



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 16, 2018 – 06:21 PM EST

PDB ID : 5Y5Y  
EMDB ID: : EMD-6811  
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, peripheral domain, rotational state 1  
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.  
Deposited on : 2017-08-10  
Resolution : 4.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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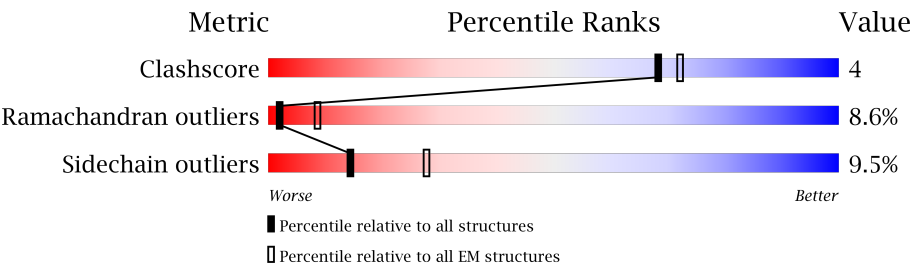
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

# 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 4.70 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	A	578	70% 23% 5% .
1	B	578	70% 24% 6% .
1	C	578	71% 23% 6% .
2	D	478	65% 23% 7% . .
2	E	478	65% 25% 5% .
2	F	478	71% 22% . .
3	G	223	63% 24% 6% . 6%
4	H	104	61% 31% . . .
5	I	120	43% 7% . 49%

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Mol	Chain	Length	Quality of chain
5	K	120	<div><div></div><div>43%6%•49%</div></div>
6	J	188	<div><div></div><div>73%7%•19%</div></div>
6	L	188	<div><div></div><div>74%7%19%</div></div>
7	M	323	<div><div></div><div>83%15%••</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32159 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	B	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	C	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	E	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	F	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	210	Total	C	N	O	S	0	0
			1642	1033	307	300	2		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	100	Total	C	N	O	S	0	0
			758	479	131	145	3		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	61	Total	C	N	O	0	0
			451	276	85	90		
5	K	61	Total	C	N	O	0	0
			451	276	85	90		

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	152	Total	C	N	O	0	0
			1043	646	203	194		
6	L	152	Total	C	N	O	0	0
			1043	646	203	194		

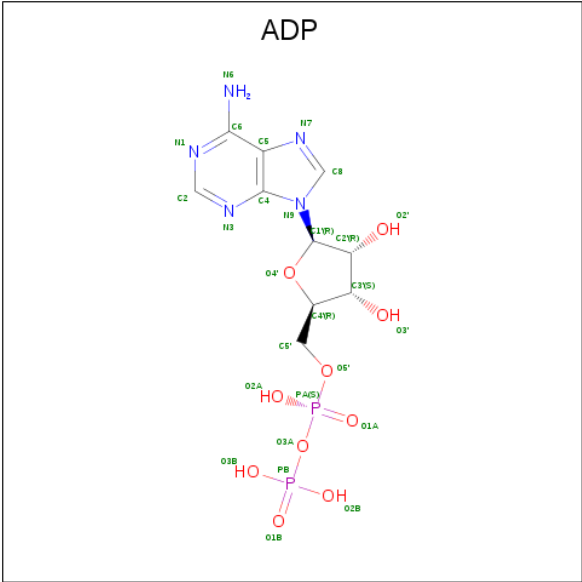
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	320	Total	C	N	O	S	0	0
			2513	1599	460	450	4		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

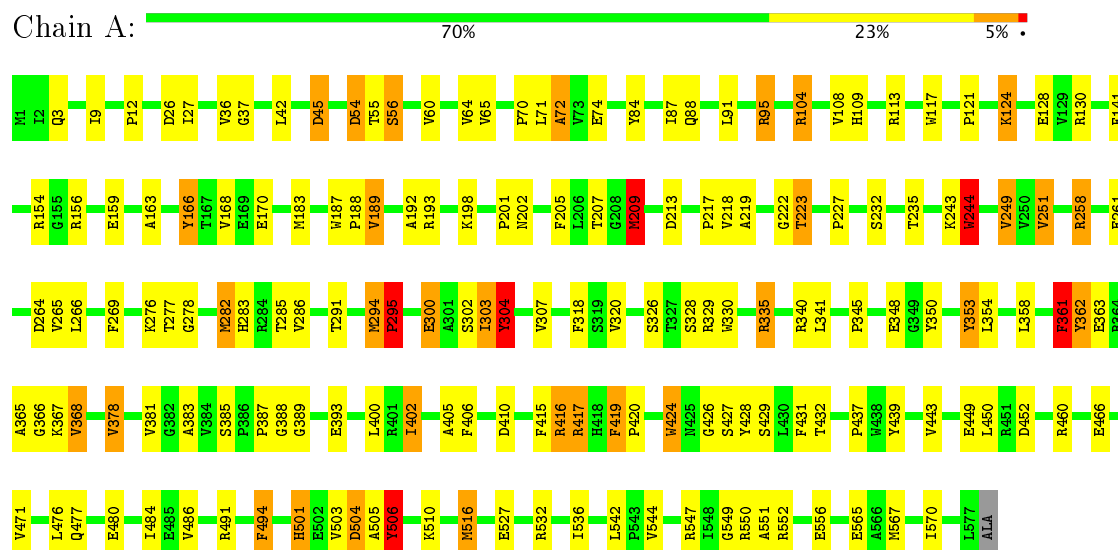


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

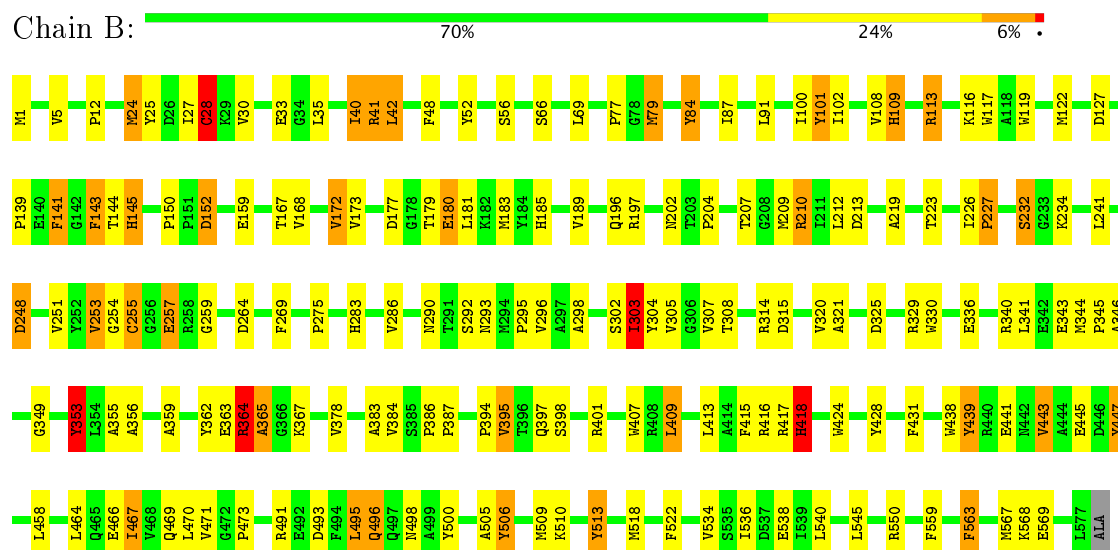
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: V-type ATP synthase alpha chain

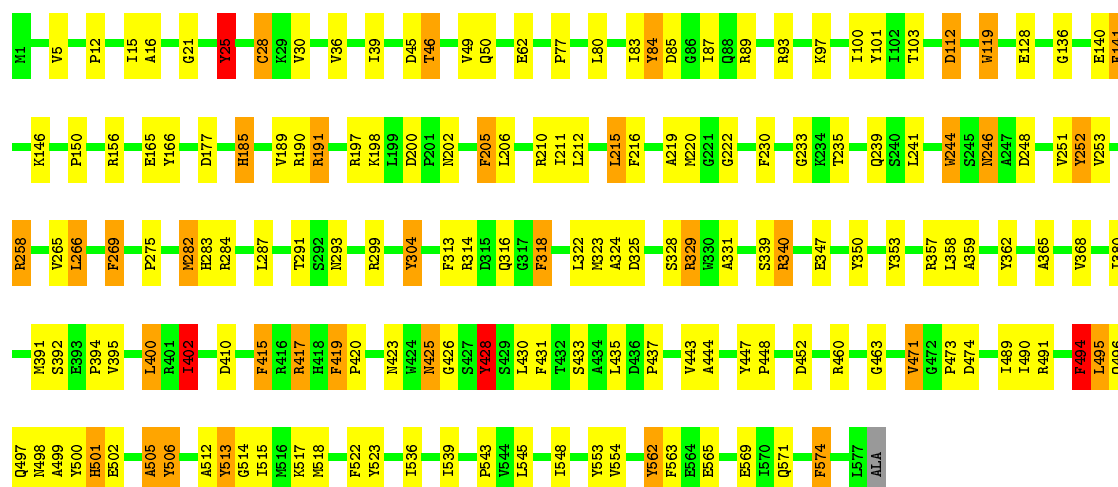


#### • Molecule 1: V-type ATP synthase alpha chain



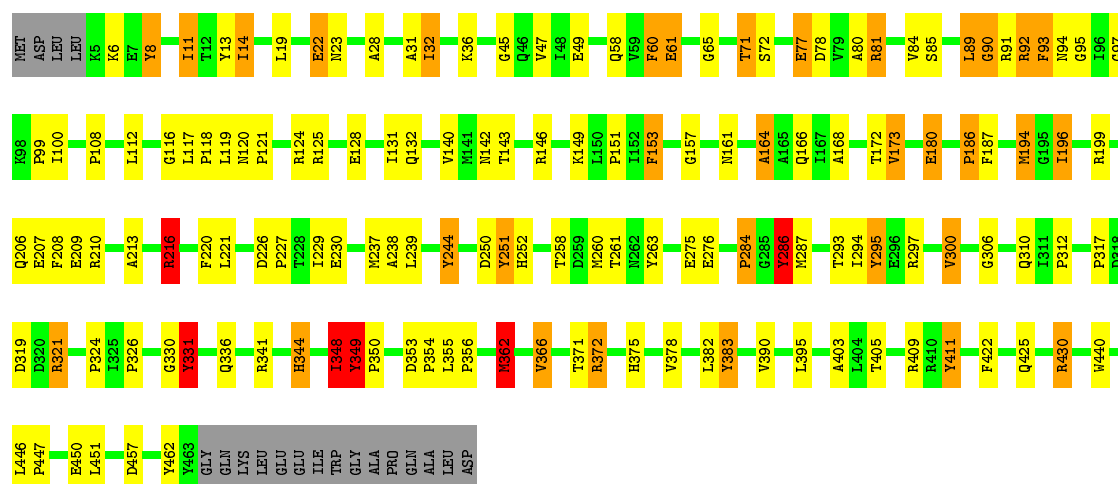
#### • Molecule 1: V-type ATP synthase alpha chain

