



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 12:17 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

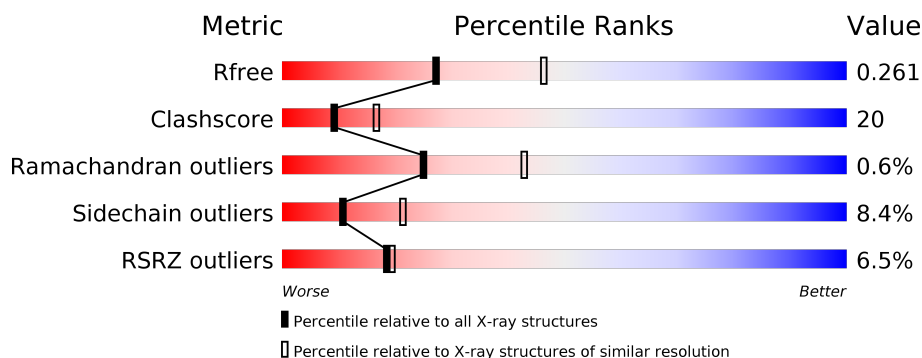
1 Overall quality at a glance

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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>2%</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>4%</div> <div> <div></div> <div>48%</div> <div>20%</div> <div>•</div> <div>29%</div> </div> </div>
1	D	736	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>21%</div> <div>•</div> <div>29%</div> </div> </div>
1	E	736	<div> <div>5%</div> <div> <div></div> <div>47%</div> <div>21%</div> <div>•</div> <div>29%</div> </div> </div>
1	F	736	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>22%</div> <div>•</div> <div>29%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	F	737	-	-	-	X
3	CYT	C	738	-	-	-	X
3	CYT	E	738	-	-	-	X
3	CYT	H	738	-	-	-	X

2 Entry composition

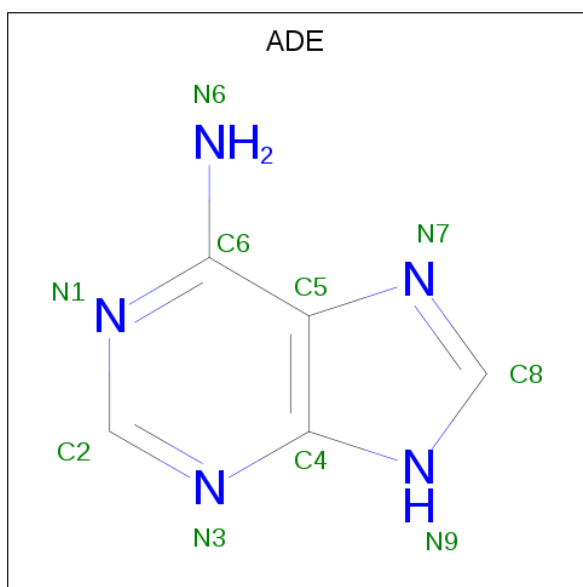
There are 4 unique types of molecules in this entry. The entry contains 42680 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

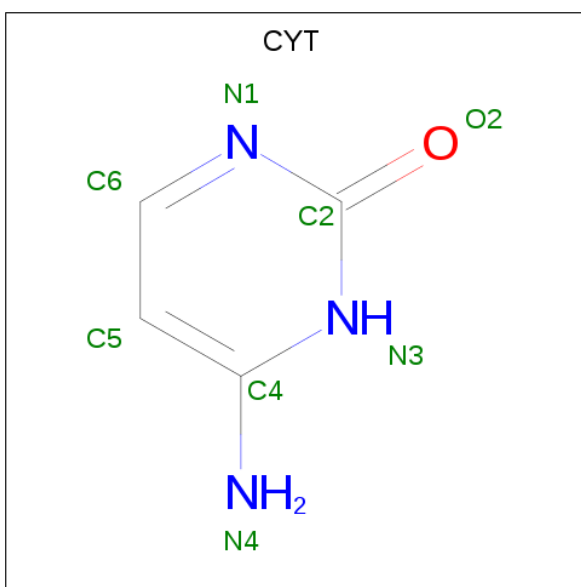
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	B	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	C	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	D	520	Total	C	N	O	S	0	0	0
			4120	2606	710	788	16			
1	E	520	Total	C	N	O	S	0	0	0
			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: C₅H₅N₅).



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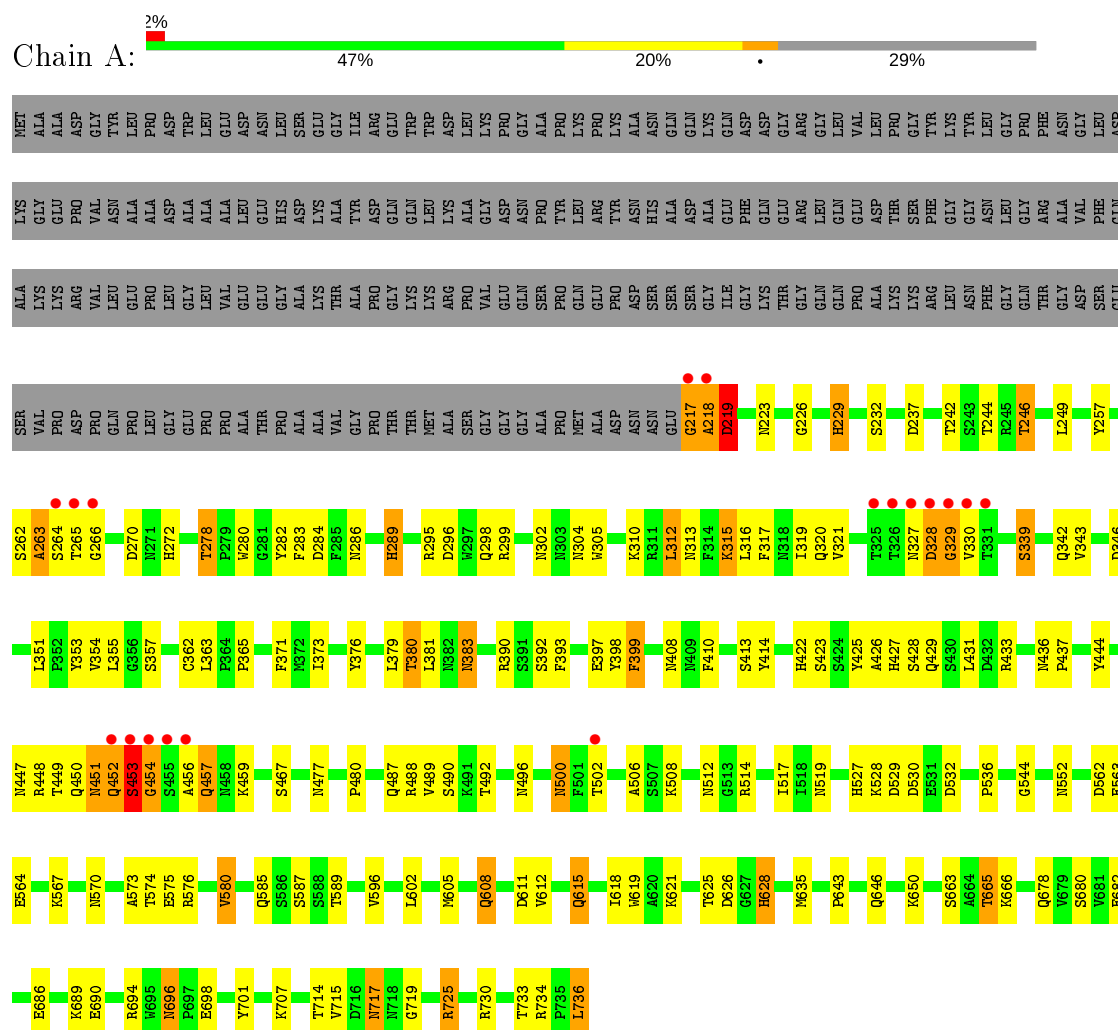
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	128	Total 128	O 128	0	0
4	D	131	Total 131	O 131	0	0
4	E	133	Total 133	O 133	0	0
4	F	131	Total 131	O 131	0	0
4	G	127	Total 127	O 127	0	0
4	H	130	Total 130	O 130	0	0
4	I	130	Total 130	O 130	0	0
4	J	129	Total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

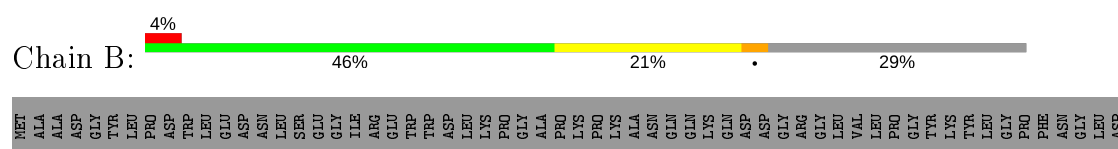
3 Residue-property plots

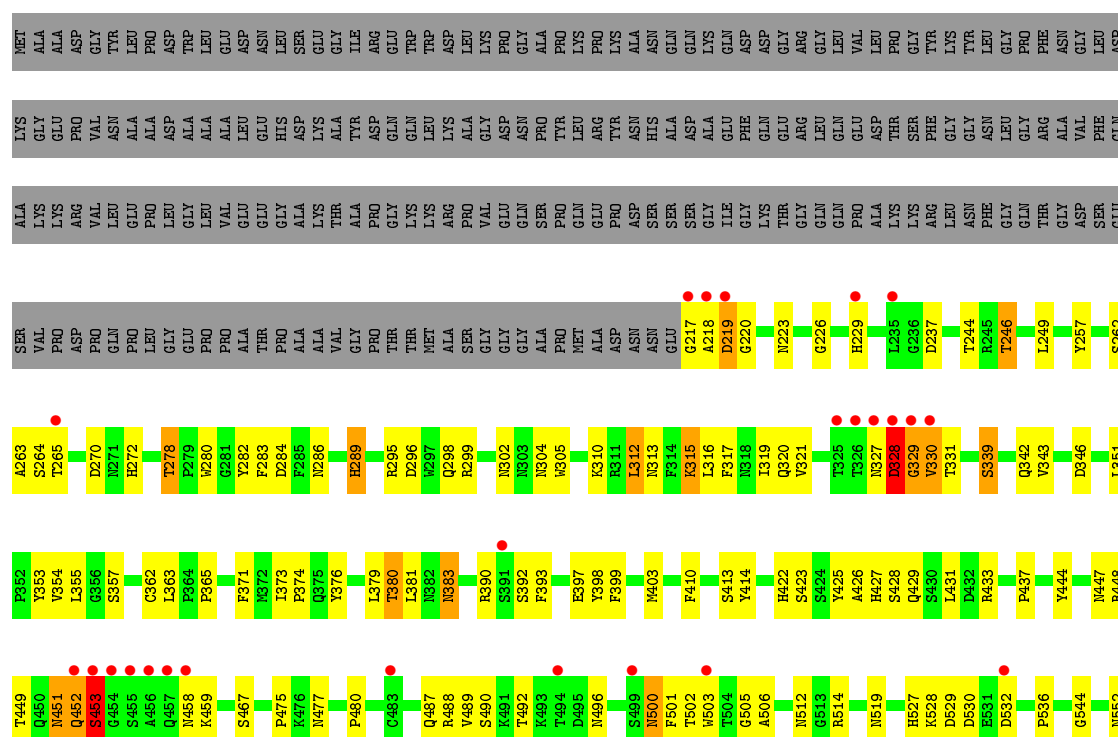
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

