



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 25, 2018 – 04:59 PM EST

PDB ID : 5NP7
EMDB ID: : EMD-8183
Title : CryoEM structure of Human Rad51 on single-stranded DNA to 4.2A resolution.
Authors : Short, J.M.; Venkitaraman, A.
Deposited on : 2017-04-13
Resolution : 4.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

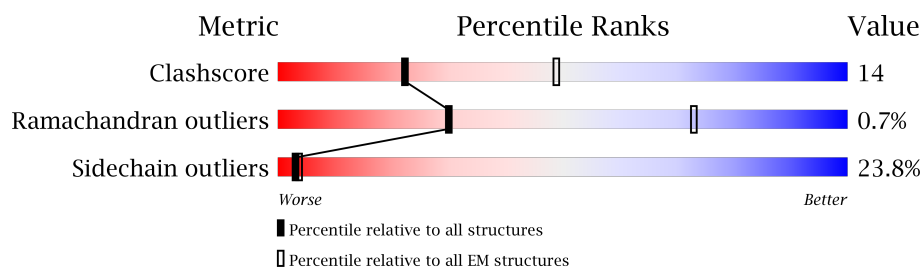
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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 ≥ 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	339	57% 24% 9% • 8%
1	B	339	56% 24% 10% • 8%
1	C	339	56% 25% 9% • 8%
1	D	339	56% 25% 9% • 8%
1	E	339	55% 25% 9% • 8%
1	F	339	56% 25% 9% • 8%
1	G	339	57% 24% 9% • 8%

2 Entry composition [i](#)

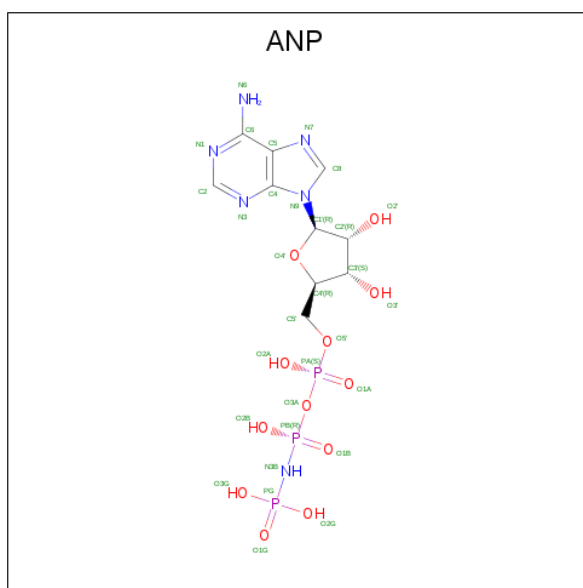
There are 2 unique types of molecules in this entry. The entry contains 16457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA repair protein RAD51 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	B	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	C	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	D	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	E	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	F	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	G	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

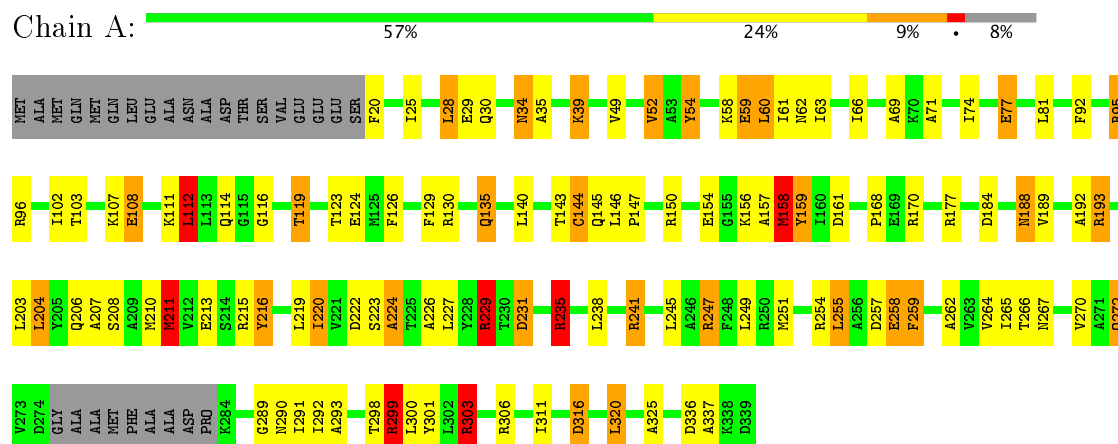


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	G	1	Total	C	N	O	P	0
			31	10	6	12	3	

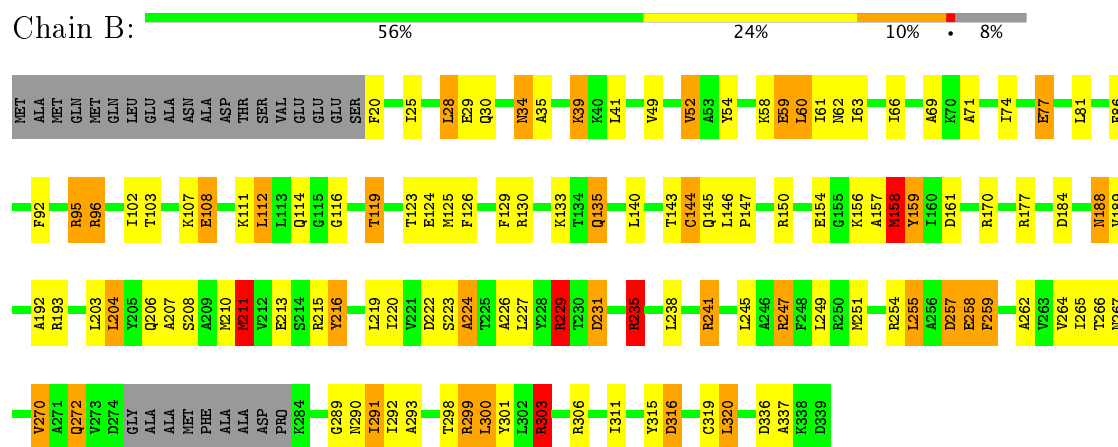
3 Residue-property plots

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.

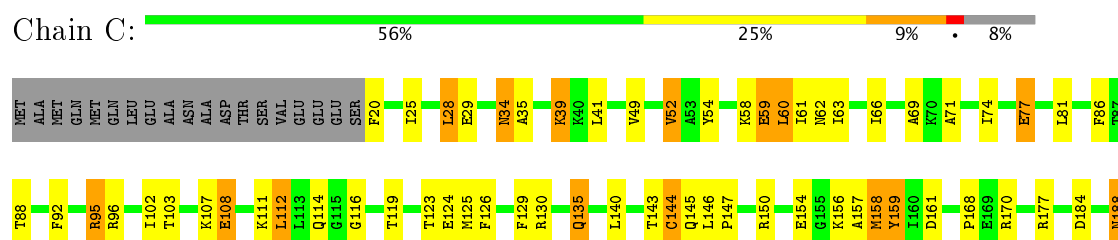
• Molecule 1: DNA repair protein RAD51 homolog 1

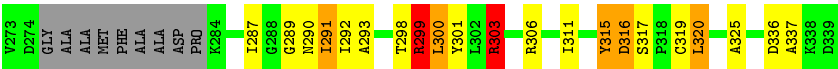


• Molecule 1: DNA repair protein RAD51 homolog 1

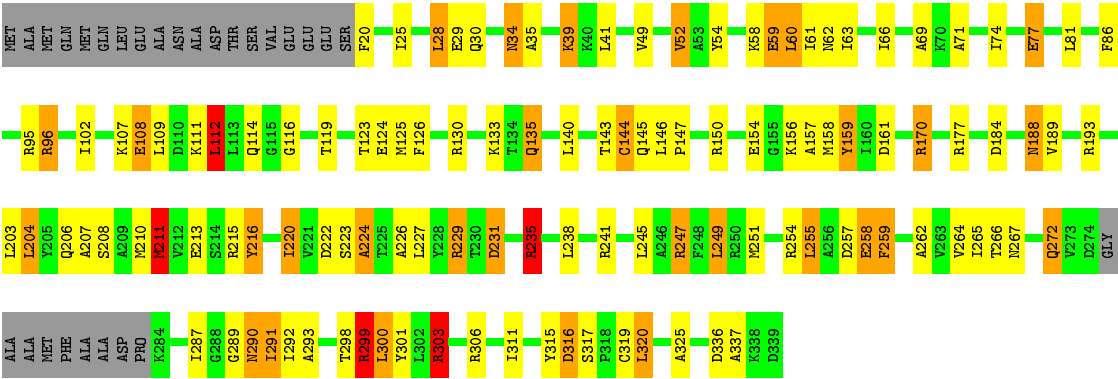


• Molecule 1: DNA repair protein RAD51 homolog 1





● Molecule 1: DNA repair protein RAD51 homolog 1



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=56.2°, rise=16.0 Å, axial sym=C1	Depositor
Number of segments used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; per segment	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104477	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: ANP

