



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:57 AM GMT

PDB ID : 3NG9  
Title : Structure to Function Correlations for Adeno-associated Virus Serotype 1  
Authors : Govindasamy, L.; Miller, E.B.; Gurda, B.; McKenna, R.; Zolotukhin, S.; Muzy-  
czka, N.; Agbandje-McKenna, M.  
Deposited on : 2010-06-11  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB 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/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

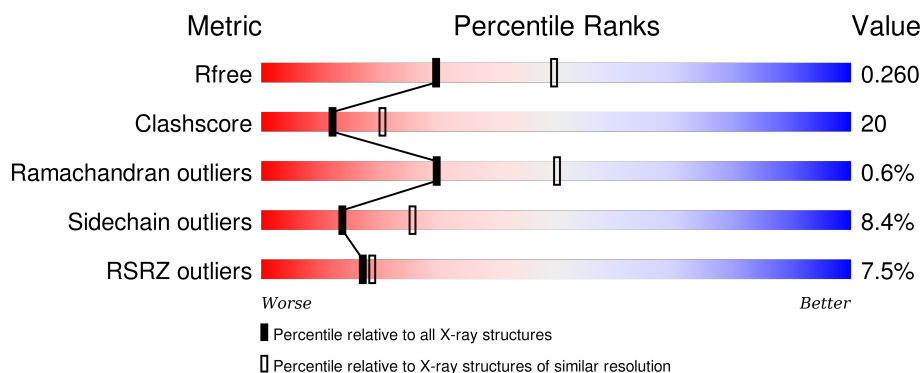
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>20%</div> <div>•</div> <div>29%</div> </div> </div>
1	B	736	<div> <div>4%</div> <div> <div></div> <div>46%</div> <div>21%</div> <div>•</div> <div>29%</div> </div> </div>
1	C	736	<div> <div>5%</div> <div> <div></div> <div>48%</div> <div>20%</div> <div>•</div> <div>29%</div> </div> </div>
1	D	736	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>21%</div> <div>•</div> <div>29%</div> </div> </div>
1	E	736	<div> <div>6%</div> <div> <div></div> <div>47%</div> <div>21%</div> <div>•</div> <div>29%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	736	
1	G	736	
1	H	736	
1	I	736	
1	J	736	

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
2	ADE	A	737	-	-	-	X
2	ADE	B	737	-	-	-	X
2	ADE	C	737	-	-	-	X
2	ADE	D	737	-	-	-	X
2	ADE	E	737	-	-	-	X
2	ADE	F	737	-	-	-	X
2	ADE	G	737	-	-	-	X
2	ADE	H	737	-	-	-	X
2	ADE	I	737	-	-	-	X
2	ADE	J	737	-	-	-	X
3	CYT	A	738	-	-	-	X
3	CYT	B	738	-	-	-	X
3	CYT	B	739	-	-	-	X
3	CYT	C	738	-	-	-	X
3	CYT	D	738	-	-	-	X
3	CYT	E	738	-	-	-	X
3	CYT	F	738	-	-	-	X
3	CYT	H	738	-	-	-	X
3	CYT	I	738	-	-	-	X
3	CYT	J	738	-	-	-	X

## 2 Entry composition

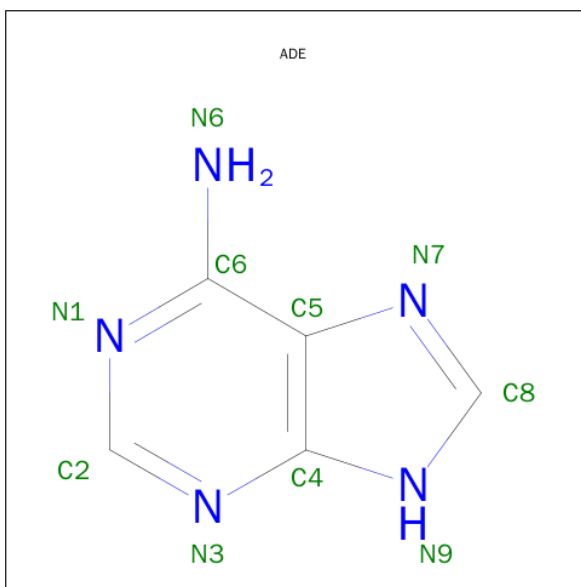
There are 4 unique types of molecules in this entry. The entry contains 42680 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Capsid protein.

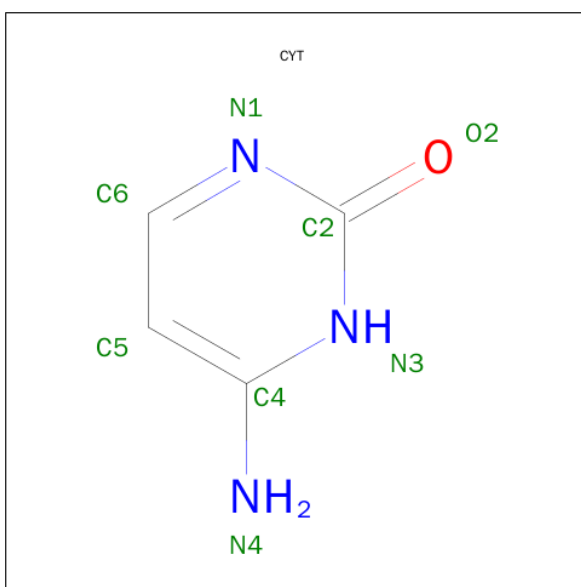
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	B	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	C	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	D	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	E	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	F	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	G	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	H	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	I	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	J	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			

- Molecule 2 is ADENINE (three-letter code: ADE) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	5	5		
2	B	1	Total	C	N	0	0
			10	5	5		
2	C	1	Total	C	N	0	0
			10	5	5		
2	D	1	Total	C	N	0	0
			10	5	5		
2	E	1	Total	C	N	0	0
			10	5	5		
2	F	1	Total	C	N	0	0
			10	5	5		
2	G	1	Total	C	N	0	0
			10	5	5		
2	H	1	Total	C	N	0	0
			10	5	5		
2	I	1	Total	C	N	0	0
			10	5	5		
2	J	1	Total	C	N	0	0
			10	5	5		

- Molecule 3 is 6-AMINOPYRIMIDIN-2(1H)-ONE (three-letter code: CYT) (formula:  $C_4H_5N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	3	1		
3	B	1	Total	C	N	O	0	0
			8	4	3	1		
3	B	1	Total	C	N	O	0	0
			8	4	3	1		
3	C	1	Total	C	N	O	0	0
			8	4	3	1		
3	D	1	Total	C	N	O	0	0
			8	4	3	1		
3	E	1	Total	C	N	O	0	0
			8	4	3	1		
3	F	1	Total	C	N	O	0	0
			8	4	3	1		
3	H	1	Total	C	N	O	0	0
			8	4	3	1		
3	I	1	Total	C	N	O	0	0
			8	4	3	1		
3	J	1	Total	C	N	O	0	0
			8	4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		
4	B	130	Total	O	0	0
			130	130		

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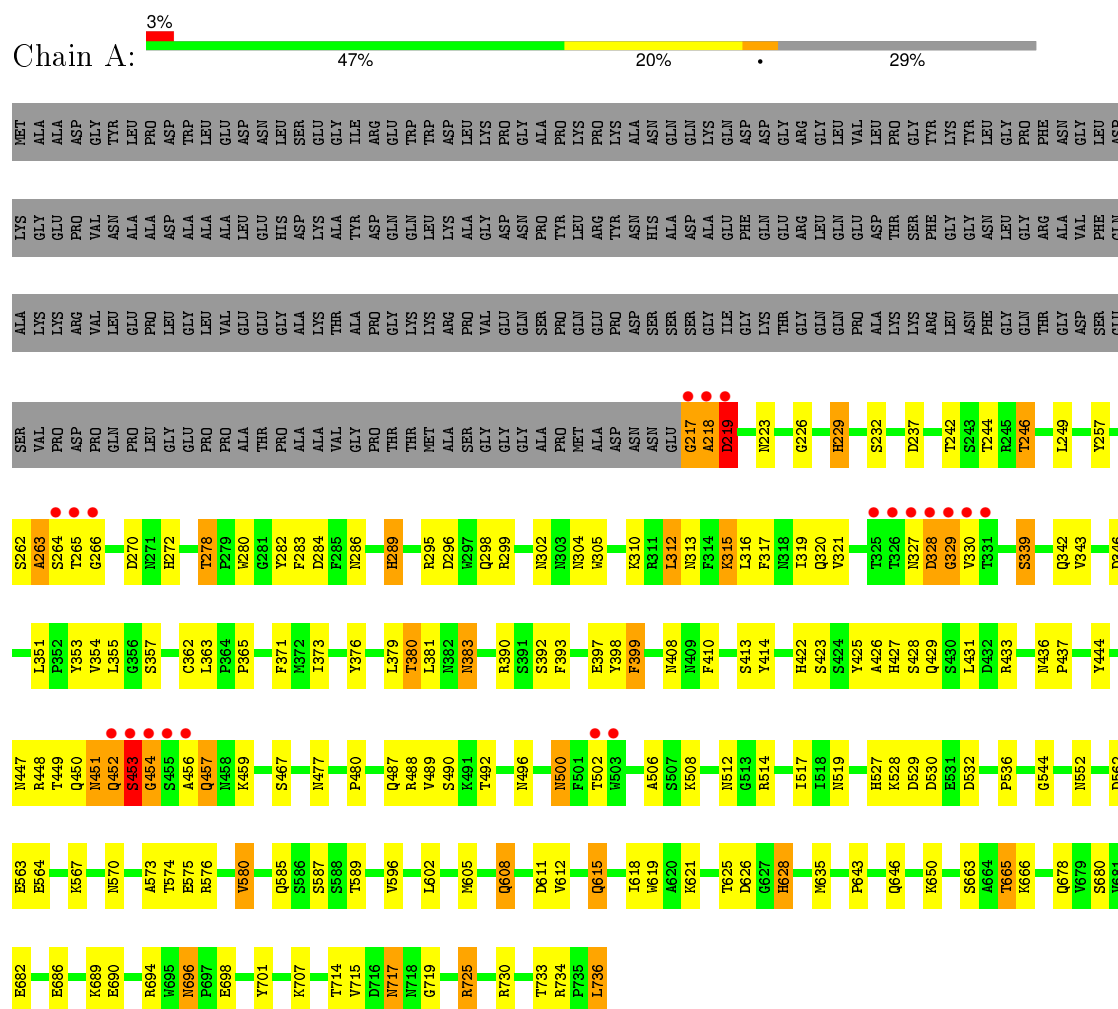
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	128	Total 128	O 128	0	0
4	D	131	Total 131	O 131	0	0
4	E	133	Total 133	O 133	0	0
4	F	131	Total 131	O 131	0	0
4	G	127	Total 127	O 127	0	0
4	H	130	Total 130	O 130	0	0
4	I	130	Total 130	O 130	0	0
4	J	129	Total 129	O 129	0	0

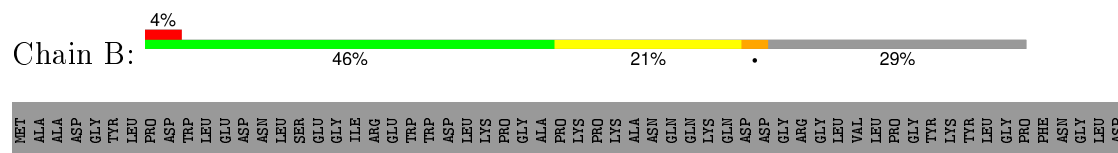
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

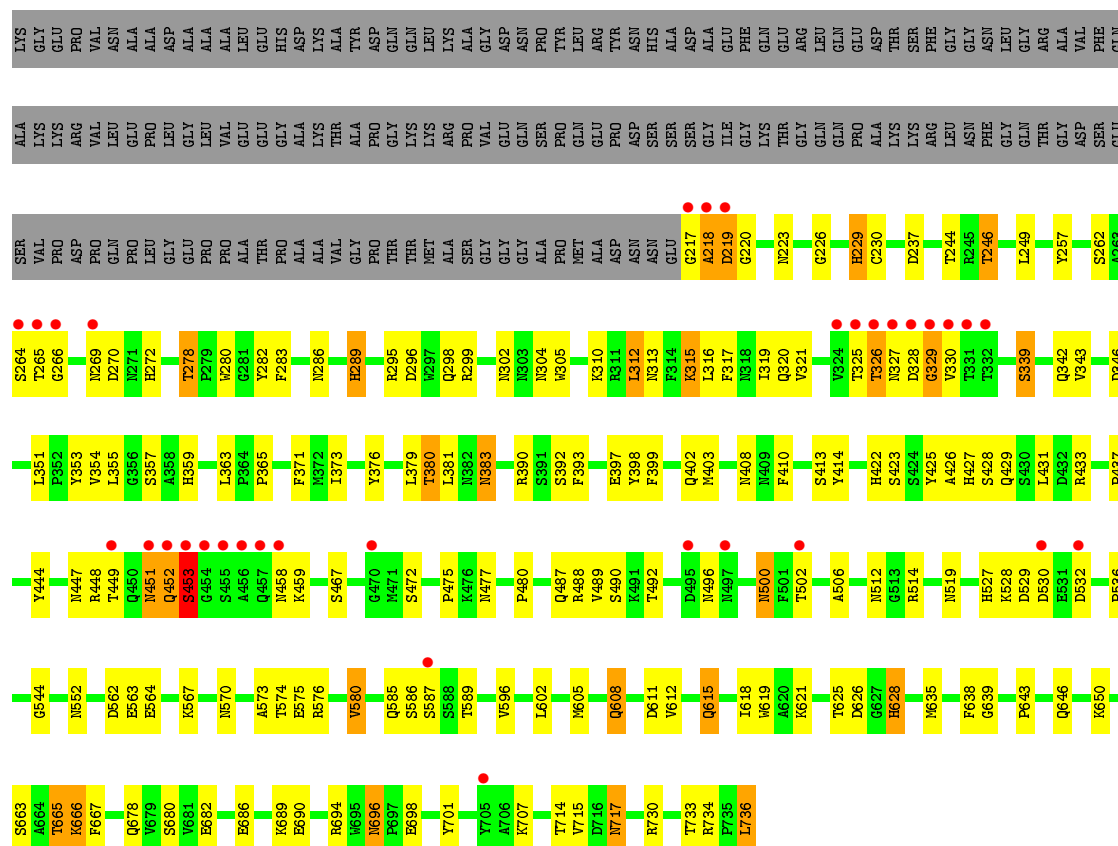
#### • Molecule 1: Capsid protein



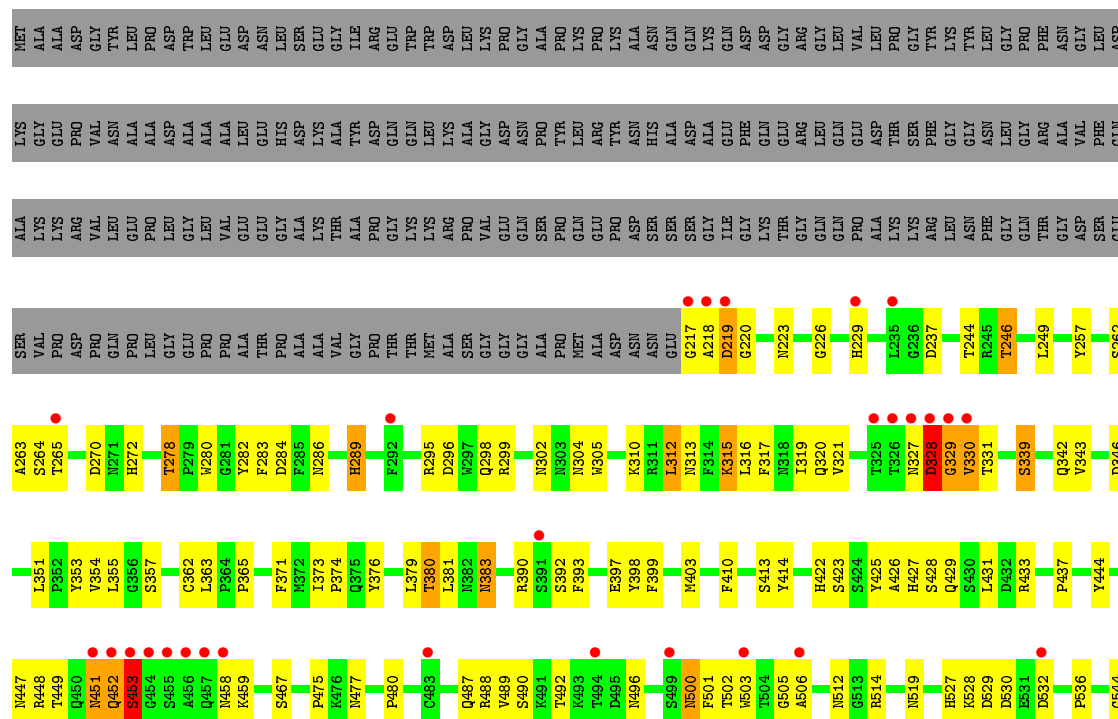
#### • Molecule 1: Capsid protein



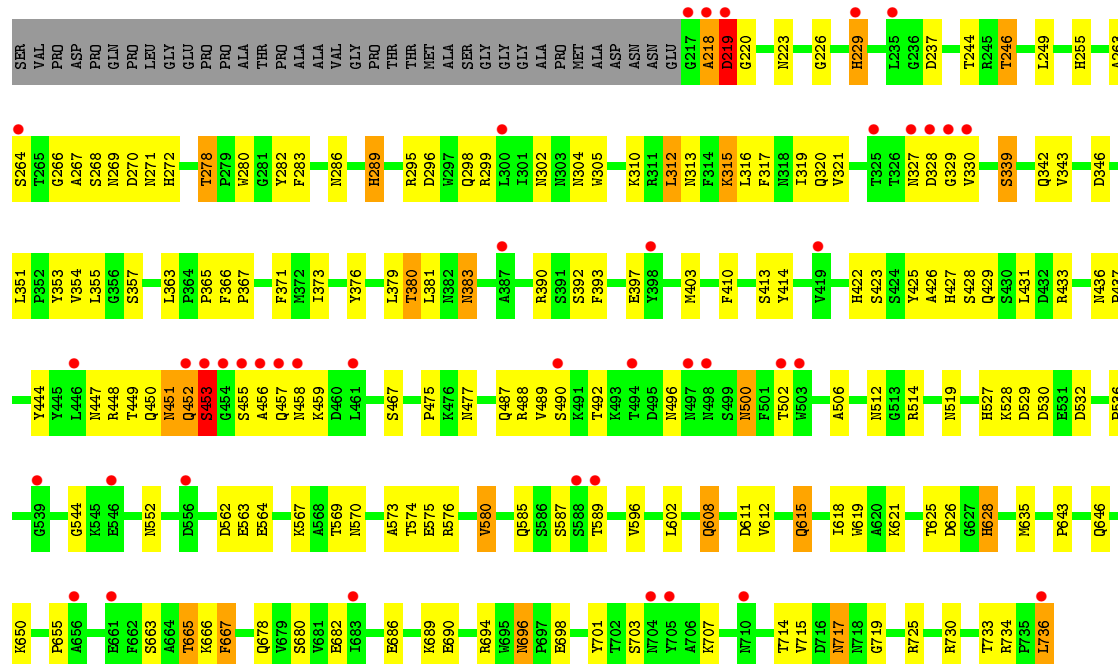




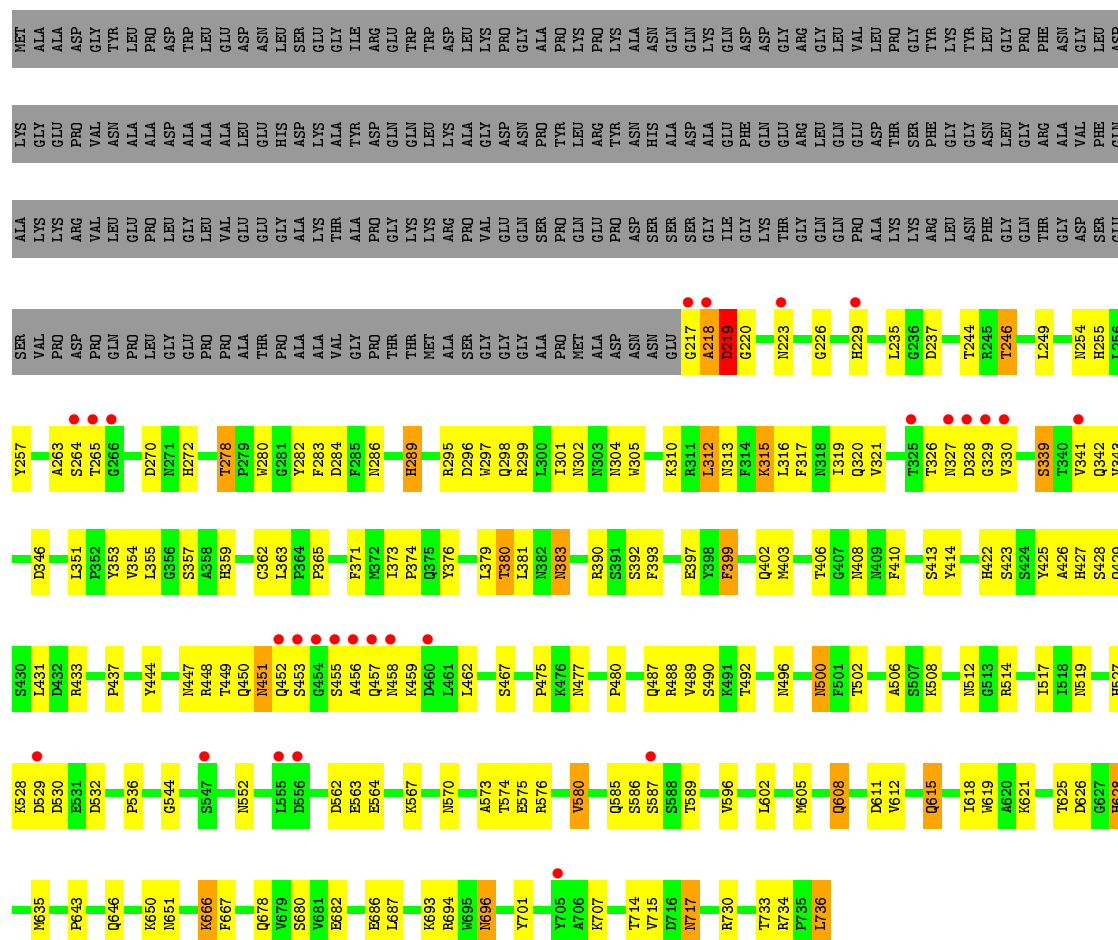
### • Molecule 1: Capsid protein



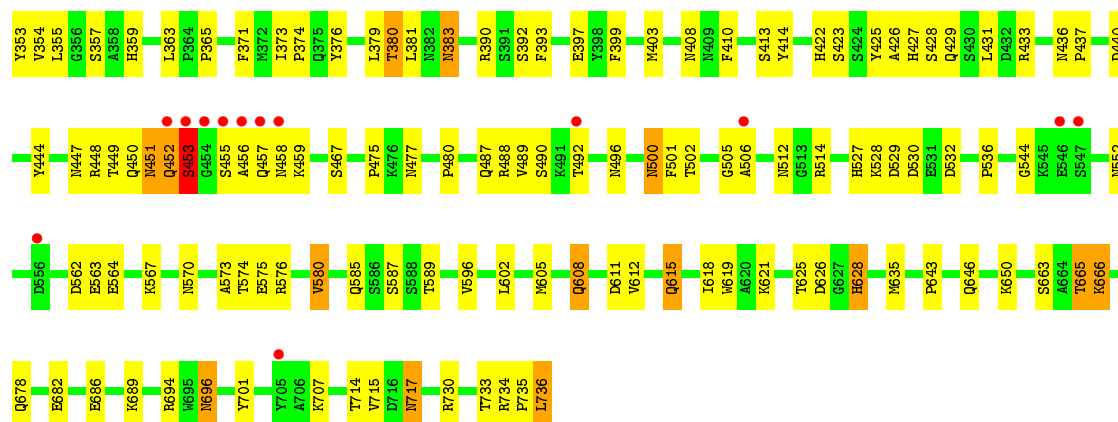




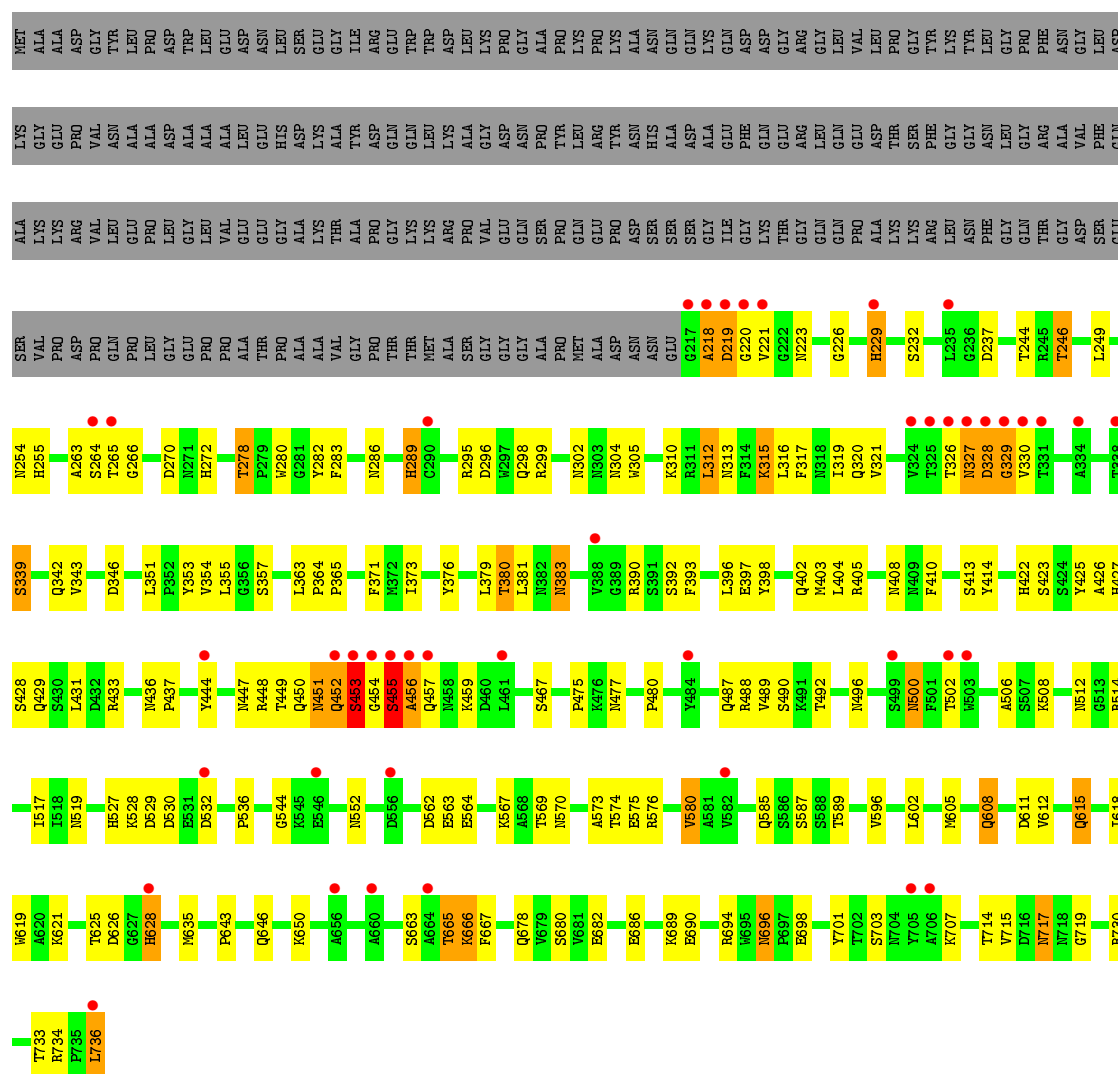
• Molecule 1: Capsid protein



[illegible][illegible]