Chain C: 



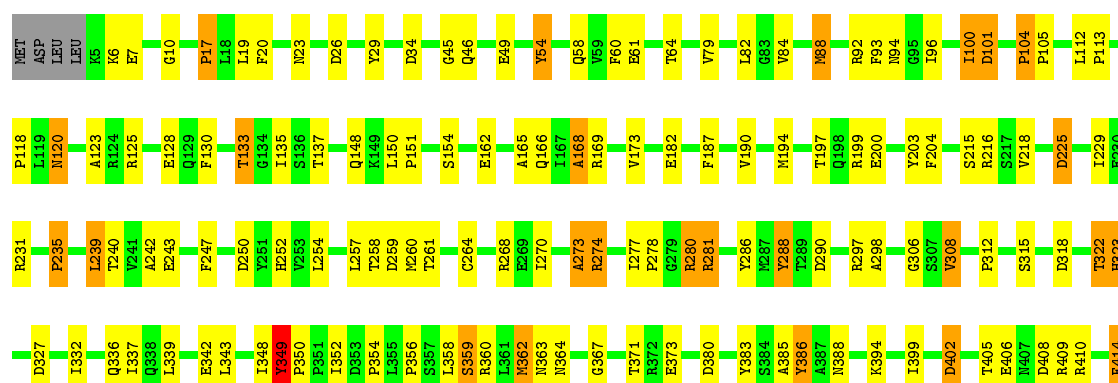
• Molecule 2: V-type ATP synthase beta chain

Chain D: 



• Molecule 2: V-type ATP synthase beta chain

Chain E: 

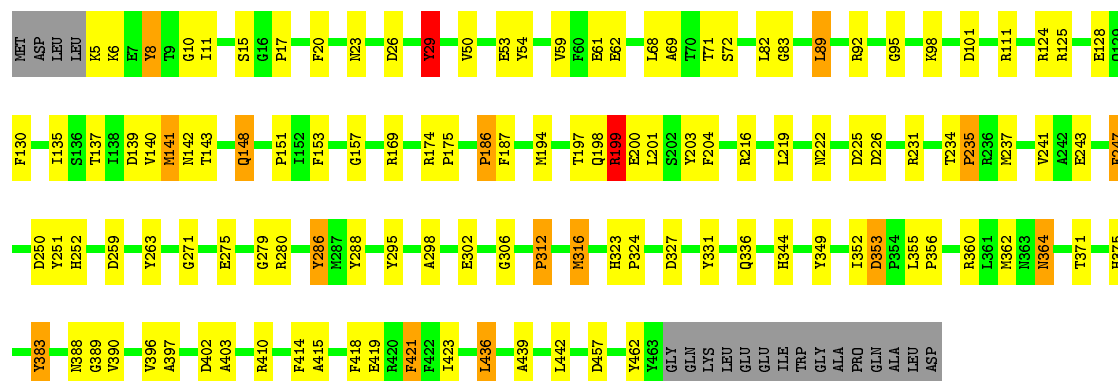






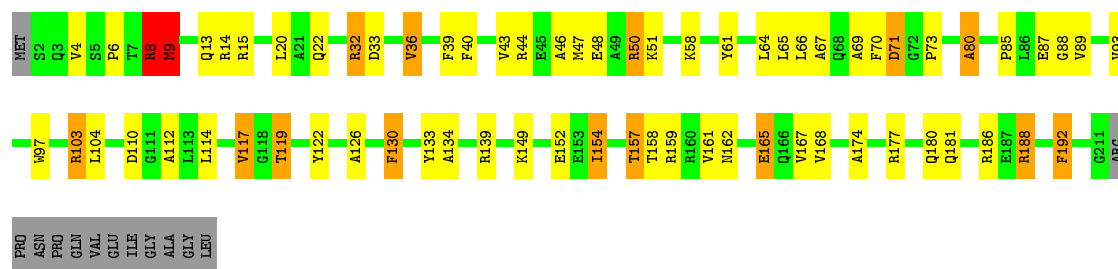
• Molecule 2: V-type ATP synthase beta chain

Chain F: 71% 22% . .



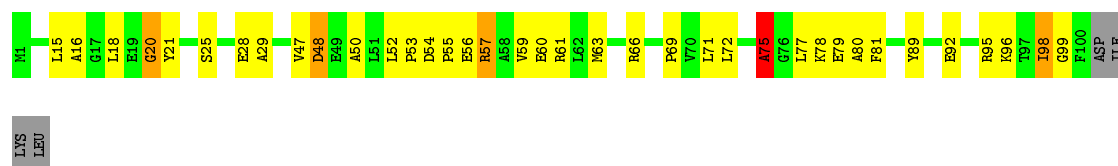
• Molecule 3: V-type ATP synthase subunit D

Chain G: 63% 24% 6% . 6%



• Molecule 4: V-type ATP synthase subunit F

Chain H: 61% 31% . . .



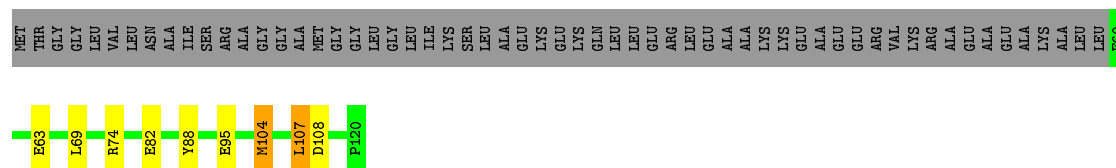
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain I: 43% 7% . 49%



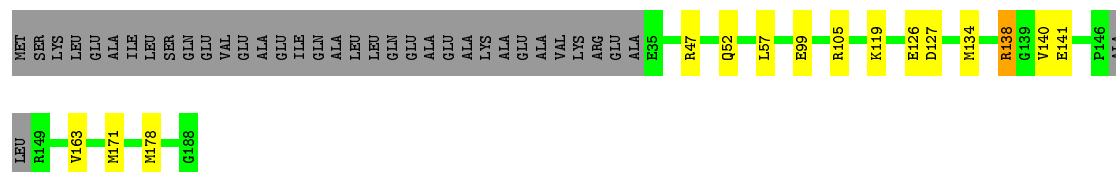
- Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

Chain K:  43% 6% 49%



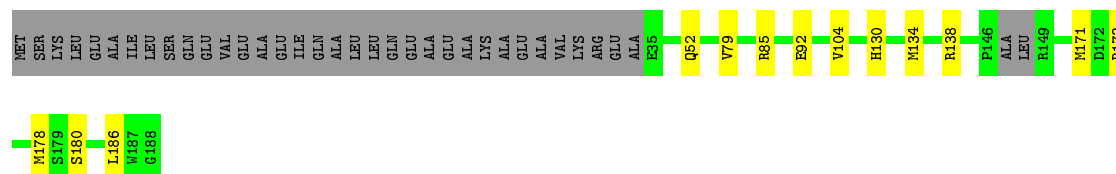
- Molecule 6: V-type ATP synthase subunit E

Chain J:  73% 7% 19%




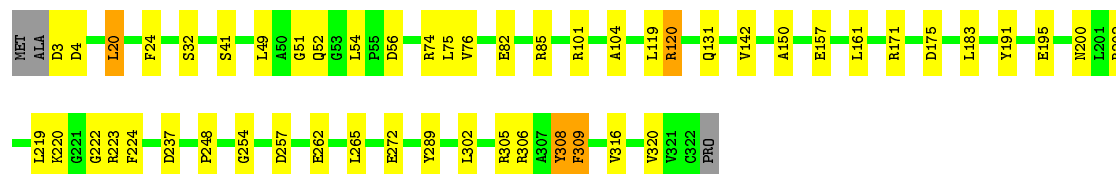
- Molecule 6: V-type ATP synthase subunit E

Chain L:  74% 7% 19%



- Molecule 7: V-type ATP synthase subunit C

Chain M:  83% 15% 2%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	26	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	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	1.38	3/4568 (0.1%)	1.45	29/6198 (0.5%)
1	B	1.31	0/4568	1.42	27/6198 (0.4%)
1	C	1.35	1/4568 (0.0%)	1.47	41/6198 (0.7%)
2	D	1.33	0/3663	1.46	29/4960 (0.6%)
2	E	1.34	1/3663 (0.0%)	1.45	30/4960 (0.6%)
2	F	1.37	1/3663 (0.0%)	1.48	25/4960 (0.5%)
3	G	1.27	0/1662	1.48	12/2235 (0.5%)
4	H	1.16	0/769	1.41	3/1039 (0.3%)
5	I	1.10	0/451	1.19	1/608 (0.2%)
5	K	1.10	0/451	1.27	3/608 (0.5%)
6	J	1.05	0/1053	1.24	1/1439 (0.1%)
6	L	1.12	0/1053	1.22	1/1439 (0.1%)
7	M	1.08	0/2552	1.20	3/3446 (0.1%)
All	All	1.30	6/32684 (0.0%)	1.41	205/44288 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	15
1	C	0	21
2	D	0	19
2	E	0	17
2	F	0	17
3	G	0	10
4	H	0	3
5	I	0	1
5	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	J	0	1
6	L	0	1
7	M	0	8
All	All	0	132

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	TYR	CB-CG	-5.66	1.43	1.51
2	E	278	PRO	CA-C	-5.53	1.41	1.52
1	A	388	GLY	CA-C	-5.51	1.43	1.51
1	C	419	PHE	C-N	-5.34	1.24	1.34
2	F	323	HIS	C-N	-5.21	1.24	1.34
1	A	358	LEU	CA-C	-5.10	1.39	1.52

