



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:17 PM UTC

PDB ID : 7CO5 / pdb_00007co5
Title : HtrA-type protease AlgW with decapeptide
Authors : Li, T.; Song, Y.J.; Bao, R.
Deposited on : 2020-08-03
Resolution : 2.35 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

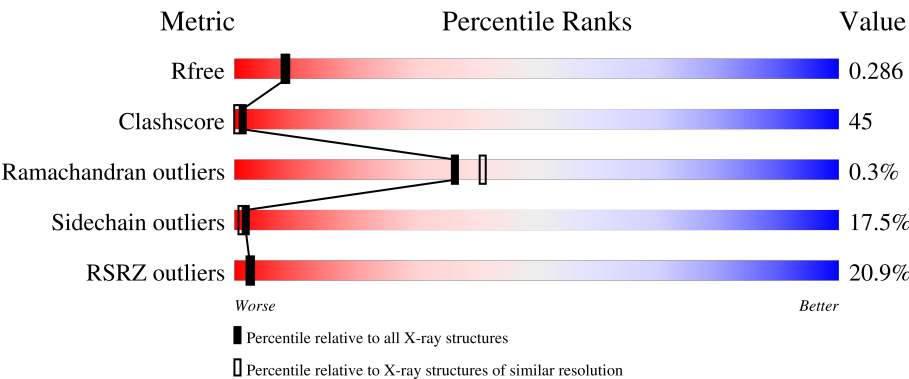
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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 of 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	10	30% 30%30%10%30%
1	C	10	30% 20%50%30%
1	E	10	50% 10%50%40%
1	G	10	30% 20%30%10%40%
1	I	10	20% 20%40%40%

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Mol	Chain	Length	Quality of chain
1	K	10	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IMD	H	401	-	-	X	-
3	IMD	L	401	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15076 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 decapeptide SVRDELRWVF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	G	6	Total	C	N	O	0	0	0
			60	42	10	8			
1	A	7	Total	C	N	O	0	0	0
			68	46	11	11			
1	C	7	Total	C	N	O	0	0	0
			68	46	11	11			
1	E	6	Total	C	N	O	0	0	0
			60	42	10	8			
1	I	6	Total	C	N	O	0	0	0
			60	42	10	8			
1	K	9	Total	C	N	O	0	0	0
			86	57	16	13			

- Molecule 2 is a protein called AlgW protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	325	Total	C	N	O	S	0	0	0
			2388	1492	427	460	9			
2	B	325	Total	C	N	O	S	0	0	0
			2388	1492	427	460	9			
2	D	325	Total	C	N	O	S	0	0	0
			2388	1492	427	460	9			
2	F	325	Total	C	N	O	S	0	0	0
			2388	1492	427	460	9			
2	J	325	Total	C	N	O	S	0	0	0
			2388	1492	427	460	9			
2	L	325	Total	C	N	O	S	0	0	0
			2388	1492	427	460	9			

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0
3	F	1	Total C N 5 3 2	0	0
3	J	1	Total C N 5 3 2	0	0
3	L	1	Total C N 5 3 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total O 2 2	0	0
4	H	51	Total O 51 51	0	0
4	B	51	Total O 51 51	0	0
4	D	51	Total O 51 51	0	0
4	F	43	Total O 43 43	0	0
4	I	2	Total O 2 2	0	0

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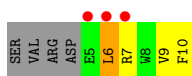
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	44	Total 44	O 44	0	0
4	K	1	Total 1	O 1	0	0
4	L	71	Total 71	O 71	0	0

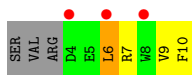
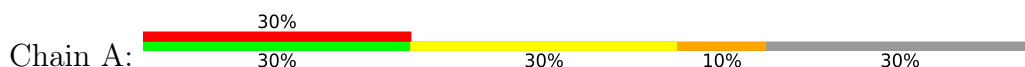
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

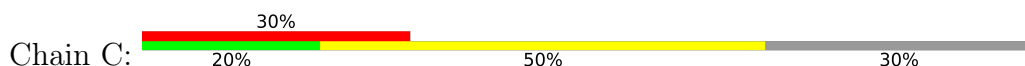
- Molecule 1: decapeptide SVRDELRWVF



- Molecule 1: decapeptide SVRDELRWVF



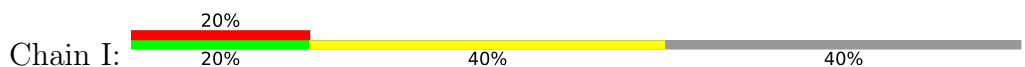
- Molecule 1: decapeptide SVRDELRWVF



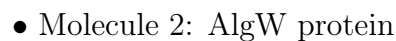
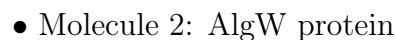
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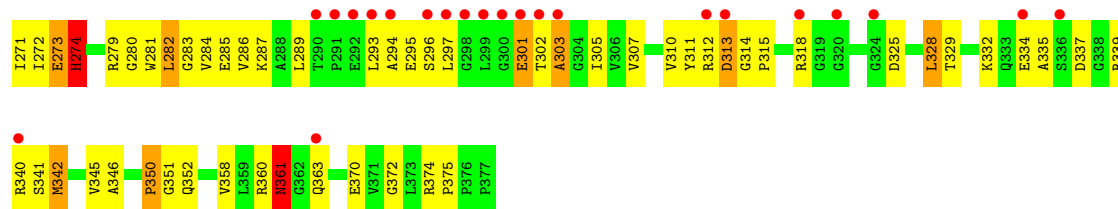


- Molecule 1: decapeptide SVRDELRWVF

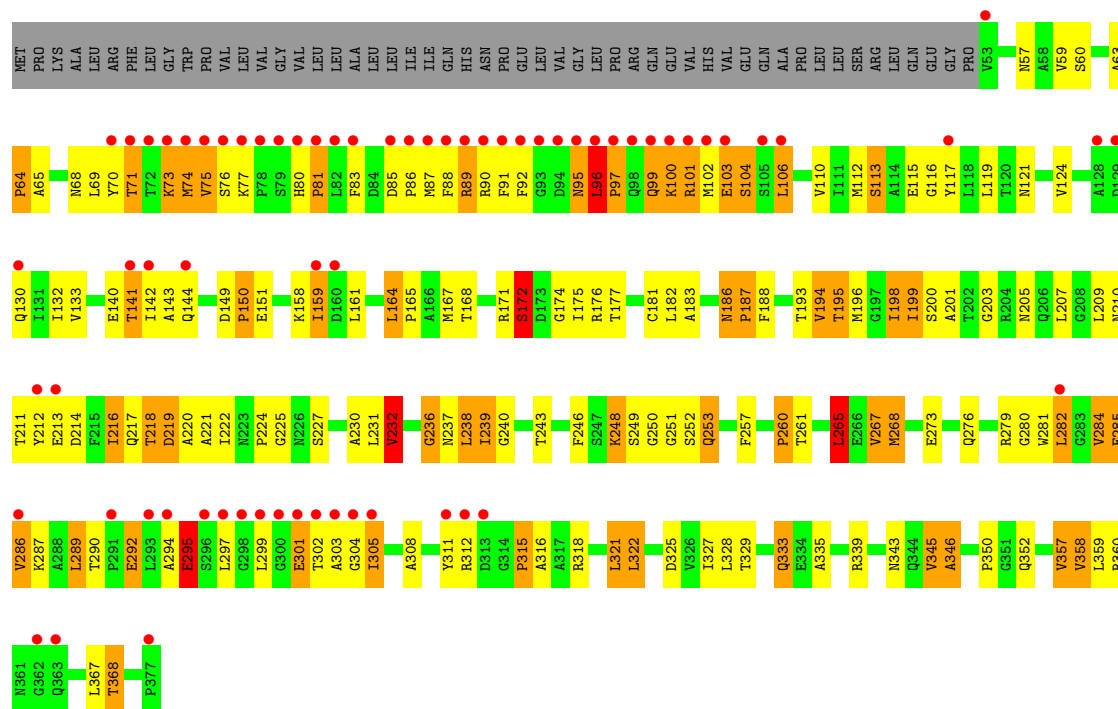


- Molecule 1: decapeptide SVRDELRWVF

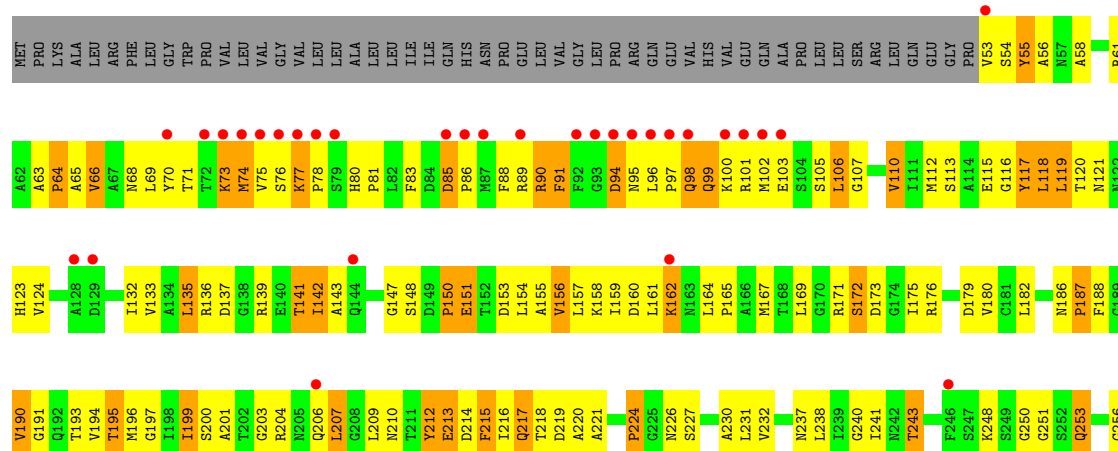


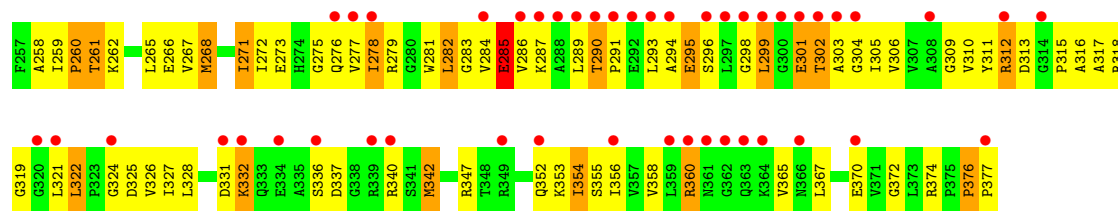


• Molecule 2: AlgW protein

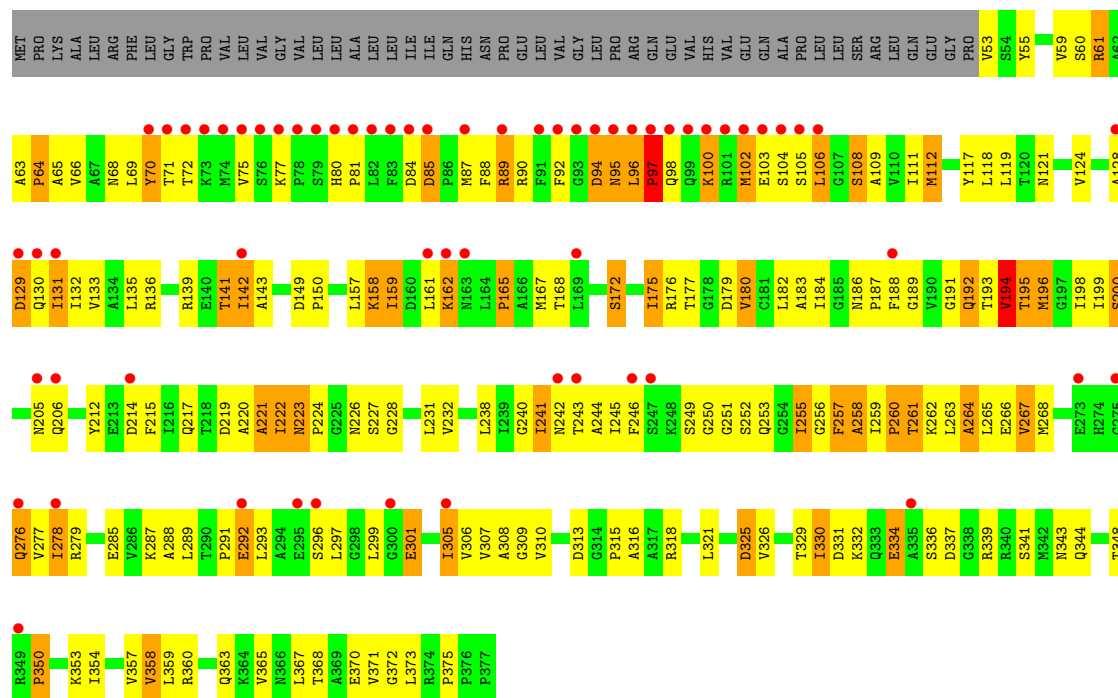


• Molecule 2: AlgW protein

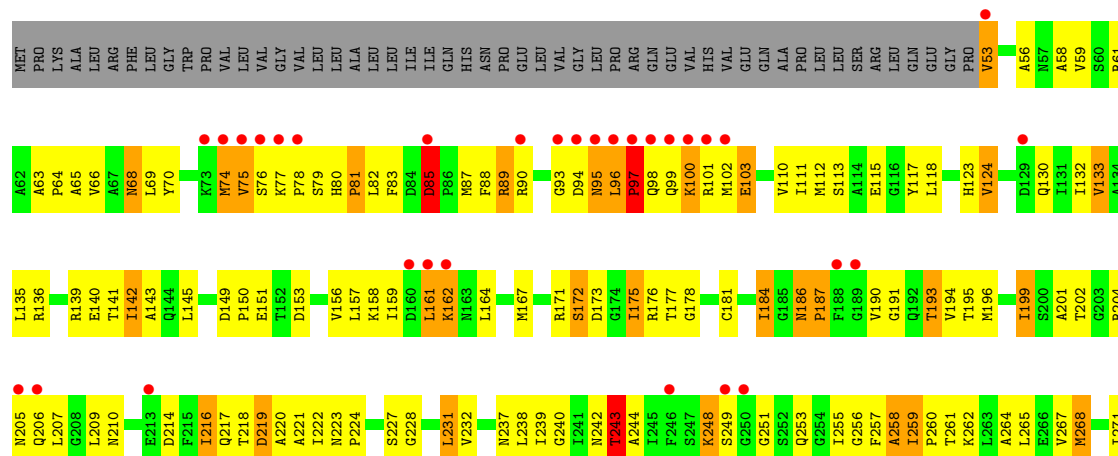


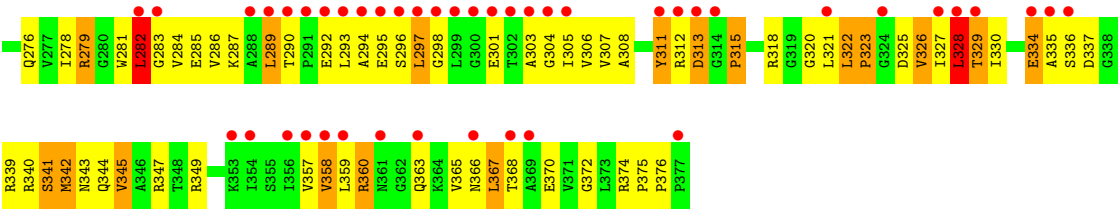


• Molecule 2: AlgW protein



• Molecule 2: AlgW protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.12Å 130.84Å 250.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.35 34.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	84.3 (34.50-2.35) 81.8 (34.50-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.268 , 0.289 0.268 , 0.286	Depositor DCC
R_{free} test set	1784 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å ²)	6.9	Xtriage
Anisotropy	2.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	15076	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: IMD

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	0.93	0/70	1.28	0/94
1	C	0.92	0/70	1.46	0/94
1	E	1.04	0/62	1.29	0/83
1	G	0.88	0/62	1.50	0/83
1	I	1.12	0/62	1.46	2/83 (2.4%)
1	K	0.85	0/88	1.74	0/118
2	B	1.60	32/2422 (1.3%)	1.56	15/3286 (0.5%)
2	D	1.59	34/2422 (1.4%)	1.60	18/3286 (0.5%)
2	F	1.59	31/2422 (1.3%)	1.58	23/3286 (0.7%)
2	H	1.65	44/2422 (1.8%)	1.55	14/3286 (0.4%)
2	J	1.60	37/2422 (1.5%)	1.56	26/3286 (0.8%)
2	L	1.63	43/2422 (1.8%)	1.58	29/3286 (0.9%)
All	All	1.60	221/14946 (1.5%)	1.57	127/20271 (0.6%)

