



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

Jul 25, 2017 – 12:38 AM EDT

PDB ID : 5VJH  
EMDB ID: : EMD-8697  
Title : Closed State CryoEM Reconstruction of Hsp104:ATPyS and FITC casein  
Authors : Gates, S.N.; Yokom, A.L.; Lin, J.-B.; Jackrel, M.E.; Rizo, A.N.; Kendsersky, N.M.; Buell, C.E.; Sweeny, E.A.; Chuang, E.; Torrente, M.P.; Mack, K.L.; Su, M.; Shorter, J.; Southworth, D.R.  
Deposited on : unknown  
Resolution : 4.00 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-20029824

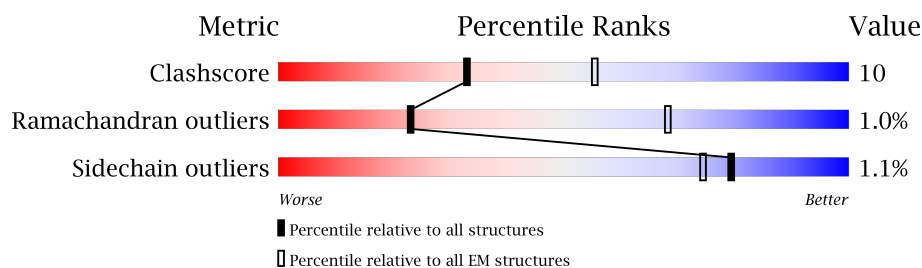
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	908	
1	B	908	
1	C	908	
1	D	908	
1	E	908	
1	F	908	
2	P	26	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AGS	B	1001	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27577 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.

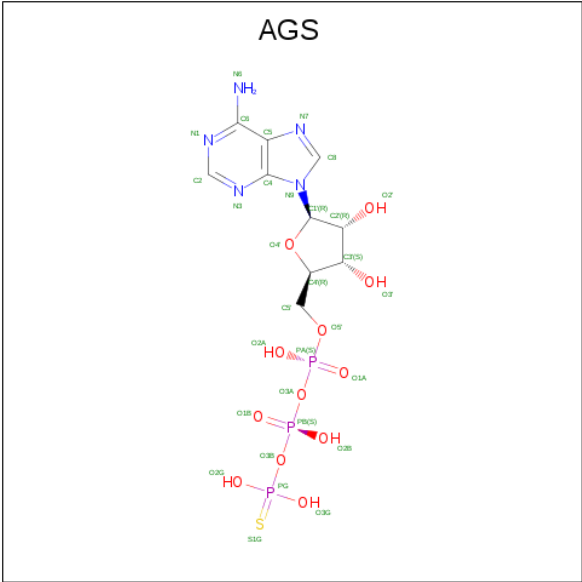
- Molecule 1 is a protein called Heat shock protein 104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	B	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	C	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	D	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	E	579	Total	C	N	O	S	0	0
			4530	2850	794	868	18		
1	F	564	Total	C	N	O	S	0	0
			4424	2782	779	845	18		

- Molecule 2 is a protein called FITC casein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	26	Total	C	N	O	0	0
			131	78	26	27		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).

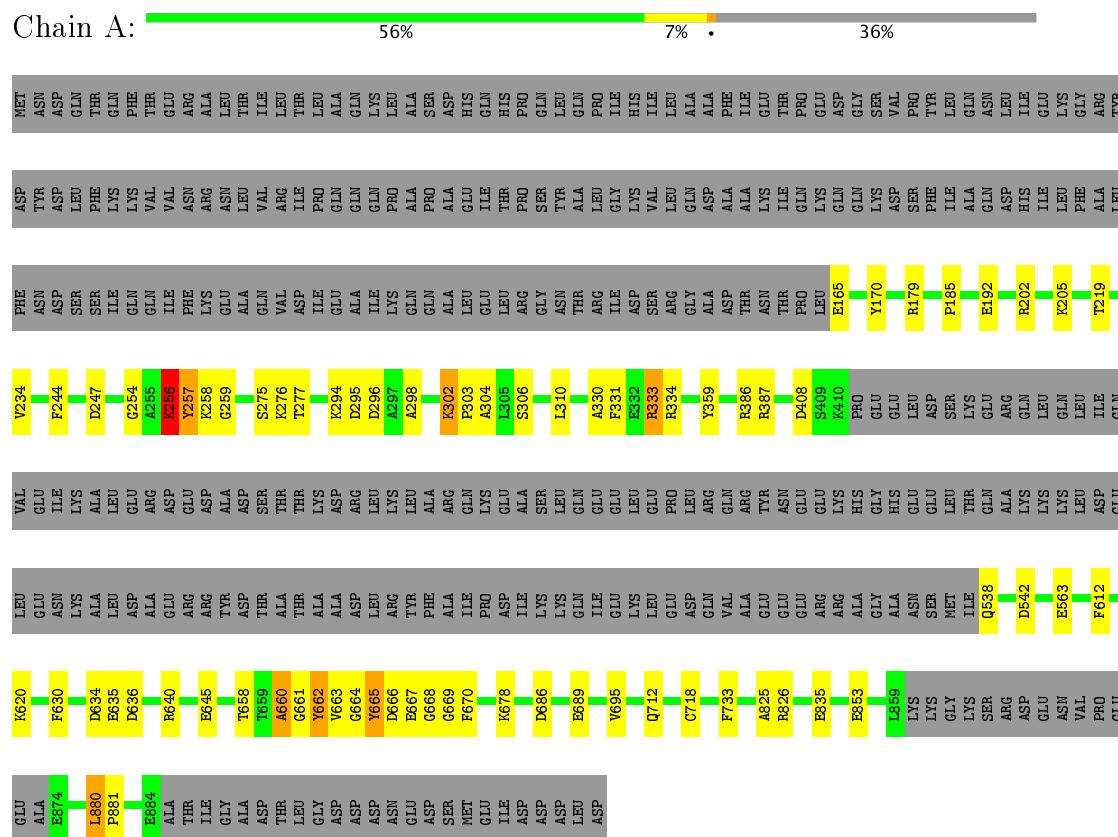


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

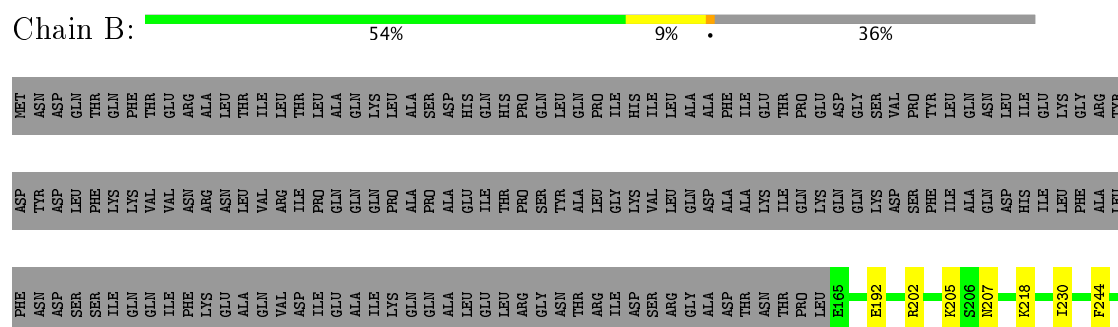
### 3 Residue-property plots

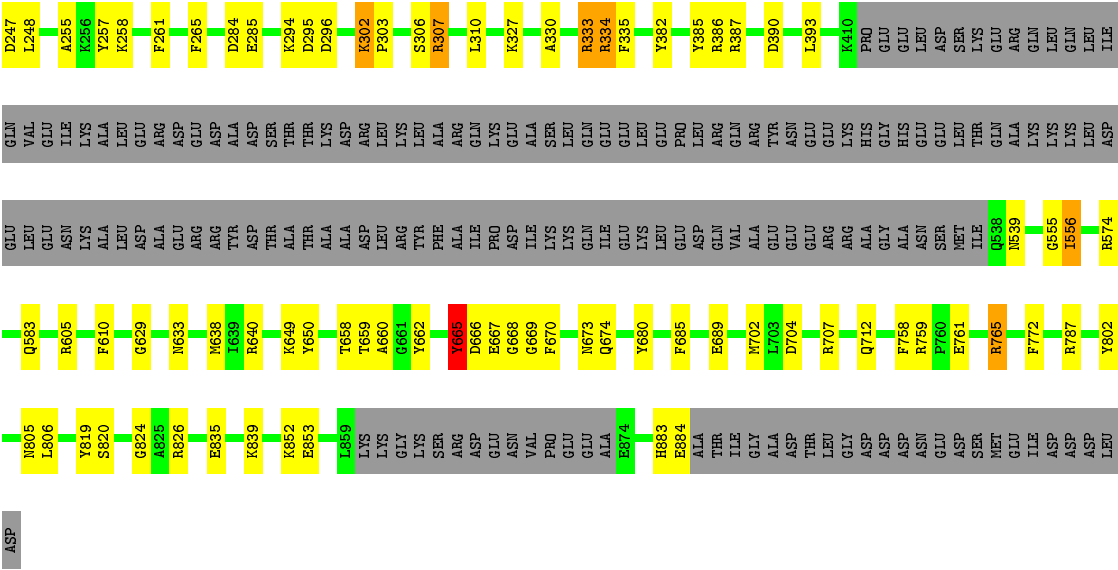
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Heat shock protein 104

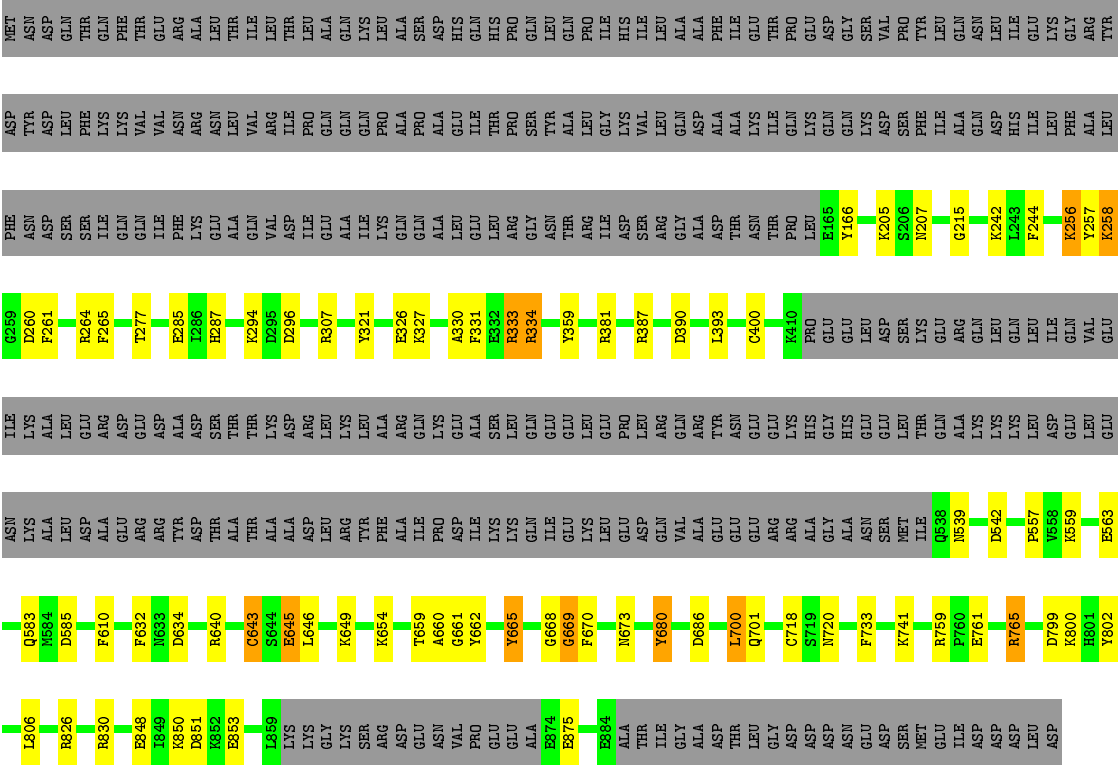


- Molecule 1: Heat shock protein 104





• Molecule 1: Heat shock protein 104



• Molecule 1: Heat shock protein 104







Diagram illustrating a linear chain of nodes:  $x_1$  (green),  $x_5$  (yellow),  $x_9$  (yellow),  $x_{22}$  (yellow), and  $x_{26}$  (green). The nodes are connected sequentially by horizontal lines.