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



RET	LYS	ALA	LYS	SER	ALA	LYS	T265	V343	A426	H527	P631	R725	W726	R730	T733	R734	P735	L736	LYS
ALA	GLY	ALA	LYS	VAL	ALA	PRO	G266	D346	H427	K528	P643	P726	I727	R730	T733	R734	P735	L736	GLY
ALA	GLU	ALA	LYS	ASP	ARG	PRO	A267	D346	H427	D529	P643	P726	I727	R730	T733	R734	P735	L736	GLU
GLY	VAL	VAL	ARG	ASP	VAL	GLN	S268	L351	Q429	D530	Q646	T733	R734	P735	L736	VAL	ASP	ASP	ASP
TRP	ASN	LEU	LEU	GLN	LEU	PRO	D270	P352	L431	D532	Q646	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	ALA	ALA	LEU	GLY	LEU	GLY	Y273	F352	L431	D532	Q646	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLU	ALA	VAL	VAL	PRO	PRO	PRO	T278	G356	L438	P536	P655	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ASN	GLU	GLU	GLU	THR	THR	THR	P279	S357	L439	E546	A660	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	ALA	VAL	VAL	PRO	PRO	PRO	W280	A358	I439	E546	B661	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	ALA	GLY	GLY	ALA	ALA	ALA	G281	H359	T449	D556	B662	T733	R734	P735	L736	LEU	ASP	ASP	ASP
HIS	GLY	GLY	GLY	PRO	PRO	PRO	Y282	Q450	T449	D556	S663	T733	R734	P735	L736	LEU	ASP	ASP	ASP
SER	ASP	ALA	ALA	ALA	ALA	ALA	F283	P364	M451	D562	A664	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	ALA	THR	THR	VAL	VAL	VAL	N286	P365	Q452	E564	T665	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ILE	TYR	ALA	GLY	GLY	GLY	GLY	H289	F366	S453	E564	K666	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	ALA	ALA	ALA	VAL	VAL	VAL	C290	G454	G454	K567	F667	T733	R734	P735	L736	LEU	ASP	ASP	ASP
PRO	GLY	GLY	GLY	PRO	PRO	PRO	R295	F371	S455	K567	S669	T733	R734	P735	L736	LEU	ASP	ASP	ASP
TRP	GLN	GLN	GLY	THR	THR	THR	D296	I373	A456	M570	P670	T733	R734	P735	L736	LEU	ASP	ASP	ASP
TRP	LEU	LYS	LYS	MET	MET	MET	G297	K376	Q457	P571	Q678	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ASP	LYS	ARG	ARG	ALA	ALA	ALA	V297	Y376	M458	V572	Q678	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	ALA	PRO	PRO	SER	SER	SER	R299	T380	D460	A673	P679	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	GLY	VAL	VAL	GLY	GLY	GLY	R302	T380	L461	T574	S680	T733	R734	P735	L736	LEU	ASP	ASP	ASP
PRO	ASN	GLY	GLY	GLY	GLY	GLY	N302	N382	F463	E575	V681	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ALA	PRO	SER	SER	ALA	ALA	ALA	N303	N383	P463	R576	E682	T733	R734	P735	L736	LEU	ASP	ASP	ASP
PRO	TYR	PRO	PRO	PRO	PRO	PRO	N304	Q384	S467	V580	B686	T733	R734	P735	L736	LEU	ASP	ASP	ASP
PRO	ARG	GLY	GLY	MET	GLN	GLY	W305	S385	P480	B689	K689	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LYS	TYR	PRO	PRO	ASP	PRO	ASP	K310	A387	Q487	S586	K693	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ALA	ASN	ASN	ASN	ASN	ASN	ASN	R311	R390	Q487	S586	K693	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ASN	HIS	SER	SER	GLY	SER	GLY	L312	S391	R488	Q585	B696	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLN	ALA	SER	SER	GLY	SER	GLY	N313	S392	V489	S587	K693	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLN	ASP	ASP	ASP	GLY	ASP	GLY	F314	S490	S490	S588	B696	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LYS	ALA	ALA	GLY	A218	ALA	ILE	K315	C395	K491	P697	B698	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLN	GLY	ILE	ILE	D219	GLY	GLY	L316	G395	T492	V596	E698	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ASP	PHE	GLY	GLY	N223	PHE	GLY	F317	L396	K493	V596	E698	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	GLN	GLY	LYS	N223	GLY	LYS	N318	E397	T494	A601	Y701	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	GLY	THR	THR	N223	GLY	THR	I319	R397	T494	A601	Y701	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ARG	LEU	ARG	GLY	G226	ARG	ARG	Q320	Y398	D495	L602	T702	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	GLN	GLY	GLY	G226	LEU	LEU	V321	Y398	M496	M605	T703	T733	R734	P735	L736	LEU	ASP	ASP	ASP
VAL	GLY	PRO	PRO	H229	VAL	VAL	K322	L404	M498	Q608	Y705	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	ASP	ALA	ALA	D237	ASP	ASP	E323	G407	S499	Q608	Y706	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LYS	THR	PRO	PRO	D237	THR	PRO	V324	M408	N500	D611	K707	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	LYS	LYS	LYS	S243	LYS	LYS	T325	M408	F501	V612	S708	T733	R734	P735	L736	LEU	ASP	ASP	ASP
TYR	PHE	ARG	ARG	T244	PHE	TYR	T326	M409	T502	V612	A709	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LYS	GLY	LEU	LEU	R245	GLY	LYS	D328	F410	M503	V613	M710	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	ASN	ASN	ASN	T246	ASN	TYR	G329	S413	G505	Q615	F713	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	ASN	PHE	PHE	T246	ASN	TYR	V330	Y414	A506	Q615	F713	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	GLY	GLY	GLY	L249	GLY	LEU	T331	Y414	S507	Q615	F713	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	GLN	GLY	GLY	T332	GLY	LEU	T332	E418	K508	Q615	F713	T733	R734	P735	L736	LEU	ASP	ASP	ASP
PRO	THR	THR	THR	N253	THR	PRO	T338	H422	R514	V618	M717	T733	R734	P735	L736	LEU	ASP	ASP	ASP
ASN	GLY	GLY	GLY	N254	GLY	PRO	S339	S423	R514	V618	M717	T733	R734	P735	L736	LEU	ASP	ASP	ASP
GLY	VAL	ALA	ALA	N254	VAL	ASN	T339	S424	R514	V618	M717	T733	R734	P735	L736	LEU	ASP	ASP	ASP
LEU	PHE	SER	SER	A263	PHE	LEU	G340	S424	T517	H628	L720	T733	R734	P735	L736	LEU	ASP	ASP	ASP

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	262.70 Å   262.70 Å   612.30 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-2.50) 89.0 (49.88-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.230 , 0.250 0.252 , 0.260	Depositor DCC
$R_{free}$ test set	12411 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.5	EDS
Estimated twinning fraction	0.004 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.009 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.017 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 247782 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	42680	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADE, CYT

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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.79	1/4246 (0.0%)	0.78	0/5790
1	B	0.79	1/4246 (0.0%)	0.79	0/5790
1	C	0.79	1/4246 (0.0%)	0.78	0/5790
1	D	0.79	1/4246 (0.0%)	0.78	0/5790
1	E	0.79	1/4246 (0.0%)	0.79	0/5790
1	F	0.78	1/4246 (0.0%)	0.77	0/5790
1	G	0.78	1/4246 (0.0%)	0.78	0/5790
1	H	0.79	1/4246 (0.0%)	0.79	0/5790
1	I	0.78	1/4246 (0.0%)	0.77	0/5790
1	J	0.78	1/4246 (0.0%)	0.78	0/5790
All	All	0.79	10/42460 (0.0%)	0.78	0/57900

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	8
1	D	0	7
1	E	0	5
1	F	0	8
1	G	0	6
1	H	0	6
1	I	0	10
1	J	0	6
All	All	0	72

All (10) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	580	VAL	CB-CG2	-5.46	1.41	1.52
1	C	580	VAL	CB-CG2	-5.46	1.41	1.52
1	J	580	VAL	CB-CG2	-5.46	1.41	1.52
1	D	580	VAL	CB-CG2	-5.45	1.41	1.52
1	H	580	VAL	CB-CG2	-5.45	1.41	1.52
1	A	580	VAL	CB-CG2	-5.44	1.41	1.52
1	G	580	VAL	CB-CG2	-5.44	1.41	1.52
1	I	580	VAL	CB-CG2	-5.44	1.41	1.52
1	E	580	VAL	CB-CG2	-5.43	1.41	1.52
1	B	580	VAL	CB-CG2	-5.43	1.41	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	GLY	Peptide
1	A	219	ASP	Peptide
1	A	263	ALA	Peptide
1	A	328	ASP	Peptide
1	A	329	GLY	Peptide
1	A	451	ASN	Peptide
1	A	453	SER	Peptide
1	A	454	GLY	Peptide
1	B	218	ALA	Peptide
1	B	219	ASP	Peptide
1	B	220	GLY	Peptide
1	B	326	THR	Peptide
1	B	329	GLY	Peptide
1	B	330	VAL	Peptide
1	B	451	ASN	Peptide
1	B	453	SER	Peptide
1	C	217	GLY	Peptide
1	C	219	ASP	Peptide
1	C	220	GLY	Peptide
1	C	328	ASP	Peptide
1	C	329	GLY	Peptide
1	C	398	TYR	Peptide
1	C	451	ASN	Peptide
1	C	453	SER	Peptide
1	D	219	ASP	Peptide
1	D	220	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	D	263	ALA	Peptide
1	D	327	ASN	Peptide
1	D	328	ASP	Peptide
1	D	451	ASN	Peptide
1	D	453	SER	Peptide
1	E	218	ALA	Peptide
1	E	219	ASP	Peptide
1	E	220	GLY	Peptide
1	E	451	ASN	Peptide
1	E	453	SER	Peptide
1	F	219	ASP	Peptide
1	F	220	GLY	Peptide
1	F	326	THR	Peptide
1	F	327	ASN	Peptide
1	F	328	ASP	Peptide
1	F	329	GLY	Peptide
1	F	451	ASN	Peptide
1	F	453	SER	Peptide
1	G	218	ALA	Peptide
1	G	220	GLY	Peptide
1	G	328	ASP	Peptide
1	G	329	GLY	Peptide
1	G	451	ASN	Peptide
1	G	453	SER	Peptide
1	H	219	ASP	Peptide
1	H	220	GLY	Peptide
1	H	328	ASP	Peptide
1	H	329	GLY	Peptide
1	H	451	ASN	Peptide
1	H	453	SER	Peptide
1	I	218	ALA	Peptide
1	I	220	GLY	Peptide
1	I	326	THR	Peptide
1	I	327	ASN	Peptide
1	I	328	ASP	Peptide
1	I	329	GLY	Peptide
1	I	451	ASN	Peptide
1	I	453	SER	Peptide
1	I	455	SER	Peptide
1	I	456	ALA	Peptide
1	J	217	GLY	Peptide
1	J	218	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	J	328	ASP	Peptide
1	J	398	TYR	Peptide
1	J	451	ASN	Peptide
1	J	453	SER	Peptide

## 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	4120	0	3884	206	0
1	B	4120	0	3884	194	0
1	C	4120	0	3884	175	0
1	D	4120	0	3884	192	0
1	E	4120	0	3884	186	0
1	F	4120	0	3884	193	0
1	G	4120	0	3884	194	0
1	H	4120	0	3884	187	0
1	I	4120	0	3884	209	0
1	J	4120	0	3884	127	0
2	A	10	0	4	0	0
2	B	10	0	4	3	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
2	G	10	0	4	0	0
2	H	10	0	4	0	0
2	I	10	0	4	0	0
2	J	10	0	4	0	0
3	A	8	0	4	3	0
3	B	16	0	8	1	0
3	C	8	0	4	3	0
3	D	8	0	4	3	0
3	E	8	0	4	1	0
3	F	8	0	4	2	0
3	H	8	0	4	3	0
3	I	8	0	4	2	0
3	J	8	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	131	0	0	6	0
4	B	130	0	0	7	0
4	C	128	0	0	4	0
4	D	131	0	0	9	0
4	E	133	0	0	9	0
4	F	131	0	0	4	0
4	G	127	0	0	7	0
4	H	130	0	0	5	0
4	I	130	0	0	6	0
4	J	129	0	0	5	0
All	All	42680	0	38920	1595	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 20.