All (221) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	197	GLY	C-O	-10.34	1.16	1.23
2	J	223	ASN	C-O	-9.62	1.16	1.24
2	B	372	GLY	C-O	-9.21	1.15	1.23
2	L	194	VAL	C-O	-9.07	1.13	1.24
2	H	63	ALA	C-O	-8.71	1.16	1.24
2	B	64	PRO	C-O	-8.65	1.13	1.24
2	J	64	PRO	C-O	-8.38	1.13	1.24
2	F	64	PRO	C-O	-8.01	1.14	1.24
2	L	184	ILE	C-O	-7.91	1.15	1.24
2	B	199	ILE	C-O	-7.81	1.14	1.23
2	L	251	GLY	C-O	-7.68	1.16	1.23
2	H	260	PRO	C-O	-7.46	1.15	1.23
2	D	150	PRO	C-O	-7.38	1.15	1.24
2	H	64	PRO	C-O	-7.36	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	281	TRP	C-O	-7.25	1.15	1.24
2	H	153	ASP	C-O	-7.22	1.14	1.23
2	D	194	VAL	C-O	-7.21	1.14	1.24
2	B	194	VAL	C-O	-7.20	1.16	1.24
2	H	187	PRO	C-O	-7.16	1.16	1.23
2	D	149	ASP	C-O	-7.15	1.18	1.24
2	F	155	ALA	C-O	-7.14	1.15	1.23
2	H	185	GLY	C-O	-6.98	1.17	1.23
2	L	376	PRO	C-O	-6.97	1.18	1.24
2	L	268	MET	C-O	-6.96	1.16	1.24
2	L	239	ILE	C-O	-6.92	1.17	1.24
2	H	258	ALA	C-O	-6.85	1.15	1.23
2	L	256	GLY	C-O	-6.83	1.15	1.23
2	H	199	ILE	C-O	-6.81	1.17	1.24
2	B	264	ALA	C-O	-6.81	1.16	1.24
2	J	260	PRO	C-O	-6.79	1.15	1.23
2	F	260	PRO	C-O	-6.76	1.15	1.23
2	F	224	PRO	C-O	-6.75	1.15	1.23
2	D	350	PRO	C-O	-6.70	1.15	1.23
2	H	315	PRO	C-O	-6.67	1.15	1.24
2	D	165	PRO	C-O	-6.64	1.16	1.23
2	J	183	ALA	C-O	-6.64	1.16	1.24
2	D	187	PRO	C-O	-6.62	1.17	1.23
2	F	58	ALA	C-O	-6.59	1.16	1.24
2	F	156	VAL	C-O	-6.57	1.16	1.24
2	D	201	ALA	C-O	-6.55	1.16	1.23
2	D	196	MET	C-O	-6.53	1.15	1.24
2	H	59	VAL	C-O	-6.53	1.16	1.24
2	B	350	PRO	C-O	-6.53	1.16	1.23
2	H	194	VAL	C-O	-6.51	1.17	1.24
2	D	199	ILE	C-O	-6.50	1.16	1.23
2	H	240	GLY	C-O	-6.49	1.17	1.23
2	F	110	VAL	C-O	-6.41	1.17	1.24
2	B	375	PRO	C-O	-6.40	1.17	1.24
2	D	267	VAL	C-O	-6.40	1.17	1.24
2	J	315	PRO	C-O	-6.39	1.16	1.24
2	H	328	LEU	C-O	-6.38	1.15	1.24
2	L	58	ALA	C-O	-6.34	1.16	1.24
2	J	261	THR	C-O	-6.28	1.16	1.24
2	D	315	PRO	C-O	-6.27	1.16	1.24
2	D	64	PRO	C-O	-6.27	1.16	1.24
2	J	288	ALA	C-O	-6.26	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	111	ILE	C-O	-6.22	1.17	1.24
2	J	350	PRO	C-O	-6.21	1.16	1.23
2	D	59	VAL	C-O	-6.21	1.17	1.24
2	H	165	PRO	C-O	-6.20	1.16	1.24
2	D	232	VAL	C-O	-6.20	1.15	1.24
2	L	224	PRO	C-O	-6.19	1.16	1.23
2	D	260	PRO	C-O	-6.18	1.16	1.23
2	J	267	VAL	C-O	-6.15	1.16	1.24
2	L	150	PRO	C-O	-6.13	1.17	1.24
2	F	376	PRO	C-O	-6.12	1.17	1.24
2	L	244	ALA	C-O	-6.07	1.16	1.23
2	H	376	PRO	C-O	-6.06	1.19	1.25
2	L	265	LEU	C-O	-6.05	1.17	1.24
2	L	231	LEU	C-O	-6.03	1.16	1.24
2	F	66	VAL	C-O	-6.03	1.17	1.24
2	B	274	HIS	CE1-NE2	-6.02	1.26	1.32
2	J	215	PHE	C-O	-6.02	1.16	1.24
2	F	187	PRO	C-O	-6.01	1.17	1.23
2	F	133	VAL	C-O	-5.96	1.17	1.24
2	L	124	VAL	C-O	-5.95	1.17	1.24
2	L	259	ILE	C-O	-5.95	1.16	1.24
2	L	323	PRO	C-O	-5.90	1.16	1.23
2	J	187	PRO	C-O	-5.88	1.17	1.23
2	L	271	ILE	C-O	-5.87	1.17	1.24
2	J	258	ALA	C-O	-5.87	1.16	1.23
2	J	194	VAL	C-O	-5.86	1.17	1.24
2	F	256	GLY	C-O	-5.86	1.16	1.23
2	J	325	ASP	C-O	-5.83	1.17	1.24
2	B	223	ASN	C-O	-5.82	1.18	1.24
2	H	333	GLN	C-O	-5.82	1.16	1.23
2	J	180	VAL	C-O	-5.82	1.16	1.24
2	H	106	LEU	C-O	-5.80	1.17	1.24
2	F	165	PRO	C-O	-5.79	1.17	1.23
2	J	244	ALA	C-O	-5.79	1.16	1.23
2	L	267	VAL	C-O	-5.78	1.17	1.24
2	H	119	LEU	C-O	-5.78	1.16	1.24
2	L	81	PRO	C-O	-5.77	1.17	1.24
2	B	341	SER	C-O	-5.76	1.17	1.24
2	D	240	GLY	C-O	-5.76	1.18	1.23
2	J	224	PRO	C-O	-5.74	1.16	1.23
2	D	216	ILE	C-O	-5.74	1.17	1.24
2	H	350	PRO	C-O	-5.74	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	187	PRO	C-O	-5.74	1.16	1.24
2	H	183	ALA	C-O	-5.73	1.17	1.24
2	L	59	VAL	C-O	-5.71	1.17	1.24
2	J	227	SER	C-O	-5.71	1.17	1.23
2	L	264	ALA	C-O	-5.70	1.17	1.24
2	F	199	ILE	C-O	-5.70	1.18	1.24
2	F	150	PRO	C-O	-5.70	1.17	1.24
2	J	150	PRO	C-O	-5.69	1.17	1.24
2	D	224	PRO	C-O	-5.68	1.15	1.23
2	H	310	VAL	C-O	-5.67	1.18	1.24
2	L	375	PRO	C-O	-5.66	1.18	1.24
2	B	261	THR	C-O	-5.66	1.17	1.24
2	J	375	PRO	C-O	-5.66	1.18	1.24
2	H	222	ILE	C-O	-5.65	1.18	1.24
2	L	149	ASP	C-O	-5.65	1.19	1.24
2	D	243	THR	C-O	-5.64	1.16	1.24
2	B	346	ALA	C-O	-5.62	1.17	1.24
2	D	238	LEU	C-O	-5.62	1.17	1.23
2	B	271	ILE	C-O	-5.62	1.17	1.24
2	B	150	PRO	C-O	-5.61	1.17	1.24
2	B	185	GLY	C-O	-5.60	1.18	1.23
2	L	258	ALA	C-O	-5.60	1.17	1.24
2	L	343	ASN	C-O	-5.59	1.17	1.24
2	H	117	TYR	C-O	-5.58	1.17	1.24
2	J	257	PHE	C-O	-5.58	1.17	1.23
2	H	56	ALA	C-O	-5.58	1.17	1.24
2	F	56	ALA	C-O	-5.58	1.17	1.24
2	F	271	ILE	C-O	-5.57	1.17	1.24
2	B	351	GLY	C-O	-5.57	1.17	1.24
2	L	191	GLY	C-O	-5.57	1.17	1.23
2	D	172	SER	C-O	-5.56	1.17	1.24
2	F	217	GLN	C-O	-5.56	1.17	1.24
2	L	201	ALA	C-O	-5.56	1.17	1.23
2	J	341	SER	C-O	-5.55	1.17	1.24
2	J	221	ALA	C-O	-5.54	1.17	1.24
2	H	156	VAL	C-O	-5.54	1.18	1.24
2	H	149	ASP	C-O	-5.54	1.17	1.24
2	L	261	THR	C-O	-5.54	1.17	1.24
2	F	117	TYR	C-O	-5.52	1.17	1.23
2	H	233	ASP	CG-OD1	-5.52	1.14	1.25
2	B	156	VAL	C-O	-5.51	1.18	1.24
2	D	343	ASN	C-O	-5.50	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	66	VAL	C-O	-5.50	1.17	1.24
2	H	221	ALA	C-O	-5.48	1.17	1.23
2	H	233	ASP	C-O	-5.47	1.17	1.23
2	J	240	GLY	C-O	-5.46	1.18	1.23
2	H	233	ASP	CG-OD2	-5.46	1.15	1.25
2	D	195	THR	C-O	-5.45	1.17	1.23
2	D	183	ALA	C-O	-5.45	1.17	1.24
2	F	63	ALA	C-O	-5.45	1.19	1.24
2	L	232	VAL	C-O	-5.44	1.17	1.23
2	L	240	GLY	C-O	-5.44	1.18	1.23
2	J	330	ILE	C-O	-5.43	1.18	1.24
2	B	118	LEU	C-O	-5.42	1.17	1.24
2	D	236	GLY	C-O	-5.42	1.17	1.24
2	H	237	ASN	C-O	-5.42	1.17	1.23
2	L	341	SER	CA-CB	-5.42	1.44	1.53
2	B	110	VAL	C-O	-5.41	1.18	1.24
2	B	241	ILE	C-O	-5.41	1.18	1.24
2	F	253	GLN	C-O	-5.41	1.16	1.24
2	F	309	GLY	C-O	-5.41	1.18	1.23
2	D	268	MET	C-O	-5.41	1.17	1.24
2	F	200	SER	C-O	-5.41	1.16	1.24
2	H	150	PRO	C-O	-5.41	1.17	1.24
2	L	315	PRO	C-O	-5.38	1.17	1.24
2	D	265	LEU	C-O	-5.38	1.17	1.24
2	B	140	GLU	C-O	-5.35	1.17	1.24
2	F	201	ALA	C-O	-5.35	1.18	1.23
2	D	168	THR	C-O	-5.34	1.17	1.23
2	D	57	ASN	C-O	-5.34	1.17	1.24
2	L	216	ILE	C-O	-5.33	1.18	1.24
2	J	165	PRO	C-O	-5.32	1.18	1.23
2	F	261	THR	C-O	-5.32	1.18	1.24
2	L	69	LEU	C-O	-5.30	1.17	1.23
2	J	291	PRO	C-O	-5.28	1.17	1.24
2	J	108	SER	C-O	-5.28	1.17	1.23
2	H	151	GLU	C-O	-5.28	1.18	1.24
2	B	260	PRO	C-O	-5.27	1.17	1.23
2	J	232	VAL	C-O	-5.26	1.17	1.23
2	J	255	ILE	C-O	-5.25	1.17	1.24
2	B	178	GLY	C-O	-5.24	1.16	1.24
2	B	165	PRO	C-O	-5.24	1.17	1.23
2	L	117	TYR	C-O	-5.24	1.17	1.24
2	L	311	TYR	C-O	-5.23	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	341	SER	C-O	-5.21	1.18	1.24
2	B	181	CYS	C-O	-5.19	1.17	1.23
2	J	219	ASP	CG-OD2	-5.19	1.15	1.25
2	J	241	ILE	C-O	-5.18	1.18	1.24
2	L	243	THR	C-O	-5.17	1.17	1.24
2	F	195	THR	C-O	-5.16	1.17	1.24
2	H	175	ILE	C-O	-5.15	1.17	1.24
2	J	372	GLY	C-O	-5.15	1.18	1.23
2	F	241	ILE	C-O	-5.14	1.18	1.24
2	D	239	ILE	C-O	-5.14	1.18	1.24
2	B	57	ASN	C-O	-5.14	1.18	1.24
2	D	345	VAL	C-O	-5.14	1.18	1.24
2	B	187	PRO	C-O	-5.14	1.17	1.24
2	B	242	ASN	C-O	-5.13	1.17	1.24
2	H	369	ALA	C-O	-5.12	1.17	1.23
2	H	123	HIS	C-O	-5.12	1.17	1.24
2	D	219	ASP	C-O	-5.11	1.17	1.24
2	L	133	VAL	C-O	-5.11	1.18	1.24
2	H	326	VAL	C-O	-5.11	1.18	1.24
2	H	124	VAL	C-O	-5.10	1.18	1.24
2	D	181	CYS	C-O	-5.10	1.17	1.23
2	J	308	ALA	C-O	-5.10	1.17	1.24
2	B	265	LEU	C-O	-5.10	1.18	1.24
2	H	271	ILE	C-O	-5.09	1.19	1.24
2	B	149	ASP	C-O	-5.09	1.18	1.24
2	F	268	MET	C-O	-5.08	1.18	1.24
2	J	310	VAL	C-O	-5.08	1.18	1.24
2	B	154	LEU	C-O	-5.08	1.17	1.23
2	F	218	THR	C-O	-5.07	1.17	1.23
2	H	306	VAL	C-O	-5.06	1.17	1.24
2	J	196	MET	C-O	-5.06	1.17	1.23
2	L	178	GLY	C-O	-5.06	1.16	1.24
2	L	56	ALA	C-O	-5.05	1.18	1.24
2	J	238	LEU	C-O	-5.03	1.17	1.23
2	H	110	VAL	C-O	-5.03	1.18	1.24
2	F	240	GLY	C-O	-5.02	1.18	1.23
2	H	157	LEU	C-O	-5.01	1.17	1.24
2	L	181	CYS	C-O	-5.01	1.17	1.23
2	B	259	ILE	C-O	-5.00	1.18	1.24

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	213	GLU	CA-C-N	-9.74	107.40	123.37
2	F	213	GLU	C-N-CA	-9.74	107.40	123.37
2	D	81	PRO	N-CA-C	9.02	126.06	113.53
2	L	376	PRO	CB-CA-C	-8.73	102.97	111.17
2	H	295	GLU	N-CA-C	-8.52	103.02	113.50
2	D	97	PRO	CB-CA-C	-8.02	105.13	111.87
2	J	128	ALA	CA-C-N	8.01	131.33	120.44
2	J	128	ALA	C-N-CA	8.01	131.33	120.44
2	F	290	THR	CB-CA-C	-7.63	97.67	109.11
2	L	313	ASP	CA-CB-CG	7.26	119.86	112.60
2	L	85	ASP	CA-CB-CG	7.19	119.79	112.60
2	B	294	ALA	CA-C-N	7.16	130.59	120.28
2	B	294	ALA	C-N-CA	7.16	130.59	120.28
2	D	218	THR	CA-C-N	6.96	130.88	120.31
2	D	218	THR	C-N-CA	6.96	130.88	120.31
2	H	325	ASP	CB-CA-C	6.95	121.16	109.48
2	B	55	TYR	N-CA-C	-6.95	103.14	112.94
2	L	97	PRO	N-CA-C	-6.93	98.19	112.47
2	J	85	ASP	CA-CB-CG	6.86	119.46	112.60
2	F	172	SER	CA-C-N	6.84	130.13	120.28
2	F	172	SER	C-N-CA	6.84	130.13	120.28
2	F	215	PHE	N-CA-C	6.49	120.09	110.48
2	F	212	TYR	CA-C-N	-6.46	113.64	123.07
2	F	212	TYR	C-N-CA	-6.46	113.64	123.07
2	H	334	GLU	N-CA-C	6.35	118.20	111.28
2	F	55	TYR	CA-C-N	6.31	128.73	120.28
2	F	55	TYR	C-N-CA	6.31	128.73	120.28
2	L	191	GLY	CA-C-O	-6.29	117.55	122.52
2	L	345	VAL	CA-C-N	6.27	128.69	120.28
2	L	345	VAL	C-N-CA	6.27	128.69	120.28
2	D	315	PRO	CB-CA-C	-6.24	101.79	112.64
2	J	179	ASP	CA-CB-CG	6.22	118.82	112.60
2	F	107	GLY	N-CA-C	6.21	118.24	110.29
2	J	97	PRO	N-CA-CB	-6.17	96.77	103.25
2	J	350	PRO	CB-CA-C	-6.16	103.51	111.46
2	B	282	LEU	N-CA-C	-6.10	106.81	114.56
2	J	189	GLY	CA-C-N	6.08	128.79	120.46
2	J	189	GLY	C-N-CA	6.08	128.79	120.46
2	L	171	ARG	CA-C-N	6.06	128.40	120.28
2	L	171	ARG	C-N-CA	6.06	128.40	120.28
1	I	8	TRP	CA-C-N	-6.03	115.05	123.13
1	I	8	TRP	C-N-CA	-6.03	115.05	123.13
2	F	98	GLN	CA-C-N	-6.01	114.63	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	98	GLN	C-N-CA	-6.01	114.63	123.05
2	J	264	ALA	CA-C-N	6.00	128.32	120.28
2	J	264	ALA	C-N-CA	6.00	128.32	120.28
2	F	94	ASP	CB-CA-C	5.93	121.55	109.76
2	H	368	THR	CA-CB-OG1	-5.91	100.74	109.60
2	J	334	GLU	CB-CA-C	5.91	119.12	110.26
2	L	279	ARG	CA-C-N	5.91	126.57	120.60
2	L	279	ARG	C-N-CA	5.91	126.57	120.60
2	B	375	PRO	N-CA-C	5.89	117.89	110.70
2	H	273	GLU	CB-CA-C	-5.85	101.66	110.90
2	L	219	ASP	CA-CB-CG	5.83	118.43	112.60
2	J	103	GLU	CB-CA-C	5.80	119.33	109.53
2	L	228	GLY	CA-C-N	5.72	129.13	121.01
2	L	228	GLY	C-N-CA	5.72	129.13	121.01
2	L	85	ASP	CB-CA-C	-5.70	100.36	109.08
2	F	191	GLY	CA-C-O	-5.69	118.02	122.52
2	D	211	THR	CA-CB-OG1	-5.65	101.12	109.60
2	D	237	ASN	CB-CA-C	5.64	119.04	109.84
2	F	90	ARG	CA-C-N	-5.64	112.86	122.56
2	F	90	ARG	C-N-CA	-5.64	112.86	122.56
2	J	191	GLY	CA-C-O	-5.61	117.56	122.16
2	B	233	ASP	CA-CB-CG	5.60	118.20	112.60
2	J	60	SER	CA-C-N	5.57	128.21	120.29
2	J	60	SER	C-N-CA	5.57	128.21	120.29
2	L	218	THR	CA-CB-OG1	-5.56	101.26	109.60
2	J	276	GLN	CA-C-N	-5.56	113.99	121.66
2	J	276	GLN	C-N-CA	-5.56	113.99	121.66
2	F	99	GLN	CB-CA-C	5.52	119.25	110.19
2	H	189	GLY	CA-C-N	5.51	128.24	120.42
2	H	189	GLY	C-N-CA	5.51	128.24	120.42
2	J	149	ASP	CA-C-N	5.50	125.02	119.19
2	J	149	ASP	C-N-CA	5.50	125.02	119.19
2	L	218	THR	CA-C-N	5.49	132.28	121.58
2	L	218	THR	C-N-CA	5.49	132.28	121.58
2	L	360	ARG	CB-CA-C	-5.48	101.21	110.19
2	B	191	GLY	CA-C-O	-5.46	118.39	122.37
2	F	299	LEU	N-CA-C	-5.43	100.06	108.90
2	D	295	GLU	N-CA-C	-5.42	106.50	113.01
2	L	282	LEU	N-CA-C	-5.42	107.68	114.56
2	D	248	LYS	N-CA-C	-5.41	106.74	113.55
2	L	328	LEU	N-CA-C	-5.37	107.27	113.88
2	J	313	ASP	CA-CB-CG	-5.34	107.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	68	ASN	CB-CA-C	5.34	119.28	109.46
2	F	298	GLY	O-C-N	5.33	126.41	122.62
2	B	85	ASP	CA-C-N	5.32	124.82	119.19
2	B	85	ASP	C-N-CA	5.32	124.82	119.19
2	J	195	THR	CB-CA-C	5.30	119.78	109.33
2	H	334	GLU	CA-C-O	-5.28	114.95	120.55
2	H	230	ALA	CA-C-N	-5.28	114.75	122.19
2	H	230	ALA	C-N-CA	-5.28	114.75	122.19
2	D	276	GLN	CB-CA-C	-5.28	101.45	110.95
2	D	333	GLN	CB-CA-C	5.26	118.99	109.37
2	J	344	GLN	CA-C-N	5.26	127.89	120.42
2	J	344	GLN	C-N-CA	5.26	127.89	120.42
2	F	237	ASN	CB-CA-C	5.25	118.49	109.51
2	L	214	ASP	CA-C-N	-5.25	114.23	122.73
2	L	214	ASP	C-N-CA	-5.25	114.23	122.73
2	D	346	ALA	CA-C-N	5.23	128.25	120.31
2	D	346	ALA	C-N-CA	5.23	128.25	120.31
2	D	282	LEU	N-CA-C	-5.22	106.87	114.12
2	B	294	ALA	O-C-N	5.21	128.75	122.35
2	F	266	GLU	CB-CG-CD	5.20	121.44	112.60
2	B	266	GLU	CB-CA-C	5.17	120.61	110.67
2	L	110	VAL	CA-C-N	-5.15	116.30	122.90
2	L	110	VAL	C-N-CA	-5.15	116.30	122.90
2	D	273	GLU	CA-C-N	-5.14	114.16	122.23
2	D	273	GLU	C-N-CA	-5.14	114.16	122.23
2	F	285	GLU	N-CA-CB	-5.14	102.53	110.65
2	J	55	TYR	N-CA-C	-5.13	105.71	112.94
2	B	361	ASN	CB-CA-C	5.12	119.33	111.39
2	B	255	ILE	CA-C-N	5.12	125.55	121.61
2	B	255	ILE	C-N-CA	5.12	125.55	121.61
2	H	206	GLN	CA-C-N	5.12	127.14	120.28
2	H	206	GLN	C-N-CA	5.12	127.14	120.28
2	H	97	PRO	CA-C-N	5.10	127.12	120.28
2	H	97	PRO	C-N-CA	5.10	127.12	120.28
2	D	73	LYS	CA-C-N	-5.10	114.39	121.99
2	D	73	LYS	C-N-CA	-5.10	114.39	121.99
2	L	95	ASN	CA-C-N	5.08	127.98	123.10
2	L	95	ASN	C-N-CA	5.08	127.98	123.10
2	L	248	LYS	N-CA-C	-5.06	105.95	112.68
2	J	231	LEU	N-CA-C	-5.03	100.98	109.07
2	J	318	ARG	CB-CA-C	5.01	119.36	110.85
2	B	303	ALA	CA-C-O	-5.01	115.93	122.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	68	0	61	6	0
1	C	68	0	61	10	0
1	E	60	0	57	7	0
1	G	60	0	57	11	0
1	I	60	0	57	0	0
1	K	86	0	83	33	0
2	B	2388	0	2435	222	2
2	D	2388	0	2434	248	0
2	F	2388	0	2434	286	0
2	H	2388	0	2435	204	1
2	J	2388	0	2435	210	1
2	L	2388	0	2435	250	0
3	B	5	0	5	1	0
3	D	5	0	5	3	0
3	F	5	0	5	3	0
3	H	5	0	5	8	0
3	J	5	0	5	1	0
3	L	5	0	5	4	0
4	B	51	0	0	43	0
4	D	51	0	0	32	0
4	F	43	0	0	42	0
4	G	2	0	0	0	0
4	H	51	0	0	26	0
4	I	2	0	0	0	0
4	J	44	0	0	23	0
4	K	1	0	0	2	0
4	L	71	0	0	58	0
All	All	15076	0	15014	1349	2

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 45.