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146463	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 ( $e^-/\text{\AA}^2$ )	0.8	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	GATAN K2 SUMMIT (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: AGS

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	1.10	12/4586 (0.3%)	0.93	7/6171 (0.1%)
1	B	1.22	14/4586 (0.3%)	0.94	14/6171 (0.2%)
1	C	1.26	23/4586 (0.5%)	0.94	6/6171 (0.1%)
1	D	1.26	27/4586 (0.6%)	0.95	11/6171 (0.2%)
1	E	1.20	18/4586 (0.4%)	0.93	10/6171 (0.2%)
1	F	1.10	14/4476 (0.3%)	0.93	7/6020 (0.1%)
All	All	1.19	108/27406 (0.4%)	0.94	55/36875 (0.1%)

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	610	PHE	CB-CG	-8.12	1.37	1.51
1	E	610	PHE	CB-CG	-7.92	1.37	1.51
1	E	670	PHE	CB-CG	-7.67	1.38	1.51
1	C	207	ASN	CB-CG	-7.35	1.34	1.51
1	D	610	PHE	CB-CG	-7.32	1.39	1.51
1	C	733	PHE	CB-CG	-7.28	1.39	1.51
1	D	643	CYS	CB-SG	-7.22	1.70	1.82
1	E	802	TYR	CB-CG	-7.16	1.41	1.51
1	B	244	PHE	CB-CG	-6.99	1.39	1.51
1	B	610	PHE	CB-CG	-6.95	1.39	1.51
1	C	662	TYR	CB-CG	-6.73	1.41	1.51
1	F	853	GLU	CD-OE1	-6.69	1.18	1.25
1	D	848	GLU	CD-OE1	-6.64	1.18	1.25
1	A	234	VAL	CB-CG1	-6.51	1.39	1.52
1	D	166	TYR	CB-CG	-6.42	1.42	1.51
1	C	670	PHE	CB-CG	-6.40	1.40	1.51
1	B	207	ASN	CB-CG	-6.39	1.36	1.51
1	B	382	TYR	CB-CG	-6.31	1.42	1.51
1	A	359	TYR	CB-CG	-6.30	1.42	1.51
1	D	265	PHE	CB-CG	-6.25	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	PHE	CB-CG	-6.12	1.41	1.51
1	B	662	TYR	CB-CG	-6.10	1.42	1.51
1	A	853	GLU	CD-OE1	-6.01	1.19	1.25
1	E	209	CYS	CB-SG	-5.97	1.72	1.81
1	F	265	PHE	CB-CG	-5.96	1.41	1.51
1	C	359	TYR	CB-CG	-5.94	1.42	1.51
1	B	265	PHE	CB-CG	-5.93	1.41	1.51
1	C	285	GLU	CD-OE1	-5.92	1.19	1.25
1	E	790	GLU	CG-CD	-5.92	1.43	1.51
1	D	685	PHE	CB-CG	-5.92	1.41	1.51
1	D	689	GLU	CD-OE1	-5.91	1.19	1.25
1	C	848	GLU	CD-OE1	-5.88	1.19	1.25
1	F	610	PHE	CB-CG	-5.87	1.41	1.51
1	B	853	GLU	CD-OE2	-5.85	1.19	1.25
1	C	265	PHE	CB-CG	-5.85	1.41	1.51
1	C	853	GLU	CD-OE2	-5.83	1.19	1.25
1	D	853	GLU	CG-CD	-5.82	1.43	1.51
1	A	835	GLU	CD-OE1	-5.80	1.19	1.25
1	E	761	GLU	CG-CD	-5.79	1.43	1.51
1	D	721	CYS	CB-SG	-5.77	1.72	1.81
1	B	667	GLU	CG-CD	-5.75	1.43	1.51
1	F	581	VAL	CB-CG1	-5.74	1.40	1.52
1	A	170	TYR	CB-CG	-5.74	1.43	1.51
1	C	287	HIS	CB-CG	-5.74	1.39	1.50
1	E	689	GLU	CG-CD	-5.72	1.43	1.51
1	E	667	GLU	CD-OE1	-5.63	1.19	1.25
1	D	244	PHE	CB-CG	-5.61	1.41	1.51
1	F	579	GLU	CD-OE1	-5.61	1.19	1.25
1	C	875	GLU	CD-OE2	-5.60	1.19	1.25
1	E	667	GLU	CD-OE2	-5.60	1.19	1.25
1	A	244	PHE	CB-CG	-5.59	1.41	1.51
1	A	612	PHE	CB-CG	-5.59	1.41	1.51
1	E	244	PHE	CB-CG	-5.58	1.41	1.51
1	E	321	TYR	CB-CG	-5.58	1.43	1.51
1	F	383	LEU	CB-CG	-5.56	1.36	1.52
1	B	685	PHE	CB-CG	-5.52	1.42	1.51
1	E	207	ASN	CB-CG	-5.49	1.38	1.51
1	B	689	GLU	CD-OE1	-5.48	1.19	1.25
1	F	680	TYR	CB-CG	-5.47	1.43	1.51
1	B	758	PHE	CB-CG	-5.46	1.42	1.51
1	E	680	TYR	CB-CG	-5.45	1.43	1.51
1	B	802	TYR	CB-CG	-5.44	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	875	GLU	CD-OE2	-5.43	1.19	1.25
1	A	331	PHE	CB-CG	-5.42	1.42	1.51
1	D	324	ILE	CB-CG1	-5.37	1.39	1.54
1	F	643	CYS	CB-SG	-5.36	1.73	1.81
1	C	645	GLU	CD-OE1	-5.35	1.19	1.25
1	D	667	GLU	CD-OE2	-5.34	1.19	1.25
1	F	875	GLU	CD-OE2	-5.34	1.19	1.25
1	C	632	PHE	CB-CG	-5.33	1.42	1.51
1	D	262	GLU	CD-OE2	-5.33	1.19	1.25
1	D	809	GLU	CD-OE2	-5.33	1.19	1.25
1	C	400	CYS	CB-SG	-5.32	1.73	1.81
1	C	166	TYR	CB-CG	-5.31	1.43	1.51
1	E	632	PHE	CB-CG	-5.29	1.42	1.51
1	C	326	GLU	CD-OE1	-5.28	1.19	1.25
1	E	689	GLU	CD-OE1	-5.27	1.19	1.25
1	F	234	VAL	CB-CG2	-5.27	1.41	1.52
1	F	762	PHE	CB-CG	-5.26	1.42	1.51
1	D	853	GLU	CD-OE1	-5.26	1.19	1.25
1	E	757	HIS	CB-CG	-5.25	1.40	1.50
1	D	733	PHE	CB-CG	-5.24	1.42	1.51
1	D	282	PHE	CB-CG	-5.24	1.42	1.51
1	A	733	PHE	CB-CG	-5.21	1.42	1.51
1	D	677	TYR	CG-CD2	-5.18	1.32	1.39
1	B	382	TYR	CG-CD2	-5.18	1.32	1.39
1	D	285	GLU	CD-OE2	-5.18	1.20	1.25
1	D	622	GLU	CD-OE2	-5.17	1.20	1.25
1	D	875	GLU	CD-OE1	-5.17	1.20	1.25
1	A	718	CYS	CB-SG	-5.17	1.73	1.81
1	F	400	CYS	CB-SG	-5.17	1.73	1.81
1	D	339	GLU	CD-OE1	-5.15	1.20	1.25
1	D	332	GLU	CD-OE1	-5.14	1.20	1.25
1	B	335	PHE	CB-CG	-5.12	1.42	1.51
1	C	326	GLU	CD-OE2	-5.11	1.20	1.25
1	C	700	LEU	CB-CG	-5.10	1.37	1.52
1	C	673	ASN	CB-CG	-5.08	1.39	1.51
1	E	687	GLU	CD-OE2	-5.08	1.20	1.25
1	D	835	GLU	CD-OE1	-5.07	1.20	1.25
1	E	165	GLU	CD-OE1	-5.06	1.20	1.25
1	A	689	GLU	CD-OE1	-5.06	1.20	1.25
1	F	630	PHE	CB-CG	-5.03	1.42	1.51
1	D	677	TYR	CB-CG	-5.03	1.44	1.51
1	F	612	PHE	CG-CD1	-5.02	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	650	TYR	CB-CG	-5.02	1.44	1.51
1	C	321	TYR	CB-CG	-5.01	1.44	1.51
1	C	563	GLU	CD-OE2	-5.01	1.20	1.25
1	A	695	VAL	CB-CG2	-5.01	1.42	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	407	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	707	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	D	322	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	202	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	C	759	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	826	ARG	NE-CZ-NH2	7.67	124.13	120.30
1	A	386	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	E	228	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	F	386	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	C	381	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	386	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	202	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	640	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	D	707	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	D	677	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	B	640	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	E	307	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	C	830	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	E	203	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	385	TYR	CB-CG-CD1	-6.14	117.31	121.00
1	F	787	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	D	794	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	D	202	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	640	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	F	707	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	B	386	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	665	TYR	N-CA-C	-5.82	95.29	111.00
1	F	202	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	170	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	B	787	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	E	650	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	202	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	F	769	ILE	N-CA-C	-5.35	96.55	111.00
1	B	202	ARG	NE-CZ-NH1	5.35	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	640	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	E	194	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	E	575	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	179	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	787	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	B	826	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	787	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	F	580	VAL	N-CA-C	-5.25	96.82	111.00
1	E	265	PHE	CB-CG-CD2	5.23	124.46	120.80
1	B	662	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	B	605	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	C	632	PHE	CB-CG-CD2	-5.22	117.14	120.80
1	B	574	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	830	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	408	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	680	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	C	662	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	D	324	ILE	CB-CA-C	-5.09	101.43	111.60
1	D	202	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	F	187	ILE	N-CA-C	5.00	124.51	111.00
1	E	189	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	4530	0	4645	119	0
1	B	4530	0	4647	139	0
1	C	4530	0	4643	113	0
1	D	4530	0	4642	158	0
1	E	4530	0	4646	111	0
1	F	4424	0	4553	46	0
2	P	131	0	40	4	0
3	A	62	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	62	0	24	13	0
3	C	62	0	24	8	0
3	D	62	0	24	6	0
3	E	62	0	24	8	0
3	F	62	0	24	5	0
All	All	27577	0	27960	582	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 10.