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	0.99	3/2354 (0.1%)	1.39	24/3182 (0.8%)
1	B	0.99	5/2354 (0.2%)	1.39	25/3182 (0.8%)
1	C	0.99	5/2354 (0.2%)	1.41	27/3182 (0.8%)
1	D	0.99	5/2354 (0.2%)	1.40	27/3182 (0.8%)
1	E	0.99	4/2354 (0.2%)	1.40	24/3182 (0.8%)
1	F	0.99	5/2354 (0.2%)	1.40	27/3182 (0.8%)
1	G	1.00	5/2354 (0.2%)	1.40	24/3182 (0.8%)
All	All	0.99	32/16478 (0.2%)	1.40	178/22274 (0.8%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	54	TYR	CE1-CZ	6.85	1.47	1.38
1	B	54	TYR	CE1-CZ	6.36	1.46	1.38
1	G	54	TYR	CE1-CZ	5.98	1.46	1.38
1	E	54	TYR	CG-CD2	5.91	1.46	1.39
1	A	258	GLU	CG-CD	-5.83	1.43	1.51
1	C	54	TYR	CE1-CZ	5.75	1.46	1.38
1	D	258	GLU	CG-CD	-5.73	1.43	1.51
1	B	258	GLU	CG-CD	-5.71	1.43	1.51
1	G	54	TYR	CG-CD2	5.70	1.46	1.39
1	G	258	GLU	CG-CD	-5.69	1.43	1.51
1	E	258	GLU	CG-CD	-5.67	1.43	1.51
1	B	54	TYR	CG-CD2	5.67	1.46	1.39
1	D	54	TYR	CE1-CZ	5.65	1.45	1.38
1	F	258	GLU	CG-CD	-5.63	1.43	1.51
1	C	258	GLU	CG-CD	-5.63	1.43	1.51
1	D	54	TYR	CG-CD2	5.61	1.46	1.39
1	C	54	TYR	CG-CD2	5.45	1.46	1.39
1	F	54	TYR	CG-CD2	5.31	1.46	1.39
1	A	54	TYR	CG-CD1	5.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	315	TYR	CE1-CZ	5.25	1.45	1.38
1	F	54	TYR	CE1-CZ	5.19	1.45	1.38
1	C	211	MET	CG-SD	-5.17	1.67	1.81
1	B	211	MET	CG-SD	-5.12	1.67	1.81
1	E	211	MET	CG-SD	-5.12	1.67	1.81
1	A	211	MET	CG-SD	-5.12	1.67	1.81
1	D	211	MET	CG-SD	-5.10	1.67	1.81
1	F	315	TYR	CE1-CZ	5.06	1.45	1.38
1	G	315	TYR	CE1-CZ	5.06	1.45	1.38
1	B	315	TYR	CE1-CZ	5.05	1.45	1.38
1	G	211	MET	CG-SD	-5.05	1.68	1.81
1	C	315	TYR	CE1-CZ	5.04	1.45	1.38
1	F	211	MET	CG-SD	-5.04	1.68	1.81

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	231	ASP	CB-CG-OD2	11.79	128.91	118.30
1	A	231	ASP	CB-CG-OD2	11.42	128.58	118.30
1	B	231	ASP	CB-CG-OD2	11.37	128.53	118.30
1	D	231	ASP	CB-CG-OD2	11.12	128.31	118.30
1	F	231	ASP	CB-CG-OD2	11.10	128.29	118.30
1	C	231	ASP	CB-CG-OD2	10.97	128.17	118.30
1	E	231	ASP	CB-CG-OD2	10.88	128.09	118.30
1	D	247	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	E	247	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	F	247	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	G	229	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	C	247	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	G	247	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	193	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	D	193	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	B	247	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	A	247	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	C	193	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	F	193	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	193	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	E	193	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	E	229	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	F	229	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	229	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	D	241	ARG	NE-CZ-NH1	7.99	124.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	C	241	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	D	229	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	241	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	E	241	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	F	254	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	229	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	G	254	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	D	254	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	254	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	254	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	E	254	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	254	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	G	259	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	B	259	PHE	CB-CG-CD2	-7.08	115.85	120.80
1	C	259	PHE	CB-CG-CD2	-7.07	115.85	120.80
1	A	96	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	259	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	G	170	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	C	219	LEU	CB-CG-CD1	7.00	122.90	111.00
1	E	259	PHE	CB-CG-CD2	-6.99	115.91	120.80
1	D	259	PHE	CB-CG-CD2	-6.98	115.91	120.80
1	A	303	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	B	303	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	F	259	PHE	CB-CG-CD2	-6.84	116.01	120.80
1	D	303	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	F	247	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	G	193	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	E	247	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	247	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	G	249	LEU	CB-CG-CD2	-6.63	99.74	111.00
1	E	303	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	G	247	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	G	303	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	303	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	247	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	249	LEU	CB-CG-CD2	-6.39	100.14	111.00
1	A	241	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	F	303	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	D	249	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	C	96	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	249	LEU	CB-CG-CD2	-6.22	100.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	216	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	E	249	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	B	170	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	B	216	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	F	249	LEU	CB-CG-CD2	-6.09	100.65	111.00
1	C	216	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	D	216	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	B	249	LEU	CB-CG-CD1	6.02	121.24	111.00
1	A	249	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	C	249	LEU	CB-CG-CD1	5.96	121.14	111.00
1	D	215	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	G	216	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	95	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	F	96	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	170	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	F	215	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	G	96	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	216	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	E	96	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	170	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	E	215	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	215	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	247	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	G	95	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	E	170	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	E	95	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	D	170	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	F	170	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	F	249	LEU	CB-CG-CD1	5.82	120.90	111.00
1	B	96	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	E	249	LEU	CB-CG-CD1	5.81	120.88	111.00
1	G	235	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	95	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	215	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	F	216	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	D	249	LEU	CB-CG-CD1	5.78	120.82	111.00
1	B	241	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	F	95	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	G	249	LEU	CB-CG-CD1	5.75	120.78	111.00
1	C	241	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	299	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	247	ARG	NE-CZ-NH2	-5.73	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	215	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	G	215	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	235	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	95	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	235	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	96	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	235	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	F	219	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	235	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	F	235	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	95	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	229	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	D	247	ARG	CD-NE-CZ	5.48	131.27	123.60
1	D	241	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	E	299	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	247	ARG	CD-NE-CZ	5.46	131.24	123.60
1	B	41	LEU	CB-CG-CD2	5.46	120.27	111.00
1	A	231	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	C	41	LEU	CB-CG-CD2	5.44	120.24	111.00
1	G	287	ILE	CG1-CB-CG2	5.42	123.33	111.40
1	E	247	ARG	CD-NE-CZ	5.40	131.17	123.60
1	B	231	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	C	247	ARG	CD-NE-CZ	5.35	131.09	123.60
1	F	41	LEU	CB-CG-CD2	5.31	120.03	111.00
1	F	112	LEU	CB-CG-CD2	5.31	120.03	111.00
1	G	231	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	E	41	LEU	CB-CG-CD2	5.30	120.01	111.00
1	F	287	ILE	CG1-CB-CG2	5.30	123.06	111.40
1	A	249	LEU	CB-CG-CD1	5.29	119.99	111.00
1	G	112	LEU	CB-CG-CD2	5.29	119.99	111.00
1	F	231	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	F	299	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	D	229	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	112	LEU	CB-CG-CD2	5.26	119.94	111.00
1	F	241	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	299	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	112	LEU	CB-CG-CD2	5.25	119.92	111.00
1	D	299	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	E	229	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	G	247	ARG	CD-NE-CZ	5.19	130.87	123.60
1	G	109	LEU	CB-CG-CD1	5.18	119.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	LEU	CB-CG-CD1	5.18	119.81	111.00
1	A	112	LEU	CB-CG-CD2	5.17	119.79	111.00
1	E	216	TYR	CB-CG-CD1	5.17	124.10	121.00
1	F	306	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	G	306	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	219	LEU	CA-CB-CG	5.13	127.11	115.30
1	C	231	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	A	247	ARG	CD-NE-CZ	5.12	130.77	123.60
1	D	41	LEU	CB-CG-CD2	5.11	119.69	111.00
1	A	158	MET	CB-CA-C	5.11	120.62	110.40
1	E	241	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	216	TYR	CB-CG-CD1	5.11	124.06	121.00
1	C	216	TYR	CB-CG-CD1	5.10	124.06	121.00
1	G	41	LEU	CB-CG-CD2	5.10	119.67	111.00
1	A	306	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	306	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	112	LEU	CB-CG-CD2	5.09	119.65	111.00
1	E	306	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	306	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	231	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	B	247	ARG	CD-NE-CZ	5.05	130.67	123.60
1	F	109	LEU	CB-CG-CD1	5.05	119.58	111.00
1	F	177	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	299	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	216	TYR	CB-CG-CD1	5.04	124.02	121.00
1	C	306	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	158	MET	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2320	0	2268	68	0
1	B	2320	0	2268	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2320	0	2268	72	0
1	D	2320	0	2268	73	0
1	E	2320	0	2268	74	0
1	F	2320	0	2268	65	0
1	G	2320	0	2268	70	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	1	0
2	F	31	0	13	1	0
2	G	31	0	13	0	0
All	All	16457	0	15967	467	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 14.