All (1349) 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)
2:L:305:ILE:HD11	2:L:327:ILE:CB	1.29	1.60
2:L:305:ILE:CD1	2:L:327:ILE:HB	1.26	1.58
1:K:6:LEU:CD2	2:L:287:LYS:HB3	1.35	1.51
2:B:74:MET:CG	2:B:101:ARG:HE	1.28	1.46
2:J:180:VAL:HA	4:J:518:HOH:O	1.21	1.39
2:F:95:ASN:ND2	2:J:296:SER:O	1.57	1.38
2:J:77:LYS:HE2	2:J:100:LYS:CB	1.50	1.38
2:F:251:GLY:HA3	2:J:253:GLN:NE2	1.41	1.36
2:J:287:LYS:HE2	4:J:521:HOH:O	1.19	1.35
2:J:68:ASN:ND2	2:J:186:ASN:HB2	1.38	1.34
2:F:94:ASP:CG	2:F:96:LEU:HD21	1.52	1.34
2:H:301:GLU:HG3	2:H:336:SER:O	1.19	1.33
2:H:151:GLU:HG2	4:H:504:HOH:O	1.19	1.33
2:D:297:LEU:HD21	4:D:541:HOH:O	1.14	1.31
2:B:172:SER:HB3	4:B:521:HOH:O	1.29	1.29
2:F:154:LEU:HA	4:F:505:HOH:O	1.11	1.28
2:D:141:THR:HG23	4:D:537:HOH:O	1.11	1.27
2:F:94:ASP:OD2	2:F:96:LEU:HD21	1.35	1.27
2:F:142:ILE:HG22	4:F:516:HOH:O	1.28	1.26
2:J:70:TYR:HE1	2:J:132:ILE:CD1	1.49	1.26
2:H:219:ASP:HB3	4:H:503:HOH:O	1.13	1.26
2:B:93:GLY:HA3	4:B:526:HOH:O	1.31	1.25
2:J:117:TYR:CE1	2:J:158:LYS:HD3	1.71	1.25
2:F:284:VAL:HB	4:F:523:HOH:O	1.23	1.25
2:H:97:PRO:HG3	4:D:538:HOH:O	1.38	1.24
1:C:7:ARG:NH1	2:D:287:LYS:HE2	1.51	1.23
2:L:83:PHE:O	2:L:90:ARG:HD2	1.27	1.23
2:F:172:SER:HB2	4:F:520:HOH:O	1.11	1.23
2:F:83:PHE:HE1	4:L:541:HOH:O	1.22	1.23
2:L:99:GLN:HA	4:L:518:HOH:O	1.08	1.22
2:J:61:ARG:HG2	4:J:515:HOH:O	1.06	1.20
2:L:102:MET:CE	4:L:562:HOH:O	1.84	1.20
1:G:6:LEU:CD1	4:H:518:HOH:O	1.87	1.20
2:L:172:SER:HB2	4:L:521:HOH:O	1.05	1.20
1:K:6:LEU:CD2	2:L:287:LYS:CB	2.20	1.19
2:L:293:LEU:HD21	4:L:561:HOH:O	1.02	1.18
2:F:71:THR:HG22	2:F:106:LEU:CD2	1.72	1.18
2:D:299:LEU:HB2	2:D:302:THR:OG1	1.40	1.18
2:J:70:TYR:CE1	2:J:132:ILE:CD1	2.26	1.17
1:K:6:LEU:HD23	2:L:287:LYS:HB3	1.25	1.17
1:G:6:LEU:HD13	4:H:518:HOH:O	1.45	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:ASN:ND2	4:B:501:HOH:O	1.77	1.16
2:D:68:ASN:HB3	4:D:524:HOH:O	1.45	1.16
2:D:325:ASP:OD1	2:D:360:ARG:HD3	1.46	1.16
2:D:188:PHE:CE2	4:L:534:HOH:O	1.98	1.15
2:F:94:ASP:CG	2:F:96:LEU:CD2	2.19	1.15
2:J:70:TYR:CE1	2:J:132:ILE:HB	1.81	1.15
2:H:279:ARG:NH1	3:H:401:IMD:C5	2.10	1.15
1:K:6:LEU:HD23	2:L:287:LYS:CB	1.76	1.14
2:D:76:SER:HA	2:D:99:GLN:HB3	1.23	1.14
2:D:318:ARG:NH1	4:D:502:HOH:O	1.80	1.14
2:B:74:MET:HG3	2:B:101:ARG:NE	1.61	1.14
2:D:299:LEU:HD12	2:D:302:THR:HG21	1.28	1.14
2:D:103:GLU:OE2	1:K:3:ARG:HB2	1.48	1.13
2:H:301:GLU:CG	2:H:336:SER:O	1.94	1.13
2:J:77:LYS:CE	2:J:100:LYS:CG	2.27	1.13
2:H:94:ASP:HB2	2:H:96:LEU:HG	1.27	1.12
2:H:293:LEU:CB	4:H:501:HOH:O	1.96	1.12
2:F:95:ASN:HB2	2:J:296:SER:HB2	1.30	1.12
2:D:174:GLY:N	4:D:501:HOH:O	1.82	1.12
2:J:68:ASN:ND2	2:J:186:ASN:CB	2.12	1.12
2:J:77:LYS:HE2	2:J:100:LYS:CG	1.79	1.12
2:B:172:SER:CB	4:B:521:HOH:O	1.90	1.11
2:D:115:GLU:O	2:D:158:LYS:HE3	1.50	1.11
2:B:53:VAL:HB	4:B:543:HOH:O	1.49	1.10
2:J:77:LYS:CE	2:J:100:LYS:HG2	1.81	1.10
1:K:6:LEU:HD22	2:L:287:LYS:HB3	1.10	1.10
2:B:325:ASP:OD2	2:B:360:ARG:NH1	1.85	1.10
2:J:102:MET:HE3	2:J:102:MET:HA	1.24	1.10
2:H:293:LEU:O	2:H:295:GLU:OE1	1.68	1.09
2:J:77:LYS:CE	2:J:100:LYS:HB2	1.81	1.09
2:B:196:MET:HE1	2:J:196:MET:HE1	1.30	1.09
2:B:74:MET:CG	2:B:101:ARG:NE	2.13	1.09
2:L:329:THR:CG2	4:L:511:HOH:O	1.98	1.09
2:H:68:ASN:HB3	4:H:525:HOH:O	0.93	1.08
2:J:72:THR:HG22	2:J:130:GLN:OE1	1.53	1.08
2:B:74:MET:HG3	2:B:101:ARG:HE	0.92	1.08
2:D:294:ALA:HB2	4:D:504:HOH:O	1.51	1.08
2:J:353:LYS:HE3	2:J:370:GLU:HG3	1.32	1.08
2:B:246:PHE:HE1	4:B:541:HOH:O	1.32	1.08
2:F:325:ASP:HB3	2:F:358:VAL:HG11	1.36	1.08
2:J:77:LYS:HE3	2:J:100:LYS:HD3	1.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:MET:HE3	2:H:119:LEU:HB3	1.35	1.07
2:F:95:ASN:HB2	2:J:296:SER:CB	1.81	1.07
2:D:141:THR:CG2	4:D:537:HOH:O	1.73	1.07
2:B:312:ARG:HB3	4:D:531:HOH:O	1.55	1.07
2:H:279:ARG:NH1	3:H:401:IMD:N1	2.03	1.07
2:D:205:ASN:HB3	4:D:528:HOH:O	1.55	1.07
2:L:75:VAL:HG23	2:L:100:LYS:O	1.53	1.07
2:L:102:MET:HE3	4:L:562:HOH:O	1.45	1.07
2:D:368:THR:CG2	4:D:533:HOH:O	2.03	1.07
2:F:295:GLU:OE2	2:F:296:SER:N	1.87	1.07
2:D:297:LEU:CD2	4:D:541:HOH:O	1.76	1.06
2:H:139:ARG:NH2	2:H:162:LYS:O	1.89	1.06
2:D:102:MET:HE2	4:K:101:HOH:O	1.54	1.06
2:L:85:ASP:HB2	2:L:90:ARG:HH12	1.15	1.06
2:D:85:ASP:OD1	2:D:86:PRO:CD	2.04	1.05
2:J:80:HIS:CD2	2:J:81:PRO:HD2	1.90	1.05
2:B:205:ASN:ND2	2:B:213:GLU:O	1.89	1.05
2:D:100:LYS:HE3	1:K:4:ASP:OD2	1.54	1.05
2:J:77:LYS:HE2	2:J:100:LYS:HB2	1.05	1.05
2:F:95:ASN:HB3	2:J:296:SER:HA	1.38	1.04
2:H:83:PHE:O	2:H:90:ARG:HD2	1.57	1.04
2:D:115:GLU:O	2:D:158:LYS:CE	2.05	1.04
2:D:299:LEU:CD1	2:D:302:THR:HG21	1.88	1.04
2:D:100:LYS:CE	1:K:4:ASP:OD2	2.05	1.03
2:D:74:MET:HE2	2:D:74:MET:HA	1.39	1.03
2:D:171:ARG:O	4:D:501:HOH:O	1.76	1.02
2:J:96:LEU:H	2:J:97:PRO:HD3	1.14	1.02
2:L:93:GLY:CA	4:L:516:HOH:O	2.05	1.02
2:D:294:ALA:CB	4:D:504:HOH:O	2.02	1.02
2:F:83:PHE:CE1	4:L:541:HOH:O	2.00	1.02
2:B:212:TYR:CD2	2:B:279:ARG:NH1	2.28	1.02
2:J:70:TYR:CE1	2:J:132:ILE:HD13	1.94	1.02
2:D:368:THR:HG22	4:D:533:HOH:O	1.56	1.02
2:F:150:PRO:HD2	4:F:517:HOH:O	0.85	1.02
2:F:303:ALA:HB1	2:F:328:LEU:HA	1.35	1.02
2:L:307:VAL:HG11	4:L:548:HOH:O	1.57	1.01
2:D:65:ALA:HB3	2:D:167:MET:HE2	1.42	1.01
1:K:10:PHE:O	2:L:282:LEU:N	1.92	1.01
2:H:163:ASN:HB2	4:H:507:HOH:O	1.58	1.01
2:D:70:TYR:CE1	2:D:103:GLU:HB3	1.95	1.01
2:L:303:ALA:HB2	2:L:328:LEU:HD23	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:GLU:HG3	4:D:513:HOH:O	1.59	1.01
2:L:85:ASP:HB2	2:L:90:ARG:NH1	1.76	1.01
2:L:195:THR:HB	4:L:515:HOH:O	0.83	1.00
2:F:322:LEU:HD23	2:F:360:ARG:HH12	1.24	1.00
2:H:94:ASP:HB2	2:H:96:LEU:CG	1.90	1.00
2:J:70:TYR:CE1	2:J:132:ILE:HD12	1.96	1.00
2:B:339:ARG:HD3	4:B:517:HOH:O	1.61	0.99
2:D:325:ASP:CG	2:D:360:ARG:HD3	1.87	0.99
2:H:70:TYR:CZ	2:H:132:ILE:HG21	1.98	0.99
2:L:53:VAL:HG22	4:L:546:HOH:O	1.61	0.99
2:L:70:TYR:CE2	2:L:132:ILE:HD12	1.97	0.99
2:F:75:VAL:HG22	2:F:100:LYS:O	1.63	0.99
2:L:366:ASN:HB3	4:L:530:HOH:O	0.80	0.98
2:F:251:GLY:HA3	2:J:253:GLN:HE21	1.23	0.98
2:L:329:THR:HG23	4:L:511:HOH:O	1.60	0.98
2:B:74:MET:HG2	2:B:101:ARG:HE	1.27	0.98
2:L:77:LYS:HG3	2:L:78:PRO:HD2	1.47	0.97
2:J:77:LYS:CE	2:J:100:LYS:CB	2.37	0.97
2:L:74:MET:HA	2:L:74:MET:CE	1.94	0.97
2:D:89:ARG:HH11	2:D:89:ARG:HG2	1.27	0.97
2:F:95:ASN:CB	2:J:296:SER:HA	1.93	0.97
2:H:94:ASP:CG	2:H:96:LEU:CD2	2.38	0.97
2:D:96:LEU:N	2:D:97:PRO:HD2	1.80	0.96
2:J:102:MET:HA	2:J:102:MET:CE	1.94	0.96
2:J:117:TYR:CD1	2:J:158:LYS:HD3	2.00	0.96
2:H:188:PHE:HE1	2:D:248:LYS:HE2	1.27	0.96
2:L:74:MET:HA	2:L:74:MET:HE2	1.47	0.96
2:D:115:GLU:O	2:D:158:LYS:NZ	1.99	0.96
2:J:226:ASN:OD1	4:J:501:HOH:O	1.84	0.95
2:D:85:ASP:OD1	2:D:86:PRO:HD2	1.66	0.95
2:D:188:PHE:CD2	4:L:534:HOH:O	2.15	0.95
2:D:96:LEU:H	2:D:97:PRO:HD2	1.31	0.95
2:F:74:MET:HE3	2:F:74:MET:HA	1.48	0.94
2:F:360:ARG:HH11	2:F:360:ARG:HG3	1.31	0.94
2:H:299:LEU:H	2:H:302:THR:HG21	1.29	0.94
2:F:169:LEU:HD13	2:F:265:LEU:HD11	1.48	0.94
2:J:77:LYS:HE3	2:J:100:LYS:CD	1.97	0.94
1:C:7:ARG:HH12	2:D:287:LYS:HE2	1.25	0.93
2:B:259:ILE:O	4:B:502:HOH:O	1.86	0.93
2:D:303:ALA:HB1	2:D:328:LEU:HD23	1.50	0.93
2:L:322:LEU:HG	2:L:360:ARG:HH21	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:TYR:HE1	2:D:103:GLU:HB3	1.29	0.93
2:B:96:LEU:N	2:B:97:PRO:HD2	1.83	0.92
2:F:71:THR:HG22	2:F:106:LEU:HD21	1.48	0.92
2:L:83:PHE:O	2:L:90:ARG:CD	2.18	0.92
2:J:80:HIS:CG	2:J:81:PRO:HD2	2.04	0.92
2:J:68:ASN:HD21	2:J:186:ASN:HB2	0.94	0.92
2:H:188:PHE:CE1	2:D:248:LYS:HE2	2.05	0.92
2:J:141:THR:HG22	4:J:505:HOH:O	1.69	0.92
2:B:200:SER:O	4:B:503:HOH:O	1.88	0.92
2:F:194:VAL:O	2:J:200:SER:OG	1.86	0.92
2:B:212:TYR:CE2	2:B:279:ARG:NH1	2.36	0.91
2:H:70:TYR:CE1	2:H:132:ILE:HG21	2.05	0.91
2:F:71:THR:HG22	2:F:106:LEU:HD22	1.50	0.91
2:F:295:GLU:HB3	4:F:526:HOH:O	1.70	0.91
2:H:198:ILE:HG12	4:H:503:HOH:O	1.70	0.91
2:H:293:LEU:N	4:H:501:HOH:O	2.00	0.91
2:L:205:ASN:HD22	2:L:339:ARG:CD	1.83	0.91
2:D:218:THR:O	4:D:503:HOH:O	1.86	0.91
2:H:279:ARG:HH11	3:H:401:IMD:C5	1.80	0.91
2:J:68:ASN:HD22	2:J:186:ASN:CB	1.84	0.90
2:D:250:GLY:O	2:L:248:LYS:CD	2.19	0.90
2:H:279:ARG:HH12	3:H:401:IMD:HN1	0.94	0.90
1:C:7:ARG:NH1	2:D:287:LYS:CE	2.35	0.90
2:D:250:GLY:O	2:L:248:LYS:HD2	1.71	0.90
2:F:71:THR:CG2	2:F:106:LEU:CD2	2.50	0.90
1:K:7:ARG:HG3	1:K:7:ARG:HH11	1.33	0.90
2:F:295:GLU:HA	4:F:526:HOH:O	1.71	0.90
2:L:344:GLN:NE2	4:L:502:HOH:O	2.02	0.90
2:L:96:LEU:HD11	4:L:559:HOH:O	1.69	0.90
2:L:75:VAL:CG2	2:L:100:LYS:O	2.18	0.89
2:D:195:THR:HG21	2:D:221:ALA:N	1.86	0.89
2:J:70:TYR:CE1	2:J:132:ILE:CB	2.55	0.89
2:L:77:LYS:CG	2:L:78:PRO:HD2	2.03	0.89
2:D:212:TYR:OH	2:D:279:ARG:HD3	1.73	0.88
2:F:65:ALA:HB3	2:F:167:MET:HE2	1.55	0.88
2:B:74:MET:SD	2:B:74:MET:N	2.46	0.88
2:L:53:VAL:HG12	4:L:538:HOH:O	1.72	0.88
2:J:77:LYS:HE3	2:J:100:LYS:CG	2.04	0.88
2:B:315:PRO:HA	2:B:318:ARG:HH12	1.39	0.88
2:D:85:ASP:OD1	2:D:86:PRO:HD3	1.70	0.88
2:B:96:LEU:H	2:B:97:PRO:CD	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:TYR:HE1	2:D:103:GLU:CB	1.86	0.88
2:L:307:VAL:HG21	4:L:548:HOH:O	1.74	0.87
2:D:299:LEU:HB2	2:D:302:THR:CB	2.03	0.87
2:J:245:ILE:HG22	2:J:256:GLY:HA2	1.55	0.87
2:B:81:PRO:O	2:B:90:ARG:HD3	1.75	0.87
2:F:250:GLY:HA2	4:F:531:HOH:O	1.73	0.87
2:J:70:TYR:HE1	2:J:132:ILE:HD13	1.28	0.87
2:L:289:LEU:HD23	2:L:306:VAL:CG2	2.05	0.87
2:J:278:ILE:HG23	2:J:373:LEU:HD11	1.56	0.87
2:F:279:ARG:NH1	3:F:401:IMD:C4	2.38	0.87
2:H:279:ARG:NH1	3:H:401:IMD:H5	1.87	0.86
2:D:161:LEU:HB2	2:D:164:LEU:HD13	1.57	0.86
2:D:325:ASP:OD1	2:D:360:ARG:CD	2.23	0.86
2:B:53:VAL:CB	4:B:543:HOH:O	2.11	0.86
2:L:85:ASP:CB	2:L:90:ARG:HH12	1.87	0.86
2:D:80:HIS:CD2	2:D:81:PRO:HD2	2.09	0.86
2:F:195:THR:HG21	2:F:221:ALA:N	1.90	0.86
2:H:94:ASP:CG	2:H:96:LEU:HD21	1.98	0.86
2:B:350:PRO:HB3	4:B:514:HOH:O	1.73	0.86
2:D:195:THR:HG22	2:D:220:ALA:HB1	1.56	0.86
2:J:96:LEU:N	2:J:97:PRO:HD3	1.89	0.86
2:F:210:ASN:N	2:F:213:GLU:OE1	2.07	0.86
2:B:193:THR:HG22	2:F:204:ARG:HH21	1.40	0.85
2:D:65:ALA:CB	2:D:167:MET:HE2	2.05	0.85
2:J:72:THR:CG2	2:J:130:GLN:OE1	2.24	0.85
2:D:106:LEU:H	2:D:106:LEU:HD22	1.40	0.85
2:H:218:THR:HG22	2:H:220:ALA:H	1.40	0.85
2:H:295:GLU:HG2	4:H:527:HOH:O	1.76	0.85
2:F:95:ASN:HB2	2:J:296:SER:CA	2.07	0.85
2:L:79:SER:HB2	4:L:523:HOH:O	1.76	0.85
2:B:86:PRO:HA	2:D:312:ARG:HH12	1.38	0.85
2:F:96:LEU:HD23	2:F:96:LEU:H	1.39	0.85
2:B:246:PHE:CE1	4:B:541:HOH:O	2.15	0.85
1:C:7:ARG:HH12	2:D:287:LYS:CE	1.90	0.84
2:L:93:GLY:HA3	4:L:516:HOH:O	1.66	0.84
2:F:74:MET:HA	2:F:74:MET:CE	2.04	0.84
2:H:249:SER:HB3	2:L:249:SER:HB2	1.58	0.83
2:H:94:ASP:CG	2:H:96:LEU:HD23	2.03	0.83
2:B:53:VAL:CG2	4:B:543:HOH:O	2.27	0.83
2:F:267:VAL:HG13	2:F:277:VAL:HG21	1.60	0.83
2:F:352:GLN:NE2	4:F:501:HOH:O	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:LYS:HE3	2:F:162:LYS:HA	1.61	0.83
1:C:8:TRP:HB2	2:D:286:VAL:HG23	1.59	0.83
2:F:162:LYS:HA	2:F:162:LYS:CE	2.09	0.83
2:L:328:LEU:HD12	2:L:357:VAL:HG12	1.59	0.83
2:L:321:LEU:HG	4:L:548:HOH:O	1.77	0.82
2:H:211:THR:HG22	2:H:212:TYR:CD2	2.13	0.82
2:F:325:ASP:HB3	2:F:358:VAL:CG1	2.09	0.82
2:J:85:ASP:O	2:L:312:ARG:NH2	2.11	0.82
2:B:108:SER:O	2:B:228:GLY:C	2.23	0.82
2:H:94:ASP:HB2	2:H:96:LEU:CD2	2.10	0.82
2:D:70:TYR:CE1	2:D:103:GLU:CB	2.61	0.82
2:D:76:SER:CA	2:D:99:GLN:HB3	2.07	0.82
2:F:71:THR:CG2	2:F:106:LEU:HD21	2.08	0.82
2:H:91:PHE:HZ	2:F:324:GLY:CA	1.92	0.82
2:F:322:LEU:HD23	2:F:360:ARG:NH1	1.95	0.82
2:L:318:ARG:NH2	4:L:501:HOH:O	1.90	0.82
2:H:72:THR:O	2:H:73:LYS:HE2	1.78	0.82
2:J:139:ARG:NH2	2:J:162:LYS:O	2.12	0.82
2:L:89:ARG:HG2	2:L:89:ARG:HH11	1.44	0.82
2:J:142:ILE:HG12	4:J:504:HOH:O	1.79	0.81
2:F:251:GLY:HA3	2:J:253:GLN:HE22	1.44	0.81
2:J:70:TYR:CD1	2:J:132:ILE:HB	2.15	0.81
2:L:325:ASP:OD1	2:L:360:ARG:HG3	1.81	0.81
2:B:96:LEU:H	2:B:97:PRO:HD2	1.38	0.81
2:H:299:LEU:H	2:H:302:THR:CG2	1.93	0.81
2:B:315:PRO:CA	2:B:318:ARG:HH12	1.94	0.80
2:H:94:ASP:OD2	2:H:96:LEU:HD23	1.82	0.80
2:F:319:GLY:O	4:F:502:HOH:O	2.00	0.80
2:J:330:ILE:HB	4:J:517:HOH:O	1.80	0.80
2:D:70:TYR:HB3	2:D:132:ILE:HB	1.63	0.80
2:L:176:ARG:HD3	4:L:535:HOH:O	1.82	0.80
2:L:205:ASN:ND2	2:L:339:ARG:NE	2.29	0.80
2:D:96:LEU:H	2:D:97:PRO:CD	1.94	0.79
2:J:70:TYR:HE1	2:J:132:ILE:CB	1.94	0.79
2:F:95:ASN:CB	2:J:296:SER:CA	2.59	0.79
2:J:65:ALA:HB3	2:J:167:MET:HE2	1.62	0.79
2:L:279:ARG:HE	3:L:401:IMD:H4	1.45	0.79
2:F:295:GLU:CB	4:F:526:HOH:O	2.27	0.79
2:J:212:TYR:CE2	2:J:279:ARG:NH1	2.51	0.79
2:D:299:LEU:HB2	2:D:302:THR:CG2	2.12	0.79
2:L:205:ASN:HD22	2:L:339:ARG:NE	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:313:ASP:OD1	2:F:318:ARG:NH1	2.17	0.78
2:B:315:PRO:HA	2:B:318:ARG:NH1	1.97	0.78
2:F:85:ASP:HB2	2:F:90:ARG:HH12	1.47	0.78
2:J:180:VAL:HG22	4:J:518:HOH:O	1.83	0.78
2:D:193:THR:HG22	2:L:204:ARG:HH21	1.48	0.78
2:B:289:LEU:O	2:B:289:LEU:HD12	1.83	0.78
2:L:177:THR:HA	2:L:199:ILE:HG22	1.63	0.78
2:F:71:THR:CG2	2:F:106:LEU:HD22	2.14	0.78
2:D:186:ASN:O	2:D:225:GLY:O	2.02	0.77
2:B:96:LEU:N	2:B:97:PRO:CD	2.43	0.77
2:H:87:MET:SD	2:F:311:TYR:CE1	2.78	0.77
2:J:70:TYR:HE1	2:J:132:ILE:CG1	1.98	0.77
3:B:401:IMD:H2	4:B:531:HOH:O	1.84	0.77
2:D:143:ALA:HB2	2:D:159:ILE:CD1	2.14	0.76
2:H:219:ASP:CB	4:H:503:HOH:O	1.92	0.76
2:D:195:THR:HG21	2:D:221:ALA:H	1.46	0.76
2:H:94:ASP:CB	2:H:96:LEU:CD2	2.64	0.76
2:L:70:TYR:CE2	2:L:103:GLU:OE1	2.39	0.76
2:B:325:ASP:CG	2:B:360:ARG:HH11	1.94	0.76
1:K:6:LEU:HD21	2:L:287:LYS:HZ3	1.51	0.75
2:F:77:LYS:HE3	2:F:96:LEU:CD1	2.16	0.75
2:F:139:ARG:NH2	2:F:162:LYS:O	2.19	0.75
2:L:70:TYR:CE2	2:L:132:ILE:CD1	2.70	0.75
2:L:328:LEU:HD12	2:L:357:VAL:CG1	2.16	0.75
2:D:186:ASN:O	2:D:186:ASN:ND2	2.20	0.75
2:F:74:MET:HE1	2:F:101:ARG:CA	2.17	0.75
2:F:123:HIS:ND1	2:F:153:ASP:OD2	2.16	0.75
2:B:196:MET:HE1	2:J:196:MET:CE	2.15	0.74
2:H:87:MET:SD	2:F:311:TYR:OH	2.43	0.74
2:H:299:LEU:C	2:H:302:THR:HG22	2.12	0.74
2:H:68:ASN:OD1	2:H:186:ASN:HB2	1.87	0.74
2:B:80:HIS:CD2	2:B:81:PRO:HD2	2.22	0.74
2:D:75:VAL:HG21	2:D:102:MET:HE3	1.69	0.74
2:L:77:LYS:CD	2:L:78:PRO:HD2	2.17	0.74
2:L:330:ILE:HB	4:L:502:HOH:O	1.86	0.74
2:B:139:ARG:NH2	2:B:162:LYS:O	2.20	0.74
2:D:303:ALA:CB	2:D:328:LEU:HD23	2.18	0.74
2:B:89:ARG:HG2	2:B:89:ARG:HH11	1.51	0.74
2:L:175:ILE:HD13	2:L:199:ILE:HG12	1.69	0.74
2:L:243:THR:HG21	2:L:259:ILE:CD1	2.18	0.74
2:F:135:LEU:N	2:F:135:LEU:HD23	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:PHE:HE2	2:D:286:VAL:HG21	1.52	0.73
2:H:85:ASP:HB2	2:H:86:PRO:CD	2.17	0.73
2:D:76:SER:HA	2:D:99:GLN:CB	2.11	0.73
2:J:71:THR:OG1	2:J:129:ASP:OD1	2.06	0.73
2:F:77:LYS:NZ	2:F:100:LYS:HG2	2.03	0.73
2:B:54:SER:OG	2:F:179:ASP:OD1	2.05	0.73
2:B:108:SER:O	2:B:228:GLY:O	2.07	0.73
2:F:96:LEU:CD2	2:F:96:LEU:H	2.00	0.73
2:F:301:GLU:O	2:F:336:SER:HB2	1.89	0.73
2:L:322:LEU:CG	2:L:360:ARG:HH21	2.02	0.73
2:B:312:ARG:HD3	2:D:87:MET:HA	1.70	0.73
2:D:116:GLY:HA3	2:D:159:ILE:O	1.89	0.73
2:J:69:LEU:HD11	2:J:109:ALA:HB2	1.69	0.73
2:H:293:LEU:HB2	4:H:501:HOH:O	1.71	0.72
2:B:177:THR:HA	2:B:199:ILE:HG22	1.71	0.72
2:D:74:MET:HA	2:D:74:MET:CE	2.18	0.72
2:F:68:ASN:HB3	4:F:514:HOH:O	1.87	0.72
2:L:305:ILE:HD12	2:L:305:ILE:O	1.89	0.72
2:D:282:LEU:O	2:D:316:ALA:HB2	1.90	0.72
2:D:305:ILE:HD13	2:D:335:ALA:HB1	1.71	0.72
2:F:289:LEU:HD21	2:F:294:ALA:HB2	1.71	0.72
2:J:316:ALA:HB1	2:J:321:LEU:HB2	1.72	0.72
1:K:6:LEU:HD23	2:L:287:LYS:HD3	1.71	0.72
2:B:361:ASN:N	2:B:361:ASN:HD22	1.88	0.72
2:F:284:VAL:HG13	2:F:316:ALA:CB	2.19	0.72
2:B:134:ALA:HB2	2:B:140:GLU:HG2	1.71	0.72
2:D:121:ASN:HB2	2:D:124:VAL:HG23	1.71	0.72
2:F:74:MET:HE1	2:F:100:LYS:C	2.14	0.72
2:F:261:THR:HG22	2:F:265:LEU:HD12	1.72	0.72
2:H:87:MET:SD	2:F:311:TYR:CZ	2.83	0.72
2:B:74:MET:HG2	2:B:101:ARG:HH11	1.54	0.72
2:B:121:ASN:ND2	2:B:153:ASP:O	2.23	0.72
2:J:250:GLY:HA2	4:J:519:HOH:O	1.90	0.72
2:H:74:MET:HA	2:H:101:ARG:HA	1.72	0.71
2:H:153:ASP:OD2	4:H:502:HOH:O	2.06	0.71
2:F:77:LYS:HE3	2:F:96:LEU:HD12	1.72	0.71
2:J:98:GLN:NE2	2:J:98:GLN:HA	2.03	0.71
1:K:6:LEU:HD13	1:K:6:LEU:O	1.90	0.71
2:L:325:ASP:OD1	2:L:360:ARG:CG	2.37	0.71
2:F:74:MET:HE1	2:F:101:ARG:N	2.04	0.71
2:L:175:ILE:HD11	2:L:202:THR:HG22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:226:ASN:OD1	4:F:503:HOH:O	2.08	0.71
2:J:96:LEU:N	2:J:97:PRO:CD	2.52	0.71
2:B:350:PRO:CB	4:B:514:HOH:O	2.36	0.71
2:H:299:LEU:N	2:H:302:THR:HG21	2.01	0.71
4:F:511:HOH:O	2:L:82:LEU:CD1	2.38	0.71
2:D:294:ALA:N	4:D:504:HOH:O	2.23	0.71
2:F:71:THR:CB	2:F:106:LEU:HD21	2.21	0.71
2:J:94:ASP:OD1	2:J:94:ASP:N	2.23	0.71
2:D:65:ALA:HB3	2:D:167:MET:CE	2.19	0.71
1:E:8:TRP:HH2	2:F:206:GLN:HG2	1.54	0.71
2:B:72:THR:OG1	2:B:130:GLN:NE2	2.24	0.71
2:B:68:ASN:OD1	2:B:108:SER:OG	2.08	0.71
2:F:286:VAL:HG12	4:F:523:HOH:O	1.90	0.70
2:H:94:ASP:CB	2:H:96:LEU:HD23	2.21	0.70
2:B:231:LEU:HB2	2:B:242:ASN:HD21	1.56	0.70
2:F:74:MET:HE3	2:F:74:MET:CA	2.20	0.70
2:H:70:TYR:CE1	2:H:132:ILE:CG2	2.74	0.70
2:F:77:LYS:HD2	2:F:100:LYS:HG3	1.72	0.70
2:F:301:GLU:O	2:F:336:SER:CB	2.39	0.70
2:D:75:VAL:HG21	2:D:102:MET:SD	2.31	0.70
2:F:94:ASP:CG	2:F:96:LEU:HD23	2.12	0.70
4:B:503:HOH:O	2:J:192:GLN:O	2.09	0.70
2:D:195:THR:CG2	2:D:221:ALA:H	2.05	0.70
2:F:77:LYS:CE	2:F:96:LEU:HD12	2.22	0.70
2:J:325:ASP:OD2	2:J:360:ARG:NH2	2.23	0.70
2:H:279:ARG:NH1	3:H:401:IMD:HN1	1.73	0.70
2:H:70:TYR:HE1	2:H:132:ILE:HD13	1.57	0.70
2:D:75:VAL:HG21	2:D:102:MET:CE	2.21	0.69
2:D:282:LEU:O	2:D:316:ALA:CB	2.40	0.69
2:F:331:ASP:CG	2:F:354:ILE:HG21	2.17	0.69
2:J:96:LEU:H	2:J:97:PRO:CD	1.96	0.69
2:L:96:LEU:CD1	4:L:559:HOH:O	2.31	0.69
2:L:289:LEU:HD23	2:L:306:VAL:HG23	1.74	0.69
2:L:293:LEU:HD12	2:L:295:GLU:OE2	1.92	0.69
2:B:301:GLU:OE2	2:B:302:THR:N	2.25	0.69
2:B:313:ASP:O	2:B:318:ARG:NH2	2.25	0.69
1:G:6:LEU:HD12	1:G:6:LEU:O	1.93	0.69
2:H:81:PRO:O	2:H:90:ARG:HD3	1.92	0.69
2:D:103:GLU:OE2	1:K:3:ARG:CB	2.35	0.69
2:F:301:GLU:N	2:F:301:GLU:OE2	2.24	0.69
2:J:112:MET:CE	2:J:119:LEU:HB2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:212:TYR:CZ	2:D:279:ARG:HD3	2.27	0.69
2:F:132:ILE:HG21	4:F:541:HOH:O	1.92	0.69
2:L:243:THR:HG21	2:L:259:ILE:HG13	1.75	0.69
2:B:200:SER:HB3	2:J:193:THR:HG23	1.73	0.69
2:D:175:ILE:HD11	2:D:216:ILE:HD12	1.74	0.69
2:D:299:LEU:CB	2:D:302:THR:CG2	2.70	0.69
1:K:7:ARG:HG3	1:K:7:ARG:NH1	1.95	0.69
2:D:290:THR:O	4:D:504:HOH:O	2.10	0.69
2:F:94:ASP:CB	2:F:96:LEU:HD21	2.23	0.69
2:J:184:ILE:HG12	2:J:194:VAL:HG13	1.73	0.69
2:B:112:MET:HE3	2:B:119:LEU:HB2	1.75	0.68
2:D:83:PHE:HA	2:D:92:PHE:O	1.93	0.68
2:H:299:LEU:O	2:H:302:THR:HG22	1.93	0.68
2:B:259:ILE:HB	4:B:502:HOH:O	1.92	0.68
2:D:140:GLU:HB2	4:D:517:HOH:O	1.92	0.68
2:F:94:ASP:CB	2:F:96:LEU:CD2	2.71	0.68
2:J:95:ASN:HB2	2:J:96:LEU:HD22	1.73	0.68
2:L:289:LEU:CD2	2:L:306:VAL:CG2	2.71	0.68
2:H:70:TYR:HD2	4:H:545:HOH:O	1.75	0.68
4:F:542:HOH:O	2:J:246:PHE:HD2	1.76	0.68
2:H:214:ASP:O	2:H:260:PRO:CD	2.41	0.68
2:H:296:SER:HB3	4:H:527:HOH:O	1.93	0.68
2:F:173:ASP:O	4:F:504:HOH:O	2.11	0.68
2:J:112:MET:HE1	2:J:119:LEU:HB2	1.75	0.68
2:H:85:ASP:HB2	2:H:86:PRO:HD3	1.76	0.68
2:H:295:GLU:CG	4:H:527:HOH:O	2.37	0.68
2:F:212:TYR:CE2	2:F:279:ARG:NH1	2.62	0.68
2:J:198:ILE:HG22	4:J:518:HOH:O	1.94	0.68
2:H:293:LEU:HB3	4:H:501:HOH:O	1.73	0.68
2:F:325:ASP:CB	2:F:358:VAL:HG11	2.18	0.68
2:J:77:LYS:NZ	2:J:100:LYS:HG2	2.09	0.68
2:L:217:GLN:HG3	2:L:257:PHE:CE1	2.29	0.68
2:B:74:MET:HG3	2:B:101:ARG:CD	2.24	0.67
2:B:289:LEU:N	4:B:509:HOH:O	2.26	0.67
2:J:63:ALA:N	2:J:64:PRO:HD2	2.09	0.67
2:L:136:ARG:NH1	4:L:505:HOH:O	2.26	0.67
2:F:96:LEU:HD23	2:F:96:LEU:N	2.10	0.67
2:L:205:ASN:ND2	2:L:339:ARG:CD	2.57	0.67
2:F:132:ILE:CG2	4:F:541:HOH:O	2.43	0.67
2:F:169:LEU:CD1	2:F:265:LEU:HD11	2.24	0.67
2:B:112:MET:CA	2:B:112:MET:HE2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:360:ARG:HE	2:F:365:VAL:HG21	1.59	0.67
