



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:40 PM UTC

PDB ID : 5D9A / pdb_00005d9a
Title : Influenza C Virus RNA-dependent RNA Polymerase - Space group P212121
Authors : Hengrung, N.; El Omari, K.; Serna Martin, I.; Vreede, F.T.; Cusack, S.; Rambo, R.P.; Vonrhein, C.; Bricogne, G.; Stuart, D.I.; Grimes, J.M.; Fodor, E.
Deposited on : 2015-08-18
Resolution : 4.30 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
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

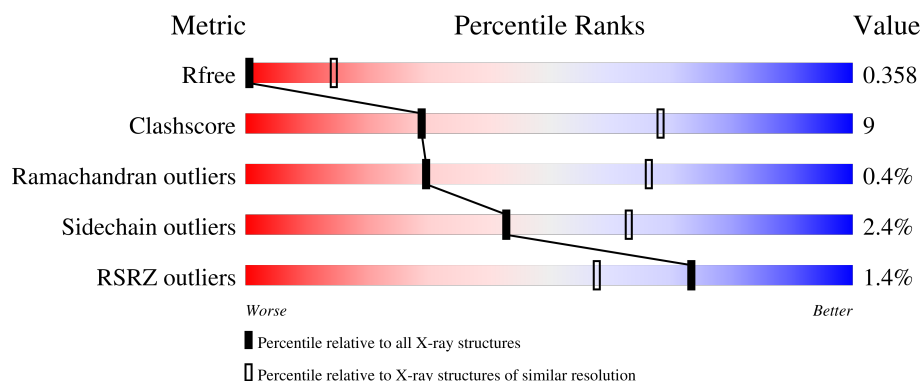
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	709	79% 18% ..
1	D	709	2% 73% 23% ..
1	G	709	80% 17% ..
1	J	709	81% 15% ..
2	B	754	80% 13% 6%

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Mol	Chain	Length	Quality of chain
2	E	754	% 80% 13% • 6%
2	H	754	% 79% 15% • 6%
2	K	754	82% 12% • 6%
3	C	782	2% 85% 10% • •
3	F	782	4% 81% 15% • •
3	I	782	% 83% 14% • •
3	L	782	2% 86% 11% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 69371 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	D	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	G	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			
1	J	693	Total	C	N	O	S	0	0	0
			5630	3589	954	1043	44			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	E	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	H	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			
2	K	711	Total	C	N	O	S	0	0	0
			5652	3587	956	1056	53			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	754	Total	C	N	O	S	0	0	0
			6015	3806	1056	1117	36			
3	F	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			
3	I	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			
3	L	762	Total	C	N	O	S	0	0	0
			6076	3845	1066	1128	37			

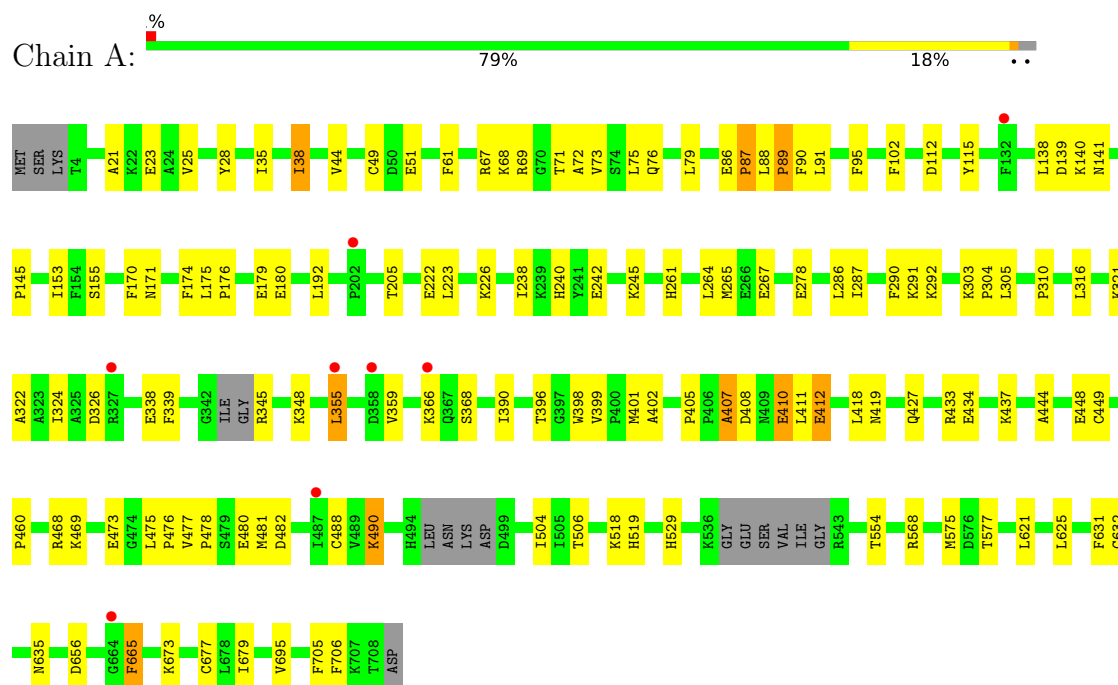
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	775	ALA	-	expression tag	UNP Q9IMP3
C	776	ARG	-	expression tag	UNP Q9IMP3
C	777	GLU	-	expression tag	UNP Q9IMP3
C	778	ASN	-	expression tag	UNP Q9IMP3
C	779	LEU	-	expression tag	UNP Q9IMP3
C	780	TYR	-	expression tag	UNP Q9IMP3
C	781	PHE	-	expression tag	UNP Q9IMP3
C	782	GLN	-	expression tag	UNP Q9IMP3
F	775	ALA	-	expression tag	UNP Q9IMP3
F	776	ARG	-	expression tag	UNP Q9IMP3
F	777	GLU	-	expression tag	UNP Q9IMP3
F	778	ASN	-	expression tag	UNP Q9IMP3
F	779	LEU	-	expression tag	UNP Q9IMP3
F	780	TYR	-	expression tag	UNP Q9IMP3
F	781	PHE	-	expression tag	UNP Q9IMP3
F	782	GLN	-	expression tag	UNP Q9IMP3
I	775	ALA	-	expression tag	UNP Q9IMP3
I	776	ARG	-	expression tag	UNP Q9IMP3
I	777	GLU	-	expression tag	UNP Q9IMP3
I	778	ASN	-	expression tag	UNP Q9IMP3
I	779	LEU	-	expression tag	UNP Q9IMP3
I	780	TYR	-	expression tag	UNP Q9IMP3
I	781	PHE	-	expression tag	UNP Q9IMP3
I	782	GLN	-	expression tag	UNP Q9IMP3
L	775	ALA	-	expression tag	UNP Q9IMP3
L	776	ARG	-	expression tag	UNP Q9IMP3
L	777	GLU	-	expression tag	UNP Q9IMP3
L	778	ASN	-	expression tag	UNP Q9IMP3
L	779	LEU	-	expression tag	UNP Q9IMP3
L	780	TYR	-	expression tag	UNP Q9IMP3
L	781	PHE	-	expression tag	UNP Q9IMP3
L	782	GLN	-	expression tag	UNP Q9IMP3

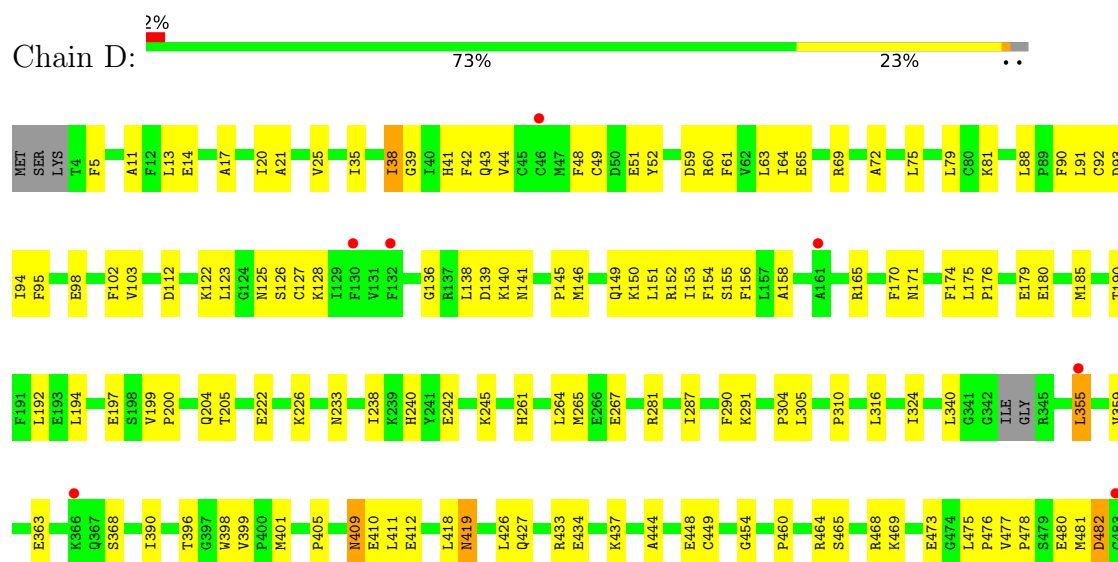
3 Residue-property plots

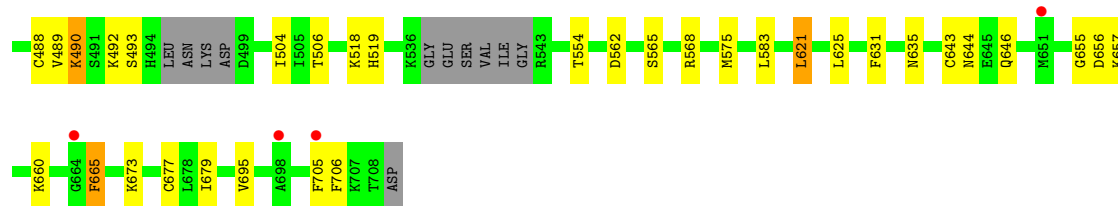
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

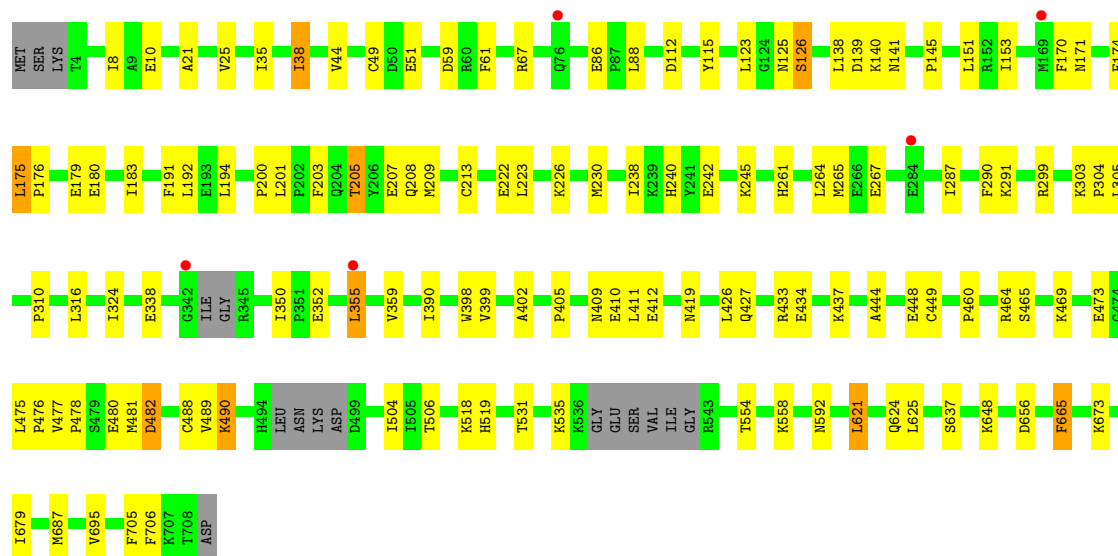
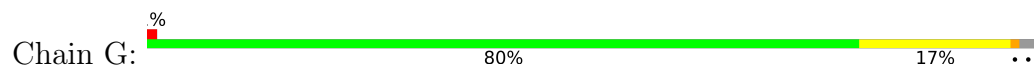


• Molecule 1: Polymerase acidic protein

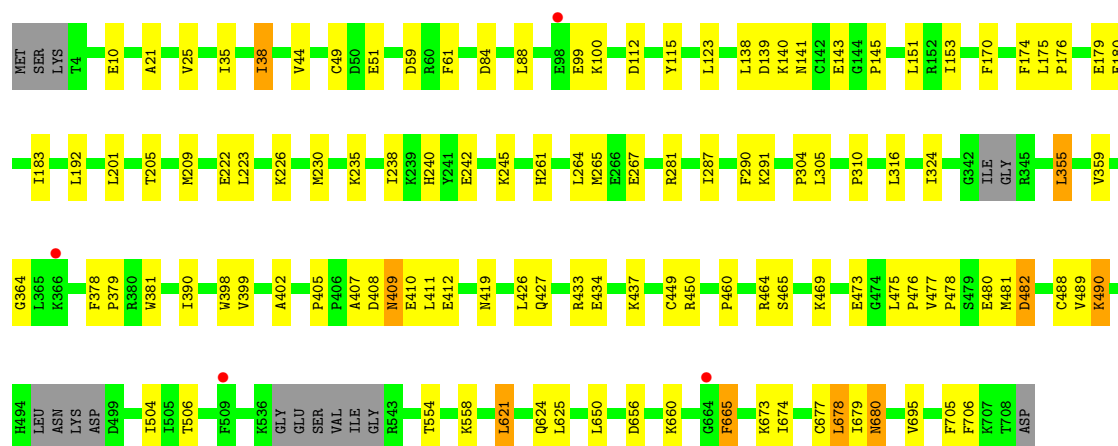
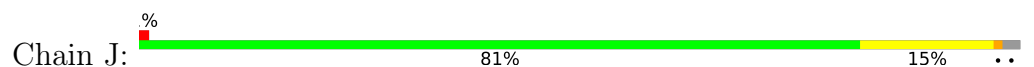




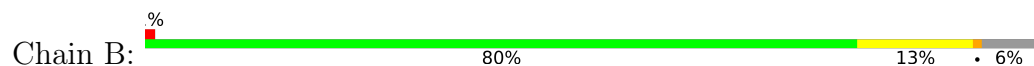
• Molecule 1: Polymerase acidic protein



• Molecule 1: Polymerase acidic protein

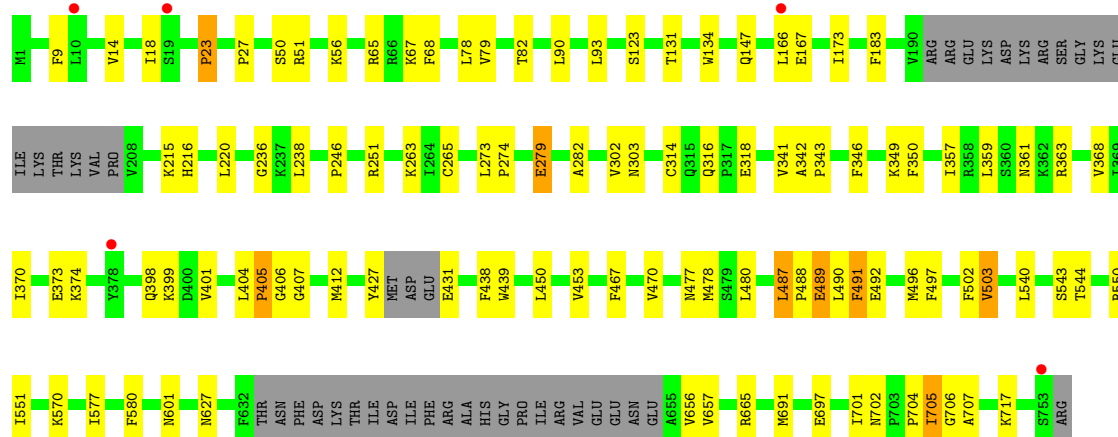
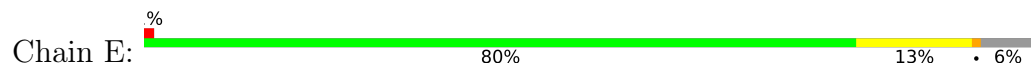


