59	1.31
1:D:40:HIS:CG	1:E:166:TYR:HB2	1.66	1.30
1:D:40:HIS:HD2	1:E:166:TYR:CD1	1.35	1.28
1:D:243:PRO:C	1:E:324:THR:CG2	2.04	1.25
1:D:244:ASP:N	1:E:324:THR:HG21	1.50	1.25
1:D:243:PRO:CA	1:E:324:THR:HG21	1.58	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:MET:O	1:E:169:TYR:CD1	1.91	1.24
1:D:64:ILE:HG21	1:E:166:TYR:CE1	1.71	1.23
1:D:40:HIS:CG	1:E:166:TYR:CD1	2.26	1.23
1:D:39:ARG:HH21	1:E:286:ASP:CG	1.41	1.23
1:D:64:ILE:CG2	1:E:166:TYR:HE1	1.52	1.20
1:D:63:GLY:N	1:E:288:ASP:HB3	1.57	1.19
1:D:63:GLY:HA2	1:E:286:ASP:OD2	1.39	1.18
1:B:195:GLU:CG	1:E:110:LEU:HB3	1.73	1.18
1:D:44:MET:H	1:E:169:TYR:HA	1.05	1.17
1:D:64:ILE:CG2	1:E:166:TYR:CE1	2.28	1.16
1:D:243:PRO:O	1:E:324:THR:CB	1.94	1.15
1:D:40:HIS:HB2	1:E:166:TYR:CD1	1.83	1.12
1:D:40:HIS:CB	1:E:166:TYR:CD1	2.32	1.12
1:D:43:VAL:CG1	1:E:139:VAL:CG2	2.27	1.11
1:D:43:VAL:HG11	1:E:139:VAL:CG2	1.80	1.11
1:D:64:ILE:HD13	1:E:289:ILE:HG21	1.13	1.10
1:D:43:VAL:HG13	1:E:139:VAL:HG22	1.29	1.10
1:D:244:ASP:HB3	1:E:290:ARG:NH1	1.67	1.10
1:D:40:HIS:CD2	1:E:166:TYR:CG	2.40	1.08
1:D:40:HIS:CG	1:E:166:TYR:CB	2.36	1.07
1:D:64:ILE:HD13	1:E:289:ILE:HD13	1.30	1.06
1:D:243:PRO:HB2	1:E:324:THR:HB	1.37	1.06
1:D:243:PRO:O	1:E:324:THR:HB	1.54	1.06
1:D:63:GLY:HA2	1:E:286:ASP:CG	1.75	1.06
1:D:64:ILE:HG12	1:E:289:ILE:HG12	1.10	1.05
1:D:41:GLN:HB3	1:E:171:LEU:O	1.54	1.05
1:D:243:PRO:CA	1:E:324:THR:HG22	1.82	1.04
1:D:40:HIS:CG	1:E:166:TYR:HD1	1.64	1.03
1:D:63:GLY:CA	1:E:286:ASP:OD2	1.98	1.03
1:D:46:GLY:N	1:E:167:GLU:O	1.89	1.02
1:D:64:ILE:HD11	1:E:289:ILE:HG23	1.04	1.01
1:D:243:PRO:HA	1:E:324:THR:HG22	1.35	1.00
1:D:62:ARG:HB2	1:E:288:ASP:HB2	1.42	1.00
1:D:43:VAL:HB	1:E:165:ILE:HB	1.45	0.99
1:D:64:ILE:HG21	1:E:166:TYR:HE1	0.82	0.98
1:D:64:ILE:HG12	1:E:289:ILE:CG1	1.90	0.98
1:D:39:ARG:NH2	1:E:286:ASP:CG	2.16	0.98
1:D:43:VAL:HG11	1:E:139:VAL:HG22	0.98	0.97
1:D:63:GLY:H	1:E:288:ASP:HB3	1.23	0.97
1:D:44:MET:N	1:E:169:TYR:HA	1.67	0.96
1:D:47:MET:C	1:E:167:GLU:CG	2.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:CG	1:E:166:TYR:CG	2.53	0.95
1:B:195:GLU:HG2	1:E:110:LEU:HB3	0.96	0.95
1:D:44:MET:HA	1:E:166:TYR:O	1.67	0.95
1:D:243:PRO:C	1:E:324:THR:CB	2.29	0.95
1:D:47:MET:O	1:E:167:GLU:OE2	1.85	0.95
1:D:62:ARG:HB2	1:E:288:ASP:CB	1.97	0.95