All (1595) 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:G:328:ASP:HB3	1:G:329:GLY:C	1.41	1.40
1:C:328:ASP:HB3	1:C:329:GLY:C	1.41	1.39
1:H:328:ASP:HB3	1:H:329:GLY:C	1.41	1.37
1:D:328:ASP:CB	1:D:329:GLY:HA3	1.42	1.29
1:B:328:ASP:OD1	1:B:329:GLY:HA2	1.28	1.28
1:B:451:ASN:HA	1:B:452:GLN:HB2	1.17	1.16
1:E:451:ASN:HA	1:E:452:GLN:HB2	1.17	1.15
1:A:451:ASN:HB2	1:A:452:GLN:HB3	1.29	1.15
1:H:451:ASN:HA	1:H:452:GLN:HB2	1.17	1.15
1:D:328:ASP:HB3	1:D:329:GLY:HA3	1.21	1.14
1:I:397:GLU:OE1	1:I:650:LYS:HE2	1.42	1.14
1:D:328:ASP:HB2	1:D:329:GLY:HA3	1.14	1.12
1:J:451:ASN:HA	1:J:452:GLN:HB2	1.17	1.12
1:D:328:ASP:CB	1:D:329:GLY:CA	2.29	1.10
1:D:451:ASN:HA	1:D:452:GLN:HB2	1.17	1.10
1:G:451:ASN:HA	1:G:452:GLN:HB2	1.17	1.10
1:F:451:ASN:CB	1:F:452:GLN:HB3	1.83	1.08
1:C:451:ASN:HA	1:C:452:GLN:HB2	1.18	1.08
1:A:502:THR:O	1:A:506:ALA:HB2	1.55	1.06
1:A:330:VAL:HG11	1:B:327:ASN:OD1	1.55	1.06
1:J:380:THR:HG21	1:J:392:SER:H	1.06	1.06
1:F:502:THR:O	1:F:506:ALA:HB2	1.55	1.06
1:C:502:THR:O	1:C:506:ALA:HB2	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:THR:HG23	4:C:843:HOH:O	1.54	1.05
1:F:451:ASN:HA	1:F:452:GLN:CB	1.85	1.05
1:G:380:THR:HG21	1:G:392:SER:H	1.21	1.05
1:I:502:THR:O	1:I:506:ALA:HB2	1.55	1.05
1:B:380:THR:HG21	1:B:392:SER:H	1.21	1.05
1:B:502:THR:O	1:B:506:ALA:HB2	1.55	1.05
1:J:502:THR:O	1:J:506:ALA:HB2	1.56	1.04
1:B:663:SER:OG	1:B:665:THR:HG23	1.58	1.04
1:G:502:THR:O	1:G:506:ALA:HB2	1.55	1.04
1:H:502:THR:O	1:H:506:ALA:HB2	1.55	1.04
1:I:380:THR:HG21	1:I:392:SER:H	1.21	1.04
1:B:328:ASP:OD1	1:B:329:GLY:CA	2.05	1.03
1:D:502:THR:O	1:D:506:ALA:HB2	1.55	1.03
1:G:328:ASP:HB3	1:G:329:GLY:CA	1.88	1.03
1:E:380:THR:HG21	1:E:392:SER:H	1.21	1.02
1:E:502:THR:O	1:E:506:ALA:HB2	1.56	1.02
1:A:380:THR:HG21	1:A:392:SER:H	1.21	1.02
1:C:328:ASP:HB3	1:C:329:GLY:CA	1.88	1.02
1:B:326:THR:HG22	1:B:327:ASN:O	1.58	1.02
1:F:380:THR:HG21	1:F:392:SER:H	1.21	1.01
1:C:380:THR:HG21	1:C:392:SER:H	1.21	1.01
1:D:380:THR:HG21	1:D:392:SER:H	1.21	1.01
1:I:451:ASN:HB2	1:I:452:GLN:HB3	1.38	1.00
1:D:393:PHE:H	1:H:696:ASN:HD21	1.09	1.00
1:H:380:THR:HG21	1:H:392:SER:H	1.21	1.00
1:C:393:PHE:H	1:F:696:ASN:HD21	1.10	0.99
1:H:328:ASP:HB3	1:H:329:GLY:CA	1.88	0.98
1:H:328:ASP:CB	1:H:329:GLY:C	2.32	0.98
1:C:696:ASN:HD21	1:I:393:PHE:H	1.12	0.98
1:G:328:ASP:CB	1:G:329:GLY:C	2.31	0.97
1:C:328:ASP:CB	1:C:329:GLY:C	2.32	0.97
1:A:451:ASN:CB	1:A:452:GLN:HB3	1.94	0.96
1:H:451:ASN:CA	1:H:452:GLN:HB2	1.96	0.96
1:B:269:ASN:HA	1:B:272:HIS:HD2	1.31	0.96
1:D:451:ASN:CA	1:D:452:GLN:HB2	1.96	0.96
1:E:278:THR:HG22	1:E:280:TRP:H	1.31	0.96
1:D:328:ASP:HB2	1:D:329:GLY:CA	1.95	0.95
1:F:451:ASN:HA	1:F:452:GLN:HB2	1.44	0.95
1:I:278:THR:HG22	1:I:280:TRP:H	1.31	0.95
1:A:393:PHE:H	1:D:696:ASN:HD21	1.10	0.95
1:B:278:THR:HG22	1:B:280:TRP:H	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:THR:HG22	1:C:280:TRP:H	1.31	0.95
1:G:278:THR:HG22	1:G:280:TRP:H	1.31	0.95
1:B:312:LEU:HD23	1:B:312:LEU:C	1.88	0.95
1:A:696:ASN:HD21	1:H:393:PHE:H	1.10	0.95
1:F:278:THR:HG22	1:F:280:TRP:H	1.31	0.94
1:A:312:LEU:HD23	1:A:312:LEU:C	1.88	0.94
1:B:451:ASN:CA	1:B:452:GLN:HB2	1.96	0.94
1:G:451:ASN:CA	1:G:452:GLN:HB2	1.96	0.94
1:E:451:ASN:CA	1:E:452:GLN:HB2	1.96	0.94
1:F:451:ASN:CA	1:F:452:GLN:HB3	1.96	0.94
1:I:312:LEU:HD23	1:I:312:LEU:C	1.88	0.94
1:E:663:SER:OG	1:E:665:THR:HG23	1.65	0.94
1:J:312:LEU:HD23	1:J:312:LEU:C	1.88	0.94
1:C:451:ASN:CA	1:C:452:GLN:HB2	1.98	0.94
1:C:312:LEU:HD23	1:C:312:LEU:C	1.88	0.94
1:J:451:ASN:CA	1:J:452:GLN:HB2	1.96	0.94
1:D:278:THR:HG22	1:D:280:TRP:H	1.31	0.94
1:F:312:LEU:HD23	1:F:312:LEU:C	1.88	0.94
1:H:312:LEU:HD23	1:H:312:LEU:C	1.88	0.94
1:D:312:LEU:HD23	1:D:312:LEU:C	1.87	0.93
1:J:278:THR:HG22	1:J:280:TRP:H	1.31	0.93
1:E:312:LEU:HD23	1:E:312:LEU:C	1.88	0.93
1:F:393:PHE:H	1:I:696:ASN:HD21	1.09	0.93
1:G:312:LEU:C	1:G:312:LEU:HD23	1.88	0.93
1:B:393:PHE:H	1:E:696:ASN:HD21	1.10	0.93
1:F:451:ASN:CA	1:F:452:GLN:CB	2.47	0.92
1:H:278:THR:HG22	1:H:280:TRP:H	1.31	0.92
1:J:327:ASN:O	1:J:328:ASP:HB2	1.67	0.92
1:A:278:THR:HG22	1:A:280:TRP:H	1.31	0.92
1:J:218:ALA:HB3	1:J:407:GLY:O	1.69	0.92
1:B:696:ASN:HD21	1:G:393:PHE:H	1.11	0.91
1:E:393:PHE:H	1:G:696:ASN:HD21	1.10	0.91
1:G:239:VAL:CG1	1:G:685:TRP:HB2	2.01	0.91
1:G:328:ASP:HB3	1:G:329:GLY:O	1.71	0.90
1:D:328:ASP:HB3	1:D:329:GLY:CA	1.99	0.90
1:J:312:LEU:HD22	1:J:414:TYR:HB3	1.53	0.90
1:B:312:LEU:HD22	1:B:414:TYR:HB3	1.53	0.90
1:I:451:ASN:CB	1:I:452:GLN:HB3	2.02	0.90
1:F:312:LEU:HD22	1:F:414:TYR:HB3	1.53	0.90
1:D:312:LEU:HD22	1:D:414:TYR:HB3	1.53	0.90
1:B:326:THR:CG2	1:B:327:ASN:O	2.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:LEU:HD22	1:G:414:TYR:HB3	1.53	0.89
1:A:451:ASN:HA	1:A:452:GLN:HB2	1.53	0.89
1:C:328:ASP:HB3	1:C:329:GLY:O	1.71	0.89
1:I:328:ASP:HA	1:I:329:GLY:C	1.92	0.88
1:A:328:ASP:OD1	1:A:329:GLY:CA	2.21	0.88
1:D:246:THR:HB	1:D:678:GLN:HE21	1.39	0.88
1:I:280:TRP:CE2	1:I:650:LYS:HD3	2.08	0.88
1:C:312:LEU:HD22	1:C:414:TYR:HB3	1.53	0.88
1:A:312:LEU:HD22	1:A:414:TYR:HB3	1.53	0.88
1:B:246:THR:HB	1:B:678:GLN:HE21	1.39	0.88
1:H:328:ASP:HB3	1:H:329:GLY:O	1.71	0.88
1:J:451:ASN:HA	1:J:452:GLN:CB	2.04	0.88
1:I:312:LEU:HD22	1:I:414:TYR:HB3	1.53	0.88
1:E:312:LEU:HD22	1:E:414:TYR:HB3	1.53	0.88
1:C:246:THR:HB	1:C:678:GLN:HE21	1.39	0.88
1:F:246:THR:HB	1:F:678:GLN:HE21	1.39	0.88
1:E:246:THR:HB	1:E:678:GLN:HE21	1.39	0.87
1:H:246:THR:HB	1:H:678:GLN:HE21	1.39	0.87
1:G:246:THR:HB	1:G:678:GLN:HE21	1.39	0.87
1:H:312:LEU:HD22	1:H:414:TYR:HB3	1.53	0.86
1:H:451:ASN:HA	1:H:452:GLN:CB	2.04	0.86
1:H:570:ASN:HD21	1:H:608:GLN:H	1.24	0.86
1:B:451:ASN:HA	1:B:452:GLN:CB	2.04	0.86
1:J:246:THR:HB	1:J:678:GLN:HE21	1.39	0.86
1:I:452:GLN:O	1:I:454:GLY:HA3	1.75	0.86
1:D:451:ASN:HA	1:D:452:GLN:CB	2.03	0.86
1:G:451:ASN:HA	1:G:452:GLN:CB	2.04	0.86
1:A:696:ASN:ND2	1:H:393:PHE:H	1.75	0.85
1:D:393:PHE:H	1:H:696:ASN:ND2	1.74	0.85
1:F:456:ALA:C	1:F:457:GLN:OE1	2.15	0.85
1:A:393:PHE:H	1:D:696:ASN:ND2	1.75	0.85
1:E:451:ASN:HA	1:E:452:GLN:CB	2.04	0.85
1:F:393:PHE:H	1:I:696:ASN:ND2	1.74	0.85
1:I:246:THR:HB	1:I:678:GLN:HE21	1.39	0.84
1:A:246:THR:HB	1:A:678:GLN:HE21	1.39	0.84
1:B:393:PHE:H	1:E:696:ASN:ND2	1.74	0.84
1:B:696:ASN:ND2	1:G:393:PHE:H	1.75	0.84
1:B:269:ASN:HA	1:B:272:HIS:CD2	2.13	0.84
1:I:570:ASN:HD21	1:I:608:GLN:H	1.24	0.84
1:E:393:PHE:H	1:G:696:ASN:ND2	1.75	0.84
1:J:570:ASN:HD21	1:J:608:GLN:H	1.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:570:ASN:HD21	1:G:608:GLN:H	1.24	0.84
1:G:327:ASN:O	1:G:328:ASP:HB2	1.77	0.84
1:C:451:ASN:HA	1:C:452:GLN:CB	2.04	0.84
1:B:570:ASN:HD21	1:B:608:GLN:H	1.24	0.84
1:A:570:ASN:HD21	1:A:608:GLN:H	1.24	0.84
1:F:451:ASN:HB2	1:F:452:GLN:HB3	1.59	0.83
1:C:393:PHE:H	1:F:696:ASN:ND2	1.75	0.83
1:C:570:ASN:HD21	1:C:608:GLN:H	1.24	0.83
1:E:570:ASN:HD21	1:E:608:GLN:H	1.24	0.83
1:A:328:ASP:OD1	1:A:329:GLY:HA3	1.77	0.83
1:E:328:ASP:HA	1:E:329:GLY:C	1.96	0.83
1:H:327:ASN:O	1:H:328:ASP:HB2	1.77	0.83
1:A:328:ASP:CG	1:A:329:GLY:N	2.30	0.83
1:A:451:ASN:HA	1:A:452:GLN:CB	2.09	0.83
1:C:696:ASN:ND2	1:I:393:PHE:H	1.75	0.83
1:C:585:GLN:HE22	1:I:496:ASN:HD22	1.27	0.83
1:A:585:GLN:HE22	1:H:496:ASN:HD22	1.27	0.83
1:F:570:ASN:HD21	1:F:608:GLN:H	1.24	0.83
1:C:327:ASN:O	1:C:328:ASP:HB2	1.77	0.82
1:D:496:ASN:HD22	1:H:585:GLN:HE22	1.27	0.82
1:B:496:ASN:HD22	1:E:585:GLN:HE22	1.27	0.82
1:A:496:ASN:HD22	1:D:585:GLN:HE22	1.27	0.82
1:B:512:ASN:HD21	1:E:529:ASP:H	1.28	0.81
1:D:570:ASN:HD21	1:D:608:GLN:H	1.24	0.81
1:D:512:ASN:HD21	1:H:529:ASP:H	1.28	0.81
1:C:496:ASN:HD22	1:F:585:GLN:HE22	1.27	0.81
1:I:451:ASN:HA	1:I:452:GLN:HB2	1.61	0.81
1:D:714:THR:HG22	1:D:715:VAL:N	1.96	0.81
1:B:585:GLN:HE22	1:G:496:ASN:HD22	1.28	0.81
1:B:490:SER:H	1:B:496:ASN:HD21	1.29	0.80
1:A:451:ASN:CA	1:A:452:GLN:CB	2.60	0.80
1:J:380:THR:HG21	1:J:392:SER:N	1.91	0.80
1:A:490:SER:H	1:A:496:ASN:HD21	1.29	0.80
1:G:237:ASP:O	1:G:687:LEU:HG	1.80	0.80
1:F:330:VAL:HG12	1:F:330:VAL:O	1.80	0.80
1:C:490:SER:H	1:C:496:ASN:HD21	1.29	0.80
1:C:512:ASN:HD21	1:F:529:ASP:H	1.29	0.80
1:H:490:SER:H	1:H:496:ASN:HD21	1.29	0.80
1:C:529:ASP:H	1:I:512:ASN:HD21	1.26	0.80
1:E:496:ASN:HD22	1:G:585:GLN:HE22	1.27	0.80
1:F:512:ASN:HD21	1:I:529:ASP:H	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:490:SER:H	1:J:496:ASN:HD21	1.29	0.79
1:I:451:ASN:HA	1:I:452:GLN:CB	2.12	0.79
1:I:453:SER:HA	1:I:455:SER:H	1.45	0.79
1:E:512:ASN:HD21	1:G:529:ASP:H	1.28	0.79
1:A:457:GLN:NE2	1:A:457:GLN:N	2.30	0.79
1:C:696:ASN:HD22	1:C:696:ASN:H	1.30	0.79
1:E:490:SER:H	1:E:496:ASN:HD21	1.29	0.79
1:A:714:THR:HG22	1:A:715:VAL:N	1.96	0.79
1:B:380:THR:HG23	4:B:842:HOH:O	1.82	0.79
1:F:496:ASN:HD22	1:I:585:GLN:HE22	1.27	0.79
1:C:714:THR:HG22	1:C:715:VAL:N	1.96	0.79
1:F:714:THR:HG22	1:F:715:VAL:N	1.96	0.79
1:B:714:THR:HG22	1:B:715:VAL:N	1.96	0.78
1:J:714:THR:HG22	1:J:715:VAL:N	1.96	0.78
1:E:696:ASN:H	1:E:696:ASN:HD22	1.30	0.78
1:I:490:SER:H	1:I:496:ASN:HD21	1.29	0.78
1:A:529:ASP:H	1:H:512:ASN:HD21	1.29	0.78
1:A:512:ASN:HD21	1:D:529:ASP:H	1.29	0.78
1:E:714:THR:HG22	1:E:715:VAL:N	1.96	0.78
1:B:696:ASN:HD22	1:B:696:ASN:H	1.30	0.78
1:I:714:THR:HG22	1:I:715:VAL:N	1.96	0.78
1:B:663:SER:HG	1:B:665:THR:HG23	1.49	0.78
1:F:490:SER:H	1:F:496:ASN:HD21	1.29	0.78
1:G:714:THR:HG22	1:G:715:VAL:N	1.96	0.78
1:G:451:ASN:CA	1:G:452:GLN:CB	2.62	0.78
1:D:490:SER:H	1:D:496:ASN:HD21	1.29	0.78
1:G:490:SER:H	1:G:496:ASN:HD21	1.29	0.78
1:F:696:ASN:H	1:F:696:ASN:HD22	1.30	0.77
1:B:218:ALA:HB1	1:B:219:ASP:OD1	1.83	0.77
1:B:529:ASP:H	1:G:512:ASN:HD21	1.29	0.77
1:B:451:ASN:CA	1:B:452:GLN:CB	2.62	0.77
1:A:696:ASN:HD22	1:A:696:ASN:H	1.30	0.77
1:H:714:THR:HG22	1:H:715:VAL:N	1.96	0.77
1:D:696:ASN:HD22	1:D:696:ASN:H	1.30	0.77
1:G:239:VAL:HG13	1:G:685:TRP:HB2	1.67	0.76
1:F:456:ALA:O	1:F:457:GLN:OE1	2.03	0.76
1:B:328:ASP:HA	1:B:329:GLY:C	2.04	0.76
1:B:663:SER:OG	1:B:665:THR:CG2	2.34	0.76
1:G:696:ASN:HD22	1:G:696:ASN:H	1.30	0.76
1:H:696:ASN:HD22	1:H:696:ASN:H	1.30	0.76
1:I:696:ASN:HD22	1:I:696:ASN:H	1.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:ASN:CA	1:J:452:GLN:CB	2.62	0.75
1:J:696:ASN:H	1:J:696:ASN:HD22	1.32	0.75
1:D:380:THR:HG23	4:D:845:HOH:O	1.84	0.75
1:A:328:ASP:CG	1:A:329:GLY:CA	2.55	0.75
1:D:451:ASN:CA	1:D:452:GLN:CB	2.62	0.75
1:I:454:GLY:O	1:I:455:SER:CB	2.35	0.75
1:H:451:ASN:CA	1:H:452:GLN:CB	2.62	0.75
1:C:312:LEU:O	1:C:312:LEU:HD23	1.87	0.75
1:E:451:ASN:CA	1:E:452:GLN:CB	2.62	0.74
1:D:312:LEU:HD23	1:D:312:LEU:O	1.87	0.74
1:J:328:ASP:HB3	1:J:329:GLY:C	2.08	0.74
1:I:312:LEU:HD23	1:I:312:LEU:O	1.87	0.74
1:C:451:ASN:CA	1:C:452:GLN:CB	2.63	0.74
1:H:380:THR:HG21	1:H:392:SER:N	2.02	0.74
1:B:312:LEU:O	1:B:312:LEU:HD23	1.87	0.74
1:F:312:LEU:O	1:F:312:LEU:HD23	1.87	0.74
1:I:451:ASN:CA	1:I:452:GLN:CB	2.65	0.74
1:F:450:GLN:HB2	1:F:458:ASN:O	1.87	0.74
1:G:380:THR:HG23	4:G:845:HOH:O	1.88	0.74
1:J:380:THR:HG23	4:J:847:HOH:O	1.88	0.74
1:G:312:LEU:O	1:G:312:LEU:HD23	1.87	0.74
1:I:663:SER:OG	1:I:665:THR:HG23	1.87	0.73
1:E:312:LEU:HD23	1:E:312:LEU:O	1.87	0.73
1:D:427:HIS:CD2	1:D:736:LEU:HD13	2.24	0.73
1:H:427:HIS:CD2	1:H:736:LEU:HD13	2.24	0.73
1:E:427:HIS:CD2	1:E:736:LEU:HD13	2.24	0.73
1:I:427:HIS:CD2	1:I:736:LEU:HD13	2.24	0.73
1:C:427:HIS:CD2	1:C:736:LEU:HD13	2.24	0.73
1:F:427:HIS:CD2	1:F:736:LEU:HD13	2.24	0.73
1:H:312:LEU:HD23	1:H:312:LEU:O	1.87	0.73
1:F:527:HIS:NE2	1:F:532:ASP:OD2	2.22	0.73
1:H:380:THR:HG23	4:H:845:HOH:O	1.88	0.73
1:H:304:ASN:HD21	1:H:689:LYS:NZ	1.87	0.73
1:H:218:ALA:O	1:H:219:ASP:CB	2.37	0.73
1:J:427:HIS:CD2	1:J:736:LEU:HD13	2.24	0.73
1:F:218:ALA:O	1:F:219:ASP:CB	2.36	0.73
1:C:451:ASN:HD21	1:C:458:ASN:HB2	1.54	0.73
1:J:312:LEU:HD23	1:J:312:LEU:O	1.87	0.73
1:G:527:HIS:NE2	1:G:532:ASP:OD2	2.22	0.73
1:E:527:HIS:NE2	1:E:532:ASP:OD2	2.22	0.73
1:B:380:THR:HG21	1:B:392:SER:N	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:VAL:HG12	1:G:685:TRP:HB2	1.69	0.72
1:J:527:HIS:NE2	1:J:532:ASP:OD2	2.22	0.72
1:I:380:THR:HG23	4:I:847:HOH:O	1.88	0.72
1:E:380:THR:HG23	4:E:845:HOH:O	1.88	0.72
1:G:427:HIS:CD2	1:G:736:LEU:HD13	2.24	0.72
1:C:304:ASN:HD21	1:C:689:LYS:NZ	1.87	0.72
1:H:527:HIS:NE2	1:H:532:ASP:OD2	2.22	0.72
1:D:527:HIS:NE2	1:D:532:ASP:OD2	2.22	0.72
1:J:304:ASN:HD21	1:J:689:LYS:NZ	1.87	0.72
1:C:527:HIS:NE2	1:C:532:ASP:OD2	2.22	0.72
1:F:380:THR:HG21	1:F:392:SER:N	2.02	0.72
1:D:304:ASN:HD21	1:D:689:LYS:NZ	1.87	0.72
1:B:527:HIS:NE2	1:B:532:ASP:OD2	2.22	0.72
1:A:304:ASN:HD21	1:A:689:LYS:NZ	1.87	0.72
1:B:427:HIS:CD2	1:B:736:LEU:HD13	2.24	0.72
1:A:312:LEU:O	1:A:312:LEU:HD23	1.87	0.72
1:B:304:ASN:HD21	1:B:689:LYS:NZ	1.87	0.72
1:A:217:GLY:HA3	1:A:408:ASN:HA	1.72	0.72
1:A:427:HIS:CD2	1:A:736:LEU:HD13	2.24	0.72
1:A:527:HIS:NE2	1:A:532:ASP:OD2	2.22	0.72
1:E:304:ASN:HD21	1:E:689:LYS:NZ	1.87	0.72
1:A:380:THR:HG23	4:A:842:HOH:O	1.88	0.72
1:I:304:ASN:HD21	1:I:689:LYS:NZ	1.87	0.72
1:G:304:ASN:HD21	1:G:689:LYS:NZ	1.87	0.71
1:I:527:HIS:NE2	1:I:532:ASP:OD2	2.22	0.71
1:A:451:ASN:CA	1:A:452:GLN:HB3	2.20	0.71
1:I:380:THR:HG21	1:I:392:SER:N	2.02	0.71
1:A:457:GLN:HE21	1:A:457:GLN:N	1.87	0.71
1:A:218:ALA:O	1:A:219:ASP:CB	2.38	0.71
1:C:380:THR:HG21	1:C:392:SER:N	2.02	0.70
1:I:453:SER:HA	1:I:455:SER:N	2.06	0.70
1:F:218:ALA:O	1:F:219:ASP:CG	2.30	0.70
1:E:218:ALA:O	1:E:219:ASP:CG	2.30	0.70
1:F:380:THR:HG23	4:F:844:HOH:O	1.88	0.70
1:J:564:GLU:O	1:J:567:LYS:HG2	1.92	0.70
1:E:564:GLU:O	1:E:567:LYS:HG2	1.92	0.70
1:I:564:GLU:O	1:I:567:LYS:HG2	1.92	0.70
1:E:380:THR:HG21	1:E:392:SER:N	2.02	0.70
1:I:456:ALA:C	1:I:457:GLN:OE1	2.30	0.70
1:A:457:GLN:H	1:A:457:GLN:HE21	1.39	0.70
1:F:217:GLY:HA3	1:F:408:ASN:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:GLU:O	1:F:567:LYS:HG2	1.92	0.70
1:H:564:GLU:O	1:H:567:LYS:HG2	1.92	0.70
1:H:218:ALA:O	1:H:219:ASP:CG	2.30	0.69
1:A:218:ALA:O	1:A:219:ASP:CG	2.30	0.69
1:A:564:GLU:O	1:A:567:LYS:HG2	1.92	0.69
1:F:714:THR:CG2	1:F:715:VAL:N	2.56	0.69
1:D:564:GLU:O	1:D:567:LYS:HG2	1.92	0.69
1:B:564:GLU:O	1:B:567:LYS:HG2	1.92	0.69
1:C:329:GLY:O	1:C:330:VAL:HG12	1.93	0.69
1:C:428:SER:O	1:I:380:THR:HG22	1.93	0.69
1:A:380:THR:HG22	1:D:428:SER:O	1.93	0.69
1:I:451:ASN:CA	1:I:452:GLN:HB3	2.23	0.69
1:I:456:ALA:O	1:I:457:GLN:CD	2.30	0.69
1:D:714:THR:CG2	1:D:715:VAL:N	2.56	0.69
1:D:429:GLN:HE21	1:D:736:LEU:H	1.41	0.69
1:F:429:GLN:HE21	1:F:736:LEU:H	1.41	0.69
1:D:698:GLU:H	1:I:298:GLN:HE22	1.41	0.69
1:J:714:THR:CG2	1:J:715:VAL:N	2.56	0.69
1:H:329:GLY:O	1:H:330:VAL:HG12	1.93	0.68
1:F:380:THR:HG22	1:I:428:SER:O	1.93	0.68
1:B:380:THR:HG22	1:E:428:SER:O	1.93	0.68
1:A:428:SER:O	1:H:380:THR:HG22	1.92	0.68
1:H:714:THR:CG2	1:H:715:VAL:N	2.56	0.68
1:C:564:GLU:O	1:C:567:LYS:HG2	1.92	0.68
1:B:428:SER:O	1:G:380:THR:HG22	1.93	0.68
1:C:714:THR:CG2	1:C:715:VAL:N	2.56	0.68
1:D:298:GLN:HE22	1:I:698:GLU:H	1.41	0.68
1:A:298:GLN:HE22	1:E:698:GLU:H	1.41	0.68
1:B:298:GLN:HE22	1:J:698:GLU:H	1.41	0.68
1:G:217:GLY:HA2	1:G:408:ASN:HA	1.75	0.68
1:H:451:ASN:HD21	1:H:458:ASN:HB2	1.59	0.68
1:E:380:THR:HG22	1:G:428:SER:O	1.93	0.68
1:A:380:THR:HG21	1:A:392:SER:N	2.02	0.68
1:B:286:ASN:HD21	1:B:619:TRP:H	1.42	0.68
1:A:714:THR:CG2	1:A:715:VAL:N	2.56	0.68
1:I:714:THR:CG2	1:I:715:VAL:N	2.56	0.68
1:D:286:ASN:HD21	1:D:619:TRP:H	1.42	0.68
1:G:380:THR:HG21	1:G:392:SER:N	2.02	0.68
1:E:286:ASN:HD21	1:E:619:TRP:H	1.42	0.68
1:C:380:THR:HG22	1:F:428:SER:O	1.93	0.68
1:E:429:GLN:HE21	1:E:736:LEU:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:429:GLN:HE21	1:I:736:LEU:H	1.41	0.68
1:E:714:THR:CG2	1:E:715:VAL:N	2.56	0.68
1:F:217:GLY:O	1:F:218:ALA:HB2	1.94	0.68
1:G:429:GLN:HE21	1:G:736:LEU:H	1.41	0.68
1:D:265:THR:HG21	1:D:267:ALA:HB2	1.74	0.68
1:B:429:GLN:HE21	1:B:736:LEU:H	1.41	0.68
1:A:429:GLN:HE21	1:A:736:LEU:H	1.41	0.68
1:D:278:THR:CG2	1:D:280:TRP:H	2.07	0.68
1:B:714:THR:CG2	1:B:715:VAL:N	2.56	0.68
1:G:714:THR:CG2	1:G:715:VAL:N	2.56	0.68
1:C:286:ASN:HD21	1:C:619:TRP:H	1.42	0.68
1:G:451:ASN:HD21	1:G:458:ASN:HB2	1.59	0.67
1:J:310:LYS:HD2	1:J:686:GLU:HB2	1.77	0.67
1:J:451:ASN:HD21	1:J:458:ASN:HB2	1.59	0.67
1:J:429:GLN:HE21	1:J:736:LEU:H	1.41	0.67
1:G:286:ASN:HD21	1:G:619:TRP:H	1.42	0.67
1:G:329:GLY:O	1:G:330:VAL:HG12	1.93	0.67
1:D:380:THR:HG21	1:D:392:SER:N	2.02	0.67
1:H:310:LYS:HD2	1:H:686:GLU:HB2	1.77	0.67
1:I:310:LYS:HD2	1:I:686:GLU:HB2	1.77	0.67
1:A:666:LYS:NZ	1:I:719:GLY:O	2.27	0.67
1:I:286:ASN:HD21	1:I:619:TRP:H	1.42	0.67
1:H:429:GLN:HE21	1:H:736:LEU:H	1.41	0.67
1:D:451:ASN:HD21	1:D:458:ASN:HB2	1.59	0.67
1:D:310:LYS:HD2	1:D:686:GLU:HB2	1.77	0.67
1:H:696:ASN:ND2	1:H:696:ASN:H	1.93	0.67
1:B:310:LYS:HD2	1:B:686:GLU:HB2	1.77	0.67
1:G:310:LYS:HD2	1:G:686:GLU:HB2	1.77	0.67
1:E:451:ASN:HD21	1:E:458:ASN:HB2	1.59	0.67
1:D:380:THR:HG22	1:H:428:SER:O	1.93	0.67
1:E:310:LYS:HD2	1:E:686:GLU:HB2	1.77	0.67
1:A:330:VAL:CG1	1:B:327:ASN:OD1	2.40	0.67
1:G:312:LEU:C	1:G:312:LEU:CD2	2.62	0.67
1:B:698:GLU:H	1:J:298:GLN:HE22	1.41	0.67
1:C:278:THR:CG2	1:C:280:TRP:H	2.07	0.66
1:J:278:THR:CG2	1:J:280:TRP:H	2.07	0.66
1:E:696:ASN:ND2	1:E:696:ASN:H	1.93	0.66
1:E:218:ALA:O	1:E:219:ASP:CB	2.43	0.66
1:G:564:GLU:O	1:G:567:LYS:HG2	1.94	0.66
1:A:698:GLU:H	1:E:298:GLN:HE22	1.41	0.66
1:F:502:THR:O	1:F:506:ALA:CB	2.40	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:ASN:HD21	1:J:619:TRP:H	1.42	0.66
1:H:286:ASN:HD21	1:H:619:TRP:H	1.42	0.66
1:A:310:LYS:HD2	1:A:686:GLU:HB2	1.77	0.66
1:H:278:THR:CG2	1:H:280:TRP:H	2.07	0.66
1:J:696:ASN:ND2	1:J:696:ASN:H	1.93	0.66
1:F:310:LYS:HD2	1:F:686:GLU:HB2	1.77	0.66
1:J:327:ASN:O	1:J:328:ASP:CB	2.40	0.66
1:A:328:ASP:CG	1:A:329:GLY:HA3	2.16	0.66
1:A:286:ASN:HD21	1:A:619:TRP:H	1.42	0.66
1:C:383:ASN:C	1:C:383:ASN:HD22	1.99	0.66
1:B:451:ASN:HD21	1:B:458:ASN:HB2	1.59	0.66
1:G:696:ASN:H	1:G:696:ASN:ND2	1.93	0.66
1:C:429:GLN:HE21	1:C:736:LEU:H	1.41	0.66
1:F:217:GLY:O	1:F:218:ALA:CB	2.44	0.66
1:J:502:THR:O	1:J:506:ALA:CB	2.40	0.66
1:H:502:THR:O	1:H:506:ALA:CB	2.40	0.66
1:B:696:ASN:ND2	1:B:696:ASN:H	1.93	0.66
1:F:696:ASN:ND2	1:F:696:ASN:H	1.93	0.65
1:I:278:THR:CG2	1:I:280:TRP:H	2.07	0.65
1:D:696:ASN:H	1:D:696:ASN:ND2	1.93	0.65
1:A:696:ASN:H	1:A:696:ASN:ND2	1.93	0.65
1:B:628:HIS:O	3:B:739:CYT:N1	2.29	0.65
1:I:383:ASN:HD22	1:I:383:ASN:C	1.99	0.65
1:I:696:ASN:ND2	1:I:696:ASN:H	1.93	0.65
1:F:354:VAL:H	1:F:646:GLN:NE2	1.95	0.65
1:G:354:VAL:H	1:G:646:GLN:NE2	1.95	0.65
1:B:354:VAL:H	1:B:646:GLN:NE2	1.95	0.65
1:F:383:ASN:C	1:F:383:ASN:HD22	1.99	0.65
1:A:383:ASN:HD22	1:A:383:ASN:C	1.99	0.65
1:G:383:ASN:HD22	1:G:383:ASN:C	1.99	0.65
1:C:502:THR:O	1:C:506:ALA:CB	2.40	0.65
1:A:354:VAL:H	1:A:646:GLN:NE2	1.95	0.65
1:G:663:SER:OG	1:G:665:THR:HG23	1.97	0.65
1:E:383:ASN:HD22	1:E:383:ASN:C	1.99	0.65
1:A:278:THR:CG2	1:A:280:TRP:H	2.07	0.65
1:A:608:GLN:HE22	1:H:625:THR:HA	1.62	0.65
1:E:354:VAL:H	1:E:646:GLN:NE2	1.95	0.65
3:A:738:CYT:N1	1:H:628:HIS:O	2.30	0.65
1:J:383:ASN:HD22	1:J:383:ASN:C	1.99	0.65
1:A:502:THR:O	1:A:506:ALA:CB	2.40	0.65
1:F:255:HIS:ND1	4:F:795:HOH:O	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LYS:HD2	1:C:686:GLU:HB2	1.77	0.65
1:I:354:VAL:H	1:I:646:GLN:NE2	1.95	0.65
1:B:625:THR:HA	1:E:608:GLN:HE22	1.62	0.65
1:J:354:VAL:H	1:J:646:GLN:NE2	1.95	0.65
1:I:218:ALA:HB1	1:I:219:ASP:CG	2.17	0.65
1:G:502:THR:O	1:G:506:ALA:CB	2.40	0.65
1:I:457:GLN:OE1	1:I:457:GLN:N	2.30	0.65
1:G:563:GLU:OE2	1:G:611:ASP:N	2.27	0.65
1:C:264:SER:OG	1:C:265:THR:N	2.30	0.65
1:C:696:ASN:H	1:C:696:ASN:ND2	1.93	0.65
1:F:286:ASN:HD21	1:F:619:TRP:H	1.42	0.65
1:A:454:GLY:O	1:A:456:ALA:N	2.30	0.65
1:F:302:ASN:HD21	1:F:701:TYR:H	1.45	0.65
1:H:354:VAL:H	1:H:646:GLN:NE2	1.95	0.64
1:B:383:ASN:HD22	1:B:383:ASN:C	1.99	0.64
1:C:328:ASP:CB	1:C:329:GLY:O	2.42	0.64
1:C:625:THR:HA	1:F:608:GLN:HE22	1.62	0.64
1:A:628:HIS:O	3:D:738:CYT:N1	2.30	0.64
1:D:354:VAL:H	1:D:646:GLN:NE2	1.95	0.64
1:C:397:GLU:N	1:C:397:GLU:OE1	2.30	0.64
1:D:218:ALA:O	1:D:219:ASP:HB2	1.96	0.64
1:D:383:ASN:HD22	1:D:383:ASN:C	1.99	0.64
1:I:502:THR:O	1:I:506:ALA:CB	2.40	0.64
1:H:312:LEU:CD2	1:H:312:LEU:C	2.62	0.64
1:D:312:LEU:CD2	1:D:312:LEU:C	2.62	0.64
1:D:625:THR:HA	1:H:608:GLN:HE22	1.61	0.64
1:D:628:HIS:O	3:H:738:CYT:N1	2.30	0.64
1:A:312:LEU:C	1:A:312:LEU:CD2	2.62	0.64
1:E:663:SER:HG	1:E:665:THR:HG23	1.62	0.64
1:G:304:ASN:HD21	1:G:689:LYS:HZ1	1.46	0.64
1:D:719:GLY:O	1:F:666:LYS:NZ	2.31	0.64
1:D:397:GLU:OE1	1:D:397:GLU:N	2.30	0.64
1:H:383:ASN:C	1:H:383:ASN:HD22	1.99	0.64
1:H:327:ASN:O	1:H:328:ASP:CB	2.46	0.64
1:B:502:THR:O	1:B:506:ALA:CB	2.40	0.64
1:H:304:ASN:HD21	1:H:689:LYS:HZ1	1.46	0.64
1:C:628:HIS:O	3:F:738:CYT:N1	2.30	0.64
1:I:563:GLU:OE2	1:I:611:ASP:N	2.27	0.64
1:E:278:THR:CG2	1:E:280:TRP:H	2.07	0.64
1:F:278:THR:CG2	1:F:280:TRP:H	2.07	0.64
1:E:625:THR:HA	1:G:608:GLN:HE22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:628:HIS:O	3:I:738:CYT:N1	2.30	0.64
1:C:327:ASN:O	1:C:328:ASP:CB	2.46	0.64
1:F:457:GLN:OE1	1:F:457:GLN:N	2.30	0.64
3:C:738:CYT:N1	1:I:628:HIS:O	2.31	0.64
1:F:452:GLN:O	1:F:452:GLN:HG2	1.97	0.63
1:C:354:VAL:H	1:C:646:GLN:NE2	1.95	0.63
1:G:278:THR:CG2	1:G:280:TRP:H	2.07	0.63
1:D:286:ASN:ND2	1:D:618:ILE:H	1.97	0.63
1:D:502:THR:O	1:D:506:ALA:CB	2.40	0.63
1:I:286:ASN:ND2	1:I:618:ILE:H	1.97	0.63
1:F:625:THR:HA	1:I:608:GLN:HE22	1.62	0.63
1:G:286:ASN:ND2	1:G:618:ILE:H	1.97	0.63
1:H:286:ASN:ND2	1:H:618:ILE:H	1.97	0.63
1:I:327:ASN:O	1:I:330:VAL:N	2.28	0.63
1:B:286:ASN:ND2	1:B:618:ILE:H	1.97	0.63
1:D:563:GLU:OE2	1:D:611:ASP:N	2.26	0.63
1:J:380:THR:CG2	1:J:392:SER:H	1.98	0.63
1:E:502:THR:O	1:E:506:ALA:CB	2.40	0.63
1:I:454:GLY:O	1:I:455:SER:HB2	1.97	0.63
1:A:625:THR:HA	1:D:608:GLN:HE22	1.62	0.63
1:E:286:ASN:ND2	1:E:618:ILE:H	1.97	0.63
1:J:286:ASN:ND2	1:J:618:ILE:H	1.97	0.63
1:A:286:ASN:ND2	1:A:618:ILE:H	1.97	0.63
1:E:264:SER:O	1:E:266:GLY:N	2.32	0.63
1:G:328:ASP:CB	1:G:329:GLY:O	2.42	0.63
1:B:608:GLN:HE22	1:G:625:THR:HA	1.62	0.63
1:B:563:GLU:OE2	1:B:611:ASP:N	2.27	0.63
1:H:328:ASP:CB	1:H:329:GLY:O	2.42	0.62
1:A:452:GLN:O	1:A:452:GLN:HG2	1.99	0.62
1:F:450:GLN:CB	1:F:458:ASN:O	2.47	0.62
1:I:570:ASN:HD21	1:I:608:GLN:N	1.97	0.62
1:C:608:GLN:HE22	1:I:625:THR:HA	1.61	0.62
1:C:286:ASN:ND2	1:C:618:ILE:H	1.97	0.62
1:G:570:ASN:HD21	1:G:608:GLN:N	1.97	0.62
1:C:570:ASN:HD21	1:C:608:GLN:N	1.97	0.62
1:B:278:THR:CG2	1:B:280:TRP:H	2.07	0.62
1:A:327:ASN:O	1:A:330:VAL:N	2.33	0.62
1:J:328:ASP:HB3	1:J:329:GLY:CA	2.29	0.62
1:J:570:ASN:HD21	1:J:608:GLN:N	1.97	0.62
1:H:570:ASN:HD21	1:H:608:GLN:N	1.97	0.62
1:D:552:ASN:ND2	1:H:447:ASN:HD22	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:ASN:ND2	1:F:447:ASN:HD22	1.98	0.62
1:B:552:ASN:ND2	1:E:447:ASN:HD22	1.98	0.62
1:A:328:ASP:CB	1:A:329:GLY:HA3	2.30	0.61
1:F:552:ASN:ND2	1:I:447:ASN:HD22	1.98	0.61
1:A:563:GLU:OE2	1:A:611:ASP:N	2.27	0.61
1:G:282:TYR:O	1:G:373:ILE:HG23	2.00	0.61
1:B:264:SER:O	1:B:266:GLY:N	2.31	0.61
1:A:282:TYR:O	1:A:373:ILE:HG23	2.00	0.61
1:F:459:LYS:HZ1	1:F:587:SER:HB3	1.63	0.61
1:A:663:SER:OG	1:A:665:THR:HG23	2.00	0.61
1:J:282:TYR:O	1:J:373:ILE:HG23	2.00	0.61
1:B:282:TYR:O	1:B:373:ILE:HG23	2.00	0.61
1:C:447:ASN:HD22	1:I:552:ASN:ND2	1.98	0.61
1:I:282:TYR:O	1:I:373:ILE:HG23	2.00	0.61
1:D:282:TYR:O	1:D:373:ILE:HG23	2.00	0.61
1:E:304:ASN:HD21	1:E:689:LYS:HZ1	1.48	0.61
1:F:286:ASN:ND2	1:F:618:ILE:H	1.97	0.61