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

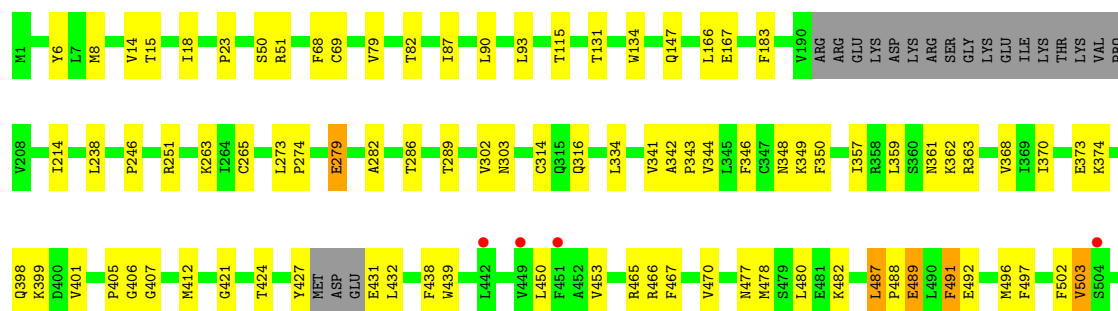
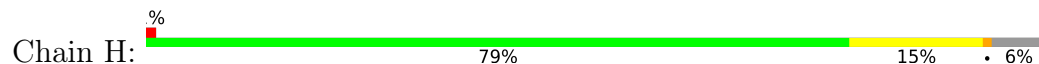


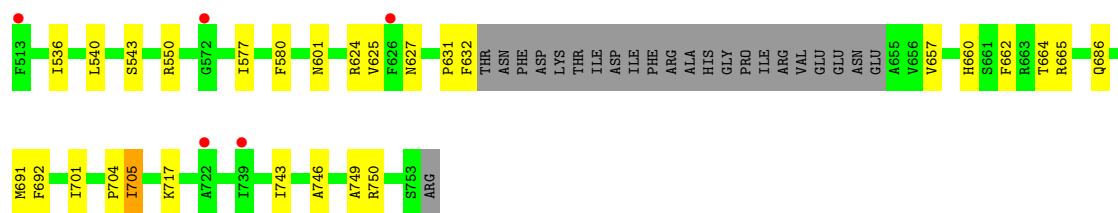


• Molecule 2: RNA-directed RNA polymerase catalytic subunit



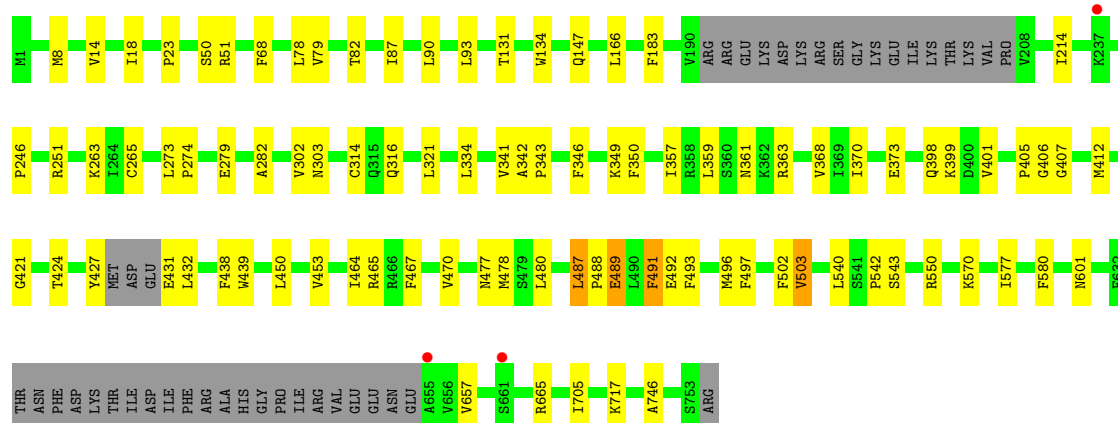
• Molecule 2: RNA-directed RNA polymerase catalytic subunit





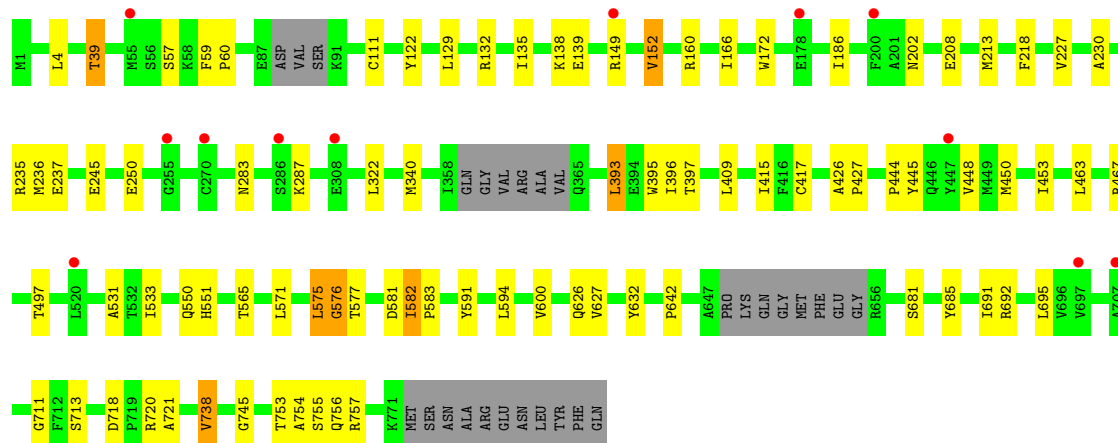
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain K: 82% 12% 6%



• Molecule 3: Polymerase basic protein 2

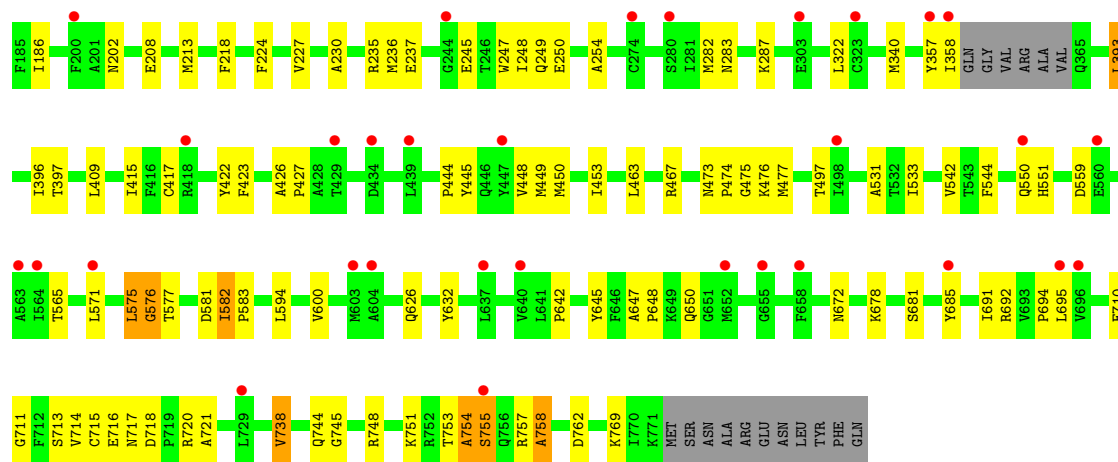
Chain C: 2% 85% 10%



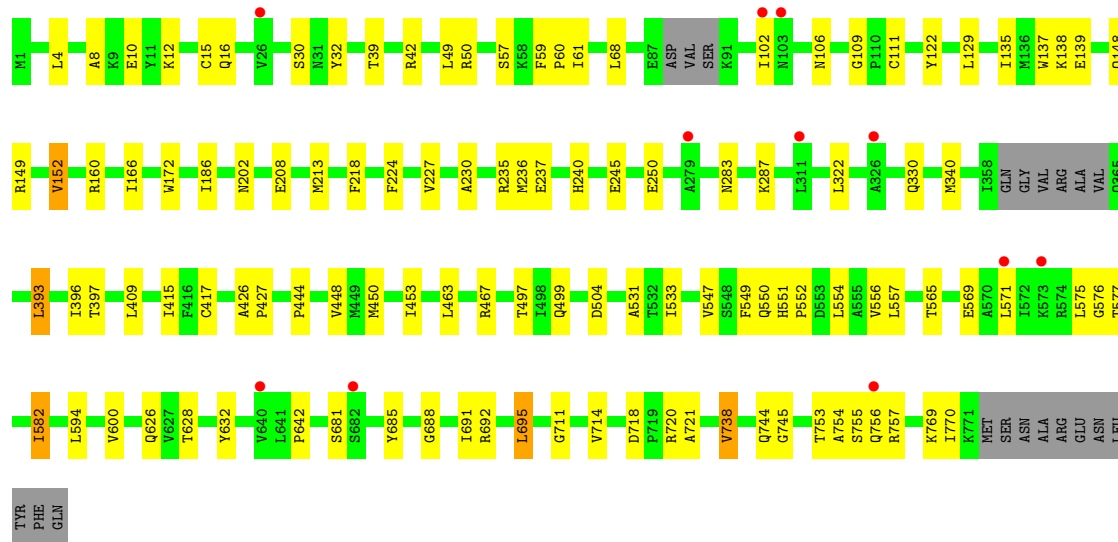
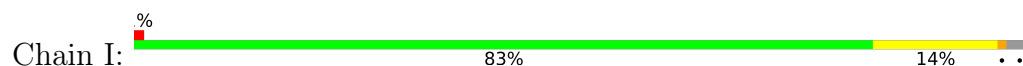
• Molecule 3: Polymerase basic protein 2

Chain F: 4% 81% 15%

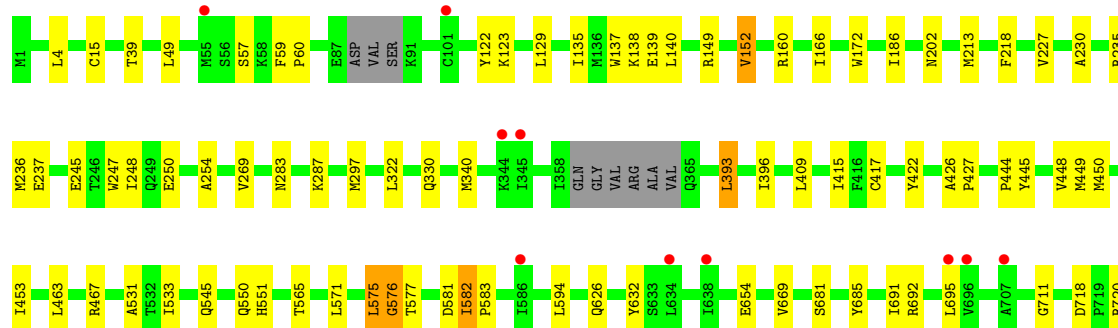
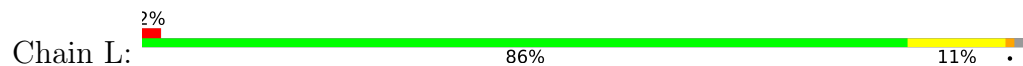




• Molecule 3: Polymerase basic protein 2



• Molecule 3: Polymerase basic protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.28Å 217.50Å 597.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 4.30 50.01 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-4.30) 98.8 (50.01-4.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 4.30Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.316 , 0.368 0.312 , 0.358	Depositor DCC
R_{free} test set	4744 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	146.0	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 158.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	69371	wwPDB-VP
Average B, all atoms (Å ²)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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

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	0.63	0/5746	0.94	7/7717 (0.1%)
1	D	0.63	0/5746	0.93	4/7717 (0.1%)
1	G	0.63	0/5746	0.92	6/7717 (0.1%)
1	J	0.62	0/5746	0.92	3/7717 (0.0%)
2	B	0.61	0/5749	0.92	5/7723 (0.1%)
2	E	0.61	0/5749	0.91	4/7723 (0.1%)
2	H	0.61	0/5749	0.91	4/7723 (0.1%)
2	K	0.60	0/5749	0.91	4/7723 (0.1%)
3	C	0.65	0/6121	0.93	6/8236 (0.1%)
3	F	0.65	0/6185	0.93	9/8322 (0.1%)
3	I	0.65	0/6185	0.94	7/8322 (0.1%)
3	L	0.64	0/6185	0.93	6/8322 (0.1%)
All	All	0.63	0/70656	0.92	65/94962 (0.1%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	GLU	N-CA-C	10.02	122.20	111.28
1	J	409	ASN	N-CA-C	7.26	119.20	111.28
1	G	409	ASN	N-CA-C	7.24	119.17	111.28
1	D	409	ASN	N-CA-C	7.23	119.16	111.28
1	J	481	MET	N-CA-C	7.19	119.09	108.60
1	A	481	MET	N-CA-C	7.17	119.07	108.60
1	G	481	MET	N-CA-C	7.14	119.02	108.60
1	D	481	MET	N-CA-C	7.12	119.00	108.60
3	F	718	ASP	CA-C-N	-6.75	113.73	120.21
3	F	718	ASP	C-N-CA	-6.75	113.73	120.21
3	L	718	ASP	CA-C-N	-6.71	113.76	120.21
3	L	718	ASP	C-N-CA	-6.71	113.76	120.21
3	I	718	ASP	CA-C-N	-6.69	113.78	120.21
3	I	718	ASP	C-N-CA	-6.69	113.78	120.21
3	C	718	ASP	CA-C-N	-6.67	113.80	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	718	ASP	C-N-CA	-6.67	113.80	120.21
3	F	755	SER	N-CA-C	-6.48	101.10	110.24
1	A	407	ALA	N-CA-C	6.42	119.96	109.24
3	I	556	VAL	N-CA-C	6.23	116.97	110.62
1	A	89	PRO	CA-C-N	-6.11	114.57	123.00
1	A	89	PRO	C-N-CA	-6.11	114.57	123.00
1	A	89	PRO	N-CA-C	-6.11	106.10	113.98
3	F	575	LEU	N-CA-C	6.04	118.70	110.55
3	L	575	LEU	N-CA-C	5.99	118.64	110.55
3	I	245	GLU	N-CA-C	5.94	119.63	112.38
3	C	245	GLU	N-CA-C	5.94	119.63	112.38
3	C	575	LEU	N-CA-C	5.94	118.57	110.55
3	L	245	GLU	N-CA-C	5.94	119.63	112.38
3	F	245	GLU	N-CA-C	5.93	119.62	112.38
3	F	754	ALA	N-CA-C	-5.78	102.49	110.35
1	G	665	PHE	N-CA-C	5.70	117.17	111.07
3	F	202	ASN	N-CA-C	5.62	117.48	111.36
3	I	202	ASN	N-CA-C	5.61	117.48	111.36
1	J	665	PHE	N-CA-C	5.56	117.02	111.07
3	I	576	GLY	N-CA-C	5.55	122.13	114.92
2	B	489	GLU	N-CA-C	5.53	117.31	111.28
3	C	202	ASN	N-CA-C	5.51	117.37	111.36
3	F	576	GLY	N-CA-C	5.50	122.92	115.32
2	E	489	GLU	N-CA-C	5.49	117.27	111.28
2	H	489	GLU	N-CA-C	5.49	117.26	111.28
3	I	756	GLN	N-CA-C	-5.45	102.72	110.35
2	E	246	PRO	N-CA-C	5.40	119.06	111.33
2	H	246	PRO	N-CA-C	5.40	119.06	111.33
3	C	576	GLY	N-CA-C	5.40	122.77	115.32
1	A	665	PHE	N-CA-C	5.40	116.84	111.07
3	L	202	ASN	N-CA-C	5.38	117.22	111.36
2	K	246	PRO	N-CA-C	5.36	118.99	111.33
1	D	665	PHE	N-CA-C	5.35	116.80	111.07
2	B	487	LEU	N-CA-C	-5.35	102.25	110.01
2	K	489	GLU	N-CA-C	5.33	117.09	111.28
2	B	246	PRO	N-CA-C	5.32	118.93	111.33
3	L	576	GLY	N-CA-C	5.32	122.66	115.32
2	H	487	LEU	N-CA-C	-5.29	102.34	110.01
2	E	487	LEU	N-CA-C	-5.27	102.37	110.01
2	E	406	GLY	N-CA-C	5.20	120.34	113.37
1	G	126	SER	N-CA-C	5.19	117.84	111.82
2	K	406	GLY	N-CA-C	5.19	120.33	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	710	GLU	N-CA-C	5.18	116.62	109.15
2	H	406	GLY	N-CA-C	5.15	120.27	113.37
2	K	487	LEU	N-CA-C	-5.13	102.57	110.01
1	D	125	ASN	N-CA-C	5.10	119.14	113.02
2	B	384	GLU	N-CA-C	5.04	116.86	111.36
1	G	175	LEU	CA-C-N	5.01	126.11	119.84
1	G	175	LEU	C-N-CA	5.01	126.11	119.84
2	B	406	GLY	N-CA-C	5.01	120.08	113.37

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	5630	0	5632	149	1
1	D	5630	0	5632	200	5
1	G	5630	0	5632	171	2
1	J	5630	0	5632	119	6
2	B	5652	0	5749	126	6
2	E	5652	0	5749	109	4
2	H	5652	0	5749	137	0
2	K	5652	0	5749	80	0
3	C	6015	0	6124	58	0
3	F	6076	0	6183	178	8
3	I	6076	0	6183	125	4
3	L	6076	0	6183	87	0
All	All	69371	0	70197	1213	18

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 9.