2:J:222:ILE:O	2:J:252:SER:HB2	1.94	0.67
1:K:6:LEU:CD2	2:L:287:LYS:HD3	2.25	0.67
2:L:292:GLU:O	2:L:295:GLU:OE1	2.12	0.67
2:B:209:LEU:HB2	2:B:213:GLU:OE1	1.93	0.67
1:C:10:PHE:CE2	2:D:286:VAL:HG21	2.30	0.67
2:L:80:HIS:CG	2:L:81:PRO:HD2	2.29	0.67
2:L:296:SER:OG	2:L:297:LEU:HD12	1.93	0.67
2:H:94:ASP:OD2	2:H:96:LEU:CD2	2.43	0.67
2:F:180:VAL:HG13	2:F:196:MET:HE2	1.77	0.67
2:D:299:LEU:CB	2:D:302:THR:HG23	2.25	0.67
2:F:77:LYS:HD2	2:F:100:LYS:CG	2.25	0.67
2:L:296:SER:C	2:L:297:LEU:HD12	2.20	0.67
2:H:70:TYR:CZ	2:H:132:ILE:CG2	2.77	0.66
2:D:299:LEU:CB	2:D:302:THR:OG1	2.31	0.66
2:H:204:ARG:HB2	2:H:215:PHE:HB2	1.75	0.66
2:F:106:LEU:N	2:F:106:LEU:HD23	2.10	0.66
2:F:331:ASP:HB2	2:F:354:ILE:HG21	1.77	0.66
2:B:98:GLN:HG3	2:B:99:GLN:HG3	1.76	0.66
2:F:303:ALA:CB	2:F:328:LEU:HA	2.19	0.66
2:H:96:LEU:HD12	2:H:96:LEU:O	1.96	0.66
2:H:91:PHE:CZ	2:F:324:GLY:CA	2.77	0.66
2:H:163:ASN:CB	4:H:507:HOH:O	2.27	0.66
2:H:303:ALA:O	2:H:328:LEU:HA	1.95	0.66
2:D:70:TYR:CZ	2:D:103:GLU:HB3	2.31	0.66
2:L:303:ALA:HB2	2:L:328:LEU:CD2	2.20	0.66
2:D:177:THR:HA	2:D:199:ILE:HG22	1.77	0.66
2:H:83:PHE:O	2:H:90:ARG:CD	2.41	0.66
2:H:188:PHE:HE1	2:D:248:LYS:CE	2.04	0.66
2:H:217:GLN:HE22	2:L:193:THR:CG2	2.08	0.66
2:D:71:THR:HG22	2:D:104:SER:O	1.96	0.66
2:D:80:HIS:CD2	2:D:81:PRO:CD	2.79	0.66
2:L:53:VAL:HA	4:L:538:HOH:O	1.95	0.66
4:F:542:HOH:O	2:J:246:PHE:CD2	2.49	0.66
2:B:241:ILE:N	4:B:502:HOH:O	2.05	0.66
2:D:232:VAL:HG13	2:D:236:GLY:HA2	1.77	0.65
2:F:85:ASP:HB2	2:F:90:ARG:NH1	2.11	0.65
2:F:195:THR:HG22	2:F:220:ALA:HB1	1.77	0.65
2:B:53:VAL:HG21	4:B:543:HOH:O	1.93	0.65
2:F:286:VAL:CG1	4:F:523:HOH:O	2.43	0.65
2:L:321:LEU:HD12	2:L:358:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:278:ILE:HG23	2:J:373:LEU:CD1	2.27	0.65
2:J:305:ILE:HD13	2:J:305:ILE:N	2.11	0.65
1:K:6:LEU:HD21	2:L:287:LYS:NZ	2.11	0.65
2:F:322:LEU:CD2	2:F:360:ARG:HH12	2.05	0.65
2:J:180:VAL:CG2	4:J:518:HOH:O	2.42	0.65
2:D:75:VAL:CG2	2:D:102:MET:HE3	2.26	0.65
2:D:112:MET:HG2	2:D:268:MET:HE1	1.78	0.65
2:F:141:THR:OG1	2:F:161:LEU:HD11	1.96	0.65
2:F:203:GLY:HA2	2:F:214:ASP:OD1	1.96	0.65
2:L:279:ARG:HE	3:L:401:IMD:C4	2.09	0.65
2:B:169:LEU:HD13	2:B:265:LEU:HD11	1.78	0.65
2:D:106:LEU:H	2:D:106:LEU:CD2	2.10	0.65
1:E:9:VAL:HG22	2:F:285:GLU:HG2	1.79	0.65
2:F:188:PHE:HE1	2:F:224:PRO:HG2	1.62	0.65
2:L:293:LEU:HD11	4:L:561:HOH:O	1.97	0.65
2:B:289:LEU:HG	4:B:509:HOH:O	1.97	0.65
2:H:116:GLY:O	2:H:118:LEU:HD12	1.97	0.64
2:B:241:ILE:HB	4:B:502:HOH:O	1.96	0.64
2:B:289:LEU:HD12	4:B:509:HOH:O	1.97	0.64
2:D:100:LYS:HD2	2:D:101:ARG:H	1.63	0.64
2:F:195:THR:CG2	2:F:221:ALA:N	2.59	0.64
2:B:217:GLN:HG3	2:B:257:PHE:CE1	2.33	0.64
2:D:251:GLY:HA3	2:L:253:GLN:NE2	2.12	0.64
2:D:279:ARG:NE	3:D:401:IMD:HN3	1.95	0.64
2:B:74:MET:HG2	2:B:101:ARG:NH1	2.12	0.64
2:L:143:ALA:HB2	2:L:159:ILE:HD11	1.79	0.64
2:F:195:THR:CG2	2:F:221:ALA:H	2.10	0.64
2:L:307:VAL:CG1	4:L:548:HOH:O	2.30	0.64
2:B:297:LEU:N	2:B:297:LEU:HD12	2.13	0.64
2:D:284:VAL:HG21	4:D:548:HOH:O	1.97	0.64
2:J:70:TYR:CD1	2:J:132:ILE:HD12	2.33	0.64
2:D:100:LYS:NZ	1:K:4:ASP:OD2	2.31	0.64
2:D:143:ALA:HB2	2:D:159:ILE:HD11	1.80	0.64
2:D:210:ASN:N	2:D:213:GLU:OE2	2.19	0.64
2:F:243:THR:HG21	2:F:259:ILE:HG13	1.79	0.64
1:K:10:PHE:HA	4:L:514:HOH:O	1.97	0.64
2:L:312:ARG:NH1	4:L:507:HOH:O	2.29	0.64
1:K:6:LEU:HD23	2:L:287:LYS:HB2	1.74	0.64
2:H:279:ARG:HH12	3:H:401:IMD:C5	1.92	0.64
2:H:282:LEU:O	2:H:316:ALA:HB2	1.98	0.64
1:C:9:VAL:HG22	2:D:285:GLU:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:71:THR:CG2	2:J:106:LEU:HD21	2.27	0.64
2:F:106:LEU:HD23	2:F:106:LEU:H	1.63	0.64
2:B:90:ARG:NH2	2:D:285:GLU:OE2	2.31	0.63
2:B:112:MET:HE2	2:B:112:MET:N	2.12	0.63
2:J:262:LYS:O	4:J:502:HOH:O	2.15	0.63
2:L:83:PHE:C	2:L:90:ARG:HB2	2.23	0.63
2:B:74:MET:HG2	2:B:101:ARG:NE	1.95	0.63
2:H:214:ASP:O	2:H:260:PRO:HD3	1.98	0.63
2:B:168:THR:OG1	4:B:505:HOH:O	2.11	0.63
2:D:289:LEU:HD12	2:D:304:GLY:HA2	1.81	0.63
2:F:360:ARG:HG3	2:F:360:ARG:NH1	2.07	0.63
2:F:75:VAL:HG23	2:F:100:LYS:HB2	1.81	0.63
2:B:69:LEU:HD11	2:B:109:ALA:HB2	1.81	0.63
2:B:122:ASN:ND2	2:B:150:PRO:HG3	2.14	0.63
2:L:77:LYS:HG3	2:L:78:PRO:CD	2.26	0.63
2:H:307:VAL:HG12	2:H:323:PRO:HA	1.81	0.63
2:D:112:MET:HE3	2:D:119:LEU:HB2	1.81	0.63
2:D:301:GLU:O	2:D:301:GLU:HG2	1.95	0.63
2:F:207:LEU:HD13	4:F:513:HOH:O	1.97	0.63
2:L:219:ASP:OD1	4:L:503:HOH:O	2.15	0.63
2:D:96:LEU:N	2:D:97:PRO:CD	2.46	0.63
2:B:289:LEU:CD1	4:B:509:HOH:O	2.47	0.63
2:J:175:ILE:HD12	2:J:199:ILE:HD13	1.80	0.63
2:J:309:GLY:HA2	2:L:89:ARG:O	1.99	0.63
2:L:315:PRO:HB3	2:L:370:GLU:O	1.98	0.63
4:B:503:HOH:O	2:J:193:THR:HA	1.99	0.62
2:F:278:ILE:HD12	2:F:278:ILE:C	2.24	0.62
2:J:278:ILE:CG2	2:J:373:LEU:CD1	2.76	0.62
2:L:77:LYS:HD2	2:L:78:PRO:HD2	1.80	0.62
2:H:181:CYS:SG	2:H:218:THR:HG23	2.39	0.62
2:D:89:ARG:HG2	2:D:89:ARG:NH1	2.06	0.62
2:H:290:THR:HB	4:H:501:HOH:O	2.00	0.62
1:K:10:PHE:C	2:L:282:LEU:H	2.03	0.62
2:D:116:GLY:HA2	2:D:164:LEU:CD2	2.29	0.62
2:F:151:GLU:HG2	4:F:517:HOH:O	1.98	0.62
2:J:94:ASP:HB2	2:J:97:PRO:HD2	1.82	0.62
2:L:360:ARG:CZ	4:L:513:HOH:O	2.47	0.62
2:F:305:ILE:HG13	2:F:327:ILE:HB	1.81	0.62
2:J:214:ASP:O	2:J:260:PRO:CD	2.48	0.62
2:L:285:GLU:HG2	2:L:308:ALA:HB3	1.80	0.62
1:K:6:LEU:CD2	2:L:287:LYS:CG	2.76	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:283:GLY:HA3	2:L:311:TYR:HB2	1.82	0.62
2:B:68:ASN:OD1	2:B:186:ASN:HB2	2.00	0.62
2:F:74:MET:SD	2:F:101:ARG:HB3	2.39	0.62
2:F:291:PRO:HA	2:F:294:ALA:HB3	1.81	0.62
2:J:214:ASP:O	2:J:260:PRO:HD3	2.00	0.62
2:H:87:MET:O	2:F:311:TYR:HA	2.00	0.62
2:B:80:HIS:CG	2:B:81:PRO:HD2	2.35	0.62
2:D:161:LEU:HB2	2:D:164:LEU:CD1	2.28	0.62
2:D:279:ARG:HE	3:D:401:IMD:HN3	1.48	0.62
2:F:278:ILE:HD12	2:F:278:ILE:O	1.98	0.62
2:F:293:LEU:O	2:F:293:LEU:HG	1.98	0.62
2:D:205:ASN:HD22	2:D:339:ARG:NE	1.98	0.61
2:H:182:LEU:HB2	2:H:232:VAL:HG12	1.82	0.61
2:H:299:LEU:HB2	2:H:302:THR:CG2	2.30	0.61
2:B:82:LEU:N	2:B:82:LEU:HD23	2.15	0.61
2:L:80:HIS:CE1	2:L:81:PRO:HD2	2.35	0.61
2:H:143:ALA:HB2	2:H:159:ILE:HD13	1.82	0.61
2:F:94:ASP:OD2	2:F:96:LEU:CD2	2.28	0.61
2:F:279:ARG:NH1	3:F:401:IMD:H4	2.16	0.61
2:F:279:ARG:HH12	3:F:401:IMD:C4	2.13	0.61
2:F:282:LEU:O	2:F:316:ALA:HB2	2.00	0.61
2:D:195:THR:HG23	2:L:219:ASP:OD1	2.00	0.61
2:B:251:GLY:HA3	2:F:253:GLN:NE2	2.15	0.61
2:L:80:HIS:CG	2:L:81:PRO:CD	2.84	0.61
2:B:63:ALA:N	2:B:64:PRO:HD2	2.15	0.61
2:H:65:ALA:O	2:H:111:ILE:HG13	2.00	0.61
2:H:151:GLU:N	4:H:504:HOH:O	2.16	0.61
2:J:71:THR:HB	2:J:106:LEU:HD21	1.83	0.61
2:L:177:THR:HA	2:L:199:ILE:CG2	2.29	0.61
2:F:251:GLY:CA	2:J:253:GLN:HE21	2.07	0.60
2:B:61:ARG:NH2	2:B:168:THR:HG21	2.16	0.60
2:D:299:LEU:HB3	2:D:302:THR:HG23	1.83	0.60
2:J:329:THR:HB	2:J:357:VAL:CG2	2.31	0.60
2:J:331:ASP:HB2	2:J:354:ILE:HB	1.83	0.60
2:L:303:ALA:CB	2:L:328:LEU:HD23	2.23	0.60
2:D:187:PRO:HA	2:D:225:GLY:HA3	1.84	0.60
2:F:71:THR:HB	2:F:106:LEU:HD21	1.83	0.60
1:G:6:LEU:HD11	4:H:518:HOH:O	1.72	0.60
2:B:82:LEU:HD12	2:B:92:PHE:CE2	2.37	0.60
2:L:282:LEU:HB3	2:L:284:VAL:HG23	1.84	0.60
2:H:83:PHE:CD2	2:H:94:ASP:OD1	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:THR:CG2	2:D:104:SER:O	2.49	0.60
2:D:284:VAL:HB	4:D:548:HOH:O	2.01	0.60
2:F:188:PHE:CE1	2:F:224:PRO:HG2	2.37	0.60
2:H:83:PHE:O	2:H:90:ARG:HB2	2.01	0.60
2:B:121:ASN:HB2	2:B:124:VAL:HG23	1.83	0.60
2:L:80:HIS:ND1	2:L:81:PRO:HD2	2.15	0.60
2:L:141:THR:OG1	2:L:161:LEU:HD21	2.02	0.60
2:H:91:PHE:HZ	2:F:324:GLY:HA2	1.66	0.60
2:B:188:PHE:HE1	2:F:248:LYS:HE2	1.66	0.60
2:B:195:THR:HG21	2:B:221:ALA:HB3	1.82	0.60
1:K:10:PHE:HD2	2:L:342:MET:HG3	1.66	0.60
2:D:207:LEU:HB3	2:D:209:LEU:HD12	1.84	0.60
2:F:120:THR:O	4:F:505:HOH:O	2.15	0.59
2:J:131:ILE:HG22	2:J:143:ALA:HB3	1.82	0.59
2:L:243:THR:HG21	2:L:259:ILE:CG1	2.32	0.59
2:D:141:THR:OG1	2:D:161:LEU:HD11	2.02	0.59
2:F:172:SER:CB	4:F:520:HOH:O	1.95	0.59
2:D:172:SER:C	4:D:501:HOH:O	2.45	0.59
2:D:212:TYR:HH	2:D:279:ARG:HD3	1.67	0.59
2:H:71:THR:HB	2:H:106:LEU:HD11	1.85	0.59
2:F:91:PHE:N	2:F:91:PHE:CD1	2.71	0.59
2:J:195:THR:HG21	2:J:221:ALA:O	2.02	0.59
2:L:293:LEU:HD12	2:L:293:LEU:O	2.02	0.59
2:B:95:ASN:HB3	2:B:97:PRO:HD2	1.85	0.59
2:F:74:MET:HE3	2:F:75:VAL:H	1.66	0.59
2:L:283:GLY:CA	2:L:311:TYR:HB2	2.33	0.59
2:H:112:MET:HE3	2:H:119:LEU:CB	2.23	0.59
2:D:279:ARG:NE	3:D:401:IMD:N3	2.50	0.59
2:J:176:ARG:HG2	2:J:176:ARG:HH11	1.68	0.59
2:H:96:LEU:HD12	2:H:96:LEU:C	2.28	0.59
2:H:196:MET:HB2	2:D:198:ILE:HG12	1.85	0.59
2:D:115:GLU:HB3	2:D:158:LYS:HZ1	1.68	0.59
2:B:193:THR:HG22	2:F:204:ARG:NH2	2.12	0.59
2:F:77:LYS:HE2	2:F:97:PRO:O	2.03	0.59
2:F:243:THR:CG2	2:F:259:ILE:HG13	2.32	0.58
2:F:331:ASP:CG	2:F:354:ILE:CG2	2.75	0.58
2:H:68:ASN:CB	4:H:525:HOH:O	1.76	0.58
2:F:295:GLU:CA	4:F:526:HOH:O	2.32	0.58
2:F:331:ASP:CB	2:F:354:ILE:HG21	2.31	0.58
2:L:262:LYS:HD3	4:L:557:HOH:O	2.02	0.58
2:H:261:THR:CG2	2:H:265:LEU:HD12	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:LEU:CD1	2:B:297:LEU:H	2.16	0.58
2:H:261:THR:O	2:H:265:LEU:HB2	2.03	0.58
2:J:117:TYR:CD1	2:J:158:LYS:CD	2.82	0.58
2:H:152:THR:HG21	2:H:263:LEU:HD11	1.86	0.58
2:D:193:THR:HG21	2:L:217:GLN:HE22	1.69	0.58
2:D:214:ASP:O	2:D:260:PRO:HD3	2.04	0.58
2:L:305:ILE:HD11	2:L:327:ILE:CA	2.24	0.58
2:B:335:ALA:HB2	4:B:522:HOH:O	2.03	0.58
2:L:242:ASN:HD22	2:L:258:ALA:HB2	1.69	0.58
2:D:182:LEU:HD23	2:D:194:VAL:CG1	2.34	0.58
2:L:231:LEU:HB2	2:L:242:ASN:HD21	1.69	0.58
2:F:94:ASP:HB2	2:F:96:LEU:CD2	2.33	0.58
2:J:118:LEU:HB2	2:J:157:LEU:HB2	1.86	0.58
2:B:289:LEU:HD12	2:B:289:LEU:C	2.29	0.57
2:D:328:LEU:HB2	2:D:357:VAL:HG12	1.86	0.57
2:F:136:ARG:N	4:F:508:HOH:O	2.37	0.57
2:J:195:THR:CG2	2:J:221:ALA:N	2.67	0.57
1:G:6:LEU:HB3	2:H:287:LYS:CB	2.34	0.57
2:D:96:LEU:HD23	2:D:96:LEU:C	2.28	0.57
2:F:118:LEU:HB2	2:F:157:LEU:HB2	1.85	0.57
2:F:175:ILE:O	4:F:504:HOH:O	2.17	0.57
2:J:184:ILE:O	4:J:501:HOH:O	2.17	0.57
2:H:78:PRO:HD3	2:H:100:LYS:HZ1	1.70	0.57
2:D:70:TYR:OH	2:D:103:GLU:HB3	2.04	0.57
1:E:7:ARG:NH1	2:F:287:LYS:HB2	2.19	0.57
2:F:299:LEU:HD13	2:F:302:THR:HB	1.84	0.57
2:F:356:ILE:O	2:F:367:LEU:HB2	2.03	0.57
2:J:129:ASP:OD1	2:J:129:ASP:N	2.36	0.57
2:B:198:ILE:HG12	2:J:196:MET:HB2	1.86	0.57
2:B:289:LEU:CG	4:B:509:HOH:O	2.52	0.57
2:D:106:LEU:HD22	2:D:106:LEU:N	2.15	0.57
2:L:337:ASP:HB3	2:L:340:ARG:HG3	1.86	0.57
2:B:315:PRO:N	2:B:318:ARG:HH12	2.02	0.57
2:D:143:ALA:CB	2:D:159:ILE:CD1	2.81	0.57
2:D:284:VAL:CB	4:D:548:HOH:O	2.52	0.57
2:F:85:ASP:CB	2:F:90:ARG:HH12	2.13	0.57
2:J:84:ASP:OD1	2:J:90:ARG:N	2.29	0.57
2:J:175:ILE:CD1	2:J:199:ILE:HD13	2.34	0.57
1:G:6:LEU:HB3	2:H:287:LYS:HB3	1.87	0.57
2:H:211:THR:HG22	2:H:212:TYR:CE2	2.38	0.57
2:J:95:ASN:OD1	2:J:95:ASN:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:334:GLU:O	2:L:334:GLU:HG2	1.99	0.57
2:H:85:ASP:CB	2:H:86:PRO:CD	2.81	0.57
2:H:198:ILE:HD13	2:L:196:MET:HB2	1.87	0.57
2:B:74:MET:HG2	2:B:101:ARG:CZ	2.35	0.57
2:H:72:THR:C	2:H:73:LYS:HE2	2.30	0.57
2:F:154:LEU:HD23	4:F:505:HOH:O	2.04	0.57
2:L:304:GLY:HA3	2:L:336:SER:O	2.05	0.57
2:H:193:THR:HG23	2:D:200:SER:HB3	1.86	0.57
2:D:284:VAL:CG2	4:D:548:HOH:O	2.50	0.57
2:B:311:TYR:HD1	2:D:88:PHE:CE1	2.23	0.56
2:D:321:LEU:CD2	2:D:367:LEU:HD22	2.34	0.56
2:B:68:ASN:CG	2:B:186:ASN:HB2	2.30	0.56
2:B:86:PRO:CA	2:D:312:ARG:HH12	2.12	0.56
2:L:293:LEU:CD1	4:L:561:HOH:O	2.53	0.56
2:H:217:GLN:HE22	2:L:193:THR:HG21	1.70	0.56
2:B:169:LEU:HD11	2:B:265:LEU:HD21	1.86	0.56
2:F:115:GLU:O	2:F:158:LYS:HE2	2.05	0.56
2:J:70:TYR:C	2:J:70:TYR:HD1	2.14	0.56
1:K:6:LEU:CD2	2:L:287:LYS:CD	2.83	0.56
2:L:293:LEU:CD2	4:L:561:HOH:O	1.87	0.56
2:L:305:ILE:HD13	2:L:327:ILE:HD12	1.87	0.56
2:H:110:VAL:HG13	2:H:167:MET:HE3	1.88	0.56
2:H:299:LEU:N	2:H:302:THR:CG2	2.65	0.56
2:B:211:THR:HG22	2:B:342:MET:HE1	1.88	0.56
2:J:175:ILE:HD12	2:J:199:ILE:CD1	2.35	0.56
2:D:69:LEU:O	2:D:106:LEU:HD22	2.05	0.56
2:F:75:VAL:O	2:F:99:GLN:HA	2.06	0.56
2:L:85:ASP:CG	2:L:90:ARG:HH12	2.13	0.56
2:H:94:ASP:OD1	2:H:94:ASP:N	2.39	0.56
2:D:299:LEU:CD1	2:D:302:THR:CG2	2.73	0.56
2:F:207:LEU:CD1	4:F:513:HOH:O	2.53	0.56
2:D:69:LEU:HB3	2:D:106:LEU:HD21	1.88	0.56
2:F:347:ARG:HG2	2:F:347:ARG:HH11	1.71	0.56
2:H:223:ASN:HB3	2:H:224:PRO:HD2	1.86	0.56
2:B:167:MET:HG2	2:B:238:LEU:HD13	1.88	0.56
2:B:249:SER:HB3	2:J:249:SER:HB2	1.86	0.56
2:D:115:GLU:CB	2:D:158:LYS:HZ1	2.19	0.56
2:D:195:THR:CG2	2:D:221:ALA:N	2.62	0.56
2:J:68:ASN:HD22	2:J:186:ASN:CG	2.13	0.56
2:J:121:ASN:HB2	2:J:124:VAL:HG23	1.86	0.56
2:D:113:SER:HB3	2:D:117:TYR:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:70:TYR:CD1	2:J:70:TYR:C	2.84	0.55
2:J:77:LYS:HE2	2:J:100:LYS:HG2	1.57	0.55
2:L:139:ARG:NH2	2:L:162:LYS:O	2.40	0.55
2:H:149:ASP:OD2	2:H:279:ARG:NH2	2.38	0.55
2:H:276:GLN:HE21	2:H:278:ILE:HD11	1.70	0.55
2:H:302:THR:HG23	2:H:302:THR:O	2.05	0.55
2:F:77:LYS:HG3	2:F:100:LYS:HG3	1.88	0.55
2:F:303:ALA:CB	2:F:328:LEU:HD23	2.36	0.55
1:K:2:VAL:HG23	1:K:2:VAL:O	2.06	0.55
2:L:341:SER:O	2:L:345:VAL:HG23	2.06	0.55
2:B:111:ILE:HD11	2:B:135:LEU:HD22	1.89	0.55
2:J:77:LYS:CD	2:J:100:LYS:HB2	2.36	0.55
2:L:172:SER:CB	4:L:521:HOH:O	1.87	0.55
2:H:299:LEU:HB2	2:H:302:THR:HG21	1.86	0.55
2:F:77:LYS:NZ	2:F:96:LEU:HD12	2.21	0.55
2:F:77:LYS:CE	2:F:96:LEU:CD1	2.83	0.55
2:F:80:HIS:CG	2:F:81:PRO:HD2	2.41	0.55
2:L:289:LEU:HG	2:L:303:ALA:O	2.07	0.55
2:H:329:THR:CG2	2:H:357:VAL:HG23	2.36	0.55
2:B:337:ASP:HB2	2:B:340:ARG:HH21	1.71	0.55
2:F:68:ASN:OD1	2:F:186:ASN:HB2	2.07	0.55
2:B:195:THR:CG2	2:B:221:ALA:H	2.20	0.55
2:D:102:MET:CE	4:K:101:HOH:O	2.30	0.55
2:D:325:ASP:CG	2:D:360:ARG:CD	2.72	0.55
2:F:77:LYS:CD	2:F:100:LYS:HG3	2.36	0.55
2:L:89:ARG:HH11	2:L:89:ARG:CG	2.19	0.55
2:D:329:THR:OG1	2:D:357:VAL:HB	2.06	0.55
2:F:106:LEU:O	2:F:124:VAL:HG13	2.07	0.55
2:H:53:VAL:HG21	4:L:546:HOH:O	2.08	0.54
2:F:77:LYS:CB	2:F:78:PRO:CD	2.85	0.54
2:F:282:LEU:O	2:F:316:ALA:CB	2.56	0.54
2:L:93:GLY:HA2	4:L:516:HOH:O	1.92	0.54
2:H:77:LYS:HB2	2:H:98:GLN:O	2.08	0.54
2:F:77:LYS:HZ2	2:F:100:LYS:HG2	1.72	0.54
2:L:243:THR:CG2	2:L:259:ILE:HG13	2.36	0.54
2:B:169:LEU:CD1	2:B:265:LEU:HD11	2.37	0.54
2:B:303:ALA:O	2:B:328:LEU:HD22	2.08	0.54
2:D:83:PHE:HZ	2:J:92:PHE:CE2	2.26	0.54
2:D:83:PHE:HZ	2:J:92:PHE:HE2	1.55	0.54
2:D:89:ARG:HH11	2:D:89:ARG:CG	2.07	0.54
2:D:303:ALA:CB	2:D:328:LEU:CD2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:295:GLU:CD	2:F:296:SER:H	2.11	0.54
2:J:70:TYR:CB	2:J:105:SER:HA	2.36	0.54
2:H:56:ALA:HB1	2:D:176:ARG:HH11	1.71	0.54
2:J:358:VAL:HG12	2:J:365:VAL:HB	1.89	0.54
2:L:80:HIS:CB	4:L:541:HOH:O	2.55	0.54
2:H:55:TYR:CE1	2:H:180:VAL:HG11	2.43	0.54
2:B:293:LEU:HG	2:B:293:LEU:O	2.06	0.54
2:H:195:THR:HG21	2:H:221:ALA:N	2.22	0.54
2:B:315:PRO:HB3	2:B:370:GLU:O	2.08	0.54
2:D:95:ASN:HB3	2:D:97:PRO:HD2	1.89	0.54
2:B:231:LEU:HB2	2:B:242:ASN:ND2	2.23	0.54
2:B:297:LEU:HD12	2:B:297:LEU:H	1.73	0.54
2:B:315:PRO:CA	2:B:318:ARG:NH1	2.64	0.54
2:J:241:ILE:O	2:J:258:ALA:HB1	2.07	0.54
2:L:303:ALA:HB1	2:L:326:VAL:HG13	1.89	0.54
1:G:10:PHE:HB3	2:H:342:MET:HG3	1.90	0.54
2:F:70:TYR:HD2	4:F:541:HOH:O	1.89	0.54
2:F:332:LYS:O	2:F:332:LYS:HG2	2.07	0.54
2:J:70:TYR:HB2	2:J:105:SER:HA	1.89	0.54
2:H:303:ALA:HA	2:H:334:GLU:HG3	1.90	0.54
2:B:162:LYS:HA	4:B:534:HOH:O	2.08	0.54
2:D:321:LEU:HD22	2:D:367:LEU:HD22	1.90	0.54
2:F:110:VAL:HB	2:F:112:MET:HE1	1.90	0.54
2:J:143:ALA:HA	2:J:159:ILE:CD1	2.38	0.54
2:H:219:ASP:OD1	2:L:195:THR:HG23	2.07	0.53
2:J:195:THR:HG21	2:J:221:ALA:N	2.23	0.53
2:H:163:ASN:ND2	4:H:507:HOH:O	2.32	0.53
2:B:314:GLY:C	2:B:318:ARG:NH1	2.67	0.53
2:J:119:LEU:HD23	2:J:241:ILE:HD11	1.90	0.53
2:H:303:ALA:O	2:H:328:LEU:HD23	2.08	0.53
2:B:86:PRO:HA	2:D:312:ARG:NH1	2.17	0.53
2:F:281:TRP:CE3	2:F:374:ARG:HG3	2.43	0.53
2:J:135:LEU:HD12	2:J:139:ARG:HB2	1.89	0.53
2:D:207:LEU:HB2	2:D:213:GLU:OE1	2.08	0.53
2:L:89:ARG:HG2	2:L:89:ARG:NH1	2.21	0.53
2:B:162:LYS:H	2:B:162:LYS:HD3	1.74	0.53
2:J:71:THR:HG22	2:J:106:LEU:HD21	1.90	0.53
2:J:321:LEU:HD22	2:J:367:LEU:HD12	1.91	0.53
1:A:7:ARG:HD2	2:B:285:GLU:OE2	2.08	0.53
2:D:305:ILE:CD1	2:D:335:ALA:HB1	2.38	0.53
2:J:243:THR:OG1	2:J:259:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:116:GLY:CA	2:H:159:ILE:HG22	2.39	0.53
2:B:313:ASP:O	2:B:318:ARG:CZ	2.57	0.53
2:F:310:VAL:CG1	2:F:317:ALA:HB2	2.39	0.53
2:B:89:ARG:HG2	2:B:89:ARG:NH1	2.23	0.53
2:H:350:PRO:HA	2:H:371:VAL:HG12	1.90	0.53
2:F:315:PRO:HB3	2:F:370:GLU:O	2.09	0.53
2:B:141:THR:HB	2:B:159:ILE:HD11	1.91	0.53
2:F:75:VAL:CG2	2:F:100:LYS:O	2.46	0.53
2:J:325:ASP:HB3	2:J:358:VAL:CG2	2.39	0.53
2:L:66:VAL:HG11	2:L:184:ILE:HG22	1.91	0.52
2:D:69:LEU:CB	2:D:106:LEU:HD21	2.39	0.52
2:F:303:ALA:HB1	2:F:328:LEU:CA	2.25	0.52
2:L:70:TYR:CD2	2:L:132:ILE:HD12	2.43	0.52
2:L:74:MET:HA	2:L:74:MET:HE3	1.87	0.52
2:B:82:LEU:HD12	2:B:92:PHE:HE2	1.74	0.52
2:B:172:SER:HB2	4:B:521:HOH:O	1.80	0.52
2:H:186:ASN:O	2:H:225:GLY:HA3	2.09	0.52
1:A:10:PHE:CE1	2:B:284:VAL:CG2	2.93	0.52
2:D:203:GLY:HA2	2:D:214:ASP:OD1	2.10	0.52
2:J:98:GLN:NE2	4:J:509:HOH:O	2.42	0.52
2:L:195:THR:HG21	2:L:221:ALA:N	2.25	0.52
2:B:255:ILE:HD11	2:J:223:ASN:ND2	2.25	0.52
2:D:175:ILE:CD1	2:D:216:ILE:HD12	2.38	0.52
2:H:83:PHE:HE1	2:B:83:PHE:CE1	2.27	0.52
2:H:287:LYS:HG2	2:H:306:VAL:HB	1.92	0.52
2:H:295:GLU:CD	4:H:527:HOH:O	2.52	0.52
2:B:307:VAL:HG23	2:B:325:ASP:O	2.09	0.52
2:F:113:SER:HB3	2:F:117:TYR:HB2	1.90	0.52
2:H:83:PHE:CE2	2:H:94:ASP:OD1	2.62	0.52
2:F:85:ASP:OD1	2:F:86:PRO:HD2	2.10	0.52
2:J:119:LEU:HD21	2:J:264:ALA:HB1	1.92	0.52
2:L:53:VAL:CG1	4:L:538:HOH:O	2.45	0.52
1:A:10:PHE:CE1	2:B:284:VAL:HG21	2.45	0.52
2:F:353:LYS:CE	2:F:370:GLU:HB2	2.40	0.52
2:B:89:ARG:NH1	2:B:89:ARG:CG	2.72	0.51
2:B:281:TRP:HB2	2:B:374:ARG:HA	1.93	0.51
2:D:74:MET:SD	2:D:75:VAL:N	2.83	0.51
2:L:321:LEU:CD1	2:L:358:VAL:HG21	2.41	0.51
2:J:285:GLU:HB2	2:L:88:PHE:CE1	2.46	0.51
2:B:241:ILE:CA	4:B:502:HOH:O	2.54	0.51
2:D:279:ARG:HA	2:D:346:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:ARG:NH2	4:F:506:HOH:O	2.32	0.51
2:L:195:THR:HG22	2:L:220:ALA:HB1	1.92	0.51
2:L:365:VAL:HG12	2:L:367:LEU:CD1	2.40	0.51
2:H:69:LEU:CD2	2:H:133:VAL:HG22	2.40	0.51
2:F:251:GLY:CA	2:J:253:GLN:NE2	2.38	0.51
2:B:138:GLY:HA2	4:B:508:HOH:O	2.11	0.51
2:B:184:ILE:CG2	2:B:192:GLN:HE21	2.22	0.51
2:F:77:LYS:HZ3	2:F:100:LYS:HG2	1.74	0.51
2:J:70:TYR:HA	2:J:106:LEU:HG	1.91	0.51
2:L:320:GLY:O	2:L:360:ARG:NH2	2.43	0.51
2:B:173:ASP:HB2	4:B:528:HOH:O	2.10	0.51
2:B:310:VAL:HG22	2:D:89:ARG:HB3	1.92	0.51
2:J:266:GLU:HG3	4:J:502:HOH:O	2.11	0.51
2:B:325:ASP:OD1	2:B:360:ARG:HD2	2.11	0.51
2:F:353:LYS:HE3	2:F:370:GLU:HB2	1.91	0.51
2:L:123:HIS:CE1	2:L:227:SER:HB3	2.45	0.51
2:L:175:ILE:HD11	2:L:202:THR:CG2	2.37	0.51
2:L:294:ALA:HB1	2:L:298:GLY:HA3	1.92	0.51
2:H:195:THR:HG23	2:D:219:ASP:OD1	2.10	0.51
2:B:216:ILE:HD11	2:B:260:PRO:HB3	1.93	0.51
2:H:222:ILE:HG23	2:H:226:ASN:CB	2.41	0.51
2:D:85:ASP:HB2	2:D:90:ARG:NH1	2.25	0.51
2:D:250:GLY:O	2:L:248:LYS:HD3	2.05	0.51
2:D:100:LYS:HE3	1:K:4:ASP:CG	2.32	0.51
2:D:174:GLY:CA	4:D:501:HOH:O	2.46	0.51
1:K:10:PHE:CD1	2:L:345:VAL:HG21	2.46	0.51
2:L:283:GLY:HA3	2:L:311:TYR:CB	2.40	0.51
2:L:322:LEU:HD11	2:L:360:ARG:HE	1.76	0.51
2:B:85:ASP:OD1	2:B:86:PRO:CD	2.59	0.50
2:B:350:PRO:CA	4:B:514:HOH:O	2.56	0.50
2:F:70:TYR:HB2	4:F:541:HOH:O	2.11	0.50
2:J:108:SER:O	2:J:228:GLY:HA3	2.11	0.50
2:L:94:ASP:N	4:L:516:HOH:O	2.42	0.50
2:H:65:ALA:HB3	2:H:167:MET:HE2	1.93	0.50
2:H:329:THR:HG21	2:H:357:VAL:HG23	1.94	0.50
2:B:286:VAL:HG11	2:B:305:ILE:HD12	1.93	0.50
2:D:217:GLN:HG3	2:D:257:PHE:CE1	2.46	0.50
2:L:68:ASN:CG	2:L:186:ASN:ND2	2.69	0.50
2:F:312:ARG:HD2	2:F:312:ARG:O	2.09	0.50
1:E:8:TRP:CH2	2:F:206:GLN:HG2	2.41	0.50