All (467) 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:207:ALA:O	1:D:211:MET:SD	2.06	1.13
1:C:207:ALA:O	1:C:211:MET:SD	2.06	1.13
1:F:207:ALA:O	1:F:211:MET:SD	2.06	1.13
1:B:207:ALA:O	1:B:211:MET:SD	2.06	1.12
1:A:207:ALA:O	1:A:211:MET:SD	2.06	1.12
1:E:207:ALA:O	1:E:211:MET:SD	2.06	1.12
1:G:207:ALA:O	1:G:211:MET:SD	2.06	1.12
1:A:223:SER:HB3	1:A:226:ALA:HB3	1.37	1.07
1:D:223:SER:HB3	1:D:226:ALA:HB3	1.37	1.06
1:E:223:SER:HB3	1:E:226:ALA:HB3	1.37	1.06
1:F:223:SER:HB3	1:F:226:ALA:HB3	1.37	1.05
1:G:223:SER:HB3	1:G:226:ALA:HB3	1.38	1.05
1:C:223:SER:HB3	1:C:226:ALA:HB3	1.37	1.05
1:B:223:SER:HB3	1:B:226:ALA:HB3	1.37	1.04
1:G:227:LEU:O	1:G:231:ASP:OD1	1.79	1.00
1:F:227:LEU:O	1:F:231:ASP:OD1	1.80	1.00
1:A:227:LEU:O	1:A:231:ASP:OD1	1.80	0.99
1:C:227:LEU:O	1:C:231:ASP:OD1	1.81	0.99
1:E:227:LEU:O	1:E:231:ASP:OD1	1.81	0.98
1:B:227:LEU:O	1:B:231:ASP:OD1	1.81	0.98
1:D:227:LEU:O	1:D:231:ASP:OD1	1.81	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:ASP:O	1:G:188:ASN:OD1	1.90	0.90
1:F:184:ASP:O	1:F:188:ASN:OD1	1.91	0.89
1:E:184:ASP:O	1:E:188:ASN:OD1	1.91	0.89
1:D:184:ASP:O	1:D:188:ASN:OD1	1.91	0.89
1:C:184:ASP:O	1:C:188:ASN:OD1	1.91	0.89
1:B:184:ASP:O	1:B:188:ASN:OD1	1.91	0.87
1:A:184:ASP:O	1:A:188:ASN:OD1	1.91	0.87
1:E:140:LEU:HA	1:E:143:THR:HG22	1.59	0.85
1:E:135:GLN:HE21	1:E:135:GLN:HA	1.41	0.85
1:F:140:LEU:HA	1:F:143:THR:HG22	1.59	0.85
1:D:135:GLN:HA	1:D:135:GLN:HE21	1.42	0.84
1:A:140:LEU:HA	1:A:143:THR:HG22	1.59	0.84
1:G:140:LEU:HA	1:G:143:THR:HG22	1.60	0.84
1:A:135:GLN:HA	1:A:135:GLN:HE21	1.40	0.83
1:D:140:LEU:HA	1:D:143:THR:HG22	1.59	0.83
1:C:135:GLN:HA	1:C:135:GLN:HE21	1.40	0.83
1:F:135:GLN:HA	1:F:135:GLN:HE21	1.41	0.83
1:B:140:LEU:HA	1:B:143:THR:HG22	1.60	0.82
1:G:135:GLN:HA	1:G:135:GLN:HE21	1.44	0.82
1:B:135:GLN:HE21	1:B:135:GLN:HA	1.42	0.81
1:C:140:LEU:HA	1:C:143:THR:HG22	1.61	0.81
1:G:223:SER:H	1:G:266:THR:HB	1.47	0.79
1:E:223:SER:H	1:E:266:THR:HB	1.48	0.78
1:C:135:GLN:HA	1:C:135:GLN:NE2	1.99	0.78
1:A:135:GLN:HA	1:A:135:GLN:NE2	1.99	0.78
1:B:135:GLN:NE2	1:B:135:GLN:HA	1.99	0.78
1:B:223:SER:H	1:B:266:THR:HB	1.50	0.77
1:F:135:GLN:HA	1:F:135:GLN:NE2	1.99	0.77
1:E:135:GLN:NE2	1:E:135:GLN:HA	1.99	0.77
1:F:140:LEU:HA	1:F:143:THR:CG2	2.15	0.77
1:D:135:GLN:HA	1:D:135:GLN:NE2	2.00	0.76
1:E:140:LEU:HA	1:E:143:THR:CG2	2.15	0.76
1:B:140:LEU:HA	1:B:143:THR:CG2	2.15	0.76
1:C:223:SER:H	1:C:266:THR:HB	1.49	0.76
1:F:223:SER:H	1:F:266:THR:HB	1.49	0.76
1:A:140:LEU:HA	1:A:143:THR:CG2	2.16	0.76
1:D:223:SER:H	1:D:266:THR:HB	1.50	0.76
1:G:135:GLN:HA	1:G:135:GLN:NE2	1.99	0.76
1:G:140:LEU:HA	1:G:143:THR:CG2	2.16	0.75
1:D:140:LEU:HA	1:D:143:THR:CG2	2.16	0.74
1:C:140:LEU:HA	1:C:143:THR:CG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:SER:H	1:A:266:THR:HB	1.53	0.72
1:C:229:ARG:HH22	1:C:270:VAL:HG23	1.56	0.71
1:D:229:ARG:HH22	1:D:270:VAL:HG23	1.57	0.69
1:B:229:ARG:HH22	1:B:270:VAL:HG23	1.59	0.68
1:D:145:GLN:HE22	1:D:156:LYS:HA	1.58	0.68
1:E:145:GLN:HE22	1:E:156:LYS:HA	1.58	0.68
1:G:204:LEU:HD12	1:G:251:MET:HG2	1.76	0.67
1:C:145:GLN:HE22	1:C:156:LYS:HA	1.60	0.67
1:F:145:GLN:HE22	1:F:156:LYS:HA	1.60	0.67
1:E:204:LEU:HD12	1:E:251:MET:HG2	1.77	0.66
1:D:192:ALA:HB2	1:E:86:PHE:H	1.61	0.65
1:C:192:ALA:HB2	1:D:86:PHE:H	1.61	0.65
1:B:145:GLN:HE22	1:B:156:LYS:HA	1.61	0.65
1:E:192:ALA:HB2	1:F:86:PHE:H	1.61	0.65
1:F:192:ALA:HB2	1:G:86:PHE:H	1.61	0.65
1:B:192:ALA:HB2	1:C:86:PHE:H	1.61	0.65
1:F:204:LEU:HD12	1:F:251:MET:HG2	1.78	0.65
1:E:210:MET:HB3	1:E:216:TYR:OH	1.97	0.65
1:A:145:GLN:HE22	1:A:156:LYS:HA	1.62	0.64
1:B:204:LEU:HD12	1:B:251:MET:HG2	1.79	0.64
1:C:204:LEU:HD12	1:C:251:MET:HG2	1.79	0.64
1:E:229:ARG:HH22	1:E:270:VAL:HG23	1.63	0.64
1:A:192:ALA:HB2	1:B:86:PHE:H	1.61	0.64
1:E:299:ARG:HB2	1:E:316:ASP:H	1.63	0.64
1:G:145:GLN:HE22	1:G:156:LYS:HA	1.61	0.64
1:C:210:MET:HB3	1:C:216:TYR:OH	1.98	0.64
1:D:204:LEU:HD12	1:D:251:MET:HG2	1.79	0.64
1:F:210:MET:HB3	1:F:216:TYR:OH	1.98	0.63
1:D:210:MET:HB3	1:D:216:TYR:OH	1.98	0.63
1:G:210:MET:HB3	1:G:216:TYR:OH	1.98	0.63
1:B:210:MET:HB3	1:B:216:TYR:OH	1.98	0.63
1:A:210:MET:HB3	1:A:216:TYR:OH	1.98	0.62
1:G:208:SER:HA	1:G:211:MET:SD	2.40	0.62
1:F:299:ARG:HB2	1:F:316:ASP:H	1.64	0.61
1:B:299:ARG:HB2	1:B:316:ASP:H	1.63	0.61
1:A:204:LEU:HD12	1:A:251:MET:HG2	1.80	0.61
1:F:211:MET:N	1:F:211:MET:SD	2.69	0.61
1:A:255:LEU:HA	1:A:258:GLU:HG2	1.81	0.61
1:D:255:LEU:HA	1:D:258:GLU:HG2	1.83	0.61
1:E:211:MET:SD	1:E:211:MET:N	2.69	0.61
1:G:255:LEU:HA	1:G:258:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:ARG:HB2	1:G:316:ASP:H	1.65	0.61
1:D:299:ARG:HB2	1:D:316:ASP:H	1.65	0.61
1:D:223:SER:O	1:D:226:ALA:N	2.33	0.60
1:A:208:SER:HA	1:A:211:MET:SD	2.42	0.60
1:E:223:SER:O	1:E:226:ALA:N	2.33	0.60
1:G:289:GLY:O	1:G:292:ILE:HD11	2.01	0.60
1:E:208:SER:HA	1:E:211:MET:SD	2.41	0.60
1:D:208:SER:HA	1:D:211:MET:SD	2.41	0.60
1:A:223:SER:O	1:A:226:ALA:N	2.33	0.60
1:C:255:LEU:HA	1:C:258:GLU:HG2	1.83	0.60
1:C:299:ARG:HB2	1:C:316:ASP:H	1.65	0.60
1:B:255:LEU:HA	1:B:258:GLU:HG2	1.83	0.60
1:E:124:GLU:HB2	1:E:265:ILE:O	2.01	0.60
1:B:208:SER:HA	1:B:211:MET:SD	2.42	0.59
1:G:124:GLU:HB2	1:G:265:ILE:O	2.02	0.59
1:C:208:SER:HA	1:C:211:MET:SD	2.42	0.59
1:F:255:LEU:HA	1:F:258:GLU:HG2	1.83	0.59
1:F:208:SER:HA	1:F:211:MET:SD	2.42	0.59
1:E:255:LEU:HA	1:E:258:GLU:HG2	1.83	0.59
1:B:124:GLU:HB2	1:B:265:ILE:O	2.04	0.58
1:D:211:MET:N	1:D:211:MET:SD	2.69	0.58
1:G:223:SER:O	1:G:226:ALA:N	2.35	0.58
1:B:223:SER:O	1:B:226:ALA:N	2.34	0.58
1:C:258:GLU:HG3	1:C:259:PHE:N	2.19	0.58
1:D:124:GLU:HB2	1:D:265:ILE:O	2.03	0.58
1:G:211:MET:N	1:G:211:MET:SD	2.69	0.57
1:C:211:MET:HG3	1:C:259:PHE:CE2	2.40	0.57
1:C:235:ARG:HE	1:C:235:ARG:H	1.53	0.57
1:B:235:ARG:H	1:B:235:ARG:HE	1.51	0.57
1:D:235:ARG:HE	1:D:235:ARG:H	1.53	0.57
1:F:258:GLU:HG3	1:F:259:PHE:N	2.19	0.57
1:G:235:ARG:H	1:G:235:ARG:HE	1.50	0.57
1:G:258:GLU:HG3	1:G:259:PHE:N	2.19	0.57
1:B:258:GLU:HG3	1:B:259:PHE:N	2.19	0.57
1:E:129:PHE:HB3	1:F:293:ALA:HB1	1.86	0.57
1:E:258:GLU:HG3	1:E:259:PHE:N	2.20	0.57
1:A:211:MET:HG3	1:A:259:PHE:CE2	2.39	0.57
1:D:211:MET:HG3	1:D:259:PHE:CE2	2.40	0.57
1:D:289:GLY:O	1:D:292:ILE:HD11	2.05	0.57
1:E:211:MET:HG3	1:E:259:PHE:CE2	2.40	0.57
1:D:258:GLU:HG3	1:D:259:PHE:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HD2	1:A:311:ILE:HB	1.87	0.56
1:C:289:GLY:O	1:C:292:ILE:HD11	2.05	0.56
1:B:303:ARG:HD2	1:B:311:ILE:HB	1.88	0.56
1:F:289:GLY:O	1:F:292:ILE:HD11	2.06	0.56
1:B:289:GLY:O	1:B:292:ILE:HD11	2.05	0.56
1:C:114:GLN:HG2	1:C:320:LEU:HD23	1.88	0.56
1:F:223:SER:O	1:F:226:ALA:N	2.34	0.56
1:F:235:ARG:HE	1:F:235:ARG:H	1.51	0.56
1:B:129:PHE:HB3	1:C:293:ALA:HB1	1.88	0.56
1:A:211:MET:SD	1:A:211:MET:N	2.69	0.56
1:A:258:GLU:HG3	1:A:259:PHE:N	2.20	0.55
1:F:211:MET:HG3	1:F:259:PHE:CE2	2.42	0.55
1:C:223:SER:O	1:C:226:ALA:N	2.34	0.55
1:E:235:ARG:H	1:E:235:ARG:HE	1.54	0.55