All (1213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:CZ	1:D:91:LEU:HD11	1.14	1.55
2:B:180:GLU:HG2	1:G:203:PHE:CE1	1.47	1.50
3:I:577:THR:HG23	3:I:754:ALA:CB	1.43	1.49
2:H:363:ARG:HA	1:J:409:ASN:ND2	1.20	1.42
1:D:69:ARG:NE	1:D:91:LEU:HD11	1.33	1.41
3:I:575:LEU:CD1	3:I:582:ILE:HD12	1.55	1.36
2:H:363:ARG:CA	1:J:409:ASN:HD22	1.35	1.35
1:A:355:LEU:HD11	1:A:366:LYS:NZ	1.38	1.34
1:J:674:ILE:O	1:J:678:LEU:HD13	1.23	1.34
2:B:180:GLU:OE2	2:B:215:LYS:HD3	1.24	1.31
2:E:68:PHE:CE1	2:E:316:GLN:OE1	1.83	1.31
2:B:68:PHE:CE1	2:B:316:GLN:OE1	1.82	1.30
2:H:68:PHE:CE1	2:H:316:GLN:OE1	1.83	1.29
2:K:68:PHE:CE1	2:K:316:GLN:OE1	1.84	1.29
1:D:69:ARG:CZ	1:D:91:LEU:CD1	2.09	1.28
2:K:18:ILE:HD12	2:K:497:PHE:CD1	1.68	1.26
2:E:18:ILE:HD12	2:E:497:PHE:CD1	1.69	1.26
2:B:180:GLU:CG	1:G:203:PHE:CE1	2.17	1.25
3:F:358:ILE:HA	3:F:423:PHE:CB	1.65	1.24
3:I:577:THR:CG2	3:I:754:ALA:HB2	1.67	1.23
1:J:674:ILE:O	1:J:678:LEU:CD1	1.90	1.20
3:F:474:PRO:HD3	1:G:126:SER:HA	1.25	1.16
3:I:575:LEU:HD13	3:I:582:ILE:HD12	1.17	1.16
3:F:474:PRO:CD	1:G:126:SER:HA	1.75	1.16
3:I:554:LEU:HD11	3:I:557:LEU:HG	1.17	1.16
2:B:180:GLU:OE2	2:B:215:LYS:CD	1.94	1.14
2:K:18:ILE:CD1	2:K:497:PHE:CD1	2.29	1.14
2:E:18:ILE:CD1	2:E:497:PHE:CD1	2.30	1.14
3:C:575:LEU:HD13	3:C:582:ILE:HD12	1.30	1.13
1:D:396:THR:HG21	1:D:468:ARG:HD2	1.30	1.13
1:A:366:LYS:HE3	2:B:359:LEU:CD1	1.79	1.12
3:F:575:LEU:HD13	3:F:582:ILE:HD12	1.30	1.11
1:J:408:ASP:N	1:J:412:GLU:HG3	1.65	1.11
1:J:408:ASP:H	1:J:412:GLU:CG	1.63	1.11
1:A:396:THR:HG21	1:A:468:ARG:HD2	1.29	1.10
3:F:477:MET:CE	1:G:88:LEU:HD11	1.81	1.10
1:D:69:ARG:NE	1:D:91:LEU:CD1	2.09	1.10
1:D:90:PHE:CZ	1:D:122:LYS:HB3	1.85	1.10
3:F:477:MET:HE1	1:G:88:LEU:HD11	1.19	1.10
3:L:575:LEU:HD13	3:L:582:ILE:HD12	1.31	1.10
2:H:363:ARG:CA	1:J:409:ASN:ND2	1.99	1.10
1:A:407:ALA:HB1	1:A:412:GLU:HB3	1.14	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ARG:NH2	3:F:139:GLU:OE2	1.85	1.08
3:C:575:LEU:CD1	3:C:582:ILE:HD12	1.84	1.07
3:F:358:ILE:CA	3:F:423:PHE:HB3	1.83	1.07
3:F:575:LEU:CD1	3:F:582:ILE:HD12	1.83	1.07
3:L:575:LEU:CD1	3:L:582:ILE:HD12	1.84	1.06
1:D:90:PHE:HB2	1:D:123:LEU:HD11	1.31	1.06
1:A:407:ALA:CB	1:A:412:GLU:HB3	1.85	1.05
1:D:152:ARG:NH2	3:F:757:ARG:O	1.89	1.04
3:F:474:PRO:CG	1:G:126:SER:HA	1.86	1.04
1:A:396:THR:HG21	1:A:468:ARG:CD	1.88	1.04
3:C:692:ARG:NH2	3:C:755:SER:OG	1.91	1.03
3:F:692:ARG:NH2	3:F:755:SER:OG	1.89	1.03
3:I:547:VAL:HG13	3:I:688:GLY:HA2	1.35	1.03
3:I:575:LEU:HD13	3:I:582:ILE:CD1	1.88	1.03
3:I:554:LEU:HD11	3:I:557:LEU:CG	1.89	1.03
3:I:692:ARG:NH2	3:I:755:SER:OG	1.92	1.02
1:D:396:THR:HG21	1:D:468:ARG:CD	1.88	1.02
3:L:576:GLY:HA2	3:L:583:PRO:HG3	1.42	1.02
1:A:407:ALA:HB1	1:A:412:GLU:CB	1.90	1.01
3:L:692:ARG:NH2	3:L:755:SER:OG	1.91	1.01
1:A:355:LEU:CD1	1:A:366:LYS:NZ	2.24	1.00
3:C:576:GLY:HA2	3:C:583:PRO:HG3	1.44	1.00
2:B:180:GLU:HB2	1:G:203:PHE:CD1	1.96	0.99
1:D:90:PHE:CB	1:D:123:LEU:HD11	1.92	0.99
3:I:755:SER:O	3:I:757:ARG:HG3	1.63	0.98
1:J:408:ASP:H	1:J:412:GLU:HG3	0.84	0.98
3:C:575:LEU:HD13	3:C:582:ILE:CD1	1.94	0.98
3:F:575:LEU:HD13	3:F:582:ILE:CD1	1.92	0.98
3:F:576:GLY:HA2	3:F:583:PRO:HG3	1.42	0.98
2:K:487:LEU:HD23	2:K:488:PRO:N	1.79	0.98
3:L:575:LEU:HD13	3:L:582:ILE:CD1	1.94	0.98
3:F:477:MET:SD	1:G:88:LEU:HD13	2.04	0.98
1:A:326:ASP:HB3	3:F:542:VAL:HG23	1.44	0.97
2:H:686:GLN:OE1	3:I:39:THR:CG2	2.12	0.97
1:G:203:PHE:HB3	1:G:208:GLN:HE21	1.28	0.97
1:A:76:GLN:HB2	1:A:91:LEU:CD2	1.94	0.97
2:E:487:LEU:HD23	2:E:488:PRO:N	1.79	0.97
3:C:755:SER:O	3:C:757:ARG:HG3	1.65	0.97
2:H:487:LEU:HD23	2:H:488:PRO:N	1.79	0.97
3:I:575:LEU:CD1	3:I:582:ILE:CD1	2.44	0.96
3:L:755:SER:O	3:L:757:ARG:HG3	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:HD11	1:A:366:LYS:HZ1	1.16	0.95
3:F:576:GLY:HA2	3:F:583:PRO:CG	1.96	0.95
1:A:76:GLN:HB2	1:A:91:LEU:HD21	1.48	0.95
1:A:366:LYS:CE	2:B:359:LEU:CD1	2.44	0.95
2:K:68:PHE:HE1	2:K:316:GLN:OE1	1.32	0.94
3:I:552:PRO:HG2	3:I:554:LEU:HG	1.47	0.93
1:G:412:GLU:N	1:G:412:GLU:OE1	2.00	0.93
1:D:412:GLU:N	1:D:412:GLU:OE1	2.00	0.93
3:F:358:ILE:HA	3:F:423:PHE:HB3	0.96	0.93
3:F:474:PRO:HB3	1:G:126:SER:OG	1.69	0.93
2:B:182:LYS:NZ	1:G:205:THR:HG23	1.84	0.92
2:H:686:GLN:OE1	3:I:39:THR:HG21	1.69	0.92
2:H:363:ARG:HG2	1:J:409:ASN:HB2	1.50	0.92
3:C:576:GLY:HA2	3:C:583:PRO:CG	1.99	0.92
3:L:576:GLY:HA2	3:L:583:PRO:CG	1.97	0.92
2:B:180:GLU:HG2	1:G:203:PHE:CZ	2.05	0.91
3:I:577:THR:HG23	3:I:754:ALA:HB1	1.51	0.91
3:F:474:PRO:HD3	1:G:126:SER:CA	2.00	0.91
1:A:355:LEU:HD11	1:A:366:LYS:HZ2	1.10	0.90
1:D:92:CYS:SG	1:D:102:PHE:HD2	1.93	0.90
1:D:410:GLU:HB3	3:F:137:TRP:HB3	1.53	0.90
2:H:363:ARG:HA	1:J:409:ASN:CG	1.97	0.89
2:H:701:ILE:HD11	3:I:208:GLU:HA	1.54	0.89
1:A:410:GLU:OE1	1:A:411:LEU:HB2	1.72	0.89
1:D:69:ARG:NH1	1:D:91:LEU:HD11	1.88	0.88
3:F:577:THR:HG23	3:F:754:ALA:HB2	1.55	0.88
2:E:68:PHE:HE1	2:E:316:GLN:OE1	1.31	0.88
1:D:59:ASP:OD2	3:F:769:LYS:NZ	2.07	0.88
2:H:363:ARG:C	1:J:409:ASN:ND2	2.31	0.88
2:H:68:PHE:HE1	2:H:316:GLN:OE1	1.31	0.87
2:B:179:LYS:HB2	1:G:203:PHE:CZ	2.09	0.87
3:F:477:MET:HE1	1:G:88:LEU:CD1	2.05	0.87
2:K:50:SER:HB3	2:K:68:PHE:CE1	2.10	0.87
3:F:358:ILE:HA	3:F:423:PHE:CA	2.03	0.87
2:H:50:SER:HB3	2:H:68:PHE:CE1	2.09	0.86
2:B:180:GLU:CB	1:G:203:PHE:CE1	2.58	0.86
2:B:50:SER:OG	2:B:68:PHE:CZ	2.29	0.86
2:B:487:LEU:CD1	2:B:488:PRO:HD2	2.05	0.86
3:F:358:ILE:C	3:F:423:PHE:O	2.04	0.86
2:K:50:SER:OG	2:K:68:PHE:CZ	2.29	0.85
2:H:50:SER:OG	2:H:68:PHE:CZ	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:686:GLN:NE2	3:I:39:THR:OG1	2.09	0.85
2:B:50:SER:HB3	2:B:68:PHE:CE1	2.11	0.85
2:E:50:SER:HB3	2:E:68:PHE:CE1	2.10	0.85
1:J:408:ASP:O	1:J:412:GLU:HB2	1.75	0.85
2:E:50:SER:OG	2:E:68:PHE:CZ	2.29	0.85
3:F:576:GLY:HA2	3:F:583:PRO:CD	2.06	0.85
2:K:18:ILE:HD12	2:K:497:PHE:CE1	2.12	0.85
1:D:410:GLU:HG2	3:F:137:TRP:CE3	2.11	0.84
3:I:577:THR:CG2	3:I:754:ALA:CB	2.39	0.84
2:B:68:PHE:HE1	2:B:316:GLN:OE1	1.30	0.84
2:H:487:LEU:HG	2:H:488:PRO:HD2	1.59	0.84
1:D:52:TYR:CD2	1:D:146:MET:HE3	2.13	0.84
3:I:577:THR:HG23	3:I:754:ALA:HB2	0.84	0.83
2:K:487:LEU:HG	2:K:488:PRO:HD2	1.59	0.83
2:B:487:LEU:HD12	2:B:488:PRO:CD	2.08	0.83
1:D:92:CYS:HG	1:D:102:PHE:HD2	0.85	0.83
2:E:18:ILE:HD12	2:E:497:PHE:CE1	2.13	0.83
3:I:554:LEU:CD1	3:I:557:LEU:H	1.91	0.83
1:A:529:HIS:CE1	3:F:678:LYS:HE2	2.14	0.83
2:B:180:GLU:CG	1:G:203:PHE:CD1	2.62	0.83
3:I:554:LEU:HD12	3:I:554:LEU:O	1.79	0.83
3:F:477:MET:CE	1:G:88:LEU:CD1	2.57	0.82
3:L:576:GLY:HA2	3:L:583:PRO:CD	2.10	0.82
2:E:487:LEU:HG	2:E:488:PRO:HD2	1.60	0.82
1:A:72:ALA:O	1:A:91:LEU:HD21	1.78	0.81
1:J:419:ASN:ND2	2:K:543:SER:OG	2.13	0.81
3:L:138:LYS:HB3	3:L:250:GLU:HB2	1.60	0.81
2:B:363:ARG:CD	3:F:139:GLU:OE2	2.28	0.81
1:D:90:PHE:CE2	1:D:122:LYS:HB3	2.14	0.81
1:G:419:ASN:ND2	2:H:543:SER:OG	2.14	0.81
3:I:552:PRO:CG	3:I:557:LEU:HD12	2.10	0.81
3:F:138:LYS:HB3	3:F:250:GLU:HB2	1.63	0.81
1:A:355:LEU:CD1	1:A:366:LYS:HZ2	1.86	0.80
2:B:180:GLU:HB2	1:G:203:PHE:HD1	1.40	0.80
2:B:180:GLU:HG2	1:G:203:PHE:HE1	1.35	0.80
1:D:11:ALA:O	3:F:184:LYS:NZ	2.15	0.80
1:A:338:GLU:HG2	3:F:254:ALA:HB1	1.64	0.80
3:F:477:MET:SD	1:G:88:LEU:CD1	2.69	0.80
1:A:396:THR:CG2	1:A:468:ARG:HD2	2.12	0.79
3:C:576:GLY:HA2	3:C:583:PRO:CD	2.11	0.79
3:I:552:PRO:HG3	3:I:557:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:469:LYS:HD3	1:G:475:LEU:HD13	1.64	0.79
1:A:286:LEU:HD11	1:A:482:ASP:OD2	1.81	0.79
1:D:396:THR:CG2	1:D:468:ARG:HD2	2.12	0.79
1:G:171:ASN:ND2	2:H:167:GLU:OE2	2.15	0.79
1:J:469:LYS:HD3	1:J:475:LEU:HD13	1.65	0.79
2:K:50:SER:CB	2:K:68:PHE:CZ	2.66	0.79
2:B:180:GLU:CB	1:G:203:PHE:CD1	2.66	0.79
2:H:627:ASN:ND2	3:I:111:CYS:SG	2.56	0.78
2:B:50:SER:CB	2:B:68:PHE:CZ	2.67	0.78
1:A:469:LYS:HD3	1:A:475:LEU:HD13	1.64	0.78
2:E:50:SER:HB3	2:E:68:PHE:CZ	2.19	0.78
2:K:50:SER:HB3	2:K:68:PHE:CZ	2.19	0.78
2:B:363:ARG:HA	1:D:409:ASN:ND2	1.99	0.77
2:E:50:SER:CB	2:E:68:PHE:CZ	2.67	0.77
3:L:575:LEU:HD13	3:L:582:ILE:CG1	2.15	0.77
1:D:410:GLU:OE1	1:D:411:LEU:HB2	1.85	0.77
1:G:209:MET:SD	1:G:213:CYS:SG	2.82	0.77
1:D:575:MET:HG2	2:E:544:THR:HA	1.67	0.77
2:H:50:SER:HB3	2:H:68:PHE:CZ	2.19	0.77
2:H:50:SER:CB	2:H:68:PHE:CZ	2.66	0.77
1:A:355:LEU:CD1	1:A:366:LYS:HZ1	1.90	0.77
1:A:326:ASP:HB3	3:F:542:VAL:CG2	2.15	0.77
2:B:50:SER:HB3	2:B:68:PHE:CZ	2.19	0.77
1:D:90:PHE:HB2	1:D:123:LEU:CD1	2.14	0.77
1:D:52:TYR:CG	1:D:146:MET:HE3	2.19	0.76
1:D:469:LYS:HD3	1:D:475:LEU:HD13	1.65	0.76
3:F:577:THR:HG23	3:F:754:ALA:CB	2.14	0.76
3:F:575:LEU:HD13	3:F:582:ILE:CG1	2.14	0.76
3:I:575:LEU:HD11	3:I:582:ILE:HD12	1.67	0.76
1:G:410:GLU:OE1	1:G:411:LEU:HB2	1.86	0.76
1:A:366:LYS:CE	2:B:359:LEU:HD11	2.15	0.75
1:A:366:LYS:HE3	2:B:359:LEU:HD13	1.68	0.75
3:C:575:LEU:HD13	3:C:582:ILE:CG1	2.16	0.75
2:B:487:LEU:HG	2:B:488:PRO:HD2	1.68	0.75