2:F:261:THR:HG22	2:F:265:LEU:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:195:THR:CG2	2:J:221:ALA:H	2.25	0.50
2:H:110:VAL:HB	2:H:112:MET:HE1	1.94	0.50
2:B:87:MET:HG3	2:D:311:TYR:CE1	2.46	0.50
2:B:241:ILE:CB	4:B:502:HOH:O	2.57	0.50
2:D:69:LEU:HB2	2:D:106:LEU:HD23	1.94	0.50
2:J:89:ARG:CD	4:L:507:HOH:O	2.58	0.50
2:J:325:ASP:OD2	2:J:360:ARG:NE	2.42	0.50
2:J:330:ILE:HD12	4:J:517:HOH:O	2.11	0.50
1:K:6:LEU:HD23	2:L:287:LYS:CD	2.39	0.50
2:F:74:MET:CE	2:F:100:LYS:O	2.60	0.50
2:B:122:ASN:HD21	2:B:150:PRO:HG3	1.77	0.50
2:F:110:VAL:HG13	2:F:167:MET:HE3	1.93	0.50
2:L:205:ASN:C	2:L:206:GLN:HG3	2.37	0.50
1:G:9:VAL:HG23	1:G:9:VAL:O	2.12	0.50
2:B:117:TYR:CE1	2:B:158:LYS:HD3	2.47	0.50
2:B:297:LEU:N	2:B:297:LEU:CD1	2.73	0.50
2:F:141:THR:OG1	2:F:161:LEU:CD1	2.60	0.50
2:H:70:TYR:OH	2:H:132:ILE:HG21	2.10	0.49
2:H:78:PRO:HD3	2:H:100:LYS:NZ	2.26	0.49
2:D:251:GLY:HA3	2:L:253:GLN:CD	2.36	0.49
2:F:193:THR:HG21	2:J:217:GLN:HE22	1.76	0.49
2:F:321:LEU:CD1	2:F:358:VAL:HG21	2.42	0.49
2:L:231:LEU:HB2	2:L:242:ASN:ND2	2.27	0.49
2:H:141:THR:HG22	2:H:142:ILE:O	2.11	0.49
2:J:112:MET:HE3	2:J:119:LEU:HB2	1.94	0.49
2:J:175:ILE:CG1	2:J:199:ILE:HD13	2.43	0.49
2:L:216:ILE:HD11	2:L:260:PRO:HB3	1.93	0.49
2:H:223:ASN:HB3	2:H:224:PRO:CD	2.42	0.49
2:L:65:ALA:HB3	2:L:167:MET:HE2	1.94	0.49
2:L:74:MET:HA	2:L:101:ARG:HA	1.94	0.49
2:L:156:VAL:HG22	2:L:268:MET:HG3	1.94	0.49
2:H:295:GLU:HG2	2:H:296:SER:N	2.25	0.49
2:D:106:LEU:CD2	2:D:106:LEU:N	2.72	0.49
2:F:142:ILE:HG23	2:F:142:ILE:O	2.12	0.49
2:J:71:THR:CB	2:J:106:LEU:HD21	2.42	0.49
2:B:95:ASN:HD22	2:B:96:LEU:HD12	1.77	0.49
2:B:312:ARG:HG3	2:B:312:ARG:O	2.13	0.49
2:J:64:PRO:HD3	2:J:136:ARG:NH2	2.28	0.49
2:J:141:THR:CG2	4:J:505:HOH:O	2.43	0.49
2:L:284:VAL:HG12	2:L:286:VAL:HG13	1.94	0.49
2:B:209:LEU:HD21	4:B:541:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:LEU:O	2:D:297:LEU:HG	2.11	0.49
2:F:95:ASN:CB	2:J:296:SER:CB	2.71	0.49
2:F:281:TRP:N	2:F:372:GLY:O	2.42	0.49
2:F:360:ARG:NH1	2:F:360:ARG:CG	2.72	0.49
2:B:268:MET:HG2	2:B:272:ILE:HD12	1.94	0.49
2:F:213:GLU:HG2	2:F:215:PHE:HE2	1.77	0.49
2:J:89:ARG:HD3	4:L:507:HOH:O	2.11	0.49
2:H:83:PHE:CZ	2:B:80:HIS:CE1	3.00	0.49
2:D:69:LEU:HB2	2:D:106:LEU:CD2	2.42	0.49
2:D:115:GLU:C	2:D:158:LYS:NZ	2.70	0.49
2:F:142:ILE:C	2:F:142:ILE:HD13	2.37	0.49
2:H:96:LEU:C	2:H:96:LEU:CD1	2.85	0.49
2:H:279:ARG:HH11	3:H:401:IMD:H5	1.57	0.49
2:F:73:LYS:HB2	2:F:73:LYS:NZ	2.28	0.49
2:J:143:ALA:HA	2:J:159:ILE:HD13	1.94	0.49
2:J:180:VAL:CB	4:J:518:HOH:O	2.43	0.49
2:B:216:ILE:CD1	2:B:216:ILE:N	2.76	0.49
2:H:222:ILE:O	2:H:252:SER:HB2	2.13	0.48
2:D:133:VAL:HG12	2:D:133:VAL:O	2.12	0.48
2:F:75:VAL:O	2:F:100:LYS:N	2.46	0.48
2:F:287:LYS:CG	2:F:306:VAL:HB	2.43	0.48
2:J:180:VAL:CA	4:J:518:HOH:O	2.02	0.48
2:L:85:ASP:HB3	2:L:88:PHE:H	1.77	0.48
2:L:374:ARG:NH2	4:L:514:HOH:O	2.42	0.48
1:G:7:ARG:O	1:G:7:ARG:HD3	2.13	0.48
2:B:134:ALA:CB	2:B:140:GLU:HG2	2.42	0.48
2:J:68:ASN:ND2	2:J:186:ASN:CG	2.68	0.48
1:K:6:LEU:HD21	2:L:287:LYS:CD	2.42	0.48
2:D:195:THR:HG22	2:D:220:ALA:CB	2.36	0.48
2:D:249:SER:H	2:D:253:GLN:HE22	1.61	0.48
2:F:74:MET:CE	2:F:100:LYS:C	2.83	0.48
2:L:347:ARG:HG3	3:L:401:IMD:H5	1.94	0.48
2:B:85:ASP:CB	2:B:86:PRO:CD	2.91	0.48
2:F:85:ASP:HB3	2:F:88:PHE:H	1.78	0.48
2:F:112:MET:HE3	2:F:119:LEU:HB2	1.95	0.48
2:J:329:THR:HB	2:J:357:VAL:HG23	1.95	0.48
2:D:74:MET:SD	2:D:74:MET:C	2.97	0.48
1:E:10:PHE:HD2	2:F:342:MET:HG2	1.78	0.48
2:F:135:LEU:N	2:F:135:LEU:CD2	2.74	0.48
2:F:299:LEU:CD1	2:F:302:THR:HB	2.43	0.48
2:J:111:ILE:HA	2:J:118:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:80:HIS:HB2	4:L:541:HOH:O	2.12	0.48
2:B:334:GLU:O	2:B:335:ALA:HB3	2.14	0.48
2:F:74:MET:HE1	2:F:101:ARG:HA	1.91	0.48
2:H:281:TRP:HB3	2:H:372:GLY:O	2.13	0.48
2:B:170:GLY:O	2:B:261:THR:HG21	2.14	0.48
2:B:361:ASN:HD22	2:B:361:ASN:H	1.61	0.48
2:H:261:THR:HG22	2:H:265:LEU:HD12	1.96	0.48
2:B:280:GLY:HA2	4:B:514:HOH:O	2.13	0.48
1:E:7:ARG:CZ	2:F:287:LYS:HE3	2.43	0.48
2:F:71:THR:N	2:F:106:LEU:HD21	2.29	0.48
2:D:112:MET:HE3	2:D:119:LEU:CB	2.43	0.48
2:J:66:VAL:HG11	2:J:184:ILE:HG22	1.95	0.48
2:J:111:ILE:HG13	2:J:118:LEU:CD2	2.44	0.48
1:G:6:LEU:CB	2:H:287:LYS:HB3	2.42	0.47
2:H:116:GLY:HA2	2:H:164:LEU:CD1	2.44	0.47
2:H:299:LEU:O	2:H:302:THR:CG2	2.61	0.47
1:A:6:LEU:HD12	1:A:6:LEU:O	2.14	0.47
2:J:177:THR:HA	2:J:199:ILE:HG22	1.96	0.47
2:L:367:LEU:N	2:L:367:LEU:HD13	2.29	0.47
2:D:195:THR:CG2	2:D:220:ALA:HB1	2.37	0.47
2:F:287:LYS:HG3	2:F:306:VAL:HB	1.96	0.47
2:L:68:ASN:CG	2:L:186:ASN:HD22	2.21	0.47
2:B:69:LEU:CD2	2:B:133:VAL:HG22	2.44	0.47
2:B:212:TYR:HD2	2:B:279:ARG:HH12	1.56	0.47
2:D:69:LEU:O	2:D:106:LEU:CD2	2.62	0.47
2:D:214:ASP:O	2:D:260:PRO:CD	2.61	0.47
2:F:112:MET:HG2	2:F:268:MET:SD	2.54	0.47
2:F:175:ILE:HD12	2:F:199:ILE:HD12	1.96	0.47
2:L:248:LYS:H	2:L:253:GLN:HE21	1.62	0.47
2:H:94:ASP:CB	2:H:96:LEU:HG	2.20	0.47
2:B:162:LYS:H	2:B:162:LYS:CD	2.27	0.47
2:D:115:GLU:C	2:D:158:LYS:HZ1	2.22	0.47
2:J:326:VAL:HB	2:J:359:LEU:HB3	1.96	0.47
2:J:348:THR:HG21	2:J:371:VAL:HG21	1.96	0.47
2:H:303:ALA:HA	2:H:334:GLU:O	2.15	0.47
2:H:329:THR:HB	2:H:357:VAL:HB	1.96	0.47
2:B:255:ILE:HD13	2:J:188:PHE:CD2	2.50	0.47
2:D:70:TYR:CE1	2:D:103:GLU:HB2	2.47	0.47
2:F:150:PRO:CD	4:F:517:HOH:O	1.73	0.47
2:F:230:ALA:HB1	2:F:238:LEU:HD12	1.96	0.47
2:J:112:MET:HG2	2:J:268:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:321:LEU:HD22	2:J:367:LEU:CD1	2.44	0.47
2:H:94:ASP:HB2	2:H:96:LEU:HD23	1.87	0.47
2:H:196:MET:CB	2:D:198:ILE:HG12	2.45	0.47
2:D:207:LEU:HD22	2:D:246:PHE:CZ	2.50	0.47
2:F:74:MET:HE3	2:F:75:VAL:N	2.29	0.47
2:F:331:ASP:HB2	2:F:354:ILE:CG2	2.45	0.47
2:J:332:LYS:N	4:J:508:HOH:O	2.40	0.47
1:K:10:PHE:CD2	2:L:342:MET:HA	2.49	0.47
2:L:102:MET:HE1	4:L:562:HOH:O	1.81	0.47
2:L:223:ASN:N	4:L:509:HOH:O	2.47	0.47
2:L:243:THR:HG21	2:L:259:ILE:HD11	1.94	0.47
2:H:299:LEU:CA	2:H:302:THR:CG2	2.92	0.47
2:F:121:ASN:HB2	2:F:124:VAL:HG23	1.97	0.47
2:F:175:ILE:HD11	2:F:216:ILE:HD12	1.96	0.47
2:F:212:TYR:CD2	2:F:279:ARG:NH1	2.82	0.47
2:L:322:LEU:CD2	2:L:360:ARG:NH2	2.77	0.47
2:F:162:LYS:HA	2:F:162:LYS:HE2	1.94	0.47
2:J:70:TYR:HD1	2:J:70:TYR:O	1.97	0.47
2:J:175:ILE:HG13	2:J:199:ILE:HD13	1.96	0.47
2:H:211:THR:CG2	2:H:212:TYR:CE2	2.98	0.46
2:H:333:GLN:HB2	4:H:515:HOH:O	2.15	0.46
2:H:91:PHE:HZ	2:F:324:GLY:HA3	1.76	0.46
2:H:299:LEU:CA	2:H:302:THR:HG22	2.45	0.46
2:F:213:GLU:HG2	2:F:215:PHE:CE2	2.50	0.46
2:F:305:ILE:CG1	2:F:327:ILE:HB	2.45	0.46
2:L:305:ILE:HD12	2:L:305:ILE:C	2.40	0.46
2:B:196:MET:CE	2:J:196:MET:HE1	2.22	0.46
2:B:242:ASN:HD22	2:B:258:ALA:HB2	1.80	0.46
2:D:267:VAL:HG22	4:D:544:HOH:O	2.15	0.46
2:J:353:LYS:CE	2:J:370:GLU:HG3	2.23	0.46
2:H:219:ASP:CG	2:L:195:THR:HG23	2.40	0.46
2:B:214:ASP:O	2:B:260:PRO:HD3	2.15	0.46
1:C:5:GLU:O	1:C:5:GLU:HG3	2.14	0.46
2:D:212:TYR:CE2	2:D:279:ARG:NE	2.83	0.46
2:F:74:MET:CE	2:F:101:ARG:HA	2.45	0.46
2:L:321:LEU:CD2	4:L:548:HOH:O	2.63	0.46
2:H:271:ILE:O	2:H:274:HIS:O	2.33	0.46
2:H:287:LYS:CG	2:H:306:VAL:HB	2.45	0.46
2:B:64:PRO:HD3	2:B:136:ARG:NH1	2.31	0.46
2:D:158:LYS:HD2	2:D:159:ILE:H	1.79	0.46
2:H:335:ALA:HA	2:H:341:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:THR:HG21	2:B:221:ALA:N	2.30	0.46
2:J:252:SER:HA	4:J:506:HOH:O	2.14	0.46
2:L:118:LEU:HB2	2:L:157:LEU:HB2	1.97	0.46
2:L:153:ASP:HB2	2:L:210:ASN:OD1	2.15	0.46
2:D:89:ARG:NH1	2:D:89:ARG:CG	2.71	0.46
2:D:112:MET:HG2	2:D:268:MET:CE	2.45	0.46
2:F:376:PRO:CB	4:F:519:HOH:O	2.63	0.46
2:L:328:LEU:O	2:L:335:ALA:HB3	2.14	0.46
2:D:252:SER:HB3	2:L:253:GLN:O	2.16	0.46
2:L:305:ILE:CD1	2:L:327:ILE:CB	2.22	0.46
2:B:85:ASP:OD1	2:B:86:PRO:HD3	2.16	0.46
2:B:301:GLU:O	2:B:302:THR:C	2.59	0.46
2:F:196:MET:HB2	2:J:198:ILE:HD13	1.96	0.46
2:J:71:THR:HG22	2:J:106:LEU:CD2	2.46	0.46
2:L:101:ARG:O	2:L:101:ARG:HG2	2.16	0.46
2:B:227:SER:HA	2:B:242:ASN:O	2.16	0.46
2:D:230:ALA:HB1	2:D:238:LEU:HD12	1.97	0.46
2:F:310:VAL:HG12	2:F:317:ALA:HB2	1.98	0.46
2:J:325:ASP:HB3	2:J:358:VAL:HG21	1.98	0.46
2:H:303:ALA:HB1	2:H:328:LEU:HB3	1.98	0.45
2:D:186:ASN:ND2	2:D:186:ASN:C	2.75	0.45
2:J:172:SER:O	2:J:175:ILE:HG23	2.16	0.45
2:J:242:ASN:ND2	4:J:501:HOH:O	2.49	0.45
2:L:296:SER:O	2:L:297:LEU:HD12	2.16	0.45
1:C:8:TRP:HB2	2:D:286:VAL:CG2	2.39	0.45
2:B:137:ASP:HB3	4:B:516:HOH:O	2.17	0.45
2:B:289:LEU:CD1	2:B:289:LEU:C	2.89	0.45
2:F:85:ASP:CG	2:F:90:ARG:HH12	2.24	0.45
2:F:284:VAL:CG1	2:F:316:ALA:CB	2.92	0.45
2:B:138:GLY:C	4:B:508:HOH:O	2.60	0.45
2:B:209:LEU:N	2:B:213:GLU:OE1	2.48	0.45
2:B:251:GLY:HA3	2:F:253:GLN:CD	2.42	0.45
2:D:85:ASP:CG	2:D:86:PRO:HD2	2.38	0.45
2:D:265:LEU:HD12	2:D:265:LEU:HA	1.80	0.45
2:F:121:ASN:HA	4:F:505:HOH:O	2.16	0.45
2:F:216:ILE:HD11	2:F:260:PRO:HB3	1.98	0.45
2:J:159:ILE:HD13	2:J:159:ILE:HA	1.75	0.45
2:H:145:LEU:HA	2:H:145:LEU:HD12	1.83	0.45
2:H:195:THR:HG21	2:H:221:ALA:HB3	1.98	0.45
2:H:303:ALA:HB1	2:H:328:LEU:O	2.17	0.45
2:D:292:GLU:H	2:D:292:GLU:HG2	1.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:112:MET:CE	2:H:119:LEU:HB3	2.25	0.45
2:B:181:CYS:SG	2:B:199:ILE:HD12	2.56	0.45
2:D:231:LEU:HD12	2:D:231:LEU:HA	1.75	0.45
2:F:214:ASP:O	2:F:260:PRO:HD3	2.17	0.45
2:F:267:VAL:HG13	2:F:277:VAL:CG2	2.39	0.45
2:F:303:ALA:HB1	2:F:328:LEU:HD23	1.98	0.45
2:F:304:GLY:H	2:F:336:SER:HA	1.82	0.45
2:L:305:ILE:HD11	2:L:327:ILE:CG2	2.27	0.45
2:H:91:PHE:CZ	2:F:324:GLY:N	2.84	0.45
2:H:151:GLU:OE1	2:H:211:THR:CB	2.65	0.45
2:H:289:LEU:HD12	2:H:293:LEU:HD23	1.97	0.45
2:B:259:ILE:CA	4:B:502:HOH:O	2.65	0.45
2:F:193:THR:CG2	2:J:217:GLN:HE22	2.29	0.45
2:F:331:ASP:CB	2:F:354:ILE:CG2	2.95	0.45
2:L:307:VAL:CG2	4:L:548:HOH:O	2.43	0.45
2:H:91:PHE:CZ	2:F:324:GLY:HA3	2.50	0.45
2:B:281:TRP:CZ2	2:B:283:GLY:HA2	2.51	0.45
2:F:75:VAL:CG2	2:F:100:LYS:HB2	2.46	0.45
2:F:231:LEU:HD22	2:F:258:ALA:HB3	1.99	0.45
2:L:142:ILE:HD13	4:L:549:HOH:O	2.16	0.45
2:D:299:LEU:HD13	2:D:302:THR:HG21	1.88	0.45
2:F:187:PRO:O	2:F:187:PRO:HG2	2.16	0.45
2:F:284:VAL:HG13	2:F:316:ALA:HB2	1.99	0.45
2:J:267:VAL:HG13	2:J:277:VAL:CG2	2.47	0.45
2:H:214:ASP:O	2:H:260:PRO:HG3	2.17	0.45
2:B:312:ARG:NH2	2:D:87:MET:CE	2.78	0.45
2:J:217:GLN:HG3	2:J:257:PHE:CE1	2.52	0.45
2:L:322:LEU:CD2	2:L:360:ARG:HH21	2.29	0.45
2:L:325:ASP:OD1	2:L:360:ARG:HG2	2.13	0.45
2:H:309:GLY:HA2	2:H:323:PRO:HB3	2.00	0.44
2:B:119:LEU:HA	2:B:119:LEU:HD12	1.82	0.44
2:D:101:ARG:HE	2:D:101:ARG:HB2	1.67	0.44
2:H:85:ASP:HB2	2:H:86:PRO:HD2	1.98	0.44
2:D:175:ILE:HD12	2:D:199:ILE:HD13	1.99	0.44
2:F:116:GLY:O	2:F:159:ILE:HB	2.17	0.44
2:F:347:ARG:HG2	2:F:347:ARG:NH1	2.33	0.44
2:L:115:GLU:O	2:L:158:LYS:HE2	2.18	0.44
2:H:186:ASN:C	2:H:186:ASN:HD22	2.25	0.44
2:H:299:LEU:HD13	2:H:299:LEU:HA	1.79	0.44
2:B:87:MET:HE2	2:B:87:MET:HB2	1.77	0.44
2:D:141:THR:HG22	4:D:537:HOH:O	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:PHE:CE1	2:B:83:PHE:CE1	3.04	0.44
2:D:76:SER:CB	2:D:99:GLN:HB3	2.46	0.44
2:D:83:PHE:CZ	2:J:92:PHE:CE2	3.06	0.44
1:K:4:ASP:OD1	1:K:4:ASP:N	2.50	0.44
2:B:314:GLY:HA3	4:B:511:HOH:O	2.17	0.44
2:D:96:LEU:HD23	2:D:97:PRO:N	2.32	0.44
2:L:187:PRO:HD2	2:L:193:THR:HG23	1.99	0.44
2:B:89:ARG:HD2	2:B:89:ARG:HA	1.79	0.44
2:D:95:ASN:HD22	2:D:95:ASN:HA	1.49	0.44
2:B:85:ASP:OD1	2:B:86:PRO:HD2	2.18	0.44
2:L:289:LEU:CD2	2:L:306:VAL:HG22	2.45	0.44
2:H:263:LEU:HD12	2:H:263:LEU:O	2.18	0.44
2:B:74:MET:HG3	2:B:101:ARG:HD3	2.00	0.44
2:D:110:VAL:HG13	2:D:167:MET:HE3	2.00	0.44
2:L:70:TYR:OH	2:L:140:GLU:OE2	2.35	0.44
2:L:321:LEU:CG	4:L:548:HOH:O	2.52	0.44
2:F:119:LEU:HD12	2:F:119:LEU:HA	1.60	0.44
2:F:326:VAL:O	2:F:358:VAL:HG13	2.18	0.44
2:H:70:TYR:CE1	2:H:132:ILE:HD13	2.44	0.43
2:H:282:LEU:O	2:H:316:ALA:CB	2.66	0.43
2:B:111:ILE:HG21	2:B:165:PRO:O	2.18	0.43
2:D:150:PRO:HD2	4:D:513:HOH:O	2.18	0.43
2:D:315:PRO:HD3	4:D:534:HOH:O	2.18	0.43
2:J:325:ASP:CG	2:J:360:ARG:HE	2.24	0.43
2:L:112:MET:HE1	2:L:238:LEU:CD2	2.47	0.43
2:L:164:LEU:HD23	2:L:164:LEU:HA	1.83	0.43
2:L:307:VAL:HG12	2:L:323:PRO:HA	2.00	0.43
2:H:326:VAL:HB	2:H:359:LEU:HB3	2.01	0.43
2:B:106:LEU:O	2:B:124:VAL:HG13	2.18	0.43
2:J:133:VAL:CG2	2:J:143:ALA:HB2	2.49	0.43
2:J:176:ARG:HG2	2:J:176:ARG:NH1	2.31	0.43
2:J:297:LEU:CD1	2:J:306:VAL:HG21	2.48	0.43
2:L:118:LEU:HD11	2:L:159:ILE:CG1	2.48	0.43
2:L:281:TRP:HB3	2:L:372:GLY:HA3	2.00	0.43
2:B:118:LEU:HB2	2:B:157:LEU:HB2	2.01	0.43
2:B:153:ASP:OD2	2:B:243:THR:CG2	2.65	0.43
2:B:186:ASN:O	2:B:225:GLY:HA3	2.18	0.43
2:J:195:THR:HG21	2:J:221:ALA:CA	2.48	0.43
2:L:96:LEU:N	2:L:97:PRO:HD3	2.33	0.43
2:L:135:LEU:N	2:L:135:LEU:HD12	2.33	0.43
2:L:74:MET:HE2	2:L:74:MET:CA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:223:ASN:O	2:H:226:ASN:HB2	2.19	0.43
2:D:69:LEU:CD2	2:D:133:VAL:HG22	2.48	0.43
2:D:103:GLU:H	2:D:103:GLU:HG3	1.55	0.43
2:D:182:LEU:HD23	2:D:194:VAL:HG11	2.00	0.43
2:F:337:ASP:HB3	2:F:340:ARG:HB2	1.99	0.43
2:J:245:ILE:HG22	2:J:256:GLY:CA	2.39	0.43
2:D:69:LEU:CB	2:D:106:LEU:CD2	2.96	0.43
2:F:119:LEU:CD1	2:F:156:VAL:HG22	2.49	0.43
2:F:182:LEU:HD23	2:F:194:VAL:HG12	2.01	0.43
2:J:161:LEU:HD23	2:J:161:LEU:HA	1.64	0.43
2:J:325:ASP:HB3	2:J:358:VAL:HG22	2.00	0.43
2:L:162:LYS:HD3	2:L:162:LYS:HA	1.61	0.43
2:B:223:ASN:O	2:B:226:ASN:HB2	2.19	0.43
2:B:325:ASP:OD1	2:B:360:ARG:CD	2.66	0.43
2:F:77:LYS:CG	2:F:100:LYS:HG3	2.49	0.43
2:F:147:GLY:HA3	2:F:271:ILE:HG23	2.00	0.43
2:J:65:ALA:CB	2:J:167:MET:HE2	2.41	0.43
2:L:281:TRP:HA	2:L:281:TRP:CE3	2.54	0.43
2:H:68:ASN:CA	4:H:525:HOH:O	2.41	0.43
2:H:72:THR:O	2:H:72:THR:OG1	2.30	0.43
2:J:158:LYS:HD2	2:J:158:LYS:HA	1.64	0.43
2:L:63:ALA:N	2:L:64:PRO:CD	2.82	0.43
2:L:80:HIS:CD2	2:L:81:PRO:HD2	2.54	0.43
2:L:93:GLY:C	4:L:516:HOH:O	2.53	0.43
2:L:151:GLU:OE1	2:L:151:GLU:HA	2.19	0.43
2:B:253:GLN:CD	2:J:251:GLY:HA3	2.44	0.43
2:D:63:ALA:N	2:D:64:PRO:CD	2.82	0.43
2:D:143:ALA:HA	2:D:159:ILE:HD12	1.99	0.43
2:D:205:ASN:CB	4:D:528:HOH:O	2.35	0.43
2:F:143:ALA:HB2	2:F:159:ILE:HD11	1.99	0.43
2:F:281:TRP:HB2	2:F:374:ARG:HA	2.00	0.43
1:K:6:LEU:HD21	2:L:287:LYS:CG	2.49	0.43
2:L:347:ARG:CG	3:L:401:IMD:H5	2.49	0.43
2:H:151:GLU:OE2	2:H:377:PRO:HG3	2.19	0.43
2:B:195:THR:HG22	2:B:221:ALA:H	1.84	0.43
2:D:96:LEU:HD23	2:D:97:PRO:CD	2.49	0.43
2:D:96:LEU:HD23	2:D:97:PRO:HD3	2.00	0.43
2:F:98:GLN:OE1	2:F:98:GLN:HA	2.19	0.43
2:J:143:ALA:HB2	2:J:159:ILE:HD11	2.01	0.43
2:L:118:LEU:HD11	2:L:159:ILE:HG13	2.01	0.43
2:B:193:THR:HG21	2:F:217:GLN:HE22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:LYS:HB3	2:F:78:PRO:CD	2.48	0.42
2:F:281:TRP:CZ2	2:F:283:GLY:HA2	2.54	0.42
2:L:321:LEU:CD1	2:L:358:VAL:CG2	2.97	0.42
1:A:9:VAL:HA	2:B:284:VAL:O	2.18	0.42
2:D:110:VAL:HB	2:D:112:MET:HE1	2.01	0.42
1:E:7:ARG:NH2	2:F:287:LYS:HE3	2.35	0.42
2:F:74:MET:HE3	2:F:100:LYS:O	2.18	0.42
2:F:77:LYS:HB3	2:F:78:PRO:HD2	2.00	0.42
2:F:137:ASP:N	4:F:508:HOH:O	2.42	0.42
1:K:7:ARG:HH11	1:K:7:ARG:CG	2.12	0.42
2:L:337:ASP:HB3	2:L:340:ARG:CG	2.48	0.42
2:D:295:GLU:O	2:D:295:GLU:HG2	2.16	0.42
2:F:65:ALA:CB	2:F:167:MET:HE2	2.37	0.42
2:J:343:ASN:HD22	3:J:401:IMD:HN3	1.66	0.42
2:L:124:VAL:CG2	2:L:227:SER:HB2	2.49	0.42
2:B:280:GLY:HA3	2:B:345:VAL:O	2.19	0.42
2:F:136:ARG:HB3	4:F:508:HOH:O	2.19	0.42
2:L:89:ARG:CG	2:L:89:ARG:NH1	2.80	0.42
2:B:325:ASP:CG	2:B:360:ARG:HD3	2.43	0.42
2:D:322:LEU:HD12	2:D:360:ARG:HD2	2.01	0.42
2:J:69:LEU:CD1	2:J:109:ALA:HB2	2.44	0.42
2:H:112:MET:HG2	2:H:268:MET:SD	2.60	0.42
2:H:269:GLN:H	2:H:269:GLN:HG2	1.69	0.42
2:J:292:GLU:H	2:J:292:GLU:HG3	1.74	0.42
2:L:103:GLU:H	2:L:103:GLU:HG2	1.54	0.42
2:H:204:ARG:HB2	2:H:215:PHE:CB	2.44	0.42
2:L:159:ILE:CG2	2:L:161:LEU:HG	2.50	0.42
1:G:6:LEU:HB3	2:H:287:LYS:HB2	2.01	0.42
2:H:281:TRP:H	2:H:371:VAL:HG13	1.84	0.42
2:B:90:ARG:HG2	2:D:308:ALA:O	2.19	0.42
2:B:111:ILE:O	2:B:111:ILE:HG22	2.19	0.42
2:F:117:TYR:CE1	2:F:272:ILE:HD13	2.55	0.42
2:L:75:VAL:HG22	2:L:100:LYS:O	2.15	0.42
2:B:172:SER:OG	2:B:261:THR:HG22	2.19	0.42
2:B:195:THR:HG21	2:B:221:ALA:H	1.81	0.42
2:B:310:VAL:HG22	2:D:89:ARG:CB	2.50	0.42
2:F:123:HIS:HD1	2:F:153:ASP:CG	2.17	0.42
2:F:248:LYS:HB2	2:F:253:GLN:HE22	1.85	0.42
2:H:87:MET:SD	2:F:311:TYR:HE1	2.38	0.41
2:D:280:GLY:HA3	2:D:345:VAL:O	2.19	0.41
4:F:511:HOH:O	2:L:82:LEU:HD12	2.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:80:HIS:CG	2:J:81:PRO:CD	2.91	0.41
2:B:230:ALA:HB1	2:B:238:LEU:CD1	2.50	0.41
2:F:55:TYR:CE2	2:F:180:VAL:HG11	2.56	0.41
2:F:69:LEU:N	4:F:514:HOH:O	2.52	0.41
2:F:70:TYR:HD1	2:F:105:SER:HA	1.85	0.41
2:L:204:ARG:HG2	2:L:204:ARG:HH11	1.85	0.41
2:H:299:LEU:CB	2:H:302:THR:CG2	2.98	0.41
2:B:182:LEU:HA	2:B:195:THR:O	2.20	0.41
2:D:302:THR:O	2:D:303:ALA:HB3	2.20	0.41
2:L:96:LEU:HD13	2:L:96:LEU:O	2.19	0.41
2:L:289:LEU:HD21	2:L:306:VAL:HG22	2.01	0.41
2:H:80:HIS:HB3	2:H:83:PHE:HB2	2.01	0.41
2:B:133:VAL:O	2:B:140:GLU:HA	2.20	0.41
2:B:216:ILE:HD12	4:B:506:HOH:O	2.20	0.41
2:B:312:ARG:O	2:B:312:ARG:CG	2.68	0.41
2:J:325:ASP:OD2	2:J:360:ARG:CZ	2.68	0.41
2:H:169:LEU:HD13	2:H:265:LEU:HD11	2.01	0.41
2:H:280:GLY:HA3	2:H:345:VAL:O	2.20	0.41
2:B:226:ASN:ND2	4:B:504:HOH:O	1.93	0.41
2:L:94:ASP:HB3	2:L:97:PRO:CD	2.51	0.41
2:H:69:LEU:HD21	2:H:133:VAL:HG22	2.01	0.41
2:B:337:ASP:HB3	2:B:340:ARG:HE	1.86	0.41
2:F:85:ASP:OD1	2:F:86:PRO:CD	2.69	0.41
2:F:353:LYS:HE3	2:F:370:GLU:HG3	2.02	0.41
2:J:63:ALA:N	2:J:64:PRO:CD	2.81	0.41
2:J:186:ASN:C	2:J:186:ASN:ND2	2.78	0.41
2:L:158:LYS:HD2	2:L:159:ILE:H	1.85	0.41
2:L:195:THR:CB	4:L:515:HOH:O	1.75	0.41
2:L:205:ASN:HD22	2:L:339:ARG:HD2	1.74	0.41
2:L:360:ARG:NE	4:L:513:HOH:O	2.53	0.41
2:H:214:ASP:O	2:H:260:PRO:CG	2.67	0.41
2:H:283:GLY:O	2:H:311:TYR:HB2	2.21	0.41
2:B:181:CYS:HB3	2:B:199:ILE:HD11	2.01	0.41
2:F:116:GLY:HA2	2:F:164:LEU:CD1	2.51	0.41
2:J:253:GLN:N	4:J:506:HOH:O	2.35	0.41
2:B:177:THR:HG23	2:B:199:ILE:O	2.20	0.41
2:B:361:ASN:ND2	2:B:361:ASN:N	2.59	0.41
2:D:161:LEU:CB	2:D:164:LEU:HD13	2.38	0.41
2:J:98:GLN:HA	2:J:98:GLN:HE21	1.83	0.41
2:L:68:ASN:OD1	2:L:186:ASN:ND2	2.52	0.41
2:B:273:GLU:HG2	2:B:274:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:164:LEU:HD23	2:F:164:LEU:HA	1.72	0.41
2:F:243:THR:HG21	2:F:259:ILE:CG1	2.48	0.41
2:L:133:VAL:O	2:L:140:GLU:HA	2.21	0.41
2:H:151:GLU:OE1	2:H:211:THR:HB	2.21	0.40
2:H:376:PRO:HA	2:H:377:PRO:HD3	1.87	0.40
2:B:82:LEU:HD12	2:B:92:PHE:CD2	2.56	0.40
2:B:221:ALA:HA	2:B:252:SER:OG	2.21	0.40
2:D:327:ILE:HA	2:D:358:VAL:HG23	2.03	0.40
2:F:291:PRO:HA	2:F:294:ALA:CB	2.50	0.40
4:F:511:HOH:O	2:L:82:LEU:HD11	2.12	0.40
2:J:195:THR:HG22	2:J:220:ALA:HB1	2.03	0.40
2:J:331:ASP:CB	2:J:354:ILE:HB	2.51	0.40
2:L:156:VAL:CG2	2:L:268:MET:HG3	2.50	0.40
2:L:260:PRO:HB2	4:L:521:HOH:O	2.21	0.40
2:L:349:ARG:HH21	2:L:349:ARG:HD3	1.66	0.40
2:H:271:ILE:C	2:H:274:HIS:O	2.64	0.40
2:B:66:VAL:HG11	2:B:184:ILE:HG22	2.04	0.40
2:F:96:LEU:HB2	2:F:97:PRO:HD2	2.03	0.40
2:F:275:GLY:C	2:F:276:GLN:HG3	2.47	0.40
2:F:377:PRO:CD	4:F:519:HOH:O	2.69	0.40
2:J:85:ASP:HB3	2:J:88:PHE:HB2	2.04	0.40
2:J:98:GLN:NE2	2:J:98:GLN:CA	2.74	0.40
2:L:173:ASP:OD2	2:L:262:LYS:HE2	2.21	0.40
2:D:175:ILE:N	4:D:501:HOH:O	2.46	0.40
2:D:251:GLY:HA3	2:L:253:GLN:HE22	1.86	0.40
2:F:190:VAL:O	2:F:190:VAL:CG1	2.70	0.40
2:J:64:PRO:O	2:J:165:PRO:HG2	2.21	0.40
2:D:186:ASN:O	2:D:225:GLY:C	2.64	0.40
2:D:232:VAL:CG1	2:D:236:GLY:HA2	2.48	0.40
2:L:96:LEU:CD1	2:L:96:LEU:O	2.69	0.40
1:A:6:LEU:HD12	1:A:6:LEU:C	2.47	0.40
2:B:85:ASP:HB2	2:B:90:ARG:HH12	1.86	0.40
2:B:182:LEU:O	2:B:231:LEU:HD12	2.21	0.40
2:D:100:LYS:HD2	2:D:101:ARG:N	2.33	0.40
2:F:121:ASN:HD21	2:F:243:THR:HG22	1.86	0.40
2:L:222:ILE:HD13	2:L:242:ASN:HB3	2.02	0.40
2:L:305:ILE:CD1	2:L:327:ILE:CG1	2.96	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:ARG:NH1	2:B:296:SER:O[1_655]	1.87	0.33
2:B:61:ARG:NH1	2:J:301:GLU:OE2[3_545]	2.17	0.03