All (582) 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:A:205:LYS:HZ3	1:A:306:SER:CA	1.05	1.59
1:A:258:LYS:NZ	1:B:261:PHE:CE2	1.70	1.55
1:D:205:LYS:CE	1:D:333:ARG:HH21	1.13	1.52
1:A:205:LYS:NZ	1:A:306:SER:CB	1.78	1.44
1:A:330:ALA:HB1	1:A:334:ARG:NH1	1.32	1.44
1:A:258:LYS:NZ	1:B:261:PHE:CD2	1.84	1.44
1:D:256:LYS:O	1:D:257:TYR:CD2	1.71	1.40
1:D:205:LYS:HE2	1:D:333:ARG:NH2	1.34	1.38
1:D:765:ARG:NH1	3:E:1002:AGS:S1G	1.99	1.35
1:A:205:LYS:NZ	1:A:306:SER:CA	1.82	1.35
1:A:258:LYS:HB3	1:B:255:ALA:CB	1.54	1.34
1:A:333:ARG:NH2	3:B:1001:AGS:H5'2	1.05	1.34
1:C:765:ARG:NH2	3:E:1001:AGS:S1G	1.99	1.34
1:D:205:LYS:NZ	1:D:333:ARG:HH21	1.25	1.33
1:D:660:ALA:HB2	1:D:665:TYR:OH	1.18	1.32
1:A:205:LYS:HZ3	1:A:306:SER:CB	1.34	1.29
1:B:330:ALA:HB1	1:B:334:ARG:NH1	1.45	1.29
1:B:660:ALA:HB2	1:B:665:TYR:OH	1.15	1.27
1:A:205:LYS:CE	1:A:306:SER:CB	2.13	1.26
1:A:333:ARG:NH2	3:B:1001:AGS:C5'	1.98	1.25
1:A:258:LYS:HB2	2:P:9:UNK:CB	1.66	1.25
1:D:765:ARG:HE	1:E:826:ARG:NH1	1.36	1.24
1:B:333:ARG:HD3	1:C:390:ASP:OD2	1.35	1.24
1:D:205:LYS:CE	1:D:333:ARG:NH2	1.91	1.20
1:B:660:ALA:CB	1:B:665:TYR:OH	1.89	1.20
1:A:205:LYS:CE	1:A:306:SER:HB2	1.71	1.17
1:D:258:LYS:HD3	1:E:261:PHE:CE2	1.79	1.16
1:A:205:LYS:NZ	1:A:306:SER:HB3	1.46	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:ALA:HB2	1:C:665:TYR:OH	1.42	1.16
1:D:660:ALA:HB2	1:D:665:TYR:CZ	1.82	1.14
1:A:205:LYS:NZ	1:A:306:SER:HA	1.52	1.14
1:B:333:ARG:CD	1:C:390:ASP:OD2	1.96	1.12
1:C:660:ALA:HA	1:C:665:TYR:CZ	1.85	1.11
1:A:205:LYS:HE2	1:A:306:SER:CB	1.77	1.10
1:D:258:LYS:CG	1:E:261:PHE:HZ	1.63	1.10
1:D:258:LYS:CG	1:E:261:PHE:CZ	2.34	1.10
1:B:659:THR:C	1:B:665:TYR:HE1	1.54	1.08
1:C:660:ALA:CB	1:C:665:TYR:OH	2.02	1.07
1:D:205:LYS:NZ	1:D:333:ARG:NH2	1.99	1.07
1:A:333:ARG:HH21	3:B:1001:AGS:C5'	1.61	1.06
1:D:660:ALA:CB	1:D:665:TYR:OH	2.01	1.06
1:A:205:LYS:CE	1:A:306:SER:CA	2.32	1.05
1:A:258:LYS:HB3	1:B:255:ALA:HB3	1.07	1.04
1:A:205:LYS:CE	1:A:306:SER:HA	1.86	1.04
1:A:330:ALA:CB	1:A:334:ARG:HH12	1.69	1.04
1:A:205:LYS:HE2	1:A:306:SER:HB2	1.07	1.03
1:F:330:ALA:O	1:F:334:ARG:HG2	1.57	1.03
1:C:660:ALA:CA	1:C:665:TYR:OH	2.06	1.03
1:E:662:TYR:OH	1:F:650:TYR:CE1	2.11	1.02
1:B:330:ALA:HB1	1:B:334:ARG:HH12	0.85	1.00
1:B:333:ARG:HD2	1:C:390:ASP:CG	1.82	1.00
1:D:700:LEU:HD12	1:D:765:ARG:HD2	1.44	1.00
1:F:826:ARG:HB2	1:F:827:PRO:HD3	1.40	1.00
1:B:330:ALA:CB	1:B:334:ARG:HH12	1.76	0.99
1:D:660:ALA:N	1:D:665:TYR:CE1	2.31	0.99
1:D:256:LYS:C	1:D:257:TYR:CD2	2.34	0.98
1:A:333:ARG:HH22	3:B:1001:AGS:H5'2	1.26	0.98
1:D:765:ARG:NE	1:E:826:ARG:NH1	2.12	0.98
1:A:665:TYR:HE2	1:B:666:ASP:OD2	1.44	0.97
1:A:205:LYS:HZ1	1:A:306:SER:HB3	1.15	0.96
1:B:660:ALA:CA	1:B:665:TYR:CZ	2.48	0.96
1:C:660:ALA:HB2	1:C:665:TYR:HH	1.19	0.96
1:A:254:GLY:O	1:A:256:LYS:HD2	1.66	0.96
1:C:660:ALA:CA	1:C:665:TYR:CZ	2.48	0.96
1:C:258:LYS:HG2	1:D:255:ALA:HB3	1.47	0.95
1:B:205:LYS:HD3	1:B:333:ARG:NH1	1.80	0.95
1:B:660:ALA:HA	1:B:665:TYR:CZ	2.00	0.95
1:A:330:ALA:CB	1:A:334:ARG:NH1	2.27	0.95
1:B:660:ALA:HA	1:B:665:TYR:CE1	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NE	1:B:390:ASP:OD2	2.00	0.95
1:D:258:LYS:CD	1:E:261:PHE:CZ	2.50	0.95
1:B:660:ALA:N	1:B:665:TYR:CE1	2.35	0.95
1:D:258:LYS:HD3	1:E:261:PHE:CZ	2.01	0.94
1:A:258:LYS:CB	1:B:255:ALA:CB	2.44	0.94
1:E:826:ARG:HB2	1:E:827:PRO:HD3	1.50	0.94
1:A:205:LYS:HZ3	1:A:306:SER:N	1.65	0.94
1:A:333:ARG:CD	1:B:390:ASP:OD2	2.16	0.94
1:D:765:ARG:HE	1:E:826:ARG:HH12	1.06	0.93
1:D:256:LYS:O	1:D:257:TYR:HD2	1.22	0.93
1:D:258:LYS:HG3	1:E:261:PHE:HZ	1.31	0.92
1:D:660:ALA:CA	1:D:665:TYR:CE1	2.52	0.92
1:C:205:LYS:NZ	1:D:390:ASP:CG	2.23	0.92
1:D:660:ALA:N	1:D:665:TYR:HE1	1.66	0.91
1:D:258:LYS:HD3	1:E:261:PHE:HE2	1.33	0.91
1:A:205:LYS:CD	1:A:306:SER:HA	1.99	0.91
1:B:765:ARG:HH11	1:B:765:ARG:HG3	1.36	0.91
1:E:186:VAL:HG13	1:E:186:VAL:O	1.68	0.91
1:A:205:LYS:HD3	1:A:306:SER:HA	1.52	0.91
1:E:665:TYR:OH	1:E:712:GLN:HG2	1.69	0.91
1:C:258:LYS:CG	1:D:255:ALA:CB	2.48	0.91
1:D:765:ARG:NE	1:E:826:ARG:HH12	1.66	0.90
1:D:660:ALA:CB	1:D:665:TYR:CZ	2.54	0.90
1:D:660:ALA:HA	1:D:665:TYR:CE1	2.06	0.90
1:C:257:TYR:CG	1:D:256:LYS:HG2	2.07	0.90
1:B:659:THR:C	1:B:665:TYR:CE1	2.44	0.90
1:A:258:LYS:CB	1:B:255:ALA:HB3	2.00	0.90
1:B:333:ARG:HH21	1:B:334:ARG:NH2	1.70	0.90
1:D:333:ARG:HD2	1:E:215:GLY:CA	2.02	0.89
1:C:258:LYS:HG3	1:D:255:ALA:CB	2.02	0.89
1:C:645:GLU:O	1:C:645:GLU:CD	2.10	0.89
1:B:660:ALA:CA	1:B:665:TYR:CE1	2.55	0.89
1:A:258:LYS:HB3	1:B:255:ALA:HB1	1.54	0.89
1:E:662:TYR:CZ	1:F:650:TYR:CE1	2.24	0.89
1:B:761:GLU:N	1:B:761:GLU:OE1	2.05	0.89
1:C:258:LYS:CG	1:D:255:ALA:HB3	2.03	0.89
1:B:333:ARG:CD	1:C:390:ASP:CG	2.40	0.89
1:D:660:ALA:HB2	1:D:665:TYR:HH	1.07	0.89
1:B:660:ALA:N	1:B:665:TYR:HE1	1.72	0.88
1:F:310:LEU:HG	1:F:310:LEU:O	1.73	0.88
1:B:660:ALA:CA	1:B:665:TYR:OH	2.22	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:HD3	1:D:215:GLY:CA	2.03	0.88
1:C:333:ARG:HD3	1:D:215:GLY:HA3	1.56	0.88
1:C:645:GLU:O	1:C:645:GLU:OE1	1.90	0.87
1:D:809:GLU:N	1:D:809:GLU:OE1	2.05	0.87
3:D:1001:AGS:O1B	3:D:1001:AGS:O2G	1.92	0.87
1:D:256:LYS:O	1:D:257:TYR:CG	2.26	0.87
1:A:258:LYS:NZ	1:B:261:PHE:HE2	1.63	0.87
3:D:1002:AGS:O1A	3:D:1002:AGS:O2G	1.93	0.86
1:C:718:CYS:O	1:C:718:CYS:SG	2.32	0.86
1:E:761:GLU:OE1	1:E:761:GLU:N	2.09	0.86
1:A:333:ARG:CG	1:B:390:ASP:OD2	2.24	0.85
1:D:256:LYS:HB2	1:D:257:TYR:CE2	2.11	0.85
1:E:665:TYR:CZ	1:E:712:GLN:HG2	2.11	0.85
1:B:333:ARG:HH21	1:B:334:ARG:HH21	1.24	0.85
1:E:643:CYS:SG	1:E:699:MET:HE2	2.15	0.85
1:A:662:TYR:OH	1:B:649:LYS:O	1.94	0.85
1:C:205:LYS:HD3	1:C:333:ARG:NH2	1.90	0.85
1:C:660:ALA:N	1:C:665:TYR:OH	2.10	0.85
3:E:1002:AGS:O1B	3:E:1002:AGS:O2G	1.94	0.85
1:D:258:LYS:CD	1:E:261:PHE:CE2	2.60	0.84
1:A:258:LYS:CB	2:P:9:UNK:CB	2.53	0.84
1:E:330:ALA:O	1:E:334:ARG:HG2	1.78	0.84
1:C:557:PRO:HG3	1:C:680:TYR:CE2	2.11	0.84
1:D:712:GLN:NE2	1:E:666:ASP:OD2	2.11	0.83
1:B:660:ALA:HB2	1:B:665:TYR:HH	1.02	0.83
1:A:665:TYR:OH	1:A:712:GLN:HG3	1.79	0.83
1:D:258:LYS:HG2	1:E:261:PHE:CZ	2.12	0.83
1:A:192:GLU:N	1:A:192:GLU:OE1	2.11	0.82
1:C:660:ALA:HA	1:C:665:TYR:CE1	2.13	0.82
1:C:258:LYS:HG3	1:D:255:ALA:HB2	1.59	0.82
1:B:704:ASP:OD2	1:B:765:ARG:NE	2.13	0.82
1:C:761:GLU:N	1:C:761:GLU:OE1	2.13	0.82
1:A:219:THR:HG21	1:F:333:ARG:HH22	1.43	0.82
3:A:1001:AGS:O2G	3:A:1001:AGS:O1B	1.92	0.81
1:E:333:ARG:HD3	1:E:333:ARG:O	1.79	0.81
1:B:205:LYS:HD3	1:B:333:ARG:HH12	1.41	0.81
1:A:662:TYR:CD2	1:B:650:TYR:CE2	2.69	0.81
1:C:330:ALA:HB1	1:C:334:ARG:HH12	1.45	0.80
1:C:205:LYS:NZ	1:D:390:ASP:OD2	2.13	0.80
1:A:660:ALA:O	1:B:658:THR:CG2	2.29	0.80
1:B:306:SER:C	1:B:307:ARG:HE	1.84	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:660:ALA:CA	1:D:665:TYR:CZ	2.63	0.80
1:C:557:PRO:HG3	1:C:680:TYR:CZ	2.17	0.80
1:D:256:LYS:C	1:D:257:TYR:CG	2.51	0.80
1:A:661:GLY:O	2:P:22:UNK:CB	2.30	0.80
3:F:1002:AGS:O1B	3:F:1002:AGS:O2G	1.99	0.79
1:E:809:GLU:OE1	1:E:809:GLU:N	2.16	0.79
1:B:307:ARG:N	1:B:307:ARG:HE	1.80	0.79
3:D:1002:AGS:O1B	3:D:1002:AGS:O2G	1.93	0.79
3:B:1002:AGS:S1G	3:B:1002:AGS:O2B	2.41	0.78
1:D:205:LYS:HE2	1:D:333:ARG:HH22	1.43	0.78
1:C:327:LYS:NZ	1:D:712:GLN:HE22	1.82	0.78
1:E:643:CYS:SG	1:E:699:MET:CE	2.72	0.78
1:A:712:GLN:NE2	1:B:666:ASP:OD2	2.17	0.78
1:D:205:LYS:HZ1	1:D:333:ARG:NH2	1.78	0.78
1:F:819:TYR:O	1:F:819:TYR:CD2	2.37	0.78
1:D:258:LYS:CD	1:E:261:PHE:HZ	1.91	0.77
1:B:333:ARG:HD2	1:C:390:ASP:OD1	1.84	0.77
3:C:1001:AGS:H5'2	3:C:1001:AGS:H8	1.65	0.77
1:D:300:ILE:HG23	1:D:300:ILE:O	1.84	0.76
1:A:665:TYR:CE2	1:B:666:ASP:OD2	2.36	0.76
3:A:1001:AGS:O1A	3:A:1001:AGS:O2B	1.99	0.76
1:D:256:LYS:CB	1:D:257:TYR:CE2	2.69	0.76
1:D:333:ARG:HD2	1:E:215:GLY:HA3	1.66	0.76
1:A:662:TYR:CE2	1:B:650:TYR:CE2	2.73	0.76
1:D:661:GLY:HA2	1:E:662:TYR:HB3	1.68	0.76
1:D:205:LYS:NZ	1:D:333:ARG:HE	1.83	0.75
1:B:333:ARG:NH2	1:B:334:ARG:HE	1.83	0.75
1:D:333:ARG:HD2	1:E:215:GLY:HA2	1.69	0.75
1:A:310:LEU:O	1:A:310:LEU:HG	1.85	0.74
1:E:826:ARG:HB2	1:E:827:PRO:CD	2.17	0.74
1:E:387:ARG:NE	1:E:387:ARG:HA	2.03	0.74
3:C:1001:AGS:H8	3:C:1001:AGS:C5'	2.17	0.74
1:D:205:LYS:HZ3	1:D:333:ARG:HE	1.36	0.73
1:B:660:ALA:HB2	1:B:665:TYR:CZ	2.23	0.73
1:D:258:LYS:HG3	1:E:261:PHE:CZ	2.15	0.73
1:A:258:LYS:HD3	1:B:255:ALA:HB1	1.69	0.72
1:C:257:TYR:HB3	1:D:256:LYS:CG	2.19	0.72
1:A:333:ARG:HH21	3:B:1001:AGS:H5'2	0.91	0.72
1:E:583:GLN:OE1	1:E:583:GLN:HA	1.90	0.72
1:C:257:TYR:CD1	1:D:256:LYS:HG2	2.23	0.72
3:C:1001:AGS:C8	3:C:1001:AGS:C5'	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:NH1	1:D:390:ASP:CG	2.42	0.72
1:B:765:ARG:HG3	1:B:765:ARG:NH1	2.04	0.72
1:B:680:TYR:O	1:B:680:TYR:CD2	2.43	0.71