1:B:195:GLU:OE1	1:E:111:ASN:C	2.06	0.94
1:D:64:ILE:CG1	1:E:289:ILE:HG12	1.98	0.93
1:D:243:PRO:O	1:E:324:THR:OG1	1.85	0.93
1:D:63:GLY:O	1:E:286:ASP:HB3	1.67	0.93
1:D:40:HIS:CD2	1:E:166:TYR:CB	2.54	0.90
1:D:63:GLY:C	1:E:286:ASP:HB3	1.92	0.90
1:D:243:PRO:CB	1:E:324:THR:HG22	2.02	0.90
1:D:43:VAL:HG12	1:E:165:ILE:HG12	1.53	0.89
1:D:47:MET:C	1:E:167:GLU:HG3	1.93	0.89
1:D:63:GLY:HA3	1:E:289:ILE:N	1.86	0.89
1:D:43:VAL:HG13	1:E:139:VAL:CG2	1.97	0.88
1:D:39:ARG:NH2	1:E:286:ASP:OD1	2.08	0.87
1:D:64:ILE:HD13	1:E:289:ILE:CD1	2.04	0.87
1:D:47:MET:O	1:E:167:GLU:CG	2.23	0.86
1:D:39:ARG:CZ	1:E:286:ASP:HB2	2.05	0.85
1:D:243:PRO:CB	1:E:324:THR:CG2	2.54	0.85
1:D:243:PRO:HA	1:E:324:THR:HG21	1.26	0.85
1:D:41:GLN:O	1:E:170:ALA:CB	2.24	0.85
1:D:40:HIS:ND1	1:E:166:TYR:HB2	1.93	0.84
1:D:63:GLY:HA2	1:E:286:ASP:CB	2.08	0.84
1:D:243:PRO:HB2	1:E:324:THR:CB	2.09	0.82
1:D:39:ARG:NE	1:E:286:ASP:HB2	1.95	0.81
1:D:47:MET:O	1:E:167:GLU:CD	2.21	0.79
1:D:64:ILE:CD1	1:E:289:ILE:HG23	1.86	0.79
1:D:244:ASP:HB3	1:E:290:ARG:HH12	1.46	0.78
1:D:44:MET:H	1:E:169:TYR:CA	1.91	0.78
1:D:64:ILE:CG1	1:E:289:ILE:CG1	2.59	0.77
1:D:40:HIS:CB	1:E:166:TYR:CG	2.66	0.77
1:B:195:GLU:OE1	1:E:111:ASN:O	2.03	0.77
1:D:40:HIS:NE2	1:E:149:THR:HG23	2.00	0.77
1:D:46:GLY:HA3	1:E:148:THR:HB	1.66	0.76
1:D:44:MET:O	1:E:169:TYR:HD1	1.69	0.75
1:D:48:GLY:N	1:E:167:GLU:HG3	2.02	0.75
1:D:41:GLN:HA	1:E:171:LEU:H	1.52	0.75
1:D:64:ILE:CD1	1:E:289:ILE:HD13	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:PRO:CB	1:E:324:THR:HB	2.16	0.74
1:D:39:ARG:NH2	1:E:286:ASP:CB	2.51	0.74
1:D:43:VAL:HG12	1:E:165:ILE:CG1	2.18	0.73
1:D:45:VAL:CG2	1:E:139:VAL:HG13	2.18	0.73
1:D:40:HIS:NE2	1:E:166:TYR:HA	2.03	0.73
1:D:63:GLY:CA	1:E:286:ASP:HB3	2.18	0.73
1:D:244:ASP:HB3	1:E:290:ARG:HH11	1.55	0.72
1:D:39:ARG:NH2	1:E:286:ASP:HB2	2.06	0.71
1:D:43:VAL:CG1	1:E:165:ILE:HD13	2.19	0.71
1:D:63:GLY:N	1:E:288:ASP:CB	2.47	0.71
1:D:46:GLY:CA	1:E:167:GLU:HA	2.22	0.70
1:D:44:MET:O	1:E:169:TYR:CG	2.44	0.69
1:D:64:ILE:HG23	1:E:166:TYR:CE1	2.23	0.69
1:D:63:GLY:HA3	1:E:288:ASP:C	2.12	0.69
1:D:45:VAL:HG21	1:E:139:VAL:HG13	1.76	0.68
1:D:64:ILE:HD13	1:E:289:ILE:CG2	1.89	0.68
1:B:195:GLU:HG2	1:E:110:LEU:HB2	1.71	0.68
1:D:47:MET:O	1:E:167:GLU:HG3	1.92	0.67