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	5/10 (50%)	5 (100%)	0	0	100	100
1	C	5/10 (50%)	5 (100%)	0	0	100	100
1	E	4/10 (40%)	4 (100%)	0	0	100	100
1	G	4/10 (40%)	4 (100%)	0	0	100	100
1	I	4/10 (40%)	4 (100%)	0	0	100	100
1	K	7/10 (70%)	7 (100%)	0	0	100	100
2	B	323/377 (86%)	316 (98%)	6 (2%)	1 (0%)	36	41
2	D	323/377 (86%)	318 (98%)	4 (1%)	1 (0%)	36	41
2	F	323/377 (86%)	318 (98%)	5 (2%)	0	100	100
2	H	323/377 (86%)	309 (96%)	14 (4%)	0	100	100
2	J	323/377 (86%)	316 (98%)	5 (2%)	2 (1%)	21	22
2	L	323/377 (86%)	318 (98%)	3 (1%)	2 (1%)	21	22
All	All	1967/2322 (85%)	1924 (98%)	37 (2%)	6 (0%)	36	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	97	PRO
2	B	96	LEU
2	J	96	LEU
2	D	96	LEU
2	L	97	PRO
2	L	186	ASN

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	7/10 (70%)	6 (86%)	1 (14%)	3	2
1	C	7/10 (70%)	7 (100%)	0	100	100
1	E	6/10 (60%)	5 (83%)	1 (17%)	2	1
1	G	6/10 (60%)	5 (83%)	1 (17%)	2	1
1	I	6/10 (60%)	3 (50%)	3 (50%)	0	0
1	K	9/10 (90%)	6 (67%)	3 (33%)	0	0
2	B	253/298 (85%)	213 (84%)	40 (16%)	2	2
2	D	253/298 (85%)	204 (81%)	49 (19%)	1	1
2	F	253/298 (85%)	205 (81%)	48 (19%)	1	1
2	H	253/298 (85%)	226 (89%)	27 (11%)	6	5
2	J	253/298 (85%)	201 (79%)	52 (21%)	1	1
2	L	253/298 (85%)	205 (81%)	48 (19%)	1	1
All	All	1559/1848 (84%)	1286 (82%)	273 (18%)	2	1