1:A:254:GLY:O	1:A:256:LYS:CD	2.36	0.71
1:B:310:LEU:HG	1:B:310:LEU:O	1.90	0.71
1:C:765:ARG:NH2	3:E:1001:AGS:PG	2.64	0.71
3:B:1001:AGS:O2A	3:B:1001:AGS:O1B	2.04	0.70
1:E:397:ASP:HA	1:E:400:CYS:SG	2.32	0.70
1:C:258:LYS:HG2	1:D:255:ALA:CB	2.15	0.70
1:C:257:TYR:CD2	1:D:256:LYS:HE2	2.27	0.70
1:B:759:ARG:HA	1:B:759:ARG:NE	2.06	0.70
1:E:186:VAL:O	1:E:186:VAL:CG1	2.40	0.70
1:D:205:LYS:NZ	1:D:333:ARG:CZ	2.54	0.69
1:B:660:ALA:N	1:B:665:TYR:OH	2.26	0.69
1:D:583:GLN:HA	1:D:583:GLN:OE1	1.91	0.69
1:D:765:ARG:CZ	1:E:826:ARG:HH12	2.04	0.69
1:D:680:TYR:HB2	1:D:720:ASN:O	1.92	0.69
1:B:660:ALA:CB	1:B:665:TYR:CZ	2.75	0.69
1:E:662:TYR:OH	1:F:650:TYR:CZ	2.11	0.69
1:F:819:TYR:O	1:F:819:TYR:CG	2.45	0.69
1:B:556:ILE:O	1:B:556:ILE:HG13	1.91	0.69
1:C:205:LYS:HD3	1:C:333:ARG:HH22	1.58	0.69
3:E:1001:AGS:O1B	3:E:1001:AGS:O2G	2.07	0.68
1:D:698:VAL:HG22	1:E:645:GLU:HG3	1.75	0.68
1:C:333:ARG:HD3	1:D:215:GLY:HA2	1.74	0.68
1:C:659:THR:C	1:C:665:TYR:HE1	1.96	0.68
1:D:390:ASP:OD1	1:D:394:ASP:OD1	2.11	0.68
1:D:697:THR:CG2	1:E:644:SER:HB2	2.23	0.68
1:A:333:ARG:NH2	3:B:1001:AGS:O1A	2.27	0.68
1:B:333:ARG:HH21	1:B:334:ARG:CZ	2.06	0.68
1:D:205:LYS:NZ	1:D:333:ARG:NE	2.42	0.68
1:D:258:LYS:O	1:D:258:LYS:HG3	1.94	0.68
1:A:665:TYR:O	1:A:667:GLU:N	2.28	0.67
1:A:538:GLN:N	1:A:538:GLN:OE1	2.28	0.67
1:E:826:ARG:CB	1:E:827:PRO:HD3	2.21	0.67
1:C:330:ALA:HB1	1:C:334:ARG:NH1	2.10	0.66
3:C:1002:AGS:O1B	3:C:1002:AGS:O2G	2.11	0.66
1:E:192:GLU:N	1:E:192:GLU:OE1	2.25	0.66
1:B:307:ARG:HE	1:B:307:ARG:CA	2.08	0.66
1:B:330:ALA:O	1:B:334:ARG:HG2	1.95	0.66
1:B:330:ALA:CB	1:B:334:ARG:NH1	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HG2	1:B:390:ASP:OD2	1.95	0.66
1:F:559:LYS:HG2	1:F:559:LYS:O	1.96	0.66
1:F:823:MET:O	1:F:826:ARG:HG2	1.96	0.66
1:D:765:ARG:NH1	1:E:826:ARG:HH12	1.94	0.66
3:F:1001:AGS:H5'2	3:F:1001:AGS:H8	1.76	0.66
1:D:333:ARG:CD	1:E:215:GLY:CA	2.73	0.65
1:D:809:GLU:H	1:D:809:GLU:CD	1.92	0.65
1:C:327:LYS:HZ1	1:D:712:GLN:HE22	1.45	0.65
1:E:397:ASP:O	1:E:400:CYS:SG	2.53	0.65
1:B:333:ARG:NH2	1:B:334:ARG:NE	2.45	0.65
1:C:557:PRO:CG	1:C:680:TYR:CE2	2.80	0.65
1:D:765:ARG:HE	1:E:826:ARG:HH11	1.43	0.65
1:A:205:LYS:HE2	1:A:306:SER:CA	2.16	0.65
1:E:330:ALA:O	1:E:334:ARG:CG	2.44	0.65
1:A:258:LYS:HD3	1:B:255:ALA:CB	2.26	0.64
3:D:1002:AGS:O1A	3:D:1002:AGS:O1B	2.15	0.64
1:D:700:LEU:HD12	1:D:765:ARG:CD	2.25	0.64
1:C:257:TYR:HB3	1:D:256:LYS:HG3	1.79	0.64
1:E:680:TYR:N	1:E:680:TYR:CD1	2.64	0.64
1:A:645:GLU:O	1:A:645:GLU:HG3	1.98	0.64
3:C:1001:AGS:O1B	3:C:1001:AGS:O2A	2.11	0.64
1:A:258:LYS:NZ	1:B:261:PHE:HD2	1.88	0.63
3:D:1001:AGS:O1B	3:D:1001:AGS:O1A	2.15	0.63
3:C:1001:AGS:H5'1	3:C:1001:AGS:C8	2.28	0.63
1:C:583:GLN:OE1	1:C:583:GLN:HA	1.99	0.63
1:B:704:ASP:CG	1:B:765:ARG:HE	2.02	0.63
1:C:257:TYR:CB	1:D:256:LYS:CG	2.77	0.63
1:D:718:CYS:O	1:D:718:CYS:SG	2.55	0.63
1:D:698:VAL:CG2	1:E:645:GLU:HG3	2.29	0.62
1:D:700:LEU:CD1	1:D:765:ARG:HD2	2.22	0.62
1:B:387:ARG:NE	1:B:387:ARG:HA	2.14	0.62
1:C:701:GLN:OE1	1:C:701:GLN:HA	1.99	0.62
1:D:765:ARG:HH11	1:E:826:ARG:HH12	1.48	0.62
1:C:205:LYS:HZ2	1:D:390:ASP:CG	1.94	0.62
1:B:333:ARG:NH2	1:B:334:ARG:HH21	1.97	0.62
1:E:643:CYS:SG	1:E:691:ALA:HB2	2.39	0.62
1:E:826:ARG:CG	1:E:826:ARG:HH21	2.12	0.62
3:B:1001:AGS:O2G	3:B:1001:AGS:O1B	2.17	0.61
1:B:257:TYR:HB3	1:C:256:LYS:HG3	1.82	0.61
1:C:257:TYR:CB	1:D:256:LYS:HG2	2.31	0.61
1:C:700:LEU:CD1	1:C:765:ARG:HD2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:HA	1:A:387:ARG:NE	2.15	0.61
1:D:659:THR:C	1:D:665:TYR:HE1	2.04	0.61
1:A:205:LYS:NZ	1:A:334:ARG:HG2	2.16	0.61
1:D:698:VAL:HG22	1:E:645:GLU:HB2	1.82	0.61
1:C:334:ARG:CG	1:C:334:ARG:HH11	2.14	0.60
1:C:387:ARG:NE	1:C:387:ARG:HA	2.16	0.60
1:E:202:ARG:O	1:E:206:SER:HB3	2.01	0.60
1:A:219:THR:HG21	1:F:333:ARG:NH2	2.12	0.60
1:B:660:ALA:N	1:B:665:TYR:CZ	2.63	0.60
1:F:310:LEU:CG	1:F:310:LEU:O	2.44	0.60
1:D:256:LYS:O	1:D:257:TYR:CB	2.48	0.60
1:D:333:ARG:CD	1:E:215:GLY:HA2	2.32	0.60
1:D:698:VAL:HG22	1:E:645:GLU:CG	2.32	0.60
1:D:205:LYS:HZ1	1:D:333:ARG:CZ	2.12	0.60
1:C:258:LYS:CE	1:D:255:ALA:HB1	2.32	0.59
1:D:668:GLY:O	1:D:669:GLY:C	2.40	0.59
1:A:333:ARG:NH2	3:B:1001:AGS:PA	2.75	0.59
1:E:665:TYR:CZ	1:E:712:GLN:CG	2.85	0.59
1:B:192:GLU:N	1:B:192:GLU:OE1	2.33	0.59
1:A:330:ALA:HB1	1:A:334:ARG:HH11	1.57	0.59
1:B:638:MET:C	1:B:638:MET:SD	2.81	0.59
1:C:765:ARG:HH22	3:E:1001:AGS:PG	2.25	0.59
1:A:662:TYR:N	1:A:662:TYR:HD1	2.01	0.58
1:E:387:ARG:HE	1:E:387:ARG:HA	1.65	0.58
1:A:333:ARG:HH21	3:B:1001:AGS:PA	2.27	0.58
1:C:660:ALA:CA	1:C:665:TYR:CE1	2.82	0.58
1:B:258:LYS:NZ	1:C:296:ASP:OD2	2.36	0.58
1:E:302:LYS:NZ	1:E:328:ASP:OD1	2.37	0.58
1:C:258:LYS:HE2	1:D:255:ALA:HB1	1.86	0.58
1:D:378:LEU:HD23	1:D:378:LEU:C	2.24	0.58
1:A:712:GLN:HE21	1:B:666:ASP:CB	2.16	0.58
1:E:643:CYS:HG	1:E:699:MET:HE2	1.68	0.57
1:A:257:TYR:HD1	1:A:257:TYR:N	2.01	0.57
1:C:659:THR:C	1:C:665:TYR:CE1	2.76	0.57
1:E:202:ARG:CZ	1:F:398:ILE:CG1	2.83	0.57
1:E:583:GLN:OE1	1:E:583:GLN:CA	2.53	0.57
1:D:785:ASP:OD2	1:D:789:LYS:NZ	2.37	0.57
1:C:761:GLU:O	1:C:765:ARG:CG	2.53	0.57
1:E:700:LEU:C	1:E:700:LEU:HD23	2.25	0.57
1:D:700:LEU:CD1	1:D:765:ARG:CD	2.83	0.57
1:A:330:ALA:HB1	1:A:334:ARG:HH12	0.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:CD	1:D:215:GLY:HA3	2.32	0.57
1:C:645:GLU:OE1	1:C:654:LYS:NZ	2.38	0.56
1:D:390:ASP:OD1	1:D:394:ASP:CG	2.43	0.56
1:D:300:ILE:CG2	1:D:300:ILE:O	2.52	0.56
1:D:205:LYS:HZ3	1:D:333:ARG:NE	2.00	0.56
1:B:306:SER:OG	1:B:307:ARG:CZ	2.54	0.56
1:C:257:TYR:CB	1:D:256:LYS:HG3	2.36	0.56
1:A:258:LYS:CB	1:B:255:ALA:HB1	2.25	0.56
1:A:662:TYR:CD2	1:B:650:TYR:HE2	2.23	0.56
1:F:410:LYS:HG3	1:F:410:LYS:O	2.06	0.56
1:A:219:THR:CB	1:F:333:ARG:HH12	2.19	0.56
1:A:257:TYR:H	1:A:257:TYR:HD1	1.54	0.56
1:C:327:LYS:NZ	1:D:712:GLN:NE2	2.53	0.56
3:A:1002:AGS:O2G	3:A:1002:AGS:O3A	2.24	0.55
1:C:643:CYS:SG	1:C:686:ASP:N	2.80	0.55
1:C:700:LEU:HD12	1:C:765:ARG:HD2	1.88	0.55
1:A:257:TYR:CD1	1:A:257:TYR:N	2.73	0.55
1:A:662:TYR:CD1	1:A:662:TYR:N	2.73	0.55
1:A:259:GLY:H	1:B:255:ALA:HB3	1.71	0.55
1:D:583:GLN:OE1	1:D:583:GLN:CA	2.55	0.55
1:C:257:TYR:HB3	1:D:256:LYS:HG2	1.87	0.55
1:B:327:LYS:NZ	1:D:666:ASP:OD2	2.39	0.55
1:A:219:THR:HB	1:F:333:ARG:HH12	1.71	0.55
1:A:712:GLN:HE21	1:B:666:ASP:HB3	1.71	0.54
1:D:660:ALA:N	1:D:665:TYR:CZ	2.75	0.54
1:D:660:ALA:HA	1:D:665:TYR:CZ	2.36	0.54
1:D:702:MET:SD	1:D:702:MET:C	2.86	0.54
1:D:387:ARG:HA	1:D:387:ARG:NE	2.23	0.54
1:C:660:ALA:N	1:C:665:TYR:CE1	2.75	0.54
1:D:258:LYS:HG2	1:E:261:PHE:CE2	2.41	0.54
1:E:305:LEU:HB3	1:E:334:ARG:HD3	1.89	0.54
1:C:205:LYS:NZ	1:D:390:ASP:OD1	2.40	0.54
1:F:826:ARG:CB	1:F:827:PRO:HD3	2.19	0.54
1:B:333:ARG:HH21	1:B:334:ARG:NE	2.05	0.54
1:B:680:TYR:O	1:B:680:TYR:CG	2.61	0.54
1:D:698:VAL:HG22	1:E:645:GLU:CB	2.38	0.54
1:C:307:ARG:HA	1:C:307:ARG:NE	2.23	0.53
1:A:205:LYS:HZ1	1:A:334:ARG:HG2	1.74	0.53
1:B:668:GLY:O	1:B:669:GLY:C	2.44	0.53
1:E:668:GLY:O	1:E:670:PHE:N	2.42	0.53
1:C:668:GLY:O	1:C:669:GLY:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ARG:CZ	1:F:398:ILE:HG12	2.39	0.53
1:A:165:GLU:OE2	1:A:276:LYS:NZ	2.42	0.53
1:D:256:LYS:HB3	1:D:257:TYR:CE2	2.43	0.53
1:E:386:ARG:HD3	1:E:390:ASP:OD2	2.09	0.53
1:A:258:LYS:CD	1:B:255:ALA:HB1	2.37	0.53
1:E:387:ARG:NE	1:E:387:ARG:CA	2.72	0.52
1:B:765:ARG:NE	1:C:826:ARG:NH2	2.58	0.52
1:A:668:GLY:O	1:A:670:PHE:N	2.43	0.52
1:C:257:TYR:CG	1:D:256:LYS:CG	2.88	0.52
1:D:258:LYS:CD	1:E:261:PHE:HE2	2.13	0.52
1:E:826:ARG:HG3	1:E:826:ARG:NH2	2.24	0.52
1:B:247:ASP:OD1	1:B:248:LEU:N	2.43	0.52
1:F:559:LYS:O	1:F:559:LYS:CG	2.57	0.52
1:F:826:ARG:HB2	1:F:827:PRO:CD	2.28	0.52
1:C:802:TYR:C	1:C:802:TYR:CD1	2.83	0.52
1:D:656:LEU:HD12	1:E:645:GLU:OE2	2.09	0.52
1:E:643:CYS:SG	1:E:699:MET:HE1	2.49	0.52
1:B:294:LYS:O	1:B:296:ASP:N	2.42	0.52
1:B:307:ARG:CA	1:B:307:ARG:NE	2.73	0.52
1:C:643:CYS:SG	1:C:686:ASP:O	2.67	0.52
1:F:826:ARG:NH1	3:F:1002:AGS:H5'1	2.25	0.51
1:E:700:LEU:O	1:E:700:LEU:HD23	2.09	0.51
1:F:735:ASN:C	1:F:735:ASN:OD1	2.45	0.51
1:A:294:LYS:O	1:A:296:ASP:N	2.43	0.51
1:A:334:ARG:NH2	3:B:1001:AGS:S1G	2.83	0.51
1:A:658:THR:OG1	1:A:664:GLY:O	2.29	0.51
1:C:660:ALA:N	1:C:665:TYR:CZ	2.75	0.51
1:E:247:ASP:OD1	1:E:248:LEU:N	2.43	0.51
1:C:542:ASP:C	1:C:542:ASP:OD1	2.47	0.51
1:E:644:SER:HB3	1:E:687:GLU:HB2	1.93	0.51
1:E:826:ARG:CB	1:E:827:PRO:CD	2.78	0.51
1:E:689:GLU:OE1	1:E:689:GLU:N	2.35	0.51
1:D:205:LYS:HZ1	1:D:333:ARG:NE	2.08	0.51
1:A:660:ALA:HB1	1:B:658:THR:HG23	1.92	0.50
1:C:261:PHE:CD1	1:C:261:PHE:C	2.85	0.50
1:E:238:LEU:HD23	1:E:238:LEU:H	1.75	0.50
1:B:704:ASP:CG	1:B:765:ARG:NE	2.60	0.50