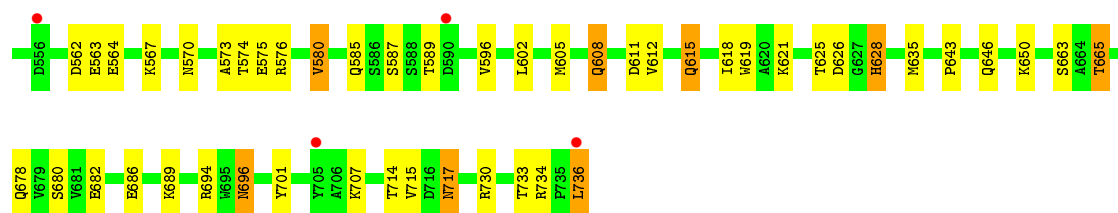
• Molecule 1: Capsid protein



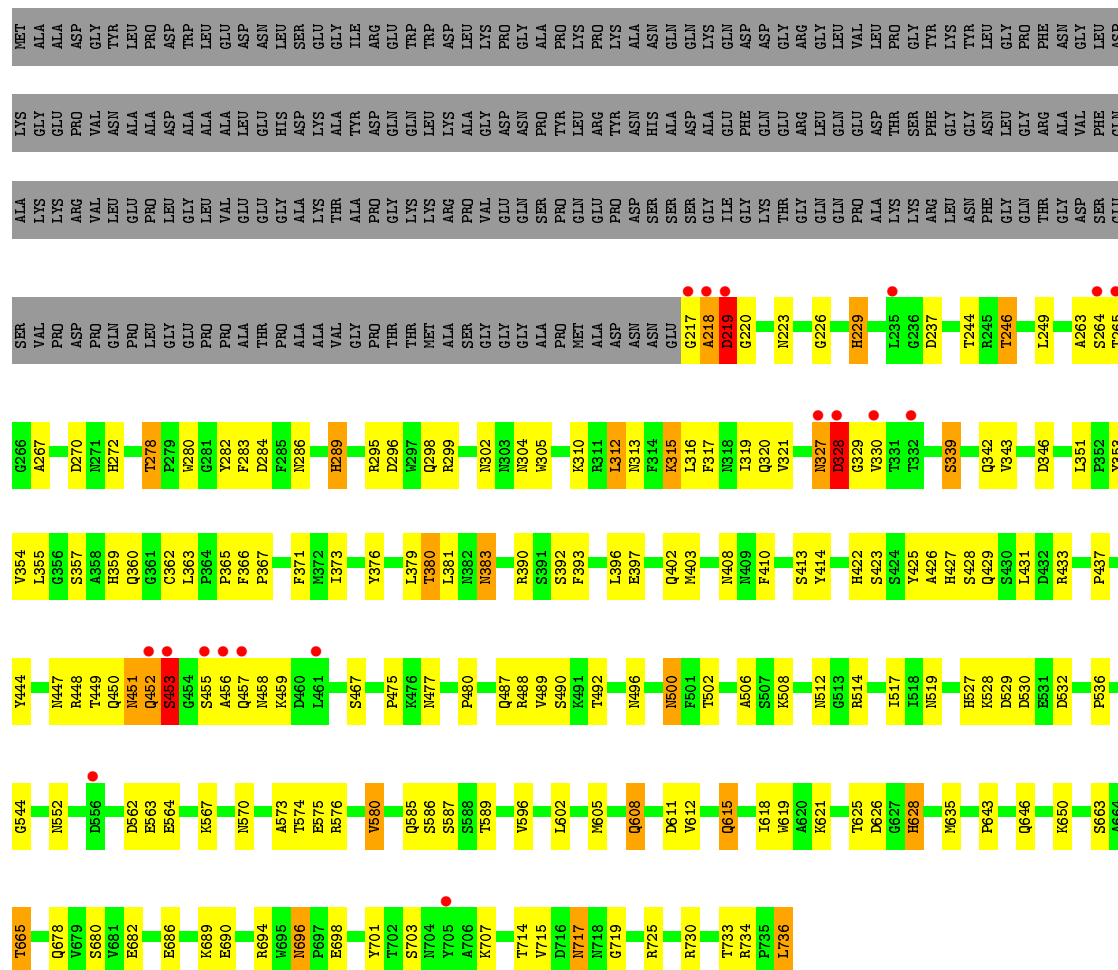
• Molecule 1: Capsid protein



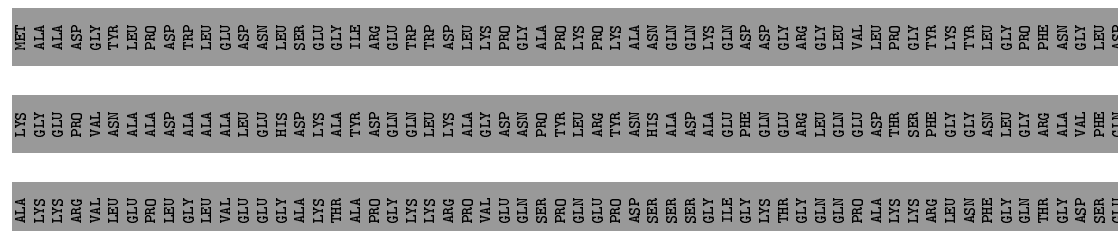


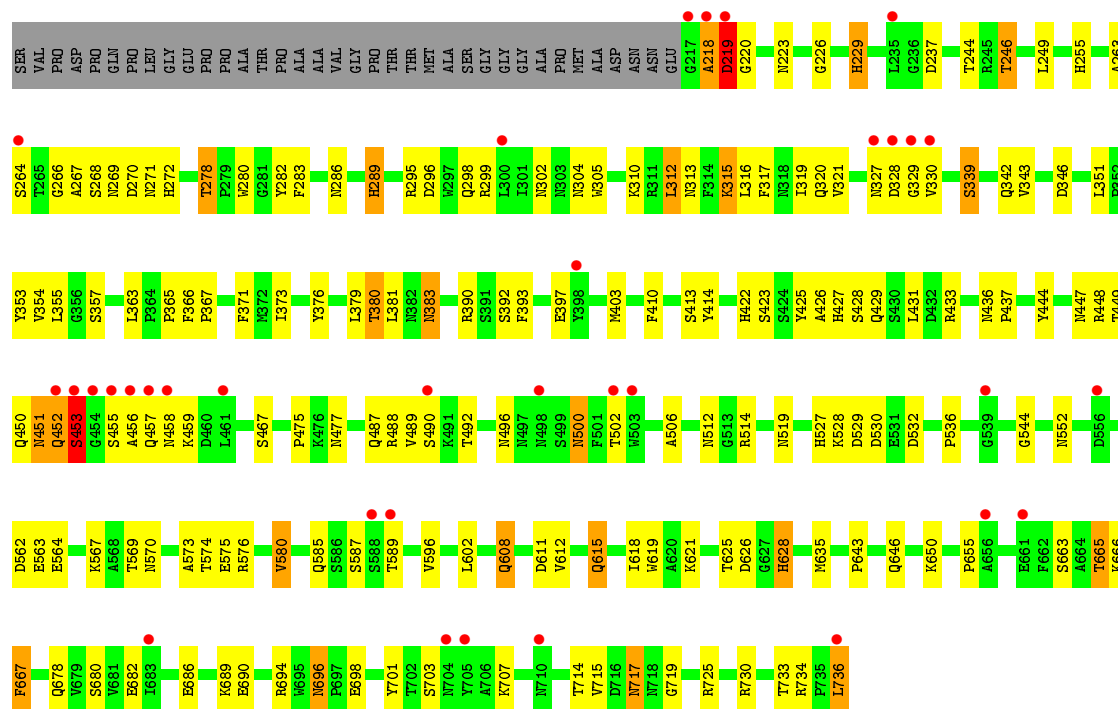


• Molecule 1: Capsid protein

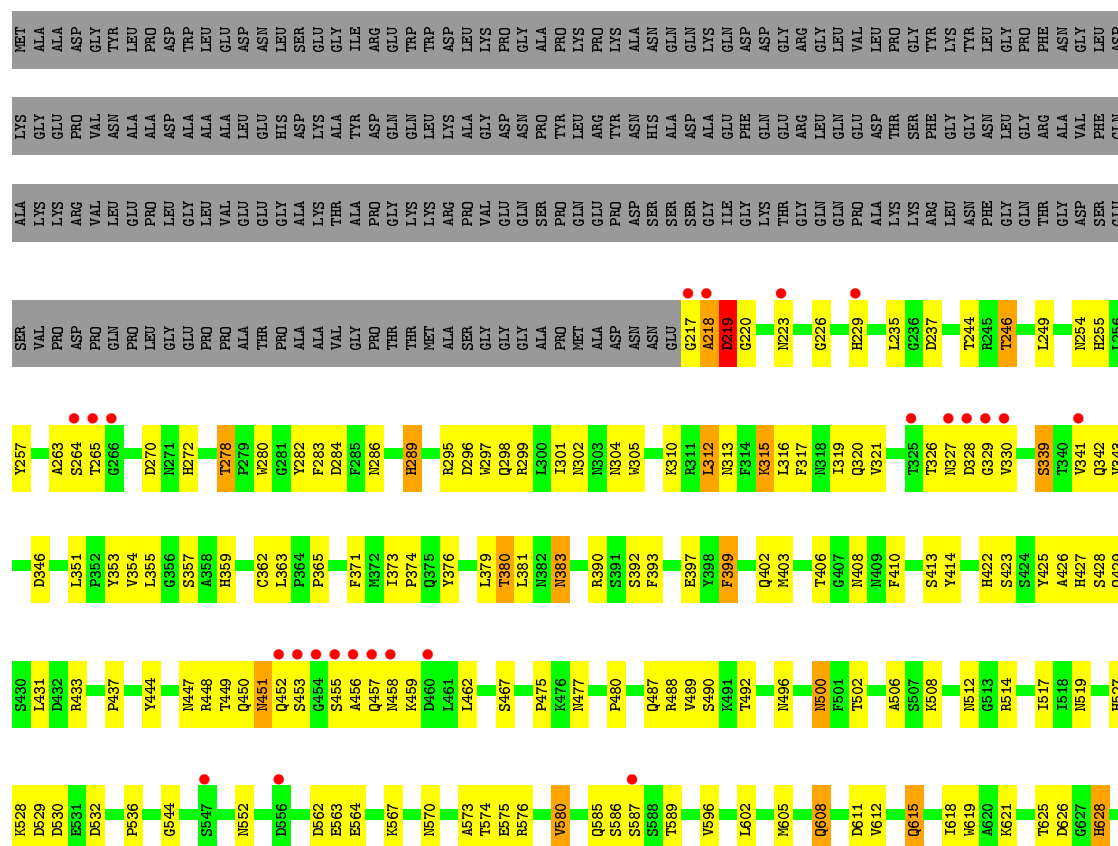


• Molecule 1: Capsid protein



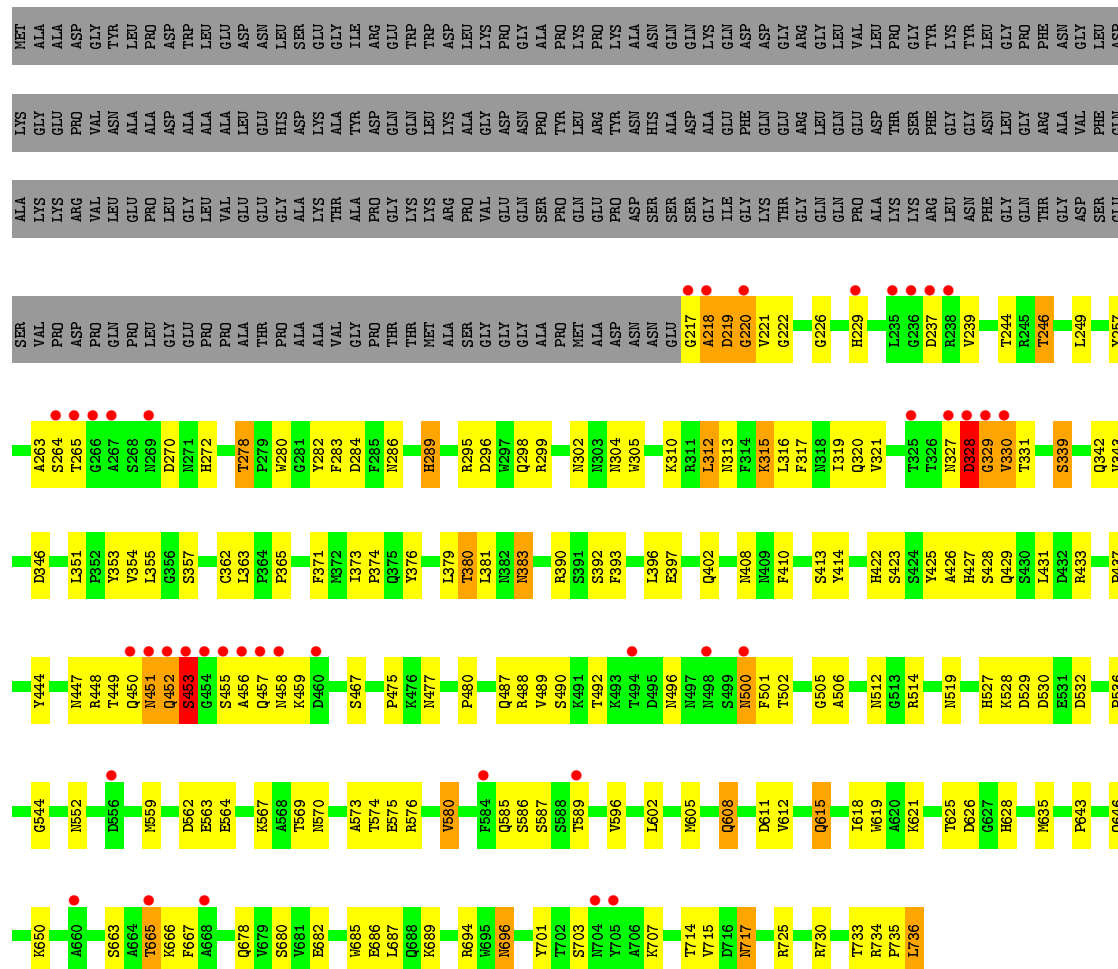


• Molecule 1: Capsid protein

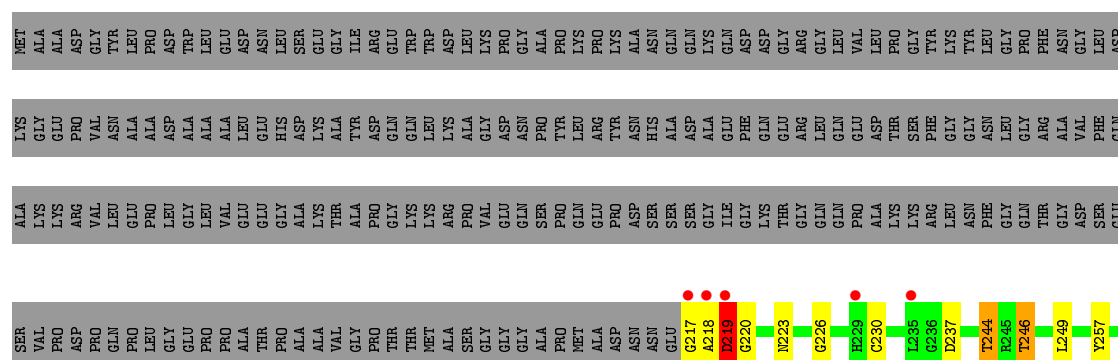


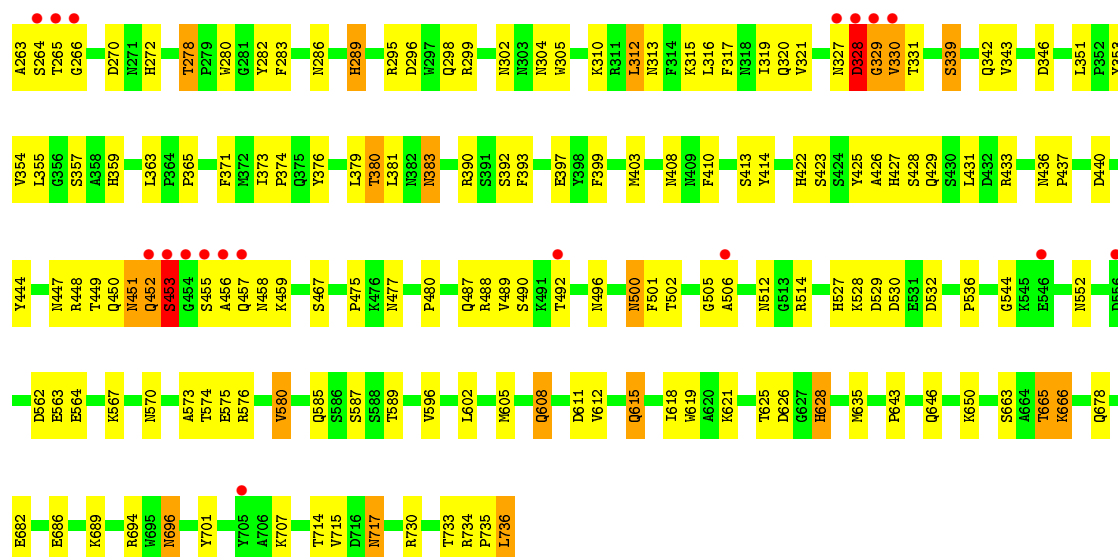


• Molecule 1: Capsid protein

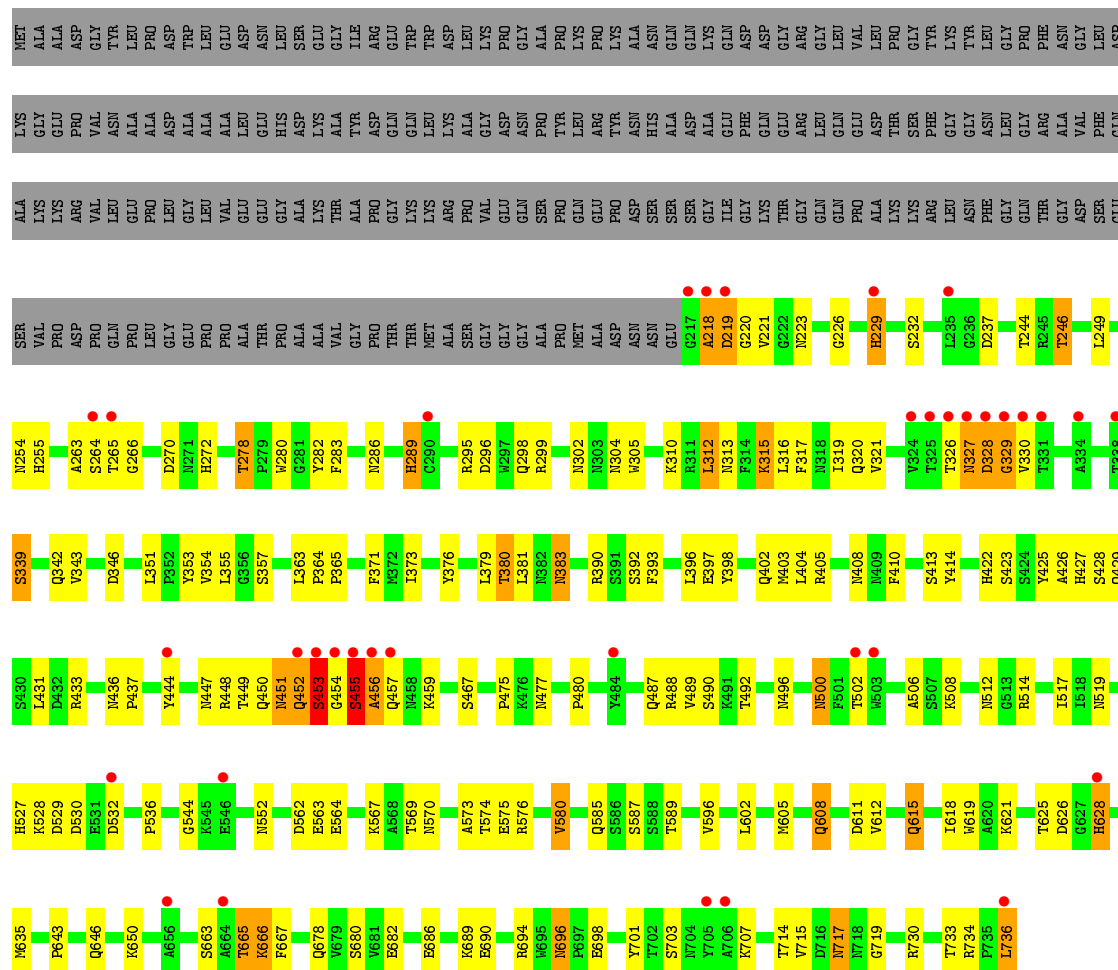


• Molecule 1: Capsid protein





• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.250 0.257 , 0.261	Depositor DCC
R_{free} test set	12421 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
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
F_o, F_c correlation	0.88	EDS
Total number of atoms	42680	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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:C:502:THR:O	1:C:506:ALA:HB2	1.55	1.06
1:F:502:THR:O	1:F: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:B:380:THR:HG21	1:B:392:SER:H	1.21	1.05
1:I:502:THR:O	1:I:506:ALA:HB2	1.55	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:D:380:THR:HG21	1:D:392:SER:H	1.21	1.01
1:C:380:THR:HG21	1:C: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:B:269:ASN:HA	1:B:272:HIS:HD2	1.31	0.96
1:H:451:ASN:CA	1:H:452:GLN:HB2	1.96	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: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
1:I:278:THR:HG22	1:I: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:A:312:LEU:HD23	1:A:312:LEU:C	1.88	0.94
1:F:278:THR:HG22	1:F:280:TRP:H	1.31	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:E:663:SER:OG	1:E:665:THR:HG23	1.65	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:J:312:LEU:HD23	1:J:312:LEU:C	1.88	0.94
1:C:312:LEU:HD23	1:C:312:LEU:C	1.88	0.94
1:C:451:ASN:CA	1:C:452:GLN:HB2	1.98	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:J:451:ASN:CA	1:J:452:GLN:HB2	1.96	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:E:312:LEU:HD23	1:E:312:LEU:C	1.88	0.93
1:J:278:THR:HG22	1:J:280:TRP:H	1.31	0.93
1:G:312:LEU:C	1:G:312:LEU:HD23	1.88	0.93
1:F:393:PHE:H	1:I:696:ASN:HD21	1.09	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:D:312:LEU:HD22	1:D:414:TYR:HB3	1.53	0.90
1:F:312:LEU:HD22	1:F:414:TYR:HB3	1.53	0.90
1:I:451:ASN:CB	1:I:452:GLN:HB3	2.02	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:C:312:LEU:HD22	1:C:414:TYR:HB3	1.53	0.88
1:I:280:TRP:CE2	1:I:650:LYS:HD3	2.08	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:C:246:THR:HB	1:C:678:GLN:HE21	1.39	0.88
1:E:312:LEU:HD22	1:E:414:TYR:HB3	1.53	0.88
1:F:246:THR:HB	1:F:678:GLN:HE21	1.39	0.88
1:I:312:LEU:HD22	1:I:414:TYR:HB3	1.53	0.88
1:J:451:ASN:HA	1:J:452:GLN:CB	2.04	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:F:456:ALA:C	1:F:457:GLN:OE1	2.15	0.85
1:D:393:PHE:H	1:H:696:ASN:ND2	1.74	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:G:570:ASN:HD21	1:G:608:GLN:H	1.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:570:ASN:HD21	1:J:608:GLN:H	1.24	0.84
1:A:570:ASN:HD21	1:A:608:GLN:H	1.24	0.84
1:B:570:ASN:HD21	1:B:608:GLN:H	1.24	0.84
1:C:451:ASN:HA	1:C:452:GLN:CB	2.04	0.84
1:G:327:ASN:O	1:G:328:ASP:HB2	1.77	0.84
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:F:451:ASN:HB2	1:F:452:GLN:HB3	1.59	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:A:328:ASP:CG	1:A:329:GLY:N	2.30	0.83
1:H:327:ASN:O	1:H:328:ASP:HB2	1.77	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:F:570:ASN:HD21	1:F:608:GLN:H	1.24	0.83
1:A:585:GLN:HE22	1:H:496:ASN:HD22	1.27	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:D:714:THR:HG22	1:D:715:VAL:N	1.96	0.81
1:I:451:ASN:HA	1:I:452:GLN:HB2	1.61	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:F:330:VAL:HG12	1:F:330:VAL:O	1.80	0.80
1:G:237:ASP:O	1:G:687:LEU:HG	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:F:512:ASN:HD21	1:I:529:ASP:H	1.29	0.80
1:E:496:ASN:HD22	1:G:585:GLN:HE22	1.27	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:A:457:GLN:NE2	1:A:457:GLN:N	2.30	0.79
1:E:512:ASN:HD21	1:G:529:ASP:H	1.28	0.79
1:A:714:THR:HG22	1:A:715:VAL:N	1.96	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: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: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:A:529:ASP:H	1:H:512:ASN:HD21	1.29	0.78
1:I:490:SER:H	1:I:496:ASN:HD21	1.29	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:D:490:SER:H	1:D:496:ASN:HD21	1.29	0.78
1:G:451:ASN:CA	1:G:452:GLN:CB	2.62	0.78
1:G:490:SER:H	1:G:496:ASN:HD21	1.29	0.78
1:B:218:ALA:HB1	1:B:219:ASP:OD1	1.83	0.77
1:F:696:ASN:H	1:F:696:ASN:HD22	1.30	0.77
1:B:529:ASP:H	1:G:512:ASN:HD21	1.29	0.77
1:A:696:ASN:HD22	1:A:696:ASN:H	1.30	0.77
1:B:451:ASN:CA	1:B:452:GLN:CB	2.62	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:F:456:ALA:O	1:F:457:GLN:OE1	2.03	0.76
1:G:239:VAL:HG13	1:G:685:TRP:HB2	1.67	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:H	1:H:696:ASN:HD22	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:A:328:ASP:CG	1:A:329:GLY:CA	2.55	0.75
1:D:380:THR:HG23	4:D:845:HOH:O	1.84	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:C:312:LEU:HD23	1:C:312:LEU:O	1.87	0.75
1:H:451:ASN:CA	1:H:452:GLN:CB	2.62	0.75
1:D:312:LEU:O	1:D:312:LEU:HD23	1.87	0.74
1:E:451:ASN:CA	1:E:452:GLN:CB	2.62	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:B:312:LEU:O	1:B:312:LEU:HD23	1.87	0.74
1:C:451:ASN:CA	1:C:452:GLN:CB	2.63	0.74
1:F:312:LEU:O	1:F:312:LEU:HD23	1.87	0.74
1:H:380:THR:HG21	1:H:392:SER:N	2.02	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:G:312:LEU:O	1:G:312:LEU:HD23	1.87	0.74
1:J:380:THR:HG23	4:J:847:HOH:O	1.88	0.74
1:I:663:SER:OG	1:I:665:THR:HG23	1.87	0.73
1:D:427:HIS:CD2	1:D:736:LEU:HD13	2.24	0.73
1:E:312:LEU:HD23	1:E:312:LEU:O	1.87	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: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:I:427:HIS:CD2	1:I:736:LEU:HD13	2.24	0.73
1:F:527:HIS:NE2	1:F:532:ASP:OD2	2.22	0.73
1:H:312:LEU:HD23	1:H:312:LEU:O	1.87	0.73
1:F:218:ALA:O	1:F:219:ASP:CB	2.36	0.73
1:H:218:ALA:O	1:H:219:ASP:CB	2.37	0.73
1:H:304:ASN:HD21	1:H:689:LYS:NZ	1.87	0.73
1:H:380:THR:HG23	4:H:845:HOH:O	1.88	0.73