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	6	LEU
2	H	53	VAL
2	H	84	ASP
2	H	94	ASP
2	H	121	ASN
2	H	132	ILE
2	H	144	GLN
2	H	148	SER
2	H	175	ILE
2	H	190	VAL
2	H	209	LEU
2	H	211	THR
2	H	232	VAL
2	H	248	LYS

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Mol	Chain	Res	Type
2	H	263	LEU
2	H	265	LEU
2	H	266	GLU
2	H	269	GLN
2	H	274	HIS
2	H	286	VAL
2	H	292	GLU
2	H	302	THR
2	H	310	VAL
2	H	329	THR
2	H	336	SER
2	H	340	ARG
2	H	358	VAL
2	H	368	THR
1	A	6	LEU
2	B	53	VAL
2	B	71	THR
2	B	72	THR
2	B	74	MET
2	B	77	LYS
2	B	82	LEU
2	B	85	ASP
2	B	87	MET
2	B	89	ARG
2	B	98	GLN
2	B	100	LYS
2	B	113	SER
2	B	132	ILE
2	B	135	LEU
2	B	136	ARG
2	B	151	GLU
2	B	162	LYS
2	B	176	ARG
2	B	196	MET
2	B	199	ILE
2	B	211	THR
2	B	216	ILE
2	B	227	SER
2	B	232	VAL
2	B	261	THR
2	B	273	GLU
2	B	274	HIS

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Mol	Chain	Res	Type
2	B	282	LEU
2	B	287	LYS
2	B	295	GLU
2	B	301	GLU
2	B	313	ASP
2	B	328	LEU
2	B	329	THR
2	B	332	LYS
2	B	342	MET
2	B	352	GLN
2	B	358	VAL
2	B	361	ASN
2	B	363	GLN
2	D	60	SER
2	D	71	THR
2	D	73	LYS
2	D	74	MET
2	D	75	VAL
2	D	77	LYS
2	D	89	ARG
2	D	91	PHE
2	D	95	ASN
2	D	96	LEU
2	D	99	GLN
2	D	100	LYS
2	D	101	ARG
2	D	103	GLU
2	D	104	SER
2	D	106	LEU
2	D	113	SER
2	D	130	GLN
2	D	141	THR
2	D	142	ILE
2	D	144	GLN
2	D	159	ILE
2	D	164	LEU
2	D	172	SER
2	D	186	ASN
2	D	198	ILE
2	D	222	ILE
2	D	227	SER
2	D	232	VAL