1:A:662:TYR:CE2	1:B:650:TYR:CZ	3.00	0.50
1:E:826:ARG:CG	1:E:826:ARG:NH2	2.72	0.50
1:A:620:LYS:NZ	1:A:686:ASP:OD1	2.44	0.50
3:C:1001:AGS:PA	3:C:1001:AGS:C3'	2.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ARG:CG	1:C:334:ARG:NH1	2.73	0.50
1:F:367:ILE:N	1:F:367:ILE:HD12	2.27	0.50
1:A:256:LYS:NZ	1:A:257:TYR:CE1	2.80	0.50
1:B:702:MET:C	1:B:702:MET:SD	2.90	0.49
1:B:712:GLN:O	1:B:712:GLN:HG2	2.12	0.49
1:D:635:GLU:CD	1:D:635:GLU:H	2.15	0.49
1:D:665:TYR:OH	1:D:712:GLN:HG3	2.12	0.49
1:A:258:LYS:CG	1:B:255:ALA:CB	2.90	0.49
1:E:809:GLU:CD	1:E:809:GLU:N	2.65	0.49
1:A:712:GLN:O	1:A:712:GLN:HG2	2.12	0.49
1:B:387:ARG:HA	1:B:387:ARG:HE	1.78	0.49
1:A:660:ALA:O	1:B:658:THR:HG22	2.08	0.49
1:D:258:LYS:CG	1:E:261:PHE:CE2	2.86	0.49
1:B:668:GLY:O	1:B:670:PHE:N	2.45	0.49
1:D:301:LEU:HG	1:D:301:LEU:O	2.13	0.49
1:E:274:GLU:HG3	1:E:274:GLU:O	2.12	0.49
1:C:583:GLN:OE1	1:C:583:GLN:CA	2.61	0.49
1:E:165:GLU:OE2	1:E:276:LYS:NZ	2.46	0.49
1:E:668:GLY:O	1:E:669:GLY:C	2.51	0.48
1:A:205:LYS:HE3	1:A:333:ARG:NH1	2.28	0.48
1:C:850:LYS:NZ	1:C:851:ASP:OD2	2.43	0.48
1:D:880:LEU:HB3	1:D:881:PRO:HD3	1.95	0.48
1:E:616:SER:OG	1:E:826:ARG:NH2	2.45	0.48
1:F:826:ARG:HA	1:F:826:ARG:HE	1.79	0.48
1:C:559:LYS:HA	1:C:559:LYS:HE2	1.94	0.48
1:B:884:GLU:O	1:B:884:GLU:HG3	2.14	0.48
1:E:238:LEU:HD23	1:E:238:LEU:N	2.28	0.48
1:E:294:LYS:O	1:E:296:ASP:N	2.46	0.48
1:B:666:ASP:OD1	1:B:666:ASP:N	2.40	0.48
1:B:759:ARG:HE	1:B:759:ARG:HA	1.76	0.48
1:C:585:ASP:OD2	1:C:741:LYS:NZ	2.46	0.48
1:F:672:THR:OG1	1:F:673:ASN:N	2.46	0.48
1:F:826:ARG:N	1:F:827:PRO:CD	2.77	0.48
1:A:542:ASP:N	1:A:542:ASP:OD1	2.44	0.47
1:B:629:GLY:O	1:B:633:ASN:N	2.46	0.47
1:C:327:LYS:HZ1	1:D:712:GLN:NE2	2.11	0.47
1:D:645:GLU:OE1	1:D:654:LYS:NZ	2.47	0.47
1:E:202:ARG:O	1:E:206:SER:CB	2.62	0.47
1:D:742:ILE:HG23	1:D:742:ILE:O	2.13	0.47
1:C:539:ASN:N	1:C:539:ASN:OD1	2.44	0.47
1:E:825:ALA:O	1:E:826:ARG:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:CD	1:D:215:GLY:CA	2.84	0.47
1:C:260:ASP:OD2	1:C:264:ARG:NH1	2.47	0.47
1:C:680:TYR:HB2	1:C:720:ASN:O	2.14	0.47
1:E:397:ASP:CA	1:E:400:CYS:SG	3.03	0.47
1:F:230:ILE:HD13	1:F:230:ILE:HA	1.70	0.47
1:A:665:TYR:OH	1:A:712:GLN:CG	2.58	0.47
1:E:662:TYR:CZ	1:F:650:TYR:HE1	1.85	0.47
1:B:761:GLU:O	1:B:765:ARG:NH1	2.48	0.47
1:A:333:ARG:HD3	1:A:333:ARG:O	2.15	0.46
1:D:660:ALA:CA	1:D:665:TYR:OH	2.61	0.46
1:A:185:PRO:O	3:A:1001:AGS:H2	2.16	0.46
1:C:258:LYS:CE	1:D:255:ALA:CB	2.93	0.46
1:A:660:ALA:O	1:B:658:THR:HG23	2.15	0.46
1:D:378:LEU:HD23	1:D:378:LEU:O	2.14	0.46
1:A:247:ASP:C	1:A:247:ASP:OD1	2.54	0.46
1:A:660:ALA:C	1:B:658:THR:CG2	2.84	0.46
1:B:805:ASN:O	1:B:806:LEU:C	2.54	0.46
1:C:799:ASP:OD2	1:C:800:LYS:NZ	2.48	0.46
1:F:789:LYS:NZ	1:F:793:GLU:OE2	2.45	0.46
1:A:302:LYS:HB3	1:A:303:PRO:HD3	1.98	0.46
1:E:202:ARG:CZ	1:F:398:ILE:HG13	2.46	0.45
1:C:257:TYR:HA	2:P:5:UNK:O	2.16	0.45
1:C:387:ARG:HE	1:C:387:ARG:HA	1.80	0.45
1:C:649:LYS:HE2	1:C:649:LYS:HB2	1.78	0.45
3:E:1002:AGS:O1B	3:E:1002:AGS:O2A	2.27	0.45
1:A:634:ASP:OD1	1:A:635:GLU:N	2.50	0.45
1:D:256:LYS:CB	1:D:257:TYR:CD2	3.00	0.45
1:D:880:LEU:CB	1:D:881:PRO:CD	2.95	0.45
1:D:326:GLU:HA	1:D:326:GLU:OE1	2.16	0.45
1:F:826:ARG:NE	1:F:826:ARG:HA	2.31	0.45
1:C:660:ALA:CB	1:C:665:TYR:CZ	2.88	0.45
1:C:331:PHE:HD1	1:C:331:PHE:HA	1.71	0.45
1:E:667:GLU:OE1	1:E:712:GLN:OE1	2.34	0.45
1:E:643:CYS:HG	1:E:699:MET:CE	2.24	0.44
1:A:660:ALA:CB	1:B:658:THR:HG23	2.47	0.44
1:F:167:LEU:C	1:F:167:LEU:HD12	2.38	0.44
1:B:704:ASP:OD1	1:B:765:ARG:HD3	2.17	0.44
1:B:820:SER:O	1:B:824:GLY:N	2.51	0.44
1:D:629:GLY:O	1:D:633:ASN:N	2.47	0.44
1:D:680:TYR:CG	1:D:680:TYR:O	2.70	0.44
1:E:185:PRO:O	1:E:186:VAL:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:568:LYS:O	1:E:572:MET:N	2.50	0.44
1:A:880:LEU:HB2	1:A:881:PRO:HD2	2.00	0.44
1:C:387:ARG:NE	1:C:387:ARG:CA	2.80	0.44
1:E:728:ASN:C	1:E:728:ASN:OD1	2.55	0.44
1:D:751:MET:HA	1:D:751:MET:CE	2.48	0.44
3:F:1001:AGS:H5'2	3:F:1001:AGS:C8	2.47	0.44
1:F:602:ALA:O	1:F:603:ASN:C	2.53	0.44
1:A:712:GLN:NE2	1:B:666:ASP:CB	2.81	0.43
1:A:665:TYR:HD1	1:A:665:TYR:HA	1.67	0.43
1:B:307:ARG:HA	1:B:307:ARG:HE	1.78	0.43
1:B:539:ASN:N	1:B:539:ASN:OD1	2.51	0.43
1:E:774:LYS:NZ	1:E:822:ASP:OD1	2.50	0.43
1:F:802:TYR:C	1:F:802:TYR:CD1	2.91	0.43
1:B:883:HIS:O	1:B:884:GLU:C	2.57	0.43
1:A:302:LYS:O	1:A:304:ALA:N	2.52	0.43
1:F:382:TYR:CD1	1:F:383:LEU:HG	2.54	0.43
1:D:635:GLU:N	1:D:635:GLU:OE1	2.35	0.43
1:D:662:TYR:N	1:D:662:TYR:CD1	2.86	0.43
1:A:219:THR:CG2	1:F:333:ARG:HH12	2.32	0.43
1:A:880:LEU:CB	1:A:881:PRO:CD	2.97	0.43
1:B:673:ASN:OD1	1:B:674:GLN:N	2.51	0.43
1:B:772:PHE:CD1	1:B:772:PHE:N	2.87	0.43
1:A:302:LYS:HB3	1:A:303:PRO:CD	2.49	0.43
1:D:293:GLY:O	1:D:294:LYS:HB2	2.19	0.43
1:B:302:LYS:HB2	1:B:303:PRO:HD3	2.01	0.42
1:C:393:LEU:HD23	1:C:393:LEU:HA	1.79	0.42
1:C:806:LEU:HD12	1:C:806:LEU:C	2.39	0.42
1:E:408:ASP:OD1	1:E:409:SER:N	2.52	0.42
1:E:660:ALA:HA	1:E:665:TYR:CE1	2.54	0.42
1:E:704:ASP:O	1:E:705:ASP:CB	2.66	0.42
1:A:825:ALA:O	1:A:826:ARG:C	2.57	0.42
1:B:555:GLY:O	1:B:556:ILE:C	2.56	0.42
1:B:306:SER:C	1:B:307:ARG:NE	2.64	0.42
1:B:659:THR:O	1:B:665:TYR:CE1	2.71	0.42
3:E:1001:AGS:O2A	3:E:1001:AGS:O2B	2.38	0.42
1:A:563:GLU:CD	1:A:563:GLU:H	2.19	0.42
1:A:258:LYS:CD	1:B:255:ALA:CB	2.95	0.42
1:B:852:LYS:HD2	1:B:852:LYS:N	2.34	0.42
1:C:327:LYS:HZ3	1:D:712:GLN:HE22	1.63	0.42
1:F:588:LYS:HE2	1:F:588:LYS:HB2	1.83	0.42
1:D:255:ALA:O	1:D:256:LYS:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:LYS:HB3	1:F:218:LYS:HE2	1.81	0.42
1:F:261:PHE:C	1:F:261:PHE:CD1	2.93	0.42
1:F:583:GLN:OE1	1:F:583:GLN:HA	2.20	0.42
1:A:333:ARG:HH22	3:B:1001:AGS:C5'	1.98	0.42
3:C:1001:AGS:PA	3:C:1001:AGS:H3'	2.60	0.42
1:B:302:LYS:CB	1:B:303:PRO:CD	2.98	0.42
1:D:256:LYS:HB3	1:D:257:TYR:CZ	2.55	0.42
1:B:230:ILE:HD13	1:B:230:ILE:HA	1.83	0.42
1:B:307:ARG:HA	1:B:307:ARG:NE	2.33	0.42
1:C:334:ARG:NH1	1:C:334:ARG:HG2	2.35	0.42
1:D:665:TYR:CZ	1:D:712:GLN:HG3	2.55	0.42
1:E:270:LYS:NZ	1:E:274:GLU:OE1	2.48	0.42
3:D:1001:AGS:H8	3:D:1001:AGS:H5'1	2.01	0.42
1:D:805:ASN:O	1:D:806:LEU:C	2.55	0.42
1:D:826:ARG:N	1:D:827:PRO:CD	2.83	0.42
1:A:310:LEU:O	1:A:310:LEU:CG	2.53	0.41
1:B:835:GLU:OE1	1:B:839:LYS:NZ	2.53	0.41
1:D:665:TYR:CE2	1:D:712:GLN:CD	2.94	0.41
1:B:218:LYS:HE2	1:B:218:LYS:HB2	1.81	0.41
1:C:761:GLU:O	1:C:765:ARG:HG3	2.21	0.41
1:C:800:LYS:HD3	1:C:800:LYS:HA	1.85	0.41
1:B:765:ARG:HE	1:C:826:ARG:NH2	2.18	0.41
1:A:302:LYS:CB	1:A:303:PRO:CD	2.98	0.41
1:B:306:SER:O	1:B:307:ARG:NH2	2.43	0.41
1:B:819:TYR:C	1:B:819:TYR:CD2	2.93	0.41
1:E:585:ASP:OD2	1:E:741:LYS:NZ	2.53	0.41
1:F:678:LYS:HB3	1:F:681:SER:HB3	2.01	0.41
1:B:638:MET:SD	1:B:638:MET:O	2.78	0.41
1:B:765:ARG:CG	1:B:765:ARG:NH1	2.73	0.41
1:C:333:ARG:NH1	1:D:390:ASP:OD2	2.49	0.41
1:D:712:GLN:HG2	1:D:712:GLN:O	2.20	0.41
1:B:284:ASP:O	1:B:285:GLU:C	2.59	0.41
1:D:665:TYR:HD1	1:D:665:TYR:HA	1.62	0.41
1:C:680:TYR:CG	1:C:680:TYR:O	2.70	0.41
1:C:643:CYS:HA	1:C:646:LEU:CD1	2.51	0.41
1:D:668:GLY:CA	1:D:672:THR:HB	2.50	0.41
1:A:630:PHE:C	1:A:630:PHE:CD2	2.92	0.41
1:B:759:ARG:CA	1:B:759:ARG:NE	2.77	0.41
1:B:704:ASP:OD1	1:B:765:ARG:CD	2.68	0.41
1:C:634:ASP:OD1	1:C:634:ASP:C	2.59	0.41
1:E:302:LYS:HB2	1:E:303:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:644:SER:HB3	1:F:687:GLU:HB3	2.03	0.41
1:C:242:LYS:HB3	1:C:242:LYS:HE3	1.88	0.41
1:C:294:LYS:O	1:C:296:ASP:N	2.54	0.41
1:B:306:SER:HB2	1:B:307:ARG:NH2	2.36	0.41
1:C:661:GLY:N	1:D:663:VAL:O	2.52	0.41
1:D:660:ALA:N	1:D:665:TYR:OH	2.54	0.41
1:E:249:ALA:O	1:E:250:ALA:C	2.59	0.41
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.86	0.41
1:E:649:LYS:HA	1:E:649:LYS:HD3	1.81	0.41
1:F:172:ILE:HD12	1:F:172:ILE:N	2.36	0.41
1:D:242:LYS:HE3	1:D:242:LYS:HB3	1.94	0.40
1:F:568:LYS:O	1:F:572:MET:N	2.54	0.40
1:B:306:SER:CB	1:B:307:ARG:NH2	2.85	0.40
1:E:255:ALA:O	1:E:256:LYS:C	2.58	0.40
1:B:302:LYS:HB2	1:B:303:PRO:CD	2.52	0.40
1:B:333:ARG:HD3	1:C:215:GLY:HA2	2.03	0.40
1:E:799:ASP:OD2	1:E:850:LYS:NZ	2.42	0.40
1:A:636:ASP:OD2	1:A:678:LYS:NZ	2.48	0.40
1:B:583:GLN:HA	1:B:583:GLN:OE1	2.22	0.40
3:F:1001:AGS:O2G	3:F:1001:AGS:O1B	2.39	0.40
1:F:352:LEU:O	1:F:356:GLN:N	2.55	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	573/908 (63%)	533 (93%)	28 (5%)	12 (2%)	8	48
1	B	573/908 (63%)	552 (96%)	18 (3%)	3 (0%)	32	73
1	C	573/908 (63%)	548 (96%)	22 (4%)	3 (0%)	32	73
1	D	573/908 (63%)	547 (96%)	20 (4%)	6 (1%)	18	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	573/908 (63%)	544 (95%)	22 (4%)	7 (1%)	15	58
1	F	556/908 (61%)	535 (96%)	19 (3%)	2 (0%)	38	77
All	All	3421/5448 (63%)	3259 (95%)	129 (4%)	33 (1%)	23	61