1:D:48:PHE:O	1:D:149:GLN:NE2	2.20	0.75
1:D:69:ARG:HE	1:D:91:LEU:HD21	1.52	0.75
3:F:577:THR:CG2	3:F:754:ALA:HB2	2.16	0.75
3:I:575:LEU:HD13	3:I:582:ILE:CG1	2.17	0.75
3:I:552:PRO:HG3	3:I:557:LEU:CD1	2.17	0.74
1:D:410:GLU:OE1	1:D:411:LEU:CB	2.36	0.74
1:D:477:VAL:HG11	1:D:480:GLU:OE2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:363:ARG:HA	1:J:409:ASN:HD22	0.61	0.74
2:B:182:LYS:HE2	1:G:205:THR:OG1	1.87	0.74
1:A:366:LYS:HE3	2:B:359:LEU:HD12	1.69	0.74
1:D:44:VAL:HG13	1:D:153:ILE:HD11	1.70	0.74
1:D:410:GLU:HG2	3:F:137:TRP:CD2	2.22	0.74
1:D:477:VAL:HG12	1:D:478:PRO:O	1.88	0.74
1:J:477:VAL:HG11	1:J:480:GLU:OE2	1.88	0.73
1:A:286:LEU:HD21	1:A:482:ASP:OD2	1.88	0.73
3:F:358:ILE:CA	3:F:423:PHE:C	2.57	0.73
1:A:89:PRO:HG2	1:A:90:PHE:CD1	2.24	0.73
1:G:477:VAL:HG12	1:G:478:PRO:O	1.88	0.73
1:G:44:VAL:HG13	1:G:153:ILE:HD11	1.71	0.73
1:A:477:VAL:HG11	1:A:480:GLU:OE2	1.88	0.73
2:K:487:LEU:CD2	2:K:488:PRO:HD2	2.18	0.73
2:K:487:LEU:CG	2:K:488:PRO:HD2	2.19	0.73
1:G:477:VAL:HG11	1:G:480:GLU:OE2	1.88	0.73
2:H:487:LEU:CD2	2:H:488:PRO:HD2	2.19	0.73
2:B:487:LEU:HD12	2:B:488:PRO:HD3	1.70	0.72
2:E:282:ALA:HB3	3:F:149:ARG:HD3	1.71	0.72
3:I:552:PRO:CG	3:I:557:LEU:CD1	2.67	0.72
2:K:18:ILE:CD1	2:K:497:PHE:HD1	2.02	0.72
2:B:487:LEU:CG	2:B:488:PRO:HD2	2.20	0.72
1:G:203:PHE:CB	1:G:208:GLN:HE21	2.02	0.72
1:G:350:ILE:HB	2:H:368:VAL:HG22	1.69	0.72
1:G:410:GLU:OE1	1:G:411:LEU:CB	2.37	0.72
1:A:44:VAL:HG13	1:A:153:ILE:HD11	1.70	0.72
1:A:477:VAL:HG12	1:A:478:PRO:O	1.89	0.72
2:H:487:LEU:CG	2:H:488:PRO:HD2	2.20	0.72
1:J:477:VAL:HG12	1:J:478:PRO:O	1.88	0.72
2:E:487:LEU:CD2	2:E:488:PRO:HD2	2.18	0.72
2:H:15:THR:HA	2:H:18:ILE:CD1	2.20	0.72
2:B:487:LEU:HD12	2:B:488:PRO:HD2	1.70	0.72
2:E:50:SER:CB	2:E:68:PHE:CE1	2.73	0.72
1:A:76:GLN:NE2	1:A:88:LEU:O	2.23	0.71
2:E:487:LEU:HD23	2:E:488:PRO:CD	2.20	0.71
2:E:487:LEU:CG	2:E:488:PRO:HD2	2.20	0.71
1:J:138:LEU:HD11	1:J:140:LYS:HE3	1.72	0.71
1:J:44:VAL:HG13	1:J:153:ILE:HD11	1.70	0.71
2:B:50:SER:CB	2:B:68:PHE:CE1	2.74	0.71
1:G:138:LEU:HD11	1:G:140:LYS:HE3	1.72	0.71
1:A:76:GLN:HB2	1:A:91:LEU:HD23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:680:ASN:H	1:J:680:ASN:HD22	1.35	0.71
2:K:50:SER:CB	2:K:68:PHE:CE1	2.73	0.71
2:B:15:THR:HA	2:B:18:ILE:CD1	2.21	0.71
1:A:401:MET:HE1	2:B:551:ILE:HD11	1.72	0.71
2:K:487:LEU:HD23	2:K:488:PRO:CD	2.20	0.71
2:B:182:LYS:HZ1	1:G:205:THR:HG23	1.56	0.70
2:H:50:SER:CB	2:H:68:PHE:CE1	2.73	0.70
2:H:14:VAL:O	2:H:18:ILE:HG13	1.91	0.70
3:I:692:ARG:HH22	3:I:755:SER:CB	2.04	0.70
2:H:487:LEU:HD23	2:H:488:PRO:CD	2.20	0.70
1:J:410:GLU:OE1	1:J:411:LEU:HB2	1.90	0.70
1:A:366:LYS:HE2	2:B:381:LEU:HD21	1.74	0.70
1:A:366:LYS:HE2	2:B:381:LEU:CD2	2.22	0.70
2:B:363:ARG:HA	1:D:409:ASN:HD22	1.57	0.70
3:F:475:GLY:C	1:G:86:GLU:HG3	2.17	0.70
2:B:14:VAL:O	2:B:18:ILE:HG13	1.92	0.70
1:A:23:GLU:OE1	1:A:68:LYS:HD3	1.91	0.69
1:A:345:ARG:HD3	3:F:136:MET:HE3	1.74	0.69
1:A:138:LEU:HD11	1:A:140:LYS:HE3	1.73	0.69
3:F:474:PRO:CB	1:G:126:SER:HA	2.22	0.69
1:A:73:VAL:HA	1:A:91:LEU:HD11	1.73	0.69
1:D:69:ARG:CD	1:D:91:LEU:CD1	2.70	0.69
2:B:182:LYS:HZ3	1:G:205:THR:HG23	1.55	0.69
3:C:692:ARG:HH22	3:C:755:SER:CB	2.06	0.69
1:D:52:TYR:CE2	1:D:146:MET:HE3	2.27	0.69
3:F:575:LEU:CD1	3:F:582:ILE:CD1	2.61	0.69
1:D:138:LEU:HD11	1:D:140:LYS:HE3	1.74	0.69
1:G:477:VAL:HG13	1:G:478:PRO:HD2	1.75	0.69
1:D:477:VAL:HG13	1:D:478:PRO:HD2	1.76	0.68
2:H:363:ARG:HD3	3:L:139:GLU:OE2	1.93	0.68
2:B:180:GLU:HB2	1:G:203:PHE:CE1	2.25	0.68
3:F:358:ILE:C	3:F:423:PHE:C	2.61	0.68
1:J:408:ASP:N	1:J:412:GLU:CG	2.40	0.68
1:A:477:VAL:HG13	1:A:478:PRO:HD2	1.76	0.68
2:K:487:LEU:CD2	2:K:489:GLU:H	2.07	0.68
1:D:21:ALA:HA	1:D:38:ILE:HD11	1.75	0.68
1:D:69:ARG:NH2	1:D:91:LEU:HD11	1.99	0.68
3:I:547:VAL:HG13	3:I:688:GLY:CA	2.18	0.67
1:A:366:LYS:CE	2:B:359:LEU:HD13	2.22	0.67
3:L:692:ARG:HH22	3:L:755:SER:CB	2.06	0.67
1:A:89:PRO:HG2	1:A:90:PHE:HD1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:477:VAL:HG13	1:J:478:PRO:HD2	1.76	0.67
1:A:366:LYS:HE2	2:B:359:LEU:HD11	1.74	0.67
1:D:304:PRO:HG3	1:D:310:PRO:HB3	1.76	0.67
1:G:299:ARG:NE	3:L:545:GLN:HE22	1.92	0.67
1:J:304:PRO:HG3	1:J:310:PRO:HB3	1.77	0.67
1:A:322:ALA:HA	3:F:544:PHE:CD1	2.29	0.67
1:J:678:LEU:N	1:J:678:LEU:HD12	2.10	0.67
3:F:474:PRO:HG3	1:G:126:SER:HA	1.75	0.66
1:D:103:VAL:HG22	1:D:128:LYS:HB2	1.77	0.66
1:D:151:LEU:CD2	3:F:715:CYS:HB2	2.24	0.66
2:H:282:ALA:HB2	3:I:148:GLN:HG2	1.76	0.66
2:H:664:THR:HG23	3:I:42:ARG:HH11	1.59	0.66
1:D:69:ARG:CD	1:D:91:LEU:HD11	2.25	0.66
1:D:155:SER:HB3	3:F:713:SER:OG	1.95	0.66
3:I:575:LEU:HD22	3:I:582:ILE:H	1.60	0.66
2:B:180:GLU:N	1:G:203:PHE:HE1	1.93	0.66
2:H:363:ARG:O	1:J:409:ASN:ND2	2.28	0.66
1:J:410:GLU:OE1	1:J:411:LEU:CB	2.44	0.66
2:B:180:GLU:OE2	2:B:215:LYS:CE	2.43	0.66
3:F:358:ILE:HA	3:F:423:PHE:C	2.18	0.66
1:A:67:ARG:HD3	1:A:71:THR:CG2	2.26	0.65
1:A:304:PRO:HG3	1:A:310:PRO:HB3	1.77	0.65
3:I:552:PRO:CG	3:I:554:LEU:HG	2.26	0.65
2:E:18:ILE:CD1	2:E:497:PHE:HD1	2.03	0.65
1:G:304:PRO:HG3	1:G:310:PRO:HB3	1.77	0.65
1:D:154:PHE:CD2	3:F:715:CYS:O	2.49	0.65
1:G:10:GLU:HB2	3:I:330:GLN:HE22	1.61	0.65
1:J:230:MET:SD	2:K:465:ARG:HB3	2.37	0.65
1:D:151:LEU:HD23	3:F:715:CYS:HB2	1.76	0.65
2:K:349:LYS:NZ	2:K:407:GLY:O	2.25	0.65
1:D:52:TYR:CZ	1:D:146:MET:HB2	2.33	0.64
2:K:487:LEU:HD23	2:K:489:GLU:H	1.61	0.64
2:H:487:LEU:CD2	2:H:489:GLU:H	2.09	0.64
1:D:233:ASN:HA	2:E:78:LEU:HD12	1.80	0.64
3:L:753:THR:HG22	3:L:754:ALA:N	2.13	0.64
1:D:88:LEU:HD12	1:D:123:LEU:HD22	1.78	0.64
2:B:179:LYS:CB	1:G:203:PHE:CZ	2.80	0.64
2:B:180:GLU:CD	2:B:215:LYS:HD3	2.17	0.64
3:L:575:LEU:HD12	3:L:582:ILE:HD12	1.79	0.64
3:F:474:PRO:HB3	1:G:126:SER:CA	2.28	0.64
1:G:230:MET:SD	2:H:465:ARG:HB3	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:487:LEU:HD23	2:H:489:GLU:H	1.63	0.64
2:B:349:LYS:NZ	2:B:407:GLY:O	2.25	0.63
2:E:349:LYS:NZ	2:E:407:GLY:O	2.25	0.63
2:H:349:LYS:NZ	2:H:407:GLY:O	2.25	0.63
1:A:88:LEU:HD23	1:A:102:PHE:CZ	2.32	0.63
1:D:88:LEU:HD21	1:D:126:SER:OG	1.99	0.63
1:D:368:SER:HB2	2:E:359:LEU:HD23	1.81	0.63
2:E:14:VAL:O	2:E:18:ILE:HG23	1.98	0.63
3:L:575:LEU:CD1	3:L:582:ILE:CD1	2.62	0.63
3:I:753:THR:HG22	3:I:754:ALA:N	2.14	0.63
2:E:487:LEU:CD2	2:E:489:GLU:H	2.11	0.63
3:C:415:ILE:HD11	3:C:453:ILE:HD13	1.80	0.63
3:I:554:LEU:CD1	3:I:557:LEU:HG	2.11	0.63
1:D:665:PHE:HB2	2:E:480:LEU:O	1.99	0.62
1:A:412:GLU:HG2	2:B:601:ASN:ND2	2.14	0.62
3:L:139:GLU:O	3:L:140:LEU:HG	1.99	0.62
3:C:753:THR:HG22	3:C:754:ALA:N	2.13	0.62
1:D:90:PHE:CE1	1:D:122:LYS:O	2.52	0.62
2:K:14:VAL:O	2:K:18:ILE:HG23	1.99	0.62
3:L:415:ILE:HD11	3:L:453:ILE:HD13	1.80	0.62
3:F:474:PRO:HB3	1:G:126:SER:CB	2.28	0.62
3:I:415:ILE:HD11	3:I:453:ILE:HD13	1.80	0.62
1:D:64:ILE:N	1:D:93:ASP:O	2.30	0.62
1:D:102:PHE:O	1:D:128:LYS:N	2.26	0.62
1:G:183:ILE:HD13	2:H:334:LEU:HD22	1.80	0.62
1:G:151:LEU:HD13	3:I:753:THR:OG1	1.99	0.62
1:A:477:VAL:HG12	1:A:478:PRO:N	2.15	0.61
3:I:554:LEU:HD13	3:I:557:LEU:H	1.65	0.61
3:F:757:ARG:O	3:F:758:ALA:HB3	1.99	0.61
3:I:549:PHE:CE1	3:I:569:GLU:OE1	2.53	0.61
2:B:487:LEU:CD1	2:B:488:PRO:CD	2.73	0.61
1:D:410:GLU:CD	1:D:411:LEU:N	2.58	0.61
2:H:282:ALA:HB2	3:I:148:GLN:CG	2.30	0.61
2:B:363:ARG:HD3	3:F:139:GLU:OE2	1.99	0.61
1:D:154:PHE:CG	3:F:715:CYS:O	2.53	0.61
3:F:474:PRO:HD3	1:G:126:SER:N	2.14	0.61
3:I:554:LEU:HD11	3:I:557:LEU:CB	2.31	0.61
3:F:415:ILE:HD11	3:F:453:ILE:HD13	1.80	0.61
3:F:692:ARG:HH22	3:F:755:SER:CB	2.14	0.61
1:G:410:GLU:CD	1:G:411:LEU:N	2.59	0.61
2:B:180:GLU:CB	1:G:203:PHE:HE1	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:531:THR:HG21	3:L:669:VAL:HG22	1.82	0.61
3:C:575:LEU:HD12	3:C:582:ILE:HD12	1.81	0.61
1:D:69:ARG:CD	1:D:91:LEU:HD13	2.31	0.61
1:G:67:ARG:NH2	3:I:770:ILE:HG22	2.16	0.61
1:J:477:VAL:HG12	1:J:478:PRO:N	2.15	0.61
1:G:477:VAL:HG12	1:G:478:PRO:N	2.16	0.61
2:E:487:LEU:HD23	2:E:489:GLU:H	1.66	0.60
1:J:410:GLU:CD	1:J:411:LEU:N	2.59	0.60
1:D:476:PRO:O	1:D:477:VAL:HG23	2.02	0.60
1:G:410:GLU:OE1	1:G:411:LEU:N	2.35	0.60
2:H:303:ASN:ND2	2:H:488:PRO:O	2.33	0.60
2:H:362:LYS:O	1:J:409:ASN:HB3	2.01	0.60
1:D:477:VAL:CG1	1:D:478:PRO:HD2	2.32	0.60
1:G:477:VAL:CG1	1:G:478:PRO:HD2	2.32	0.60
1:A:477:VAL:CG1	1:A:478:PRO:HD2	2.32	0.60
2:E:701:ILE:HD11	3:F:208:GLU:HA	1.83	0.60
2:H:686:GLN:CD	3:I:39:THR:OG1	2.45	0.60
1:A:171:ASN:ND2	2:B:167:GLU:OE2	2.35	0.60
1:D:52:TYR:CG	1:D:146:MET:CE	2.84	0.60
1:A:73:VAL:CA	1:A:91:LEU:HD11	2.31	0.59
1:A:396:THR:HG21	1:A:468:ARG:CG	2.31	0.59
2:B:303:ASN:ND2	2:B:488:PRO:O	2.35	0.59
3:C:575:LEU:CD1	3:C:582:ILE:CD1	2.62	0.59
1:D:477:VAL:HG12	1:D:478:PRO:N	2.16	0.59
3:F:576:GLY:CA	3:F:583:PRO:HG3	2.25	0.59
1:G:476:PRO:O	1:G:477:VAL:HG23	2.02	0.59
1:D:48:PHE:HA	1:D:149:GLN:HE21	1.66	0.59
1:D:410:GLU:OE1	1:D:411:LEU:N	2.35	0.59
2:E:303:ASN:ND2	2:E:488:PRO:O	2.34	0.59