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Mol	Chain	Res	Type
2	D	239	ILE
2	D	253	GLN
2	D	261	THR
2	D	265	LEU
2	D	284	VAL
2	D	285	GLU
2	D	286	VAL
2	D	289	LEU
2	D	292	GLU
2	D	295	GLU
2	D	301	GLU
2	D	305	ILE
2	D	321	LEU
2	D	322	LEU
2	D	333	GLN
2	D	352	GLN
2	D	357	VAL
2	D	358	VAL
2	D	359	LEU
2	D	368	THR
1	E	6	LEU
2	F	53	VAL
2	F	54	SER
2	F	61	ARG
2	F	64	PRO
2	F	66	VAL
2	F	73	LYS
2	F	74	MET
2	F	76	SER
2	F	77	LYS
2	F	85	ASP
2	F	91	PHE
2	F	102	MET
2	F	103	GLU
2	F	106	LEU
2	F	118	LEU
2	F	119	LEU
2	F	135	LEU
2	F	141	THR
2	F	142	ILE
2	F	148	SER
2	F	151	GLU

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Mol	Chain	Res	Type
2	F	160	ASP
2	F	162	LYS
2	F	171	ARG
2	F	176	ARG
2	F	190	VAL
2	F	207	LEU
2	F	209	LEU
2	F	219	ASP
2	F	227	SER
2	F	232	VAL
2	F	243	THR
2	F	262	LYS
2	F	273	GLU
2	F	278	ILE
2	F	282	LEU
2	F	285	GLU
2	F	290	THR
2	F	295	GLU
2	F	301	GLU
2	F	302	THR
2	F	312	ARG
2	F	322	LEU
2	F	332	LYS
2	F	342	MET
2	F	354	ILE
2	F	355	SER
2	F	360	ARG
1	I	5	GLU
1	I	6	LEU
1	I	9	VAL
2	J	53	VAL
2	J	59	VAL
2	J	61	ARG
2	J	70	TYR
2	J	75	VAL
2	J	87	MET
2	J	89	ARG
2	J	94	ASP
2	J	95	ASN
2	J	100	LYS
2	J	102	MET
2	J	104	SER

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Mol	Chain	Res	Type
2	J	106	LEU
2	J	112	MET
2	J	129	ASP
2	J	131	ILE
2	J	141	THR
2	J	142	ILE
2	J	158	LYS
2	J	159	ILE
2	J	162	LYS
2	J	168	THR
2	J	172	SER
2	J	175	ILE
2	J	182	LEU
2	J	192	GLN
2	J	194	VAL
2	J	200	SER
2	J	205	ASN
2	J	206	GLN
2	J	222	ILE
2	J	255	ILE
2	J	261	THR
2	J	263	LEU
2	J	265	LEU
2	J	276	GLN
2	J	278	ILE
2	J	289	LEU
2	J	292	GLU
2	J	293	LEU
2	J	299	LEU
2	J	301	GLU
2	J	305	ILE
2	J	307	VAL
2	J	334	GLU
2	J	336	SER
2	J	337	ASP
2	J	339	ARG
2	J	350	PRO
2	J	358	VAL
2	J	363	GLN
2	J	368	THR
1	K	4	ASP
1	K	6	LEU

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Mol	Chain	Res	Type
1	K	7	ARG
2	L	53	VAL
2	L	61	ARG
2	L	74	MET
2	L	75	VAL
2	L	76	SER
2	L	85	ASP
2	L	87	MET
2	L	89	ARG
2	L	95	ASN
2	L	96	LEU
2	L	98	GLN
2	L	100	LYS
2	L	103	GLU
2	L	113	SER
2	L	130	GLN
2	L	142	ILE
2	L	145	LEU
2	L	161	LEU
2	L	162	LYS
2	L	172	SER
2	L	175	ILE
2	L	190	VAL
2	L	193	THR
2	L	199	ILE
2	L	207	LEU
2	L	209	LEU
2	L	237	ASN
2	L	243	THR
2	L	255	ILE
2	L	276	GLN
2	L	278	ILE
2	L	282	LEU
2	L	289	LEU
2	L	290	THR
2	L	297	LEU
2	L	301	GLU
2	L	313	ASP
2	L	322	LEU
2	L	326	VAL
2	L	328	LEU
2	L	329	THR

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Mol	Chain	Res	Type
2	L	334	GLU
2	L	342	MET
2	L	358	VAL
2	L	359	LEU
2	L	363	GLN
2	L	367	LEU
2	L	368	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	95	ASN
2	H	98	GLN
2	H	186	ASN
2	H	205	ASN
2	H	217	GLN
2	H	237	ASN
2	H	253	GLN
2	H	276	GLN
2	H	344	GLN
2	B	80	HIS
2	B	95	ASN
2	B	122	ASN
2	B	130	GLN
2	B	144	GLN
2	B	163	ASN
2	B	223	ASN
2	B	237	ASN
2	B	242	ASN
2	B	276	GLN
2	B	343	ASN
2	B	344	GLN
2	B	361	ASN
2	B	363	GLN
2	D	80	HIS
2	D	95	ASN
2	D	186	ASN
2	D	276	GLN
2	D	343	ASN
2	D	361	ASN
2	F	121	ASN
2	F	122	ASN

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Mol	Chain	Res	Type
2	F	226	ASN
2	F	276	GLN
2	F	343	ASN
2	F	361	ASN
2	J	68	ASN
2	J	98	GLN
2	J	186	ASN
2	J	223	ASN
2	J	242	ASN
2	J	276	GLN
2	J	343	ASN
2	J	344	GLN
2	L	57	ASN
2	L	99	GLN
2	L	122	ASN
2	L	186	ASN
2	L	205	ASN
2	L	223	ASN
2	L	242	ASN
2	L	253	GLN
2	L	276	GLN
2	L	361	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	IMD	L	401	-	5,5,5	0.65	0	5,5,5	0.71	0
3	IMD	H	401	-	5,5,5	0.55	0	5,5,5	0.19	0
3	IMD	F	401	-	5,5,5	0.60	0	5,5,5	0.46	0
3	IMD	D	401	-	5,5,5	0.49	0	5,5,5	0.78	0
3	IMD	B	401	-	5,5,5	0.56	0	5,5,5	0.30	0
3	IMD	J	401	-	5,5,5	0.51	0	5,5,5	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	L	401	-	-	-	0/1/1/1
3	IMD	H	401	-	-	-	0/1/1/1
3	IMD	F	401	-	-	-	0/1/1/1
3	IMD	D	401	-	-	-	0/1/1/1
3	IMD	B	401	-	-	-	0/1/1/1
3	IMD	J	401	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	401	IMD	4	0
3	H	401	IMD	8	0
3	F	401	IMD	3	0
3	D	401	IMD	3	0
3	B	401	IMD	1	0
3	J	401	IMD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	7/10 (70%)	2.13	3 (42%) 0 0	20, 41, 53, 70	0
1	C	7/10 (70%)	1.67	3 (42%) 0 0	18, 33, 67, 72	0
1	E	6/10 (60%)	3.08	5 (83%) 0 0	32, 45, 66, 69	0
1	G	6/10 (60%)	2.79	3 (50%) 0 0	20, 34, 59, 64	0
1	I	6/10 (60%)	1.65	2 (33%) 1 1	19, 29, 40, 71	0
1	K	9/10 (90%)	3.82	6 (66%) 0 0	29, 69, 85, 94	0
2	B	325/377 (86%)	1.24	56 (17%) 4 4	9, 27, 77, 101	0
2	D	325/377 (86%)	1.33	68 (20%) 2 3	6, 27, 76, 116	0
2	F	325/377 (86%)	1.25	77 (23%) 2 1	8, 31, 63, 97	0
2	H	325/377 (86%)	1.12	56 (17%) 4 4	8, 25, 70, 100	0
2	J	325/377 (86%)	1.16	62 (19%) 3 3	9, 27, 65, 114	0
2	L	325/377 (86%)	1.27	75 (23%) 2 2	7, 27, 73, 99	0
All	All	1991/2322 (85%)	1.26	416 (20%) 2 3	6, 27, 73, 116	0

All (416) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	96	LEU	13.9
2	B	297	LEU	11.7
2	B	94	ASP	9.2
2	L	297	LEU	9.1
2	D	96	LEU	9.0
2	L	303	ALA	8.8
2	D	74	MET	8.3
2	L	96	LEU	8.0
2	L	304	GLY	7.9
2	D	93	GLY	7.9
2	J	78	PRO	7.8

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Mol	Chain	Res	Type	RSRZ
2	F	299	LEU	7.8
2	H	297	LEU	7.8
2	B	303	ALA	7.6
2	J	99	GLN	7.5
2	B	98	GLN	7.4
2	H	299	LEU	7.3
2	B	299	LEU	7.3
2	J	95	ASN	7.2
1	K	2	VAL	7.1
2	H	98	GLN	7.1
2	B	96	LEU	7.0
2	H	87	MET	7.0
2	H	78	PRO	7.0
2	H	95	ASN	6.8
2	J	74	MET	6.8
2	L	300	GLY	6.7
2	F	300	GLY	6.7
2	L	299	LEU	6.6
2	F	301	GLU	6.5
2	D	75	VAL	6.5
2	D	94	ASP	6.5
2	J	93	GLY	6.4
2	B	97	PRO	6.4
2	D	73	LYS	6.1
2	B	302	THR	6.1
2	L	95	ASN	6.1
2	F	302	THR	6.0
2	H	303	ALA	5.9
2	J	97	PRO	5.9
1	E	6	LEU	5.9
2	D	297	LEU	5.9
2	D	97	PRO	5.9
2	J	75	VAL	5.9
2	D	299	LEU	5.9
1	K	6	LEU	5.8
2	L	302	THR	5.8
2	H	97	PRO	5.8
2	B	298	GLY	5.7
2	D	304	GLY	5.7
2	L	290	THR	5.6
2	D	78	PRO	5.6
2	B	75	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
2	D	77	LYS	5.6
2	H	76	SER	5.6
2	D	302	THR	5.6
2	F	303	ALA	5.5
2	J	100	LYS	5.5
2	B	93	GLY	5.3
2	D	70	TYR	5.2
2	D	102	MET	5.2
2	B	76	SER	5.2
2	H	77	LYS	5.1
2	D	95	ASN	5.1
2	H	94	ASP	5.1
2	H	74	MET	5.1
1	G	7	ARG	5.1
1	I	5	GLU	5.0
2	H	102	MET	5.0
2	L	335	ALA	5.0
2	H	300	GLY	5.0
2	B	79	SER	4.9
2	F	95	ASN	4.9
2	D	99	GLN	4.8
2	B	78	PRO	4.8
2	B	95	ASN	4.8
2	L	97	PRO	4.8
2	L	76	SER	4.7
1	K	4	ASP	4.7
2	F	96	LEU	4.7
2	H	91	PHE	4.7
2	D	91	PHE	4.6
2	H	298	GLY	4.6
2	D	87	MET	4.6
2	D	92	PHE	4.5
2	J	79	SER	4.5
2	L	291	PRO	4.5
2	D	72	THR	4.5
2	B	300	GLY	4.5
1	K	7	ARG	4.5
2	D	129	ASP	4.4
2	L	292	GLU	4.4
2	L	301	GLU	4.4
2	L	334	GLU	4.4
2	D	100	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
2	L	73	LYS	4.4
2	J	76	SER	4.4
2	D	101	ARG	4.3
2	J	102	MET	4.3
2	F	75	VAL	4.3
1	A	4	ASP	4.3
2	L	77	LYS	4.3
2	D	98	GLN	4.3
2	H	79	SER	4.2
2	L	78	PRO	4.2
2	B	77	LYS	4.2
2	D	303	ALA	4.2
2	L	305	ILE	4.2
2	H	73	LYS	4.2
2	F	289	LEU	4.2
2	B	102	MET	4.1
2	B	100	LYS	4.1
2	J	77	LYS	4.1
2	B	296	SER	4.1
2	F	291	PRO	4.1
1	G	6	LEU	4.0
2	F	298	GLY	4.0
2	F	76	SER	4.0
2	D	88	PHE	4.0
2	L	313	ASP	4.0
2	H	53	VAL	4.0
2	L	298	GLY	4.0
2	J	276	GLN	4.0
2	H	75	VAL	4.0
2	B	101	ARG	4.0
2	D	82	LEU	4.0
2	D	80	HIS	3.9
2	H	302	THR	3.9
1	G	5	GLU	3.9
2	J	70	TYR	3.9
2	L	293	LEU	3.9
2	F	290	THR	3.9
2	D	313	ASP	3.8
2	H	92	PHE	3.8
2	D	76	SER	3.8
2	J	98	GLN	3.8
2	J	73	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	94	ASP	3.8
2	L	205	ASN	3.8
2	B	70	TYR	3.8
2	H	99	GLN	3.8
2	B	301	GLU	3.8
2	D	83	PHE	3.8
2	F	292	GLU	3.7
2	F	363	GLN	3.7
2	J	128	ALA	3.7
2	B	129	ASP	3.7
2	H	100	LYS	3.7
1	K	5	GLU	3.6
2	F	293	LEU	3.6
2	L	361	ASN	3.6
2	D	212	TYR	3.6
2	L	75	VAL	3.6
2	L	296	SER	3.5
2	H	93	GLY	3.5
2	J	101	ARG	3.5
2	B	336	SER	3.5
2	L	102	MET	3.5
2	L	359	LEU	3.5
2	L	366	ASN	3.5
1	K	3	ARG	3.5
2	B	81	PRO	3.4
2	J	104	SER	3.4
2	H	301	GLU	3.4
2	H	101	ARG	3.4
2	D	293	LEU	3.4
2	F	89	ARG	3.4
2	F	276	GLN	3.4
2	F	79	SER	3.4
2	L	294	ALA	3.4
2	F	87	MET	3.4
2	F	102	MET	3.4
2	F	362	GLY	3.4
2	L	100	LYS	3.4
2	L	282	LEU	3.3
2	J	83	PHE	3.3
2	J	71	THR	3.3
2	J	72	THR	3.3
2	B	99	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	89	ARG	3.3
2	F	246	PHE	3.3
2	B	363	GLN	3.3
2	H	129	ASP	3.3
2	D	79	SER	3.3
2	D	298	GLY	3.2
1	A	6	LEU	3.2
2	H	83	PHE	3.2
2	J	246	PHE	3.2
2	F	324	GLY	3.2
2	D	160	ASP	3.2
2	L	328	LEU	3.2
2	L	363	GLN	3.2
2	F	100	LYS	3.1
2	B	83	PHE	3.1
2	D	300	GLY	3.1
2	L	358	VAL	3.1
2	F	98	GLN	3.1
2	L	101	ARG	3.1
1	E	5	GLU	3.1
2	H	115	GLU	3.1
2	J	94	ASP	3.1
2	F	206	GLN	3.1
2	F	97	PRO	3.1
2	L	295	GLU	3.1
2	H	96	LEU	3.1
2	J	81	PRO	3.1
1	C	5	GLU	3.1
2	F	352	GLN	3.1
2	J	92	PHE	3.1
2	F	312	ARG	3.1
2	D	103	GLU	3.0
2	F	370	GLU	3.0
1	C	4	ASP	3.0
2	D	71	THR	3.0
2	D	130	GLN	3.0
2	D	296	SER	3.0
2	D	128	ALA	3.0
2	F	297	LEU	3.0
2	F	339	ARG	3.0
2	F	73	LYS	2.9
2	F	332	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	101	ARG	2.9
2	L	368	THR	2.9
2	B	334	GLU	2.9
2	J	103	GLU	2.9
2	J	129	ASP	2.9
2	J	163	ASN	2.9
2	L	357	VAL	2.9
2	H	290	THR	2.9
2	L	98	GLN	2.9
2	D	213	GLU	2.9
2	B	74	MET	2.9
2	L	160	ASP	2.9
2	L	336	SER	2.8
2	B	293	LEU	2.8
2	F	321	LEU	2.8
2	F	277	VAL	2.8
2	F	129	ASP	2.8
2	F	296	SER	2.8
2	F	70	TYR	2.8
2	B	92	PHE	2.8
2	F	334	GLU	2.8
2	F	94	ASP	2.8
2	H	275	GLY	2.8
2	D	362	GLY	2.8
2	H	291	PRO	2.8
2	L	74	MET	2.8
2	B	269	GLN	2.8
2	J	91	PHE	2.8
2	D	53	VAL	2.8
2	J	243	THR	2.7
2	F	77	LYS	2.7
2	B	85	ASP	2.7
2	F	361	ASN	2.7
2	D	301	GLU	2.7
2	B	141	THR	2.7
2	J	84	ASP	2.7
2	F	93	GLY	2.7
1	E	8	TRP	2.7
2	D	294	ALA	2.7
2	F	128	ALA	2.7
2	H	292	GLU	2.7
2	H	127	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	296	SER	2.7
2	B	291	PRO	2.7
2	J	105	SER	2.7
1	A	8	TRP	2.7
2	L	249	SER	2.6
2	H	160	ASP	2.6
1	E	7	ARG	2.6
2	F	86	PRO	2.6
2	L	321	LEU	2.6
2	H	88	PHE	2.6
2	B	91	PHE	2.6
2	D	81	PRO	2.6
2	L	93	GLY	2.6
2	L	99	GLN	2.6
2	B	82	LEU	2.6
2	F	314	GLY	2.6
2	L	188	PHE	2.6
2	L	329	THR	2.6
2	L	353	LYS	2.6
2	L	161	LEU	2.5
2	L	289	LEU	2.5
2	L	129	ASP	2.5
2	F	359	LEU	2.5
2	J	82	LEU	2.5
2	F	74	MET	2.5
2	F	294	ALA	2.5
2	L	314	GLY	2.5
2	L	324	GLY	2.5
2	H	246	PHE	2.5
2	F	356	ILE	2.5
2	B	89	ARG	2.5
1	I	6	LEU	2.5
2	H	128	ALA	2.5
2	J	335	ALA	2.5
2	J	206	GLN	2.5
1	E	9	VAL	2.5
2	H	318	ARG	2.5
2	L	354	ILE	2.5
2	D	106	LEU	2.5
2	J	80	HIS	2.5
2	L	369	ALA	2.5
2	B	292	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	53	VAL	2.4
2	J	188	PHE	2.4
2	D	311	TYR	2.4
2	L	85	ASP	2.4
2	H	89	ARG	2.4
2	H	250	GLY	2.4
2	D	86	PRO	2.4
2	J	161	LEU	2.4
2	J	214	ASP	2.4
2	B	294	ALA	2.4
2	L	377	PRO	2.4
2	F	320	GLY	2.4
2	J	275	GLY	2.4
2	J	106	LEU	2.4
2	L	206	GLN	2.4
2	L	311	TYR	2.4
2	F	331	ASP	2.4
2	D	141	THR	2.4
2	F	162	LYS	2.4
2	D	305	ILE	2.4
2	F	278	ILE	2.4
2	D	144	GLN	2.4
2	J	296	SER	2.3
2	L	53	VAL	2.3
2	B	312	ARG	2.3
2	H	206	GLN	2.3
2	H	219	ASP	2.3
2	B	313	ASP	2.3
2	B	73	LYS	2.3
2	F	377	PRO	2.3
2	D	142	ILE	2.3
2	H	293	LEU	2.3
2	F	366	ASN	2.3
2	J	162	LYS	2.3
2	B	320	GLY	2.3
2	H	113	SER	2.3
2	F	360	ARG	2.3
2	J	247	SER	2.3
2	L	356	ILE	2.3
2	H	209	LEU	2.3
2	B	205	ASN	2.3
2	F	85	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	291	PRO	2.3
2	L	189	GLY	2.3
2	J	305	ILE	2.3
2	L	327	ILE	2.3
2	L	246	PHE	2.2
2	B	340	ARG	2.2
2	J	89	ARG	2.2
2	H	70	TYR	2.2
2	B	290	THR	2.2
2	J	278	ILE	2.2
2	F	284	VAL	2.2
2	H	186	ASN	2.2
2	J	300	GLY	2.2
2	J	295	GLU	2.2
2	F	144	GLN	2.2
2	J	169	LEU	2.2
2	F	92	PHE	2.2
2	D	90	ARG	2.2
2	J	87	MET	2.2
2	B	162	LYS	2.2
2	F	287	LYS	2.2
2	D	117	TYR	2.2
2	J	142	ILE	2.2
2	B	318	ARG	2.2
2	D	282	LEU	2.2
2	J	349	ARG	2.2
2	H	173	ASP	2.2
2	D	377	PRO	2.2
2	H	103	GLU	2.2
2	F	364	LYS	2.2
2	J	273	GLU	2.2
2	F	340	ARG	2.1
2	J	85	ASP	2.1
2	F	78	PRO	2.1
2	B	324	GLY	2.1
2	L	250	GLY	2.1
2	L	283	GLY	2.1
2	D	105	SER	2.1
2	F	308	ALA	2.1
2	D	159	ILE	2.1
2	J	131	ILE	2.1
2	J	205	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	312	ARG	2.1
2	F	349	ARG	2.1
1	C	6	LEU	2.1
2	F	103	GLU	2.1
2	D	85	ASP	2.1
2	J	242	ASN	2.1
2	F	286	VAL	2.1
2	B	127	GLY	2.1
2	F	304	GLY	2.1
2	B	248	LYS	2.1
2	B	103	GLU	2.1
2	L	213	GLU	2.1
2	H	85	ASP	2.1
2	B	214	ASP	2.1
2	L	90	ARG	2.1
2	L	312	ARG	2.1
2	H	72	THR	2.0
2	F	72	THR	2.0
2	F	288	ALA	2.0
2	D	363	GLN	2.0
2	J	130	GLN	2.0
2	D	286	VAL	2.0
2	L	162	LYS	2.0
2	F	336	SER	2.0
2	J	292	GLU	2.0
2	L	288	ALA	2.0
2	H	333	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	IMD	L	401	5/5	0.81	0.24	24,26,32,34	0
3	IMD	B	401	5/5	0.86	0.17	29,29,39,43	0
3	IMD	H	401	5/5	0.86	0.14	32,33,39,42	0
3	IMD	D	401	5/5	0.88	0.13	24,26,31,31	0
3	IMD	F	401	5/5	0.89	0.12	25,32,36,38	0
3	IMD	J	401	5/5	0.90	0.16	24,25,41,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.