1:J:427:HIS:CD2	1:J:736:LEU:HD13	2.24	0.73
1:C:451:ASN:HD21	1:C:458:ASN:HB2	1.54	0.73
1:G:527:HIS:NE2	1:G:532:ASP:OD2	2.22	0.73
1:J:312:LEU:HD23	1:J:312:LEU:O	1.87	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:C:304:ASN:HD21	1:C:689:LYS:NZ	1.87	0.72
1:D:527:HIS:NE2	1:D:532:ASP:OD2	2.22	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:H:527:HIS:NE2	1:H:532:ASP:OD2	2.22	0.72
1:I:380:THR:HG23	4:I:847:HOH:O	1.88	0.72
1:C:527:HIS:NE2	1:C:532:ASP:OD2	2.22	0.72
1:J:304:ASN:HD21	1:J:689:LYS:NZ	1.87	0.72
1:A:304:ASN:HD21	1:A:689:LYS:NZ	1.87	0.72
1:B:527:HIS:NE2	1:B:532:ASP:OD2	2.22	0.72
1:D:304:ASN:HD21	1:D:689:LYS:NZ	1.87	0.72
1:F:380:THR:HG21	1:F:392:SER:N	2.02	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: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:B:304:ASN:HD21	1:B:689:LYS:NZ	1.87	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:E:218:ALA:O	1:E:219:ASP:CG	2.30	0.70
1:F:218:ALA:O	1:F:219:ASP:CG	2.30	0.70
1:I:453:SER:HA	1:I:455:SER:N	2.06	0.70
1:E:564:GLU:O	1:E:567:LYS:HG2	1.92	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:I:564:GLU:O	1:I:567:LYS:HG2	1.92	0.70
1:A:457:GLN:HE21	1:A:457:GLN:H	1.39	0.70
1:E:380:THR:HG21	1:E:392:SER:N	2.02	0.70
1:F:217:GLY:HA3	1:F:408:ASN:HA	1.73	0.70
1:I:456:ALA:C	1:I:457:GLN:OE1	2.30	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:A:218:ALA:O	1:A:219:ASP:CG	2.30	0.69
1:H:218:ALA:O	1:H: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:B:564:GLU:O	1:B:567:LYS:HG2	1.92	0.69
1:D:564:GLU:O	1:D:567:LYS:HG2	1.92	0.69
1:A:380:THR:HG22	1:D:428:SER:O	1.93	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: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:C:329:GLY:O	1:C:330:VAL:HG12	1.93	0.69
1:D:698:GLU:H	1:I:298:GLN:HE22	1.41	0.69
1:D:714:THR:CG2	1:D:715:VAL:N	2.56	0.69
1:C:428:SER:O	1:I:380:THR:HG22	1.93	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:C:564:GLU:O	1:C:567:LYS:HG2	1.92	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:B:298:GLN:HE22	1:J:698:GLU:H	1.41	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:A:298:GLN:HE22	1:E:698:GLU:H	1.41	0.68
1:G:217:GLY:HA2	1:G:408:ASN:HA	1.75	0.68
1:D:298:GLN:HE22	1:I:698:GLU:H	1.41	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:E:380:THR:HG22	1:G:428:SER:O	1.93	0.68
1:H:451:ASN:HD21	1:H:458:ASN:HB2	1.59	0.68
1:A:714:THR:CG2	1:A:715:VAL:N	2.56	0.68
1:D:286:ASN:HD21	1:D:619:TRP:H	1.42	0.68
1:I:714:THR:CG2	1:I:715:VAL:N	2.56	0.68
1:E:286:ASN:HD21	1:E:619:TRP:H	1.42	0.68
1:G:380:THR:HG21	1:G:392:SER:N	2.02	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:D:265:THR:HG21	1:D:267:ALA:HB2	1.74	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:A:429:GLN:HE21	1:A:736:LEU:H	1.41	0.68
1:B:429:GLN:HE21	1:B:736:LEU:H	1.41	0.68
1:B:714:THR:CG2	1:B:715:VAL:N	2.56	0.68
1:C:286:ASN:HD21	1:C:619:TRP:H	1.42	0.68
1:D:278:THR:CG2	1:D:280:TRP:H	2.07	0.68
1:G:714:THR:CG2	1:G:715:VAL:N	2.56	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:G:286:ASN:HD21	1:G:619:TRP:H	1.42	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:D:380:THR:HG21	1:D:392:SER:N	2.02	0.67
1:G:329:GLY:O	1:G:330:VAL:HG12	1.93	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: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:H:696:ASN:ND2	1:H:696:ASN:H	1.93	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:E:451:ASN:HD21	1:E:458:ASN:HB2	1.59	0.67
1:A:330:VAL:CG1	1:B:327:ASN:OD1	2.40	0.67
1:B:698:GLU:H	1:J:298:GLN:HE22	1.41	0.67
1:G:312:LEU:C	1:G:312:LEU:CD2	2.62	0.67
1:C:278:THR:CG2	1:C:280:TRP:H	2.07	0.66
1:E:218:ALA:O	1:E:219:ASP:CB	2.43	0.66
1:E:696:ASN:ND2	1:E:696:ASN:H	1.93	0.66
1:G:564:GLU:O	1:G:567:LYS:HG2	1.94	0.66
1:J:278:THR:CG2	1:J:280:TRP:H	2.07	0.66
1:A:698:GLU:H	1:E:298:GLN:HE22	1.41	0.66
1:A:310:LYS:HD2	1:A:686:GLU:HB2	1.77	0.66

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:HIS:ND1	4:F:795:HOH:O	2.25	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:I:218:ALA:HB1	1:I:219:ASP:CG	2.17	0.65
1:J:354:VAL:H	1:J:646:GLN:NE2	1.95	0.65
1:C:264:SER:OG	1:C:265:THR:N	2.30	0.65
1:G:502:THR:O	1:G:506:ALA:CB	2.40	0.65
1:G:563:GLU:OE2	1:G:611:ASP:N	2.27	0.65
1:I:457:GLN:OE1	1:I:457:GLN:N	2.30	0.65
1:A:454:GLY:O	1:A:456:ALA:N	2.30	0.65
1:C:696:ASN:H	1:C:696:ASN:ND2	1.93	0.65
1:F:302:ASN:HD21	1:F:701:TYR:H	1.45	0.65
1:F:286:ASN:HD21	1:F:619:TRP:H	1.42	0.65
1:B:383:ASN:HD22	1:B:383:ASN:C	1.99	0.64
1:H:354:VAL:H	1:H:646:GLN:NE2	1.95	0.64
1:C:328:ASP:CB	1:C:329:GLY:O	2.42	0.64
1:C:397:GLU:N	1:C:397:GLU:OE1	2.30	0.64
1:C:625:THR:HA	1:F:608:GLN:HE22	1.62	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:D:354:VAL:H	1:D:646:GLN:NE2	1.95	0.64
1:A:628:HIS:O	3:D:738:CYT:N1	2.30	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:H:312:LEU:CD2	1:H:312:LEU:C	2.62	0.64
1:I:502:THR:O	1:I:506:ALA:CB	2.40	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:397:GLU:OE1	1:D:397:GLU:N	2.30	0.64
1:D:719:GLY:O	1:F:666:LYS:NZ	2.31	0.64
1:H:383:ASN:C	1:H:383:ASN:HD22	1.99	0.64
1:B:502:THR:O	1:B:506:ALA:CB	2.40	0.64
1:C:628:HIS:O	3:F:738:CYT:N1	2.30	0.64
1:H:304:ASN:HD21	1:H:689:LYS:HZ1	1.46	0.64
1:H:327:ASN:O	1:H:328:ASP:CB	2.46	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:C:354:VAL:H	1:C:646:GLN:NE2	1.95	0.63
1:F:452:GLN:O	1:F:452:GLN:HG2	1.97	0.63
1:D:286:ASN:ND2	1:D:618:ILE:H	1.97	0.63
1:G:278:THR:CG2	1:G:280:TRP:H	2.07	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: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:I:327:ASN:O	1:I:330:VAL:N	2.28	0.63
1:A:286:ASN:ND2	1:A:618:ILE:H	1.97	0.63
1:A:625:THR:HA	1:D:608:GLN:HE22	1.62	0.63
1:E:502:THR:O	1:E:506:ALA:CB	2.40	0.63
1:E:286:ASN:ND2	1:E:618:ILE:H	1.97	0.63
1:I:454:GLY:O	1:I:455:SER:HB2	1.97	0.63
1:J:286:ASN:ND2	1:J:618:ILE:H	1.97	0.63
1:J:380:THR:CG2	1:J:392:SER:H	1.98	0.63
1:E:264:SER:O	1:E:266:GLY:N	2.32	0.63
1:B:563:GLU:OE2	1:B:611:ASP:N	2.27	0.63
1:B:608:GLN:HE22	1:G:625:THR:HA	1.62	0.63
1:G:328:ASP:CB	1:G:329:GLY:O	2.42	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:C:608:GLN:HE22	1:I:625:THR:HA	1.61	0.62
1:I:570:ASN:HD21	1:I:608:GLN:N	1.97	0.62
1:C:286:ASN:ND2	1:C:618:ILE:H	1.97	0.62
1:C:570:ASN:HD21	1:C:608:GLN:N	1.97	0.62
1:G:570:ASN:HD21	1:G: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:B:552:ASN:ND2	1:E:447:ASN:HD22	1.98	0.62
1:C:552:ASN:ND2	1:F:447:ASN:HD22	1.98	0.62