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	88	TYR	CB-CG-CD2	-10.45	114.73	121.00
1	C	84	TYR	CB-CG-CD2	-10.43	114.74	121.00
2	F	383	TYR	CB-CG-CD1	-9.94	115.03	121.00
2	F	286	TYR	CB-CG-CD2	-9.94	115.04	121.00
5	K	88	TYR	CB-CG-CD1	9.39	126.64	121.00
2	D	286	TYR	CB-CG-CD2	-9.12	115.53	121.00
2	D	153	PHE	CB-CG-CD2	-8.99	114.51	120.80
1	C	282	MET	CG-SD-CE	-8.70	86.29	100.20
3	G	46	ALA	N-CA-C	8.57	134.13	111.00
1	C	494	PHE	CB-CG-CD2	-8.46	114.88	120.80
2	D	286	TYR	CB-CG-CD1	8.30	125.98	121.00
1	C	269	PHE	CB-CG-CD2	-8.22	115.04	120.80
2	E	20	PHE	CB-CG-CD1	7.94	126.36	120.80
1	C	500	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	B	364	ARG	N-CA-C	-7.89	89.69	111.00
1	A	420	PRO	N-CA-C	-7.84	91.72	112.10
1	A	362	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	C	269	PHE	CB-CG-CD1	7.75	126.23	120.80
1	C	205	PHE	N-CA-C	-7.71	90.17	111.00
2	E	288	TYR	CB-CG-CD2	-7.68	116.39	121.00
2	D	295	TYR	CB-CG-CD2	-7.60	116.44	121.00
1	C	494	PHE	CB-CG-CD1	7.59	126.11	120.80
2	F	141	MET	CG-SD-CE	-7.55	88.12	100.20
1	C	471	VAL	CB-CA-C	7.33	125.33	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	153	PHE	CB-CG-CD1	7.22	125.85	120.80
2	E	247	PHE	CB-CG-CD1	-7.22	115.75	120.80
1	C	304	TYR	CB-CG-CD2	-7.13	116.72	121.00
2	D	263	TYR	CB-CG-CD1	-7.10	116.74	121.00
1	A	494	PHE	CB-CG-CD1	7.09	125.76	120.80
2	D	331	TYR	CB-CG-CD2	-7.07	116.76	121.00
1	C	185	HIS	C-N-CA	7.01	139.22	121.70
2	D	383	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	C	523	TYR	CB-CG-CD2	-6.91	116.86	121.00
2	F	286	TYR	CB-CG-CD1	6.83	125.10	121.00
2	F	237	MET	CG-SD-CE	-6.79	89.34	100.20
2	F	98	LYS	N-CA-C	-6.77	92.72	111.00
1	A	494	PHE	CB-CG-CD2	-6.77	116.06	120.80
7	M	309	PHE	CB-CG-CD1	6.76	125.53	120.80
1	C	251	VAL	N-CA-C	-6.74	92.80	111.00
2	E	19	LEU	C-N-CA	6.74	138.54	121.70
1	A	258	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	388	GLY	N-CA-C	-6.71	96.34	113.10
2	F	295	TYR	CB-CG-CD1	6.70	125.02	121.00
2	F	295	TYR	CB-CG-CD2	-6.68	116.99	121.00
2	F	316	MET	CG-SD-CE	-6.63	89.59	100.20
2	F	153	PHE	CB-CG-CD2	-6.59	116.18	120.80
1	C	506	TYR	N-CA-C	-6.58	93.23	111.00
2	E	386	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	A	424	TRP	CB-CG-CD2	-6.52	118.13	126.60
3	G	119	THR	CA-C-N	6.52	135.35	117.10
4	H	75	ALA	N-CA-CB	6.49	119.18	110.10
1	C	574	PHE	CB-CG-CD1	-6.47	116.27	120.80
2	F	29	TYR	CB-CG-CD2	-6.45	117.13	121.00
2	F	252	HIS	CA-CB-CG	-6.40	102.72	113.60
2	E	280	ARG	C-N-CA	6.37	137.63	121.70
3	G	165	GLU	CB-CA-C	-6.37	97.65	110.40
2	E	247	PHE	CB-CG-CD2	6.36	125.25	120.80
1	A	361	PHE	CB-CG-CD1	-6.32	116.37	120.80
1	A	506	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	A	258	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	D	13	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	251	VAL	N-CA-C	-6.25	94.13	111.00
2	D	331	TYR	CB-CG-CD1	6.24	124.75	121.00
2	D	90	GLY	N-CA-C	-6.21	97.58	113.10
1	A	294	MET	CG-SD-CE	-6.18	90.31	100.20
1	C	420	PRO	N-CA-C	-6.10	96.23	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	CYS	CA-CB-SG	-6.07	103.07	114.00
7	M	51	GLY	N-CA-C	-5.96	98.19	113.10
1	A	476	LEU	N-CA-C	-5.96	94.90	111.00
1	C	425	ASN	N-CA-C	-5.96	94.91	111.00
1	A	350	TYR	CA-CB-CG	-5.96	102.08	113.40
1	A	56	SER	N-CA-CB	5.96	119.43	110.50
1	B	563	PHE	CB-CG-CD1	5.94	124.96	120.80
2	D	348	ILE	N-CA-C	-5.93	94.97	111.00
2	E	352	ILE	N-CA-C	-5.92	95.01	111.00
1	A	353	TYR	CB-CA-C	-5.90	98.61	110.40
1	C	452	ASP	CA-CB-CG	-5.89	100.44	113.40
2	E	359	SER	N-CA-C	-5.88	95.13	111.00
1	B	42	LEU	CB-CA-C	-5.87	99.04	110.20
2	F	353	ASP	CB-CA-C	-5.87	98.66	110.40
1	B	25	TYR	CB-CG-CD1	-5.85	117.49	121.00
3	G	80	ALA	N-CA-CB	5.85	118.29	110.10
6	J	138	ARG	C-N-CA	5.83	134.54	122.30
2	D	93	PHE	CB-CA-C	-5.81	98.78	110.40
1	C	415	PHE	CB-CA-C	5.81	122.02	110.40
1	C	553	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	B	219	ALA	N-CA-CB	5.80	118.22	110.10
1	B	447	TYR	CB-CG-CD2	-5.79	117.53	121.00
4	H	16	ALA	N-CA-CB	5.78	118.19	110.10
1	A	72	ALA	CB-CA-C	-5.76	101.46	110.10
2	F	199	ARG	NE-CZ-NH1	5.73	123.17	120.30
5	I	74	ARG	CB-CA-C	-5.72	98.95	110.40
1	B	513	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	B	24	MET	CG-SD-CE	-5.71	91.06	100.20
1	C	415	PHE	CA-CB-CG	-5.71	100.21	113.90
2	E	133	THR	N-CA-C	-5.70	95.62	111.00
1	C	574	PHE	CB-CG-CD2	5.70	124.79	120.80
1	B	365	ALA	N-CA-CB	5.68	118.05	110.10
1	B	257	GLU	N-CA-C	-5.66	95.71	111.00
1	A	426	GLY	N-CA-C	-5.66	98.96	113.10
2	E	204	PHE	CB-CA-C	-5.64	99.11	110.40
3	G	192	PHE	CB-CG-CD1	5.62	124.73	120.80
3	G	104	LEU	CB-CA-C	-5.61	99.53	110.20
1	B	102	ILE	N-CA-C	-5.60	95.88	111.00
2	D	77	GLU	C-N-CA	5.60	135.70	121.70
2	F	383	TYR	CB-CG-CD2	5.60	124.36	121.00
1	A	209	MET	N-CA-C	-5.59	95.91	111.00
3	G	36	VAL	CA-CB-CG2	5.58	119.28	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	157	THR	CA-CB-CG2	-5.58	104.58	112.40
1	B	308	THR	N-CA-CB	5.57	120.89	110.30
1	C	425	ASN	CA-CB-CG	-5.57	101.14	113.40
2	F	364	ASN	N-CA-C	-5.57	95.95	111.00
3	G	130	PHE	CA-CB-CG	-5.57	100.52	113.90
1	B	500	TYR	CB-CG-CD2	-5.57	117.66	121.00
3	G	32	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	B	28	CYS	CA-CB-SG	-5.56	103.99	114.00
1	B	341	LEU	N-CA-C	-5.55	96.00	111.00
1	B	563	PHE	CB-CG-CD2	-5.55	116.91	120.80
3	G	158	THR	N-CA-CB	5.55	120.84	110.30
1	B	353	TYR	CB-CA-C	-5.52	99.37	110.40
1	C	25	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	C	84	TYR	CB-CG-CD1	5.50	124.30	121.00
2	E	286	TYR	CB-CG-CD2	-5.50	117.70	121.00
2	D	450	GLU	CB-CA-C	-5.49	99.41	110.40
2	E	315	SER	CB-CA-C	-5.48	99.68	110.10
7	M	309	PHE	CB-CG-CD2	-5.47	116.97	120.80
2	E	359	SER	N-CA-CB	5.47	118.70	110.50
1	B	152	ASP	CA-CB-CG	-5.46	101.38	113.40
2	D	60	PHE	CB-CG-CD1	5.46	124.62	120.80
2	D	383	TYR	CB-CG-CD1	5.46	124.27	121.00
1	A	361	PHE	CB-CG-CD2	5.45	124.62	120.80
1	A	506	TYR	N-CA-C	-5.45	96.27	111.00
1	B	52	TYR	CB-CG-CD1	-5.44	117.74	121.00
6	L	92	GLU	N-CA-CB	-5.43	100.82	110.60
2	E	362	MET	N-CA-CB	5.40	120.33	110.60
2	E	242	ALA	CB-CA-C	-5.37	102.04	110.10
1	A	166	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	C	495	LEU	N-CA-C	-5.37	96.50	111.00
1	B	48	PHE	CB-CG-CD2	5.37	124.56	120.80
2	D	372	ARG	N-CA-CB	5.34	120.22	110.60
2	E	349	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	E	318	ASP	N-CA-C	-5.32	96.63	111.00
2	F	421	PHE	CA-CB-CG	-5.32	101.13	113.90
2	D	411	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	C	140	GLU	N-CA-C	-5.32	96.65	111.00
2	F	247	PHE	CA-CB-CG	-5.31	101.16	113.90
5	K	107	LEU	C-N-CA	5.30	134.96	121.70
1	C	30	VAL	N-CA-C	-5.30	96.68	111.00
1	B	254	GLY	N-CA-C	-5.28	99.90	113.10
2	E	278	PRO	N-CA-C	-5.28	98.37	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ILE	CB-CA-C	-5.28	101.04	111.60
2	E	54	TYR	CB-CG-CD2	-5.28	117.83	121.00
2	D	244	TYR	CB-CG-CD2	-5.28	117.83	121.00
2	E	388	ASN	CB-CA-C	-5.27	99.86	110.40
1	C	244	TRP	CA-CB-CG	-5.26	103.71	113.70
2	E	463	TYR	CB-CG-CD2	-5.26	117.85	121.00
2	D	28	ALA	CB-CA-C	-5.24	102.24	110.10
1	B	227	PRO	N-CA-C	-5.24	98.48	112.10
2	D	382	LEU	CB-CA-C	-5.23	100.26	110.20
2	E	364	ASN	N-CA-C	-5.23	96.87	111.00
1	B	343	GLU	N-CA-C	-5.22	96.90	111.00
2	D	321	ARG	N-CA-C	-5.22	96.90	111.00
2	F	186	PRO	N-CA-C	-5.22	98.53	112.10
2	E	169	ARG	CB-CA-C	-5.22	99.96	110.40
2	F	383	TYR	CA-CB-CG	5.21	123.30	113.40
2	F	148	GLN	N-CA-CB	5.21	119.97	110.60
1	C	190	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	518	MET	CB-CA-C	-5.20	100.01	110.40
2	E	264	CYS	CA-CB-SG	-5.20	104.65	114.00
1	C	350	TYR	CB-CG-CD1	-5.19	117.89	121.00
3	G	71	ASP	CB-CA-C	-5.17	100.05	110.40
2	D	378	VAL	CB-CA-C	-5.16	101.60	111.40
2	F	312	PRO	N-CA-C	-5.15	98.70	112.10
1	C	391	MET	N-CA-C	-5.14	97.12	111.00
1	B	143	PHE	CA-CB-CG	-5.12	101.60	113.90
1	A	449	GLU	CB-CA-C	5.12	120.64	110.40
1	A	353	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	381	VAL	N-CA-C	-5.12	97.19	111.00
1	C	252	TYR	CB-CG-CD1	-5.11	117.93	121.00
2	D	120	ASN	N-CA-C	-5.11	97.20	111.00
1	C	89	ARG	N-CA-C	-5.11	97.21	111.00
1	A	415	PHE	CB-CA-C	-5.10	100.21	110.40
1	C	97	LYS	CB-CA-C	-5.09	100.22	110.40
1	C	266	LEU	CB-CA-C	-5.09	100.53	110.20
2	D	92	ARG	N-CA-C	-5.08	97.28	111.00
1	C	554	VAL	N-CA-C	-5.08	97.29	111.00
1	A	419	PHE	N-CA-CB	5.08	119.74	110.60
1	B	545	LEU	CB-CA-C	-5.08	100.56	110.20
1	C	103	THR	N-CA-C	-5.07	97.32	111.00
1	A	26	ASP	CA-CB-CG	-5.05	102.28	113.40
2	D	350	PRO	N-CA-C	-5.05	98.96	112.10
2	F	20	PHE	CB-CA-C	-5.05	100.30	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	569	GLU	CB-CA-C	-5.05	100.30	110.40
2	E	290	ASP	CA-CB-CG	-5.05	102.30	113.40
2	F	8	TYR	CB-CA-C	-5.04	100.32	110.40
4	H	99	GLY	N-CA-C	-5.04	100.50	113.10
2	E	168	ALA	N-CA-CB	5.04	117.15	110.10
1	B	506	TYR	CB-CG-CD1	-5.03	117.98	121.00
2	D	355	LEU	CA-C-N	5.03	131.17	117.10
2	E	79	VAL	N-CA-C	-5.03	97.43	111.00
2	F	243	GLU	CB-CA-C	-5.02	100.36	110.40
1	C	501	HIS	N-CA-C	-5.02	97.44	111.00
2	E	445	MET	CG-SD-CE	-5.01	92.18	100.20
2	D	194	MET	N-CA-CB	5.00	119.61	110.60
2	E	218	VAL	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	304	TYR	Sidechain
1	A	335	ARG	Sidechain
1	A	340	ARG	Sidechain
1	A	361	PHE	Sidechain
1	A	362	TYR	Sidechain
1	A	416	ARG	Sidechain
1	A	417	ARG	Sidechain
1	A	439	TYR	Sidechain
1	A	460	ARG	Sidechain
1	A	491	ARG	Sidechain
1	A	501	HIS	Sidechain
1	A	506	TYR	Sidechain
1	A	532	ARG	Sidechain
1	A	547	ARG	Sidechain
1	A	552	ARG	Sidechain
1	A	84	TYR	Sidechain
1	A	95	ARG	Sidechain
1	B	101	TYR	Sidechain
1	B	113	ARG	Sidechain
1	B	143	PHE	Sidechain
1	B	314	ARG	Sidechain
1	B	362	TYR	Sidechain
1	B	387	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	B	401	ARG	Sidechain
1	B	41	ARG	Sidechain
1	B	415	PHE	Sidechain
1	B	416	ARG	Sidechain
1	B	428	TYR	Sidechain
1	B	491	ARG	Sidechain
1	B	506	TYR	Sidechain
1	B	513	TYR	Sidechain
1	B	84	TYR	Sidechain
1	C	101	TYR	Sidechain
1	C	191	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	25	TYR	Sidechain
1	C	252	TYR	Sidechain
1	C	258	ARG	Sidechain
1	C	299	ARG	Sidechain
1	C	304	TYR	Sidechain
1	C	318	PHE	Sidechain
1	C	329	ARG	Sidechain
1	C	340	ARG	Sidechain
1	C	353	TYR	Sidechain
1	C	357	ARG	Sidechain
1	C	362	TYR	Sidechain
1	C	415	PHE	Sidechain
1	C	428	TYR	Sidechain
1	C	460	ARG	Sidechain
1	C	513	TYR	Sidechain
1	C	562	TYR	Sidechain
1	C	84	TYR	Sidechain
1	C	93	ARG	Sidechain
2	D	124	ARG	Sidechain
2	D	153	PHE	Sidechain
2	D	187	PHE	Sidechain
2	D	216	ARG	Sidechain
2	D	331	TYR	Sidechain
2	D	341	ARG	Sidechain
2	D	344	HIS	Sidechain
2	D	349	TYR	Sidechain
2	D	356	PRO	Mainchain
2	D	383	TYR	Sidechain
2	D	409	ARG	Sidechain
2	D	411	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	D	422	PHE	Sidechain
2	D	430	ARG	Sidechain
2	D	462	TYR	Sidechain
2	D	6	LYS	Peptide
2	D	8	TYR	Sidechain
2	D	91	ARG	Sidechain
2	D	93	PHE	Sidechain
2	E	125	ARG	Sidechain
2	E	130	PHE	Sidechain
2	E	187	PHE	Sidechain
2	E	231	ARG	Sidechain
2	E	268	ARG	Sidechain
2	E	274	ARG	Sidechain
2	E	280	ARG	Sidechain
2	E	288	TYR	Sidechain
2	E	29	TYR	Sidechain
2	E	349	TYR	Sidechain
2	E	383	TYR	Sidechain
2	E	414	PHE	Sidechain
2	E	458	HIS	Sidechain
2	E	463	TYR	Sidechain
2	E	6	LYS	Peptide
2	E	92	ARG	Mainchain,Peptide
2	F	111	ARG	Sidechain
2	F	124	ARG	Sidechain
2	F	169	ARG	Sidechain
2	F	203	TYR	Sidechain
2	F	216	ARG	Sidechain
2	F	247	PHE	Sidechain
2	F	271	GLY	Mainchain
2	F	288	TYR	Sidechain
2	F	29	TYR	Sidechain
2	F	331	TYR	Sidechain
2	F	349	TYR	Sidechain
2	F	383	TYR	Sidechain
2	F	421	PHE	Sidechain
2	F	462	TYR	Sidechain
2	F	54	TYR	Sidechain
2	F	6	LYS	Peptide
2	F	8	TYR	Sidechain
3	G	130	PHE	Sidechain
3	G	133	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	G	139	ARG	Sidechain
3	G	15	ARG	Sidechain
3	G	159	ARG	Sidechain
3	G	188	ARG	Sidechain
3	G	40	PHE	Sidechain
3	G	47	MET	Mainchain
3	G	50	ARG	Sidechain
3	G	8	ARG	Sidechain
4	H	21	TYR	Sidechain
4	H	61	ARG	Sidechain
4	H	89	TYR	Sidechain
5	I	76	ARG	Sidechain
6	J	47	ARG	Sidechain
5	K	74	ARG	Sidechain
6	L	85	ARG	Sidechain
7	M	120	ARG	Sidechain
7	M	183	LEU	Peptide
7	M	191	TYR	Sidechain
7	M	223	ARG	Sidechain
7	M	289	TYR	Sidechain
7	M	3	ASP	Peptide
7	M	308	TYR	Sidechain
7	M	85	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	A	4472	0	4491	48	0
1	B	4472	0	4491	42	0
1	C	4472	0	4491	47	0
2	D	3596	0	3624	41	0
2	E	3596	0	3624	34	0
2	F	3596	0	3624	27	0
3	G	1642	0	1718	18	0
4	H	758	0	764	9	0
5	I	451	0	429	3	0
5	K	451	0	429	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1043	0	936	3	0
6	L	1043	0	936	6	0
7	M	2513	0	2587	12	0
8	A	27	0	12	4	0
8	C	27	0	12	4	0
All	All	32159	0	32168	280	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 4.