1:G:114:GLN:HG2	1:G:320:LEU:HD23	1.88	0.55
1:C:129:PHE:HB3	1:D:293:ALA:HB1	1.88	0.55
1:F:123:THR:O	1:F:264:VAL:HA	2.07	0.55
1:F:124:GLU:HB2	1:F:265:ILE:O	2.06	0.55
1:G:207:ALA:C	1:G:211:MET:SD	2.85	0.55
1:A:207:ALA:C	1:A:211:MET:SD	2.85	0.55
1:C:211:MET:N	1:C:211:MET:SD	2.69	0.55
1:E:303:ARG:HD2	1:E:311:ILE:HB	1.89	0.55
1:D:158:MET:SD	1:D:219:LEU:HG	2.47	0.55
1:D:129:PHE:HB3	1:E:293:ALA:HB1	1.88	0.55
1:B:211:MET:HG3	1:B:259:PHE:CE2	2.43	0.54
1:B:123:THR:O	1:B:264:VAL:HA	2.07	0.54
1:A:123:THR:O	1:A:264:VAL:HA	2.08	0.54
1:A:299:ARG:HB2	1:A:316:ASP:H	1.72	0.54
1:F:114:GLN:HG2	1:F:320:LEU:HD23	1.89	0.54
1:E:289:GLY:O	1:E:292:ILE:HD11	2.07	0.54
1:B:211:MET:N	1:B:211:MET:SD	2.69	0.54
1:E:123:THR:O	1:E:264:VAL:HA	2.08	0.54
1:F:188:ASN:N	1:F:188:ASN:OD1	2.41	0.54
1:C:158:MET:SD	1:C:219:LEU:HG	2.48	0.54
1:A:124:GLU:HB2	1:A:265:ILE:O	2.08	0.54
1:B:207:ALA:C	1:B:211:MET:SD	2.85	0.54
1:G:188:ASN:OD1	1:G:188:ASN:N	2.40	0.54
1:A:235:ARG:H	1:A:235:ARG:HE	1.54	0.53
1:E:188:ASN:OD1	1:E:188:ASN:N	2.41	0.53
1:F:60:LEU:O	1:F:63:ILE:HG12	2.08	0.53
1:A:129:PHE:HB3	1:B:293:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:OD1	1:A:188:ASN:N	2.41	0.53
1:C:124:GLU:HB2	1:C:265:ILE:O	2.08	0.53
1:A:289:GLY:O	1:A:292:ILE:HD11	2.08	0.53
1:B:114:GLN:HG2	1:B:320:LEU:HD23	1.91	0.53
1:E:158:MET:SD	1:E:219:LEU:HG	2.48	0.53
1:B:188:ASN:N	1:B:188:ASN:OD1	2.41	0.52
1:C:211:MET:CG	1:C:259:PHE:CE2	2.93	0.52
1:A:119:THR:HB	1:A:262:ALA:HB2	1.90	0.52
1:G:211:MET:HG3	1:G:259:PHE:CE2	2.44	0.52
1:C:188:ASN:OD1	1:C:188:ASN:N	2.41	0.52
1:G:123:THR:O	1:G:264:VAL:HA	2.10	0.52
1:C:123:THR:O	1:C:264:VAL:HA	2.08	0.52
1:D:188:ASN:OD1	1:D:188:ASN:N	2.41	0.52
1:A:158:MET:SD	1:A:219:LEU:HG	2.50	0.52
1:E:60:LEU:O	1:E:63:ILE:HG12	2.10	0.52
1:D:102:ILE:O	1:D:116:GLY:HA3	2.09	0.52
1:B:102:ILE:O	1:B:116:GLY:HA3	2.10	0.51
1:A:157:ALA:HB3	1:A:189:VAL:HG22	1.93	0.51
1:C:207:ALA:C	1:C:211:MET:SD	2.85	0.51
1:C:60:LEU:O	1:C:63:ILE:HG12	2.10	0.51
1:D:159:TYR:HE1	1:D:222:ASP:HB2	1.76	0.51
1:G:159:TYR:HE1	1:G:222:ASP:HB2	1.76	0.51
1:A:114:GLN:HG2	1:A:320:LEU:HD23	1.93	0.51
1:E:211:MET:CG	1:E:259:PHE:CE2	2.93	0.51
1:A:211:MET:CG	1:A:259:PHE:CE2	2.94	0.51
1:B:158:MET:SD	1:B:219:LEU:HG	2.50	0.51
1:C:303:ARG:HD2	1:C:311:ILE:HB	1.93	0.51
1:D:303:ARG:HD2	1:D:311:ILE:HB	1.93	0.51
1:B:211:MET:CG	1:B:259:PHE:CE2	2.94	0.51
1:D:211:MET:CG	1:D:259:PHE:CE2	2.94	0.51
1:G:60:LEU:O	1:G:63:ILE:HG12	2.10	0.51
1:C:159:TYR:HE1	1:C:222:ASP:HB2	1.75	0.51
1:D:207:ALA:C	1:D:211:MET:SD	2.85	0.51
1:B:60:LEU:O	1:B:63:ILE:HG12	2.11	0.51
1:D:114:GLN:HG2	1:D:320:LEU:HD23	1.92	0.51
1:D:60:LEU:O	1:D:63:ILE:HG12	2.11	0.50
1:F:303:ARG:HD2	1:F:311:ILE:HB	1.93	0.50
1:F:129:PHE:HB3	1:G:293:ALA:HB1	1.93	0.50
1:A:60:LEU:O	1:A:63:ILE:HG12	2.12	0.50
1:D:123:THR:O	1:D:264:VAL:HA	2.12	0.50
1:E:207:ALA:C	1:E:211:MET:SD	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ILE:O	1:E:116:GLY:HA3	2.11	0.50
1:E:119:THR:HB	1:E:262:ALA:HB2	1.93	0.50
1:F:211:MET:CG	1:F:259:PHE:CE2	2.95	0.50
1:A:102:ILE:O	1:A:116:GLY:HA3	2.12	0.50
1:C:102:ILE:O	1:C:116:GLY:HA3	2.12	0.50
1:D:157:ALA:HB3	1:D:189:VAL:HG22	1.94	0.50
1:E:114:GLN:HG2	1:E:320:LEU:HD23	1.94	0.50
1:F:207:ALA:C	1:F:211:MET:SD	2.85	0.50
1:B:157:ALA:HB3	1:B:189:VAL:HG22	1.94	0.49
1:A:235:ARG:N	1:A:235:ARG:HE	2.10	0.49
1:E:144:CYS:SG	1:E:157:ALA:HB2	2.53	0.49
1:G:235:ARG:HE	1:G:235:ARG:N	2.10	0.49
1:B:235:ARG:HE	1:B:235:ARG:N	2.10	0.49
1:G:211:MET:CG	1:G:259:PHE:CE2	2.96	0.49
1:D:157:ALA:O	1:D:189:VAL:HA	2.13	0.49
1:A:49:VAL:HA	1:A:52:VAL:HG12	1.95	0.49
1:B:229:ARG:CZ	1:C:291:ILE:HD11	2.43	0.49
1:F:157:ALA:HB3	1:F:189:VAL:HG22	1.95	0.49
1:C:235:ARG:HE	1:C:235:ARG:N	2.10	0.49
1:E:157:ALA:HB3	1:E:189:VAL:HG22	1.94	0.49
1:B:34:ASN:OD1	1:B:34:ASN:N	2.46	0.48
1:C:34:ASN:OD1	1:C:34:ASN:N	2.46	0.48
1:D:144:CYS:SG	1:D:157:ALA:HB2	2.53	0.48
1:D:66:ILE:HG22	1:D:69:ALA:H	1.77	0.48
1:F:235:ARG:HE	1:F:235:ARG:N	2.10	0.48
1:G:157:ALA:O	1:G:189:VAL:HA	2.13	0.48
1:G:303:ARG:HD2	1:G:311:ILE:HB	1.95	0.48
1:F:119:THR:HB	1:F:262:ALA:HB2	1.94	0.48
1:G:144:CYS:SG	1:G:157:ALA:HB2	2.53	0.48
1:D:235:ARG:HE	1:D:235:ARG:N	2.10	0.48
1:E:34:ASN:OD1	1:E:34:ASN:N	2.46	0.48
1:E:157:ALA:O	1:E:189:VAL:HA	2.13	0.48
1:A:66:ILE:HG22	1:A:69:ALA:H	1.77	0.48
1:A:124:GLU:OE1	1:A:299:ARG:HD3	2.14	0.48
1:F:159:TYR:HE1	1:F:222:ASP:HB2	1.79	0.48
1:G:34:ASN:OD1	1:G:34:ASN:N	2.46	0.48
1:A:293:ALA:HA	1:A:299:ARG:HH12	1.79	0.48
1:B:119:THR:HB	1:B:262:ALA:HB2	1.96	0.48
1:D:34:ASN:N	1:D:34:ASN:OD1	2.46	0.48
1:B:159:TYR:HE1	1:B:222:ASP:HB2	1.78	0.48
1:A:272:GLN:NE2	1:A:272:GLN:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:CYS:SG	1:B:157:ALA:HB2	2.54	0.48
1:E:66:ILE:HG22	1:E:69:ALA:H	1.78	0.48
1:F:35:ALA:O	1:F:39:LYS:HB2	2.14	0.48
1:D:126:PHE:HB3	1:D:267:ASN:HB3	1.95	0.47
1:F:102:ILE:O	1:F:116:GLY:HA3	2.13	0.47
1:F:147:PRO:HG2	1:F:150:ARG:HB2	1.96	0.47
1:G:102:ILE:O	1:G:116:GLY:HA3	2.13	0.47
1:G:35:ALA:O	1:G:39:LYS:HB2	2.14	0.47
1:C:157:ALA:HB3	1:C:189:VAL:HG22	1.95	0.47
1:D:119:THR:HB	1:D:262:ALA:HB2	1.95	0.47
1:A:35:ALA:O	1:A:39:LYS:HB2	2.15	0.47
1:E:235:ARG:HE	1:E:235:ARG:N	2.11	0.47
1:A:144:CYS:SG	1:A:157:ALA:HB2	2.54	0.47
1:A:157:ALA:O	1:A:189:VAL:HA	2.13	0.47
1:A:34:ASN:N	1:A:34:ASN:OD1	2.46	0.47
1:C:35:ALA:O	1:C:39:LYS:HB2	2.14	0.47
1:E:35:ALA:O	1:E:39:LYS:HB2	2.14	0.47
1:F:66:ILE:HG22	1:F:69:ALA:H	1.78	0.47
1:B:157:ALA:O	1:B:189:VAL:HA	2.14	0.47
1:F:144:CYS:SG	1:F:157:ALA:HB2	2.54	0.47
1:G:66:ILE:HG22	1:G:69:ALA:H	1.78	0.47
1:A:147:PRO:HG2	1:A:150:ARG:HB2	1.97	0.47
1:B:35:ALA:O	1:B:39:LYS:HB2	2.14	0.47
1:C:144:CYS:SG	1:C:157:ALA:HB2	2.54	0.47
1:G:147:PRO:HG2	1:G:150:ARG:HB2	1.97	0.47
1:C:157:ALA:O	1:C:189:VAL:HA	2.14	0.47
1:C:66:ILE:HG22	1:C:69:ALA:H	1.78	0.47
1:G:157:ALA:HB3	1:G:189:VAL:HG22	1.96	0.47
1:G:208:SER:CA	1:G:211:MET:SD	3.03	0.47
1:C:229:ARG:CZ	1:D:291:ILE:HD11	2.45	0.47
1:D:35:ALA:O	1:D:39:LYS:HB2	2.14	0.47
1:F:34:ASN:OD1	1:F:34:ASN:N	2.47	0.47
1:B:126:PHE:HB3	1:B:267:ASN:HB3	1.95	0.47
1:D:147:PRO:HG2	1:D:150:ARG:HB2	1.97	0.47
1:B:66:ILE:HG22	1:B:69:ALA:H	1.79	0.47
1:C:147:PRO:HG2	1:C:150:ARG:HB2	1.97	0.47
1:A:229:ARG:HH22	1:A:270:VAL:HG23	1.80	0.46
1:E:147:PRO:HG2	1:E:150:ARG:HB2	1.98	0.46
1:A:208:SER:CA	1:A:211:MET:SD	3.04	0.46
1:A:28:LEU:HD13	1:A:77:GLU:HB2	1.98	0.46
1:E:126:PHE:HB3	1:E:267:ASN:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:HB3	1:A:267:ASN:HB3	1.96	0.46
1:E:208:SER:CA	1:E:211:MET:SD	3.04	0.46
1:B:147:PRO:HG2	1:B:150:ARG:HB2	1.98	0.46
1:C:223:SER:O	1:C:224:ALA:C	2.55	0.46
1:C:126:PHE:HB3	1:C:267:ASN:HB3	1.97	0.46
1:D:208:SER:CA	1:D:211:MET:SD	3.04	0.46
1:F:158:MET:SD	1:F:219:LEU:HG	2.56	0.46
1:C:208:SER:CA	1:C:211:MET:SD	3.04	0.46
1:D:28:LEU:HD13	1:D:77:GLU:HB2	1.97	0.46
1:G:119:THR:HB	1:G:262:ALA:HB2	1.98	0.46
1:B:223:SER:O	1:B:224:ALA:C	2.54	0.45