1:F:282:TYR:O	1:F:373:ILE:HG23	2.00	0.61
1:J:563:GLU:OE2	1:J:611:ASP:N	2.27	0.61
1:G:237:ASP:O	1:G:687:LEU:CG	2.49	0.61
1:A:447:ASN:HD22	1:H:552:ASN:ND2	1.98	0.61
1:B:312:LEU:CD2	1:B:312:LEU:C	2.62	0.61
1:E:570:ASN:HD21	1:E:608:GLN:N	1.97	0.61
1:B:448:ARG:HA	1:G:500:ASN:HD21	1.66	0.61
1:E:563:GLU:OE2	1:E:611:ASP:N	2.27	0.61
1:E:552:ASN:ND2	1:G:447:ASN:HD22	1.98	0.60
1:I:703:SER:HB2	4:I:743:HOH:O	1.99	0.60
1:H:563:GLU:OE2	1:H:611:ASP:N	2.26	0.60
1:B:500:ASN:HD21	1:E:448:ARG:HA	1.66	0.60
1:A:500:ASN:HD21	1:D:448:ARG:HA	1.66	0.60
1:F:563:GLU:OE2	1:F:611:ASP:N	2.27	0.60
1:H:282:TYR:O	1:H:373:ILE:HG23	2.00	0.60
1:A:552:ASN:ND2	1:D:447:ASN:HD22	1.98	0.60
1:I:452:GLN:O	1:I:452:GLN:HG2	2.01	0.60
1:D:500:ASN:HD21	1:H:448:ARG:HA	1.66	0.60
1:C:327:ASN:O	1:C:330:VAL:N	2.34	0.60
1:G:327:ASN:O	1:G:330:VAL:N	2.34	0.60
1:F:500:ASN:HD21	1:I:448:ARG:HA	1.66	0.60
1:F:289:HIS:CE1	1:F:365:PRO:HG3	2.37	0.60
1:C:282:TYR:O	1:C:373:ILE:HG23	2.00	0.60
1:B:299:ARG:NH2	1:J:690:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ASN:HD21	1:F:448:ARG:HA	1.66	0.60
1:G:218:ALA:HB1	1:G:219:ASP:CG	2.22	0.60
1:C:448:ARG:HA	1:I:500:ASN:HD21	1.67	0.60
1:A:299:ARG:NH2	1:E:690:GLU:OE2	2.34	0.60
1:C:289:HIS:CE1	1:C:365:PRO:HG3	2.37	0.60
1:E:282:TYR:O	1:E:373:ILE:HG23	2.00	0.60
1:E:500:ASN:HD21	1:G:448:ARG:HA	1.66	0.60
1:G:327:ASN:O	1:G:328:ASP:CB	2.46	0.60
1:A:450:GLN:OE1	1:A:457:GLN:HB3	2.01	0.60
1:B:289:HIS:CE1	1:B:365:PRO:HG3	2.37	0.60
1:D:452:GLN:O	1:D:453:SER:C	2.41	0.60
1:D:278:THR:HB	1:D:376:TYR:O	2.02	0.60
1:A:448:ARG:HA	1:H:500:ASN:HD21	1.66	0.60
1:A:289:HIS:CE1	1:A:365:PRO:HG3	2.37	0.60
1:B:328:ASP:OD1	1:B:329:GLY:N	2.35	0.59
1:I:289:HIS:CE1	1:I:365:PRO:HG3	2.37	0.59
1:I:278:THR:HB	1:I:376:TYR:O	2.02	0.59
1:E:278:THR:HB	1:E:376:TYR:O	2.02	0.59
1:B:278:THR:HB	1:B:376:TYR:O	2.02	0.59
1:F:459:LYS:NZ	1:F:587:SER:HB3	2.16	0.59
1:D:299:ARG:NH2	1:I:690:GLU:OE2	2.35	0.59
1:A:422:HIS:CE1	1:A:612:VAL:HG22	2.38	0.59
1:H:422:HIS:CE1	1:H:612:VAL:HG22	2.38	0.59
1:H:289:HIS:CE1	1:H:365:PRO:HG3	2.37	0.59
1:A:278:THR:HB	1:A:376:TYR:O	2.02	0.59
1:B:447:ASN:HD22	1:G:552:ASN:ND2	1.99	0.59
1:I:452:GLN:O	1:I:453:SER:C	2.40	0.59
1:G:422:HIS:CE1	1:G:612:VAL:HG22	2.38	0.59
1:I:405:ARG:H	1:I:408:ASN:ND2	2.00	0.59
1:J:289:HIS:CE1	1:J:365:PRO:HG3	2.37	0.59
1:G:397:GLU:OE2	1:G:650:LYS:NZ	2.25	0.59
1:C:422:HIS:CE1	1:C:612:VAL:HG22	2.38	0.59
1:J:422:HIS:CE1	1:J:612:VAL:HG22	2.38	0.59
1:E:327:ASN:O	1:E:330:VAL:HG12	2.03	0.59
1:D:289:HIS:CE1	1:D:365:PRO:HG3	2.37	0.59
1:B:422:HIS:CE1	1:B:612:VAL:HG22	2.38	0.59
1:I:422:HIS:CE1	1:I:612:VAL:HG22	2.38	0.59
1:F:218:ALA:O	1:F:219:ASP:HB2	2.01	0.59
1:J:304:ASN:HD21	1:J:689:LYS:HZ1	1.50	0.59
1:E:289:HIS:CE1	1:E:365:PRO:HG3	2.37	0.59
1:B:638:PHE:HA	2:B:737:ADE:H61	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:327:ASN:O	1:H:330:VAL:N	2.34	0.59
1:B:452:GLN:O	1:B:453:SER:C	2.41	0.59
1:F:263:ALA:O	1:F:264:SER:HB3	2.02	0.59
1:G:289:HIS:CE1	1:G:365:PRO:HG3	2.37	0.59
1:H:452:GLN:O	1:H:453:SER:C	2.41	0.59
1:C:452:GLN:O	1:C:453:SER:C	2.41	0.59
1:C:278:THR:HB	1:C:376:TYR:O	2.02	0.59
1:F:570:ASN:HD21	1:F:608:GLN:N	1.97	0.59
1:D:570:ASN:HD21	1:D:608:GLN:N	1.97	0.58
1:B:365:PRO:HD2	4:B:756:HOH:O	2.02	0.58
1:B:690:GLU:OE2	1:J:299:ARG:NH2	2.34	0.58
1:G:278:THR:HB	1:G:376:TYR:O	2.02	0.58
1:A:570:ASN:HD21	1:A:608:GLN:N	1.97	0.58
1:D:690:GLU:OE2	1:I:299:ARG:NH2	2.35	0.58
1:E:452:GLN:O	1:E:453:SER:C	2.41	0.58
1:F:312:LEU:C	1:F:312:LEU:CD2	2.62	0.58
1:I:402:GLN:HG2	1:I:404:LEU:CD1	2.33	0.58
1:G:452:GLN:O	1:G:453:SER:C	2.41	0.58
1:H:218:ALA:O	1:H:219:ASP:HB2	2.02	0.58
1:E:719:GLY:O	1:H:666:LYS:NZ	2.35	0.58
1:D:422:HIS:CE1	1:D:612:VAL:HG22	2.38	0.58
1:H:278:THR:HB	1:H:376:TYR:O	2.02	0.58
1:B:570:ASN:HD21	1:B:608:GLN:N	1.97	0.58
1:A:690:GLU:OE2	1:E:299:ARG:NH2	2.34	0.58
1:F:304:ASN:ND2	1:F:687:LEU:HB3	2.18	0.58
1:F:278:THR:HB	1:F:376:TYR:O	2.02	0.58
1:J:278:THR:HB	1:J:376:TYR:O	2.02	0.58
1:F:552:ASN:HD21	1:I:447:ASN:HD22	1.52	0.58
1:F:422:HIS:CE1	1:F:612:VAL:HG22	2.38	0.58
1:E:422:HIS:CE1	1:E:612:VAL:HG22	2.38	0.58
1:E:312:LEU:CD2	1:E:312:LEU:C	2.62	0.58
1:A:330:VAL:HG11	1:B:327:ASN:CG	2.21	0.58
1:I:312:LEU:C	1:I:312:LEU:CD2	2.62	0.57
1:J:452:GLN:O	1:J:453:SER:C	2.41	0.57
1:A:217:GLY:HA3	1:A:408:ASN:CA	2.34	0.57
1:I:280:TRP:CD2	1:I:650:LYS:HD3	2.39	0.57
1:D:532:ASP:OD2	1:D:562:ASP:OD2	2.23	0.57
1:J:218:ALA:CB	1:J:407:GLY:O	2.48	0.57
1:B:217:GLY:HA2	1:B:408:ASN:HA	1.86	0.57
1:B:304:ASN:HD21	1:B:689:LYS:HZ1	1.50	0.57
1:A:532:ASP:OD2	1:A:562:ASP:OD2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:ALA:O	1:E:264:SER:HB3	2.03	0.57
1:A:552:ASN:HD21	1:D:447:ASN:HD22	1.52	0.57
1:F:452:GLN:OE1	1:F:462:LEU:HD11	2.05	0.57
1:I:254:ASN:O	1:I:255:HIS:HB2	2.04	0.57
1:H:381:LEU:HD12	1:H:390:ARG:HB3	1.87	0.57
1:C:608:GLN:HE22	1:I:625:THR:CA	2.18	0.57
1:B:381:LEU:HD12	1:B:390:ARG:HB3	1.87	0.57
1:H:532:ASP:OD2	1:H:562:ASP:OD2	2.23	0.57
1:J:381:LEU:HD12	1:J:390:ARG:HB3	1.87	0.57
1:F:399:PHE:CD1	1:F:399:PHE:N	2.72	0.57
1:F:532:ASP:OD2	1:F:562:ASP:OD2	2.23	0.56
1:B:447:ASN:HD22	1:G:552:ASN:HD21	1.53	0.56
1:I:381:LEU:HD12	1:I:390:ARG:HB3	1.87	0.56
1:E:532:ASP:OD2	1:E:562:ASP:OD2	2.23	0.56
1:J:532:ASP:OD2	1:J:562:ASP:OD2	2.23	0.56
1:A:218:ALA:O	1:A:219:ASP:HB2	2.04	0.56
1:I:304:ASN:HD21	1:I:689:LYS:HZ1	1.53	0.56
1:E:218:ALA:C	1:E:219:ASP:OD1	2.44	0.56
1:D:552:ASN:HD21	1:H:447:ASN:HD22	1.52	0.56
1:C:552:ASN:HD21	1:F:447:ASN:HD22	1.52	0.56
1:B:552:ASN:HD21	1:E:447:ASN:HD22	1.52	0.56
1:E:552:ASN:HD21	1:G:447:ASN:HD22	1.52	0.56
1:C:381:LEU:HD12	1:C:390:ARG:HB3	1.87	0.56
1:E:381:LEU:HD12	1:E:390:ARG:HB3	1.87	0.56
1:J:717:ASN:ND2	1:J:717:ASN:H	2.04	0.56
1:J:312:LEU:CD2	1:J:312:LEU:C	2.62	0.56
1:C:312:LEU:C	1:C:312:LEU:CD2	2.62	0.56
1:H:296:ASP:OD1	1:H:299:ARG:NH1	2.38	0.56
1:D:381:LEU:HD12	1:D:390:ARG:HB3	1.87	0.56
1:A:264:SER:O	1:A:266:GLY:N	2.34	0.56
1:A:381:LEU:HD12	1:A:390:ARG:HB3	1.87	0.56
1:F:456:ALA:O	1:F:457:GLN:CD	2.44	0.56
1:I:532:ASP:OD2	1:I:562:ASP:OD2	2.23	0.56
1:D:625:THR:CA	1:H:608:GLN:HE22	2.18	0.56
1:C:625:THR:CA	1:F:608:GLN:HE22	2.19	0.56
1:F:341:VAL:HG12	1:F:651:ASN:HD22	1.71	0.56
1:E:625:THR:CA	1:G:608:GLN:HE22	2.18	0.56
1:C:532:ASP:OD2	1:C:562:ASP:OD2	2.23	0.56
1:A:447:ASN:HD22	1:H:552:ASN:HD21	1.52	0.56
1:C:563:GLU:OE2	1:C:611:ASP:N	2.27	0.56
1:F:625:THR:CA	1:I:608:GLN:HE22	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:THR:CA	1:E:608:GLN:HE22	2.18	0.55
1:G:717:ASN:H	1:G:717:ASN:ND2	2.04	0.55
1:A:380:THR:CG2	1:A:392:SER:H	2.09	0.55
1:B:608:GLN:HE22	1:G:625:THR:CA	2.19	0.55
1:C:447:ASN:HD22	1:I:552:ASN:HD21	1.53	0.55
1:F:295:ARG:HH11	1:F:298:GLN:HE21	1.54	0.55
1:F:381:LEU:HD12	1:F:390:ARG:HB3	1.87	0.55
1:G:381:LEU:HD12	1:G:390:ARG:HB3	1.87	0.55
1:I:397:GLU:OE1	1:I:650:LYS:CE	2.35	0.55
1:F:512:ASN:ND2	1:I:529:ASP:H	2.03	0.55
1:D:304:ASN:HD21	1:D:689:LYS:HZ1	1.54	0.55
1:B:532:ASP:OD2	1:B:562:ASP:OD2	2.23	0.55
1:E:302:ASN:HD21	1:E:701:TYR:H	1.54	0.55
1:E:615:GLN:HE21	1:E:615:GLN:H	1.55	0.55
1:I:615:GLN:H	1:I:615:GLN:HE21	1.54	0.55
1:G:451:ASN:HB2	1:G:452:GLN:HB3	1.89	0.55
1:D:302:ASN:HD21	1:D:701:TYR:H	1.54	0.55
1:D:615:GLN:HE21	1:D:615:GLN:H	1.55	0.55
1:G:532:ASP:OD2	1:G:562:ASP:OD2	2.23	0.55
1:F:563:GLU:HG3	4:F:775:HOH:O	2.07	0.55
1:A:302:ASN:HD21	1:A:701:TYR:H	1.54	0.55
1:I:717:ASN:H	1:I:717:ASN:ND2	2.04	0.55
1:I:450:GLN:OE1	1:I:457:GLN:HB3	2.07	0.55
1:B:529:ASP:H	1:G:512:ASN:ND2	2.03	0.55
1:D:265:THR:CG2	1:D:267:ALA:HB2	2.36	0.55
1:F:254:ASN:O	1:F:255:HIS:HB2	2.07	0.55
1:B:270:ASP:HA	1:B:514:ARG:HG2	1.88	0.55
1:B:717:ASN:H	1:B:717:ASN:ND2	2.03	0.55
1:H:451:ASN:HB2	1:H:452:GLN:HB3	1.88	0.55
1:A:608:GLN:HE22	1:H:625:THR:CA	2.18	0.55
1:I:328:ASP:HA	1:I:329:GLY:O	2.05	0.55
1:A:615:GLN:H	1:A:615:GLN:HE21	1.55	0.55
1:E:717:ASN:H	1:E:717:ASN:ND2	2.04	0.55
1:F:615:GLN:H	1:F:615:GLN:HE21	1.55	0.55
1:D:327:ASN:O	1:D:328:ASP:HB2	2.07	0.55
1:E:451:ASN:HB2	1:E:452:GLN:HB3	1.89	0.55
1:J:451:ASN:HB2	1:J:452:GLN:HB3	1.89	0.55
1:A:625:THR:CA	1:D:608:GLN:HE22	2.18	0.55
1:J:663:SER:OG	1:J:665:THR:HG23	2.07	0.55
1:H:615:GLN:HE21	1:H:615:GLN:H	1.55	0.55
1:F:217:GLY:HA3	1:F:408:ASN:CA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:563:GLU:HG3	4:H:776:HOH:O	2.07	0.54
1:C:635:MET:H	1:F:477:ASN:HD22	1.55	0.54
1:A:717:ASN:H	1:A:717:ASN:ND2	2.04	0.54
1:D:717:ASN:ND2	1:D:717:ASN:H	2.03	0.54
1:J:296:ASP:OD1	1:J:299:ARG:NH1	2.38	0.54
1:B:302:ASN:HD21	1:B:701:TYR:H	1.54	0.54
1:J:480:PRO:O	1:J:605:MET:HG2	2.08	0.54
1:D:663:SER:OG	1:D:665:THR:HG23	2.07	0.54
1:I:480:PRO:O	1:I:605:MET:HG2	2.08	0.54
1:C:717:ASN:H	1:C:717:ASN:ND2	2.04	0.54
1:F:304:ASN:HD22	1:F:687:LEU:HB3	1.72	0.54
1:C:663:SER:OG	1:C:665:THR:HG23	2.07	0.54
1:I:302:ASN:HD21	1:I:701:TYR:H	1.54	0.54
1:A:477:ASN:HD22	1:H:635:MET:H	1.56	0.54
1:F:635:MET:H	1:I:477:ASN:HD22	1.55	0.54
1:B:451:ASN:HB2	1:B:452:GLN:HB3	1.89	0.54
1:C:451:ASN:HB2	1:C:452:GLN:HB3	1.89	0.54
1:G:302:ASN:HD21	1:G:701:TYR:H	1.55	0.54
1:A:480:PRO:O	1:A:605:MET:HG2	2.08	0.54
1:J:302:ASN:HD21	1:J:701:TYR:H	1.54	0.54
1:D:480:PRO:O	1:D:605:MET:HG2	2.08	0.54
1:D:451:ASN:HB2	1:D:452:GLN:HB3	1.89	0.54
1:D:563:GLU:HG3	4:D:775:HOH:O	2.07	0.54
1:A:296:ASP:OD1	1:A:299:ARG:NH1	2.38	0.54
1:G:480:PRO:O	1:G:605:MET:HG2	2.08	0.54
1:A:451:ASN:CB	1:A:452:GLN:CB	2.78	0.54
1:A:563:GLU:HG3	4:A:773:HOH:O	2.07	0.54
1:E:635:MET:H	1:G:477:ASN:HD22	1.56	0.54
1:G:296:ASP:OD1	1:G:299:ARG:NH1	2.38	0.54
1:B:477:ASN:HD22	1:G:635:MET:H	1.56	0.54
1:C:496:ASN:ND2	1:F:585:GLN:HE22	2.03	0.54
1:C:512:ASN:ND2	1:F:529:ASP:H	2.03	0.54
1:H:480:PRO:O	1:H:605:MET:HG2	2.08	0.54
1:H:717:ASN:ND2	1:H:717:ASN:H	2.04	0.54
1:I:280:TRP:NE1	1:I:650:LYS:HD3	2.22	0.54
1:A:328:ASP:HB3	1:A:329:GLY:HA3	1.89	0.54
1:C:480:PRO:O	1:C:605:MET:HG2	2.08	0.54
1:F:717:ASN:ND2	1:F:717:ASN:H	2.04	0.54
1:I:452:GLN:O	1:I:454:GLY:CA	2.53	0.54
1:E:512:ASN:ND2	1:G:529:ASP:H	2.03	0.54
1:I:296:ASP:OD1	1:I:299:ARG:NH1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:615:GLN:H	1:G:615:GLN:HE21	1.55	0.54
1:B:512:ASN:ND2	1:E:529:ASP:H	2.03	0.54
1:G:666:LYS:NZ	1:J:719:GLY:O	2.41	0.54
1:F:480:PRO:O	1:F:605:MET:HG2	2.08	0.54
1:C:380:THR:CG2	1:C:392:SER:H	2.09	0.53
1:C:563:GLU:HG3	4:C:773:HOH:O	2.07	0.53
1:B:635:MET:H	1:E:477:ASN:HD22	1.55	0.53
1:B:615:GLN:H	1:B:615:GLN:HE21	1.55	0.53
1:C:615:GLN:HE21	1:C:615:GLN:H	1.55	0.53
1:I:570:ASN:ND2	1:I:608:GLN:H	2.02	0.53
1:F:353:TYR:CE2	1:F:355:LEU:HB2	2.44	0.53
1:G:353:TYR:CE2	1:G:355:LEU:HB2	2.44	0.53
1:J:353:TYR:CE2	1:J:355:LEU:HB2	2.44	0.53
1:C:477:ASN:HD22	1:I:635:MET:H	1.56	0.53
1:B:563:GLU:HG3	4:B:773:HOH:O	2.07	0.53
1:B:639:GLY:O	2:B:737:ADE:C2	2.61	0.53
1:E:353:TYR:CE2	1:E:355:LEU:HB2	2.44	0.53
1:C:302:ASN:HD21	1:C:701:TYR:H	1.54	0.53
1:C:585:GLN:HE22	1:I:496:ASN:ND2	2.02	0.53
1:A:353:TYR:CE2	1:A:355:LEU:HB2	2.44	0.53
1:C:353:TYR:CE2	1:C:355:LEU:HB2	2.44	0.53
1:F:380:THR:CG2	1:F:392:SER:H	2.09	0.53
1:H:302:ASN:HD21	1:H:701:TYR:H	1.54	0.53
1:B:626:ASP:H	1:E:608:GLN:NE2	2.07	0.53
1:F:270:ASP:HA	1:F:514:ARG:HG2	1.91	0.53
1:C:280:TRP:CE2	1:C:650:LYS:HD3	2.44	0.53
1:A:433:ARG:NH1	1:H:272:HIS:O	2.42	0.53
1:D:280:TRP:CE2	1:D:650:LYS:HD3	2.44	0.53
1:A:280:TRP:CE2	1:A:650:LYS:HD3	2.44	0.53
1:A:500:ASN:ND2	1:D:449:THR:H	2.07	0.53
1:H:353:TYR:CE2	1:H:355:LEU:HB2	2.44	0.53
1:J:264:SER:O	1:J:266:GLY:N	2.37	0.53
1:B:380:THR:CG2	1:B:392:SER:H	2.09	0.53
1:A:635:MET:H	1:D:477:ASN:HD22	1.55	0.53
1:B:480:PRO:O	1:B:605:MET:HG2	2.08	0.53
1:J:270:ASP:HA	1:J:514:ARG:HG2	1.91	0.53
1:I:264:SER:O	1:I:266:GLY:N	2.37	0.53
1:J:615:GLN:H	1:J:615:GLN:HE21	1.55	0.53
1:A:626:ASP:H	1:D:608:GLN:NE2	2.07	0.52
1:A:457:GLN:NE2	1:A:457:GLN:H	2.01	0.52
1:D:272:HIS:O	1:H:433:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:TYR:CE2	1:B:355:LEU:HB2	2.44	0.52
1:C:270:ASP:HA	1:C:514:ARG:HG2	1.91	0.52
1:H:280:TRP:CE2	1:H:650:LYS:HD3	2.44	0.52
1:C:608:GLN:NE2	1:I:626:ASP:H	2.07	0.52
1:D:296:ASP:OD1	1:D:299:ARG:NH1	2.38	0.52
1:A:270:ASP:HA	1:A:514:ARG:HG2	1.91	0.52
1:B:433:ARG:NH1	1:G:272:HIS:O	2.42	0.52
1:F:272:HIS:O	1:I:433:ARG:NH1	2.43	0.52
1:D:353:TYR:CE2	1:D:355:LEU:HB2	2.44	0.52
1:D:512:ASN:ND2	1:H:529:ASP:H	2.02	0.52
1:C:500:ASN:ND2	1:F:449:THR:H	2.07	0.52
1:J:280:TRP:CE2	1:J:650:LYS:HD3	2.44	0.52
1:F:626:ASP:H	1:I:608:GLN:NE2	2.07	0.52
1:C:626:ASP:H	1:F:608:GLN:NE2	2.07	0.52
1:D:496:ASN:ND2	1:H:585:GLN:HE22	2.02	0.52
1:F:496:ASN:ND2	1:I:585:GLN:HE22	2.03	0.52
1:I:270:ASP:HA	1:I:514:ARG:HG2	1.91	0.52
1:E:280:TRP:CE2	1:E:650:LYS:HD3	2.44	0.52
1:F:500:ASN:ND2	1:I:449:THR:H	2.07	0.52
1:G:612:VAL:HA	4:G:842:HOH:O	2.10	0.52
1:I:402:GLN:HG2	1:I:404:LEU:HD12	1.91	0.52
1:E:626:ASP:H	1:G:608:GLN:NE2	2.07	0.52
4:E:843:HOH:O	1:G:735:PRO:HD3	2.10	0.52
1:D:270:ASP:HA	1:D:514:ARG:HG2	1.91	0.52
1:B:280:TRP:CE2	1:B:650:LYS:HD3	2.44	0.52
1:B:608:GLN:NE2	1:G:626:ASP:H	2.07	0.52
1:B:449:THR:H	1:G:500:ASN:ND2	2.07	0.52
1:C:433:ARG:NH2	4:C:869:HOH:O	2.43	0.52
1:F:280:TRP:CE2	1:F:650:LYS:HD3	2.44	0.52
1:A:304:ASN:HD21	1:A:689:LYS:HZ1	1.54	0.52
1:I:353:TYR:CE2	1:I:355:LEU:HB2	2.44	0.52
1:D:635:MET:H	1:H:477:ASN:HD22	1.55	0.52
1:A:272:HIS:O	1:D:433:ARG:NH1	2.43	0.52
1:B:552:ASN:HD21	1:E:447:ASN:ND2	2.08	0.52
1:B:500:ASN:ND2	1:E:449:THR:H	2.07	0.52
1:A:449:THR:H	1:H:500:ASN:ND2	2.07	0.52
1:E:272:HIS:O	1:G:433:ARG:NH1	2.42	0.52
1:J:217:GLY:HA3	1:J:408:ASN:HA	1.92	0.52
1:E:270:ASP:HA	1:E:514:ARG:HG2	1.91	0.52
1:C:449:THR:H	1:I:500:ASN:ND2	2.08	0.52
1:C:433:ARG:NH1	1:I:272:HIS:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ASN:ND2	1:A:608:GLN:H	2.02	0.51
1:H:218:ALA:C	1:H:219:ASP:OD1	2.49	0.51
1:A:249:LEU:HB2	1:A:373:ILE:HD12	1.93	0.51
1:A:447:ASN:ND2	1:H:552:ASN:HD21	2.08	0.51
1:D:626:ASP:H	1:H:608:GLN:NE2	2.07	0.51
1:A:552:ASN:HD21	1:D:447:ASN:ND2	2.08	0.51
1:H:433:ARG:NH2	4:H:871:HOH:O	2.43	0.51
1:G:270:ASP:HA	1:G:514:ARG:HG2	1.91	0.51
1:B:451:ASN:CB	1:B:452:GLN:HB3	2.41	0.51
1:G:280:TRP:CG	1:G:396:LEU:HD22	2.45	0.51
1:E:500:ASN:ND2	1:G:449:THR:H	2.07	0.51
1:F:264:SER:O	1:F:265:THR:HB	2.11	0.51
1:I:433:ARG:NH2	4:I:873:HOH:O	2.43	0.51
1:H:270:ASP:HA	1:H:514:ARG:HG2	1.91	0.51
1:F:218:ALA:C	1:F:219:ASP:OD1	2.49	0.51
1:A:286:ASN:ND2	1:A:618:ILE:HB	2.26	0.51
1:C:529:ASP:H	1:I:512:ASN:ND2	2.01	0.51
1:B:286:ASN:ND2	1:B:618:ILE:HB	2.26	0.51
1:C:286:ASN:ND2	1:C:618:ILE:HB	2.26	0.51
1:F:249:LEU:HB2	1:F:373:ILE:HD12	1.93	0.51
1:E:563:GLU:HG3	4:E:775:HOH:O	2.10	0.51
1:G:433:ARG:NH2	4:G:871:HOH:O	2.43	0.51
1:B:451:ASN:CB	1:B:452:GLN:CB	2.89	0.51
1:E:451:ASN:CB	1:E:452:GLN:HB3	2.41	0.51
1:D:451:ASN:CB	1:D:452:GLN:HB3	2.41	0.51
1:C:529:ASP:O	1:C:530:ASP:HB2	2.11	0.51
1:D:286:ASN:ND2	1:D:618:ILE:HB	2.26	0.51
1:B:447:ASN:ND2	1:G:552:ASN:HD21	2.09	0.51
1:A:433:ARG:NH2	4:A:868:HOH:O	2.43	0.51
1:H:451:ASN:CB	1:H:452:GLN:CB	2.89	0.51
1:J:451:ASN:CB	1:J:452:GLN:HB3	2.41	0.51
1:B:326:THR:HG23	1:B:327:ASN:O	2.07	0.51
1:E:433:ARG:NH2	4:E:871:HOH:O	2.43	0.51
1:G:529:ASP:O	1:G:530:ASP:HB2	2.11	0.51
1:J:249:LEU:HB2	1:J:373:ILE:HD12	1.93	0.51
1:J:433:ARG:NH2	4:J:873:HOH:O	2.43	0.51
1:I:249:LEU:HB2	1:I:373:ILE:HD12	1.92	0.51
1:G:451:ASN:CB	1:G:452:GLN:HB3	2.41	0.51
1:A:608:GLN:NE2	1:H:626:ASP:H	2.08	0.51
1:F:552:ASN:HD21	1:I:447:ASN:ND2	2.08	0.51
1:G:280:TRP:CD1	1:G:396:LEU:HD22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:ASN:HD21	1:F:447:ASN:ND2	2.08	0.51
1:G:249:LEU:HB2	1:G:373:ILE:HD12	1.93	0.51
1:C:249:LEU:HB2	1:C:373:ILE:HD12	1.93	0.51
1:H:217:GLY:O	1:H:408:ASN:ND2	2.34	0.51
1:D:536:PRO:HG3	1:D:573:ALA:HB3	1.93	0.51
1:A:536:PRO:HG3	1:A:573:ALA:HB3	1.93	0.51
1:E:529:ASP:O	1:E:530:ASP:HB2	2.11	0.51
1:G:286:ASN:ND2	1:G:618:ILE:HB	2.26	0.51
1:I:563:GLU:OE2	1:I:611:ASP:CB	2.59	0.51
1:B:249:LEU:HB2	1:B:373:ILE:HD12	1.93	0.51
1:C:536:PRO:HG3	1:C:573:ALA:HB3	1.93	0.51
1:E:286:ASN:ND2	1:E:618:ILE:HB	2.26	0.50
1:J:286:ASN:ND2	1:J:618:ILE:HB	2.26	0.50
1:D:552:ASN:HD21	1:H:447:ASN:ND2	2.08	0.50
1:H:563:GLU:OE2	1:H:611:ASP:CB	2.59	0.50
1:C:270:ASP:OD2	1:C:503:TRP:HZ2	1.94	0.50
1:C:272:HIS:O	1:F:433:ARG:NH1	2.43	0.50
1:G:563:GLU:OE2	1:G:611:ASP:CB	2.59	0.50
1:F:286:ASN:ND2	1:F:618:ILE:HB	2.26	0.50
1:D:249:LEU:HB2	1:D:373:ILE:HD12	1.92	0.50
1:I:404:LEU:HA	1:I:408:ASN:HD22	1.74	0.50
1:G:559:MET:SD	1:G:725:ARG:HA	2.51	0.50
1:B:663:SER:HG	1:B:665:THR:CG2	2.16	0.50
1:B:496:ASN:ND2	1:E:585:GLN:HE22	2.03	0.50
1:A:529:ASP:O	1:A:530:ASP:HB2	2.11	0.50
1:H:501:PHE:O	1:H:505:GLY:N	2.31	0.50
1:F:563:GLU:OE2	1:F:611:ASP:CB	2.59	0.50
1:E:296:ASP:OD1	1:E:299:ARG:NH1	2.38	0.50
1:G:703:SER:HB2	4:G:742:HOH:O	2.11	0.50
1:J:529:ASP:O	1:J:530:ASP:HB2	2.11	0.50
1:H:451:ASN:CB	1:H:452:GLN:HB3	2.41	0.50
1:I:455:SER:HB3	1:I:456:ALA:HB2	1.92	0.50
1:B:585:GLN:HE22	1:G:496:ASN:ND2	2.03	0.50
1:D:529:ASP:O	1:D:530:ASP:HB2	2.11	0.50
1:D:500:ASN:ND2	1:H:449:THR:H	2.08	0.50
1:E:249:LEU:HB2	1:E:373:ILE:HD12	1.93	0.50
1:D:451:ASN:CB	1:D:452:GLN:CB	2.89	0.50
1:C:451:ASN:ND2	1:C:458:ASN:HB2	2.23	0.50
1:I:451:ASN:O	1:I:451:ASN:OD1	2.30	0.50
1:B:563:GLU:OE2	1:B:611:ASP:CB	2.60	0.50
1:H:536:PRO:HG3	1:H:573:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:ASN:CB	1:E:452:GLN:CB	2.89	0.50
1:F:451:ASN:HA	1:F:452:GLN:HB3	1.65	0.50
1:I:529:ASP:O	1:I:530:ASP:HB2	2.11	0.50
1:E:552:ASN:HD21	1:G:447:ASN:ND2	2.08	0.50
1:D:433:ARG:NH2	4:D:871:HOH:O	2.43	0.50
1:F:297:TRP:O	1:F:301:ILE:HG12	2.12	0.50
1:I:280:TRP:CE2	1:I:650:LYS:CD	2.90	0.50
1:J:451:ASN:CB	1:J:452:GLN:CB	2.89	0.50
1:F:218:ALA:O	1:F:219:ASP:OD1	2.30	0.50
1:H:286:ASN:ND2	1:H:618:ILE:HB	2.26	0.50
1:J:563:GLU:OE2	1:J:611:ASP:CB	2.59	0.50
1:E:268:SER:O	1:E:269:ASN:C	2.48	0.50
1:E:703:SER:HB2	4:E:741:HOH:O	2.12	0.50
1:A:496:ASN:ND2	1:D:585:GLN:HE22	2.03	0.50
1:H:529:ASP:O	1:H:530:ASP:HB2	2.11	0.50
1:E:218:ALA:O	1:E:219:ASP:HB2	2.12	0.50
1:D:563:GLU:OE2	1:D:611:ASP:CB	2.59	0.50
1:C:447:ASN:ND2	1:I:552:ASN:HD21	2.08	0.50
1:B:570:ASN:ND2	1:B:608:GLN:H	2.02	0.49
1:I:286:ASN:ND2	1:I:618:ILE:HB	2.26	0.49
1:H:354:VAL:O	1:H:354:VAL:HG13	2.12	0.49
1:B:296:ASP:OD1	1:B:299:ARG:NH1	2.38	0.49
1:B:433:ARG:NH2	4:B:868:HOH:O	2.43	0.49
1:F:536:PRO:HG3	1:F:573:ALA:HB3	1.93	0.49
1:D:715:VAL:HG21	1:F:257:TYR:O	2.12	0.49
1:E:563:GLU:OE2	1:E:611:ASP:CB	2.60	0.49
1:C:563:GLU:OE2	1:C:611:ASP:CB	2.59	0.49
1:J:536:PRO:HG3	1:J:573:ALA:HB3	1.94	0.49
1:F:529:ASP:O	1:F:530:ASP:HB2	2.11	0.49
1:E:715:VAL:HG21	1:H:257:TYR:O	2.12	0.49
1:G:714:THR:HG22	1:G:715:VAL:O	2.12	0.49
1:A:563:GLU:OE2	1:A:611:ASP:CB	2.59	0.49
1:H:249:LEU:HB2	1:H:373:ILE:HD12	1.93	0.49
1:J:580:VAL:HG23	1:J:596:VAL:CG2	2.43	0.49
1:J:714:THR:HG22	1:J:715:VAL:O	2.12	0.49
1:B:529:ASP:O	1:B:530:ASP:HB2	2.11	0.49
1:C:304:ASN:HD21	1:C:689:LYS:HZ1	1.57	0.49
1:B:536:PRO:HG3	1:B:573:ALA:HB3	1.93	0.49
1:D:714:THR:HG22	1:D:715:VAL:O	2.13	0.49
1:E:496:ASN:ND2	1:G:585:GLN:HE22	2.03	0.49
1:B:714:THR:HG22	1:B:715:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:354:VAL:HG13	1:I:354:VAL:O	2.12	0.49
1:J:264:SER:OG	1:J:265:THR:N	2.46	0.49
1:G:536:PRO:HG3	1:G:573:ALA:HB3	1.93	0.49
1:A:451:ASN:OD1	1:A:451:ASN:O	2.30	0.49
1:G:451:ASN:CB	1:G:452:GLN:CB	2.89	0.49
1:H:570:ASN:ND2	1:H:608:GLN:H	2.02	0.49
1:C:304:ASN:HD21	1:C:689:LYS:HZ3	1.58	0.49
1:C:270:ASP:OD2	1:C:503:TRP:CZ2	2.65	0.49
1:I:396:LEU:HD12	1:I:396:LEU:N	2.27	0.49
1:H:580:VAL:HG23	1:H:596:VAL:CG2	2.43	0.49
1:E:580:VAL:HG23	1:E:596:VAL:CG2	2.42	0.49
1:D:615:GLN:NE2	1:D:615:GLN:H	2.11	0.49
1:E:536:PRO:HG3	1:E:573:ALA:HB3	1.93	0.49
1:H:316:LEU:HB2	1:H:410:PHE:HB3	1.95	0.49
1:I:580:VAL:HG23	1:I:596:VAL:CG2	2.43	0.49
1:J:283:PHE:CZ	1:J:316:LEU:HD21	2.48	0.49
1:J:316:LEU:HB2	1:J:410:PHE:HB3	1.95	0.49
1:G:283:PHE:CZ	1:G:316:LEU:HD21	2.48	0.49
1:I:316:LEU:HB2	1:I:410:PHE:HB3	1.95	0.49
1:G:278:THR:HG23	1:G:280:TRP:HD1	1.78	0.49
1:A:715:VAL:HG21	1:B:257:TYR:O	2.13	0.49
1:E:714:THR:HG22	1:E:715:VAL:O	2.12	0.49
1:I:714:THR:HG22	1:I:715:VAL:O	2.12	0.49
1:B:615:GLN:NE2	1:B:615:GLN:H	2.11	0.49
1:J:615:GLN:NE2	1:J:615:GLN:H	2.11	0.49
1:H:283:PHE:CZ	1:H:316:LEU:HD21	2.48	0.49
1:D:283:PHE:CZ	1:D:316:LEU:HD21	2.48	0.49
1:C:316:LEU:HB2	1:C:410:PHE:HB3	1.95	0.49
1:H:264:SER:O	1:H:266:GLY:N	2.36	0.49
1:A:283:PHE:CZ	1:A:316:LEU:HD21	2.48	0.49
1:A:580:VAL:HG23	1:A:596:VAL:CG2	2.43	0.49
1:C:714:THR:HG22	1:C:715:VAL:O	2.12	0.49
1:G:316:LEU:HB2	1:G:410:PHE:HB3	1.95	0.49
1:G:580:VAL:HG23	1:G:596:VAL:CG2	2.43	0.49
1:A:354:VAL:HG13	1:A:354:VAL:O	2.12	0.49
1:G:218:ALA:HB1	1:G:219:ASP:OD1	2.13	0.49
1:D:327:ASN:O	1:D:330:VAL:N	2.43	0.48
1:A:529:ASP:H	1:H:512:ASN:ND2	2.03	0.48
1:F:580:VAL:HG23	1:F:596:VAL:CG2	2.43	0.48
1:C:296:ASP:OD1	1:C:299:ARG:NH1	2.38	0.48
1:H:714:THR:HG22	1:H:715:VAL:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:PHE:CZ	1:I:316:LEU:HD21	2.48	0.48
1:B:580:VAL:HG23	1:B:596:VAL:CG2	2.43	0.48
1:B:316:LEU:HB2	1:B:410:PHE:HB3	1.95	0.48
1:E:283:PHE:CZ	1:E:316:LEU:HD21	2.48	0.48
1:J:357:SER:HB3	1:J:359:HIS:CE1	2.49	0.48
1:A:328:ASP:CB	1:A:329:GLY:CA	2.91	0.48
1:A:714:THR:HG22	1:A:715:VAL:O	2.12	0.48
1:G:257:TYR:O	1:J:715:VAL:HG21	2.13	0.48
1:B:354:VAL:HG13	1:B:354:VAL:O	2.12	0.48
1:E:354:VAL:O	1:E:354:VAL:HG13	2.13	0.48
1:E:615:GLN:NE2	1:E:615:GLN:H	2.11	0.48
1:I:615:GLN:H	1:I:615:GLN:NE2	2.11	0.48
1:C:283:PHE:CZ	1:C:316:LEU:HD21	2.48	0.48
1:B:283:PHE:CZ	1:B:316:LEU:HD21	2.48	0.48
1:D:580:VAL:HG23	1:D:596:VAL:CG2	2.43	0.48
1:I:380:THR:CG2	1:I:392:SER:H	2.09	0.48
1:F:714:THR:HG22	1:F:715:VAL:O	2.12	0.48
1:J:354:VAL:O	1:J:354:VAL:HG13	2.12	0.48
1:A:615:GLN:H	1:A:615:GLN:NE2	2.11	0.48
1:D:703:SER:HB2	4:D:741:HOH:O	2.13	0.48
1:D:304:ASN:HD21	1:D:689:LYS:HZ3	1.61	0.48
1:F:354:VAL:O	1:F:354:VAL:HG13	2.12	0.48
1:D:218:ALA:O	1:D:219:ASP:CB	2.61	0.48
1:B:639:GLY:O	2:B:737:ADE:H2	1.95	0.48
1:H:230:CYS:HB2	1:H:244:THR:CG2	2.43	0.48
1:C:580:VAL:HG23	1:C:596:VAL:CG2	2.43	0.48
1:B:437:PRO:HG3	1:G:379:LEU:HG	1.95	0.48
1:F:283:PHE:CZ	1:F:316:LEU:HD21	2.48	0.48
1:F:316:LEU:HB2	1:F:410:PHE:HB3	1.95	0.48
1:B:326:THR:HG22	1:B:327:ASN:C	2.30	0.48
1:A:585:GLN:HE22	1:H:496:ASN:ND2	2.03	0.48
1:H:666:LYS:O	1:H:666:LYS:HG2	2.12	0.48
1:H:615:GLN:NE2	1:H:615:GLN:H	2.11	0.48
1:C:615:GLN:NE2	1:C:615:GLN:H	2.11	0.48
1:C:218:ALA:O	1:C:219:ASP:OD1	2.30	0.48
1:C:379:LEU:HG	1:F:437:PRO:HG3	1.96	0.48
1:A:379:LEU:HG	1:D:437:PRO:HG3	1.96	0.48
1:I:536:PRO:HG3	1:I:573:ALA:HB3	1.93	0.48
3:J:738:CYT:N4	4:J:769:HOH:O	2.23	0.48
1:D:354:VAL:O	1:D:354:VAL:HG13	2.12	0.48
1:C:264:SER:HG	1:C:265:THR:H	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:615:GLN:H	1:F:615:GLN:NE2	2.11	0.48
1:G:615:GLN:H	1:G:615:GLN:NE2	2.11	0.48
1:A:399:PHE:N	1:A:399:PHE:CD1	2.82	0.48
1:E:380:THR:CG2	1:E:392:SER:H	2.09	0.48
1:F:570:ASN:ND2	1:F:608:GLN:H	2.02	0.48
1:A:257:TYR:O	1:I:715:VAL:HG21	2.13	0.48
1:G:354:VAL:O	1:G:354:VAL:HG13	2.12	0.48
1:E:316:LEU:HB2	1:E:410:PHE:HB3	1.95	0.48
1:A:346:ASP:OD2	1:A:351:LEU:HB2	2.14	0.48
1:B:346:ASP:OD2	1:B:351:LEU:HB2	2.14	0.48
1:A:257:TYR:OH	1:A:397:GLU:OE1	2.28	0.47
1:D:635:MET:HB2	1:H:477:ASN:ND2	2.29	0.47
1:I:249:LEU:HD21	1:I:650:LYS:HA	1.97	0.47
1:H:380:THR:CG2	1:H:392:SER:H	2.09	0.47
1:C:635:MET:HB2	1:F:477:ASN:ND2	2.30	0.47
1:G:342:GLN:C	1:G:343:VAL:HG23	2.35	0.47