All (280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASP:HA	1:B:383:ALA:HB3	1.65	0.77
6:L:178:MET:CG	6:L:178:MET:CE	2.63	0.77
5:I:104:MET:CG	5:I:104:MET:CE	2.64	0.75
2:D:131:ILE:HG22	2:D:132:GLN:O	1.91	0.71
6:J:178:MET:CE	6:J:178:MET:CG	2.68	0.71
6:L:134:MET:CG	6:L:134:MET:CE	2.69	0.70
6:J:171:MET:CE	6:J:171:MET:CG	2.70	0.69
3:G:64:LEU:HD22	3:G:126:ALA:HB2	1.75	0.69
1:A:303:ILE:HD12	1:A:304:TYR:H	1.59	0.67
5:K:104:MET:CE	5:K:104:MET:CG	2.73	0.67
1:A:198:LYS:HA	1:A:368:VAL:HG12	1.77	0.66
6:J:134:MET:CG	6:J:134:MET:CE	2.74	0.65
2:E:257:LEU:HD12	2:E:257:LEU:H	1.60	0.64
1:A:366:GLY:O	1:A:368:VAL:HG13	1.98	0.64
1:B:30:VAL:H	1:B:35:LEU:H	1.44	0.64
2:F:5:LYS:HG3	6:L:173:ARG:HH21	1.64	0.63
2:F:141:MET:HB2	2:F:142:ASN:HD22	1.62	0.63
1:A:300:GLU:HG2	1:A:330:TRP:HE1	1.66	0.61
2:F:148:GLN:HE22	2:F:360:ARG:H	1.48	0.61
1:A:365:ALA:HB3	1:A:378:VAL:HB	1.84	0.60
1:B:367:LYS:HA	1:B:367:LYS:HZ3	1.66	0.60
1:C:235:THR:HG21	2:E:360:ARG:HH12	1.66	0.60
2:D:22:GLU:CD	2:D:23:ASN:H	2.05	0.60
1:C:322:LEU:HD23	1:C:380:ILE:HD11	1.83	0.60
1:A:141:PHE:CD2	1:A:283:HIS:CE1	2.90	0.59
1:A:419:PHE:CG	8:A:600:ADP:C5	2.91	0.58
1:A:91:LEU:H	1:A:91:LEU:HD12	1.68	0.58
1:A:419:PHE:CD2	8:A:600:ADP:C8	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:VAL:HG12	2:F:61:GLU:H	1.68	0.57
2:E:373:GLU:CD	2:E:373:GLU:H	2.08	0.57
1:A:258:ARG:HA	1:A:291:THR:HG23	1.87	0.56
1:A:326:SER:H	1:A:383:ALA:HB3	1.68	0.56
1:A:501:HIS:CE1	1:A:503:VAL:H	2.24	0.56
1:B:251:VAL:HG13	1:B:286:VAL:HG13	1.88	0.56
1:C:266:LEU:HD21	1:C:287:LEU:HD13	1.88	0.55
1:B:77:PRO:HA	1:B:145:HIS:CE1	2.42	0.55
1:C:211:ILE:HG23	1:C:212:LEU:H	1.73	0.55
1:A:542:LEU:HB3	1:A:544:VAL:HG12	1.88	0.54
1:C:215:LEU:HD13	1:C:216:PHE:CE2	2.42	0.54
1:C:198:LYS:HA	1:C:368:VAL:HG12	1.89	0.54
1:A:124:LYS:H	1:A:124:LYS:HE3	1.72	0.54
3:G:8:ARG:NE	3:G:9:MET:H	2.05	0.54
2:E:45:GLY:HA2	2:E:60:PHE:CE1	2.43	0.53
2:F:418:PHE:CE1	2:F:423:ILE:HD11	2.44	0.53
2:E:165:ALA:O	2:E:168:ALA:HB3	2.09	0.53
1:B:295:PRO:O	1:B:298:ALA:HB3	2.09	0.52
2:E:45:GLY:HA2	2:E:60:PHE:CD1	2.45	0.52
1:C:293:ASN:HD21	2:E:118:PRO:HA	1.74	0.52
2:D:11:ILE:H	2:D:11:ILE:HD13	1.73	0.52
6:L:171:MET:CG	6:L:171:MET:CE	2.88	0.52
1:C:146:LYS:H	1:C:316:GLN:NE2	2.06	0.52
2:E:194:MET:H	2:E:258:THR:HG22	1.74	0.52
1:C:219:ALA:HB2	1:C:431:PHE:CG	2.44	0.52
2:D:446:LEU:HD11	2:D:451:LEU:HD21	1.92	0.52
2:D:131:ILE:HA	2:D:173:VAL:HG12	1.92	0.52
2:F:197:THR:HG22	2:F:198:GLN:H	1.75	0.52
1:A:419:PHE:CD1	8:A:600:ADP:C4	2.97	0.51
1:B:234:LYS:HZ3	1:B:409:LEU:HB3	1.75	0.51
2:E:46:GLN:H	2:E:58:GLN:HB3	1.74	0.51
1:B:418:HIS:CE1	1:B:495:LEU:HG	2.45	0.51
2:D:31:ALA:H	2:D:47:VAL:HB	1.76	0.51
2:D:239:LEU:HD21	2:D:310:GLN:HE22	1.76	0.51
1:B:439:TYR:CD1	1:B:447:TYR:CE2	2.98	0.50
1:B:172:VAL:HG23	1:B:173:VAL:H	1.77	0.50
1:B:168:VAL:HA	1:B:183:MET:SD	2.51	0.50
1:B:150:PRO:HB3	1:B:185:HIS:CG	2.47	0.50
2:E:197:THR:H	2:E:200:GLU:HB2	1.76	0.50
1:A:249:VAL:HG23	1:A:320:VAL:HA	1.94	0.50
1:B:234:LYS:HZ3	1:B:409:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:440:TRP:CE3	2:E:443:LEU:HD12	2.47	0.50
7:M:224:PHE:CE2	7:M:248:PRO:HD2	2.47	0.50
1:A:219:ALA:HB2	1:A:431:PHE:CD2	2.48	0.49
1:B:320:VAL:HG12	1:B:321:ALA:H	1.76	0.49
2:D:31:ALA:HB3	2:D:47:VAL:HG21	1.94	0.49
7:M:104:ALA:HB3	7:M:161:LEU:HD22	1.94	0.49
2:D:440:TRP:HA	2:D:440:TRP:CE3	2.47	0.49
2:E:17:PRO:HG3	2:E:273:ALA:HB1	1.95	0.49
1:B:568:LYS:H	1:B:568:LYS:HD2	1.77	0.49
3:G:8:ARG:HE	3:G:9:MET:H	1.59	0.49
5:I:91:ARG:HH21	5:I:95:GLU:HB2	1.77	0.49
2:E:150:LEU:O	2:E:312:PRO:HD2	2.12	0.49
1:C:328:SER:O	1:C:331:ALA:HB3	2.13	0.49
1:A:556:GLU:H	1:A:556:GLU:CD	2.16	0.49
2:D:161:ASN:O	2:D:164:ALA:HB3	2.13	0.49
2:D:252:HIS:CE1	2:D:306:GLY:HA2	2.48	0.49
2:E:84:VAL:HG12	2:E:112:LEU:HD21	1.95	0.49
2:D:196:ILE:HD13	2:D:196:ILE:H	1.76	0.48
2:D:344:HIS:C	2:D:344:HIS:CD2	2.86	0.48
2:E:349:TYR:CD1	2:E:350:PRO:HA	2.48	0.48
2:F:436:LEU:O	2:F:439:ALA:HB3	2.12	0.48
2:D:60:PHE:CD1	2:D:229:ILE:HG21	2.47	0.48
2:D:32:ILE:HD12	2:D:80:ALA:HB2	1.95	0.48
7:M:302:LEU:O	7:M:302:LEU:HD23	2.12	0.48
1:C:423:ASN:C	1:C:425:ASN:H	2.16	0.48
1:C:522:PHE:CZ	1:C:545:LEU:HD21	2.48	0.48
2:E:348:ILE:HG23	2:E:424:ASN:HB2	1.95	0.48
1:C:428:TYR:CE2	2:F:157:GLY:HA2	2.49	0.48
2:D:425:GLN:HB3	2:D:430:ARG:HH12	1.78	0.48
2:F:251:TYR:O	2:F:306:GLY:HA2	2.12	0.48
1:A:117:TRP:H	1:A:166:TYR:H	1.62	0.48
2:E:154:SER:HA	2:E:339:LEU:HD12	1.95	0.48
1:C:119:TRP:CZ3	1:C:136:GLY:HA3	2.49	0.48
6:L:130:HIS:CD2	6:L:130:HIS:N	2.81	0.48
1:C:25:TYR:H	1:C:39:ILE:HB	1.78	0.47
3:G:65:LEU:HD12	3:G:69:ALA:HA	1.96	0.47
2:D:390:VAL:HG12	2:D:390:VAL:O	2.14	0.47
2:E:298:ALA:HB1	2:E:308:VAL:HB	1.96	0.47
1:A:265:VAL:HG13	1:A:269:PHE:CG	2.49	0.47
1:B:303:ILE:HD11	1:B:330:TRP:CZ2	2.48	0.47
5:I:109:GLU:CD	5:I:109:GLU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:MET:HE2	1:B:84:TYR:CE1	2.50	0.47
2:D:366:VAL:HG21	2:D:375:HIS:CG	2.50	0.47
1:A:243:LYS:O	1:A:244:TRP:CD2	2.68	0.47
1:A:294:MET:HB3	1:A:295:PRO:HD2	1.96	0.46
2:E:402:ASP:CG	2:E:409:ARG:HH22	2.18	0.46
1:A:251:VAL:HG22	1:A:286:VAL:HG21	1.98	0.46
1:A:109:HIS:CG	1:A:113:ARG:HE	2.33	0.46
1:C:314:ARG:HH11	1:C:368:VAL:HG21	1.79	0.46
2:D:220:PHE:CD2	2:D:238:ALA:HB2	2.50	0.46
4:H:56:GLU:HG3	4:H:71:LEU:HD11	1.96	0.46
1:B:141:PHE:CE2	1:B:283:HIS:CD2	3.04	0.46
1:C:419:PHE:CE1	8:C:600:ADP:C4	3.03	0.46
2:E:203:TYR:C	2:E:203:TYR:CD2	2.89	0.46
2:F:148:GLN:HE22	2:F:360:ARG:N	2.13	0.46
2:F:125:ARG:HB2	2:F:302:GLU:HA	1.97	0.46
2:F:352:ILE:HG22	2:F:353:ASP:N	2.31	0.46
1:B:418:HIS:O	1:B:418:HIS:CG	2.69	0.46
1:C:253:VAL:HG13	1:C:324:ALA:HB2	1.96	0.46
1:B:28:CYS:SG	1:B:66:SER:HA	2.56	0.46
2:D:146:ARG:HH11	2:D:252:HIS:CE1	2.34	0.46
1:A:168:VAL:HA	1:A:183:MET:SD	2.56	0.45
1:B:42:LEU:HD12	1:B:42:LEU:H	1.80	0.45
1:C:419:PHE:CZ	8:C:600:ADP:C4	3.04	0.45
1:A:400:LEU:HD11	1:A:406:PHE:CE2	2.51	0.45
2:D:229:ILE:HG23	2:D:230:GLU:N	2.32	0.45
2:E:406:GLU:C	2:E:408:ASP:H	2.19	0.45
3:G:161:VAL:HG12	3:G:165:GLU:CD	2.36	0.45
1:A:205:PHE:HB3	1:A:218:VAL:HG23	1.99	0.45
1:B:204:PRO:HG3	1:B:438:TRP:CZ2	2.51	0.45
1:C:359:ALA:HA	1:C:402:ILE:HD13	1.98	0.45
2:D:84:VAL:HG11	2:D:244:TYR:CD1	2.51	0.45
1:A:424:TRP:CD1	1:A:424:TRP:O	2.70	0.45
1:C:447:TYR:H	1:C:448:PRO:HD2	1.81	0.45
1:A:128:GLU:HB3	1:A:156:ARG:HE	1.82	0.44
1:B:251:VAL:HG22	1:B:286:VAL:HG12	1.99	0.44
1:B:307:VAL:HG12	1:B:364:ARG:HH21	1.82	0.44
3:G:161:VAL:HG12	3:G:165:GLU:OE2	2.16	0.44
4:H:71:LEU:O	4:H:71:LEU:HD12	2.16	0.44