1:D:244:ASP:N	1:E:324:THR:CG2	2.39	0.67
1:D:243:PRO:CB	1:E:324:THR:CB	2.72	0.65
1:B:195:GLU:HG2	1:E:110:LEU:CA	2.24	0.65
1:D:40:HIS:CD2	1:E:166:TYR:HA	2.30	0.65
1:D:64:ILE:CD1	1:E:289:ILE:CD1	2.72	0.64
1:D:62:ARG:CB	1:E:288:ASP:HB2	2.24	0.64
1:D:244:ASP:CB	1:E:290:ARG:NH1	2.55	0.63
1:C:40:HIS:CE1	1:D:170:ALA:HA	2.33	0.63
1:D:63:GLY:HA2	1:E:286:ASP:HB3	1.74	0.63
1:D:45:VAL:HG21	1:E:139:VAL:CG1	2.31	0.61
1:D:39:ARG:HH21	1:E:286:ASP:CB	2.07	0.61
1:D:40:HIS:CD2	1:E:166:TYR:CA	2.84	0.60
1:D:42:GLY:HA3	1:E:164:PRO:O	2.02	0.60
1:D:46:GLY:HA3	1:E:167:GLU:HA	1.82	0.60
1:D:40:HIS:CE1	1:E:165:ILE:C	2.75	0.59
1:D:41:GLN:O	1:E:170:ALA:HB2	2.01	0.59
1:D:44:MET:O	1:E:169:TYR:HA	2.03	0.59
1:D:43:VAL:HG21	1:E:163:VAL:HG11	1.85	0.58
1:D:244:ASP:HA	1:E:324:THR:OG1	2.04	0.58
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.85	0.57
1:D:53:TYR:OH	1:E:166:TYR:OH	2.05	0.57
1:D:45:VAL:CG2	1:E:139:VAL:CG1	2.82	0.57
1:D:40:HIS:HB2	1:E:166:TYR:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:TYR:CZ	3:D:401:ADP:H2	2.23	0.56
1:C:212:ILE:HG12	1:C:240:TYR:CE2	2.41	0.56
1:D:47:MET:N	1:E:167:GLU:OE2	2.36	0.56
1:D:48:GLY:CA	1:E:167:GLU:HG3	2.35	0.56
1:C:136:ILE:HD12	1:C:136:ILE:N	2.21	0.56
1:D:64:ILE:CD1	1:E:289:ILE:CG1	2.82	0.55
1:D:244:ASP:OD1	1:E:287:ILE:HG23	2.08	0.54
1:D:45:VAL:HB	1:E:142:LEU:HD23	1.90	0.54
1:D:40:HIS:HB3	1:E:166:TYR:CG	2.42	0.54
1:D:45:VAL:C	1:E:167:GLU:O	2.45	0.54
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.91	0.53
1:D:44:MET:O	1:E:169:TYR:CA	2.56	0.53
1:D:43:VAL:CB	1:E:165:ILE:HB	2.25	0.53
1:B:202:THR:HG21	1:E:270:GLU:HG2	1.91	0.53
1:B:9:VAL:HG21	1:B:344:SER:HA	1.91	0.53
1:D:243:PRO:C	1:E:324:THR:HB	2.12	0.52
1:E:173:HIS:CG	1:E:174:ALA:H	2.26	0.52
1:E:43:VAL:HG12	1:E:44:MET:H	1.74	0.52
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.91	0.52
1:D:171:LEU:HD13	1:D:173:HIS:HB3	1.91	0.52
1:A:43:VAL:HG12	1:A:44:MET:H	1.74	0.52
1:D:46:GLY:CA	1:E:148:THR:HB	2.37	0.52
1:D:9:VAL:HG23	1:D:22:ALA:HA	1.91	0.52
1:D:40:HIS:CE1	1:E:166:TYR:CA	2.93	0.51
1:A:173:HIS:CG	1:A:174:ALA:H	2.26	0.51
1:D:40:HIS:NE2	1:E:166:TYR:CA	2.72	0.51
1:D:62:ARG:CB	1:E:288:ASP:CB	2.81	0.51
1:D:244:ASP:CG	1:E:287:ILE:HG23	2.30	0.51
1:A:173:HIS:CD2	1:A:174:ALA:H	2.30	0.50