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
1	A	669	GLY
1	B	302	LYS
1	E	186	VAL
1	E	274	GLU
1	E	669	GLY
1	F	187	ILE
1	F	819	TYR
1	A	256	LYS
1	A	277	THR
1	A	660	ALA
1	A	666	ASP
1	B	295	ASP
1	C	669	GLY
1	D	277	THR
1	D	669	GLY
1	E	257	TYR
1	E	277	THR
1	A	295	ASP
1	A	298	ALA
1	C	258	LYS
1	C	277	THR
1	D	275	SER
1	E	295	ASP
1	A	257	TYR
1	A	275	SER
1	D	880	LEU
1	A	880	LEU
1	D	257	TYR
1	D	301	LEU
1	A	663	VAL
1	B	556	ILE
1	E	705	ASP

### 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	497/783 (64%)	493 (99%)	4 (1%)	85	93
1	B	497/783 (64%)	492 (99%)	5 (1%)	80	90
1	C	497/783 (64%)	490 (99%)	7 (1%)	71	87
1	D	497/783 (64%)	490 (99%)	7 (1%)	71	87
1	E	497/783 (64%)	491 (99%)	6 (1%)	75	89
1	F	488/783 (62%)	485 (99%)	3 (1%)	89	95
All	All	2973/4698 (63%)	2941 (99%)	32 (1%)	79	89