7:M:41:SER:HB3	7:M:49:LEU:HD22	1.99	0.44
1:C:141:PHE:CE2	1:C:283:HIS:CE1	3.05	0.44
1:C:244:TRP:CE2	1:C:505:ALA:HB1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ILE:HD12	1:C:539:ILE:H	1.82	0.44
2:D:116:GLY:HA3	2:D:297:ARG:HH21	1.82	0.44
2:F:234:THR:HB	2:F:235:PRO:HD3	1.99	0.44
2:F:82:LEU:HD12	2:F:83:GLY:H	1.82	0.44
7:M:202:ARG:HH21	7:M:265:LEU:HD13	1.82	0.44
1:C:435:LEU:HA	1:C:435:LEU:HD23	1.82	0.44
2:D:94:ASN:HB2	2:D:100:ILE:HG13	2.00	0.44
4:H:59:VAL:HG12	4:H:63:MET:SD	2.57	0.44
1:A:428:TYR:CD2	2:D:157:GLY:HA3	2.52	0.44
1:C:253:VAL:O	1:C:324:ALA:HA	2.17	0.44
1:C:419:PHE:CE2	8:C:600:ADP:C8	3.05	0.44
2:D:81:ARG:HB2	2:D:112:LEU:O	2.18	0.44
2:D:143:THR:H	2:D:362:MET:HG3	1.82	0.44
2:D:446:LEU:HD12	2:D:447:PRO:O	2.17	0.44
2:D:14:ILE:HG23	2:D:19:LEU:HD13	1.99	0.44
2:E:323:HIS:CE1	3:G:181:GLN:CD	2.91	0.44
3:G:66:LEU:O	3:G:66:LEU:HD13	2.18	0.44
1:A:400:LEU:HD21	1:A:406:PHE:CE1	2.53	0.44
1:C:314:ARG:NH1	1:C:368:VAL:HG21	2.33	0.44
7:M:200:ASN:HD21	7:M:219:LEU:H	1.66	0.44
1:B:320:VAL:HG12	1:B:321:ALA:N	2.33	0.43
1:B:536:ILE:C	1:B:538:GLU:H	2.20	0.43
1:C:21:GLY:H	2:F:68:LEU:HB2	1.81	0.43
3:G:48:GLU:HA	3:G:51:LYS:HE2	1.99	0.43
1:C:83:ILE:HA	1:C:287:LEU:HB2	1.99	0.43
2:F:396:VAL:HG13	2:F:397:ALA:N	2.33	0.43
3:G:33:ASP:O	3:G:36:VAL:HG22	2.18	0.43
1:A:3:GLN:HB3	1:A:65:VAL:HG13	2.00	0.43
1:B:251:VAL:HG13	1:B:286:VAL:CG1	2.48	0.43
1:C:219:ALA:HB2	1:C:431:PHE:CD2	2.53	0.43
2:D:186:PRO:HG2	2:D:251:TYR:CE2	2.54	0.43
2:D:294:ILE:O	2:D:295:TYR:CD1	2.71	0.43
1:B:116:LYS:HG2	1:B:167:THR:HG23	2.00	0.43
1:C:340:ARG:HD3	1:C:340:ARG:HA	1.90	0.43
2:F:442:LEU:HA	2:F:442:LEU:HD23	1.91	0.43
7:M:101:ARG:HA	7:M:161:LEU:HD21	2.00	0.43
7:M:54:LEU:HD21	7:M:305:ARG:HG2	2.00	0.43
1:B:443:VAL:HG21	1:B:447:TYR:CE2	2.54	0.43
3:G:103:ARG:HH21	3:G:149:LYS:HD3	1.83	0.43
1:B:353:TYR:C	1:B:355:ALA:H	2.22	0.43
1:B:363:GLU:HA	1:B:363:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:TRP:CD2	1:C:505:ALA:O	2.72	0.43
3:G:58:LYS:HA	3:G:61:TYR:CD2	2.54	0.43
1:A:354:LEU:H	1:A:354:LEU:HD12	1.83	0.42
2:F:174:ARG:NE	2:F:174:ARG:HA	2.34	0.42
1:A:494:PHE:CG	1:A:494:PHE:O	2.72	0.42
2:D:140:VAL:O	2:D:375:HIS:HE1	2.01	0.42
4:H:98:ILE:H	4:H:98:ILE:HD13	1.82	0.42
1:A:424:TRP:CG	1:A:424:TRP:O	2.72	0.42
2:E:60:PHE:CD1	2:E:229:ILE:HG21	2.54	0.42
3:G:64:LEU:HD22	3:G:126:ALA:CB	2.45	0.42
7:M:150:ALA:HB1	7:M:171:ARG:HE	1.85	0.42
1:B:77:PRO:HB3	1:B:145:HIS:CE1	2.55	0.42
1:C:515:ILE:HA	1:C:518:MET:HG2	2.02	0.42
2:D:45:GLY:HA2	2:D:60:PHE:CE1	2.54	0.42
2:F:89:LEU:HD23	2:F:89:LEU:HA	1.87	0.42
1:C:265:VAL:HG13	1:C:269:PHE:CE2	2.54	0.42
1:C:16:ALA:O	1:C:46:THR:HA	2.19	0.42
2:D:32:ILE:CD1	2:D:80:ALA:HB2	2.50	0.42
1:A:27:ILE:HA	1:A:37:GLY:O	2.19	0.42
1:C:165:GLU:O	1:C:166:TYR:CD1	2.72	0.42
1:A:235:THR:HG21	1:A:261:GLU:OE1	2.20	0.42
1:A:503:VAL:HG12	1:A:504:ASP:H	1.85	0.42
1:C:489:ILE:C	1:C:491:ARG:H	2.23	0.42
2:D:125:ARG:NH2	2:D:300:VAL:HG11	2.34	0.42
2:E:281:ARG:HG3	2:E:281:ARG:H	1.54	0.42
2:F:199:ARG:NH1	2:F:200:GLU:HA	2.34	0.42
1:B:344:MET:HB2	3:G:192:PHE:CE1	2.55	0.42
1:B:418:HIS:HB2	1:B:496:GLN:HE21	1.84	0.42
2:E:252:HIS:CE1	2:E:306:GLY:HA2	2.54	0.42
2:F:199:ARG:C	2:F:199:ARG:HH11	2.23	0.42
2:F:241:VAL:HG12	2:F:241:VAL:O	2.20	0.42
2:F:362:MET:C	2:F:364:ASN:H	2.23	0.42
4:H:48:ASP:HB2	4:H:50:ALA:H	1.84	0.42
4:H:57:ARG:HE	4:H:57:ARG:H	1.67	0.42
7:M:308:TYR:CD2	7:M:309:PHE:CE1	3.08	0.42
2:E:194:MET:H	2:E:258:THR:CG2	2.33	0.41
2:E:385:ALA:HB1	2:E:414:PHE:CE1	2.53	0.41
3:G:154:ILE:HD13	3:G:154:ILE:HA	1.93	0.41
3:G:20:LEU:HA	3:G:20:LEU:HD23	1.94	0.41
1:B:109:HIS:CD2	1:B:113:ARG:HE	2.37	0.41
2:D:84:VAL:HG21	2:D:244:TYR:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:48:ASP:HA	4:H:75:ALA:H	1.85	0.41
1:A:187:TRP:CE2	1:A:193:ARG:HG3	2.55	0.41
1:A:366:GLY:HA2	1:A:378:VAL:H	1.85	0.41
1:B:336:GLU:OE1	2:D:286:TYR:HA	2.20	0.41
1:B:84:TYR:N	1:B:84:TYR:CD2	2.88	0.41
2:F:199:ARG:HH11	2:F:199:ARG:HG2	1.85	0.41
1:A:223:THR:O	1:A:405:ALA:HB3	2.20	0.41
1:B:424:TRP:NE1	1:B:458:LEU:HD13	2.36	0.41
1:C:128:GLU:HA	1:C:156:ARG:HE	1.86	0.41
2:E:254:LEU:HA	2:E:254:LEU:HD23	1.90	0.41
2:F:71:THR:HG22	2:F:72:SER:N	2.36	0.41
1:A:209:MET:N	1:A:209:MET:SD	2.93	0.41
1:B:209:MET:HB2	1:B:212:LEU:HB2	2.02	0.41
1:C:150:PRO:HB3	1:C:185:HIS:CG	2.55	0.41
1:A:419:PHE:CD1	8:A:600:ADP:C5	3.08	0.41
1:B:212:LEU:HD22	1:B:407:TRP:CZ2	2.55	0.41
1:C:15:ILE:HG22	1:C:16:ALA:H	1.85	0.41
1:C:562:TYR:N	1:C:562:TYR:CD1	2.89	0.41
2:F:11:ILE:HG12	2:F:11:ILE:H	1.60	0.41
7:M:20:LEU:HD23	7:M:24:PHE:CD2	2.55	0.41
1:A:402:ILE:O	1:A:402:ILE:HG22	2.21	0.41
1:C:235:THR:O	1:C:235:THR:HG22	2.20	0.41
1:C:283:HIS:N	1:C:283:HIS:CD2	2.88	0.41
2:D:161:ASN:ND2	2:D:161:ASN:H	2.19	0.41
1:C:100:ILE:C	2:E:120:ASN:HD21	2.25	0.41
7:M:306:ARG:HG3	7:M:316:VAL:HG21	2.03	0.41
1:A:494:PHE:CE2	1:A:516:MET:HG3	2.56	0.41
3:G:192:PHE:N	3:G:192:PHE:CD1	2.88	0.41
1:A:328:SER:HB2	1:A:385:SER:H	1.85	0.40
1:B:329:ARG:HH21	2:D:331:TYR:HB3	1.86	0.40
2:E:94:ASN:HB2	2:E:100:ILE:HD11	2.03	0.40
2:E:100:ILE:HG22	2:E:101:ASP:H	1.86	0.40
2:E:104:PRO:HB2	2:E:105:PRO:HD2	2.02	0.40
2:E:135:ILE:HG23	2:E:425:GLN:OE1	2.21	0.40
4:H:18:LEU:C	4:H:20:GLY:H	2.24	0.40
1:A:405:ALA:HA	1:A:429:SER:HA	2.03	0.40
1:C:419:PHE:CD1	8:C:600:ADP:C5	3.09	0.40
1:A:113:ARG:HA	1:A:168:VAL:HG21	2.03	0.40
1:C:206:LEU:H	1:C:246:ASN:ND2	2.20	0.40
2:D:45:GLY:HA2	2:D:58:GLN:O	2.21	0.40
2:E:112:LEU:HB2	2:E:113:PRO:CD	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:HIS:O	2:F:344:HIS:CG	2.75	0.40
3:G:64:LEU:HA	3:G:122:TYR:CD1	2.56	0.40
1:B:467:ILE:HD12	1:B:467:ILE:H	1.85	0.40
2:D:348:ILE:HG22	2:D:349:TYR:H	1.86	0.40
4:H:47:VAL:HG12	4:H:48:ASP:N	2.37	0.40
6:L:79:VAL:HG11	6:L:186:LEU:HD13	2.03	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	575/578 (100%)	423 (74%)	97 (17%)	55 (10%)	1	13
1	B	575/578 (100%)	408 (71%)	100 (17%)	67 (12%)	0	8
1	C	575/578 (100%)	426 (74%)	102 (18%)	47 (8%)	1	16
2	D	457/478 (96%)	317 (69%)	93 (20%)	47 (10%)	0	11
2	E	457/478 (96%)	321 (70%)	92 (20%)	44 (10%)	1	13
2	F	457/478 (96%)	337 (74%)	83 (18%)	37 (8%)	1	17
3	G	208/223 (93%)	157 (76%)	33 (16%)	18 (9%)	1	15
4	H	98/104 (94%)	65 (66%)	18 (18%)	15 (15%)	0	4
5	I	59/120 (49%)	57 (97%)	1 (2%)	1 (2%)	11	51
5	K	59/120 (49%)	55 (93%)	2 (3%)	2 (3%)	4	36
6	J	148/188 (79%)	115 (78%)	24 (16%)	9 (6%)	2	23
6	L	148/188 (79%)	129 (87%)	15 (10%)	4 (3%)	6	41
7	M	318/323 (98%)	293 (92%)	15 (5%)	10 (3%)	5	38
All	All	4134/4434 (93%)	3103 (75%)	675 (16%)	356 (9%)	2	16