1:F:125:MET:HB3	1:F:300:LEU:HD12	1.98	0.45
1:G:290:ASN:O	1:G:293:ALA:HB3	2.16	0.45
1:G:126:PHE:HB3	1:G:267:ASN:HB3	1.96	0.45
1:G:28:LEU:HD13	1:G:77:GLU:HB2	1.98	0.45
1:B:71:ALA:O	1:B:74:ILE:HG22	2.16	0.45
1:D:223:SER:O	1:D:224:ALA:C	2.55	0.45
1:G:245:LEU:HD21	1:G:292:ILE:HG23	1.98	0.45
1:E:223:SER:O	1:E:224:ALA:C	2.55	0.45
1:F:208:SER:CA	1:F:211:MET:SD	3.04	0.45
1:F:223:SER:O	1:F:224:ALA:C	2.55	0.45
1:B:245:LEU:HD21	1:B:292:ILE:HG23	1.98	0.45
1:C:28:LEU:HD13	1:C:77:GLU:HB2	1.98	0.45
1:D:245:LEU:HD21	1:D:292:ILE:HG23	1.99	0.45
1:E:159:TYR:HE1	1:E:222:ASP:HB2	1.81	0.45
1:F:126:PHE:HB3	1:F:267:ASN:HB3	1.98	0.45
1:A:71:ALA:O	1:A:74:ILE:HG22	2.17	0.45
1:B:208:SER:CA	1:B:211:MET:SD	3.04	0.45
1:C:71:ALA:O	1:C:74:ILE:HG22	2.17	0.45
1:E:49:VAL:HA	1:E:52:VAL:HG12	1.99	0.45
1:G:223:SER:O	1:G:224:ALA:C	2.55	0.44
1:D:59:GLU:HA	1:D:62:ASN:ND2	2.33	0.44
1:C:49:VAL:HA	1:C:52:VAL:HG12	2.00	0.44
1:D:71:ALA:O	1:D:74:ILE:HG22	2.17	0.44
1:E:71:ALA:O	1:E:74:ILE:HG22	2.17	0.44
1:A:229:ARG:NH2	1:A:270:VAL:HG23	2.32	0.44
1:C:272:GLN:NE2	1:C:272:GLN:O	2.49	0.44
1:B:272:GLN:O	1:B:272:GLN:NE2	2.49	0.44
1:D:291:ILE:HD12	1:D:291:ILE:HA	1.85	0.44
1:D:49:VAL:HA	1:D:52:VAL:HG12	2.00	0.44
1:E:133:LYS:HB2	1:E:133:LYS:HE2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:SER:O	1:A:224:ALA:C	2.55	0.44
1:E:247:ARG:HG3	1:E:247:ARG:HH11	1.83	0.44
1:F:71:ALA:O	1:F:74:ILE:HG22	2.18	0.44
2:D:600:ANP:H8	1:E:317:SER:O	2.18	0.43
1:B:49:VAL:HA	1:B:52:VAL:HG12	2.00	0.43
1:B:59:GLU:HA	1:B:62:ASN:ND2	2.33	0.43
1:E:28:LEU:HD13	1:E:77:GLU:HB2	1.99	0.43
1:F:49:VAL:HA	1:F:52:VAL:HG12	2.00	0.43
1:B:291:ILE:HD12	1:B:291:ILE:HA	1.73	0.43
1:F:157:ALA:O	1:F:189:VAL:HA	2.18	0.43
1:G:49:VAL:HA	1:G:52:VAL:HG12	2.00	0.43
1:C:220:ILE:H	1:C:220:ILE:HG12	1.74	0.43
1:F:28:LEU:HD13	1:F:77:GLU:HB2	1.99	0.43
1:C:119:THR:HB	1:C:262:ALA:HB2	1.99	0.43
1:E:59:GLU:HA	1:E:62:ASN:ND2	2.33	0.43
1:G:133:LYS:HB2	1:G:133:LYS:HE2	1.83	0.43
1:G:291:ILE:HD12	1:G:291:ILE:HA	1.75	0.43
1:G:59:GLU:HA	1:G:62:ASN:ND2	2.33	0.43
1:A:245:LEU:HD21	1:A:292:ILE:HG23	2.01	0.43
1:C:59:GLU:HA	1:C:62:ASN:ND2	2.33	0.43
1:D:272:GLN:NE2	1:D:272:GLN:O	2.50	0.43
1:E:125:MET:HB3	1:E:300:LEU:HD12	1.99	0.43
1:F:59:GLU:HA	1:F:62:ASN:ND2	2.33	0.43
1:G:71:ALA:O	1:G:74:ILE:HG22	2.18	0.43
1:A:293:ALA:HA	1:A:299:ARG:NH1	2.33	0.43
1:A:59:GLU:HA	1:A:62:ASN:ND2	2.34	0.43
1:G:258:GLU:HG3	1:G:259:PHE:H	1.84	0.43
1:D:112:LEU:HG	1:D:325:ALA:HB2	2.00	0.42
1:B:28:LEU:HD13	1:B:77:GLU:HB2	2.01	0.42
1:C:210:MET:HA	1:C:210:MET:CE	2.50	0.42
1:E:245:LEU:HD21	1:E:292:ILE:HG23	2.01	0.42
1:A:220:ILE:H	1:A:220:ILE:HG12	1.74	0.42
1:B:258:GLU:HG3	1:B:259:PHE:H	1.85	0.42
1:G:124:GLU:OE1	1:G:299:ARG:HD3	2.20	0.42
1:F:168:PRO:HD2	1:G:96:ARG:HD3	2.01	0.42
1:A:292:ILE:HD12	1:A:293:ALA:N	2.35	0.42
1:A:229:ARG:CZ	1:B:291:ILE:HD11	2.49	0.42
2:C:600:ANP:H8	1:D:317:SER:O	2.19	0.42
1:F:247:ARG:HG3	1:F:247:ARG:HH11	1.83	0.42
1:B:210:MET:CE	1:B:210:MET:HA	2.50	0.42
1:D:247:ARG:HG3	1:D:247:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LEU:HG	1:E:325:ALA:HB2	2.01	0.42
2:F:600:ANP:H8	1:G:317:SER:O	2.20	0.42
1:A:112:LEU:HG	1:A:325:ALA:HB2	2.01	0.42
1:A:210:MET:CE	1:A:210:MET:HA	2.50	0.42
1:B:133:LYS:HE2	1:B:133:LYS:HB2	1.85	0.42
1:C:245:LEU:HD21	1:C:292:ILE:HG23	2.01	0.42
1:E:220:ILE:H	1:E:220:ILE:HG12	1.73	0.42
1:A:159:TYR:HE1	1:A:222:ASP:HB2	1.85	0.42
1:G:292:ILE:HD12	1:G:293:ALA:N	2.35	0.42
1:C:168:PRO:HD2	1:D:96:ARG:HD3	2.02	0.42
1:D:229:ARG:CZ	1:E:291:ILE:HD11	2.50	0.42
1:B:211:MET:HG2	1:B:259:PHE:CE2	2.55	0.41
1:C:291:ILE:HD12	1:C:291:ILE:HA	1.83	0.41
1:E:168:PRO:HD2	1:F:96:ARG:HD3	2.02	0.41
1:G:125:MET:HB3	1:G:300:LEU:HD12	2.01	0.41
1:G:59:GLU:HA	1:G:62:ASN:HD21	1.85	0.41
1:E:258:GLU:HG3	1:E:259:PHE:H	1.85	0.41
1:D:168:PRO:HD2	1:E:96:ARG:HD3	2.02	0.41
1:F:108:GLU:HA	1:F:108:GLU:OE1	2.21	0.41
1:B:30:GLN:OE1	1:B:30:GLN:HA	2.21	0.41
1:D:249:LEU:HD21	1:D:292:ILE:HA	2.03	0.41
1:D:210:MET:CE	1:D:210:MET:HA	2.50	0.41
1:E:30:GLN:OE1	1:E:30:GLN:HA	2.21	0.41
1:F:220:ILE:HG12	1:F:220:ILE:H	1.74	0.41
1:G:108:GLU:OE1	1:G:108:GLU:HA	2.21	0.41
1:G:210:MET:CE	1:G:210:MET:HA	2.50	0.41
1:E:210:MET:CE	1:E:210:MET:HA	2.50	0.41
2:E:600:ANP:H8	1:F:317:SER:O	2.21	0.41
1:C:247:ARG:HG3	1:C:247:ARG:HH11	1.86	0.41
1:D:258:GLU:HG3	1:D:259:PHE:H	1.85	0.41
1:F:258:GLU:HG3	1:F:259:PHE:H	1.85	0.41
1:F:59:GLU:HA	1:F:62:ASN:HD21	1.86	0.41
1:C:159:TYR:CE1	1:C:222:ASP:HB2	2.55	0.41
1:D:193:ARG:HH21	1:E:257:ASP:CG	2.24	0.41
1:G:220:ILE:H	1:G:220:ILE:HG12	1.75	0.41
1:A:30:GLN:OE1	1:A:30:GLN:HA	2.21	0.41
1:B:108:GLU:OE1	1:B:108:GLU:HA	2.21	0.41
2:B:600:ANP:H8	1:C:317:SER:O	2.21	0.41
1:C:125:MET:HB3	1:C:300:LEU:HD12	2.02	0.41
1:D:293:ALA:HA	1:D:299:ARG:NH1	2.36	0.41
1:E:59:GLU:HA	1:E:62:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:LEU:HG	1:G:325:ALA:HB2	2.01	0.41
1:A:59:GLU:HA	1:A:62:ASN:HD21	1.86	0.41
1:C:206:GLN:OE1	1:C:206:GLN:HA	2.21	0.41
1:E:108:GLU:HA	1:E:108:GLU:OE1	2.21	0.41
1:F:112:LEU:HG	1:F:325:ALA:HB2	2.01	0.41
1:F:30:GLN:HA	1:F:30:GLN:OE1	2.21	0.41
1:G:249:LEU:HD21	1:G:292:ILE:HA	2.02	0.41
1:G:30:GLN:HA	1:G:30:GLN:OE1	2.21	0.41
1:A:193:ARG:HH21	1:B:257:ASP:CG	2.25	0.41
1:C:211:MET:HG2	1:C:259:PHE:CE2	2.56	0.41
1:E:206:GLN:OE1	1:E:206:GLN:HA	2.21	0.41
1:G:170:ARG:HH21	1:G:170:ARG:HA	1.85	0.41
1:B:59:GLU:HA	1:B:62:ASN:HD21	1.86	0.41
1:C:290:ASN:O	1:C:293:ALA:HB3	2.22	0.41
1:D:108:GLU:OE1	1:D:108:GLU:HA	2.21	0.41
1:D:59:GLU:HA	1:D:62:ASN:HD21	1.85	0.41
1:G:293:ALA:HA	1:G:299:ARG:NH1	2.36	0.41
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.21	0.40
1:A:92:PHE:O	1:A:95:ARG:HB2	2.21	0.40
1:C:108:GLU:OE1	1:C:108:GLU:HA	2.21	0.40
1:D:292:ILE:HD12	1:D:293:ALA:N	2.36	0.40
1:E:292:ILE:H	1:E:292:ILE:HG13	1.68	0.40
1:G:227:LEU:HD12	1:G:227:LEU:HA	2.01	0.40
1:B:125:MET:HB3	1:B:300:LEU:HD12	2.02	0.40
1:B:92:PHE:O	1:B:95:ARG:HB2	2.22	0.40
1:C:292:ILE:HD12	1:C:293:ALA:N	2.35	0.40
1:C:92:PHE:O	1:C:95:ARG:HB2	2.22	0.40
1:F:210:MET:CE	1:F:210:MET:HA	2.51	0.40
1:G:272:GLN:NE2	1:G:272:GLN:O	2.55	0.40
1:A:168:PRO:HD2	1:B:96:ARG:HD3	2.02	0.40
1:D:290:ASN:O	1:D:293:ALA:HB3	2.22	0.40
1:B:293:ALA:HA	1:B:299:ARG:NH1	2.37	0.40
1:C:59:GLU:HA	1:C:62:ASN:HD21	1.86	0.40
1:D:230:THR:HG22	1:E:246:ALA:HB1	2.04	0.40
1:E:293:ALA:HA	1:E:299:ARG:NH1	2.37	0.40
1:E:229:ARG:CZ	1:F:291:ILE:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/339 (91%)	263 (86%)	42 (14%)	2 (1%)	25	68
1	B	307/339 (91%)	263 (86%)	42 (14%)	2 (1%)	25	68
1	C	307/339 (91%)	265 (86%)	39 (13%)	3 (1%)	18	61
1	D	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	25	68
1	E	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	25	68
1	F	307/339 (91%)	265 (86%)	40 (13%)	2 (1%)	25	68
1	G	307/339 (91%)	266 (87%)	39 (13%)	2 (1%)	25	68
All	All	2149/2373 (91%)	1850 (86%)	284 (13%)	15 (1%)	30	68