1:H:346:ASP:OD2	1:H:351:LEU:HB2	2.14	0.47
1:E:346:ASP:OD2	1:E:351:LEU:HB2	2.14	0.47
1:B:379:LEU:HG	1:E:437:PRO:HG3	1.96	0.47
1:F:379:LEU:HG	1:I:437:PRO:HG3	1.96	0.47
1:J:383:ASN:ND2	1:J:383:ASN:C	2.68	0.47
1:C:354:VAL:O	1:C:354:VAL:HG13	2.12	0.47
1:F:635:MET:HB2	1:I:477:ASN:ND2	2.29	0.47
1:G:346:ASP:OD2	1:G:351:LEU:HB2	2.14	0.47
1:C:451:ASN:CB	1:C:452:GLN:HB3	2.45	0.47
1:I:454:GLY:O	1:I:455:SER:OG	2.30	0.47
1:E:570:ASN:ND2	1:E:608:GLN:H	2.02	0.47
1:A:262:SER:O	1:A:265:THR:HB	2.14	0.47
1:B:635:MET:HB2	1:E:477:ASN:ND2	2.29	0.47
1:D:316:LEU:HB2	1:D:410:PHE:HB3	1.95	0.47
1:E:379:LEU:HG	1:G:437:PRO:HG3	1.96	0.47
1:B:262:SER:O	1:B:265:THR:HB	2.13	0.47
1:J:425:TYR:O	1:J:730:ARG:HG2	2.15	0.47
1:F:397:GLU:OE2	1:F:650:LYS:NZ	2.32	0.47
1:D:264:SER:O	1:D:265:THR:HB	2.14	0.47
1:I:218:ALA:HB1	1:I:219:ASP:OD1	2.13	0.47
1:B:383:ASN:C	1:B:383:ASN:ND2	2.68	0.47
1:A:449:THR:HG21	1:H:501:PHE:CZ	2.50	0.47
1:A:477:ASN:ND2	1:H:635:MET:HB2	2.29	0.47
1:E:635:MET:HB2	1:G:477:ASN:ND2	2.30	0.47
1:E:342:GLN:C	1:E:343:VAL:HG23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:TYR:O	1:B:730:ARG:HG2	2.15	0.47
1:C:330:VAL:CG2	1:C:331:THR:N	2.78	0.47
1:H:330:VAL:CG2	1:H:331:THR:N	2.78	0.47
1:F:295:ARG:HH11	1:F:298:GLN:NE2	2.13	0.47
1:C:477:ASN:ND2	1:I:635:MET:HB2	2.30	0.47
1:A:635:MET:HB2	1:D:477:ASN:ND2	2.30	0.47
1:D:379:LEU:HG	1:H:437:PRO:HG3	1.96	0.47
1:G:425:TYR:O	1:G:730:ARG:HG2	2.15	0.47
1:G:264:SER:OG	1:G:265:THR:N	2.47	0.47
1:C:425:TYR:O	1:C:730:ARG:HG2	2.15	0.47
1:I:346:ASP:OD2	1:I:351:LEU:HB2	2.14	0.47
1:D:346:ASP:OD2	1:D:351:LEU:HB2	2.14	0.47
1:G:383:ASN:ND2	1:G:383:ASN:C	2.68	0.47
1:H:342:GLN:C	1:H:343:VAL:HG23	2.35	0.47
1:J:346:ASP:OD2	1:J:351:LEU:HB2	2.14	0.47
1:F:635:MET:HB2	1:I:477:ASN:HD21	1.80	0.47
1:A:316:LEU:HB2	1:A:410:PHE:HB3	1.95	0.47
1:A:425:TYR:O	1:A:730:ARG:HG2	2.15	0.47
1:H:425:TYR:O	1:H:730:ARG:HG2	2.15	0.47
1:J:342:GLN:C	1:J:343:VAL:HG23	2.35	0.47
1:A:383:ASN:C	1:A:383:ASN:ND2	2.68	0.47
1:D:383:ASN:ND2	1:D:383:ASN:C	2.68	0.47
1:H:383:ASN:C	1:H:383:ASN:ND2	2.68	0.47
1:F:425:TYR:O	1:F:730:ARG:HG2	2.15	0.47
1:I:342:GLN:C	1:I:343:VAL:HG23	2.35	0.47
1:A:437:PRO:HG3	1:H:379:LEU:HG	1.96	0.47
1:I:425:TYR:O	1:I:730:ARG:HG2	2.15	0.47
1:A:328:ASP:OD1	1:A:329:GLY:HA2	2.09	0.46
1:F:217:GLY:HA3	1:F:408:ASN:CB	2.45	0.46
1:E:425:TYR:O	1:E:730:ARG:HG2	2.15	0.46
1:G:380:THR:CG2	1:G:392:SER:H	2.09	0.46
1:D:278:THR:HG22	1:D:280:TRP:N	2.15	0.46
1:D:425:TYR:O	1:D:730:ARG:HG2	2.15	0.46
1:G:330:VAL:CG2	1:G:331:THR:N	2.78	0.46
1:I:456:ALA:C	1:I:457:GLN:CD	2.74	0.46
1:B:226:GLY:HA3	1:B:317:PHE:CD2	2.51	0.46
1:I:229:HIS:HE1	4:I:810:HOH:O	1.97	0.46
1:D:570:ASN:ND2	1:D:608:GLN:H	2.02	0.46
1:F:342:GLN:C	1:F:343:VAL:HG23	2.35	0.46
1:F:346:ASP:OD2	1:F:351:LEU:HB2	2.14	0.46
1:E:459:LYS:NZ	1:E:587:SER:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ASP:OD2	1:C:351:LEU:HB2	2.14	0.46
1:G:459:LYS:NZ	1:G:587:SER:HB3	2.31	0.46
1:F:736:LEU:HA	1:F:736:LEU:HD13	1.82	0.46
1:A:217:GLY:O	1:A:218:ALA:CB	2.63	0.46
1:C:218:ALA:C	1:C:219:ASP:OD1	2.54	0.46
1:C:399:PHE:CE2	1:F:693:LYS:HG3	2.50	0.46
1:B:342:GLN:C	1:B:343:VAL:HG23	2.35	0.46
1:D:342:GLN:C	1:D:343:VAL:HG23	2.35	0.46
1:C:451:ASN:CB	1:C:452:GLN:CB	2.93	0.46
1:A:278:THR:HG22	1:A:280:TRP:N	2.15	0.46
1:J:570:ASN:ND2	1:J:608:GLN:H	2.02	0.46
1:C:263:ALA:O	1:C:264:SER:HB3	2.15	0.46
1:B:477:ASN:ND2	1:G:635:MET:HB2	2.30	0.46
1:H:226:GLY:HA3	1:H:317:PHE:CD2	2.51	0.46
1:C:342:GLN:C	1:C:343:VAL:HG23	2.35	0.46
1:I:304:ASN:HD21	1:I:689:LYS:HZ3	1.63	0.46
1:D:264:SER:OG	1:D:265:THR:N	2.49	0.46
1:G:619:TRP:C	1:G:619:TRP:CD1	2.89	0.46
1:C:262:SER:OG	1:C:272:HIS:HA	2.16	0.46
1:C:437:PRO:HG3	1:I:379:LEU:HG	1.96	0.46
1:I:459:LYS:NZ	1:I:587:SER:HB3	2.31	0.46
1:F:226:GLY:HA3	1:F:317:PHE:CD2	2.51	0.46
1:I:328:ASP:O	1:I:328:ASP:OD1	2.34	0.46
1:J:619:TRP:C	1:J:619:TRP:CD1	2.89	0.46
1:F:619:TRP:CD1	1:F:619:TRP:C	2.89	0.46
1:H:365:PRO:HD2	4:H:759:HOH:O	2.16	0.46
1:E:365:PRO:HD2	4:E:758:HOH:O	2.16	0.46
1:A:477:ASN:HD21	1:H:635:MET:HB2	1.81	0.46
1:E:635:MET:HB2	1:G:477:ASN:HD21	1.81	0.46
1:D:635:MET:HB2	1:H:477:ASN:HD21	1.80	0.46
1:E:628:HIS:O	3:E:738:CYT:N1	2.49	0.46
1:C:226:GLY:HA3	1:C:317:PHE:CD2	2.51	0.46
1:C:459:LYS:NZ	1:C:587:SER:HB3	2.31	0.46
1:I:666:LYS:HG2	1:I:666:LYS:O	2.16	0.46
1:A:619:TRP:CD1	1:A:619:TRP:C	2.89	0.46
1:A:635:MET:HB2	1:D:477:ASN:HD21	1.81	0.46
1:F:359:HIS:NE2	1:I:436:ASN:N	2.55	0.46
1:A:342:GLN:C	1:A:343:VAL:HG23	2.35	0.46
1:J:226:GLY:HA3	1:J:317:PHE:CD2	2.51	0.46
1:E:619:TRP:C	1:E:619:TRP:CD1	2.89	0.46
1:H:619:TRP:CD1	1:H:619:TRP:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:MET:HB2	1:F:477:ASN:HD21	1.81	0.46
1:D:459:LYS:NZ	1:D:587:SER:HB3	2.31	0.46
1:J:736:LEU:HA	1:J:736:LEU:HD13	1.83	0.45
1:C:619:TRP:CD1	1:C:619:TRP:C	2.89	0.45
1:G:263:ALA:O	1:G:264:SER:HB3	2.15	0.45
1:I:226:GLY:HA3	1:I:317:PHE:CD2	2.51	0.45
1:A:459:LYS:NZ	1:A:587:SER:HB3	2.31	0.45
1:I:254:ASN:O	1:I:255:HIS:CB	2.63	0.45
1:B:635:MET:HB2	1:E:477:ASN:HD21	1.80	0.45
1:H:264:SER:OG	1:H:265:THR:N	2.49	0.45
1:I:365:PRO:HD2	4:I:760:HOH:O	2.16	0.45
1:B:477:ASN:HD21	1:G:635:MET:HB2	1.81	0.45
1:J:459:LYS:NZ	1:J:587:SER:HB3	2.31	0.45
1:J:398:TYR:CG	1:J:398:TYR:O	2.69	0.45
1:G:226:GLY:HA3	1:G:317:PHE:CD2	2.51	0.45
1:H:459:LYS:NZ	1:H:587:SER:HB3	2.31	0.45
1:I:397:GLU:CD	1:I:650:LYS:HE2	2.27	0.45
1:D:380:THR:CG2	1:D:392:SER:H	2.09	0.45
1:J:263:ALA:O	1:J:264:SER:HB3	2.17	0.45
1:G:264:SER:O	1:G:265:THR:HB	2.15	0.45
1:E:267:ALA:HB1	1:E:271:ASN:HB2	1.98	0.45
1:D:226:GLY:HA3	1:D:317:PHE:CD2	2.51	0.45
1:E:226:GLY:HA3	1:E:317:PHE:CD2	2.51	0.45
1:A:226:GLY:HA3	1:A:317:PHE:CD2	2.51	0.45
1:B:619:TRP:CD1	1:B:619:TRP:C	2.89	0.45
1:D:619:TRP:C	1:D:619:TRP:CD1	2.89	0.45
1:E:286:ASN:HD21	1:E:619:TRP:N	2.13	0.45
1:C:257:TYR:OH	1:C:397:GLU:OE1	2.23	0.45
1:B:262:SER:O	1:B:265:THR:CB	2.65	0.45
1:B:272:HIS:O	1:E:433:ARG:NH1	2.49	0.45
1:G:570:ASN:ND2	1:G:608:GLN:H	2.02	0.45
1:I:619:TRP:C	1:I:619:TRP:CD1	2.89	0.45
1:H:286:ASN:HD21	1:H:619:TRP:N	2.13	0.45
1:B:459:LYS:NZ	1:B:587:SER:HB3	2.31	0.45
1:A:512:ASN:ND2	1:D:529:ASP:H	2.03	0.45
1:C:477:ASN:HD21	1:I:635:MET:HB2	1.81	0.45
1:D:396:LEU:HD12	1:D:396:LEU:N	2.31	0.45
1:I:487:GLN:NE2	1:I:488:ARG:H	2.15	0.45
1:B:512:ASN:HD21	1:E:529:ASP:N	2.07	0.45
1:E:218:ALA:C	1:E:219:ASP:CG	2.75	0.45
1:H:305:TRP:CE3	1:H:734:ARG:NH2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:ASP:OD1	1:F:299:ARG:NH1	2.41	0.45
1:A:487:GLN:NE2	1:A:488:ARG:H	2.15	0.45
1:D:217:GLY:O	1:D:218:ALA:HB3	2.15	0.45
1:F:666:LYS:HG2	1:F:666:LYS:O	2.17	0.45
1:B:305:TRP:CE3	1:B:734:ARG:NH2	2.85	0.45
1:G:305:TRP:CE3	1:G:734:ARG:NH2	2.85	0.45
1:I:305:TRP:CE3	1:I:734:ARG:NH2	2.85	0.45
1:F:621:LYS:HB2	1:F:643:PRO:HG3	1.99	0.45
1:C:444:TYR:CE1	1:I:544:GLY:HA3	2.52	0.45
1:D:487:GLN:NE2	1:D:488:ARG:H	2.15	0.45
1:B:487:GLN:NE2	1:B:488:ARG:H	2.15	0.45
1:B:379:LEU:HD21	1:E:437:PRO:HB3	1.99	0.45
1:E:379:LEU:HD21	1:G:437:PRO:HB3	1.99	0.45
1:C:621:LYS:HB2	1:C:643:PRO:HG3	1.99	0.45
1:E:305:TRP:CE3	1:E:734:ARG:NH2	2.85	0.45
1:G:315:LYS:HE2	1:G:315:LYS:HB2	1.82	0.45
1:H:278:THR:HG22	1:H:280:TRP:N	2.15	0.44
1:C:570:ASN:ND2	1:C:608:GLN:H	2.02	0.44
1:B:585:GLN:HG3	1:G:487:GLN:NE2	2.32	0.44
1:A:305:TRP:CE3	1:A:734:ARG:NH2	2.85	0.44
1:J:305:TRP:CE3	1:J:734:ARG:NH2	2.85	0.44
1:B:397:GLU:OE1	1:B:397:GLU:N	2.50	0.44
1:C:487:GLN:NE2	1:C:488:ARG:H	2.15	0.44
1:D:286:ASN:HD21	1:D:619:TRP:N	2.13	0.44
1:I:286:ASN:HD21	1:I:619:TRP:N	2.13	0.44
1:C:383:ASN:C	1:C:383:ASN:ND2	2.68	0.44
1:A:264:SER:OG	1:A:265:THR:N	2.49	0.44
1:C:379:LEU:HD21	1:F:437:PRO:HB3	1.99	0.44
1:H:423:SER:HB2	1:H:425:TYR:CE2	2.53	0.44
1:F:305:TRP:CE3	1:F:734:ARG:NH2	2.85	0.44
1:F:544:GLY:HA3	1:I:444:TYR:CE1	2.52	0.44
1:E:512:ASN:HD21	1:G:529:ASP:N	2.07	0.44
1:G:500:ASN:HD22	1:G:500:ASN:HA	1.67	0.44
1:D:316:LEU:HA	1:D:316:LEU:HD23	1.83	0.44
1:F:379:LEU:HD21	1:I:437:PRO:HB3	1.99	0.44
1:D:305:TRP:CE3	1:D:734:ARG:NH2	2.85	0.44
1:H:451:ASN:ND2	1:H:458:ASN:HB2	2.30	0.44
1:J:397:GLU:OE1	1:J:397:GLU:N	2.50	0.44
1:E:487:GLN:NE2	1:G:585:GLN:HG3	2.33	0.44
1:B:437:PRO:HB3	1:G:379:LEU:HD21	1.98	0.44
1:B:423:SER:HB2	1:B:425:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:423:SER:HB2	1:I:425:TYR:CE2	2.53	0.44
1:C:305:TRP:CE3	1:C:734:ARG:NH2	2.85	0.44
1:B:666:LYS:NZ	4:B:812:HOH:O	2.30	0.44
1:E:255:HIS:ND1	4:E:795:HOH:O	2.34	0.44
1:E:392:SER:OG	1:G:694:ARG:NH1	2.51	0.44
1:D:365:PRO:HD2	4:D:758:HOH:O	2.16	0.44
1:J:423:SER:HB2	1:J:425:TYR:CE2	2.53	0.44
1:A:423:SER:HB2	1:A:425:TYR:CE2	2.53	0.44
1:D:544:GLY:HA3	1:H:444:TYR:CE1	2.52	0.44
1:G:328:ASP:CB	1:G:329:GLY:CA	2.76	0.44
1:C:585:GLN:HG3	1:I:487:GLN:NE2	2.32	0.44
1:A:585:GLN:HG3	1:H:487:GLN:NE2	2.33	0.44
1:H:487:GLN:NE2	1:H:488:ARG:H	2.15	0.44
1:C:487:GLN:NE2	1:F:585:GLN:HG3	2.33	0.44
1:A:714:THR:CG2	1:A:715:VAL:H	2.31	0.44
1:J:217:GLY:HA3	1:J:409:ASN:H	1.82	0.44
1:F:423:SER:HB2	1:F:425:TYR:CE2	2.53	0.44
1:A:437:PRO:HB3	1:H:379:LEU:HD21	1.99	0.44
1:D:423:SER:HB2	1:D:425:TYR:CE2	2.53	0.44
1:A:398:TYR:OH	1:I:232:SER:HB2	2.17	0.44
1:B:397:GLU:C	1:B:399:PHE:H	2.20	0.44
1:G:487:GLN:NE2	1:G:488:ARG:H	2.15	0.44
1:E:544:GLY:HA3	1:G:444:TYR:CE1	2.53	0.44
1:C:544:GLY:HA3	1:F:444:TYR:CE1	2.53	0.44
1:B:359:HIS:NE2	1:E:436:ASN:N	2.56	0.44
1:B:714:THR:CG2	1:B:715:VAL:H	2.31	0.44
1:I:295:ARG:HH11	1:I:298:GLN:HE21	1.66	0.44
1:G:286:ASN:HD21	1:G:619:TRP:N	2.13	0.44
1:F:383:ASN:ND2	1:F:383:ASN:C	2.68	0.44
3:A:738:CYT:N4	4:A:768:HOH:O	2.31	0.44
1:A:365:PRO:HD2	4:A:756:HOH:O	2.16	0.44
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.83	0.44
1:D:426:ALA:O	1:D:733:THR:HA	2.18	0.44
1:D:621:LYS:HB2	1:D:643:PRO:HG3	1.99	0.44
1:E:397:GLU:OE2	1:E:650:LYS:NZ	2.41	0.44
1:J:327:ASN:O	1:J:330:VAL:HG13	2.18	0.44
1:D:295:ARG:HH11	1:D:298:GLN:HE21	1.66	0.44
1:B:295:ARG:HH11	1:B:298:GLN:HE21	1.66	0.44
1:F:254:ASN:O	1:F:255:HIS:CB	2.65	0.44
1:A:379:LEU:HD21	1:D:437:PRO:HB3	1.99	0.44
1:C:423:SER:HB2	1:C:425:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:ALA:O	1:C:733:THR:HA	2.18	0.44
1:H:426:ALA:O	1:H:733:THR:HA	2.18	0.44
1:H:621:LYS:HB2	1:H:643:PRO:HG3	1.99	0.44
1:B:392:SER:OG	1:E:694:ARG:NH1	2.51	0.43
1:F:392:SER:OG	1:I:694:ARG:NH1	2.50	0.43
1:A:487:GLN:NE2	1:D:585:GLN:HG3	2.33	0.43
1:E:487:GLN:NE2	1:E:488:ARG:H	2.15	0.43
1:B:304:ASN:HD21	1:B:689:LYS:HZ3	1.65	0.43
1:A:736:LEU:HD13	1:A:736:LEU:HA	1.83	0.43
1:J:286:ASN:HD21	1:J:619:TRP:N	2.13	0.43
1:F:286:ASN:HD21	1:F:618:ILE:H	1.66	0.43
1:G:423:SER:HB2	1:G:425:TYR:CE2	2.53	0.43
1:A:426:ALA:O	1:A:733:THR:HA	2.18	0.43
1:A:621:LYS:HB2	1:A:643:PRO:HG3	1.99	0.43
1:B:621:LYS:HB2	1:B:643:PRO:HG3	1.99	0.43
1:C:295:ARG:HH11	1:C:298:GLN:HE21	1.66	0.43
1:J:621:LYS:HB2	1:J:643:PRO:HG3	1.99	0.43
1:C:694:ARG:NH1	1:I:392:SER:OG	2.50	0.43
1:B:487:GLN:NE2	1:E:585:GLN:HG3	2.33	0.43
1:F:487:GLN:NE2	1:I:585:GLN:HG3	2.33	0.43
1:H:286:ASN:HD21	1:H:618:ILE:H	1.66	0.43
1:E:423:SER:HB2	1:E:425:TYR:CE2	2.53	0.43
1:B:444:TYR:CE1	1:G:544:GLY:HA3	2.53	0.43
1:J:426:ALA:O	1:J:733:THR:HA	2.18	0.43
1:I:621:LYS:HB2	1:I:643:PRO:HG3	1.99	0.43
1:E:451:ASN:ND2	1:E:458:ASN:HB2	2.30	0.43
1:A:392:SER:OG	1:D:694:ARG:NH1	2.51	0.43
1:D:392:SER:OG	1:H:694:ARG:NH1	2.50	0.43
1:F:487:GLN:NE2	1:F:488:ARG:H	2.15	0.43
1:E:383:ASN:ND2	1:E:383:ASN:C	2.68	0.43
1:H:663:SER:OG	1:H:665:THR:HG23	2.18	0.43
1:E:621:LYS:HB2	1:E:643:PRO:HG3	1.99	0.43
1:A:544:GLY:HA3	1:D:444:TYR:CE1	2.53	0.43
1:H:397:GLU:C	1:H:399:PHE:H	2.21	0.43
1:A:452:GLN:O	1:A:453:SER:C	2.55	0.43
1:E:286:ASN:HD21	1:E:618:ILE:H	1.66	0.43
1:E:500:ASN:HA	1:E:500:ASN:HD22	1.67	0.43
1:B:262:SER:O	1:B:265:THR:OG1	2.34	0.43
1:A:444:TYR:CE1	1:H:544:GLY:HA3	2.53	0.43
1:J:455:SER:HA	1:J:456:ALA:HA	1.70	0.43
1:B:426:ALA:O	1:B:733:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:ASN:ND2	1:J:458:ASN:HB2	2.30	0.43
1:A:694:ARG:NH1	1:H:392:SER:OG	2.51	0.43
1:C:714:THR:CG2	1:C:715:VAL:H	2.31	0.43
1:J:286:ASN:HD21	1:J:618:ILE:H	1.67	0.43
1:I:703:SER:CB	4:I:743:HOH:O	2.62	0.43
1:I:263:ALA:O	1:I:264:SER:HB3	2.18	0.43
1:F:321:VAL:HG11	1:F:339:SER:HB3	2.00	0.43
1:C:321:VAL:HG11	1:C:339:SER:HB3	2.00	0.43
1:H:363:LEU:CD2	1:H:371:PHE:CZ	3.02	0.43
1:B:278:THR:HG22	1:B:280:TRP:N	2.15	0.43
1:F:455:SER:HA	1:F:456:ALA:HA	1.66	0.43
1:C:437:PRO:HB3	1:I:379:LEU:HD21	1.99	0.43
1:A:719:GLY:O	1:B:666:LYS:NZ	2.50	0.43
1:J:363:LEU:CD2	1:J:371:PHE:CZ	3.02	0.43
1:A:321:VAL:HG11	1:A:339:SER:HB3	2.00	0.43
1:E:363:LEU:CD2	1:E:371:PHE:CZ	3.02	0.43
1:J:487:GLN:NE2	1:J:488:ARG:H	2.15	0.43
1:C:392:SER:OG	1:F:694:ARG:NH1	2.51	0.43
1:F:217:GLY:HA3	1:F:408:ASN:HB3	2.01	0.43
1:A:217:GLY:HA3	1:A:408:ASN:HB3	2.01	0.43
3:D:738:CYT:N4	4:D:770:HOH:O	2.31	0.43
1:F:399:PHE:HD1	1:F:399:PHE:N	2.15	0.43
1:B:544:GLY:HA3	1:E:444:TYR:CE1	2.52	0.43
1:E:426:ALA:O	1:E:733:THR:HA	2.18	0.43
1:I:321:VAL:HG11	1:I:339:SER:HB3	2.00	0.43
1:G:426:ALA:O	1:G:733:THR:HA	2.18	0.43
1:G:295:ARG:HH11	1:G:298:GLN:HE21	1.66	0.43
1:J:321:VAL:HG11	1:J:339:SER:HB3	2.00	0.43
1:D:487:GLN:NE2	1:H:585:GLN:HG3	2.33	0.43
1:A:263:ALA:O	1:A:264:SER:HB3	2.19	0.43
1:D:379:LEU:HD21	1:H:437:PRO:HB3	1.99	0.43
1:I:383:ASN:ND2	1:I:383:ASN:C	2.68	0.43
1:F:426:ALA:O	1:F:733:THR:HA	2.18	0.43
1:G:621:LYS:HB2	1:G:643:PRO:HG3	1.99	0.43
1:I:363:LEU:CD2	1:I:371:PHE:CZ	3.02	0.43
1:B:363:LEU:CD2	1:B:371:PHE:CZ	3.02	0.43
1:B:694:ARG:NH1	1:G:392:SER:OG	2.51	0.43
1:A:286:ASN:HD21	1:A:618:ILE:H	1.66	0.43
1:A:436:ASN:N	1:H:359:HIS:NE2	2.56	0.43
1:A:363:LEU:CD2	1:A:371:PHE:CZ	3.02	0.43
1:E:315:LYS:HE2	1:E:315:LYS:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:714:THR:CG2	1:E:715:VAL:H	2.31	0.42
1:A:304:ASN:HD21	1:A:689:LYS:HZ3	1.61	0.42
1:H:397:GLU:OE1	1:H:397:GLU:N	2.50	0.42
1:B:321:VAL:HG11	1:B:339:SER:HB3	2.00	0.42
1:I:426:ALA:O	1:I:733:THR:HA	2.18	0.42
1:I:278:THR:HG22	1:I:280:TRP:N	2.15	0.42
1:A:217:GLY:HA3	1:A:408:ASN:CB	2.48	0.42
1:A:295:ARG:HH11	1:A:298:GLN:HE21	1.66	0.42
1:A:229:HIS:HB3	4:A:833:HOH:O	2.19	0.42
1:H:321:VAL:HG11	1:H:339:SER:HB3	2.00	0.42
1:G:363:LEU:CD2	1:G:371:PHE:CZ	3.02	0.42
1:D:321:VAL:HG11	1:D:339:SER:HB3	2.00	0.42
1:G:321:VAL:HG11	1:G:339:SER:HB3	2.00	0.42
1:J:229:HIS:HB3	4:J:837:HOH:O	2.19	0.42
1:E:229:HIS:HE1	4:E:808:HOH:O	2.02	0.42
1:H:295:ARG:HH11	1:H:298:GLN:HE21	1.66	0.42
1:D:363:LEU:CD2	1:D:371:PHE:CZ	3.02	0.42
1:J:295:ARG:HH11	1:J:298:GLN:HE21	1.66	0.42
1:B:229:HIS:HB3	4:B:833:HOH:O	2.19	0.42
1:H:455:SER:HA	1:H:456:ALA:HA	1.69	0.42
1:E:321:VAL:HG11	1:E:339:SER:HB3	2.01	0.42
1:A:312:LEU:HA	1:A:682:GLU:O	2.20	0.42
1:I:286:ASN:HD21	1:I:618:ILE:H	1.66	0.42
1:E:295:ARG:HH11	1:E:298:GLN:HE21	1.66	0.42
1:J:316:LEU:HD23	1:J:316:LEU:HA	1.83	0.42
1:H:263:ALA:O	1:H:264:SER:HB3	2.19	0.42
1:F:363:LEU:CD2	1:F:371:PHE:CZ	3.02	0.42
1:E:655:PRO:HB3	1:E:667:PHE:CE1	2.55	0.42
1:J:328:ASP:HB3	1:J:330:VAL:N	2.33	0.42
1:G:703:SER:CB	4:G:742:HOH:O	2.67	0.42
1:C:363:LEU:CD2	1:C:371:PHE:CZ	3.02	0.42
1:A:725:ARG:HB3	1:A:725:ARG:HE	1.69	0.42
1:C:312:LEU:HA	1:C:682:GLU:O	2.20	0.42
1:F:330:VAL:CG1	1:F:330:VAL:O	2.53	0.42
1:I:396:LEU:C	1:I:398:TYR:H	2.21	0.42
1:B:475:PRO:HA	1:G:519:ASN:O	2.20	0.42
1:D:229:HIS:HB3	4:D:836:HOH:O	2.19	0.42
1:E:280:TRP:CE3	1:E:650:LYS:HB2	2.55	0.42
1:B:280:TRP:CE3	1:B:650:LYS:HB2	2.55	0.42
1:F:280:TRP:CE3	1:F:650:LYS:HB2	2.55	0.42
1:I:312:LEU:HA	1:I:682:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:312:LEU:HA	1:J:682:GLU:O	2.20	0.42
1:J:397:GLU:OE2	1:J:650:LYS:NZ	2.41	0.42
1:I:488:ARG:HB2	1:I:574:THR:HB	2.02	0.42
1:C:488:ARG:HB2	1:C:574:THR:HB	2.02	0.42
1:B:286:ASN:HD21	1:B:619:TRP:N	2.13	0.42
1:I:264:SER:OG	1:I:265:THR:N	2.50	0.42
1:D:725:ARG:HE	1:D:725:ARG:HB3	1.69	0.42
1:F:519:ASN:O	1:I:475:PRO:HA	2.20	0.42
1:B:312:LEU:HA	1:B:682:GLU:O	2.20	0.42
1:J:280:TRP:CE3	1:J:650:LYS:HB2	2.55	0.42
1:G:488:ARG:HB2	1:G:574:THR:HB	2.02	0.42
1:F:714:THR:CG2	1:F:715:VAL:H	2.31	0.42
1:F:500:ASN:HD22	1:F:500:ASN:HA	1.67	0.42
1:E:229:HIS:HB3	4:E:836:HOH:O	2.19	0.42
1:J:501:PHE:O	1:J:505:GLY:N	2.44	0.42
1:C:475:PRO:HA	1:I:519:ASN:O	2.20	0.42
1:E:488:ARG:HB2	1:E:574:THR:HB	2.02	0.42
1:D:218:ALA:H	1:D:408:ASN:HD22	1.67	0.42
1:J:488:ARG:HB2	1:J:574:THR:HB	2.02	0.42
1:D:312:LEU:HA	1:D:682:GLU:O	2.20	0.41
1:B:449:THR:H	1:G:500:ASN:HD22	1.68	0.41
1:E:500:ASN:HD22	1:G:449:THR:H	1.68	0.41
1:C:701:TYR:CD2	1:C:701:TYR:C	2.94	0.41
1:D:359:HIS:NE2	1:H:436:ASN:N	2.55	0.41
1:G:365:PRO:HD2	4:G:759:HOH:O	2.19	0.41
1:H:342:GLN:HG2	1:H:403:MET:HG2	2.03	0.41
1:G:451:ASN:ND2	1:G:458:ASN:HB2	2.30	0.41
1:A:327:ASN:ND2	1:I:330:VAL:HG21	2.35	0.41
1:C:278:THR:HG22	1:C:280:TRP:N	2.15	0.41
1:A:488:ARG:HB2	1:A:574:THR:HB	2.02	0.41
1:I:714:THR:CG2	1:I:715:VAL:H	2.31	0.41
1:D:286:ASN:HD21	1:D:618:ILE:H	1.66	0.41
1:F:701:TYR:C	1:F:701:TYR:CD2	2.94	0.41
1:J:339:SER:HA	4:J:835:HOH:O	2.19	0.41
1:A:519:ASN:O	1:D:475:PRO:HA	2.20	0.41
1:E:519:ASN:O	1:G:475:PRO:HA	2.20	0.41
1:J:278:THR:HG22	1:J:280:TRP:N	2.15	0.41
1:H:488:ARG:HB2	1:H:574:THR:HB	2.02	0.41
1:D:500:ASN:HD22	1:H:449:THR:H	1.69	0.41
1:B:519:ASN:O	1:E:475:PRO:HA	2.20	0.41
1:C:501:PHE:O	1:C:505:GLY:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ASN:O	1:F:475:PRO:HA	2.20	0.41
1:F:586:SER:HB2	4:F:825:HOH:O	2.21	0.41
1:D:280:TRP:CE3	1:D:650:LYS:HB2	2.55	0.41
1:B:219:ASP:OD1	1:B:219:ASP:N	2.53	0.41
1:G:286:ASN:HD21	1:G:618:ILE:H	1.67	0.41
3:C:738:CYT:N4	4:C:768:HOH:O	2.24	0.41
1:A:449:THR:H	1:H:500:ASN:HD22	1.68	0.41
1:A:701:TYR:C	1:A:701:TYR:CD2	2.94	0.41
1:J:693:LYS:HA	1:J:693:LYS:HD3	1.89	0.41
1:H:280:TRP:CE3	1:H:650:LYS:HB2	2.55	0.41
1:A:397:GLU:N	1:A:397:GLU:OE1	2.50	0.41
1:F:628:HIS:O	3:I:738:CYT:C6	2.74	0.41
1:D:701:TYR:C	1:D:701:TYR:CD2	2.94	0.41
1:G:342:GLN:C	1:G:343:VAL:CG2	2.89	0.41
1:E:342:GLN:C	1:E:343:VAL:CG2	2.89	0.41
1:F:342:GLN:C	1:F:343:VAL:CG2	2.89	0.41
1:C:342:GLN:C	1:C:343:VAL:CG2	2.89	0.41
1:G:501:PHE:O	1:G:505:GLY:N	2.44	0.41
1:E:455:SER:HA	1:E:456:ALA:HA	1.69	0.41
1:D:586:SER:HB2	4:D:825:HOH:O	2.21	0.41
1:D:519:ASN:O	1:H:475:PRO:HA	2.20	0.41
1:I:280:TRP:CD1	1:I:650:LYS:HD3	2.55	0.41
1:E:278:THR:HG22	1:E:280:TRP:N	2.15	0.41
1:F:312:LEU:HA	1:F:682:GLU:O	2.20	0.41
1:H:714:THR:CG2	1:H:715:VAL:H	2.31	0.41
1:A:500:ASN:HD22	1:D:449:THR:H	1.68	0.41
1:E:342:GLN:HG2	1:E:403:MET:HG2	2.03	0.41
1:C:342:GLN:HG2	1:C:403:MET:HG2	2.03	0.41
1:G:315:LYS:HB3	1:G:680:SER:HB2	2.03	0.41
1:I:315:LYS:HB3	1:I:680:SER:HB2	2.03	0.41
1:E:725:ARG:HE	1:E:725:ARG:HB3	1.69	0.41
1:F:451:ASN:OD1	1:F:458:ASN:HB2	2.21	0.41
1:H:312:LEU:HA	1:H:682:GLU:O	2.20	0.41
1:F:393:PHE:HB3	1:I:696:ASN:ND2	2.36	0.41
1:B:488:ARG:HB2	1:B:574:THR:HB	2.02	0.41
1:I:264:SER:O	1:I:265:THR:HB	2.21	0.41
1:A:284:ASP:O	1:A:362:CYS:HA	2.21	0.41
1:B:451:ASN:ND2	1:B:458:ASN:HB2	2.30	0.41
1:C:280:TRP:CE3	1:C:650:LYS:HB2	2.55	0.41
1:A:696:ASN:ND2	1:H:393:PHE:HB3	2.36	0.41
1:E:312:LEU:HA	1:E:682:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TRP:CE3	1:A:650:LYS:HB2	2.55	0.41
1:D:714:THR:CG2	1:D:715:VAL:H	2.30	0.41
1:G:237:ASP:OD1	1:G:237:ASP:N	2.53	0.41
1:H:218:ALA:C	1:H:219:ASP:CG	2.79	0.41
1:D:628:HIS:O	3:H:738:CYT:C6	2.74	0.41
1:F:500:ASN:HD22	1:I:449:THR:H	1.68	0.41
1:E:701:TYR:CD2	1:E:701:TYR:C	2.94	0.41
1:B:701:TYR:CD2	1:B:701:TYR:C	2.94	0.41
1:G:701:TYR:CD2	1:G:701:TYR:C	2.94	0.41
1:I:316:LEU:HD23	1:I:316:LEU:HA	1.83	0.41
1:J:342:GLN:HG2	1:J:403:MET:HG2	2.03	0.41
1:A:342:GLN:C	1:A:343:VAL:CG2	2.89	0.41
1:I:363:LEU:HA	1:I:364:PRO:HD3	1.96	0.41
1:D:508:LYS:HG2	1:D:517:ILE:HA	2.03	0.41
1:F:315:LYS:HB2	1:F:315:LYS:HE2	1.82	0.41
1:A:232:SER:HB2	1:B:398:TYR:OH	2.21	0.41
1:A:508:LYS:HG2	1:A:517:ILE:HA	2.03	0.41
1:I:508:LYS:HG2	1:I:517:ILE:HA	2.03	0.41
4:D:831:HOH:O	1:H:735:PRO:HD3	2.19	0.41
1:J:438:LEU:O	1:J:439:ILE:HD13	2.21	0.41
1:D:455:SER:HA	1:D:456:ALA:HA	1.69	0.41
1:D:284:ASP:O	1:D:362:CYS:HA	2.21	0.41
1:B:586:SER:HB2	4:B:823:HOH:O	2.21	0.41
1:E:397:GLU:OE1	1:E:397:GLU:N	2.50	0.41
1:G:312:LEU:HA	1:G:682:GLU:O	2.20	0.41
3:A:738:CYT:C6	1:H:628:HIS:O	2.73	0.41
1:I:701:TYR:C	1:I:701:TYR:CD2	2.94	0.41
1:H:342:GLN:C	1:H:343:VAL:CG2	2.89	0.41
1:E:315:LYS:HB3	1:E:680:SER:HB2	2.03	0.41
1:J:508:LYS:HG2	1:J:517:ILE:HA	2.03	0.41
1:B:393:PHE:HB3	1:E:696:ASN:ND2	2.36	0.40
1:I:569:THR:OG1	1:I:570:ASN:ND2	2.55	0.40
1:E:569:THR:OG1	1:E:570:ASN:ND2	2.55	0.40
1:G:736:LEU:HD13	1:G:736:LEU:HA	1.83	0.40
1:C:286:ASN:HD21	1:C:618:ILE:H	1.66	0.40
1:A:286:ASN:HD21	1:A:619:TRP:N	2.13	0.40
1:I:405:ARG:H	1:I:408:ASN:HD22	1.69	0.40
1:J:701:TYR:C	1:J:701:TYR:CD2	2.94	0.40
1:J:342:GLN:C	1:J:343:VAL:CG2	2.89	0.40
1:B:342:GLN:C	1:B:343:VAL:CG2	2.89	0.40
1:E:366:PHE:HA	1:E:367:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LYS:HB3	1:C:680:SER:HB2	2.03	0.40
1:G:455:SER:HA	1:G:456:ALA:HA	1.69	0.40
1:D:360:GLN:OE1	1:H:440:ASP:HB2	2.21	0.40
1:C:328:ASP:CB	1:C:329:GLY:CA	2.76	0.40
1:D:488:ARG:HB2	1:D:574:THR:HB	2.02	0.40
1:D:427:HIS:NE2	1:D:736:LEU:HD13	2.37	0.40
1:E:427:HIS:NE2	1:E:736:LEU:HD13	2.37	0.40
1:F:342:GLN:HG2	1:F:403:MET:HG2	2.03	0.40
1:D:342:GLN:C	1:D:343:VAL:CG2	2.89	0.40
1:D:315:LYS:HB3	1:D:680:SER:HB2	2.03	0.40
1:G:586:SER:HB2	4:G:826:HOH:O	2.21	0.40
1:G:220:GLY:C	1:G:222:GLY:N	2.75	0.40
1:I:280:TRP:CZ2	1:I:650:LYS:HE3	2.56	0.40
1:F:488:ARG:HB2	1:F:574:THR:HB	2.02	0.40
1:I:427:HIS:NE2	1:I:736:LEU:HD13	2.37	0.40
1:C:628:HIS:O	3:F:738:CYT:C6	2.74	0.40
1:G:282:TYR:CE1	1:G:374:PRO:HB2	2.57	0.40
1:C:449:THR:H	1:I:500:ASN:HD22	1.69	0.40
1:H:701:TYR:CD2	1:H:701:TYR:C	2.94	0.40
1:B:472:SER:HB3	1:G:270:ASP:O	2.22	0.40
1:F:315:LYS:HB3	1:F:680:SER:HB2	2.03	0.40
1:C:284:ASP:O	1:C:362:CYS:HA	2.21	0.40
1:A:315:LYS:HB3	1:A:680:SER:HB2	2.03	0.40
1:G:329:GLY:C	1:G:330:VAL:HG12	2.42	0.40
1:D:451:ASN:ND2	1:D:458:ASN:HB2	2.30	0.40
1:A:628:HIS:O	3:D:738:CYT:C6	2.74	0.40
3:C:738:CYT:C6	1:I:628:HIS:O	2.74	0.40
1:C:282:TYR:CE1	1:C:374:PRO:HB2	2.57	0.40
1:H:500:ASN:HA	1:H:500:ASN:HD22	1.67	0.40
1:G:342:GLN:HA	1:G:402:GLN:O	2.22	0.40
1:B:342:GLN:HA	1:B:402:GLN:O	2.22	0.40
1:D:342:GLN:HA	1:D:402:GLN:O	2.22	0.40
1:E:450:GLN:OE1	1:E:457:GLN:HB3	2.22	0.40
1:D:393:PHE:HB3	1:H:696:ASN:ND2	2.36	0.40
1:B:397:GLU:OE2	1:B:650:LYS:NZ	2.41	0.40
1:G:278:THR:CG2	1:G:280:TRP:HB2	2.52	0.40
1:G:569:THR:OG1	1:G:570:ASN:ND2	2.55	0.40
1:F:427:HIS:NE2	1:F:736:LEU:HD13	2.37	0.40
3:H:738:CYT:N4	4:H:771:HOH:O	2.29	0.40
1:F:282:TYR:CE1	1:F:374:PRO:HB2	2.57	0.40
1:H:282:TYR:CE1	1:H:374:PRO:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:342:GLN:HG2	1:I:403:MET:HG2	2.03	0.40
1:F:342:GLN:HA	1:F:402:GLN:O	2.22	0.40
1:B:342:GLN:HG2	1:B:403:MET:HG2	2.03	0.40
1:D:342:GLN:HG2	1:D:403:MET:HG2	2.03	0.40
1:A:229:HIS:O	1:A:242:THR:HG22	2.22	0.40
1:B:315:LYS:HB3	1:B:680:SER:HB2	2.03	0.40
1:F:284:ASP:O	1:F:362:CYS:HA	2.21	0.40
1:F:508:LYS:HG2	1:F:517:ILE:HA	2.03	0.40
1:G:450:GLN:OE1	1:G:457:GLN:HB3	2.22	0.40
1:G:284:ASP:O	1:G:362:CYS:HA	2.21	0.40
1:H:450:GLN:OE1	1:H:457:GLN:HB3	2.22	0.40
1:J:450:GLN:OE1	1:J:457:GLN:HB3	2.22	0.40
1:D:450:GLN:OE1	1:D:457:GLN:HB3	2.22	0.40
1:D:366:PHE:HA	1:D:367:PRO:HD3	1.94	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 X-ray entries followed by that with respect to entries of similar resolution.