1:A:79:LEU:HG	1:A:95:PHE:CZ	2.37	0.59
1:A:476:PRO:O	1:A:477:VAL:HG23	2.02	0.59
1:A:575:MET:HG2	2:B:544:THR:HA	1.84	0.59
1:D:396:THR:HG21	1:D:468:ARG:CG	2.31	0.59
1:D:469:LYS:HB2	1:D:475:LEU:HD12	1.85	0.59
2:H:50:SER:HB3	2:H:68:PHE:CD1	2.37	0.59
1:J:476:PRO:O	1:J:477:VAL:HG23	2.02	0.59
1:A:368:SER:HB2	2:B:359:LEU:HD23	1.85	0.59
1:D:562:ASP:HB2	3:F:49:LEU:HD13	1.83	0.59
2:H:363:ARG:HA	1:J:409:ASN:CB	2.33	0.59
1:D:64:ILE:HB	1:D:92:CYS:O	2.03	0.59
1:D:52:TYR:HE2	1:D:149:GLN:OE1	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:VAL:O	2:E:67:LYS:HD2	2.03	0.59
2:E:18:ILE:CD1	2:E:497:PHE:CG	2.86	0.59
1:G:176:PRO:HA	1:G:180:GLU:HB3	1.85	0.59
1:G:469:LYS:HB2	1:G:475:LEU:HD12	1.85	0.59
3:I:582:ILE:HG22	3:I:695:LEU:HD11	1.85	0.59
2:K:487:LEU:CD2	2:K:488:PRO:CD	2.81	0.59
1:D:185:MET:SD	2:E:173:ILE:CD1	2.91	0.58
2:H:363:ARG:CD	3:L:139:GLU:OE2	2.51	0.58
2:K:50:SER:HB3	2:K:68:PHE:CD1	2.37	0.58
1:A:366:LYS:HE2	2:B:359:LEU:CD1	2.27	0.58
2:B:50:SER:HB3	2:B:68:PHE:CD1	2.38	0.58
1:J:477:VAL:CG1	1:J:478:PRO:HD2	2.32	0.58
1:A:410:GLU:OE1	1:A:411:LEU:CB	2.48	0.58
1:D:52:TYR:CD1	1:D:146:MET:HE3	2.38	0.58
2:H:15:THR:HA	2:H:18:ILE:HD12	1.85	0.58
2:K:303:ASN:ND2	2:K:488:PRO:O	2.35	0.58
3:F:474:PRO:HG3	1:G:126:SER:O	2.02	0.58
2:K:487:LEU:HD23	2:K:487:LEU:C	2.29	0.58
1:A:469:LYS:HB2	1:A:475:LEU:HD12	1.85	0.58
1:G:464:ARG:HG2	1:G:482:ASP:HB3	1.85	0.58
2:H:51:ARG:CZ	2:H:82:THR:HG22	2.34	0.58
2:H:749:ALA:HB1	3:I:16:GLN:HA	1.86	0.58
1:J:410:GLU:OE1	1:J:411:LEU:N	2.37	0.58
3:C:576:GLY:CA	3:C:583:PRO:HG3	2.28	0.58
1:D:151:LEU:HD11	3:F:751:LYS:HE3	1.85	0.58
2:K:18:ILE:CD1	2:K:497:PHE:CG	2.85	0.58
2:K:314:CYS:SG	2:K:477:ASN:ND2	2.76	0.58
2:E:487:LEU:HD23	2:E:487:LEU:C	2.29	0.58
1:J:464:ARG:HG2	1:J:482:ASP:HB3	1.86	0.58
2:H:487:LEU:HD23	2:H:487:LEU:C	2.29	0.58
1:D:165:ARG:NH2	2:E:707:ALA:HB2	2.19	0.58
1:D:194:LEU:HD21	2:E:220:LEU:HD11	1.84	0.58
3:F:755:SER:O	3:F:757:ARG:HG3	2.03	0.58
2:H:350:PHE:HB3	2:H:401:VAL:HG21	1.86	0.58
2:H:625:VAL:HG22	3:I:106:ASN:HB3	1.86	0.58
1:D:565:SER:OG	3:F:52:ARG:NH1	2.30	0.57
2:E:314:CYS:SG	2:E:477:ASN:ND2	2.76	0.57
2:H:314:CYS:SG	2:H:477:ASN:ND2	2.77	0.57
2:K:350:PHE:HB3	2:K:401:VAL:HG21	1.86	0.57
1:D:464:ARG:HG2	1:D:482:ASP:HB3	1.86	0.57
2:E:50:SER:HB3	2:E:68:PHE:CD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:487:LEU:CD2	2:E:488:PRO:CD	2.81	0.57
2:E:656:VAL:HG13	3:F:213:MET:HE1	1.85	0.57
3:I:554:LEU:HD12	3:I:554:LEU:C	2.29	0.57
1:A:72:ALA:O	1:A:91:LEU:CD2	2.50	0.57
1:A:176:PRO:HA	1:A:180:GLU:HB3	1.85	0.57
2:H:662:PHE:CE2	3:I:102:ILE:HD13	2.40	0.57
3:I:42:ARG:CZ	3:I:50:ARG:HD2	2.35	0.57
1:J:469:LYS:HB2	1:J:475:LEU:HD12	1.85	0.57
2:H:487:LEU:HG	2:H:488:PRO:CD	2.32	0.57
3:I:393:LEU:N	3:I:417:CYS:SG	2.78	0.57
1:J:176:PRO:HA	1:J:180:GLU:HB3	1.85	0.57
2:B:18:ILE:HG21	2:B:497:PHE:CE1	2.40	0.57
2:H:686:GLN:OE1	3:I:39:THR:OG1	2.22	0.57
1:A:529:HIS:NE2	3:F:678:LYS:HG3	2.20	0.57
1:G:205:THR:OG1	1:G:208:GLN:HG3	2.04	0.57
2:H:286:THR:CG2	3:I:504:ASP:HB2	2.34	0.57
1:J:21:ALA:HA	1:J:38:ILE:HD11	1.87	0.57
1:D:90:PHE:HE1	1:D:122:LYS:O	1.88	0.57
1:G:194:LEU:HG	2:H:348:ASN:HD22	1.69	0.57
3:F:474:PRO:CG	1:G:126:SER:CA	2.75	0.56
3:I:552:PRO:HG2	3:I:557:LEU:HD12	1.87	0.56
2:B:314:CYS:SG	2:B:477:ASN:ND2	2.78	0.56
2:B:363:ARG:HD2	3:F:139:GLU:OE2	2.02	0.56
2:E:51:ARG:CZ	2:E:82:THR:HG22	2.34	0.56
1:J:151:LEU:HD13	3:L:753:THR:CG2	2.35	0.56
1:J:410:GLU:O	3:L:139:GLU:HB3	2.05	0.56
2:B:15:THR:HA	2:B:18:ILE:HD12	1.86	0.56
1:A:322:ALA:HA	3:F:544:PHE:CG	2.40	0.56
2:B:350:PHE:HB3	2:B:401:VAL:HG21	1.87	0.56
3:F:393:LEU:N	3:F:417:CYS:SG	2.78	0.56
3:F:476:LYS:N	1:G:86:GLU:HG3	2.20	0.56
2:H:286:THR:HG23	3:I:504:ASP:HB2	1.87	0.56
2:K:487:LEU:HG	2:K:488:PRO:CD	2.32	0.56
2:K:51:ARG:CZ	2:K:82:THR:HG22	2.35	0.56
1:D:63:LEU:HA	1:D:94:ILE:HG12	1.87	0.56
1:A:21:ALA:HA	1:A:38:ILE:HD11	1.88	0.56
3:F:357:TYR:CD2	3:F:358:ILE:O	2.59	0.56
1:G:200:PRO:HB3	2:H:69:CYS:HB2	1.87	0.56
2:B:51:ARG:CZ	2:B:82:THR:HG22	2.34	0.56
3:L:393:LEU:N	3:L:417:CYS:SG	2.78	0.56
1:D:176:PRO:HA	1:D:180:GLU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:393:LEU:N	3:C:417:CYS:SG	2.79	0.55
1:J:281:ARG:HD3	2:K:570:LYS:HB3	1.87	0.55
2:E:18:ILE:HD13	2:E:497:PHE:CG	2.42	0.55
2:E:350:PHE:HB3	2:E:401:VAL:HG21	1.87	0.55
2:H:18:ILE:HG21	2:H:497:PHE:CE1	2.41	0.55
3:I:39:THR:O	3:I:39:THR:HG22	2.07	0.55
1:A:635:ASN:ND2	2:B:27:PRO:O	2.40	0.55
1:G:203:PHE:HA	1:G:208:GLN:NE2	2.21	0.55
1:D:90:PHE:CZ	1:D:122:LYS:CB	2.76	0.55
1:D:204:GLN:NE2	2:E:56:LYS:HE3	2.21	0.55
1:D:340:LEU:HD22	1:D:493:SER:HB3	1.88	0.55
1:D:401:MET:HE1	2:E:551:ILE:HD11	1.88	0.55
2:K:18:ILE:HD13	2:K:497:PHE:CG	2.41	0.55
1:G:175:LEU:HB3	1:G:176:PRO:HD2	1.89	0.55
1:A:28:TYR:HE1	1:A:69:ARG:HH11	1.52	0.55
1:G:637:SER:HB2	2:H:238:LEU:HA	1.87	0.55
1:D:575:MET:CG	2:E:544:THR:HA	2.36	0.55
2:E:123:SER:HB3	3:F:34:THR:HG22	1.88	0.55
3:F:140:LEU:O	3:F:248:ILE:HG22	2.07	0.55
3:F:753:THR:HG22	3:F:754:ALA:N	2.21	0.55
2:E:487:LEU:HG	2:E:488:PRO:CD	2.32	0.55
3:F:692:ARG:CZ	3:F:755:SER:OG	2.54	0.55
1:A:175:LEU:HB3	1:A:176:PRO:HD2	1.89	0.54
2:B:179:LYS:CB	1:G:203:PHE:HZ	2.20	0.54
3:F:575:LEU:HD12	3:F:582:ILE:HD12	1.79	0.54
3:I:340:MET:HE2	3:I:409:LEU:HD23	1.89	0.54
3:L:140:LEU:O	3:L:248:ILE:HG22	2.07	0.54
2:H:487:LEU:CD2	2:H:488:PRO:CD	2.81	0.54
2:H:496:MET:HA	2:H:503:VAL:HG21	1.90	0.54
3:C:340:MET:HE2	3:C:409:LEU:HD23	1.89	0.54
2:B:701:ILE:HD11	3:C:208:GLU:HA	1.89	0.54
1:D:52:TYR:CE2	1:D:146:MET:HB2	2.42	0.54
1:G:402:ALA:HB3	2:H:550:ARG:HG2	1.90	0.54
3:F:474:PRO:HG3	1:G:126:SER:C	2.33	0.54
2:H:686:GLN:CD	3:I:39:THR:HG1	2.16	0.54
1:A:529:HIS:NE2	3:F:678:LYS:HE2	2.23	0.54
2:B:496:MET:HA	2:B:503:VAL:HG21	1.90	0.54
3:F:358:ILE:HG12	3:F:423:PHE:HA	1.90	0.54
1:J:410:GLU:HG2	3:L:137:TRP:HB3	1.89	0.54
1:G:21:ALA:HA	1:G:38:ILE:HD11	1.88	0.54
1:J:408:ASP:O	1:J:412:GLU:CB	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:ARG:HE	1:D:91:LEU:CD2	2.20	0.54
3:F:340:MET:HE2	3:F:409:LEU:HD23	1.89	0.54
1:D:175:LEU:HB3	1:D:176:PRO:HD2	1.90	0.54
1:D:185:MET:SD	2:E:173:ILE:HD13	2.48	0.54
2:H:686:GLN:OE1	3:I:39:THR:HG23	2.03	0.54
1:D:644:ASN:ND2	2:E:236:GLY:HA3	2.23	0.53
2:K:496:MET:HA	2:K:503:VAL:HG21	1.90	0.53
3:L:340:MET:HE2	3:L:409:LEU:HD23	1.90	0.53
1:D:171:ASN:ND2	2:E:167:GLU:OE2	2.41	0.53
1:D:151:LEU:HD21	3:F:751:LYS:HG2	1.90	0.53
2:K:421:GLY:O	2:K:424:THR:OG1	2.24	0.53
1:A:67:ARG:HD3	1:A:71:THR:HG22	1.91	0.53
1:J:175:LEU:HB3	1:J:176:PRO:HD2	1.89	0.53
1:A:449:CYS:SG	1:A:490:LYS:NZ	2.82	0.53
1:G:203:PHE:HB3	1:G:208:GLN:HB2	1.89	0.53
1:J:412:GLU:OE1	2:K:601:ASN:ND2	2.42	0.53
1:J:449:CYS:SG	1:J:490:LYS:NZ	2.81	0.53
2:E:496:MET:HA	2:E:503:VAL:HG21	1.90	0.53
1:D:245:LYS:HA	1:D:706:PHE:HB2	1.91	0.53
3:F:576:GLY:H	3:F:581:ASP:HB3	1.74	0.53
1:D:90:PHE:CG	1:D:123:LEU:HD11	2.41	0.52
1:G:476:PRO:O	1:G:477:VAL:CG2	2.57	0.52
2:B:487:LEU:HG	2:B:488:PRO:CD	2.38	0.52
1:A:88:LEU:C	1:A:90:PHE:N	2.66	0.52
1:A:568:ARG:HD2	2:B:555:GLU:OE2	2.08	0.52
1:D:281:ARG:HD3	2:E:570:LYS:HB3	1.89	0.52
3:F:475:GLY:C	1:G:86:GLU:CG	2.81	0.52
1:J:476:PRO:O	1:J:477:VAL:CG2	2.57	0.52
1:J:680:ASN:H	1:J:680:ASN:ND2	2.06	0.52
2:K:487:LEU:CG	2:K:488:PRO:CD	2.88	0.52
1:A:86:GLU:O	1:A:88:LEU:HD22	2.10	0.52
1:A:476:PRO:O	1:A:477:VAL:CG2	2.57	0.52
2:B:363:ARG:CZ	3:F:139:GLU:OE2	2.56	0.52
1:D:69:ARG:NH1	1:D:91:LEU:CD1	2.62	0.52
3:F:474:PRO:HD3	1:G:125:ASN:C	2.35	0.52
1:J:677:CYS:C	1:J:678:LEU:HD12	2.34	0.52
2:E:691:MET:SD	3:F:7:ILE:HG23	2.50	0.52
3:L:753:THR:CG2	3:L:754:ALA:N	2.73	0.52
1:D:476:PRO:O	1:D:477:VAL:CG2	2.57	0.52
1:J:355:LEU:HG	2:K:368:VAL:HG11	1.92	0.52
1:D:69:ARG:NE	1:D:91:LEU:HD21	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:477:MET:CE	1:G:126:SER:CB	2.87	0.52
2:H:750:ARG:HB2	3:I:15:CYS:HB2	1.92	0.52
1:D:155:SER:HA	3:F:714:VAL:CG2	2.40	0.52
2:H:357:ILE:O	2:H:370:ILE:HG22	2.10	0.52
1:J:245:LYS:HA	1:J:706:PHE:HB2	1.92	0.52
1:A:292:LYS:O	3:F:672:ASN:HB2	2.10	0.52
2:E:357:ILE:O	2:E:370:ILE:HG22	2.10	0.52
1:G:200:PRO:CB	2:H:69:CYS:HB2	2.40	0.52
1:G:398:TRP:CG	1:G:433:ARG:HA	2.45	0.52
3:I:138:LYS:HB3	3:I:250:GLU:HB2	1.92	0.52
2:K:373:GLU:HA	2:K:399:LYS:O	2.10	0.52
2:B:357:ILE:O	2:B:370:ILE:HG22	2.10	0.51
2:B:373:GLU:HA	2:B:399:LYS:O	2.10	0.51
2:B:487:LEU:CG	2:B:488:PRO:CD	2.88	0.51
1:G:303:LYS:HE2	3:L:123:LYS:HD3	1.91	0.51
2:E:373:GLU:HA	2:E:399:LYS:O	2.10	0.51
2:E:438:PHE:HB2	2:E:453:VAL:HB	1.92	0.51
2:E:702:ASN:HB2	3:F:171:MET:SD	2.50	0.51
2:H:624:ARG:HG2	3:I:109:GLY:O	2.10	0.51
1:A:245:LYS:HA	1:A:706:PHE:HB2	1.92	0.51
2:K:357:ILE:O	2:K:370:ILE:HG22	2.10	0.51
1:A:398:TRP:CG	1:A:433:ARG:HA	2.45	0.51
2:E:487:LEU:CG	2:E:488:PRO:CD	2.88	0.51
2:E:701:ILE:HD12	3:F:174:LEU:HD11	1.92	0.51
3:F:754:ALA:O	3:F:755:SER:C	2.50	0.51