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:299:ARG:NH2	1:E:690:GLU:OE2	2.34	0.60
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:E:500:ASN:HD21	1:G:448:ARG:HA	1.66	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:G:327:ASN:O	1:G:328:ASP:CB	2.46	0.60
1:A:289:HIS:CE1	1:A:365:PRO:HG3	2.37	0.60
1:A:448:ARG:HA	1:H:500:ASN:HD21	1.66	0.60
1:D:278:THR:HB	1:D:376:TYR:O	2.02	0.60
1:D:452:GLN:O	1:D:453:SER:C	2.41	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:A:422:HIS:CE1	1:A:612:VAL:HG22	2.38	0.59
1:B:278:THR:HB	1:B:376:TYR:O	2.02	0.59
1:E:278:THR:HB	1:E:376:TYR:O	2.02	0.59
1:F:459:LYS:NZ	1:F:587:SER:HB3	2.16	0.59
1:H:289:HIS:CE1	1:H:365:PRO:HG3	2.37	0.59
1:H:422:HIS:CE1	1:H:612:VAL:HG22	2.38	0.59
1:D:299:ARG:NH2	1:I:690:GLU:OE2	2.35	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:G:397:GLU:OE2	1:G:650:LYS:NZ	2.25	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:I:452:GLN:O	1:I:453:SER:C	2.40	0.59
1:J:289:HIS:CE1	1:J:365:PRO:HG3	2.37	0.59
1:C:422:HIS:CE1	1:C:612:VAL:HG22	2.38	0.59
1:E:327:ASN:O	1:E:330:VAL:HG12	2.03	0.59
1:J:422:HIS:CE1	1:J:612:VAL:HG22	2.38	0.59
1:B:422:HIS:CE1	1:B:612:VAL:HG22	2.38	0.59
1:D:289:HIS:CE1	1:D:365:PRO:HG3	2.37	0.59
1:I:422:HIS:CE1	1:I:612:VAL:HG22	2.38	0.59
1:B:638:PHE:HA	2:B:737:ADE:H61	1.68	0.59
1:E:289:HIS:CE1	1:E:365:PRO:HG3	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:327:ASN:O	1:H:330:VAL:N	2.34	0.59
1:C:278:THR:HB	1:C:376:TYR:O	2.02	0.59
1:C:452:GLN:O	1:C:453:SER:C	2.41	0.59
1:F:570:ASN:HD21	1:F:608:GLN:N	1.97	0.59
1:H:452:GLN:O	1:H:453:SER:C	2.41	0.59
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:D:570:ASN:HD21	1:D:608:GLN:N	1.97	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:G:278:THR:HB	1:G:376:TYR:O	2.02	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:D:422:HIS:CE1	1:D:612:VAL:HG22	2.38	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: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:H:278:THR:HB	1:H:376:TYR:O	2.02	0.58
1:F:278:THR:HB	1:F:376:TYR:O	2.02	0.58
1:F:552:ASN:HD21	1:I:447:ASN:HD22	1.52	0.58
1:J:278:THR:HB	1:J:376:TYR:O	2.02	0.58
1:E:422:HIS:CE1	1:E:612:VAL:HG22	2.38	0.58
1:F:422:HIS:CE1	1:F: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:A:217:GLY:HA3	1:A:408:ASN:CA	2.34	0.57
1:J:452:GLN:O	1:J:453:SER:C	2.41	0.57
1:D:532:ASP:OD2	1:D:562:ASP:OD2	2.23	0.57
1:I:280:TRP:CD2	1:I:650:LYS:HD3	2.39	0.57
1:B:217:GLY:HA2	1:B:408:ASN:HA	1.86	0.57
1:J:218:ALA:CB	1:J:407:GLY:O	2.48	0.57
1:A:532:ASP:OD2	1:A:562:ASP:OD2	2.23	0.57
1:B:304:ASN:HD21	1:B:689:LYS:HZ1	1.50	0.57