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	518/736 (70%)	499 (96%)	15 (3%)	4 (1%)	24	41
1	B	518/736 (70%)	500 (96%)	17 (3%)	1 (0%)	52	75
1	C	518/736 (70%)	498 (96%)	18 (4%)	2 (0%)	39	61
1	D	518/736 (70%)	498 (96%)	16 (3%)	4 (1%)	24	41
1	E	518/736 (70%)	500 (96%)	16 (3%)	2 (0%)	39	61
1	F	518/736 (70%)	501 (97%)	14 (3%)	3 (1%)	30	50
1	G	518/736 (70%)	498 (96%)	16 (3%)	4 (1%)	24	41
1	H	518/736 (70%)	498 (96%)	17 (3%)	3 (1%)	30	50
1	I	518/736 (70%)	501 (97%)	12 (2%)	5 (1%)	19	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	518/736 (70%)	497 (96%)	18 (4%)	3 (1%)	30	50
All	All	5180/7360 (70%)	4990 (96%)	159 (3%)	31 (1%)	30	50

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ALA
1	A	219	ASP
1	C	328	ASP
1	E	219	ASP
1	F	218	ALA
1	F	219	ASP
1	G	221	VAL
1	G	328	ASP
1	H	219	ASP
1	H	328	ASP
1	I	221	VAL
1	I	455	SER
1	J	328	ASP
1	A	453	SER
1	B	453	SER
1	C	453	SER
1	D	453	SER
1	E	453	SER
1	G	453	SER
1	H	453	SER
1	I	453	SER
1	J	453	SER
1	D	219	ASP
1	J	218	ALA
1	D	218	ALA
1	F	406	THR
1	G	219	ASP
1	I	219	ASP
1	I	452	GLN
1	A	452	GLN
1	D	328	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 X-ray entries followed by that with respect to entries of similar resolution.