1:D:244:ASP:OD1	1:E:290:ARG:HD2	2.11	0.50
1:B:102:PRO:HA	1:B:129:VAL:HG12	1.93	0.50
1:D:43:VAL:CG2	1:E:163:VAL:CG1	2.89	0.50
1:D:244:ASP:OD2	1:E:287:ILE:HG23	2.12	0.50
1:D:64:ILE:CD1	1:E:289:ILE:CB	2.86	0.49
1:D:243:PRO:HB3	1:E:324:THR:HG22	1.90	0.49
1:D:41:GLN:CA	1:E:171:LEU:H	2.24	0.49
1:D:151:ILE:HG23	1:D:297:ASN:HA	1.94	0.49
1:E:173:HIS:CD2	1:E:174:ALA:H	2.30	0.49
1:D:43:VAL:CG1	1:E:165:ILE:CD1	2.83	0.49
1:A:18:LYS:O	1:A:340:TRP:CD1	2.66	0.49
1:D:1:ASP:OD2	1:D:101:HIS:CE1	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:CE1	1:E:165:ILE:O	2.66	0.48
1:B:113:LYS:HE2	1:D:196:ARG:HH21	1.77	0.48
1:D:40:HIS:CD2	1:E:166:TYR:HB2	2.26	0.48
1:E:18:LYS:O	1:E:340:TRP:CD1	2.66	0.48
1:D:44:MET:HE1	1:E:168:GLY:HA3	1.65	0.48
1:D:64:ILE:HD13	1:E:289:ILE:CG1	2.42	0.48
1:B:121:GLN:O	1:B:125:GLU:HB2	2.14	0.48
1:D:212:ILE:HG12	1:D:240:TYR:CD2	2.49	0.48
1:D:40:HIS:CE1	1:E:166:TYR:N	2.82	0.47
1:D:40:HIS:CB	1:E:166:TYR:HB2	2.39	0.47
1:D:215:LYS:HG3	1:D:216:LEU:HD12	1.96	0.47
1:D:43:VAL:HG12	1:E:165:ILE:CD1	2.39	0.47
1:E:133:TYR:CE2	1:E:135:ALA:HA	2.50	0.47
1:B:195:GLU:OE1	1:E:111:ASN:CA	2.62	0.47
1:C:7:ALA:HB2	1:C:102:PRO:HB2	1.97	0.47
1:D:9:VAL:HG21	1:D:344:SER:HA	1.98	0.46
1:A:133:TYR:CE2	1:A:135:ALA:HA	2.50	0.46
1:B:1:ASP:OD2	1:B:101:HIS:CE1	2.68	0.46
1:E:220:ALA:HB2	1:E:255:PHE:HB2	1.98	0.46
1:C:53:TYR:HB3	1:C:58:ALA:HA	1.98	0.45
1:A:90:PHE:CD2	1:A:96:VAL:HG23	2.52	0.45
1:A:220:ALA:HB2	1:A:255:PHE:HB2	1.98	0.45
1:D:40:HIS:CE1	1:E:166:TYR:HB2	2.50	0.45
1:B:216:LEU:HD11	1:B:240:TYR:CD1	2.52	0.45
1:B:279:TYR:CZ	1:B:320:LEU:HB2	2.51	0.45
1:D:46:GLY:CA	1:E:167:GLU:CA	2.85	0.45
1:D:306:TYR:CE1	3:D:401:ADP:C2	3.04	0.45
1:C:306:TYR:O	1:C:309:ILE:HG22	2.16	0.45
1:B:117:GLU:HA	1:B:370:VAL:HG21	1.99	0.45
1:D:63:GLY:CA	1:E:286:ASP:CB	2.81	0.45
1:D:41:GLN:HE22	1:E:171:LEU:HD22	1.82	0.45
1:E:90:PHE:CD2	1:E:96:VAL:HG23	2.52	0.45
1:B:139:VAL:HG11	1:B:169:TYR:CE2	2.52	0.45
1:B:306:TYR:O	1:B:309:ILE:HG22	2.17	0.44
1:B:165:ILE:HA	1:B:165:ILE:HD12	1.79	0.44
1:D:43:VAL:CG2	1:E:163:VAL:HG11	2.48	0.44
1:C:317:ILE:O	1:C:321:ALA:HB3	2.16	0.44
1:D:220:ALA:HB2	1:D:255:PHE:HB2	1.98	0.44
1:C:159:VAL:HG11	1:C:177:ARG:HD2	2.00	0.44
1:E:113:LYS:O	1:E:371:HIS:HE1	2.01	0.44