All (356) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	56	SER
1	A	188	PRO
1	A	217	PRO
1	A	227	PRO
1	A	244	TRP
1	A	266	LEU
1	A	276	LYS
1	A	427	SER
1	A	471	VAL
1	A	480	GLU
1	B	27	ILE
1	B	101	TYR
1	B	122	MET
1	B	159	GLU
1	B	202	ASN
1	B	292	SER
1	B	303	ILE
1	B	304	TYR
1	B	305	VAL
1	B	353	TYR
1	B	364	ARG
1	B	365	ALA
1	B	418	HIS
1	B	466	GLU
1	B	505	ALA
1	C	141	PHE
1	C	191	ARG
1	C	233	GLY
1	C	417	ARG
1	C	494	PHE
1	C	498	ASN
1	C	499	ALA
1	C	505	ALA
1	C	506	TYR
2	D	49	GLU
2	D	71	THR
2	D	72	SER
2	D	78	ASP
2	D	89	LEU
2	D	118	PRO
2	D	151	PRO

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Mol	Chain	Res	Type
2	D	210	ARG
2	D	216	ARG
2	D	276	GLU
2	D	321	ARG
2	D	349	TYR
2	D	354	PRO
2	D	372	ARG
2	E	7	GLU
2	E	64	THR
2	E	96	ILE
2	E	100	ILE
2	E	137	THR
2	E	148	GLN
2	E	151	PRO
2	E	215	SER
2	E	281	ARG
2	E	354	PRO
2	E	362	MET
2	E	419	GLU
2	F	101	ASP
2	F	135	ILE
2	F	139	ASP
2	F	143	THR
2	F	151	PRO
2	F	280	ARG
2	F	327	ASP
2	F	356	PRO
3	G	6	PRO
3	G	9	MET
3	G	67	ALA
4	H	66	ARG
4	H	69	PRO
4	H	75	ALA
4	H	80	ALA
6	J	138	ARG
6	J	141	GLU
6	L	138	ARG
7	M	4	ASP
7	M	32	SER
7	M	131	GLN
1	A	36	VAL
1	A	45	ASP