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	LYS
1	A	333	ARG
1	A	662	TYR
1	A	665	TYR
1	B	307	ARG
1	B	333	ARG
1	B	334	ARG
1	B	665	TYR
1	B	765	ARG
1	C	256	LYS
1	C	333	ARG
1	C	334	ARG
1	C	643	CYS
1	C	665	TYR
1	C	680	TYR
1	C	765	ARG
1	D	257	TYR
1	D	258	LYS
1	D	333	ARG
1	D	334	ARG
1	D	665	TYR
1	D	680	TYR

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Mol	Chain	Res	Type
1	D	765	ARG
1	E	333	ARG
1	E	334	ARG
1	E	643	CYS
1	E	663	VAL
1	E	665	TYR
1	E	826	ARG
1	F	302	LYS
1	F	334	ARG
1	F	638	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	GLN
1	A	712	GLN
1	C	712	GLN
1	D	712	GLN
1	D	720	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AGS	A	1001	-	26,33,33	2.04	4 (15%)	22,52,52	2.30	8 (36%)
3	AGS	A	1002	-	26,33,33	2.20	5 (19%)	22,52,52	1.93	5 (22%)
3	AGS	B	1001	-	26,33,33	2.06	4 (15%)	22,52,52	2.11	6 (27%)
3	AGS	B	1002	-	26,33,33	2.00	5 (19%)	22,52,52	2.47	5 (22%)
3	AGS	C	1001	1	26,33,33	1.91	6 (23%)	22,52,52	2.13	6 (27%)
3	AGS	C	1002	-	26,33,33	1.93	5 (19%)	22,52,52	2.46	4 (18%)
3	AGS	D	1001	1	26,33,33	1.99	4 (15%)	22,52,52	2.18	5 (22%)
3	AGS	D	1002	1	26,33,33	2.02	3 (11%)	22,52,52	2.49	5 (22%)
3	AGS	E	1001	-	26,33,33	1.98	6 (23%)	22,52,52	2.44	5 (22%)
3	AGS	E	1002	-	26,33,33	1.97	5 (19%)	22,52,52	2.28	6 (27%)
3	AGS	F	1001	-	26,33,33	2.00	5 (19%)	22,52,52	2.15	4 (18%)
3	AGS	F	1002	-	26,33,33	2.11	6 (23%)	22,52,52	2.24	8 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	A	1001	-	-	0/17/38/38	0/3/3/3
3	AGS	A	1002	-	-	0/17/38/38	0/3/3/3
3	AGS	B	1001	-	-	0/17/38/38	0/3/3/3
3	AGS	B	1002	-	-	0/17/38/38	0/3/3/3
3	AGS	C	1001	1	-	0/17/38/38	0/3/3/3
3	AGS	C	1002	-	-	0/17/38/38	0/3/3/3
3	AGS	D	1001	1	-	0/17/38/38	0/3/3/3
3	AGS	D	1002	1	-	0/17/38/38	0/3/3/3
3	AGS	E	1001	-	-	0/17/38/38	0/3/3/3
3	AGS	E	1002	-	-	0/17/38/38	0/3/3/3
3	AGS	F	1001	-	-	0/17/38/38	0/3/3/3
3	AGS	F	1002	-	-	0/17/38/38	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1001	AGS	C2'-C1'	-3.59	1.47	1.53
3	E	1002	AGS	C2'-C1'	-3.58	1.48	1.53
3	C	1002	AGS	C2'-C1'	-2.90	1.49	1.53
3	B	1001	AGS	C2'-C1'	-2.78	1.49	1.53
3	C	1002	AGS	C5-N7	-2.59	1.30	1.39
3	E	1001	AGS	PG-O3G	-2.56	1.46	1.55
3	D	1001	AGS	C2'-C1'	-2.46	1.49	1.53
3	E	1001	AGS	C5-N7	-2.45	1.31	1.39
3	B	1002	AGS	C2'-C1'	-2.44	1.49	1.53
3	E	1002	AGS	C5-N7	-2.44	1.31	1.39
3	C	1001	AGS	C2'-C1'	-2.43	1.49	1.53
3	F	1002	AGS	C5-N7	-2.36	1.31	1.39
3	C	1001	AGS	PG-O3G	-2.31	1.47	1.55
3	D	1001	AGS	PG-O3G	-2.28	1.47	1.55
3	B	1002	AGS	C5-N7	-2.23	1.31	1.39
3	C	1001	AGS	C5-N7	-2.20	1.31	1.39
3	D	1002	AGS	PG-O3G	-2.19	1.47	1.55
3	C	1001	AGS	C4-N3	-2.17	1.32	1.35
3	E	1002	AGS	PG-O3G	-2.17	1.47	1.55
3	A	1001	AGS	C2'-C1'	-2.16	1.50	1.53
3	A	1002	AGS	C5-N7	-2.15	1.32	1.39
3	C	1002	AGS	PG-O3G	-2.14	1.47	1.55
3	B	1002	AGS	PG-O3G	-2.12	1.47	1.55
3	F	1002	AGS	PG-O3G	-2.10	1.47	1.55
3	B	1001	AGS	C5-N7	-2.00	1.32	1.39
3	F	1001	AGS	PG-O2G	2.04	1.62	1.55
3	E	1001	AGS	O4'-C1'	2.05	1.44	1.41
3	F	1001	AGS	C2-N3	2.06	1.35	1.32
3	F	1002	AGS	PG-O2G	2.09	1.62	1.55
3	A	1001	AGS	PG-O2G	2.10	1.62	1.55
3	A	1002	AGS	PG-O2G	2.11	1.62	1.55
3	F	1002	AGS	O4'-C1'	2.17	1.44	1.41
3	F	1001	AGS	O4'-C1'	2.26	1.44	1.41
3	E	1002	AGS	C5-C4	2.56	1.46	1.40
3	C	1001	AGS	C5-C4	2.60	1.46	1.40
3	D	1001	AGS	C5-C4	2.75	1.46	1.40
3	E	1001	AGS	C5-C4	2.76	1.46	1.40
3	C	1002	AGS	C5-C4	2.78	1.46	1.40
3	D	1002	AGS	C5-C4	2.83	1.46	1.40
3	A	1002	AGS	O4'-C1'	2.88	1.45	1.41
3	B	1002	AGS	C5-C4	2.89	1.47	1.40
3	B	1001	AGS	C5-C4	2.95	1.47	1.40
3	F	1001	AGS	C5-C4	2.98	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	AGS	C5-C4	3.00	1.47	1.40
3	A	1001	AGS	C5-C4	3.20	1.47	1.40
3	F	1002	AGS	C5-C4	3.39	1.48	1.40
3	E	1001	AGS	PG-S1G	7.04	2.04	1.90
3	C	1002	AGS	PG-S1G	7.33	2.04	1.90
3	C	1001	AGS	PG-S1G	7.36	2.04	1.90
3	E	1002	AGS	PG-S1G	7.39	2.04	1.90
3	B	1002	AGS	PG-S1G	7.96	2.05	1.90
3	D	1001	AGS	PG-S1G	7.97	2.05	1.90
3	A	1001	AGS	PG-S1G	8.11	2.06	1.90
3	F	1001	AGS	PG-S1G	8.24	2.06	1.90
3	D	1002	AGS	PG-S1G	8.36	2.06	1.90
3	B	1001	AGS	PG-S1G	8.41	2.06	1.90
3	F	1002	AGS	PG-S1G	8.43	2.06	1.90
3	A	1002	AGS	PG-S1G	9.16	2.08	1.90