1:G:203:PHE:CA	1:G:208:GLN:NE2	2.74	0.51
3:L:139:GLU:O	3:L:140:LEU:CG	2.58	0.51
2:B:398:GLN:HG3	2:B:399:LYS:H	1.75	0.51
3:C:753:THR:CG2	3:C:754:ALA:N	2.73	0.51
1:D:233:ASN:CG	2:E:78:LEU:HD12	2.35	0.51
1:G:245:LYS:HA	1:G:706:PHE:HB2	1.92	0.51
1:D:88:LEU:CD2	1:D:126:SER:OG	2.58	0.51
1:D:398:TRP:CG	1:D:433:ARG:HA	2.45	0.51
1:D:568:ARG:HB3	2:E:551:ILE:HD12	1.92	0.51
3:I:571:LEU:O	3:I:575:LEU:HG	2.11	0.51
3:I:711:GLY:O	3:I:753:THR:O	2.29	0.51
3:L:575:LEU:HD13	3:L:582:ILE:HG13	1.93	0.51
3:L:576:GLY:H	3:L:581:ASP:HB3	1.76	0.51
3:L:576:GLY:CA	3:L:583:PRO:HG3	2.26	0.51
1:A:407:ALA:CB	1:A:412:GLU:CB	2.70	0.51
1:G:449:CYS:SG	1:G:490:LYS:NZ	2.81	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:678:LEU:CD1	1:J:678:LEU:N	2.73	0.51
1:D:13:LEU:HD21	1:D:39:GLY:O	2.11	0.51
1:D:197:GLU:O	2:E:65:ARG:NH1	2.43	0.51
1:D:449:CYS:SG	1:D:490:LYS:NZ	2.82	0.51
1:G:624:GLN:NE2	2:H:8:MET:SD	2.80	0.51
2:H:373:GLU:HA	2:H:399:LYS:O	2.10	0.51
1:J:398:TRP:CG	1:J:433:ARG:HA	2.45	0.51
2:B:438:PHE:HB2	2:B:453:VAL:HB	1.93	0.51
1:D:112:ASP:HB2	1:D:139:ASP:HB2	1.92	0.51
1:D:419:ASN:ND2	2:E:543:SER:OG	2.42	0.51
2:H:746:ALA:HB1	3:I:15:CYS:SG	2.50	0.51
3:I:753:THR:CG2	3:I:754:ALA:N	2.73	0.51
1:J:59:ASP:OD2	3:L:769:LYS:NZ	2.44	0.51
1:J:469:LYS:HD3	1:J:475:LEU:CD1	2.40	0.51
2:H:303:ASN:ND2	2:H:488:PRO:HA	2.27	0.50
1:A:677:CYS:HA	2:B:238:LEU:HD22	1.93	0.50
3:C:138:LYS:HB3	3:C:250:GLU:HB2	1.92	0.50
2:E:18:ILE:HD13	2:E:497:PHE:CD1	2.38	0.50
2:E:398:GLN:HG3	2:E:399:LYS:H	1.76	0.50
1:G:264:LEU:HD21	1:G:267:GLU:HB2	1.94	0.50
1:G:469:LYS:CD	1:G:475:LEU:HD13	2.40	0.50
3:C:571:LEU:O	3:C:575:LEU:HG	2.11	0.50
3:C:576:GLY:H	3:C:581:ASP:HB3	1.77	0.50
1:D:264:LEU:HD21	1:D:267:GLU:HB2	1.93	0.50
2:H:90:LEU:HA	2:H:93:LEU:HD12	1.93	0.50
1:J:402:ALA:HB3	2:K:550:ARG:HG2	1.93	0.50
2:H:363:ARG:C	1:J:409:ASN:HD22	2.01	0.50
3:I:577:THR:HA	3:I:754:ALA:HA	1.92	0.50
2:B:90:LEU:HA	2:B:93:LEU:HD12	1.93	0.50
1:G:209:MET:SD	1:G:209:MET:C	2.94	0.50
2:E:282:ALA:CB	3:F:149:ARG:HD3	2.40	0.50
3:F:477:MET:HE3	1:G:126:SER:OG	2.11	0.50
3:I:57:SER:HB2	3:I:60:PRO:HG3	1.94	0.50
1:A:264:LEU:HD21	1:A:267:GLU:HB2	1.93	0.50
3:F:575:LEU:HD13	3:F:582:ILE:HG13	1.93	0.50
1:J:264:LEU:HD21	1:J:267:GLU:HB2	1.93	0.50
2:K:342:ALA:HB3	2:K:343:PRO:HD3	1.94	0.50
2:H:359:LEU:HB2	2:H:368:VAL:HB	1.94	0.50
3:L:122:TYR:CD1	3:L:213:MET:HG2	2.47	0.50
2:K:90:LEU:HA	2:K:93:LEU:HD12	1.94	0.49
3:L:138:LYS:HD3	3:L:250:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ALA:HB1	3:C:235:ARG:HD2	1.94	0.49
3:L:57:SER:HB2	3:L:60:PRO:HG3	1.94	0.49
3:L:230:ALA:HB1	3:L:235:ARG:HD2	1.95	0.49
1:D:69:ARG:NE	1:D:91:LEU:CD2	2.75	0.49
1:D:200:PRO:HG3	2:E:318:GLU:HB3	1.93	0.49
3:F:358:ILE:CA	3:F:423:PHE:CA	2.82	0.49
3:L:138:LYS:HE2	3:L:140:LEU:CD1	2.43	0.49
1:D:165:ARG:HD3	2:E:706:GLY:CA	2.42	0.49
1:D:405:PRO:HG2	2:E:601:ASN:ND2	2.28	0.49
3:I:575:LEU:HD12	3:I:582:ILE:HD12	1.77	0.49
3:L:283:ASN:O	3:L:287:LYS:NZ	2.46	0.49
3:C:57:SER:HB2	3:C:60:PRO:HG3	1.94	0.49
3:C:565:THR:HG22	3:C:685:TYR:HB3	1.95	0.49
2:H:279:GLU:HB2	3:I:224:PHE:CE2	2.47	0.49
1:A:631:PHE:CD1	2:B:23:PRO:HB3	2.48	0.49
3:C:122:TYR:CD1	3:C:213:MET:HG2	2.48	0.49
3:F:57:SER:HB2	3:F:60:PRO:HG3	1.94	0.49
2:K:438:PHE:HB2	2:K:453:VAL:HB	1.93	0.49
3:L:571:LEU:O	3:L:575:LEU:HG	2.12	0.49
1:D:233:ASN:HA	2:E:78:LEU:CG	2.42	0.49
3:F:138:LYS:HE2	3:F:140:LEU:CD1	2.43	0.49
2:H:487:LEU:CG	2:H:488:PRO:CD	2.88	0.49
3:I:575:LEU:HD13	3:I:582:ILE:CB	2.43	0.49
3:L:711:GLY:O	3:L:753:THR:O	2.30	0.49
3:L:721:ALA:HB1	3:L:738:VAL:HA	1.94	0.49
1:D:79:LEU:HG	1:D:95:PHE:CE1	2.48	0.49
3:F:122:TYR:CD1	3:F:213:MET:HG2	2.47	0.49
3:F:571:LEU:O	3:F:575:LEU:HG	2.12	0.49
3:F:757:ARG:O	3:F:758:ALA:CB	2.61	0.49
1:G:203:PHE:HA	1:G:208:GLN:HE22	1.78	0.49
1:G:648:LYS:HE3	2:H:482:LYS:O	2.13	0.49
2:H:134:TRP:HZ3	2:H:183:PHE:CE1	2.31	0.49
2:K:134:TRP:HZ3	2:K:183:PHE:CE1	2.30	0.49
1:A:345:ARG:HH11	3:F:136:MET:HB3	1.78	0.49
2:B:282:ALA:HB3	3:C:149:ARG:HD3	1.94	0.49
1:D:150:LYS:HD3	3:F:716:GLU:OE2	2.12	0.49
3:F:565:THR:HG22	3:F:685:TYR:HB3	1.94	0.49
2:H:398:GLN:HG3	2:H:399:LYS:H	1.78	0.49
2:K:359:LEU:HB2	2:K:368:VAL:HB	1.94	0.49
2:K:398:GLN:HG3	2:K:399:LYS:H	1.77	0.49
3:C:721:ALA:HB1	3:C:738:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:230:ALA:HB1	3:F:235:ARG:HD2	1.94	0.49
3:I:552:PRO:CD	3:I:557:LEU:HD12	2.43	0.49
1:J:240:HIS:NE2	1:J:656:ASP:OD2	2.46	0.49
1:J:695:VAL:HG13	1:J:705:PHE:CD1	2.48	0.49
1:G:112:ASP:HB2	1:G:139:ASP:HB2	1.95	0.48
3:I:230:ALA:HB1	3:I:235:ARG:HD2	1.95	0.48
1:D:92:CYS:SG	1:D:102:PHE:CD2	2.81	0.48
2:H:438:PHE:HB2	2:H:453:VAL:HB	1.94	0.48
2:E:90:LEU:HA	2:E:93:LEU:HD12	1.95	0.48
1:J:238:ILE:HG21	1:J:665:PHE:HA	1.95	0.48
3:L:139:GLU:O	3:L:140:LEU:HD23	2.13	0.48
1:A:695:VAL:HG13	1:A:705:PHE:CD1	2.48	0.48
2:B:180:GLU:HG3	1:G:203:PHE:CD1	2.47	0.48
1:D:473:GLU:OE2	1:D:475:LEU:HD21	2.13	0.48
3:F:357:TYR:CE2	3:F:358:ILE:O	2.65	0.48
3:F:721:ALA:HB1	3:F:738:VAL:HA	1.94	0.48
3:I:721:ALA:HB1	3:I:738:VAL:HA	1.94	0.48
1:J:677:CYS:SG	1:J:678:LEU:HD12	2.54	0.48
2:K:303:ASN:ND2	2:K:488:PRO:HA	2.28	0.48
2:B:303:ASN:ND2	2:B:488:PRO:HA	2.29	0.48
1:D:233:ASN:HA	2:E:78:LEU:CD1	2.43	0.48
1:D:240:HIS:NE2	1:D:656:ASP:OD2	2.46	0.48
1:G:240:HIS:NE2	1:G:656:ASP:OD2	2.47	0.48
1:G:477:VAL:CG1	1:G:478:PRO:CD	2.92	0.48
2:H:282:ALA:HB3	3:I:149:ARG:HD3	1.96	0.48
1:J:183:ILE:HD13	2:K:334:LEU:HD13	1.94	0.48
1:J:477:VAL:CG1	1:J:478:PRO:CD	2.92	0.48
1:J:477:VAL:CG1	1:J:478:PRO:N	2.77	0.48
1:A:240:HIS:NE2	1:A:656:ASP:OD2	2.46	0.48
2:B:342:ALA:HB3	2:B:343:PRO:HD3	1.95	0.48
2:E:359:LEU:HB2	2:E:368:VAL:HB	1.95	0.48
1:G:201:LEU:HD11	2:H:87:ILE:HD11	1.96	0.48
2:H:743:ILE:HD12	3:I:8:ALA:HB1	1.95	0.48
3:I:122:TYR:CD1	3:I:213:MET:HG2	2.47	0.48
1:A:67:ARG:HG2	1:A:71:THR:HB	1.94	0.48
1:A:469:LYS:CD	1:A:475:LEU:HD13	2.40	0.48
1:A:473:GLU:OE2	1:A:475:LEU:HD21	2.14	0.48
2:B:359:LEU:HB2	2:B:368:VAL:HB	1.94	0.48
2:B:363:ARG:NH2	3:F:139:GLU:CD	2.67	0.48
1:D:238:ILE:HG21	1:D:665:PHE:HA	1.95	0.48
1:G:473:GLU:OE2	1:G:475:LEU:HD21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:473:GLU:OE2	1:J:475:LEU:HD21	2.14	0.48
1:A:112:ASP:HB2	1:A:139:ASP:HB2	1.95	0.48
1:A:115:TYR:CZ	1:A:175:LEU:HD12	2.48	0.48
1:A:632:CYS:HA	2:B:26:GLY:HA3	1.95	0.48
1:D:69:ARG:NH2	1:D:91:LEU:CD1	2.70	0.48
1:D:583:LEU:HD13	3:F:247:TRP:CZ2	2.49	0.48
3:F:139:GLU:O	3:F:140:LEU:HG	2.14	0.48
1:G:535:LYS:NZ	3:L:654:GLU:HG2	2.29	0.48
1:D:151:LEU:CD2	3:F:751:LYS:HG2	2.44	0.48
2:H:342:ALA:HB3	2:H:343:PRO:HD3	1.95	0.48
3:L:565:THR:HG22	3:L:685:TYR:HB3	1.95	0.48
3:C:711:GLY:O	3:C:753:THR:O	2.31	0.48
1:D:677:CYS:HA	2:E:238:LEU:HD22	1.96	0.48
1:G:191:PHE:CE1	2:H:344:VAL:HG21	2.49	0.48
1:G:203:PHE:HB3	1:G:208:GLN:CB	2.44	0.48
2:B:18:ILE:HD13	2:B:497:PHE:CG	2.49	0.47
3:C:576:GLY:HA2	3:C:583:PRO:HD3	1.95	0.47
2:E:627:ASN:ND2	3:F:111:CYS:SG	2.87	0.47
3:F:711:GLY:O	3:F:753:THR:O	2.32	0.47
1:G:115:TYR:CZ	1:G:175:LEU:HD12	2.48	0.47
1:G:695:VAL:HG13	1:G:705:PHE:CD1	2.48	0.47
1:J:151:LEU:HD13	3:L:753:THR:OG1	2.14	0.47
3:L:138:LYS:HD3	3:L:250:GLU:CG	2.44	0.47
3:L:692:ARG:CZ	3:L:755:SER:OG	2.60	0.47
1:A:73:VAL:N	1:A:91:LEU:HD11	2.29	0.47
1:D:155:SER:HA	3:F:714:VAL:HG23	1.96	0.47
1:D:477:VAL:CG1	1:D:478:PRO:CD	2.92	0.47
1:G:151:LEU:HA	3:I:714:VAL:O	2.15	0.47
2:H:18:ILE:HD13	2:H:497:PHE:CG	2.49	0.47
2:E:303:ASN:ND2	2:E:488:PRO:HA	2.30	0.47
2:E:342:ALA:HB3	2:E:343:PRO:HD3	1.94	0.47
2:H:289:THR:HG21	3:I:499:GLN:HE22	1.79	0.47
1:A:477:VAL:CG1	1:A:478:PRO:CD	2.91	0.47
1:D:660:LYS:HE2	2:E:489:GLU:HB2	1.97	0.47
1:D:695:VAL:HG13	1:D:705:PHE:CD1	2.49	0.47
1:J:115:TYR:CZ	1:J:175:LEU:HD12	2.49	0.47
1:A:238:ILE:HG21	1:A:665:PHE:HA	1.96	0.47
1:D:52:TYR:HE2	1:D:149:GLN:CD	2.23	0.47
3:F:166:ILE:HD12	3:F:218:PHE:HB2	1.95	0.47
3:F:138:LYS:HD3	3:F:250:GLU:HG2	1.97	0.47
1:A:477:VAL:CG1	1:A:478:PRO:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:LYS:C	1:G:203:PHE:HE1	2.22	0.47
2:B:180:GLU:OE2	2:B:215:LYS:HE2	2.14	0.47
1:D:13:LEU:HG	1:D:43:GLN:OE1	2.15	0.47
3:F:139:GLU:O	3:F:140:LEU:HD23	2.14	0.47
3:F:283:ASN:O	3:F:287:LYS:NZ	2.45	0.47
3:F:577:THR:HG23	3:F:754:ALA:CA	2.43	0.47
1:G:338:GLU:HG2	3:L:254:ALA:HB1	1.96	0.47
3:I:565:THR:HG22	3:I:685:TYR:HB3	1.95	0.47
1:J:287:ILE:CG2	1:J:460:PRO:HB3	2.45	0.47
3:L:166:ILE:HD12	3:L:218:PHE:HB2	1.96	0.47
3:C:692:ARG:CZ	3:C:755:SER:OG	2.62	0.47
1:D:287:ILE:CG2	1:D:460:PRO:HB3	2.45	0.47
2:E:134:TRP:HZ3	2:E:183:PHE:CE1	2.32	0.47
2:B:179:LYS:HB2	1:G:203:PHE:CE1	2.49	0.47
1:G:287:ILE:CG2	1:G:460:PRO:HB3	2.45	0.47
1:D:165:ARG:HD3	2:E:706:GLY:HA2	1.97	0.47
3:F:474:PRO:HG3	1:G:126:SER:CA	2.42	0.47
1:J:10:GLU:HB2	3:L:330:GLN:HE22	1.79	0.47
1:A:88:LEU:HD23	1:A:102:PHE:CE2	2.50	0.46
1:D:199:VAL:O	2:E:67:LYS:NZ	2.43	0.46