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	451/617 (73%)	413 (92%)	38 (8%)	14	25
1	B	451/617 (73%)	411 (91%)	40 (9%)	12	23
1	C	451/617 (73%)	413 (92%)	38 (8%)	14	25
1	D	451/617 (73%)	415 (92%)	36 (8%)	15	28
1	E	451/617 (73%)	413 (92%)	38 (8%)	14	25
1	F	451/617 (73%)	413 (92%)	38 (8%)	14	25
1	G	451/617 (73%)	414 (92%)	37 (8%)	14	27
1	H	451/617 (73%)	413 (92%)	38 (8%)	14	25
1	I	451/617 (73%)	414 (92%)	37 (8%)	14	27
1	J	451/617 (73%)	413 (92%)	38 (8%)	14	25
All	All	4510/6170 (73%)	4132 (92%)	378 (8%)	14	25

All (378) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	229	HIS
1	A	237	ASP
1	A	244	THR
1	A	246	THR
1	A	278	THR
1	A	289	HIS
1	A	312	LEU
1	A	313	ASN
1	A	315	LYS
1	A	319	ILE
1	A	320	GLN
1	A	339	SER
1	A	357	SER
1	A	380	THR
1	A	383	ASN

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Mol	Chain	Res	Type
1	A	399	PHE
1	A	413	SER
1	A	431	LEU
1	A	457	GLN
1	A	467	SER
1	A	489	VAL
1	A	492	THR
1	A	500	ASN
1	A	528	LYS
1	A	575	GLU
1	A	576	ARG
1	A	589	THR
1	A	602	LEU
1	A	608	GLN
1	A	615	GLN
1	A	628	HIS
1	A	665	THR
1	A	696	ASN
1	A	707	LYS
1	A	717	ASN
1	A	725	ARG
1	A	736	LEU
1	B	223	ASN
1	B	229	HIS
1	B	230	CYS
1	B	237	ASP
1	B	244	THR
1	B	246	THR
1	B	278	THR
1	B	289	HIS
1	B	312	LEU
1	B	313	ASN
1	B	315	LYS
1	B	319	ILE
1	B	320	GLN
1	B	325	THR
1	B	339	SER
1	B	357	SER
1	B	380	THR
1	B	383	ASN
1	B	413	SER
1	B	431	LEU

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Mol	Chain	Res	Type
1	B	452	GLN
1	B	467	SER
1	B	489	VAL
1	B	492	THR
1	B	500	ASN
1	B	528	LYS
1	B	575	GLU
1	B	576	ARG
1	B	589	THR
1	B	602	LEU
1	B	608	GLN
1	B	615	GLN
1	B	628	HIS
1	B	665	THR
1	B	666	LYS
1	B	667	PHE
1	B	696	ASN
1	B	707	LYS
1	B	717	ASN
1	B	736	LEU
1	C	223	ASN
1	C	229	HIS
1	C	237	ASP
1	C	244	THR
1	C	246	THR
1	C	278	THR
1	C	289	HIS
1	C	312	LEU
1	C	313	ASN
1	C	315	LYS
1	C	319	ILE
1	C	320	GLN
1	C	328	ASP
1	C	330	VAL
1	C	339	SER
1	C	357	SER
1	C	380	THR
1	C	383	ASN
1	C	413	SER
1	C	431	LEU
1	C	452	GLN
1	C	467	SER

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Mol	Chain	Res	Type
1	C	489	VAL
1	C	492	THR
1	C	500	ASN
1	C	528	LYS
1	C	575	GLU
1	C	576	ARG
1	C	589	THR
1	C	602	LEU
1	C	608	GLN
1	C	615	GLN
1	C	628	HIS
1	C	665	THR
1	C	696	ASN
1	C	707	LYS
1	C	717	ASN
1	C	736	LEU
1	D	223	ASN
1	D	229	HIS
1	D	237	ASP
1	D	244	THR
1	D	246	THR
1	D	278	THR
1	D	289	HIS
1	D	312	LEU
1	D	313	ASN
1	D	315	LYS
1	D	319	ILE
1	D	320	GLN
1	D	339	SER
1	D	357	SER
1	D	380	THR
1	D	383	ASN
1	D	413	SER
1	D	431	LEU
1	D	452	GLN
1	D	467	SER
1	D	489	VAL
1	D	492	THR
1	D	500	ASN
1	D	528	LYS
1	D	575	GLU
1	D	576	ARG

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Mol	Chain	Res	Type
1	D	589	THR
1	D	602	LEU
1	D	608	GLN
1	D	615	GLN
1	D	628	HIS
1	D	665	THR
1	D	696	ASN
1	D	707	LYS
1	D	717	ASN
1	D	736	LEU
1	E	223	ASN
1	E	229	HIS
1	E	237	ASP
1	E	244	THR
1	E	246	THR
1	E	278	THR
1	E	289	HIS
1	E	312	LEU
1	E	313	ASN
1	E	315	LYS
1	E	319	ILE
1	E	320	GLN
1	E	339	SER
1	E	357	SER
1	E	380	THR
1	E	383	ASN
1	E	413	SER
1	E	431	LEU
1	E	452	GLN
1	E	467	SER
1	E	489	VAL
1	E	492	THR
1	E	500	ASN
1	E	528	LYS
1	E	575	GLU
1	E	576	ARG
1	E	589	THR
1	E	602	LEU
1	E	608	GLN
1	E	615	GLN
1	E	628	HIS
1	E	665	THR

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Mol	Chain	Res	Type
1	E	666	LYS
1	E	667	PHE
1	E	696	ASN
1	E	707	LYS
1	E	717	ASN
1	E	736	LEU
1	F	223	ASN
1	F	229	HIS
1	F	235	LEU
1	F	237	ASP
1	F	244	THR
1	F	246	THR
1	F	278	THR
1	F	289	HIS
1	F	312	LEU
1	F	313	ASN
1	F	315	LYS
1	F	319	ILE
1	F	320	GLN
1	F	339	SER
1	F	357	SER
1	F	380	THR
1	F	383	ASN
1	F	399	PHE
1	F	413	SER
1	F	431	LEU
1	F	467	SER
1	F	489	VAL
1	F	492	THR
1	F	500	ASN
1	F	528	LYS
1	F	575	GLU
1	F	576	ARG
1	F	589	THR
1	F	602	LEU
1	F	608	GLN
1	F	615	GLN
1	F	628	HIS
1	F	666	LYS
1	F	667	PHE
1	F	696	ASN
1	F	707	LYS

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Mol	Chain	Res	Type
1	F	717	ASN
1	F	736	LEU
1	G	229	HIS
1	G	244	THR
1	G	246	THR
1	G	278	THR
1	G	289	HIS
1	G	312	LEU
1	G	313	ASN
1	G	315	LYS
1	G	319	ILE
1	G	320	GLN
1	G	328	ASP
1	G	330	VAL
1	G	339	SER
1	G	357	SER
1	G	380	THR
1	G	383	ASN
1	G	413	SER
1	G	431	LEU
1	G	452	GLN
1	G	467	SER
1	G	489	VAL
1	G	492	THR
1	G	500	ASN
1	G	528	LYS
1	G	575	GLU
1	G	576	ARG
1	G	589	THR
1	G	602	LEU
1	G	608	GLN
1	G	615	GLN
1	G	628	HIS
1	G	665	THR
1	G	667	PHE
1	G	696	ASN
1	G	707	LYS
1	G	717	ASN
1	G	736	LEU
1	H	223	ASN
1	H	237	ASP
1	H	244	THR

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Mol	Chain	Res	Type
1	H	246	THR
1	H	278	THR
1	H	289	HIS
1	H	312	LEU
1	H	313	ASN
1	H	315	LYS
1	H	319	ILE
1	H	320	GLN
1	H	328	ASP
1	H	330	VAL
1	H	339	SER
1	H	357	SER
1	H	380	THR
1	H	383	ASN
1	H	413	SER
1	H	431	LEU
1	H	452	GLN
1	H	467	SER
1	H	489	VAL
1	H	492	THR
1	H	500	ASN
1	H	528	LYS
1	H	575	GLU
1	H	576	ARG
1	H	589	THR
1	H	602	LEU
1	H	608	GLN
1	H	615	GLN
1	H	628	HIS
1	H	665	THR
1	H	666	LYS
1	H	696	ASN
1	H	707	LYS
1	H	717	ASN
1	H	736	LEU
1	I	223	ASN
1	I	229	HIS
1	I	237	ASP
1	I	244	THR
1	I	246	THR
1	I	278	THR
1	I	289	HIS

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Mol	Chain	Res	Type
1	I	312	LEU
1	I	313	ASN
1	I	315	LYS
1	I	319	ILE
1	I	320	GLN
1	I	339	SER
1	I	357	SER
1	I	380	THR
1	I	383	ASN
1	I	413	SER
1	I	431	LEU
1	I	467	SER
1	I	489	VAL
1	I	492	THR
1	I	500	ASN
1	I	528	LYS
1	I	575	GLU
1	I	576	ARG
1	I	589	THR
1	I	602	LEU
1	I	608	GLN
1	I	615	GLN
1	I	628	HIS
1	I	665	THR
1	I	666	LYS
1	I	667	PHE
1	I	696	ASN
1	I	707	LYS
1	I	717	ASN
1	I	736	LEU
1	J	223	ASN
1	J	229	HIS
1	J	237	ASP
1	J	244	THR
1	J	246	THR
1	J	278	THR
1	J	289	HIS
1	J	312	LEU
1	J	313	ASN
1	J	315	LYS
1	J	319	ILE
1	J	320	GLN

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Mol	Chain	Res	Type
1	J	328	ASP
1	J	330	VAL
1	J	339	SER
1	J	357	SER
1	J	380	THR
1	J	383	ASN
1	J	413	SER
1	J	431	LEU
1	J	452	GLN
1	J	467	SER
1	J	489	VAL
1	J	492	THR
1	J	500	ASN
1	J	528	LYS
1	J	575	GLU
1	J	576	ARG
1	J	589	THR
1	J	602	LEU
1	J	608	GLN
1	J	615	GLN
1	J	628	HIS
1	J	665	THR
1	J	696	ASN
1	J	707	LYS
1	J	717	ASN
1	J	736	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (318) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	253	ASN
1	A	286	ASN
1	A	298	GLN
1	A	302	ASN
1	A	304	ASN
1	A	335	ASN
1	A	350	GLN
1	A	375	GLN
1	A	382	ASN
1	A	383	ASN
1	A	386	GLN

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Mol	Chain	Res	Type
1	A	402	GLN
1	A	422	HIS
1	A	429	GLN
1	A	451	ASN
1	A	457	GLN
1	A	474	GLN
1	A	477	ASN
1	A	487	GLN
1	A	496	ASN
1	A	500	ASN
1	A	512	ASN
1	A	552	ASN
1	A	570	ASN
1	A	608	GLN
1	A	615	GLN
1	A	624	HIS
1	A	646	GLN
1	A	678	GLN
1	A	691	ASN
1	A	696	ASN
1	A	717	ASN
1	B	229	HIS
1	B	253	ASN
1	B	286	ASN
1	B	298	GLN
1	B	302	ASN
1	B	304	ASN
1	B	335	ASN
1	B	350	GLN
1	B	375	GLN
1	B	382	ASN
1	B	383	ASN
1	B	386	GLN
1	B	402	GLN
1	B	422	HIS
1	B	429	GLN
1	B	451	ASN
1	B	457	GLN
1	B	474	GLN
1	B	477	ASN
1	B	487	GLN
1	B	496	ASN

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Mol	Chain	Res	Type
1	B	500	ASN
1	B	512	ASN
1	B	552	ASN
1	B	570	ASN
1	B	608	GLN
1	B	615	GLN
1	B	624	HIS
1	B	646	GLN
1	B	678	GLN
1	B	691	ASN
1	B	696	ASN
1	B	717	ASN
1	C	229	HIS
1	C	253	ASN
1	C	286	ASN
1	C	298	GLN
1	C	302	ASN
1	C	304	ASN
1	C	335	ASN
1	C	350	GLN
1	C	375	GLN
1	C	382	ASN
1	C	383	ASN
1	C	422	HIS
1	C	429	GLN
1	C	451	ASN
1	C	457	GLN
1	C	474	GLN
1	C	477	ASN
1	C	487	GLN
1	C	496	ASN
1	C	500	ASN
1	C	512	ASN
1	C	552	ASN
1	C	570	ASN
1	C	608	GLN
1	C	615	GLN
1	C	624	HIS
1	C	646	GLN
1	C	678	GLN
1	C	691	ASN
1	C	696	ASN

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Mol	Chain	Res	Type
1	C	717	ASN
1	D	229	HIS
1	D	253	ASN
1	D	286	ASN
1	D	298	GLN
1	D	302	ASN
1	D	304	ASN
1	D	335	ASN
1	D	350	GLN
1	D	375	GLN
1	D	382	ASN
1	D	383	ASN
1	D	402	GLN
1	D	422	HIS
1	D	429	GLN
1	D	451	ASN
1	D	457	GLN
1	D	474	GLN
1	D	477	ASN
1	D	487	GLN
1	D	496	ASN
1	D	500	ASN
1	D	512	ASN
1	D	552	ASN
1	D	570	ASN
1	D	608	GLN
1	D	615	GLN
1	D	624	HIS
1	D	646	GLN
1	D	678	GLN
1	D	691	ASN
1	D	696	ASN
1	D	717	ASN
1	E	229	HIS
1	E	253	ASN
1	E	286	ASN
1	E	298	GLN
1	E	302	ASN
1	E	304	ASN
1	E	335	ASN
1	E	350	GLN
1	E	375	GLN

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Mol	Chain	Res	Type
1	E	382	ASN
1	E	383	ASN
1	E	422	HIS
1	E	429	GLN
1	E	451	ASN
1	E	457	GLN
1	E	474	GLN
1	E	477	ASN
1	E	487	GLN
1	E	496	ASN
1	E	500	ASN
1	E	512	ASN
1	E	552	ASN
1	E	570	ASN
1	E	608	GLN
1	E	615	GLN
1	E	624	HIS
1	E	646	GLN
1	E	678	GLN
1	E	691	ASN
1	E	696	ASN
1	E	717	ASN
1	F	229	HIS
1	F	286	ASN
1	F	289	HIS
1	F	298	GLN
1	F	302	ASN
1	F	335	ASN
1	F	350	GLN
1	F	375	GLN
1	F	382	ASN
1	F	383	ASN
1	F	386	GLN
1	F	402	GLN
1	F	422	HIS
1	F	429	GLN
1	F	474	GLN
1	F	477	ASN
1	F	487	GLN
1	F	496	ASN
1	F	500	ASN
1	F	512	ASN

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Mol	Chain	Res	Type
1	F	552	ASN
1	F	570	ASN
1	F	608	GLN
1	F	615	GLN
1	F	624	HIS
1	F	646	GLN
1	F	651	ASN
1	F	678	GLN
1	F	688	GLN
1	F	691	ASN
1	F	696	ASN
1	F	717	ASN
1	G	229	HIS
1	G	253	ASN
1	G	286	ASN
1	G	298	GLN
1	G	302	ASN
1	G	304	ASN
1	G	335	ASN
1	G	350	GLN
1	G	375	GLN
1	G	382	ASN
1	G	383	ASN
1	G	386	GLN
1	G	422	HIS
1	G	429	GLN
1	G	451	ASN
1	G	457	GLN
1	G	474	GLN
1	G	477	ASN
1	G	487	GLN
1	G	496	ASN
1	G	500	ASN
1	G	512	ASN
1	G	552	ASN
1	G	570	ASN
1	G	608	GLN
1	G	615	GLN
1	G	624	HIS
1	G	646	GLN
1	G	678	GLN
1	G	691	ASN

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Mol	Chain	Res	Type
1	G	696	ASN
1	G	717	ASN
1	H	253	ASN
1	H	286	ASN
1	H	298	GLN
1	H	302	ASN
1	H	304	ASN
1	H	335	ASN
1	H	350	GLN
1	H	375	GLN
1	H	382	ASN
1	H	383	ASN
1	H	386	GLN
1	H	422	HIS
1	H	429	GLN
1	H	451	ASN
1	H	457	GLN
1	H	474	GLN
1	H	477	ASN
1	H	487	GLN
1	H	496	ASN
1	H	500	ASN
1	H	510	ASN
1	H	512	ASN
1	H	552	ASN
1	H	570	ASN
1	H	608	GLN
1	H	615	GLN
1	H	624	HIS
1	H	646	GLN
1	H	678	GLN
1	H	691	ASN
1	H	696	ASN
1	H	717	ASN
1	I	229	HIS
1	I	253	ASN
1	I	286	ASN
1	I	298	GLN
1	I	302	ASN
1	I	304	ASN
1	I	335	ASN
1	I	350	GLN