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1001	AGS	PB-O3B-PG	-8.20	105.85	132.35
3	D	1002	AGS	PB-O3B-PG	-8.00	106.48	132.35
3	B	1002	AGS	PB-O3B-PG	-7.81	107.09	132.35
3	C	1002	AGS	PB-O3B-PG	-7.75	107.31	132.35
3	A	1001	AGS	PB-O3B-PG	-7.27	108.87	132.35
3	D	1001	AGS	PB-O3B-PG	-6.89	110.06	132.35
3	E	1002	AGS	PB-O3B-PG	-6.66	110.82	132.35
3	C	1001	AGS	PB-O3B-PG	-6.39	111.71	132.35
3	F	1001	AGS	PB-O3B-PG	-6.10	112.63	132.35
3	B	1001	AGS	PB-O3B-PG	-5.80	113.59	132.35
3	F	1002	AGS	PB-O3B-PG	-5.77	113.69	132.35
3	F	1001	AGS	N3-C2-N1	-5.16	124.36	128.86
3	D	1002	AGS	N3-C2-N1	-5.14	124.38	128.86
3	B	1002	AGS	N3-C2-N1	-4.86	124.62	128.86
3	E	1002	AGS	N3-C2-N1	-4.74	124.73	128.86
3	A	1002	AGS	PB-O3B-PG	-4.62	117.41	132.35
3	C	1002	AGS	N3-C2-N1	-4.56	124.88	128.86
3	A	1002	AGS	N3-C2-N1	-4.55	124.89	128.86
3	E	1001	AGS	N3-C2-N1	-4.49	124.95	128.86
3	B	1001	AGS	N3-C2-N1	-4.41	125.01	128.86
3	F	1002	AGS	N3-C2-N1	-4.39	125.03	128.86
3	D	1001	AGS	N3-C2-N1	-3.89	125.47	128.86
3	C	1001	AGS	N3-C2-N1	-3.64	125.69	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	AGS	C4-C5-N7	-3.10	106.41	109.41
3	A	1001	AGS	N3-C2-N1	-3.00	126.25	128.86
3	C	1001	AGS	C4-C5-N7	-2.67	106.83	109.41
3	A	1002	AGS	C5'-C4'-C3'	-2.63	105.28	115.29
3	E	1002	AGS	C5'-C4'-C3'	-2.51	105.73	115.29
3	C	1001	AGS	O2'-C2'-C1'	-2.30	104.41	111.61
3	B	1001	AGS	C4-C5-N7	-2.29	107.20	109.41
3	D	1001	AGS	C4-C5-N7	-2.27	107.22	109.41
3	F	1002	AGS	C4-C5-N7	-2.22	107.26	109.41
3	A	1001	AGS	O5'-C5'-C4'	-2.19	101.22	109.00
3	E	1001	AGS	C5'-C4'-C3'	-2.16	107.07	115.29
3	D	1002	AGS	O5'-C5'-C4'	-2.14	101.42	109.00
3	F	1002	AGS	O2'-C2'-C1'	-2.09	105.06	111.61
3	E	1002	AGS	C4-C5-N7	-2.07	107.41	109.41
3	A	1001	AGS	C5'-C4'-C3'	-2.03	107.54	115.29
3	A	1002	AGS	C4-C5-N7	-2.02	107.46	109.41
3	E	1002	AGS	O2B-PB-O1B	2.01	122.66	112.28
3	B	1001	AGS	O2B-PB-O1B	2.02	122.72	112.28
3	F	1002	AGS	O4'-C4'-C5'	2.06	116.36	109.40
3	F	1001	AGS	O2B-PB-O1B	2.11	123.21	112.28
3	E	1001	AGS	O2B-PB-O1B	2.13	123.33	112.28
3	C	1002	AGS	C1'-N9-C4	2.14	130.33	126.64
3	D	1002	AGS	O2B-PB-O1B	2.15	123.41	112.28
3	B	1002	AGS	C2'-C3'-C4'	2.18	106.86	102.62
3	C	1001	AGS	O2A-PA-O1A	2.21	123.73	112.28
3	D	1001	AGS	O2B-PB-O1B	2.24	123.90	112.28
3	B	1001	AGS	C2'-C3'-C4'	2.25	107.00	102.62
3	A	1001	AGS	C2'-C3'-C4'	2.33	107.16	102.62
3	F	1002	AGS	O2B-PB-O1B	2.33	124.36	112.28
3	B	1002	AGS	O2B-PB-O1B	2.34	124.39	112.28
3	A	1001	AGS	O2B-PB-O1B	2.36	124.52	112.28
3	B	1001	AGS	N6-C6-N1	2.59	123.90	118.77
3	C	1001	AGS	N6-C6-N1	2.68	124.08	118.77
3	A	1001	AGS	N6-C6-N1	2.78	124.28	118.77
3	D	1002	AGS	N6-C6-N1	2.80	124.31	118.77
3	F	1002	AGS	C1'-N9-C4	3.03	131.88	126.64
3	D	1001	AGS	N6-C6-N1	3.12	124.94	118.77
3	A	1002	AGS	N6-C6-N1	3.16	125.03	118.77
3	F	1001	AGS	N6-C6-N1	3.17	125.05	118.77
3	F	1002	AGS	N6-C6-N1	3.26	125.23	118.77
3	E	1002	AGS	N6-C6-N1	3.45	125.61	118.77
3	E	1001	AGS	N6-C6-N1	3.52	125.74	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	B	1002	AGS	N6-C6-N1	3.55	125.81	118.77
3	C	1002	AGS	N6-C6-N1	3.99	126.67	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	AGS	3	0
3	A	1002	AGS	1	0
3	B	1001	AGS	12	0
3	B	1002	AGS	1	0
3	C	1001	AGS	7	0
3	C	1002	AGS	1	0
3	D	1001	AGS	3	0
3	D	1002	AGS	3	0
3	E	1001	AGS	5	0
3	E	1002	AGS	3	0
3	F	1001	AGS	3	0
3	F	1002	AGS	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.