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Mol	Chain	Res	Type
1	A	64	VAL
1	A	72	ALA
1	A	108	VAL
1	A	318	PHE
1	A	353	TYR
1	A	367	LYS
1	A	387	PRO
1	A	416	ARG
1	A	432	THR
1	A	506	TYR
1	A	551	ALA
1	B	28	CYS
1	B	100	ILE
1	B	139	PRO
1	B	152	ASP
1	B	180	GLU
1	B	210	ARG
1	B	255	CYS
1	B	259	GLY
1	B	275	PRO
1	B	293	ASN
1	B	302	SER
1	B	340	ARG
1	B	397	GLN
1	B	443	VAL
1	B	467	ILE
1	B	469	GLN
1	B	471	VAL
1	B	495	LEU
1	C	45	ASP
1	C	112	ASP
1	C	177	ASP
1	C	202	ASN
1	C	210	ARG
1	C	222	GLY
1	C	246	ASN
1	C	347	GLU
1	C	392	SER
1	C	426	GLY
1	C	497	GLN
1	C	501	HIS
1	C	512	ALA

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Mol	Chain	Res	Type
2	D	95	GLY
2	D	119	LEU
2	D	213	ALA
2	D	293	THR
2	D	330	GLY
2	D	366	VAL
2	E	10	GLY
2	E	216	ARG
2	E	239	LEU
2	E	259	ASP
2	E	274	ARG
2	E	322	THR
2	E	332	ILE
2	E	356	PRO
2	E	359	SER
2	E	363	ASN
2	E	367	GLY
2	F	15	SER
2	F	23	ASN
2	F	95	GLY
2	F	140	VAL
2	F	186	PRO
2	F	275	GLU
2	F	298	ALA
2	F	389	GLY
2	F	402	ASP
3	G	112	ALA
3	G	117	VAL
3	G	119	THR
3	G	180	GLN
4	H	15	LEU
4	H	25	SER
4	H	48	ASP
4	H	54	ASP
6	J	99	GLU
6	J	163	VAL
5	K	107	LEU
6	L	180	SER
7	M	237	ASP
7	M	320	VAL
1	A	70	PRO
1	A	201	PRO

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Mol	Chain	Res	Type
1	A	222	GLY
1	A	232	SER
1	A	278	GLY
1	A	282	MET
1	A	302	SER
1	A	304	TYR
1	A	389	GLY
1	A	417	ARG
1	B	56	SER
1	B	145	HIS
1	B	177	ASP
1	B	197	ARG
1	B	227	PRO
1	B	346	ALA
1	B	349	GLY
1	B	356	ALA
1	B	413	LEU
1	B	473	PRO
1	B	510	LYS
1	C	12	PRO
1	C	80	LEU
1	C	85	ASP
1	C	318	PHE
1	C	365	ALA
1	C	400	LEU
1	C	410	ASP
1	C	463	GLY
1	C	473	PRO
1	C	496	GLN
2	D	97	GLY
2	D	164	ALA
2	D	168	ALA
2	D	180	GLU
2	D	284	PRO
2	D	317	PRO
2	D	326	PRO
2	D	362	MET
2	D	371	THR
2	E	17	PRO
2	E	88	MET
2	E	101	ASP
2	E	123	ALA

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Mol	Chain	Res	Type
2	E	225	ASP
2	E	336	GLN
2	E	358	LEU
2	F	10	GLY
2	F	89	LEU
2	F	128	GLU
2	F	375	HIS
2	F	403	ALA
2	F	436	LEU
3	G	88	GLY
3	G	110	ASP
3	G	134	ALA
3	G	174	ALA
4	H	29	ALA
4	H	53	PRO
4	H	55	PRO
4	H	81	PHE
6	J	119	LYS
6	J	140	VAL
5	K	104	MET
1	A	71	LEU
1	A	121	PRO
1	A	163	ALA
1	A	295	PRO
1	A	510	LYS
1	B	91	LEU
1	B	179	THR
1	B	232	SER
1	B	345	PRO
1	B	386	PRO
1	B	496	GLN
1	C	25	TYR
1	C	77	PRO
1	C	275	PRO
1	C	284	ARG
1	C	428	TYR
1	C	433	SER
1	C	444	ALA
2	D	77	GLU
2	D	108	PRO
2	D	117	LEU
2	D	237	MET

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Mol	Chain	Res	Type
2	D	250	ASP
2	D	275	GLU
2	D	312	PRO
2	D	403	ALA
2	E	54	TYR
2	E	128	GLU
2	E	166	GLN
2	E	190	VAL
2	E	240	THR
2	E	277	ILE
2	E	297	ARG
2	F	69	ALA
2	F	222	ASN
2	F	263	TYR
2	F	312	PRO
2	F	415	ALA
3	G	80	ALA
3	G	85	PRO
3	G	87	GLU
3	G	168	VAL
4	H	79	GLU
5	I	104	MET
6	J	52	GLN
6	J	126	GLU
6	L	52	GLN
7	M	254	GLY
1	A	202	ASN
1	A	277	THR
1	A	345	PRO
1	A	361	PHE
1	A	477	GLN
1	A	505	ALA
1	A	516	MET
1	B	108	VAL
1	B	141	PHE
1	B	248	ASP
1	B	257	GLU
1	B	315	ASP
1	B	359	ALA
1	B	395	VAL
1	B	417	ARG
1	B	445	GLU

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Mol	Chain	Res	Type
1	B	540	LEU
1	C	402	ILE
1	C	563	PHE
2	D	8	TYR
2	D	61	GLU
2	D	336	GLN
2	E	23	ASN
2	E	49	GLU
2	E	250	ASP
2	F	137	THR
2	F	259	ASP
3	G	114	LEU
3	G	167	VAL
4	H	52	LEU
6	J	127	ASP
7	M	52	GLN
7	M	75	LEU
7	M	76	VAL
1	A	192	ALA
1	A	402	ILE
1	A	484	ILE
1	B	253	VAL
1	B	296	VAL
1	B	509	MET
1	C	248	ASP
2	D	99	PRO
2	D	128	GLU
2	E	273	ALA
2	E	399	ILE
2	F	175	PRO
2	F	226	ASP
2	F	250	ASP
4	H	20	GLY
1	A	549	GLY
1	B	40	ILE
1	C	36	VAL
2	D	121	PRO
2	D	186	PRO
2	D	348	ILE
2	E	270	ILE
2	F	17	PRO
1	A	170	GLU