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Mol	Chain	Res	Type
1	I	375	GLN
1	I	382	ASN
1	I	383	ASN
1	I	408	ASN
1	I	422	HIS
1	I	429	GLN
1	I	474	GLN
1	I	477	ASN
1	I	487	GLN
1	I	496	ASN
1	I	500	ASN
1	I	512	ASN
1	I	552	ASN
1	I	570	ASN
1	I	608	GLN
1	I	615	GLN
1	I	624	HIS
1	I	646	GLN
1	I	678	GLN
1	I	691	ASN
1	I	696	ASN
1	I	717	ASN
1	J	223	ASN
1	J	229	HIS
1	J	253	ASN
1	J	286	ASN
1	J	298	GLN
1	J	302	ASN
1	J	304	ASN
1	J	335	ASN
1	J	359	HIS
1	J	360	GLN
1	J	375	GLN
1	J	382	ASN
1	J	383	ASN
1	J	402	GLN
1	J	422	HIS
1	J	429	GLN
1	J	451	ASN
1	J	457	GLN
1	J	474	GLN
1	J	487	GLN

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Mol	Chain	Res	Type
1	J	496	ASN
1	J	500	ASN
1	J	512	ASN
1	J	552	ASN
1	J	570	ASN
1	J	608	GLN
1	J	615	GLN
1	J	646	GLN
1	J	678	GLN
1	J	691	ASN
1	J	696	ASN
1	J	717	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](#)

20 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	ADE	A	737	-	8,11,11	0.87	0	4,15,15	5.17	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CYT	A	738	-	5,8,8	1.66	1 (20%)	8,10,10	9.90	5 (62%)
2	ADE	B	737	-	8,11,11	0.87	0	4,15,15	5.14	2 (50%)
3	CYT	B	738	-	5,8,8	1.64	1 (20%)	8,10,10	9.93	5 (62%)
3	CYT	B	739	-	5,8,8	1.65	1 (20%)	8,10,10	9.91	5 (62%)
2	ADE	C	737	-	8,11,11	0.88	0	4,15,15	5.17	2 (50%)
3	CYT	C	738	-	5,8,8	1.66	1 (20%)	8,10,10	9.91	5 (62%)
2	ADE	D	737	-	8,11,11	0.87	0	4,15,15	5.17	2 (50%)
3	CYT	D	738	-	5,8,8	1.65	1 (20%)	8,10,10	9.88	5 (62%)
2	ADE	E	737	-	8,11,11	0.87	0	4,15,15	5.18	2 (50%)
3	CYT	E	738	-	5,8,8	1.64	1 (20%)	8,10,10	9.91	5 (62%)
2	ADE	F	737	-	8,11,11	0.88	0	4,15,15	5.16	2 (50%)
3	CYT	F	738	-	5,8,8	1.67	1 (20%)	8,10,10	9.85	5 (62%)
2	ADE	G	737	-	8,11,11	0.87	0	4,15,15	5.18	2 (50%)
2	ADE	H	737	-	8,11,11	0.86	0	4,15,15	5.15	2 (50%)
3	CYT	H	738	-	5,8,8	1.66	1 (20%)	8,10,10	9.87	5 (62%)
2	ADE	I	737	-	8,11,11	0.87	0	4,15,15	5.19	2 (50%)
3	CYT	I	738	-	5,8,8	1.66	1 (20%)	8,10,10	9.90	5 (62%)
2	ADE	J	737	-	8,11,11	0.86	0	4,15,15	5.14	2 (50%)
3	CYT	J	738	-	5,8,8	1.64	1 (20%)	8,10,10	9.95	5 (62%)

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	ADE	A	737	-	-	0/0/0/0	0/2/2/2
3	CYT	A	738	-	-	0/0/0/0	0/1/1/1
2	ADE	B	737	-	-	0/0/0/0	0/2/2/2
3	CYT	B	738	-	-	0/0/0/0	0/1/1/1
3	CYT	B	739	-	-	0/0/0/0	0/1/1/1
2	ADE	C	737	-	-	0/0/0/0	0/2/2/2
3	CYT	C	738	-	-	0/0/0/0	0/1/1/1
2	ADE	D	737	-	-	0/0/0/0	0/2/2/2
3	CYT	D	738	-	-	0/0/0/0	0/1/1/1
2	ADE	E	737	-	-	0/0/0/0	0/2/2/2
3	CYT	E	738	-	-	0/0/0/0	0/1/1/1
2	ADE	F	737	-	-	0/0/0/0	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYT	F	738	-	-	0/0/0/0	0/1/1/1
2	ADE	G	737	-	-	0/0/0/0	0/2/2/2
2	ADE	H	737	-	-	0/0/0/0	0/2/2/2
3	CYT	H	738	-	-	0/0/0/0	0/1/1/1
2	ADE	I	737	-	-	0/0/0/0	0/2/2/2
3	CYT	I	738	-	-	0/0/0/0	0/1/1/1
2	ADE	J	737	-	-	0/0/0/0	0/2/2/2
3	CYT	J	738	-	-	0/0/0/0	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	738	CYT	C5-C6	-2.56	1.33	1.38
3	I	738	CYT	C5-C6	-2.55	1.33	1.38
3	D	738	CYT	C5-C6	-2.54	1.33	1.38
3	A	738	CYT	C5-C6	-2.53	1.33	1.38
3	C	738	CYT	C5-C6	-2.52	1.33	1.38
3	H	738	CYT	C5-C6	-2.52	1.33	1.38
3	E	738	CYT	C5-C6	-2.51	1.33	1.38
3	J	738	CYT	C5-C6	-2.51	1.33	1.38
3	B	739	CYT	C5-C6	-2.51	1.33	1.38
3	B	738	CYT	C5-C6	-2.50	1.33	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	738	CYT	N1-C2-N3	-20.21	115.44	128.33
3	B	738	CYT	N1-C2-N3	-20.18	115.46	128.33
3	I	738	CYT	N1-C2-N3	-20.15	115.47	128.33
3	E	738	CYT	N1-C2-N3	-20.14	115.48	128.33
3	B	739	CYT	N1-C2-N3	-20.14	115.48	128.33
3	A	738	CYT	N1-C2-N3	-20.11	115.50	128.33
3	C	738	CYT	N1-C2-N3	-20.11	115.50	128.33
3	H	738	CYT	N1-C2-N3	-20.09	115.52	128.33
3	D	738	CYT	N1-C2-N3	-20.06	115.53	128.33
3	F	738	CYT	N1-C2-N3	-20.06	115.54	128.33
2	I	737	ADE	N3-C2-N1	-9.24	121.82	128.89
2	E	737	ADE	N3-C2-N1	-9.24	121.82	128.89
2	D	737	ADE	N3-C2-N1	-9.24	121.82	128.89
2	A	737	ADE	N3-C2-N1	-9.23	121.83	128.89
2	G	737	ADE	N3-C2-N1	-9.22	121.83	128.89
2	C	737	ADE	N3-C2-N1	-9.20	121.85	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	737	ADE	N3-C2-N1	-9.20	121.85	128.89
2	H	737	ADE	N3-C2-N1	-9.18	121.87	128.89
2	B	737	ADE	N3-C2-N1	-9.17	121.87	128.89
2	J	737	ADE	N3-C2-N1	-9.15	121.89	128.89
2	G	737	ADE	C4-C5-N7	-4.41	105.42	109.48
2	C	737	ADE	C4-C5-N7	-4.40	105.43	109.48
2	H	737	ADE	C4-C5-N7	-4.39	105.44	109.48
2	I	737	ADE	C4-C5-N7	-4.39	105.44	109.48
2	J	737	ADE	C4-C5-N7	-4.39	105.44	109.48
2	E	737	ADE	C4-C5-N7	-4.38	105.45	109.48
2	F	737	ADE	C4-C5-N7	-4.36	105.47	109.48
2	A	737	ADE	C4-C5-N7	-4.36	105.47	109.48
2	D	737	ADE	C4-C5-N7	-4.33	105.50	109.48
2	B	737	ADE	C4-C5-N7	-4.31	105.52	109.48
3	C	738	CYT	C5-C6-N1	-3.18	120.27	123.90
3	E	738	CYT	C5-C6-N1	-3.17	120.28	123.90
3	J	738	CYT	C5-C6-N1	-3.16	120.30	123.90
3	A	738	CYT	C5-C6-N1	-3.15	120.30	123.90
3	D	738	CYT	C5-C6-N1	-3.15	120.30	123.90
3	B	738	CYT	C5-C6-N1	-3.15	120.31	123.90
3	H	738	CYT	C5-C6-N1	-3.14	120.31	123.90
3	B	739	CYT	C5-C6-N1	-3.13	120.33	123.90
3	F	738	CYT	C5-C6-N1	-3.11	120.34	123.90
3	I	738	CYT	C5-C6-N1	-3.11	120.35	123.90
3	B	739	CYT	C5-C4-N3	2.67	125.17	121.80
3	B	738	CYT	C5-C4-N3	2.67	125.17	121.80
3	F	738	CYT	C5-C4-N3	2.68	125.17	121.80
3	J	738	CYT	C5-C4-N3	2.70	125.20	121.80
3	C	738	CYT	C5-C4-N3	2.70	125.20	121.80
3	E	738	CYT	C5-C4-N3	2.71	125.21	121.80
3	A	738	CYT	C5-C4-N3	2.72	125.22	121.80
3	D	738	CYT	C5-C4-N3	2.72	125.22	121.80
3	H	738	CYT	C5-C4-N3	2.72	125.23	121.80
3	I	738	CYT	C5-C4-N3	2.74	125.25	121.80
3	D	738	CYT	C2-N3-C4	3.38	120.38	115.61
3	A	738	CYT	C2-N3-C4	3.40	120.40	115.61
3	I	738	CYT	C2-N3-C4	3.40	120.41	115.61
3	C	738	CYT	C2-N3-C4	3.40	120.41	115.61
3	H	738	CYT	C2-N3-C4	3.41	120.43	115.61
3	F	738	CYT	C2-N3-C4	3.41	120.43	115.61
3	E	738	CYT	C2-N3-C4	3.42	120.43	115.61
3	J	738	CYT	C2-N3-C4	3.44	120.46	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	739	CYT	C2-N3-C4	3.45	120.48	115.61
3	B	738	CYT	C2-N3-C4	3.46	120.50	115.61
3	F	738	CYT	C6-N1-C2	18.44	123.47	114.40
3	H	738	CYT	C6-N1-C2	18.50	123.50	114.40
3	I	738	CYT	C6-N1-C2	18.54	123.52	114.40
3	D	738	CYT	C6-N1-C2	18.58	123.54	114.40
3	A	738	CYT	C6-N1-C2	18.59	123.55	114.40
3	B	739	CYT	C6-N1-C2	18.59	123.55	114.40
3	E	738	CYT	C6-N1-C2	18.60	123.55	114.40
3	B	738	CYT	C6-N1-C2	18.62	123.56	114.40
3	C	738	CYT	C6-N1-C2	18.64	123.57	114.40
3	J	738	CYT	C6-N1-C2	18.69	123.59	114.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	738	CYT	3	0
2	B	737	ADE	3	0
3	B	739	CYT	1	0
3	C	738	CYT	3	0
3	D	738	CYT	3	0
3	E	738	CYT	1	0
3	F	738	CYT	2	0
3	H	738	CYT	3	0
3	I	738	CYT	2	0
3	J	738	CYT	1	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.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	520/736 (70%)	0.32	20 (3%)	44	49	25, 34, 55, 92	0
1	B	520/736 (70%)	0.66	33 (6%)	23	26	25, 34, 55, 92	0
1	C	520/736 (70%)	0.90	34 (6%)	22	25	25, 34, 55, 92	0
1	D	520/736 (70%)	0.52	22 (4%)	40	45	25, 34, 55, 92	0
1	E	520/736 (70%)	0.86	42 (8%)	15	16	25, 34, 55, 92	0
1	F	520/736 (70%)	0.66	27 (5%)	31	35	25, 34, 55, 92	0
1	G	520/736 (70%)	0.84	45 (8%)	13	13	25, 34, 55, 92	0
1	H	520/736 (70%)	0.47	27 (5%)	31	35	25, 34, 55, 92	0
1	I	520/736 (70%)	0.98	44 (8%)	13	14	25, 34, 55, 92	0
1	J	520/736 (70%)	1.34	95 (18%)	2	2	25, 34, 55, 92	0
All	All	5200/7360 (70%)	0.76	389 (7%)	17	19	25, 34, 55, 92	0

All (389) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	453	SER	13.4
1	G	453	SER	11.5
1	F	453	SER	11.3
1	F	456	ALA	11.0
1	I	453	SER	10.0
1	I	217	GLY	9.5
1	J	453	SER	9.4
1	A	330	VAL	9.1
1	B	452	GLN	9.0
1	B	453	SER	8.9
1	C	218	ALA	8.8
1	J	456	ALA	8.8
1	A	454	GLY	8.7

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	8.6
1	D	456	ALA	8.5
1	E	452	GLN	8.4
1	C	217	GLY	8.4
1	I	454	GLY	8.2
1	I	455	SER	8.2
1	C	457	GLN	8.2
1	J	452	GLN	8.1
1	E	453	SER	8.1
1	G	218	ALA	8.0
1	F	452	GLN	8.0
1	B	454	GLY	8.0
1	G	457	GLN	7.9
1	B	329	GLY	7.9
1	E	456	ALA	7.7
1	H	452	GLN	7.6
1	G	456	ALA	7.6
1	J	218	ALA	7.6
1	C	453	SER	7.5
1	H	328	ASP	7.4
1	C	452	GLN	7.4
1	D	217	GLY	7.3
1	D	327	ASN	7.2
1	D	452	GLN	7.2
1	J	328	ASP	7.1
1	D	328	ASP	7.1
1	C	456	ALA	7.1
1	J	327	ASN	7.1
1	H	218	ALA	7.0
1	I	330	VAL	7.0
1	G	330	VAL	6.9
1	I	328	ASP	6.9
1	B	328	ASP	6.8
1	C	328	ASP	6.6
1	F	330	VAL	6.5
1	E	218	ALA	6.5
1	D	218	ALA	6.5
1	J	330	VAL	6.4
1	H	456	ALA	6.4
1	I	329	GLY	6.4
1	J	329	GLY	6.4
1	B	217	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	G	328	ASP	6.3
1	E	217	GLY	6.2
1	A	328	ASP	6.1
1	H	457	GLN	6.1
1	A	453	SER	6.0
1	F	454	GLY	6.0
1	A	327	ASN	5.9
1	B	327	ASN	5.9
1	J	457	GLN	5.8
1	B	456	ALA	5.8
1	C	455	SER	5.7
1	H	217	GLY	5.6
1	B	455	SER	5.6
1	D	453	SER	5.6
1	F	457	GLN	5.6
1	E	455	SER	5.5
1	E	330	VAL	5.5
1	C	329	GLY	5.5
1	H	329	GLY	5.5
1	G	452	GLN	5.4
1	G	329	GLY	5.4
1	B	330	VAL	5.4
1	I	452	GLN	5.4
1	J	705	TYR	5.3
1	J	217	GLY	5.3
1	A	455	SER	5.3
1	I	456	ALA	5.3
1	J	264	SER	5.2
1	G	220	GLY	5.2
1	J	454	GLY	5.2
1	B	457	GLN	5.2
1	A	452	GLN	5.2
1	G	327	ASN	5.0
1	I	327	ASN	5.0
1	G	217	GLY	4.9
1	I	218	ALA	4.7
1	G	265	THR	4.7
1	D	455	SER	4.6
1	J	219	ASP	4.6
1	E	327	ASN	4.5
1	E	457	GLN	4.5
1	D	457	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	327	ASN	4.5
1	D	219	ASP	4.5
1	A	456	ALA	4.5
1	J	656	ALA	4.5
1	C	330	VAL	4.4
1	E	219	ASP	4.4
1	G	235	LEU	4.4
1	A	331	THR	4.4
1	G	455	SER	4.4
1	E	328	ASP	4.4
1	F	455	SER	4.4
1	C	454	GLY	4.3
1	I	457	GLN	4.2
1	B	266	GLY	4.2
1	F	327	ASN	4.2
1	D	556	ASP	4.2
1	D	330	VAL	4.1
1	C	705	TYR	4.1
1	E	264	SER	4.1
1	J	265	THR	4.0
1	F	329	GLY	4.0
1	F	587	SER	4.0
1	A	218	ALA	4.0
1	A	217	GLY	4.0
1	H	705	TYR	3.9
1	H	229	HIS	3.9
1	G	229	HIS	3.9
1	J	451	ASN	3.9
1	I	705	TYR	3.9
1	C	327	ASN	3.9
1	B	218	ALA	3.8
1	I	502	THR	3.8
1	C	235	LEU	3.8
1	F	328	ASP	3.8
1	B	705	TYR	3.7
1	I	265	THR	3.6
1	A	325	THR	3.6
1	F	218	ALA	3.6
1	H	265	THR	3.6
1	J	449	THR	3.5
1	G	325	THR	3.4
1	G	264	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	704	ASN	3.4
1	J	266	GLY	3.4
1	C	494	THR	3.3
1	I	326	THR	3.3
1	J	493	LYS	3.3
1	C	219	ASP	3.3
1	B	264	SER	3.3
1	J	229	HIS	3.3
1	H	330	VAL	3.2
1	G	500	ASN	3.2
1	J	706	ALA	3.2
1	J	489	VAL	3.2
1	E	329	GLY	3.2
1	H	455	SER	3.2
1	J	395	CYS	3.2
1	J	461	LEU	3.2
1	J	661	GLU	3.2
1	I	628	HIS	3.1
1	H	219	ASP	3.1
1	H	506	ALA	3.1
1	A	265	THR	3.1
1	D	265	THR	3.1
1	F	265	THR	3.1
1	J	267	ALA	3.1
1	J	385	SER	3.1
1	A	266	GLY	3.1
1	H	235	LEU	3.1
1	J	703	SER	3.1
1	E	461	LEU	3.0
1	H	454	GLY	3.0
1	B	495	ASP	3.0
1	E	556	ASP	3.0
1	J	664	ALA	3.0
1	C	590	ASP	3.0
1	J	498	ASN	3.0
1	C	499	SER	3.0
1	E	705	TYR	3.0
1	I	334	ALA	3.0
1	G	458	ASN	3.0
1	J	490	SER	3.0
1	G	266	GLY	3.0
1	J	497	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	264	SER	2.9
1	F	556	ASP	2.9
1	J	455	SER	2.9
1	D	332	THR	2.9
1	G	705	TYR	2.9
1	G	584	PHE	2.9
1	I	736	LEU	2.9
1	G	237	ASP	2.9
1	F	547	SER	2.9
1	J	628	HIS	2.9
1	J	660	ALA	2.9
1	B	325	THR	2.9
1	B	332	THR	2.8
1	G	556	ASP	2.8
1	J	366	PHE	2.8
1	J	709	ALA	2.8
1	C	265	THR	2.8
1	G	494	THR	2.8
1	J	253	ASN	2.8
1	E	498	ASN	2.8
1	G	238	ARG	2.8
1	F	325	THR	2.7
1	B	451	ASN	2.7
1	J	319	ILE	2.7
1	A	326	THR	2.7
1	J	710	ASN	2.7
1	J	584	PHE	2.7
1	J	726	PRO	2.7
1	E	490	SER	2.7
1	E	736	LEU	2.7
1	J	670	PHE	2.7
1	E	589	THR	2.7
1	I	324	VAL	2.7
1	G	451	ASN	2.7
1	B	326	THR	2.7
1	J	587	SER	2.7
1	J	312	LEU	2.6
1	D	264	SER	2.6
1	I	264	SER	2.6
1	F	223	ASN	2.6
1	E	503	TRP	2.6
1	B	587	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	458	ASN	2.6
1	J	669	SER	2.6
1	C	736	LEU	2.6
1	H	266	GLY	2.6
1	B	502	THR	2.6
1	H	492	THR	2.6
1	H	556	ASP	2.5
1	F	458	ASN	2.5
1	E	235	LEU	2.5
1	G	450	GLN	2.5
1	E	656	ALA	2.5
1	I	656	ALA	2.5
1	J	662	PHE	2.5
1	G	665	THR	2.5
1	J	439	ILE	2.5
1	B	470	GLY	2.5
1	J	499	SER	2.5
1	I	331	THR	2.5
1	I	338	THR	2.5
1	E	704	ASN	2.5
1	J	680	SER	2.5
1	B	530	ASP	2.5
1	C	556	ASP	2.5
1	J	492	THR	2.5
1	F	705	TYR	2.5
1	J	263	ALA	2.5
1	H	264	SER	2.5
1	J	586	SER	2.5
1	B	324	VAL	2.5
1	C	325	THR	2.5
1	H	546	GLU	2.5
1	J	667	PHE	2.4
1	C	458	ASN	2.4
1	E	588	SER	2.4
1	G	267	ALA	2.4
1	J	459	LYS	2.4
1	F	460	ASP	2.4
1	E	454	GLY	2.4
1	E	710	ASN	2.4
1	J	463	PHE	2.4
1	J	713	PHE	2.4
1	F	217	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	236	GLY	2.4
1	J	458	ASN	2.4
1	B	219	ASP	2.4
1	I	444	TYR	2.4
1	C	532	ASP	2.4
1	I	219	ASP	2.4
1	J	503	TRP	2.4
1	F	341	VAL	2.4
1	B	331	THR	2.4
1	I	290	CYS	2.4
1	D	705	TYR	2.4
1	J	323	GLU	2.4
1	J	338	THR	2.4
1	I	503	TRP	2.3
1	G	460	ASP	2.3
1	I	532	ASP	2.3
1	D	461	LEU	2.3
1	E	502	THR	2.3
1	G	589	THR	2.3
1	I	235	LEU	2.3
1	G	660	ALA	2.3
1	E	661	GLU	2.3
1	I	546	GLU	2.3
1	C	229	HIS	2.3
1	J	501	PHE	2.3
1	E	398	TYR	2.3
1	J	387	ALA	2.3
1	J	500	ASN	2.3
1	B	265	THR	2.3
1	J	655	PRO	2.3
1	G	668	ALA	2.3
1	I	706	ALA	2.3
1	D	235	LEU	2.3
1	E	458	ASN	2.3
1	I	325	THR	2.3
1	J	273	TYR	2.3
1	J	721	TYR	2.3
1	B	269	ASN	2.2
1	E	539	GLY	2.2
1	F	266	GLY	2.2
1	J	332	THR	2.2
1	C	391	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	269	ASN	2.2
1	E	300	LEU	2.2
1	I	484	TYR	2.2
1	E	683	ILE	2.2
1	J	243	SER	2.2
1	J	418	GLU	2.2
1	J	601	ALA	2.2
1	G	269	ASN	2.2
1	G	454	GLY	2.2
1	B	532	ASP	2.2
1	I	664	ALA	2.2
1	J	254	ASN	2.2
1	J	495	ASP	2.2
1	F	264	SER	2.2
1	I	229	HIS	2.2
1	C	503	TRP	2.2
1	C	592	ALA	2.2
1	F	229	HIS	2.2
1	C	483	CYS	2.2
1	A	502	THR	2.2
1	J	702	THR	2.2
1	G	489	VAL	2.1
1	C	326	THR	2.1
1	J	359	HIS	2.1
1	J	450	GLN	2.1
1	J	534	PHE	2.1
1	G	498	ASN	2.1
1	G	546	GLU	2.1
1	J	727	ILE	2.1
1	J	588	SER	2.1
1	J	725	ARG	2.1
1	A	503	TRP	2.1
1	G	550	ALA	2.1
1	J	546	GLU	2.1
1	I	220	GLY	2.1
1	C	588	SER	2.1
1	J	613	TYR	2.1
1	D	454	GLY	2.1
1	E	446	LEU	2.1
1	F	555	LEU	2.1
1	J	283	PHE	2.1
1	B	449	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	546	GLU	2.1
1	G	244	THR	2.1
1	H	332	THR	2.1
1	H	547	SER	2.1
1	I	499	SER	2.1
1	I	556	ASP	2.1
1	C	506	ALA	2.1
1	I	660	ALA	2.1
1	B	497	ASN	2.1
1	E	419	VAL	2.1
1	I	582	VAL	2.1
1	G	483	CYS	2.1
1	D	736	LEU	2.1
1	I	461	LEU	2.1
1	J	364	PRO	2.1
1	F	529	ASP	2.1
1	J	556	ASP	2.1
1	H	223	ASN	2.0
1	I	388	VAL	2.0
1	J	290	CYS	2.0
1	J	404	LEU	2.0
1	J	571	PRO	2.0
1	E	325	THR	2.0
1	E	494	THR	2.0
1	J	325	THR	2.0
1	D	458	ASN	2.0
1	D	500	ASN	2.0
1	H	458	ASN	2.0
1	J	448	ARG	2.0
1	G	221	VAL	2.0
1	A	219	ASP	2.0
1	C	292	PHE	2.0
1	J	589	THR	2.0
1	E	387	ALA	2.0
1	E	229	HIS	2.0
1	I	221	VAL	2.0
1	J	596	VAL	2.0
1	J	631	PRO	2.0
1	C	451	ASN	2.0
1	E	497	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CYT	H	738	8/8	0.54	0.43	9.13	63,67,68,70	0
2	ADE	D	737	10/10	0.79	0.29	7.90	78,81,82,83	0
3	CYT	B	739	8/8	0.59	0.38	7.63	63,67,68,70	0
2	ADE	F	737	10/10	0.63	0.46	7.29	78,81,82,83	0
3	CYT	E	738	8/8	0.43	0.47	7.01	63,67,68,70	0
2	ADE	H	737	10/10	0.82	0.31	6.27	78,81,82,83	0
2	ADE	G	737	10/10	0.80	0.35	6.23	78,81,82,83	0
3	CYT	B	738	8/8	0.72	0.34	6.19	63,67,68,70	0
3	CYT	D	738	8/8	0.52	0.40	5.93	63,67,68,70	0
2	ADE	A	737	10/10	0.77	0.33	5.80	78,81,82,83	0
3	CYT	I	738	8/8	0.76	0.33	5.57	63,67,68,70	0
2	ADE	I	737	10/10	0.73	0.34	5.31	78,81,82,83	0
2	ADE	E	737	10/10	0.74	0.40	4.85	78,81,82,83	0
2	ADE	J	737	10/10	0.82	0.36	4.81	78,81,82,83	0
3	CYT	F	738	8/8	0.54	0.38	4.20	63,67,68,70	0
2	ADE	C	737	10/10	0.82	0.30	3.93	78,81,82,83	0
3	CYT	A	738	8/8	0.76	0.34	3.57	63,67,68,70	0
3	CYT	C	738	8/8	0.60	0.42	3.40	63,67,68,70	0
2	ADE	B	737	10/10	0.83	0.25	3.01	78,81,82,83	0
3	CYT	J	738	8/8	0.79	0.36	2.28	63,67,68,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.