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ALA
1	A	337	ALA
1	B	224	ALA
1	B	337	ALA
1	C	224	ALA
1	C	337	ALA
1	D	224	ALA
1	D	337	ALA
1	E	224	ALA
1	E	337	ALA
1	F	224	ALA
1	F	337	ALA
1	G	224	ALA
1	G	337	ALA
1	C	88	THR

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	229/269 (85%)	175 (76%)	54 (24%)	1	7
1	B	229/269 (85%)	174 (76%)	55 (24%)	1	6
1	C	229/269 (85%)	175 (76%)	54 (24%)	1	7
1	D	229/269 (85%)	175 (76%)	54 (24%)	1	7
1	E	229/269 (85%)	173 (76%)	56 (24%)	1	6
1	F	229/269 (85%)	173 (76%)	56 (24%)	1	6
1	G	229/269 (85%)	177 (77%)	52 (23%)	1	8
All	All	1603/1883 (85%)	1222 (76%)	381 (24%)	3	6

All (381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	25	ILE
1	A	28	LEU
1	A	29	GLU
1	A	34	ASN
1	A	39	LYS
1	A	52	VAL
1	A	54	TYR
1	A	58	LYS
1	A	59	GLU
1	A	60	LEU
1	A	61	ILE
1	A	77	GLU
1	A	81	LEU
1	A	103	THR
1	A	107	LYS
1	A	108	GLU
1	A	111	LYS
1	A	112	LEU
1	A	119	THR

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Mol	Chain	Res	Type
1	A	130	ARG
1	A	135	GLN
1	A	144	CYS
1	A	146	LEU
1	A	154	GLU
1	A	158	MET
1	A	159	TYR
1	A	161	ASP
1	A	177	ARG
1	A	188	ASN
1	A	203	LEU
1	A	204	LEU
1	A	206	GLN
1	A	211	MET
1	A	213	GLU
1	A	220	ILE
1	A	229	ARG
1	A	235	ARG
1	A	238	LEU
1	A	241	ARG
1	A	247	ARG
1	A	255	LEU
1	A	257	ASP
1	A	272	GLN
1	A	290	ASN
1	A	291	ILE
1	A	298	THR
1	A	299	ARG
1	A	300	LEU
1	A	301	TYR
1	A	303	ARG
1	A	316	ASP
1	A	320	LEU
1	A	336	ASP
1	B	20	PHE
1	B	25	ILE
1	B	28	LEU
1	B	29	GLU
1	B	34	ASN
1	B	39	LYS
1	B	52	VAL
1	B	58	LYS

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Mol	Chain	Res	Type
1	B	59	GLU
1	B	60	LEU
1	B	61	ILE
1	B	77	GLU
1	B	81	LEU
1	B	103	THR
1	B	107	LYS
1	B	108	GLU
1	B	111	LYS
1	B	112	LEU
1	B	119	THR
1	B	130	ARG
1	B	135	GLN
1	B	144	CYS
1	B	146	LEU
1	B	154	GLU
1	B	158	MET
1	B	159	TYR
1	B	161	ASP
1	B	177	ARG
1	B	188	ASN
1	B	203	LEU
1	B	204	LEU
1	B	206	GLN
1	B	211	MET
1	B	213	GLU
1	B	220	ILE
1	B	229	ARG
1	B	235	ARG
1	B	238	LEU
1	B	241	ARG
1	B	247	ARG
1	B	255	LEU
1	B	257	ASP
1	B	270	VAL
1	B	272	GLN
1	B	290	ASN
1	B	291	ILE
1	B	298	THR
1	B	299	ARG
1	B	300	LEU
1	B	301	TYR