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Mol	Chain	Res	Type
1	A	189	VAL
1	A	443	VAL
1	A	570	ILE
1	B	534	VAL
1	C	490	ILE
1	C	514	GLY
1	B	87	ILE
1	C	443	VAL
2	F	355	LEU
2	F	390	VAL
3	G	154	ILE
6	L	104	VAL
7	M	222	GLY
1	A	486	VAL
1	B	394	PRO
2	D	65	GLY
2	D	90	GLY
1	C	5	VAL
2	E	235	PRO
2	F	279	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	A	468/468 (100%)	419 (90%)	49 (10%)	8	34
1	B	468/468 (100%)	416 (89%)	52 (11%)	7	32
1	C	468/468 (100%)	423 (90%)	45 (10%)	10	38
2	D	386/401 (96%)	343 (89%)	43 (11%)	7	32
2	E	386/401 (96%)	350 (91%)	36 (9%)	10	39
2	F	386/401 (96%)	360 (93%)	26 (7%)	19	53
3	G	166/176 (94%)	141 (85%)	25 (15%)	3	21
4	H	76/80 (95%)	66 (87%)	10 (13%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	37/86 (43%)	32 (86%)	5 (14%)	4	26
5	K	37/86 (43%)	32 (86%)	5 (14%)	4	26
6	J	76/141 (54%)	74 (97%)	2 (3%)	51	76
6	L	76/141 (54%)	76 (100%)	0	100	100
7	M	254/256 (99%)	240 (94%)	14 (6%)	25	59
All	All	3284/3573 (92%)	2972 (90%)	312 (10%)	14	38

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	12	PRO
1	A	42	LEU
1	A	45	ASP
1	A	54	ASP
1	A	55	THR
1	A	60	VAL
1	A	74	GLU
1	A	87	ILE
1	A	88	GLN
1	A	95	ARG
1	A	104	ARG
1	A	124	LYS
1	A	130	ARG
1	A	154	ARG
1	A	159	GLU
1	A	189	VAL
1	A	207	THR
1	A	209	MET
1	A	213	ASP
1	A	223	THR
1	A	244	TRP
1	A	249	VAL
1	A	264	ASP
1	A	282	MET
1	A	285	THR
1	A	295	PRO
1	A	300	GLU
1	A	303	ILE
1	A	307	VAL

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Mol	Chain	Res	Type
1	A	329	ARG
1	A	335	ARG
1	A	341	LEU
1	A	348	GLU
1	A	361	PHE
1	A	363	GLU
1	A	368	VAL
1	A	378	VAL
1	A	393	GLU
1	A	410	ASP
1	A	437	PRO
1	A	450	LEU
1	A	452	ASP
1	A	466	GLU
1	A	504	ASP
1	A	527	GLU
1	A	550	ARG
1	A	565	GLU
1	A	567	MET
1	B	1	MET
1	B	5	VAL
1	B	12	PRO
1	B	24	MET
1	B	33	GLU
1	B	40	ILE
1	B	41	ARG
1	B	69	LEU
1	B	79	MET
1	B	109	HIS
1	B	117	TRP
1	B	119	TRP
1	B	127	ASP
1	B	144	THR
1	B	172	VAL
1	B	180	GLU
1	B	181	LEU
1	B	189	VAL
1	B	196	GLN
1	B	207	THR
1	B	210	ARG
1	B	213	ASP
1	B	223	THR

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Mol	Chain	Res	Type
1	B	226	ILE
1	B	232	SER
1	B	241	LEU
1	B	248	ASP
1	B	253	VAL
1	B	255	CYS
1	B	264	ASP
1	B	269	PHE
1	B	290	ASN
1	B	303	ILE
1	B	378	VAL
1	B	384	VAL
1	B	395	VAL
1	B	398	SER
1	B	409	LEU
1	B	418	HIS
1	B	431	PHE
1	B	439	TYR
1	B	441	GLU
1	B	464	LEU
1	B	470	LEU
1	B	493	ASP
1	B	498	ASN
1	B	522	PHE
1	B	550	ARG
1	B	559	PHE
1	B	563	PHE
1	B	567	MET
1	B	569	GLU
1	C	28	CYS
1	C	46	THR
1	C	49	VAL
1	C	50	GLN
1	C	62	GLU
1	C	87	ILE
1	C	112	ASP
1	C	119	TRP
1	C	189	VAL
1	C	200	ASP
1	C	205	PHE
1	C	215	LEU
1	C	220	MET

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Mol	Chain	Res	Type
1	C	230	PHE
1	C	239	GLN
1	C	241	LEU
1	C	258	ARG
1	C	282	MET
1	C	291	THR
1	C	313	PHE
1	C	323	MET
1	C	325	ASP
1	C	329	ARG
1	C	339	SER
1	C	358	LEU
1	C	394	PRO
1	C	395	VAL
1	C	400	LEU
1	C	402	ILE
1	C	417	ARG
1	C	430	LEU
1	C	437	PRO
1	C	471	VAL
1	C	474	ASP
1	C	494	PHE
1	C	495	LEU
1	C	502	GLU
1	C	513	TYR
1	C	517	LYS
1	C	536	ILE
1	C	543	PRO
1	C	548	ILE
1	C	565	GLU
1	C	571	GLN
1	C	574	PHE
2	D	11	ILE
2	D	14	ILE
2	D	22	GLU
2	D	32	ILE
2	D	36	LYS
2	D	61	GLU
2	D	71	THR
2	D	81	ARG
2	D	85	SER
2	D	89	LEU

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Mol	Chain	Res	Type
2	D	92	ARG
2	D	142	ASN
2	D	149	LYS
2	D	166	GLN
2	D	172	THR
2	D	173	VAL
2	D	180	GLU
2	D	194	MET
2	D	196	ILE
2	D	199	ARG
2	D	206	GLN
2	D	207	GLU
2	D	208	PHE
2	D	209	GLU
2	D	216	ARG
2	D	221	LEU
2	D	226	ASP
2	D	227	PRO
2	D	251	TYR
2	D	258	THR
2	D	260	MET
2	D	261	THR
2	D	284	PRO
2	D	286	TYR
2	D	287	MET
2	D	300	VAL
2	D	319	ASP
2	D	324	PRO
2	D	353	ASP
2	D	362	MET
2	D	395	LEU
2	D	405	THR
2	D	457	ASP
2	E	26	ASP
2	E	34	ASP
2	E	61	GLU
2	E	82	LEU
2	E	88	MET
2	E	93	PHE
2	E	104	PRO
2	E	120	ASN
2	E	133	THR

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Mol	Chain	Res	Type
2	E	162	GLU
2	E	173	VAL
2	E	182	GLU
2	E	199	ARG
2	E	225	ASP
2	E	235	PRO
2	E	239	LEU
2	E	243	GLU
2	E	260	MET
2	E	261	THR
2	E	308	VAL
2	E	322	THR
2	E	323	HIS
2	E	327	ASP
2	E	337	ILE
2	E	342	GLU
2	E	343	LEU
2	E	371	THR
2	E	380	ASP
2	E	386	TYR
2	E	394	LYS
2	E	402	ASP
2	E	405	THR
2	E	410	ARG
2	E	421	PHE
2	E	429	ASN
2	E	463	TYR
2	F	26	ASP
2	F	29	TYR
2	F	50	VAL
2	F	53	GLU
2	F	62	GLU
2	F	92	ARG
2	F	130	PHE
2	F	187	PHE
2	F	194	MET
2	F	199	ARG
2	F	201	LEU
2	F	204	PHE
2	F	219	LEU
2	F	225	ASP
2	F	231	ARG

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Mol	Chain	Res	Type
2	F	235	PRO
2	F	286	TYR
2	F	316	MET
2	F	324	PRO
2	F	336	GLN
2	F	371	THR
2	F	388	ASN
2	F	410	ARG
2	F	414	PHE
2	F	419	GLU
2	F	457	ASP
3	G	4	VAL
3	G	8	ARG
3	G	9	MET
3	G	13	GLN
3	G	14	ARG
3	G	22	GLN
3	G	32	ARG
3	G	39	PHE
3	G	43	VAL
3	G	44	ARG
3	G	50	ARG
3	G	70	PHE
3	G	71	ASP
3	G	73	PRO
3	G	89	VAL
3	G	93	VAL
3	G	97	TRP
3	G	103	ARG
3	G	117	VAL
3	G	152	GLU
3	G	157	THR
3	G	162	ASN
3	G	177	ARG
3	G	186	ARG
3	G	188	ARG
4	H	28	GLU
4	H	57	ARG
4	H	60	GLU
4	H	72	LEU
4	H	77	LEU
4	H	78	LYS

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Mol	Chain	Res	Type
4	H	92	GLU
4	H	95	ARG
4	H	96	LYS
4	H	98	ILE
5	I	61	GLU
5	I	69	LEU
5	I	75	GLU
5	I	88	TYR
5	I	91	ARG
6	J	57	LEU
6	J	105	ARG
5	K	63	GLU
5	K	69	LEU
5	K	82	GLU
5	K	95	GLU
5	K	108	ASP
7	M	20	LEU
7	M	56	ASP
7	M	74	ARG
7	M	82	GLU
7	M	119	LEU
7	M	120	ARG
7	M	142	VAL
7	M	157	GLU
7	M	175	ASP
7	M	195	GLU
7	M	220	LYS
7	M	257	ASP
7	M	262	GLU
7	M	272	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	185	HIS
1	A	283	HIS
1	A	442	ASN
1	B	145	HIS
1	B	283	HIS
1	B	316	GLN
1	B	418	HIS

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Mol	Chain	Res	Type
1	B	496	GLN
1	C	246	ASN
1	C	316	GLN
2	D	142	ASN
2	D	161	ASN
2	D	170	GLN
2	D	249	HIS
2	D	252	HIS
2	D	344	HIS
2	D	363	ASN
2	D	429	ASN
2	E	249	HIS
2	E	323	HIS
2	F	148	GLN
2	F	166	GLN
2	F	222	ASN
2	F	262	ASN
2	F	338	GLN
6	L	130	HIS
7	M	126	GLN
7	M	200	ASN
7	M	208	GLN
7	M	315	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

2 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$
8	ADP	A	600	-	25,29,29	1.79	5 (20%)	24,45,45	1.31	2 (8%)
8	ADP	C	600	-	25,29,29	1.60	3 (12%)	24,45,45	1.27	2 (8%)

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
8	ADP	A	600	-	-	0/12/32/32	0/3/3/3
8	ADP	C	600	-	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	600	ADP	C2'-C1'	-4.40	1.46	1.53
8	C	600	ADP	C2'-C1'	-3.68	1.47	1.53
8	A	600	ADP	C8-N7	-2.94	1.29	1.34
8	A	600	ADP	O4'-C1'	-2.82	1.37	1.41
8	C	600	ADP	C8-N7	-2.72	1.29	1.34
8	A	600	ADP	C4-N3	-2.36	1.32	1.35
8	A	600	ADP	PB-O3A	3.96	1.66	1.60
8	C	600	ADP	PB-O3A	4.68	1.67	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	600	ADP	C1'-N9-C4	-3.01	121.43	126.64
8	C	600	ADP	C5-C6-N6	-2.17	116.05	120.47
8	A	600	ADP	N6-C6-N1	3.94	126.58	118.77
8	C	600	ADP	N6-C6-N1	4.01	126.72	118.77

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	600	ADP	4	0
8	C	600	ADP	4	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.