1:D:22:ALA:HB1	1:D:347:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:HG3	1:A:339:VAL:HG11	2.00	0.44
1:D:49:GLN:O	1:D:50:LYS:HG2	2.17	0.44
1:E:361:GLU:HB3	1:E:369:ILE:HG12	2.00	0.44
1:E:117:GLU:OE1	1:E:371:HIS:CE1	2.71	0.43
1:C:340:TRP:CZ3	1:C:344:SER:OG	2.70	0.43
1:D:76:ILE:HG21	1:D:79:TRP:CD2	2.53	0.43
1:D:62:ARG:C	1:E:288:ASP:HB3	2.32	0.43
1:C:79:TRP:CE2	1:C:118:LYS:HG2	2.54	0.43
1:D:48:GLY:HA2	1:E:167:GLU:HG3	1.99	0.43
1:A:350:SER:O	1:A:353:GLN:HB3	2.19	0.43
1:A:113:LYS:O	1:A:371:HIS:HE1	2.01	0.43
1:A:117:GLU:OE1	1:A:371:HIS:CE1	2.71	0.43
1:E:257:CYS:HB3	1:E:258:PRO:HD3	2.01	0.43
1:E:116:ARG:HD2	1:E:371:HIS:CE1	2.54	0.43
1:D:76:ILE:HG21	1:D:79:TRP:CE3	2.53	0.43
1:D:41:GLN:CB	1:E:171:LEU:O	2.45	0.42
1:E:350:SER:O	1:E:353:GLN:HB3	2.19	0.42
1:B:90:PHE:CD2	1:B:98:PRO:HA	2.54	0.42
1:B:195:GLU:CB	1:E:110:LEU:O	2.46	0.42
1:E:137:GLN:HG3	1:E:339:VAL:HG11	2.00	0.42
1:A:116:ARG:HD2	1:A:371:HIS:CE1	2.54	0.42
1:A:361:GLU:HB3	1:A:369:ILE:HG12	2.00	0.42
1:D:62:ARG:HB2	1:E:288:ASP:CG	2.37	0.42
1:D:45:VAL:HG23	1:E:139:VAL:HG13	2.01	0.42
1:B:202:THR:CG2	1:E:270:GLU:HG2	2.50	0.42
1:B:159:VAL:HG23	1:B:161:HIS:CE1	2.54	0.42
1:C:287:ILE:HG13	1:C:287:ILE:H	1.60	0.42
1:D:44:MET:HE3	1:E:168:GLY:HA2	1.39	0.42
1:C:113:LYS:HD2	1:C:113:LYS:H	1.85	0.42
1:A:351:THR:HA	1:A:354:GLN:HG2	2.02	0.41
1:A:244:ASP:HB3	1:B:287:ILE:HG22	2.01	0.41
1:D:44:MET:CA	1:E:166:TYR:O	2.51	0.41
1:D:72:GLU:HA	1:D:72:GLU:OE1	2.20	0.41
1:D:48:GLY:N	1:E:167:GLU:HB2	2.29	0.41
1:D:64:ILE:HD13	1:E:289:ILE:CB	2.47	0.41
1:C:104:LEU:HD12	1:C:133:TYR:O	2.20	0.41
1:A:257:CYS:HB3	1:A:258:PRO:HD3	2.01	0.41
1:B:140:LEU:O	1:B:342:GLY:HA3	2.20	0.41
1:D:244:ASP:HA	1:E:324:THR:HG1	1.85	0.41
1:D:163:VAL:HA	1:D:175:ILE:HG22	2.03	0.41
1:C:136:ILE:N	1:C:136:ILE:CD1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD11	1:A:240:TYR:CD1	2.56	0.41
1:D:41:GLN:NE2	1:E:171:LEU:HD22	2.36	0.40
1:D:101:HIS:O	1:D:129:VAL:HG13	2.22	0.40
1:E:351:THR:HA	1:E:354:GLN:HG2	2.02	0.40
1:D:43:VAL:N	1:E:165:ILE:HA	2.37	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	A	373/375 (100%)	321 (86%)	40 (11%)	12 (3%)	5 41
1	B	373/375 (100%)	326 (87%)	33 (9%)	14 (4%)	4 37
1	C	373/375 (100%)	322 (86%)	39 (10%)	12 (3%)	5 41
1	D	373/375 (100%)	325 (87%)	37 (10%)	11 (3%)	6 43