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:717:ASN:H	1:G:717:ASN:ND2	2.04	0.55
1:F:625:THR:CA	1:I:608:GLN:HE22	2.18	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:B:532:ASP:OD2	1:B:562:ASP:OD2	2.23	0.55
1:D:304:ASN:HD21	1:D:689:LYS:HZ1	1.54	0.55
1:E:615:GLN:HE21	1:E:615:GLN:H	1.55	0.55
1:E:302:ASN:HD21	1:E:701:TYR:H	1.54	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:I:615:GLN:H	1:I:615:GLN:HE21	1.54	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:451:ASN:HB2	1:G:452:GLN:HB3	1.89	0.55
1:A:302:ASN:HD21	1:A:701:TYR:H	1.54	0.55
1:F:563:GLU:HG3	4:F:775:HOH:O	2.07	0.55
1:G:532:ASP:OD2	1:G:562:ASP:OD2	2.23	0.55
1:I:717:ASN:ND2	1:I:717:ASN:H	2.04	0.55
1:B:270:ASP:HA	1:B:514:ARG:HG2	1.88	0.55
1:B:529:ASP:H	1:G:512:ASN:ND2	2.03	0.55
1:B:717:ASN:H	1:B:717: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:I:450:GLN:OE1	1:I:457:GLN:HB3	2.07	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:A:615:GLN:H	1:A:615:GLN:HE21	1.55	0.55
1:I:328:ASP:HA	1:I:329:GLY:O	2.05	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:A:625:THR:CA	1:D:608:GLN:HE22	2.18	0.55
1:E:451:ASN:HB2	1:E:452:GLN:HB3	1.89	0.55
1:H:615:GLN:HE21	1:H:615:GLN:H	1.55	0.55
1:J:451:ASN:HB2	1:J:452:GLN:HB3	1.89	0.55
1:J:663:SER:OG	1:J:665:THR:HG23	2.07	0.55
1:A:717:ASN:H	1:A:717:ASN:ND2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:MET:H	1:F:477:ASN:HD22	1.55	0.54
1:D:717:ASN:ND2	1:D:717:ASN:H	2.03	0.54
1:F:217:GLY:HA3	1:F:408:ASN:CA	2.37	0.54
1:H:563:GLU:HG3	4:H:776:HOH:O	2.07	0.54
1:B:302:ASN:HD21	1:B:701:TYR:H	1.54	0.54
1:C:717:ASN:H	1:C:717:ASN:ND2	2.04	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:J:296:ASP:OD1	1:J:299:ARG:NH1	2.38	0.54
1:J:480:PRO:O	1:J:605:MET:HG2	2.08	0.54
1:C:663:SER:OG	1:C:665:THR:HG23	2.07	0.54
1:F:304:ASN:HD22	1:F:687:LEU:HB3	1.72	0.54
1:F:635:MET:H	1:I:477:ASN:HD22	1.55	0.54
1:A:477:ASN:HD22	1:H:635:MET:H	1.56	0.54
1:I:302:ASN:HD21	1:I:701:TYR:H	1.54	0.54
1:A:480:PRO:O	1:A:605:MET:HG2	2.08	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:D:480:PRO:O	1:D:605:MET:HG2	2.08	0.54
1:G:302:ASN:HD21	1:G:701:TYR:H	1.55	0.54
1:J:302:ASN:HD21	1:J:701:TYR:H	1.54	0.54
1:A:296:ASP:OD1	1:A:299:ARG:NH1	2.38	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: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:G:296:ASP:OD1	1:G:299:ARG:NH1	2.38	0.54
1:E:635:MET:H	1:G:477:ASN:HD22	1.56	0.54
1:B:477:ASN:HD22	1:G:635:MET:H	1.56	0.54
1:C:512:ASN:ND2	1:F:529:ASP:H	2.03	0.54
1:C:496:ASN:ND2	1:F:585:GLN:HE22	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: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:280:TRP:NE1	1:I:650:LYS:HD3	2.22	0.54
1:E:512:ASN:ND2	1:G:529:ASP:H	2.03	0.54
1:G:615:GLN:H	1:G:615:GLN:HE21	1.55	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:I:452:GLN:O	1:I:454:GLY:CA	2.53	0.54
1:B:512:ASN:ND2	1:E:529:ASP:H	2.03	0.54
1:F:480:PRO:O	1:F:605:MET:HG2	2.08	0.54
1:G:666:LYS:NZ	1:J:719:GLY:O	2.41	0.54
1:B:615:GLN:HE21	1:B:615:GLN:H	1.55	0.53
1:B:635:MET:H	1:E:477:ASN:HD22	1.55	0.53
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:C:615:GLN:HE21	1:C:615:GLN:H	1.55	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:I:570:ASN:ND2	1:I:608:GLN:H	2.02	0.53
1:C:477:ASN:HD22	1:I:635:MET:H	1.56	0.53
1:J:353:TYR:CE2	1:J:355:LEU:HB2	2.44	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:C:302:ASN:HD21	1:C:701:TYR:H	1.54	0.53
1:E:353:TYR:CE2	1:E:355:LEU:HB2	2.44	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:C:585:GLN:HE22	1:I:496:ASN:ND2	2.02	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:A:433:ARG:NH1	1:H:272:HIS:O	2.42	0.53
1:C:280:TRP:CE2	1:C:650:LYS:HD3	2.44	0.53
1:A:500:ASN:ND2	1:D:449:THR:H	2.07	0.53
1:A:280:TRP:CE2	1:A:650:LYS:HD3	2.44	0.53
1:D:280:TRP:CE2	1:D:650:LYS:HD3	2.44	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:A:635:MET:H	1:D:477:ASN:HD22	1.55	0.53
1:B:380:THR:CG2	1:B:392:SER:H	2.09	0.53
1:B:480:PRO:O	1:B:605:MET:HG2	2.08	0.53
1:I:264:SER:O	1:I:266:GLY:N	2.37	0.53
1:J:270:ASP:HA	1:J:514:ARG:HG2	1.91	0.53
1:J:615:GLN:H	1:J:615:GLN:HE21	1.55	0.53
1:A:457:GLN:NE2	1:A:457:GLN:H	2.01	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:HIS:O	1:H:433:ARG:NH1	2.43	0.52
1:A:626:ASP:H	1:D:608:GLN:NE2	2.07	0.52
1:A:270:ASP:HA	1:A:514:ARG:HG2	1.91	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:D:353:TYR:CE2	1:D:355:LEU:HB2	2.44	0.52
1:F:272:HIS:O	1:I:433:ARG:NH1	2.43	0.52
1:B:433:ARG:NH1	1:G:272:HIS:O	2.42	0.52
1:H:280:TRP:CE2	1:H:650:LYS:HD3	2.44	0.52
1:C:500:ASN:ND2	1:F:449:THR:H	2.07	0.52
1:D:512:ASN:ND2	1:H:529:ASP:H	2.02	0.52
1:C:626:ASP:H	1:F:608:GLN:NE2	2.07	0.52
1:F:626:ASP:H	1:I:608:GLN:NE2	2.07	0.52
1:D:496:ASN:ND2	1:H:585:GLN:HE22	2.02	0.52
1:I:270:ASP:HA	1:I:514:ARG:HG2	1.91	0.52
1:F:496:ASN:ND2	1:I:585:GLN:HE22	2.03	0.52
1:J:280:TRP:CE2	1:J:650:LYS:HD3	2.44	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:D:270:ASP:HA	1:D:514:ARG:HG2	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:B:449:THR:H	1:G:500:ASN:ND2	2.07	0.52
1:B:608:GLN:NE2	1:G:626:ASP:H	2.07	0.52
1:B:280:TRP:CE2	1:B:650:LYS:HD3	2.44	0.52
1:C:433:ARG:NH2	4:C:869:HOH:O	2.43	0.52
1:A:272:HIS:O	1:D:433:ARG:NH1	2.43	0.52
1:A:304:ASN:HD21	1:A:689:LYS:HZ1	1.54	0.52
1:D:635:MET:H	1:H:477:ASN:HD22	1.55	0.52
1:F:280:TRP:CE2	1:F:650:LYS:HD3	2.44	0.52
1:I:353:TYR:CE2	1:I:355:LEU:HB2	2.44	0.52
1:E:272:HIS:O	1:G:433:ARG:NH1	2.42	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:E:270:ASP:HA	1:E:514:ARG:HG2	1.91	0.52
1:A:449:THR:H	1:H:500:ASN:ND2	2.07	0.52
1:J:217:GLY:HA3	1:J:408:ASN:HA	1.92	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:249:LEU:HB2	1:A:373:ILE:HD12	1.93	0.51
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:447:ASN:ND2	1:H:552:ASN:HD21	2.08	0.51
1:A:552:ASN:HD21	1:D:447:ASN:ND2	2.08	0.51
1:G:270:ASP:HA	1:G:514:ARG:HG2	1.91	0.51
1:H:433:ARG:NH2	4:H:871:HOH:O	2.43	0.51
1:D:626:ASP:H	1:H:608:GLN:NE2	2.07	0.51
1:B:451:ASN:CB	1:B:452:GLN:HB3	2.41	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:G:280:TRP:CG	1:G:396:LEU:HD22	2.45	0.51
1:H:270:ASP:HA	1:H:514:ARG:HG2	1.91	0.51
1:I:433:ARG:NH2	4:I:873:HOH:O	2.43	0.51
1:A:286:ASN:ND2	1:A:618:ILE:HB	2.26	0.51
1:F:218:ALA:C	1:F:219:ASP:OD1	2.49	0.51
1:B:286:ASN:ND2	1:B:618:ILE:HB	2.26	0.51
1:C:529:ASP:H	1:I:512:ASN:ND2	2.01	0.51
1:C:286:ASN:ND2	1:C:618:ILE:HB	2.26	0.51
1:E:563:GLU:HG3	4:E:775:HOH:O	2.10	0.51
1:F:249:LEU:HB2	1:F:373:ILE:HD12	1.93	0.51
1:G:433:ARG:NH2	4:G:871:HOH:O	2.43	0.51
1:A:433:ARG:NH2	4:A:868:HOH:O	2.43	0.51
1:B:447:ASN:ND2	1:G:552:ASN:HD21	2.09	0.51
1:B:451:ASN:CB	1:B:452:GLN:CB	2.89	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:D:451:ASN:CB	1:D:452:GLN:HB3	2.41	0.51
1:E:451:ASN:CB	1:E: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:H:451:ASN:CB	1:H:452:GLN:CB	2.89	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:J:451:ASN:CB	1:J:452:GLN:HB3	2.41	0.51
1:F:552:ASN:HD21	1:I:447:ASN:ND2	2.08	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:I:249:LEU:HB2	1:I:373:ILE:HD12	1.92	0.51
1:A:536:PRO:HG3	1:A:573:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:HB2	1:C:373:ILE:HD12	1.93	0.51
1:C:552:ASN:HD21	1:F:447:ASN:ND2	2.08	0.51
1:D:536:PRO:HG3	1:D:573:ALA:HB3	1.93	0.51
1:G:280:TRP:CD1	1:G:396:LEU:HD22	2.45	0.51
1:G:249:LEU:HB2	1:G:373:ILE:HD12	1.93	0.51
1:H:217:GLY:O	1:H:408:ASN:ND2	2.34	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: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:C:270:ASP:OD2	1:C:503:TRP:HZ2	1.94	0.50
1:E:286:ASN:ND2	1:E:618:ILE:HB	2.26	0.50
1:C:272:HIS:O	1:F:433:ARG:NH1	2.43	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:J:286:ASN:ND2	1:J:618:ILE:HB	2.26	0.50
1:D:249:LEU:HB2	1:D:373:ILE:HD12	1.92	0.50
1:F:286:ASN:ND2	1:F:618:ILE:HB	2.26	0.50
1:G:559:MET:SD	1:G:725:ARG:HA	2.51	0.50
1:G:563:GLU:OE2	1:G:611:ASP:CB	2.59	0.50
1:I:404:LEU:HA	1:I:408:ASN:HD22	1.74	0.50
1:A:529:ASP:O	1:A:530:ASP:HB2	2.11	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:H:501:PHE:O	1:H:505:GLY:N	2.31	0.50
1:E:296:ASP:OD1	1:E:299:ARG:NH1	2.38	0.50
1:F:563:GLU:OE2	1:F:611:ASP:CB	2.59	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: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:E:249:LEU:HB2	1:E:373:ILE:HD12	1.93	0.50
1:D:500:ASN:ND2	1:H:449:THR:H	2.08	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:563:GLU:OE2	1:B:611:ASP:CB	2.60	0.50
1:C:451:ASN:ND2	1:C:458:ASN:HB2	2.23	0.50
1:D:451:ASN:CB	1:D:452:GLN:CB	2.89	0.50
1:H:536:PRO:HG3	1:H:573:ALA:HB3	1.93	0.50
1:I:451:ASN:O	1:I:451:ASN:OD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ARG:NH2	4:D:871:HOH:O	2.43	0.50
1:E:451:ASN:CB	1:E:452:GLN:CB	2.89	0.50
1:F:297:TRP:O	1:F:301:ILE:HG12	2.12	0.50
1:F:451:ASN:HA	1:F:452:GLN:HB3	1.65	0.50
1:E:552:ASN:HD21	1:G:447:ASN:ND2	2.08	0.50
1:I:529:ASP:O	1:I:530:ASP:HB2	2.11	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: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: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:J:563:GLU:OE2	1:J:611:ASP:CB	2.59	0.50
1:A:496:ASN:ND2	1:D:585:GLN:HE22	2.03	0.50
1:D:563:GLU:OE2	1:D:611:ASP:CB	2.59	0.50
1:E:218:ALA:O	1:E:219:ASP:HB2	2.12	0.50
1:H:529:ASP:O	1:H:530:ASP:HB2	2.11	0.50
1:C:447:ASN:ND2	1:I:552:ASN:HD21	2.08	0.50
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:B:570:ASN:ND2	1:B:608:GLN:H	2.02	0.49
1:F:536:PRO:HG3	1:F:573:ALA:HB3	1.93	0.49
1:H:354:VAL:O	1:H:354:VAL:HG13	2.12	0.49
1:I:286:ASN:ND2	1:I:618:ILE:HB	2.26	0.49
1:C:563:GLU:OE2	1:C:611:ASP:CB	2.59	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:J:536:PRO:HG3	1:J:573:ALA:HB3	1.94	0.49
1:A:563:GLU:OE2	1:A:611:ASP:CB	2.59	0.49
1:E:715:VAL:HG21	1:H:257:TYR:O	2.12	0.49
1:F:529:ASP:O	1:F:530:ASP:HB2	2.11	0.49
1:G:714:THR:HG22	1:G:715:VAL:O	2.12	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:B:529:ASP:O	1:B:530:ASP:HB2	2.11	0.49
1:B:536:PRO:HG3	1:B:573:ALA:HB3	1.93	0.49
1:C:304:ASN:HD21	1:C:689:LYS:HZ1	1.57	0.49
1:J:714:THR:HG22	1:J:715:VAL:O	2.12	0.49
1:B:714:THR:HG22	1:B:715:VAL:O	2.13	0.49
1:D:714:THR:HG22	1:D:715:VAL:O	2.13	0.49
1:G:536:PRO:HG3	1:G:573:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:ASN:ND2	1:G:585:GLN:HE22	2.03	0.49
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:A:451:ASN:OD1	1:A:451:ASN:O	2.30	0.49
1:C:270:ASP:OD2	1:C:503:TRP:CZ2	2.65	0.49
1:C:304:ASN:HD21	1:C:689:LYS:HZ3	1.58	0.49
1:E:580:VAL:HG23	1:E:596:VAL:CG2	2.42	0.49
1:G:451:ASN:CB	1:G:452:GLN:CB	2.89	0.49
1:H:580:VAL:HG23	1:H:596:VAL:CG2	2.43	0.49
1:H:570:ASN:ND2	1:H:608:GLN:H	2.02	0.49
1:I:396:LEU:HD12	1:I:396:LEU:N	2.27	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:G:283:PHE:CZ	1:G:316:LEU:HD21	2.48	0.49
1:H:316:LEU:HB2	1:H:410:PHE:HB3	1.95	0.49
1:I:316:LEU:HB2	1:I: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: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:A:715:VAL:HG21	1:B:257:TYR:O	2.13	0.49
1:B:615:GLN:NE2	1:B:615:GLN:H	2.11	0.49
1:C:316:LEU:HB2	1:C:410:PHE:HB3	1.95	0.49
1:D:283:PHE:CZ	1:D:316:LEU:HD21	2.48	0.49
1:E:714:THR:HG22	1:E:715:VAL:O	2.12	0.49
1:G:278:THR:HG23	1:G:280:TRP:HD1	1.78	0.49
1:H:264:SER:O	1:H:266:GLY:N	2.36	0.49
1:H:283:PHE:CZ	1:H:316:LEU:HD21	2.48	0.49
1:I:714:THR:HG22	1:I:715:VAL:O	2.12	0.49
1:J:615:GLN:NE2	1:J:615:GLN:H	2.11	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:A:529:ASP:H	1:H:512:ASN:ND2	2.03	0.48
1:C:296:ASP:OD1	1:C:299:ARG:NH1	2.38	0.48
1:D:327:ASN:O	1:D:330:VAL:N	2.43	0.48
1:F:580:VAL:HG23	1:F:596:VAL:CG2	2.43	0.48
1:B:316:LEU:HB2	1:B:410:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:VAL:HG23	1:B:596:VAL:CG2	2.43	0.48
1:E:283:PHE:CZ	1:E:316:LEU:HD21	2.48	0.48
1:H:714:THR:HG22	1:H:715:VAL:O	2.12	0.48
1:I:283:PHE:CZ	1:I: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:B:283:PHE:CZ	1:B:316:LEU:HD21	2.48	0.48
1:B:354:VAL:HG13	1:B:354:VAL:O	2.12	0.48
1:C:283:PHE:CZ	1:C:316:LEU:HD21	2.48	0.48
1:D:580:VAL:HG23	1:D:596:VAL:CG2	2.43	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:G:257:TYR:O	1:J:715:VAL:HG21	2.13	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:F:714:THR:HG22	1:F:715:VAL:O	2.12	0.48
1:I:380:THR:CG2	1:I:392:SER:H	2.09	0.48
1:J:354:VAL:O	1:J:354:VAL:HG13	2.12	0.48
1:B:437:PRO:HG3	1:G:379:LEU:HG	1.95	0.48
1:B:639:GLY:O	2:B:737:ADE:H2	1.95	0.48
1:C:580:VAL:HG23	1:C:596:VAL:CG2	2.43	0.48
1:D:218:ALA:O	1:D:219:ASP:CB	2.61	0.48
1:D:304:ASN:HD21	1:D:689:LYS:HZ3	1.61	0.48
1:F:283:PHE:CZ	1:F:316:LEU:HD21	2.48	0.48
1:F:354:VAL:O	1:F:354:VAL:HG13	2.12	0.48
1:F:316:LEU:HB2	1:F:410:PHE:HB3	1.95	0.48
1:H:230:CYS:HB2	1:H:244:THR:CG2	2.43	0.48
1:A:585:GLN:HE22	1:H:496:ASN:ND2	2.03	0.48
1:B:326:THR:HG22	1:B:327:ASN:C	2.30	0.48
1:C:218:ALA:O	1:C:219:ASP:OD1	2.30	0.48
1:C:615:GLN:NE2	1:C:615:GLN:H	2.11	0.48
1:A:379:LEU:HG	1:D:437:PRO:HG3	1.96	0.48
1:C:379:LEU:HG	1:F:437:PRO:HG3	1.96	0.48
1:H:615:GLN:NE2	1:H:615:GLN:H	2.11	0.48
1:H:666:LYS:O	1:H:666:LYS:HG2	2.12	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:A:399:PHE:CD1	1:A:399:PHE:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:SER:HG	1:C:265:THR:H	1.62	0.48
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: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:E:380:THR:CG2	1:E:392:SER:H	2.09	0.48
1:E:316:LEU:HB2	1:E:410:PHE:HB3	1.95	0.48
1:F:570:ASN:ND2	1:F:608:GLN:H	2.02	0.48
1:G:354:VAL:O	1:G:354:VAL:HG13	2.12	0.48
1:A:257:TYR:O	1:I:715:VAL:HG21	2.13	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:B:379:LEU:HG	1:E:437:PRO:HG3	1.96	0.47
1:C:635:MET:HB2	1:F:477:ASN:ND2	2.30	0.47
1:E:346:ASP:OD2	1:E:351:LEU:HB2	2.14	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:H:380:THR:CG2	1:H:392:SER:H	2.09	0.47
1:I:249:LEU:HD21	1:I:650:LYS:HA	1.97	0.47
1:F:379:LEU:HG	1:I:437:PRO:HG3	1.96	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:J:383:ASN:ND2	1:J:383:ASN:C	2.68	0.47
1:A:262:SER:O	1:A:265:THR:HB	2.14	0.47
1:B:262:SER:O	1:B:265:THR:HB	2.13	0.47
1:C:451:ASN:CB	1:C:452:GLN:HB3	2.45	0.47
1:D:316:LEU:HB2	1:D:410:PHE:HB3	1.95	0.47
1:B:635:MET:HB2	1:E:477:ASN:ND2	2.29	0.47
1:E:570:ASN:ND2	1:E:608:GLN:H	2.02	0.47
1:E:379:LEU:HG	1:G:437:PRO:HG3	1.96	0.47
1:I:454:GLY:O	1:I:455:SER:OG	2.30	0.47
1:J:425:TYR:O	1:J:730:ARG:HG2	2.15	0.47
1:B:383:ASN:C	1:B:383:ASN:ND2	2.68	0.47
1:B:425:TYR:O	1:B:730:ARG:HG2	2.15	0.47
1:D:264:SER:O	1:D:265:THR:HB	2.14	0.47
1:E:342:GLN:C	1:E:343:VAL:HG23	2.35	0.47
1:E:635:MET:HB2	1:G:477:ASN:ND2	2.30	0.47
1:F:397:GLU:OE2	1:F:650:LYS:NZ	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:ALA:HB1	1:I:219:ASP:OD1	2.13	0.47
1:C:425:TYR:O	1:C:730:ARG:HG2	2.15	0.47
1:F:295:ARG:HH11	1:F:298:GLN:NE2	2.13	0.47
1:G:264:SER:OG	1:G:265:THR:N	2.47	0.47
1:G:425:TYR:O	1:G:730:ARG:HG2	2.15	0.47
1:D:379:LEU:HG	1:H:437:PRO:HG3	1.96	0.47
1:I:346:ASP:OD2	1:I:351:LEU:HB2	2.14	0.47
1:A:635:MET:HB2	1:D:477:ASN:ND2	2.30	0.47
1:C:330:VAL:CG2	1:C:331:THR:N	2.78	0.47
1:C:477:ASN:ND2	1:I:635:MET:HB2	2.30	0.47
1:D:346:ASP:OD2	1:D:351:LEU:HB2	2.14	0.47
1:H:330:VAL:CG2	1:H:331:THR:N	2.78	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: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:F:635:MET:HB2	1:I:477:ASN:HD21	1.80	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:A:437:PRO:HG3	1:H:379:LEU:HG	1.96	0.47
1:D:383:ASN:ND2	1:D:383:ASN:C	2.68	0.47
1:F:425:TYR:O	1:F:730:ARG:HG2	2.15	0.47
1:H:383:ASN:C	1:H:383:ASN:ND2	2.68	0.47
1:I:342:GLN:C	1:I:343:VAL:HG23	2.35	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:E:425:TYR:O	1:E:730:ARG:HG2	2.15	0.46
1:F:217:GLY:HA3	1:F:408:ASN:CB	2.45	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:380:THR:CG2	1:G:392:SER:H	2.09	0.46
1:B:226:GLY:HA3	1:B:317:PHE:CD2	2.51	0.46
1:G:330:VAL:CG2	1:G:331:THR:N	2.78	0.46
1:I:229:HIS:HE1	4:I:810:HOH:O	1.97	0.46
1:I:456:ALA:C	1:I:457:GLN:CD	2.74	0.46
1:C:346:ASP:OD2	1:C:351:LEU:HB2	2.14	0.46
1:D:570:ASN:ND2	1:D:608:GLN:H	2.02	0.46
1:E:459:LYS:NZ	1:E:587:SER:HB3	2.31	0.46
1:F:342:GLN:C	1:F:343:VAL:HG23	2.35	0.46