1:D:410:GLU:CB	3:F:137:TRP:HB3	2.34	0.46
1:J:235:LYS:NZ	2:K:464:ILE:HG22	2.30	0.46
1:J:407:ALA:CB	1:J:412:GLU:HB3	2.46	0.46
2:E:697:GLU:N	3:F:178:GLU:OE2	2.49	0.46
1:G:477:VAL:CG1	1:G:478:PRO:N	2.77	0.46
1:J:112:ASP:HB2	1:J:139:ASP:HB2	1.95	0.46
1:J:407:ALA:HA	1:J:412:GLU:HG3	1.97	0.46
1:A:278:GLU:HG2	2:B:570:LYS:HD2	1.96	0.46
1:A:287:ILE:CG2	1:A:460:PRO:HB3	2.45	0.46
2:B:421:GLY:O	2:B:424:THR:OG1	2.24	0.46
1:D:635:ASN:ND2	2:E:27:PRO:O	2.48	0.46
2:E:14:VAL:HG12	2:E:18:ILE:HG22	1.96	0.46
3:F:576:GLY:HA2	3:F:583:PRO:HD3	1.92	0.46
1:G:291:LYS:HD3	1:G:324:ILE:HG22	1.97	0.46
1:J:624:GLN:NE2	2:K:8:MET:SD	2.84	0.46
2:B:439:TRP:HB2	2:B:450:LEU:HD11	1.98	0.46
1:D:291:LYS:HD3	1:D:324:ILE:HG22	1.97	0.46
2:E:18:ILE:HD13	2:E:497:PHE:HB2	1.97	0.46
1:G:183:ILE:HD13	2:H:334:LEU:CD2	2.46	0.46
1:G:200:PRO:HB3	2:H:69:CYS:SG	2.55	0.46
3:I:453:ILE:HG12	3:I:463:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:575:LEU:HD13	3:I:582:ILE:HB	1.97	0.46
2:K:18:ILE:HD13	2:K:497:PHE:HB2	1.97	0.46
1:A:291:LYS:HD3	1:A:324:ILE:HG22	1.98	0.46
1:G:238:ILE:HG21	1:G:665:PHE:HA	1.96	0.46
1:G:469:LYS:HD3	1:G:475:LEU:CD1	2.40	0.46
2:H:363:ARG:CG	1:J:409:ASN:HB2	2.33	0.46
1:D:469:LYS:HD3	1:D:475:LEU:CD1	2.40	0.46
1:D:477:VAL:CG1	1:D:478:PRO:N	2.78	0.46
3:F:681:SER:HB3	3:F:691:ILE:HD11	1.98	0.46
2:H:289:THR:HG21	3:I:499:GLN:OE1	2.16	0.46
3:I:283:ASN:O	3:I:287:LYS:NZ	2.46	0.46
1:A:287:ILE:HA	1:A:290:PHE:HB2	1.98	0.46
1:D:287:ILE:HA	1:D:290:PHE:HB2	1.98	0.46
3:F:152:VAL:HG13	3:F:236:MET:HE2	1.98	0.46
1:G:242:GLU:N	1:G:242:GLU:OE1	2.48	0.46
2:K:439:TRP:HB2	2:K:450:LEU:HD11	1.98	0.46
1:A:348:LYS:NZ	3:F:138:LYS:NZ	2.63	0.46
2:B:134:TRP:HZ3	2:B:183:PHE:CE1	2.32	0.46
1:D:242:GLU:N	1:D:242:GLU:OE1	2.49	0.46
2:E:439:TRP:HB2	2:E:450:LEU:HD11	1.98	0.46
3:C:166:ILE:HD12	3:C:218:PHE:HB2	1.96	0.46
1:D:69:ARG:HD3	1:D:91:LEU:CD1	2.46	0.46
2:H:439:TRP:HB2	2:H:450:LEU:HD11	1.98	0.46
3:I:166:ILE:HD12	3:I:218:PHE:HB2	1.97	0.46
1:D:17:ALA:HA	1:D:42:PHE:HE2	1.81	0.46
1:G:194:LEU:HG	2:H:348:ASN:ND2	2.29	0.46
2:H:421:GLY:O	2:H:424:THR:OG1	2.24	0.46
1:J:201:LEU:HD21	2:K:87:ILE:HD11	1.98	0.46
1:J:287:ILE:HA	1:J:290:PHE:HB2	1.98	0.46
1:G:412:GLU:N	1:G:412:GLU:CD	2.73	0.45
3:L:393:LEU:HD22	3:L:396:ILE:HD11	1.98	0.45
1:D:14:GLU:HG2	1:D:43:GLN:NE2	2.31	0.45
1:D:190:THR:HG21	2:E:216:HIS:CE1	2.50	0.45
3:F:59:PHE:N	3:F:60:PRO:HD3	2.31	0.45
3:I:59:PHE:N	3:I:60:PRO:HD3	2.32	0.45
1:J:405:PRO:HG2	2:K:601:ASN:ND2	2.32	0.45
2:K:14:VAL:HG12	2:K:18:ILE:HG22	1.98	0.45
3:L:576:GLY:HA2	3:L:583:PRO:HD3	1.94	0.45
1:A:174:PHE:HB2	1:A:179:GLU:HB2	1.98	0.45
1:A:529:HIS:NE2	3:F:678:LYS:CE	2.79	0.45
3:C:59:PHE:N	3:C:60:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:TYR:CZ	1:D:146:MET:HE3	2.51	0.45
1:A:23:GLU:OE1	1:A:68:LYS:CD	2.63	0.45
1:A:261:HIS:CD2	1:A:265:MET:HE3	2.51	0.45
1:D:355:LEU:HD13	1:D:359:VAL:HG23	1.99	0.45
1:D:655:GLY:HA2	2:E:490:LEU:HD12	1.98	0.45
3:F:474:PRO:CB	1:G:126:SER:CA	2.87	0.45
3:L:577:THR:HG23	3:L:754:ALA:HB2	1.97	0.45
1:J:174:PHE:HB2	1:J:179:GLU:HB2	1.98	0.45
1:G:558:LYS:HE3	3:I:49:LEU:HD11	1.98	0.45
2:H:691:MET:HG2	3:I:10:GLU:HG2	1.98	0.45
1:J:151:LEU:HD13	3:L:753:THR:HG21	1.99	0.45
1:J:291:LYS:HD3	1:J:324:ILE:HG22	1.97	0.45
3:L:681:SER:HB3	3:L:691:ILE:HD11	1.98	0.45
3:C:283:ASN:O	3:C:287:LYS:NZ	2.45	0.45
3:C:453:ILE:HG12	3:C:463:LEU:HD22	1.98	0.45
3:C:681:SER:HB3	3:C:691:ILE:HD11	1.98	0.45
3:F:753:THR:CG2	3:F:754:ALA:N	2.79	0.45
1:G:174:PHE:HB2	1:G:179:GLU:HB2	1.98	0.45
2:H:50:SER:HB3	2:H:68:PHE:CE2	2.52	0.45
2:H:631:PRO:HB3	3:I:68:LEU:HB2	1.99	0.45
1:J:242:GLU:N	1:J:242:GLU:OE1	2.49	0.45
3:L:59:PHE:N	3:L:60:PRO:HD3	2.32	0.45
1:A:401:MET:CE	2:B:551:ILE:HD11	2.44	0.45
1:G:287:ILE:HA	1:G:290:PHE:HB2	1.98	0.45
1:G:405:PRO:HG2	2:H:601:ASN:ND2	2.32	0.45
3:I:393:LEU:HD22	3:I:396:ILE:HD11	1.98	0.45
3:L:139:GLU:O	3:L:140:LEU:CD2	2.64	0.45
1:A:242:GLU:OE1	1:A:242:GLU:N	2.50	0.45
1:A:418:LEU:HB3	2:B:543:SER:OG	2.17	0.45
1:A:469:LYS:HB2	1:A:475:LEU:CD1	2.47	0.45
1:D:151:LEU:O	3:F:714:VAL:O	2.34	0.45
2:H:427:TYR:CD2	2:H:431:GLU:HB2	2.52	0.45
2:K:131:THR:HG21	2:K:251:ARG:HD2	1.99	0.45
3:L:138:LYS:HE2	3:L:140:LEU:HD11	1.99	0.45
1:D:152:ARG:NH1	3:F:762:ASP:OD2	2.50	0.45
1:G:8:ILE:HD11	2:H:115:THR:CG2	2.47	0.45
1:G:469:LYS:HB2	1:G:475:LEU:CD1	2.47	0.45
2:H:131:THR:HG21	2:H:251:ARG:HD2	1.99	0.45
1:A:338:GLU:CG	3:F:254:ALA:HB1	2.43	0.44
2:E:361:ASN:C	2:E:363:ARG:H	2.26	0.44
3:F:453:ILE:HG12	3:F:463:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:692:ARG:CZ	3:I:755:SER:OG	2.61	0.44
1:J:410:GLU:CD	1:J:411:LEU:H	2.25	0.44
1:J:660:LYS:HE2	2:K:489:GLU:OE2	2.17	0.44
2:B:50:SER:HB3	2:B:68:PHE:CE2	2.52	0.44
1:D:434:GLU:HA	1:D:437:LYS:HG2	2.00	0.44
1:D:488:CYS:SG	1:D:504:ILE:HD11	2.58	0.44
3:F:393:LEU:HD22	3:F:396:ILE:HD11	1.98	0.44
2:K:542:PRO:HD3	3:L:247:TRP:CZ2	2.52	0.44
1:D:140:LYS:HE2	1:D:145:PRO:HD2	2.00	0.44
1:D:657:LYS:HE3	2:E:9:PHE:O	2.17	0.44
1:J:88:LEU:HD12	1:J:123:LEU:HD22	1.99	0.44
2:K:467:PHE:O	2:K:470:VAL:HG12	2.17	0.44
1:A:469:LYS:HD3	1:A:475:LEU:CD1	2.40	0.44
3:C:393:LEU:HD21	3:C:467:ARG:CZ	2.48	0.44
3:C:577:THR:HG23	3:C:754:ALA:HB2	1.99	0.44
3:I:152:VAL:HG13	3:I:236:MET:HE2	1.99	0.44
1:J:261:HIS:CD2	1:J:265:MET:HE3	2.53	0.44
1:A:577:THR:HG21	2:B:20:THR:CG2	2.47	0.44
1:D:261:HIS:CD2	1:D:265:MET:HE3	2.53	0.44
1:D:412:GLU:N	1:D:412:GLU:CD	2.73	0.44
1:G:434:GLU:HA	1:G:437:LYS:HG2	1.99	0.44
1:J:223:LEU:HD22	2:K:432:LEU:HD23	1.99	0.44
1:A:88:LEU:C	1:A:90:PHE:H	2.24	0.44
1:A:410:GLU:OE1	1:A:411:LEU:N	2.50	0.44
2:B:68:PHE:CD1	2:B:68:PHE:O	2.71	0.44
2:E:50:SER:HB3	2:E:68:PHE:CE2	2.52	0.44
1:J:355:LEU:HD13	1:J:359:VAL:HG23	1.99	0.44
1:J:469:LYS:HB2	1:J:475:LEU:CD1	2.48	0.44
2:K:50:SER:HB3	2:K:68:PHE:CE2	2.52	0.44
2:B:627:ASN:ND2	3:C:111:CYS:SG	2.91	0.44
2:E:467:PHE:O	2:E:470:VAL:HG12	2.18	0.44
1:G:338:GLU:HG2	3:L:254:ALA:CB	2.48	0.44
1:J:364:GLY:O	2:K:361:ASN:HB3	2.17	0.44
3:L:139:GLU:OE1	3:L:139:GLU:N	2.51	0.44
3:L:152:VAL:HG13	3:L:236:MET:HE2	1.98	0.44
1:A:355:LEU:HD13	1:A:359:VAL:HG23	1.99	0.44
1:A:488:CYS:SG	1:A:504:ILE:HD11	2.58	0.44
3:F:138:LYS:HE2	3:F:140:LEU:HD11	2.00	0.44
1:G:687:MET:HE3	2:H:6:TYR:CE2	2.53	0.44
3:L:453:ILE:HG12	3:L:463:LEU:HD22	1.98	0.44
1:A:76:GLN:NE2	1:A:90:PHE:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:TYR:CD2	2:B:431:GLU:HB2	2.53	0.44
3:C:575:LEU:HD13	3:C:582:ILE:HG13	1.96	0.44
1:D:469:LYS:CD	1:D:475:LEU:HD13	2.41	0.44
3:F:477:MET:CE	1:G:126:SER:HB2	2.47	0.44
1:G:203:PHE:CB	1:G:208:GLN:NE2	2.76	0.44
1:G:352:GLU:HG3	2:H:370:ILE:CD1	2.47	0.44
1:G:355:LEU:HD13	1:G:359:VAL:HG23	1.99	0.44
2:H:746:ALA:HB2	3:I:12:LYS:HA	2.00	0.44
1:J:407:ALA:HB1	1:J:412:GLU:HB3	1.99	0.44
1:A:321:LYS:HB3	3:F:544:PHE:CZ	2.53	0.43
3:C:152:VAL:HG13	3:C:236:MET:HE2	1.99	0.43
1:G:49:CYS:HB2	1:G:61:PHE:HB2	2.00	0.43
1:G:488:CYS:SG	1:G:504:ILE:HD11	2.57	0.43
3:I:393:LEU:HD21	3:I:467:ARG:CZ	2.48	0.43
1:J:209:MET:HE1	2:K:321:LEU:HG	2.00	0.43
1:J:434:GLU:HA	1:J:437:LYS:HG2	2.00	0.43
1:J:488:CYS:SG	1:J:504:ILE:HD11	2.58	0.43
2:K:361:ASN:C	2:K:363:ARG:H	2.26	0.43
1:D:69:ARG:HD3	1:D:91:LEU:HD13	1.99	0.43
1:G:223:LEU:HD22	2:H:432:LEU:HD23	2.00	0.43
2:H:467:PHE:O	2:H:470:VAL:HG12	2.18	0.43
1:A:286:LEU:CD1	1:A:482:ASP:OD2	2.60	0.43
1:A:405:PRO:HB3	2:B:598:LEU:HG	1.99	0.43
1:A:434:GLU:HA	1:A:437:LYS:HG2	2.01	0.43
1:D:51:GLU:OE1	1:D:51:GLU:N	2.51	0.43
2:E:427:TYR:CD2	2:E:431:GLU:HB2	2.53	0.43
3:L:236:MET:O	3:L:237:GLU:C	2.62	0.43
3:L:393:LEU:HD21	3:L:467:ARG:CZ	2.48	0.43
1:A:51:GLU:N	1:A:51:GLU:OE1	2.51	0.43
3:C:393:LEU:HD22	3:C:396:ILE:HD11	1.99	0.43
1:D:52:TYR:CD1	1:D:146:MET:CE	3.01	0.43
1:D:64:ILE:HG22	1:D:72:ALA:HB1	2.00	0.43
1:G:207:GLU:HA	1:G:207:GLU:OE1	2.18	0.43
1:A:49:CYS:HB2	1:A:61:PHE:HB2	2.00	0.43
2:B:361:ASN:C	2:B:363:ARG:H	2.26	0.43
3:C:322:LEU:HD21	3:C:531:ALA:HB1	2.01	0.43
2:H:68:PHE:CD1	2:H:68:PHE:O	2.71	0.43
2:H:361:ASN:C	2:H:363:ARG:H	2.26	0.43
2:H:664:THR:HG23	3:I:42:ARG:HD3	2.00	0.43
2:K:265:CYS:HB3	2:K:274:PRO:HG3	2.01	0.43
2:B:131:THR:HG21	2:B:251:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:172:TRP:CD1	3:F:186:ILE:HD11	2.54	0.43
1:G:303:LYS:CE	3:L:123:LYS:HD3	2.49	0.43
3:I:552:PRO:CD	3:I:557:LEU:CD1	2.96	0.43
1:J:51:GLU:N	1:J:51:GLU:OE1	2.51	0.43
1:A:140:LYS:HE2	1:A:145:PRO:HD2	2.00	0.43
1:A:577:THR:HG21	2:B:20:THR:HG21	2.00	0.43
2:E:68:PHE:CD1	2:E:68:PHE:O	2.72	0.43
2:E:131:THR:HG21	2:E:251:ARG:HD2	2.00	0.43
2:E:705:ILE:H	3:F:744:GLN:HB2	1.84	0.43
3:F:357:TYR:O	3:F:423:PHE:HB3	2.19	0.43
3:F:393:LEU:HD21	3:F:467:ARG:CZ	2.48	0.43
3:F:477:MET:CE	1:G:126:SER:OG	2.65	0.43
2:H:265:CYS:HB3	2:H:274:PRO:HG3	2.01	0.43
2:H:705:ILE:O	3:I:744:GLN:HB2	2.18	0.43
1:J:49:CYS:HB2	1:J:61:PHE:HB2	2.00	0.43