1	E	373/375 (100%)	321 (86%)	40 (11%)	12 (3%)	5 41
All	All	1865/1875 (100%)	1615 (87%)	189 (10%)	61 (3%)	8 40

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	246	GLN
1	B	6	THR
1	B	39	ARG
1	B	128	ASN
1	B	173	HIS
1	B	180	LEU
1	C	6	THR
1	C	234	SER

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Mol	Chain	Res	Type
1	C	244	ASP
1	D	6	THR
1	E	6	THR
1	E	246	GLN
1	A	3	ASP
1	A	128	ASN
1	A	180	LEU
1	B	156	GLY
1	B	244	ASP
1	C	174	ALA
1	C	197	GLY
1	D	7	ALA
1	D	39	ARG
1	D	100	GLU
1	E	3	ASP
1	E	128	ASN
1	E	180	LEU
1	A	39	ARG
1	B	158	GLY
1	C	7	ALA
1	C	49	GLN
1	C	180	LEU
1	C	181	ALA
1	D	47	MET
1	D	197	GLY
1	D	238	LYS
1	E	39	ARG
1	A	51	ASP
1	A	244	ASP
1	B	3	ASP
1	B	49	GLN
1	B	234	SER
1	C	173	HIS
1	D	234	SER
1	E	51	ASP
1	E	244	ASP
1	B	194	THR
1	C	129	VAL
1	D	173	HIS
1	B	137	GLN
1	C	3	ASP
1	D	181	ALA

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Mol	Chain	Res	Type
1	A	45	VAL
1	A	322	PRO
1	B	201	VAL
1	E	45	VAL
1	E	322	PRO
1	A	243	PRO
1	E	243	PRO
1	A	15	GLY
1	D	15	GLY
1	E	15	GLY

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	A	318/318 (100%)	293 (92%)	25 (8%)	15 51
1	B	318/318 (100%)	277 (87%)	41 (13%)	5 28
1	C	318/318 (100%)	288 (91%)	30 (9%)	11 42
1	D	318/318 (100%)	288 (91%)	30 (9%)	11 42
1	E	318/318 (100%)	293 (92%)	25 (8%)	15 51
All	All	1590/1590 (100%)	1439 (90%)	151 (10%)	15 41

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	34	ILE
1	A	39	ARG
1	A	69	TYR
1	A	93	GLU
1	A	113	LYS
1	A	117	GLU
1	A	126	THR
1	A	153	LEU

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Mol	Chain	Res	Type
1	A	159	VAL
1	A	183	ARG
1	A	193	LEU
1	A	196	ARG
1	A	203	THR
1	A	219	VAL
1	A	242	LEU
1	A	264	PRO
1	A	276	GLU
1	A	291	LYS
1	A	312	ARG
1	A	315	LYS
1	A	328	LYS
1	A	334	GLU
1	A	356	TRP
1	A	372	ARG
1	B	2	GLU
1	B	25	ASP
1	B	30	VAL
1	B	38	PRO
1	B	39	ARG
1	B	41	GLN
1	B	47	MET
1	B	57	GLU
1	B	69	TYR
1	B	93	GLU
1	B	95	ARG
1	B	110	LEU
1	B	111	ASN
1	B	113	LYS
1	B	128	ASN
1	B	153	LEU
1	B	166	TYR
1	B	171	LEU
1	B	183	ARG
1	B	192	ILE
1	B	193	LEU
1	B	195	GLU
1	B	196	ARG
1	B	218	TYR
1	B	234	SER
1	B	246	GLN

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Mol	Chain	Res	Type
1	B	250	ILE
1	B	261	LEU
1	B	284	LYS
1	B	300	SER
1	B	303	THR