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:459:LYS:NZ	1:A:587:SER:HB3	2.31	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:J:736:LEU:HA	1:J:736:LEU:HD13	1.83	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:254:ASN:O	1:I:255:HIS:CB	2.63	0.45
1:B:477:ASN:HD21	1:G:635:MET:HB2	1.81	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:365:PRO:HD2	4:I:760:HOH:O	2.16	0.45
1:J:398:TYR:CG	1:J:398:TYR:O	2.69	0.45
1:J:459:LYS:NZ	1:J:587:SER:HB3	2.31	0.45
1:A:226:GLY:HA3	1:A:317:PHE:CD2	2.51	0.45
1:D:226:GLY:HA3	1:D:317:PHE:CD2	2.51	0.45
1:D:380:THR:CG2	1:D:392:SER:H	2.09	0.45
1:E:267:ALA:HB1	1:E:271:ASN:HB2	1.98	0.45
1:E:226:GLY:HA3	1:E:317:PHE:CD2	2.51	0.45
1:G:264:SER:O	1:G:265:THR:HB	2.15	0.45
1:I:397:GLU:CD	1:I:650:LYS:HE2	2.27	0.45
1:J:263:ALA:O	1:J:264:SER:HB3	2.17	0.45
1:B:262:SER:O	1:B:265:THR:CB	2.65	0.45
1:B:619:TRP:CD1	1:B:619:TRP:C	2.89	0.45
1:C:257:TYR:OH	1:C:397:GLU:OE1	2.23	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:B:459:LYS:NZ	1:B:587:SER:HB3	2.31	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:H:286:ASN:HD21	1:H:619:TRP:N	2.13	0.45
1:I:619:TRP:C	1:I:619:TRP:CD1	2.89	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:A:512:ASN:ND2	1:D:529:ASP:H	2.03	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:F:296:ASP:OD1	1:F:299:ARG:NH1	2.41	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:I:487:GLN:NE2	1:I:488:ARG:H	2.15	0.45
1:A:487:GLN:NE2	1:A:488:ARG:H	2.15	0.45
1:B:305:TRP:CE3	1:B:734:ARG:NH2	2.85	0.45
1:C:444:TYR:CE1	1:I:544:GLY:HA3	2.52	0.45
1:D:217:GLY:O	1:D:218:ALA:HB3	2.15	0.45
1:F:621:LYS:HB2	1:F:643:PRO:HG3	1.99	0.45
1:F:666:LYS:HG2	1:F:666:LYS:O	2.17	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:B:487:GLN:NE2	1:B:488:ARG:H	2.15	0.45
1:C:621:LYS:HB2	1:C:643:PRO:HG3	1.99	0.45
1:D:487:GLN:NE2	1:D:488:ARG:H	2.15	0.45
1:E:305:TRP:CE3	1:E:734:ARG:NH2	2.85	0.45
1:E:379:LEU:HD21	1:G:437:PRO:HB3	1.99	0.45
1:B:379:LEU:HD21	1:E:437:PRO:HB3	1.99	0.45
1:G:315:LYS:HB2	1:G:315:LYS:HE2	1.82	0.45
1:A:305:TRP:CE3	1:A:734:ARG:NH2	2.85	0.44
1:B:585:GLN:HG3	1:G:487:GLN:NE2	2.32	0.44
1:C:570:ASN:ND2	1:C:608:GLN:H	2.02	0.44
1:H:278:THR:HG22	1:H:280:TRP:N	2.15	0.44
1:J:305:TRP:CE3	1:J:734:ARG:NH2	2.85	0.44
1:A:264:SER:OG	1:A:265:THR:N	2.49	0.44
1:B:397:GLU:OE1	1:B:397:GLU:N	2.50	0.44
1:C:379:LEU:HD21	1:F:437:PRO:HB3	1.99	0.44
1:C:383:ASN:ND2	1:C:383:ASN:C	2.68	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: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:H:423:SER:HB2	1:H:425:TYR:CE2	2.53	0.44
1:I:286:ASN:HD21	1:I:619:TRP:N	2.13	0.44
1:D:305:TRP:CE3	1:D:734:ARG:NH2	2.85	0.44
1:D:316:LEU:HA	1:D:316:LEU:HD23	1.83	0.44
1:E:512:ASN:HD21	1:G:529:ASP:N	2.07	0.44
1:F:379:LEU:HD21	1:I:437:PRO:HB3	1.99	0.44
1:G:500:ASN:HD22	1:G:500:ASN:HA	1.67	0.44
1:B:423:SER:HB2	1:B:425:TYR:CE2	2.53	0.44
1:B:437:PRO:HB3	1:G:379:LEU:HD21	1.98	0.44
1:B:666:LYS:NZ	4:B:812:HOH:O	2.30	0.44
1:C:305:TRP:CE3	1:C:734:ARG:NH2	2.85	0.44
1:E:255:HIS:ND1	4:E:795:HOH:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:GLN:NE2	1:G:585:GLN:HG3	2.33	0.44
1:H:451:ASN:ND2	1:H:458:ASN:HB2	2.30	0.44
1:I:423:SER:HB2	1:I:425:TYR:CE2	2.53	0.44
1:J:397:GLU:OE1	1:J:397:GLU:N	2.50	0.44
1:A:423:SER:HB2	1:A:425:TYR:CE2	2.53	0.44
1:D:365:PRO:HD2	4:D:758:HOH:O	2.16	0.44
1:E:392:SER:OG	1:G:694:ARG:NH1	2.51	0.44
1:D:544:GLY:HA3	1:H:444:TYR:CE1	2.52	0.44
1:J:423:SER:HB2	1:J:425:TYR:CE2	2.53	0.44
1:A:714:THR:CG2	1:A:715:VAL:H	2.31	0.44
1:C:487:GLN:NE2	1:F:585:GLN:HG3	2.33	0.44
1:D:423:SER:HB2	1:D:425:TYR:CE2	2.53	0.44
1:F:423:SER:HB2	1:F:425:TYR:CE2	2.53	0.44
1:G:328:ASP:CB	1:G:329:GLY:CA	2.76	0.44
1:A:437:PRO:HB3	1:H:379:LEU:HD21	1.99	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:A:398:TYR:OH	1:I:232:SER:HB2	2.17	0.44
1:C:585:GLN:HG3	1:I:487:GLN:NE2	2.32	0.44
1:J:217:GLY:HA3	1:J:409:ASN:H	1.82	0.44
1:B:359:HIS:NE2	1:E:436:ASN:N	2.56	0.44
1:B:397:GLU:C	1:B:399:PHE:H	2.20	0.44
1:C:544:GLY:HA3	1:F:444:TYR:CE1	2.53	0.44
1:E:544:GLY:HA3	1:G:444:TYR:CE1	2.53	0.44
1:G:487:GLN:NE2	1:G:488:ARG:H	2.15	0.44
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.83	0.44
1:A:365:PRO:HD2	4:A:756:HOH:O	2.16	0.44
3:A:738:CYT:N4	4:A:768:HOH:O	2.31	0.44
1:B:714:THR:CG2	1:B:715:VAL:H	2.31	0.44
1:D:621:LYS:HB2	1:D:643:PRO:HG3	1.99	0.44
1:D:426:ALA:O	1:D:733:THR:HA	2.18	0.44
1:F:383:ASN:ND2	1:F:383:ASN:C	2.68	0.44
1:G:286:ASN:HD21	1:G:619:TRP:N	2.13	0.44
1:I:295:ARG:HH11	1:I:298:GLN:HE21	1.66	0.44
1:A:379:LEU:HD21	1:D:437:PRO:HB3	1.99	0.44
1:B:295:ARG:HH11	1:B:298:GLN:HE21	1.66	0.44
1:C:423:SER:HB2	1:C:425:TYR:CE2	2.53	0.44
1:C:426:ALA:O	1:C:733:THR:HA	2.18	0.44
1:D:295:ARG:HH11	1:D:298:GLN:HE21	1.66	0.44
1:E:397:GLU:OE2	1:E:650:LYS:NZ	2.41	0.44
1:F:254:ASN:O	1:F:255:HIS:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:327:ASN:O	1:J:330:VAL:HG13	2.18	0.44
1:A:621:LYS:HB2	1:A:643:PRO:HG3	1.99	0.43
1:A:426:ALA:O	1:A:733:THR:HA	2.18	0.43
1:A:736:LEU:HD13	1:A:736:LEU:HA	1.83	0.43
1:B:304:ASN:HD21	1:B:689:LYS:HZ3	1.65	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: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: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: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:J:286:ASN:HD21	1:J:619:TRP:N	2.13	0.43
1:J:621:LYS:HB2	1:J:643:PRO:HG3	1.99	0.43
1:B:444:TYR:CE1	1:G:544:GLY:HA3	2.53	0.43
1:E:423:SER:HB2	1:E:425:TYR:CE2	2.53	0.43
1:B:487:GLN:NE2	1:E:585:GLN:HG3	2.33	0.43
1:H:286:ASN:HD21	1:H:618:ILE:H	1.66	0.43
1:C:694:ARG:NH1	1:I:392:SER:OG	2.50	0.43
1:F:487:GLN:NE2	1:I:585:GLN:HG3	2.33	0.43
1:I:621:LYS:HB2	1:I:643:PRO:HG3	1.99	0.43
1:J:426:ALA:O	1:J:733:THR:HA	2.18	0.43
1:A:544:GLY:HA3	1:D:444:TYR:CE1	2.53	0.43
1:D:392:SER:OG	1:H:694:ARG:NH1	2.50	0.43
1:A:392:SER:OG	1:D:694:ARG:NH1	2.51	0.43
1:E:383:ASN:ND2	1:E:383:ASN:C	2.68	0.43
1:E:451:ASN:ND2	1:E:458:ASN:HB2	2.30	0.43
1:E:621:LYS:HB2	1:E:643:PRO:HG3	1.99	0.43
1:F:487:GLN:NE2	1:F:488:ARG:H	2.15	0.43
1:H:397:GLU:C	1:H:399:PHE:H	2.21	0.43
1:H:663:SER:OG	1:H:665:THR:HG23	2.18	0.43
1:A:452:GLN:O	1:A:453:SER:C	2.55	0.43
1:B:262:SER:O	1:B:265:THR:OG1	2.34	0.43
1:B:426:ALA:O	1:B:733:THR:HA	2.18	0.43
1:E:500:ASN:HA	1:E:500:ASN:HD22	1.67	0.43
1:E:286:ASN:HD21	1:E:618:ILE:H	1.66	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASN:HD21	1:A:689:LYS:HZ3	1.61	0.42
1:B:321:VAL:HG11	1:B:339:SER:HB3	2.00	0.42
1:E:714:THR:CG2	1:E:715:VAL:H	2.31	0.42
1:H:397:GLU:OE1	1:H:397:GLU:N	2.50	0.42
1:I:426:ALA:O	1:I:733:THR:HA	2.18	0.42
1:A:217:GLY:HA3	1:A:408:ASN:CB	2.48	0.42
1:A:229:HIS:HB3	4:A:833:HOH:O	2.19	0.42
1:A:295:ARG:HH11	1:A:298:GLN:HE21	1.66	0.42
1:D:321:VAL:HG11	1:D:339:SER:HB3	2.00	0.42
1:G:363:LEU:CD2	1:G:371:PHE:CZ	3.02	0.42
1:H:321:VAL:HG11	1:H:339:SER:HB3	2.00	0.42
1:I:278:THR:HG22	1:I:280:TRP:N	2.15	0.42
1:D:363:LEU:CD2	1:D:371:PHE:CZ	3.02	0.42
1:E:229:HIS:HE1	4:E:808:HOH:O	2.02	0.42
1:G:321:VAL:HG11	1:G:339:SER:HB3	2.00	0.42
1:H:295:ARG:HH11	1:H:298:GLN:HE21	1.66	0.42
1:J:229:HIS:HB3	4:J:837:HOH:O	2.19	0.42
1:B:229:HIS:HB3	4:B:833:HOH:O	2.19	0.42
1:E:321:VAL:HG11	1:E:339:SER:HB3	2.01	0.42
1:H:455:SER:HA	1:H:456:ALA:HA	1.69	0.42
1:J:295:ARG:HH11	1:J:298:GLN:HE21	1.66	0.42
1:A:312:LEU:HA	1:A:682:GLU:O	2.20	0.42
1:E:295:ARG:HH11	1:E:298:GLN:HE21	1.66	0.42
1:E:655:PRO:HB3	1:E:667:PHE:CE1	2.55	0.42
1:F:363:LEU:CD2	1:F:371:PHE:CZ	3.02	0.42
1:H:263:ALA:O	1:H:264:SER:HB3	2.19	0.42
1:I:286:ASN:HD21	1:I:618:ILE:H	1.66	0.42
1:J:316:LEU:HD23	1:J:316:LEU:HA	1.83	0.42
1:A:725:ARG:HB3	1:A:725:ARG:HE	1.69	0.42
1:C:363:LEU:CD2	1:C:371:PHE:CZ	3.02	0.42
1:G:703:SER:CB	4:G:742:HOH:O	2.67	0.42
1:J:328:ASP:HB3	1:J:330:VAL:N	2.33	0.42
1:B:475:PRO:HA	1:G:519:ASN:O	2.20	0.42
1:C:312:LEU:HA	1:C:682:GLU:O	2.20	0.42
1:D:229:HIS:HB3	4:D:836:HOH:O	2.19	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:280:TRP:CE3	1:B:650:LYS:HB2	2.55	0.42
1:B:286:ASN:HD21	1:B:619:TRP:N	2.13	0.42
1:C:488:ARG:HB2	1:C:574:THR:HB	2.02	0.42
1:D:725:ARG:HE	1:D:725:ARG:HB3	1.69	0.42