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Mol	Chain	Res	Type
1	B	303	ARG
1	B	316	ASP
1	B	319	CYS
1	B	320	LEU
1	B	336	ASP
1	C	20	PHE
1	C	25	ILE
1	C	28	LEU
1	C	29	GLU
1	C	34	ASN
1	C	39	LYS
1	C	52	VAL
1	C	58	LYS
1	C	59	GLU
1	C	60	LEU
1	C	61	ILE
1	C	77	GLU
1	C	81	LEU
1	C	103	THR
1	C	107	LYS
1	C	108	GLU
1	C	111	LYS
1	C	112	LEU
1	C	130	ARG
1	C	135	GLN
1	C	144	CYS
1	C	146	LEU
1	C	154	GLU
1	C	158	MET
1	C	159	TYR
1	C	161	ASP
1	C	177	ARG
1	C	188	ASN
1	C	203	LEU
1	C	204	LEU
1	C	206	GLN
1	C	211	MET
1	C	213	GLU
1	C	219	LEU
1	C	220	ILE
1	C	229	ARG
1	C	235	ARG

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Mol	Chain	Res	Type
1	C	238	LEU
1	C	241	ARG
1	C	247	ARG
1	C	255	LEU
1	C	257	ASP
1	C	272	GLN
1	C	290	ASN
1	C	291	ILE
1	C	298	THR
1	C	299	ARG
1	C	300	LEU
1	C	301	TYR
1	C	303	ARG
1	C	316	ASP
1	C	319	CYS
1	C	320	LEU
1	C	336	ASP
1	D	20	PHE
1	D	25	ILE
1	D	28	LEU
1	D	29	GLU
1	D	34	ASN
1	D	39	LYS
1	D	52	VAL
1	D	58	LYS
1	D	59	GLU
1	D	60	LEU
1	D	61	ILE
1	D	77	GLU
1	D	81	LEU
1	D	103	THR
1	D	107	LYS
1	D	108	GLU
1	D	111	LYS
1	D	112	LEU
1	D	130	ARG
1	D	135	GLN
1	D	144	CYS
1	D	146	LEU
1	D	154	GLU
1	D	158	MET
1	D	159	TYR

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Mol	Chain	Res	Type
1	D	161	ASP
1	D	177	ARG
1	D	188	ASN
1	D	203	LEU
1	D	204	LEU
1	D	206	GLN
1	D	211	MET
1	D	213	GLU
1	D	220	ILE
1	D	229	ARG
1	D	235	ARG
1	D	238	LEU
1	D	241	ARG
1	D	247	ARG
1	D	255	LEU
1	D	257	ASP
1	D	272	GLN
1	D	290	ASN
1	D	291	ILE
1	D	298	THR
1	D	299	ARG
1	D	300	LEU
1	D	301	TYR
1	D	303	ARG
1	D	315	TYR
1	D	316	ASP
1	D	319	CYS
1	D	320	LEU
1	D	336	ASP
1	E	20	PHE
1	E	25	ILE
1	E	28	LEU
1	E	29	GLU
1	E	34	ASN
1	E	39	LYS
1	E	52	VAL
1	E	58	LYS
1	E	59	GLU
1	E	60	LEU
1	E	61	ILE
1	E	77	GLU
1	E	81	LEU

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Mol	Chain	Res	Type
1	E	103	THR
1	E	107	LYS
1	E	108	GLU
1	E	111	LYS
1	E	112	LEU
1	E	119	THR
1	E	130	ARG
1	E	135	GLN
1	E	144	CYS
1	E	146	LEU
1	E	154	GLU
1	E	158	MET
1	E	159	TYR
1	E	161	ASP
1	E	177	ARG
1	E	188	ASN
1	E	203	LEU
1	E	204	LEU
1	E	206	GLN
1	E	211	MET
1	E	213	GLU
1	E	220	ILE
1	E	229	ARG
1	E	235	ARG
1	E	238	LEU
1	E	241	ARG
1	E	247	ARG
1	E	255	LEU
1	E	257	ASP
1	E	270	VAL
1	E	272	GLN
1	E	290	ASN
1	E	291	ILE
1	E	298	THR
1	E	299	ARG
1	E	300	LEU
1	E	301	TYR
1	E	303	ARG
1	E	315	TYR
1	E	316	ASP
1	E	319	CYS
1	E	320	LEU

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Mol	Chain	Res	Type
1	E	336	ASP
1	F	20	PHE
1	F	25	ILE
1	F	28	LEU
1	F	29	GLU
1	F	34	ASN
1	F	39	LYS
1	F	52	VAL
1	F	58	LYS
1	F	59	GLU
1	F	60	LEU
1	F	61	ILE
1	F	77	GLU
1	F	81	LEU
1	F	107	LYS
1	F	108	GLU
1	F	111	LYS
1	F	112	LEU
1	F	119	THR
1	F	130	ARG
1	F	135	GLN
1	F	144	CYS
1	F	146	LEU
1	F	154	GLU
1	F	158	MET
1	F	159	TYR
1	F	161	ASP
1	F	177	ARG
1	F	188	ASN
1	F	203	LEU
1	F	204	LEU
1	F	206	GLN
1	F	211	MET
1	F	213	GLU
1	F	219	LEU
1	F	220	ILE
1	F	229	ARG
1	F	235	ARG
1	F	238	LEU
1	F	241	ARG
1	F	247	ARG
1	F	255	LEU

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Mol	Chain	Res	Type
1	F	257	ASP
1	F	270	VAL
1	F	272	GLN
1	F	290	ASN
1	F	291	ILE
1	F	298	THR
1	F	299	ARG
1	F	300	LEU
1	F	301	TYR
1	F	303	ARG
1	F	315	TYR
1	F	316	ASP
1	F	319	CYS
1	F	320	LEU
1	F	336	ASP
1	G	20	PHE
1	G	25	ILE
1	G	28	LEU
1	G	29	GLU
1	G	34	ASN
1	G	39	LYS
1	G	52	VAL
1	G	58	LYS
1	G	59	GLU
1	G	60	LEU
1	G	61	ILE
1	G	77	GLU
1	G	81	LEU
1	G	107	LYS
1	G	108	GLU
1	G	111	LYS
1	G	112	LEU
1	G	130	ARG
1	G	135	GLN
1	G	144	CYS
1	G	146	LEU
1	G	154	GLU
1	G	158	MET
1	G	159	TYR
1	G	161	ASP
1	G	177	ARG
1	G	188	ASN

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Mol	Chain	Res	Type
1	G	203	LEU
1	G	204	LEU
1	G	206	GLN
1	G	211	MET
1	G	213	GLU
1	G	220	ILE
1	G	229	ARG
1	G	235	ARG
1	G	238	LEU
1	G	241	ARG
1	G	247	ARG
1	G	255	LEU
1	G	257	ASP
1	G	272	GLN
1	G	290	ASN
1	G	291	ILE
1	G	298	THR
1	G	299	ARG
1	G	300	LEU
1	G	301	TYR
1	G	303	ARG
1	G	316	ASP
1	G	319	CYS
1	G	320	LEU
1	G	336	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	145	GLN
1	A	294	HIS
1	B	135	GLN
1	B	145	GLN
1	B	294	HIS
1	C	135	GLN
1	C	145	GLN
1	C	294	HIS
1	D	135	GLN
1	D	145	GLN
1	D	294	HIS
1	E	135	GLN

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Mol	Chain	Res	Type
1	E	145	GLN
1	E	294	HIS
1	F	135	GLN
1	F	145	GLN
1	F	294	HIS
1	G	135	GLN
1	G	145	GLN
1	G	294	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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	$\# Z > 2$
2	ANP	A	600	-	29,33,33	2.44	12 (41%)	28,52,52	2.53	10 (35%)
2	ANP	B	600	-	29,33,33	2.44	11 (37%)	28,52,52	2.53	9 (32%)
2	ANP	C	600	-	29,33,33	2.45	11 (37%)	28,52,52	2.52	9 (32%)
2	ANP	D	600	-	29,33,33	2.46	11 (37%)	28,52,52	2.52	10 (35%)
2	ANP	E	600	-	29,33,33	2.47	12 (41%)	28,52,52	2.52	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	F	600	-	29,33,33	2.42	11 (37%)	28,52,52	2.50	11 (39%)
2	ANP	G	600	-	29,33,33	2.42	12 (41%)	28,52,52	2.76	12 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	600	-	-	1/13/38/38	0/3/3/3
2	ANP	B	600	-	-	1/13/38/38	0/3/3/3
2	ANP	C	600	-	-	1/13/38/38	0/3/3/3
2	ANP	D	600	-	-	1/13/38/38	0/3/3/3
2	ANP	E	600	-	-	1/13/38/38	0/3/3/3
2	ANP	F	600	-	-	1/13/38/38	0/3/3/3
2	ANP	G	600	-	-	1/13/38/38	0/3/3/3