1	B	309	ILE
1	B	312	ARG
1	B	315	LYS
1	B	326	LYS
1	B	328	LYS
1	B	334	GLU
1	B	335	ARG
1	B	353	GLN
1	B	356	TRP
1	B	372	ARG
1	C	24	ASP
1	C	30	VAL
1	C	31	PHE
1	C	39	ARG
1	C	56	ASP
1	C	69	TYR
1	C	106	THR
1	C	113	LYS
1	C	117	GLU
1	C	123	MET
1	C	151	ILE
1	C	153	LEU
1	C	159	VAL
1	C	171	LEU
1	C	183	ARG
1	C	192	ILE
1	C	196	ARG
1	C	241	GLU
1	C	250	ILE
1	C	294	TYR
1	C	311	ASP
1	C	315	LYS
1	C	326	LYS
1	C	328	LYS
1	C	335	ARG
1	C	354	GLN
1	C	356	TRP

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Mol	Chain	Res	Type
1	C	358	THR
1	C	372	ARG
1	C	374	CYS
1	D	8	LEU
1	D	30	VAL
1	D	37	ARG
1	D	39	ARG
1	D	47	MET
1	D	49	GLN
1	D	56	ASP
1	D	93	GLU
1	D	113	LYS
1	D	123	MET
1	D	151	ILE
1	D	153	LEU
1	D	159	VAL
1	D	171	LEU
1	D	184	ASP
1	D	192	ILE
1	D	195	GLU
1	D	196	ARG
1	D	202	THR
1	D	223	PHE
1	D	224	GLU
1	D	261	LEU
1	D	291	LYS
1	D	312	ARG
1	D	315	LYS
1	D	325	MET
1	D	328	LYS
1	D	334	GLU
1	D	335	ARG
1	D	356	TRP
1	E	30	VAL
1	E	34	ILE
1	E	39	ARG
1	E	69	TYR
1	E	93	GLU
1	E	113	LYS
1	E	117	GLU
1	E	126	THR
1	E	153	LEU

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Mol	Chain	Res	Type
1	E	159	VAL
1	E	183	ARG
1	E	193	LEU
1	E	196	ARG
1	E	203	THR
1	E	219	VAL
1	E	242	LEU
1	E	264	PRO
1	E	276	GLU
1	E	291	LYS
1	E	312	ARG
1	E	315	LYS
1	E	328	LYS
1	E	334	GLU
1	E	356	TRP
1	E	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	41	GLN
1	A	225	ASN
1	A	314	GLN
1	A	360	GLN
1	A	371	HIS
1	B	101	HIS
1	B	225	ASN
1	C	12	ASN
1	C	40	HIS
1	C	111	ASN
1	C	252	ASN
1	C	371	HIS
1	D	40	HIS
1	D	78	ASN
1	D	88	HIS
1	D	101	HIS
1	D	111	ASN
1	E	40	HIS
1	E	41	GLN
1	E	173	HIS
1	E	225	ASN

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Mol	Chain	Res	Type
1	E	314	GLN
1	E	360	GLN
1	E	371	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	401	-	24,29,29	1.71	5 (20%)	23,45,45	1.81	7 (30%)
3	ADP	B	401	-	24,29,29	1.32	2 (8%)	23,45,45	1.68	4 (17%)
3	ADP	C	401	-	24,29,29	1.23	2 (8%)	23,45,45	2.10	7 (30%)
3	ADP	D	401	-	24,29,29	1.39	2 (8%)	23,45,45	2.89	8 (34%)
3	ADP	E	401	-	24,29,29	1.72	5 (20%)	23,45,45	1.81	7 (30%)

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
3	ADP	A	401	-	-	0/12/32/32	0/3/3/3
3	ADP	B	401	-	-	0/12/32/32	0/3/3/3
3	ADP	C	401	-	-	0/12/32/32	0/3/3/3
3	ADP	D	401	-	-	0/12/32/32	0/3/3/3