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:488:ARG:HB2	1:H:574:THR:HB	2.02	0.41
1:J:278:THR:HG22	1:J:280:TRP:N	2.15	0.41
1:A:701:TYR:C	1:A:701:TYR:CD2	2.94	0.41
1:B:219:ASP:OD1	1:B:219:ASP:N	2.53	0.41
3:C:738:CYT:N4	4:C:768:HOH:O	2.24	0.41
1:D:280:TRP:CE3	1:D:650:LYS:HB2	2.55	0.41
1:G:286:ASN:HD21	1:G:618:ILE:H	1.67	0.41
1:A:449:THR:H	1:H:500:ASN:HD22	1.68	0.41
1:J:693:LYS:HA	1:J:693:LYS:HD3	1.89	0.41
1:A:397:GLU:N	1:A:397:GLU:OE1	2.50	0.41
1:C:342:GLN:C	1:C:343:VAL:CG2	2.89	0.41
1:D:586:SER:HB2	4:D:825:HOH:O	2.21	0.41
1:D:701:TYR:C	1:D:701:TYR:CD2	2.94	0.41
1:E:342:GLN:C	1:E:343:VAL:CG2	2.89	0.41
1:E:455:SER:HA	1:E:456:ALA:HA	1.69	0.41
1:F:342:GLN:C	1:F:343:VAL:CG2	2.89	0.41
1:F:628:HIS:O	3:I:738:CYT:C6	2.74	0.41
1:G:342:GLN:C	1:G:343:VAL:CG2	2.89	0.41
1:G:501:PHE:O	1:G:505:GLY:N	2.44	0.41
1:D:519:ASN:O	1:H:475:PRO:HA	2.20	0.41
1:H:280:TRP:CE3	1:H:650:LYS:HB2	2.55	0.41
1:A:500:ASN:HD22	1:D:449:THR:H	1.68	0.41
1:C:342:GLN:HG2	1:C:403:MET:HG2	2.03	0.41
1:E:278:THR:HG22	1:E:280:TRP:N	2.15	0.41
1:E:342:GLN:HG2	1:E:403:MET:HG2	2.03	0.41
1:E:725:ARG:HE	1:E:725:ARG:HB3	1.69	0.41
1:F:312:LEU:HA	1:F:682:GLU:O	2.20	0.41
1:G:315:LYS:HB3	1:G:680:SER:HB2	2.03	0.41
1:H:714:THR:CG2	1:H:715:VAL:H	2.31	0.41
1:I:280:TRP:CD1	1:I:650:LYS:HD3	2.55	0.41
1:I:315:LYS:HB3	1:I:680:SER:HB2	2.03	0.41
1:A:284:ASP:O	1:A:362:CYS:HA	2.21	0.41
1:B:488:ARG:HB2	1:B:574:THR:HB	2.02	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:I:264:SER:O	1:I:265:THR:HB	2.21	0.41
1:F:393:PHE:HB3	1:I:696:ASN:ND2	2.36	0.41
1:A:342:GLN:C	1:A:343:VAL:CG2	2.89	0.41
1:A:280:TRP:CE3	1:A:650:LYS:HB2	2.55	0.41
1:C:280:TRP:CE3	1:C:650:LYS:HB2	2.55	0.41
1:D:508:LYS:HG2	1:D:517:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:714:THR:CG2	1:D:715:VAL:H	2.30	0.41
1:E:312:LEU:HA	1:E:682:GLU:O	2.20	0.41
1:E:701:TYR:CD2	1:E:701:TYR:C	2.94	0.41
1:F:315:LYS:HB2	1:F:315:LYS:HE2	1.82	0.41
1:G:237:ASP:OD1	1:G:237:ASP:N	2.53	0.41
1:G:701:TYR:CD2	1:G:701:TYR:C	2.94	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: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:A:696:ASN:ND2	1:H:393:PHE:HB3	2.36	0.41
1:B:451:ASN:ND2	1:B:458:ASN:HB2	2.30	0.41
1:B:586:SER:HB2	4:B:823:HOH:O	2.21	0.41
1:B:701:TYR:CD2	1:B:701:TYR:C	2.94	0.41
1:D:284:ASP:O	1:D:362:CYS:HA	2.21	0.41
1:D:455:SER:HA	1:D:456:ALA:HA	1.69	0.41
1:H:218:ALA:C	1:H:219:ASP:CG	2.79	0.41
4:D:831:HOH:O	1:H:735:PRO:HD3	2.19	0.41
1:I:316:LEU:HD23	1:I:316:LEU:HA	1.83	0.41
1:I:363:LEU:HA	1:I:364:PRO:HD3	1.96	0.41
1:I:508:LYS:HG2	1:I:517:ILE:HA	2.03	0.41
1:J:342:GLN:HG2	1:J:403:MET:HG2	2.03	0.41
1:J:438:LEU:O	1:J:439:ILE:HD13	2.21	0.41
1:E:397:GLU:N	1:E:397:GLU:OE1	2.50	0.41
1:E:315:LYS:HB3	1:E:680:SER:HB2	2.03	0.41
1:G:312:LEU:HA	1:G:682:GLU:O	2.20	0.41
1:H:342:GLN:C	1:H:343:VAL:CG2	2.89	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:J:508:LYS:HG2	1:J:517:ILE:HA	2.03	0.41
1:A:286:ASN:HD21	1:A:619:TRP:N	2.13	0.40
1:B:342:GLN:C	1:B:343:VAL:CG2	2.89	0.40
1:B:393:PHE:HB3	1:E:696:ASN:ND2	2.36	0.40
1:C:315:LYS:HB3	1:C:680:SER:HB2	2.03	0.40
1:C:286:ASN:HD21	1:C:618:ILE:H	1.66	0.40
1:D:360:GLN:OE1	1:H:440:ASP:HB2	2.21	0.40
1:E:366:PHE:HA	1:E:367:PRO:HD3	1.94	0.40
1:E:569:THR:OG1	1:E:570:ASN:ND2	2.55	0.40
1:G:455:SER:HA	1:G:456:ALA:HA	1.69	0.40
1:G:736:LEU:HA	1:G:736:LEU:HD13	1.83	0.40
1:I:405:ARG:H	1:I:408:ASN:HD22	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:569:THR:OG1	1:I:570:ASN:ND2	2.55	0.40
1:J:342:GLN:C	1:J:343:VAL:CG2	2.89	0.40
1:J:701:TYR:C	1:J:701:TYR:CD2	2.94	0.40
1:C:328:ASP:CB	1:C:329:GLY:CA	2.76	0.40
1:D:315:LYS:HB3	1:D:680:SER:HB2	2.03	0.40
1:D:342:GLN:C	1:D:343:VAL:CG2	2.89	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:G:220:GLY:C	1:G:222:GLY:N	2.75	0.40
1:G:586:SER:HB2	4:G:826:HOH:O	2.21	0.40
1:A:315:LYS:HB3	1:A:680:SER:HB2	2.03	0.40
1:C:284:ASP:O	1:C:362:CYS:HA	2.21	0.40
1:C:449:THR:H	1:I:500:ASN:HD22	1.69	0.40
1:F:315:LYS:HB3	1:F:680:SER:HB2	2.03	0.40
1:F:488:ARG:HB2	1:F:574:THR:HB	2.02	0.40
1:C:628:HIS:O	3:F:738:CYT:C6	2.74	0.40
1:B:472:SER:HB3	1:G:270:ASP:O	2.22	0.40
1:G:282:TYR:CE1	1:G:374:PRO:HB2	2.57	0.40
1:H:701:TYR:C	1:H:701:TYR:CD2	2.94	0.40
1:I:280:TRP:CZ2	1:I:650:LYS:HE3	2.56	0.40
1:I:427:HIS:NE2	1:I:736:LEU:HD13	2.37	0.40
1:A:628:HIS:O	3:D:738:CYT:C6	2.74	0.40
1:B:342:GLN:HA	1:B:402:GLN:O	2.22	0.40
1:C:282:TYR:CE1	1:C:374:PRO:HB2	2.57	0.40
1:D:342:GLN:HA	1:D:402:GLN:O	2.22	0.40
1:D:451:ASN:ND2	1:D:458:ASN:HB2	2.30	0.40
1:E:450:GLN:OE1	1:E:457:GLN:HB3	2.22	0.40
1:G:329:GLY:C	1:G:330:VAL:HG12	2.42	0.40
1:G:342:GLN:HA	1:G:402:GLN:O	2.22	0.40
1:H:500:ASN:HA	1:H:500:ASN:HD22	1.67	0.40
3:C:738:CYT:C6	1:I:628:HIS:O	2.74	0.40
1:A:229:HIS:O	1:A:242:THR:HG22	2.22	0.40
1:B:342:GLN:HG2	1:B:403:MET:HG2	2.03	0.40
1:B:397:GLU:OE2	1:B:650:LYS:NZ	2.41	0.40
1:B:315:LYS:HB3	1:B:680:SER:HB2	2.03	0.40
1:D:366:PHE:HA	1:D:367:PRO:HD3	1.94	0.40
1:D:393:PHE:HB3	1:H:696:ASN:ND2	2.36	0.40
1:D:342:GLN:HG2	1:D:403:MET:HG2	2.03	0.40
1:D:450:GLN:OE1	1:D:457:GLN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:TYR:CE1	1:F:374:PRO:HB2	2.57	0.40
1:F:284:ASP:O	1:F:362:CYS:HA	2.21	0.40
1:F:342:GLN:HA	1:F:402:GLN:O	2.22	0.40
1:F:508:LYS:HG2	1:F:517:ILE:HA	2.03	0.40
1:F:427:HIS:NE2	1:F:736:LEU:HD13	2.37	0.40
1:G:278:THR:CG2	1:G:280:TRP:HB2	2.52	0.40
1:G:284:ASP:O	1:G:362:CYS:HA	2.21	0.40
1:G:450:GLN:OE1	1:G:457:GLN:HB3	2.22	0.40
1:G:569:THR:OG1	1:G:570:ASN:ND2	2.55	0.40
1:H:282:TYR:CE1	1:H:374:PRO:HB2	2.57	0.40
1:H:450:GLN:OE1	1:H:457:GLN:HB3	2.22	0.40
3:H:738:CYT:N4	4:H:771:HOH:O	2.29	0.40
1:I:342:GLN:HG2	1:I:403:MET:HG2	2.03	0.40
1:J:450:GLN:OE1	1:J:457:GLN:HB3	2.22	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%)	19	35
1	B	518/736 (70%)	500 (96%)	17 (3%)	1 (0%)	47	68
1	C	518/736 (70%)	498 (96%)	18 (4%)	2 (0%)	34	54
1	D	518/736 (70%)	498 (96%)	16 (3%)	4 (1%)	19	35
1	E	518/736 (70%)	500 (96%)	16 (3%)	2 (0%)	34	54
1	F	518/736 (70%)	501 (97%)	14 (3%)	3 (1%)	25	43
1	G	518/736 (70%)	498 (96%)	16 (3%)	4 (1%)	19	35
1	H	518/736 (70%)	498 (96%)	17 (3%)	3 (1%)	25	43
1	I	518/736 (70%)	501 (97%)	12 (2%)	5 (1%)	15	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	518/736 (70%)	497 (96%)	18 (4%)	3 (1%)	25	43
All	All	5180/7360 (70%)	4990 (96%)	159 (3%)	31 (1%)	25	43

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%)	11	21
1	B	451/617 (73%)	411 (91%)	40 (9%)	9	19
1	C	451/617 (73%)	413 (92%)	38 (8%)	11	21
1	D	451/617 (73%)	415 (92%)	36 (8%)	12	23
1	E	451/617 (73%)	413 (92%)	38 (8%)	11	21
1	F	451/617 (73%)	413 (92%)	38 (8%)	11	21
1	G	451/617 (73%)	414 (92%)	37 (8%)	11	22
1	H	451/617 (73%)	413 (92%)	38 (8%)	11	21
1	I	451/617 (73%)	414 (92%)	37 (8%)	11	22
1	J	451/617 (73%)	413 (92%)	38 (8%)	11	21
All	All	4510/6170 (73%)	4132 (92%)	378 (8%)	11	21

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	-	9,11,11	0.91	0	7,15,15	2.55	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADE	G	737	-	9,11,11	0.91	0	7,15,15	2.56	3 (42%)
2	ADE	D	737	-	9,11,11	0.91	0	7,15,15	2.55	3 (42%)
2	ADE	E	737	-	9,11,11	0.91	0	7,15,15	2.55	3 (42%)
2	ADE	B	737	-	9,11,11	0.91	0	7,15,15	2.54	2 (28%)
2	ADE	F	737	-	9,11,11	0.92	0	7,15,15	2.54	2 (28%)
3	CYT	B	739	-	7,8,8	1.69	1 (14%)	8,10,10	9.06	6 (75%)
3	CYT	C	738	-	7,8,8	1.68	1 (14%)	8,10,10	9.06	6 (75%)
3	CYT	B	738	-	7,8,8	1.69	1 (14%)	8,10,10	9.07	6 (75%)
3	CYT	E	738	-	7,8,8	1.68	1 (14%)	8,10,10	9.06	6 (75%)
3	CYT	D	738	-	7,8,8	1.69	1 (14%)	8,10,10	9.04	6 (75%)
3	CYT	F	738	-	7,8,8	1.70	1 (14%)	8,10,10	8.99	6 (75%)
2	ADE	C	737	-	9,11,11	0.92	0	7,15,15	2.55	2 (28%)
3	CYT	H	738	-	7,8,8	1.69	1 (14%)	8,10,10	9.02	6 (75%)
2	ADE	H	737	-	9,11,11	0.90	0	7,15,15	2.55	3 (42%)
2	ADE	I	737	-	9,11,11	0.92	0	7,15,15	2.56	2 (28%)
3	CYT	J	738	-	7,8,8	1.68	1 (14%)	8,10,10	9.09	6 (75%)
2	ADE	J	737	-	9,11,11	0.90	0	7,15,15	2.54	2 (28%)
3	CYT	A	738	-	7,8,8	1.69	1 (14%)	8,10,10	9.05	6 (75%)
3	CYT	I	738	-	7,8,8	1.69	1 (14%)	8,10,10	9.04	6 (75%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADE	C	737	-	-	-	0/2/2/2
3	CYT	H	738	-	-	-	0/1/1/1
2	ADE	H	737	-	-	-	0/2/2/2
2	ADE	I	737	-	-	-	0/2/2/2
3	CYT	J	738	-	-	-	0/1/1/1
2	ADE	J	737	-	-	-	0/2/2/2
3	CYT	A	738	-	-	-	0/1/1/1
3	CYT	I	738	-	-	-	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	-2.63	1.33	1.38
3	I	738	CYT	C5-C6	-2.63	1.33	1.38
3	D	738	CYT	C5-C6	-2.61	1.33	1.38
3	A	738	CYT	C5-C6	-2.61	1.33	1.38
3	C	738	CYT	C5-C6	-2.59	1.33	1.38
3	H	738	CYT	C5-C6	-2.59	1.33	1.38
3	E	738	CYT	C5-C6	-2.59	1.33	1.38
3	J	738	CYT	C5-C6	-2.58	1.33	1.38
3	B	739	CYT	C5-C6	-2.58	1.33	1.38
3	B	738	CYT	C5-C6	-2.57	1.33	1.38

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	738	CYT	C6-N1-C2	18.60	123.59	114.42
3	C	738	CYT	C6-N1-C2	18.55	123.57	114.42
3	B	738	CYT	C6-N1-C2	18.54	123.56	114.42
3	E	738	CYT	C6-N1-C2	18.52	123.55	114.42
3	B	739	CYT	C6-N1-C2	18.51	123.55	114.42
3	A	738	CYT	C6-N1-C2	18.51	123.55	114.42
3	D	738	CYT	C6-N1-C2	18.50	123.54	114.42
3	I	738	CYT	C6-N1-C2	18.45	123.52	114.42
3	H	738	CYT	C6-N1-C2	18.42	123.50	114.42
3	F	738	CYT	C6-N1-C2	18.35	123.47	114.42
3	J	738	CYT	N1-C2-N3	-16.35	115.44	128.43
3	B	738	CYT	N1-C2-N3	-16.32	115.46	128.43
3	I	738	CYT	N1-C2-N3	-16.30	115.47	128.43
3	E	738	CYT	N1-C2-N3	-16.29	115.48	128.43
3	B	739	CYT	N1-C2-N3	-16.28	115.48	128.43
3	A	738	CYT	N1-C2-N3	-16.26	115.50	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	738	CYT	N1-C2-N3	-16.26	115.50	128.43
3	H	738	CYT	N1-C2-N3	-16.25	115.52	128.43
3	D	738	CYT	N1-C2-N3	-16.22	115.53	128.43
3	F	738	CYT	N1-C2-N3	-16.22	115.54	128.43
2	I	737	ADE	N3-C2-N1	-4.39	121.82	128.68
2	E	737	ADE	N3-C2-N1	-4.39	121.82	128.68
2	D	737	ADE	N3-C2-N1	-4.39	121.82	128.68
2	A	737	ADE	N3-C2-N1	-4.38	121.83	128.68
2	G	737	ADE	N3-C2-N1	-4.38	121.83	128.68
2	C	737	ADE	N3-C2-N1	-4.37	121.85	128.68
2	F	737	ADE	N3-C2-N1	-4.37	121.85	128.68
2	H	737	ADE	N3-C2-N1	-4.36	121.87	128.68
2	B	737	ADE	N3-C2-N1	-4.36	121.87	128.68
2	J	737	ADE	N3-C2-N1	-4.34	121.89	128.68
3	B	738	CYT	C2-N3-C4	4.10	120.50	116.34
3	B	739	CYT	C2-N3-C4	4.08	120.48	116.34
3	J	738	CYT	C2-N3-C4	4.07	120.46	116.34
3	E	738	CYT	C2-N3-C4	4.04	120.43	116.34
3	F	738	CYT	C2-N3-C4	4.03	120.43	116.34
3	H	738	CYT	C2-N3-C4	4.03	120.43	116.34
3	C	738	CYT	C2-N3-C4	4.01	120.41	116.34
3	I	738	CYT	C2-N3-C4	4.01	120.41	116.34
3	A	738	CYT	C2-N3-C4	4.01	120.40	116.34
3	D	738	CYT	C2-N3-C4	3.98	120.38	116.34
2	G	737	ADE	C4-C5-N7	-3.81	105.42	109.40
2	C	737	ADE	C4-C5-N7	-3.81	105.43	109.40
2	H	737	ADE	C4-C5-N7	-3.80	105.44	109.40
2	I	737	ADE	C4-C5-N7	-3.80	105.44	109.40
2	J	737	ADE	C4-C5-N7	-3.79	105.44	109.40
2	E	737	ADE	C4-C5-N7	-3.79	105.45	109.40
2	F	737	ADE	C4-C5-N7	-3.77	105.47	109.40
2	A	737	ADE	C4-C5-N7	-3.77	105.47	109.40
2	D	737	ADE	C4-C5-N7	-3.74	105.50	109.40
2	B	737	ADE	C4-C5-N7	-3.73	105.52	109.40
3	B	739	CYT	C6-C5-C4	-3.30	114.99	116.91
3	I	738	CYT	C6-C5-C4	-3.30	114.99	116.91
3	B	738	CYT	C6-C5-C4	-3.28	115.00	116.91
3	H	738	CYT	C6-C5-C4	-3.28	115.00	116.91
3	J	738	CYT	C6-C5-C4	-3.27	115.01	116.91
3	D	738	CYT	C6-C5-C4	-3.27	115.01	116.91
3	A	738	CYT	C6-C5-C4	-3.26	115.02	116.91
3	E	738	CYT	C6-C5-C4	-3.23	115.03	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	738	CYT	C6-C5-C4	-3.22	115.04	116.91
3	C	738	CYT	C6-C5-C4	-3.22	115.04	116.91
3	I	738	CYT	C5-C4-N3	3.06	125.25	121.72
3	H	738	CYT	C5-C4-N3	3.05	125.23	121.72
3	D	738	CYT	C5-C4-N3	3.04	125.22	121.72
3	A	738	CYT	C5-C4-N3	3.04	125.22	121.72
3	E	738	CYT	C5-C4-N3	3.03	125.21	121.72
3	C	738	CYT	C5-C4-N3	3.02	125.20	121.72
3	J	738	CYT	C5-C4-N3	3.02	125.20	121.72
3	F	738	CYT	C5-C4-N3	3.00	125.17	121.72
3	B	738	CYT	C5-C4-N3	2.99	125.17	121.72
3	B	739	CYT	C5-C4-N3	2.99	125.17	121.72
3	C	738	CYT	C5-C6-N1	-2.97	120.27	123.96
3	E	738	CYT	C5-C6-N1	-2.96	120.28	123.96
3	J	738	CYT	C5-C6-N1	-2.95	120.30	123.96
3	A	738	CYT	C5-C6-N1	-2.94	120.30	123.96
3	D	738	CYT	C5-C6-N1	-2.94	120.30	123.96
3	B	738	CYT	C5-C6-N1	-2.94	120.31	123.96
3	H	738	CYT	C5-C6-N1	-2.94	120.31	123.96
3	B	739	CYT	C5-C6-N1	-2.92	120.33	123.96
3	F	738	CYT	C5-C6-N1	-2.91	120.34	123.96
3	I	738	CYT	C5-C6-N1	-2.90	120.35	123.96
2	D	737	ADE	C2-N3-C4	2.02	118.17	113.45
2	H	737	ADE	C2-N3-C4	2.01	118.16	113.45
2	E	737	ADE	C2-N3-C4	2.01	118.15	113.45
2	A	737	ADE	C2-N3-C4	2.00	118.14	113.45
2	G	737	ADE	C2-N3-C4	2.00	118.14	113.45