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	ANP	PG-O3G	-2.39	1.50	1.56
2	B	600	ANP	PG-O3G	-2.39	1.50	1.56
2	C	600	ANP	PG-O3G	-2.38	1.50	1.56
2	E	600	ANP	PG-O3G	-2.38	1.50	1.56
2	D	600	ANP	PG-O3G	-2.30	1.50	1.56
2	A	600	ANP	PG-O3G	-2.29	1.50	1.56
2	G	600	ANP	PG-O3G	-2.22	1.50	1.56
2	G	600	ANP	PB-O2B	-2.21	1.50	1.56
2	B	600	ANP	PB-O2B	-2.06	1.51	1.56
2	C	600	ANP	PB-O2B	-2.06	1.51	1.56
2	E	600	ANP	PB-O2B	-2.04	1.51	1.56
2	A	600	ANP	PB-O2B	-2.04	1.51	1.56
2	F	600	ANP	PB-O2B	-2.03	1.51	1.56
2	D	600	ANP	PB-O2B	-2.01	1.51	1.56
2	G	600	ANP	C2-N1	2.04	1.37	1.33
2	E	600	ANP	O4'-C1'	2.07	1.44	1.41
2	A	600	ANP	O4'-C1'	2.07	1.44	1.41
2	E	600	ANP	C4-N3	2.08	1.38	1.35
2	B	600	ANP	C4-N3	2.16	1.38	1.35
2	G	600	ANP	O4'-C1'	2.17	1.44	1.41
2	D	600	ANP	C4-N3	2.18	1.38	1.35
2	C	600	ANP	C4-N3	2.19	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	ANP	C4-N3	2.20	1.38	1.35
2	A	600	ANP	C4-N3	2.21	1.38	1.35
2	C	600	ANP	C2-N1	2.33	1.38	1.33
2	A	600	ANP	C2-N1	2.33	1.38	1.33
2	F	600	ANP	C2-N1	2.33	1.38	1.33
2	E	600	ANP	C2-N1	2.36	1.38	1.33
2	B	600	ANP	C2-N1	2.37	1.38	1.33
2	D	600	ANP	C2-N1	2.37	1.38	1.33
2	G	600	ANP	C2-N3	2.56	1.36	1.32
2	G	600	ANP	C4-N3	3.01	1.40	1.35
2	F	600	ANP	C2-N3	3.10	1.37	1.32
2	F	600	ANP	PB-O3A	3.14	1.63	1.59
2	D	600	ANP	C2-N3	3.19	1.37	1.32
2	E	600	ANP	C2-N3	3.20	1.37	1.32
2	C	600	ANP	C2-N3	3.21	1.37	1.32
2	B	600	ANP	C2-N3	3.21	1.37	1.32
2	A	600	ANP	C2-N3	3.22	1.37	1.32
2	A	600	ANP	PB-O3A	3.33	1.63	1.59
2	C	600	ANP	PB-O3A	3.40	1.63	1.59
2	G	600	ANP	PB-O3A	3.40	1.63	1.59
2	B	600	ANP	PB-O3A	3.45	1.63	1.59
2	E	600	ANP	PB-O3A	3.54	1.63	1.59
2	D	600	ANP	PB-O3A	3.56	1.63	1.59
2	F	600	ANP	C5-C4	4.25	1.50	1.40
2	F	600	ANP	PB-N3B	4.27	1.74	1.63
2	A	600	ANP	C5-C4	4.30	1.50	1.40
2	B	600	ANP	PB-O1B	4.31	1.51	1.46
2	D	600	ANP	C5-C4	4.32	1.50	1.40
2	E	600	ANP	C5-C4	4.32	1.50	1.40
2	C	600	ANP	C5-C4	4.33	1.50	1.40
2	B	600	ANP	C5-C4	4.34	1.50	1.40
2	G	600	ANP	PB-N3B	4.36	1.74	1.63
2	G	600	ANP	PB-O1B	4.36	1.51	1.46
2	E	600	ANP	PB-O1B	4.43	1.51	1.46
2	B	600	ANP	PB-N3B	4.44	1.75	1.63
2	A	600	ANP	PB-N3B	4.45	1.75	1.63
2	E	600	ANP	PB-N3B	4.47	1.75	1.63
2	C	600	ANP	PB-O1B	4.47	1.51	1.46
2	C	600	ANP	PB-N3B	4.47	1.75	1.63
2	D	600	ANP	PB-N3B	4.48	1.75	1.63
2	G	600	ANP	C5-C4	4.51	1.50	1.40
2	D	600	ANP	PB-O1B	4.53	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	ANP	PB-O1B	4.63	1.51	1.46
2	A	600	ANP	PB-O1B	4.75	1.51	1.46
2	F	600	ANP	PG-N3B	5.03	1.76	1.63
2	G	600	ANP	PG-N3B	5.14	1.77	1.63
2	A	600	ANP	PG-N3B	5.15	1.77	1.63
2	E	600	ANP	PG-N3B	5.23	1.77	1.63
2	B	600	ANP	PG-N3B	5.23	1.77	1.63
2	C	600	ANP	PG-N3B	5.25	1.77	1.63
2	D	600	ANP	PG-N3B	5.26	1.77	1.63
2	G	600	ANP	PG-O1G	5.50	1.52	1.46
2	A	600	ANP	PG-O1G	5.51	1.52	1.46
2	B	600	ANP	PG-O1G	5.77	1.52	1.46
2	C	600	ANP	PG-O1G	5.78	1.52	1.46
2	D	600	ANP	PG-O1G	5.80	1.52	1.46
2	E	600	ANP	PG-O1G	5.90	1.52	1.46
2	F	600	ANP	PG-O1G	5.94	1.52	1.46

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	600	ANP	N3-C2-N1	-9.38	120.69	128.86
2	A	600	ANP	N3-C2-N1	-8.34	121.59	128.86
2	E	600	ANP	N3-C2-N1	-8.31	121.62	128.86
2	B	600	ANP	N3-C2-N1	-8.29	121.64	128.86
2	C	600	ANP	N3-C2-N1	-8.27	121.65	128.86
2	D	600	ANP	N3-C2-N1	-8.23	121.69	128.86
2	F	600	ANP	N3-C2-N1	-8.23	121.69	128.86
2	G	600	ANP	O1G-PG-N3B	-3.98	105.84	111.79
2	G	600	ANP	C1'-N9-C4	-3.40	120.77	126.64
2	B	600	ANP	PA-O3A-PB	-3.30	120.73	132.38
2	F	600	ANP	O1G-PG-N3B	-3.30	106.86	111.79
2	F	600	ANP	PA-O3A-PB	-3.25	120.92	132.38
2	G	600	ANP	PA-O3A-PB	-3.23	120.97	132.38
2	D	600	ANP	PA-O3A-PB	-3.23	120.99	132.38
2	C	600	ANP	PA-O3A-PB	-3.21	121.06	132.38
2	A	600	ANP	PA-O3A-PB	-3.20	121.08	132.38
2	E	600	ANP	PA-O3A-PB	-3.17	121.20	132.38
2	B	600	ANP	O1G-PG-N3B	-3.14	107.09	111.79
2	D	600	ANP	O1G-PG-N3B	-2.93	107.40	111.79
2	A	600	ANP	O1G-PG-N3B	-2.92	107.42	111.79
2	E	600	ANP	O1G-PG-N3B	-2.91	107.43	111.79
2	C	600	ANP	O1G-PG-N3B	-2.89	107.47	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	ANP	O3G-PG-O2G	2.00	113.30	107.69
2	D	600	ANP	O3G-PG-O2G	2.01	113.31	107.69
2	C	600	ANP	O3'-C3'-C2'	2.02	118.29	111.83
2	B	600	ANP	O3'-C3'-C2'	2.04	118.38	111.83
2	F	600	ANP	O3'-C3'-C2'	2.05	118.39	111.83
2	F	600	ANP	O2G-PG-O1G	2.05	118.62	113.41
2	G	600	ANP	O2G-PG-O1G	2.09	118.73	113.41
2	G	600	ANP	O3'-C3'-C2'	2.11	118.58	111.83
2	A	600	ANP	O3'-C3'-C2'	2.12	118.62	111.83
2	D	600	ANP	O3'-C3'-C2'	2.20	118.88	111.83
2	A	600	ANP	O3G-PG-O2G	2.20	113.86	107.69
2	E	600	ANP	O3'-C3'-C2'	2.23	118.97	111.83
2	G	600	ANP	N6-C6-N1	2.32	123.36	118.77
2	F	600	ANP	C2-N1-C6	2.38	122.93	118.77
2	A	600	ANP	C2-N1-C6	2.40	122.97	118.77
2	D	600	ANP	C2-N1-C6	2.41	122.99	118.77
2	E	600	ANP	C2-N1-C6	2.45	123.06	118.77
2	C	600	ANP	C2-N1-C6	2.45	123.06	118.77
2	B	600	ANP	C2-N1-C6	2.45	123.06	118.77
2	G	600	ANP	O2'-C2'-C3'	2.48	119.77	111.83
2	A	600	ANP	O2'-C2'-C3'	2.52	119.90	111.83
2	F	600	ANP	O2'-C2'-C3'	2.52	119.91	111.83
2	D	600	ANP	O2'-C2'-C3'	2.57	120.07	111.83
2	E	600	ANP	O2'-C2'-C3'	2.60	120.14	111.83
2	C	600	ANP	O2'-C2'-C3'	2.60	120.16	111.83
2	B	600	ANP	O2'-C2'-C3'	2.62	120.22	111.83
2	E	600	ANP	O5'-C5'-C4'	2.74	118.72	109.00
2	A	600	ANP	O5'-C5'-C4'	2.77	118.83	109.00
2	C	600	ANP	O5'-C5'-C4'	2.86	119.14	109.00
2	B	600	ANP	O5'-C5'-C4'	2.87	119.16	109.00
2	G	600	ANP	C2-N1-C6	2.87	123.79	118.77
2	D	600	ANP	O5'-C5'-C4'	2.87	119.18	109.00
2	F	600	ANP	O5'-C5'-C4'	2.89	119.25	109.00
2	F	600	ANP	O3A-PB-N3B	2.97	114.83	106.59
2	A	600	ANP	O3A-PB-N3B	3.31	115.78	106.59
2	G	600	ANP	O3A-PB-N3B	3.40	116.02	106.59
2	G	600	ANP	O5'-C5'-C4'	3.43	121.17	109.00
2	B	600	ANP	O3A-PB-N3B	3.49	116.28	106.59
2	C	600	ANP	O3A-PB-N3B	3.59	116.54	106.59
2	D	600	ANP	O3A-PB-N3B	3.67	116.76	106.59
2	E	600	ANP	O3A-PB-N3B	3.72	116.92	106.59
2	G	600	ANP	O2B-PB-O1B	4.37	118.95	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	600	ANP	O2B-PB-O1B	4.46	119.14	109.87
2	D	600	ANP	O2B-PB-O1B	4.46	119.14	109.87
2	F	600	ANP	O2B-PB-O1B	4.51	119.25	109.87
2	B	600	ANP	O2B-PB-O1B	4.52	119.26	109.87
2	C	600	ANP	O2B-PB-O1B	4.52	119.27	109.87
2	A	600	ANP	O2B-PB-O1B	4.87	120.00	109.87

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	ANP	O1B-PB-N3B-PG
2	D	600	ANP	O1B-PB-N3B-PG
2	G	600	ANP	O1B-PB-N3B-PG
2	C	600	ANP	O1B-PB-N3B-PG
2	E	600	ANP	O1B-PB-N3B-PG
2	B	600	ANP	O1B-PB-N3B-PG
2	F	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	ANP	1	0
2	C	600	ANP	1	0
2	D	600	ANP	1	0
2	E	600	ANP	1	0
2	F	600	ANP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.