3	ADP	E	401	-	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C2'-C1'	-4.47	1.46	1.53
3	A	401	ADP	C8-N7	-3.12	1.28	1.34
3	E	401	ADP	C8-N7	-3.09	1.28	1.34
3	E	401	ADP	C5-C4	-2.64	1.34	1.40
3	A	401	ADP	C5-C4	-2.62	1.34	1.40
3	B	401	ADP	C4-N3	-2.24	1.32	1.35
3	C	401	ADP	O3'-C3'	-2.17	1.37	1.43
3	E	401	ADP	PA-O2A	-2.04	1.46	1.55
3	A	401	ADP	PA-O2A	-2.04	1.46	1.55
3	C	401	ADP	O4'-C4'	2.94	1.51	1.45
3	D	401	ADP	C4-N3	3.26	1.40	1.35
3	D	401	ADP	O2'-C2'	3.45	1.51	1.43
3	A	401	ADP	C2-N3	3.51	1.38	1.32
3	E	401	ADP	C2-N3	3.55	1.38	1.32
3	A	401	ADP	O4'-C1'	4.84	1.48	1.41
3	E	401	ADP	O4'-C1'	4.88	1.48	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	401	ADP	N3-C2-N1	-3.83	125.86	128.87
3	A	401	ADP	N3-C2-N1	-3.80	125.89	128.87
3	C	401	ADP	C5'-C4'-C3'	-3.20	102.84	115.20
3	D	401	ADP	C5'-C4'-C3'	-2.85	104.18	115.20
3	E	401	ADP	C5'-C4'-C3'	-2.55	105.34	115.20
3	A	401	ADP	C5'-C4'-C3'	-2.54	105.36	115.20
3	C	401	ADP	O4'-C4'-C3'	-2.28	100.53	105.16
3	D	401	ADP	O3'-C3'-C4'	-2.09	104.77	111.01
3	B	401	ADP	C5'-C4'-C3'	-2.02	107.38	115.20
3	E	401	ADP	C2'-C3'-C4'	2.20	107.13	102.64
3	A	401	ADP	C2'-C3'-C4'	2.21	107.15	102.64
3	A	401	ADP	C4'-O4'-C1'	2.26	112.04	109.64
3	E	401	ADP	C4'-O4'-C1'	2.29	112.07	109.64
3	D	401	ADP	O4'-C4'-C5'	2.36	117.71	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	ADP	O4'-C1'-N9	2.62	113.06	108.11
3	A	401	ADP	O3B-PB-O1B	2.71	119.47	110.63
3	E	401	ADP	O3B-PB-O1B	2.71	119.47	110.63
3	C	401	ADP	O3B-PB-O1B	2.86	119.97	110.63
3	B	401	ADP	N3-C2-N1	2.99	131.22	128.87
3	A	401	ADP	N6-C6-N1	3.36	124.14	118.52
3	E	401	ADP	N6-C6-N1	3.37	124.17	118.52
3	D	401	ADP	O3B-PB-O2B	3.44	120.06	107.44
3	D	401	ADP	C4'-O4'-C1'	3.51	113.36	109.64
3	B	401	ADP	N6-C6-N1	3.57	124.51	118.52
3	C	401	ADP	C4'-O4'-C1'	3.68	113.55	109.64
3	A	401	ADP	O4'-C1'-N9	3.73	115.16	108.11
3	E	401	ADP	O4'-C1'-N9	3.75	115.18	108.11
3	C	401	ADP	C1'-N9-C4	4.09	131.37	126.81
3	B	401	ADP	O4'-C1'-N9	4.23	116.10	108.11
3	D	401	ADP	O4'-C1'-N9	4.68	116.95	108.11
3	C	401	ADP	N6-C6-N1	5.39	127.56	118.52
3	D	401	ADP	N3-C2-N1	7.42	134.70	128.87
3	D	401	ADP	N6-C6-N1	7.74	131.51	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	ADP	2	0

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.