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
2	B	737	ADE	3	0
3	B	739	CYT	1	0
3	C	738	CYT	3	0
3	E	738	CYT	1	0
3	D	738	CYT	3	0
3	F	738	CYT	2	0
3	H	738	CYT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	738	CYT	1	0
3	A	738	CYT	3	0
3	I	738	CYT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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, 95th 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 ²)	Q<0.9
1	A	520/736 (70%)	0.26	18 (3%)	44 47	25, 34, 55, 92	0
1	B	520/736 (70%)	0.58	31 (5%)	21 22	25, 34, 55, 92	0
1	C	520/736 (70%)	0.83	29 (5%)	24 25	25, 34, 55, 92	0
1	D	520/736 (70%)	0.45	18 (3%)	44 47	25, 34, 55, 92	0
1	E	520/736 (70%)	0.79	34 (6%)	18 19	25, 34, 55, 92	0
1	F	520/736 (70%)	0.59	25 (4%)	30 32	25, 34, 55, 92	0
1	G	520/736 (70%)	0.77	39 (7%)	14 14	25, 34, 55, 92	0
1	H	520/736 (70%)	0.41	23 (4%)	34 37	25, 34, 55, 92	0
1	I	520/736 (70%)	0.90	36 (6%)	16 17	25, 34, 55, 92	0
1	J	520/736 (70%)	1.25	83 (15%)	1 1	25, 34, 55, 92	0
All	All	5200/7360 (70%)	0.68	336 (6%)	18 19	25, 34, 55, 92	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	453	SER	13.2
1	G	453	SER	11.1
1	F	453	SER	11.0
1	F	456	ALA	10.5
1	I	453	SER	9.7
1	J	453	SER	9.1
1	I	217	GLY	9.0
1	B	452	GLN	8.8
1	B	453	SER	8.7
1	A	330	VAL	8.6
1	C	218	ALA	8.5
1	J	456	ALA	8.4
1	A	454	GLY	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	8.2
1	E	452	GLN	8.2
1	C	217	GLY	8.1
1	D	456	ALA	8.0
1	I	455	SER	8.0
1	C	457	GLN	7.9
1	E	453	SER	7.8
1	J	452	GLN	7.8
1	I	454	GLY	7.8
1	G	218	ALA	7.8
1	G	457	GLN	7.7
1	F	452	GLN	7.7
1	B	454	GLY	7.6
1	B	329	GLY	7.6
1	H	452	GLN	7.4
1	E	456	ALA	7.4
1	G	456	ALA	7.3
1	J	218	ALA	7.3
1	C	453	SER	7.3
1	H	328	ASP	7.1
1	C	452	GLN	7.1
1	D	217	GLY	7.1
1	D	452	GLN	7.0
1	D	327	ASN	6.9
1	J	327	ASN	6.9
1	J	328	ASP	6.8
1	D	328	ASP	6.8
1	C	456	ALA	6.7
1	H	218	ALA	6.7
1	I	330	VAL	6.6
1	I	328	ASP	6.6
1	G	330	VAL	6.6
1	B	328	ASP	6.5
1	C	328	ASP	6.3
1	E	218	ALA	6.3
1	F	330	VAL	6.2
1	J	330	VAL	6.1
1	D	218	ALA	6.1
1	I	329	GLY	6.1
1	H	456	ALA	6.1
1	B	217	GLY	6.0
1	G	328	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
1	J	329	GLY	6.0
1	E	217	GLY	6.0
1	H	457	GLN	5.9
1	A	328	ASP	5.8
1	A	453	SER	5.8
1	F	454	GLY	5.7
1	B	327	ASN	5.7
1	A	327	ASN	5.6
1	J	457	GLN	5.6
1	C	455	SER	5.5
1	B	456	ALA	5.5
1	B	455	SER	5.4
1	D	453	SER	5.4
1	F	457	GLN	5.4
1	H	217	GLY	5.3
1	G	452	GLN	5.3
1	E	455	SER	5.3
1	I	452	GLN	5.2
1	E	330	VAL	5.2
1	J	705	TYR	5.2
1	C	329	GLY	5.2
1	H	329	GLY	5.2
1	A	455	SER	5.1
1	B	330	VAL	5.1
1	J	217	GLY	5.1
1	I	456	ALA	5.1
1	B	457	GLN	5.0
1	G	329	GLY	5.0
1	J	264	SER	5.0
1	A	452	GLN	5.0
1	J	454	GLY	5.0
1	G	220	GLY	5.0
1	G	327	ASN	4.8
1	I	327	ASN	4.8
1	G	217	GLY	4.7
1	I	218	ALA	4.5
1	D	455	SER	4.4
1	G	265	THR	4.4
1	E	327	ASN	4.4
1	J	219	ASP	4.4
1	H	327	ASN	4.3
1	D	457	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	457	GLN	4.3
1	G	235	LEU	4.3
1	A	331	THR	4.3
1	A	456	ALA	4.3
1	G	455	SER	4.2
1	D	219	ASP	4.2
1	E	219	ASP	4.2
1	J	656	ALA	4.2
1	C	330	VAL	4.2
1	E	328	ASP	4.2
1	F	455	SER	4.2
1	F	327	ASN	4.1
1	I	457	GLN	4.1
1	B	266	GLY	4.1
1	C	454	GLY	4.0
1	C	705	TYR	4.0
1	D	556	ASP	3.9
1	D	330	VAL	3.9
1	J	265	THR	3.9
1	F	587	SER	3.9
1	E	264	SER	3.9
1	A	217	GLY	3.8
1	F	329	GLY	3.8
1	H	705	TYR	3.8
1	G	229	HIS	3.8
1	H	229	HIS	3.8
1	A	218	ALA	3.7
1	I	705	TYR	3.7
1	J	451	ASN	3.7
1	I	502	THR	3.7
1	C	235	LEU	3.7
1	C	327	ASN	3.7
1	B	218	ALA	3.7
1	F	328	ASP	3.6
1	B	705	TYR	3.5
1	A	325	THR	3.5
1	I	265	THR	3.4
1	H	265	THR	3.4
1	J	449	THR	3.3
1	F	218	ALA	3.3
1	G	264	SER	3.3
1	G	704	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	325	THR	3.2
1	J	493	LYS	3.2
1	J	266	GLY	3.2
1	I	326	THR	3.1
1	C	494	THR	3.1
1	J	229	HIS	3.1
1	C	219	ASP	3.1
1	G	500	ASN	3.1
1	B	264	SER	3.1
1	H	455	SER	3.0
1	I	628	HIS	3.0
1	J	706	ALA	3.0
1	J	661	GLU	3.0
1	H	330	VAL	3.0
1	J	385	SER	3.0
1	J	489	VAL	3.0
1	E	329	GLY	3.0
1	J	461	LEU	3.0
1	H	506	ALA	3.0
1	H	219	ASP	3.0
1	J	703	SER	3.0
1	H	235	LEU	3.0
1	J	395	CYS	2.9
1	J	267	ALA	2.9
1	A	265	THR	2.9
1	F	265	THR	2.9
1	D	265	THR	2.9
1	E	461	LEU	2.9
1	J	664	ALA	2.9
1	E	705	TYR	2.9
1	G	705	TYR	2.9
1	E	556	ASP	2.9
1	I	334	ALA	2.9
1	A	266	GLY	2.8
1	C	499	SER	2.8
1	B	495	ASP	2.8
1	C	590	ASP	2.8
1	G	458	ASN	2.8
1	J	490	SER	2.8
1	J	498	ASN	2.8
1	H	454	GLY	2.8
1	G	584	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	266	GLY	2.8
1	J	497	ASN	2.8
1	J	455	SER	2.8
1	D	332	THR	2.8
1	I	736	LEU	2.8
1	J	628	HIS	2.8
1	A	264	SER	2.8
1	F	556	ASP	2.8
1	B	332	THR	2.7
1	G	237	ASP	2.7
1	B	325	THR	2.7
1	F	547	SER	2.7
1	J	660	ALA	2.7
1	G	556	ASP	2.7
1	J	366	PHE	2.7
1	J	253	ASN	2.7
1	G	494	THR	2.6
1	J	709	ALA	2.6
1	J	319	ILE	2.6
1	C	265	THR	2.6
1	B	451	ASN	2.6
1	J	584	PHE	2.6
1	G	238	ARG	2.6
1	E	490	SER	2.6
1	E	498	ASN	2.6
1	E	736	LEU	2.6
1	J	670	PHE	2.6
1	J	710	ASN	2.6
1	G	451	ASN	2.6
1	A	326	THR	2.6
1	F	325	THR	2.6
1	J	726	PRO	2.6
1	F	223	ASN	2.5
1	J	587	SER	2.5
1	E	503	TRP	2.5
1	J	312	LEU	2.5
1	D	264	SER	2.5
1	I	264	SER	2.5
1	B	326	THR	2.5
1	E	589	THR	2.5
1	I	324	VAL	2.5
1	B	587	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	669	SER	2.5
1	B	458	ASN	2.5
1	H	266	GLY	2.5
1	E	235	LEU	2.4
1	C	736	LEU	2.4
1	G	450	GLN	2.4
1	B	502	THR	2.4
1	H	492	THR	2.4
1	J	499	SER	2.4
1	F	705	TYR	2.4
1	F	458	ASN	2.4
1	J	662	PHE	2.4
1	G	665	THR	2.4
1	I	331	THR	2.4
1	I	656	ALA	2.4
1	B	470	GLY	2.4
1	J	439	ILE	2.4
1	J	667	PHE	2.4
1	E	656	ALA	2.4
1	H	556	ASP	2.4
1	I	338	THR	2.4
1	E	704	ASN	2.4
1	E	588	SER	2.4
1	J	680	SER	2.4
1	C	458	ASN	2.3
1	F	217	GLY	2.3
1	H	546	GLU	2.3
1	J	586	SER	2.3
1	J	463	PHE	2.3
1	J	713	PHE	2.3
1	C	325	THR	2.3
1	B	324	VAL	2.3
1	C	556	ASP	2.3
1	J	323	GLU	2.3
1	J	459	LYS	2.3
1	G	267	ALA	2.3
1	H	264	SER	2.3
1	J	458	ASN	2.3
1	G	236	GLY	2.3
1	J	492	THR	2.3
1	F	460	ASP	2.3
1	E	710	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	290	CYS	2.3
1	E	454	GLY	2.3
1	J	263	ALA	2.3
1	I	444	TYR	2.3
1	B	530	ASP	2.3
1	I	235	LEU	2.3
1	I	503	TRP	2.3
1	C	532	ASP	2.3
1	D	705	TYR	2.3
1	D	461	LEU	2.3
1	J	503	TRP	2.3
1	J	338	THR	2.3
1	B	331	THR	2.2
1	E	502	THR	2.2
1	B	219	ASP	2.2
1	E	661	GLU	2.2
1	I	219	ASP	2.2
1	I	532	ASP	2.2
1	F	341	VAL	2.2
1	C	229	HIS	2.2
1	E	398	TYR	2.2
1	G	660	ALA	2.2
1	J	501	PHE	2.2
1	I	546	GLU	2.2
1	G	589	THR	2.2
1	G	460	ASP	2.2
1	B	265	THR	2.2
1	J	500	ASN	2.2
1	J	273	TYR	2.1
1	I	706	ALA	2.1
1	J	387	ALA	2.1
1	E	683	ILE	2.1
1	F	266	GLY	2.1
1	D	235	LEU	2.1
1	J	243	SER	2.1
1	B	269	ASN	2.1
1	E	458	ASN	2.1
1	I	484	TYR	2.1
1	J	269	ASN	2.1
1	G	668	ALA	2.1
1	I	325	THR	2.1
1	J	655	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	721	TYR	2.1
1	E	300	LEU	2.1
1	C	391	SER	2.1
1	J	418	GLU	2.1
1	G	269	ASN	2.1
1	J	332	THR	2.1
1	C	503	TRP	2.1
1	J	254	ASN	2.1
1	E	539	GLY	2.1
1	I	664	ALA	2.1
1	I	229	HIS	2.1
1	J	359	HIS	2.1
1	J	588	SER	2.1
1	G	454	GLY	2.1
1	J	601	ALA	2.1
1	J	495	ASP	2.1
1	C	483	CYS	2.1
1	B	532	ASP	2.0
1	F	229	HIS	2.0
1	C	326	THR	2.0
1	J	702	THR	2.0
1	F	264	SER	2.0
1	G	498	ASN	2.0
1	J	534	PHE	2.0
1	J	546	GLU	2.0
1	A	502	THR	2.0
1	J	450	GLN	2.0
1	J	283	PHE	2.0
1	J	613	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
3	CYT	E	738	8/8	0.42	0.47	63,67,68,70	0
3	CYT	D	738	8/8	0.52	0.40	63,67,68,70	0
3	CYT	F	738	8/8	0.54	0.38	63,67,68,70	0
3	CYT	H	738	8/8	0.54	0.43	63,67,68,70	0
3	CYT	B	739	8/8	0.58	0.38	63,67,68,70	0
3	CYT	C	738	8/8	0.60	0.42	63,67,68,70	0
2	ADE	F	737	10/10	0.63	0.46	78,81,82,83	0
2	ADE	I	737	10/10	0.72	0.34	78,81,82,83	0
3	CYT	B	738	8/8	0.73	0.33	63,67,68,70	0
2	ADE	E	737	10/10	0.74	0.40	78,81,82,83	0
3	CYT	A	738	8/8	0.76	0.34	63,67,68,70	0
3	CYT	I	738	8/8	0.76	0.33	63,67,68,70	0
2	ADE	A	737	10/10	0.77	0.33	78,81,82,83	0
2	ADE	D	737	10/10	0.78	0.30	78,81,82,83	0
3	CYT	J	738	8/8	0.79	0.36	63,67,68,70	0
2	ADE	G	737	10/10	0.80	0.36	78,81,82,83	0
2	ADE	J	737	10/10	0.82	0.36	78,81,82,83	0
2	ADE	C	737	10/10	0.82	0.30	78,81,82,83	0
2	ADE	H	737	10/10	0.82	0.31	78,81,82,83	0
2	ADE	B	737	10/10	0.83	0.25	78,81,82,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.