1:J:265:MET:HG2	1:J:434:GLU:HG2	2.00	0.43
1:A:399:VAL:HB	1:A:427:GLN:HE22	1.84	0.43
2:B:182:LYS:HE2	1:G:205:THR:HG1	1.81	0.43
1:D:399:VAL:HB	1:D:427:GLN:HE22	1.84	0.43
2:H:746:ALA:CB	3:I:12:LYS:HA	2.49	0.43
3:L:138:LYS:CB	3:L:250:GLU:HB2	2.42	0.43
2:B:79:VAL:HB	2:B:480:LEU:HD11	2.01	0.43
2:B:467:PHE:O	2:B:470:VAL:HG12	2.18	0.43
3:C:444:PRO:O	3:C:448:VAL:HG23	2.19	0.43
2:E:577:ILE:HA	2:E:580:PHE:HB3	2.01	0.43
1:G:402:ALA:O	2:H:550:ARG:HD3	2.19	0.43
1:J:399:VAL:HB	1:J:427:GLN:HE22	1.84	0.43
1:A:265:MET:HG2	1:A:434:GLU:HG2	2.01	0.43
1:D:90:PHE:CE1	1:D:122:LYS:C	2.97	0.43
3:F:139:GLU:N	3:F:139:GLU:OE1	2.51	0.43
1:G:51:GLU:N	1:G:51:GLU:OE1	2.52	0.43
1:G:67:ARG:CZ	3:I:770:ILE:HG22	2.48	0.43
1:G:410:GLU:HG2	3:I:137:TRP:HB3	1.99	0.43
2:H:536:ILE:CG1	3:I:240:HIS:HB3	2.49	0.43
3:I:172:TRP:CD1	3:I:186:ILE:HD11	2.54	0.43
3:I:322:LEU:HD21	3:I:531:ALA:HB1	2.01	0.43
1:D:20:ILE:HD13	1:D:42:PHE:CE2	2.54	0.42
1:G:261:HIS:CD2	1:G:265:MET:HE3	2.53	0.42
2:H:289:THR:HG21	3:I:499:GLN:NE2	2.34	0.42
2:K:427:TYR:CD2	2:K:431:GLU:HB2	2.54	0.42
1:D:49:CYS:HB2	1:D:61:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:PHE:CD1	2:E:23:PRO:HB3	2.54	0.42
3:F:138:LYS:HD3	3:F:250:GLU:CG	2.48	0.42
3:F:444:PRO:O	3:F:448:VAL:HG23	2.18	0.42
1:G:226:LYS:HD2	2:H:466:ARG:NE	2.34	0.42
1:G:399:VAL:HB	1:G:427:GLN:HE22	1.84	0.42
2:H:632:PHE:CE1	3:I:102:ILE:HG23	2.53	0.42
2:H:686:GLN:CD	3:I:39:THR:HG23	2.43	0.42
1:J:407:ALA:HA	1:J:412:GLU:CG	2.49	0.42
1:J:410:GLU:CG	3:L:137:TRP:HB3	2.49	0.42
3:L:426:ALA:N	3:L:427:PRO:HD3	2.35	0.42
1:D:5:PHE:HB3	1:D:35:ILE:HD11	2.01	0.42
3:F:322:LEU:HD21	3:F:531:ALA:HB1	2.01	0.42
1:G:410:GLU:CD	1:G:411:LEU:H	2.26	0.42
2:H:577:ILE:HA	2:H:580:PHE:HB3	2.01	0.42
3:I:426:ALA:N	3:I:427:PRO:HD3	2.34	0.42
3:I:575:LEU:HD11	3:I:582:ILE:CD1	2.36	0.42
3:L:444:PRO:O	3:L:448:VAL:HG23	2.19	0.42
3:C:236:MET:O	3:C:237:GLU:C	2.63	0.42
1:D:17:ALA:HA	1:D:42:PHE:CE2	2.55	0.42
1:D:52:TYR:OH	1:D:146:MET:HB2	2.19	0.42
1:D:174:PHE:HB2	1:D:179:GLU:HB2	2.00	0.42
1:D:265:MET:HG2	1:D:434:GLU:HG2	2.01	0.42
1:D:454:GLY:H	1:D:492:LYS:HD2	1.85	0.42
3:F:426:ALA:N	3:F:427:PRO:HD3	2.34	0.42
3:F:474:PRO:CB	1:G:126:SER:O	2.67	0.42
3:F:551:HIS:O	3:F:551:HIS:ND1	2.53	0.42
1:J:558:LYS:HE3	3:L:49:LEU:HD11	2.01	0.42
1:D:233:ASN:HA	2:E:78:LEU:HG	2.01	0.42
1:D:419:ASN:CG	2:E:550:ARG:HH22	2.27	0.42
2:H:686:GLN:OE1	3:I:39:THR:CB	2.65	0.42
1:J:426:LEU:HD21	1:J:621:LEU:HD22	2.01	0.42
2:B:265:CYS:HB3	2:B:274:PRO:HG3	2.02	0.42
3:F:473:ASN:HB3	3:F:474:PRO:HD2	2.01	0.42
1:G:25:VAL:HG21	1:G:35:ILE:HG22	2.02	0.42
1:G:265:MET:HG2	1:G:434:GLU:HG2	2.02	0.42
2:K:487:LEU:HD23	2:K:489:GLU:N	2.33	0.42
1:D:20:ILE:HD13	1:D:42:PHE:CZ	2.55	0.42
1:D:102:PHE:HB3	1:D:127:CYS:SG	2.59	0.42
1:D:418:LEU:HB3	2:E:543:SER:OG	2.19	0.42
2:H:79:VAL:HB	2:H:480:LEU:HD11	2.02	0.42
1:J:140:LYS:HE2	1:J:145:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:282:ALA:HB3	3:L:149:ARG:HD3	2.01	0.42
3:L:139:GLU:C	3:L:140:LEU:HG	2.44	0.42
3:L:581:ASP:C	3:L:583:PRO:HD2	2.45	0.42
1:A:25:VAL:HG21	1:A:35:ILE:HG22	2.02	0.42
1:A:87:PRO:O	1:A:89:PRO:N	2.53	0.42
1:A:408:ASP:OD2	3:C:132:ARG:NH2	2.53	0.42
2:B:179:LYS:HB3	1:G:203:PHE:HZ	1.84	0.42
1:D:469:LYS:HB2	1:D:475:LEU:CD1	2.48	0.42
1:G:222:GLU:O	1:G:226:LYS:HB2	2.20	0.42
3:L:172:TRP:CD1	3:L:186:ILE:HD11	2.55	0.42
1:A:632:CYS:HA	2:B:26:GLY:CA	2.50	0.42
2:E:704:PRO:HA	3:F:744:GLN:HG3	2.01	0.42
3:I:549:PHE:CZ	3:I:569:GLU:OE1	2.73	0.42
3:I:551:HIS:O	3:I:551:HIS:ND1	2.53	0.42
1:J:25:VAL:HG21	1:J:35:ILE:HG22	2.02	0.42
2:K:68:PHE:CD1	2:K:68:PHE:O	2.72	0.42
1:A:67:ARG:HD3	1:A:71:THR:HG21	2.02	0.42
3:F:581:ASP:C	3:F:583:PRO:HD2	2.45	0.42
3:F:600:VAL:HG13	3:F:642:PRO:HA	2.02	0.42
3:F:626:GLN:O	3:F:632:TYR:HB3	2.20	0.42
2:H:18:ILE:HD13	2:H:497:PHE:CD2	2.55	0.42
2:H:363:ARG:HD3	3:L:139:GLU:CD	2.44	0.42
2:H:660:HIS:CE1	3:I:106:ASN:HD21	2.38	0.42
2:H:704:PRO:O	3:I:30:SER:HA	2.20	0.42
3:I:236:MET:O	3:I:237:GLU:C	2.63	0.42
3:I:444:PRO:O	3:I:448:VAL:HG23	2.19	0.42
1:J:408:ASP:N	1:J:412:GLU:CB	2.82	0.42
2:K:491:PHE:CD1	2:K:491:PHE:C	2.98	0.42
2:K:746:ALA:HB1	3:L:15:CYS:SG	2.60	0.42
1:A:410:GLU:CD	1:A:411:LEU:N	2.77	0.41
1:A:412:GLU:CG	2:B:601:ASN:ND2	2.82	0.41
3:F:475:GLY:HA2	1:G:86:GLU:HG2	2.01	0.41
1:G:59:ASP:OD2	3:I:769:LYS:NZ	2.52	0.41
1:G:140:LYS:HE2	1:G:145:PRO:HD2	2.01	0.41
1:A:88:LEU:CD2	1:A:102:PHE:CZ	3.01	0.41
1:A:345:ARG:NH1	3:F:136:MET:HB3	2.35	0.41
1:A:419:ASN:ND2	2:B:543:SER:OG	2.51	0.41
3:C:172:TRP:CD1	3:C:186:ILE:HD11	2.54	0.41
1:D:13:LEU:HD12	1:D:156:PHE:HZ	1.85	0.41
3:F:445:TYR:O	3:F:448:VAL:HB	2.20	0.41
2:H:491:PHE:CD1	2:H:491:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:245:LYS:HA	1:J:706:PHE:CB	2.51	0.41
3:L:551:HIS:O	3:L:551:HIS:ND1	2.53	0.41
1:D:25:VAL:HG21	1:D:35:ILE:HG22	2.03	0.41
1:D:245:LYS:HA	1:D:706:PHE:CB	2.50	0.41
1:D:426:LEU:HD21	1:D:621:LEU:HD22	2.02	0.41
3:F:236:MET:O	3:F:237:GLU:C	2.62	0.41
1:G:201:LEU:HD13	1:G:203:PHE:CD2	2.55	0.41
1:G:518:LYS:HG3	1:G:519:HIS:CD2	2.55	0.41
3:I:626:GLN:O	3:I:632:TYR:HB3	2.20	0.41
2:K:487:LEU:CD2	2:K:489:GLU:HG3	2.50	0.41
1:A:245:LYS:HA	1:A:706:PHE:CB	2.50	0.41
2:B:51:ARG:HH12	2:B:78:LEU:HA	1.86	0.41
2:B:577:ILE:HA	2:B:580:PHE:HB3	2.02	0.41
3:C:445:TYR:O	3:C:448:VAL:HB	2.21	0.41
1:D:398:TRP:CE3	1:D:465:SER:HB2	2.55	0.41
1:D:518:LYS:HG3	1:D:519:HIS:CD2	2.56	0.41
2:B:686:GLN:NE2	3:C:39:THR:OG1	2.49	0.41
3:F:397:THR:HA	3:F:497:THR:O	2.20	0.41
1:G:88:LEU:HD12	1:G:123:LEU:HD22	2.02	0.41
1:J:222:GLU:O	1:J:226:LYS:HB2	2.21	0.41
3:L:322:LEU:HD21	3:L:531:ALA:HB1	2.01	0.41
2:B:182:LYS:NZ	1:G:205:THR:CG2	2.71	0.41
2:B:346:PHE:HA	2:B:349:LYS:HB3	2.03	0.41
2:B:491:PHE:CD1	2:B:491:PHE:C	2.98	0.41
3:C:426:ALA:N	3:C:427:PRO:HD3	2.35	0.41
3:F:474:PRO:CG	1:G:126:SER:O	2.69	0.41
1:J:469:LYS:CD	1:J:475:LEU:HD13	2.41	0.41
1:J:650:LEU:HB3	2:K:14:VAL:HG11	2.02	0.41
2:K:577:ILE:HA	2:K:580:PHE:HB3	2.01	0.41
2:E:265:CYS:HB3	2:E:274:PRO:HG3	2.01	0.41
3:F:422:TYR:CZ	3:F:449:MET:HG3	2.56	0.41
2:H:346:PHE:HA	2:H:349:LYS:HB3	2.03	0.41
3:I:600:VAL:HG13	3:I:642:PRO:HA	2.03	0.41
1:J:316:LEU:HD21	1:J:489:VAL:HG21	2.02	0.41
3:L:626:GLN:O	3:L:632:TYR:HB3	2.20	0.41
1:A:303:LYS:NZ	3:F:120:GLU:HB3	2.36	0.41
1:A:402:ALA:N	2:B:554:GLN:OE1	2.53	0.41
3:C:551:HIS:O	3:C:551:HIS:ND1	2.53	0.41
3:C:626:GLN:O	3:C:632:TYR:HB3	2.20	0.41
1:D:69:ARG:CZ	1:D:91:LEU:CG	2.91	0.41
2:E:346:PHE:HA	2:E:349:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:ILE:CD1	2:H:334:LEU:HD22	2.50	0.41
1:G:316:LEU:HD21	1:G:489:VAL:HG21	2.02	0.41
2:H:686:GLN:CD	3:I:39:THR:CG2	2.89	0.41
1:J:378:PHE:HA	1:J:379:PRO:HD3	1.97	0.41
2:K:51:ARG:HH12	2:K:78:LEU:HA	1.86	0.41
2:K:542:PRO:HD3	3:L:247:TRP:CE2	2.56	0.41
2:B:18:ILE:HD13	2:B:497:PHE:CD2	2.55	0.41
2:B:294:ARG:HG3	3:C:395:TRP:CH2	2.55	0.41
3:C:397:THR:HA	3:C:497:THR:O	2.21	0.41
3:C:600:VAL:HG13	3:C:642:PRO:HA	2.02	0.41
1:D:136:GLY:C	3:F:717:ASN:ND2	2.79	0.41
1:D:197:GLU:O	2:E:65:ARG:CZ	2.69	0.41
1:D:410:GLU:CD	1:D:411:LEU:H	2.26	0.41
1:D:410:GLU:HB2	3:F:249:GLN:OE1	2.21	0.41
1:D:565:SER:CB	3:F:52:ARG:HH22	2.34	0.41
1:D:643:CYS:HA	1:D:646:GLN:HB3	2.03	0.41
2:E:279:GLU:HB2	3:F:224:PHE:CE2	2.56	0.41
3:F:358:ILE:N	3:F:423:PHE:HB3	2.34	0.41
1:G:426:LEU:HD21	1:G:621:LEU:HD22	2.02	0.41
2:H:662:PHE:HB3	3:I:61:ILE:CG2	2.51	0.41
3:I:681:SER:HB3	3:I:691:ILE:HD11	2.01	0.41
1:J:410:GLU:O	3:L:139:GLU:CB	2.68	0.41
3:L:269:VAL:HG21	3:L:297:MET:HE1	2.03	0.41
1:A:518:LYS:HG3	1:A:519:HIS:CD2	2.55	0.41
2:E:79:VAL:HB	2:E:480:LEU:HD11	2.02	0.41
2:E:491:PHE:CD1	2:E:491:PHE:C	2.99	0.41
1:G:245:LYS:HA	1:G:706:PHE:CB	2.51	0.41
1:J:450:ARG:NE	3:L:57:SER:OG	2.54	0.41
1:A:222:GLU:O	1:A:226:LYS:HB2	2.21	0.40
1:D:60:ARG:HG3	1:D:98:GLU:HB2	2.03	0.40
1:G:444:ALA:O	1:G:448:GLU:HG2	2.22	0.40
2:H:627:ASN:CG	3:I:111:CYS:SG	3.04	0.40
2:H:692:PHE:CD2	3:I:32:TYR:CD1	3.09	0.40
1:J:379:PRO:HB3	1:J:381:TRP:NE1	2.36	0.40
2:K:346:PHE:HA	2:K:349:LYS:HB3	2.03	0.40
1:A:67:ARG:NE	1:A:75:LEU:HD22	2.36	0.40
1:D:41:HIS:HE1	1:D:65:GLU:HG2	1.86	0.40
1:D:583:LEU:CD1	3:F:247:TRP:CZ2	3.04	0.40
1:J:398:TRP:CE3	1:J:465:SER:HB2	2.56	0.40
2:K:79:VAL:HB	2:K:480:LEU:HD11	2.02	0.40
1:A:155:SER:HB3	3:C:713:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HD22	1:A:339:PHE:CE2	2.57	0.40
1:D:316:LEU:HD21	1:D:489:VAL:HG21	2.03	0.40
2:E:51:ARG:HH12	2:E:78:LEU:HA	1.85	0.40
3:F:692:ARG:HG3	3:F:694:PRO:HD2	2.02	0.40
1:G:398:TRP:CE3	1:G:465:SER:HB2	2.56	0.40
3:I:397:THR:HA	3:I:497:THR:O	2.21	0.40
2:K:491:PHE:HE1	2:K:493:PHE:HB2	1.87	0.40
1:A:338:GLU:HG2	3:F:254:ALA:CB	2.42	0.40
2:B:370:ILE:HD11	2:B:374:LYS:HB2	2.03	0.40
3:C:591:TYR:CD2	3:C:627:VAL:HG21	2.56	0.40
1:D:158:ALA:HB1	3:F:748:ARG:NE	2.37	0.40
1:J:407:ALA:HA	1:J:412:GLU:HB3	2.02	0.40
3:L:422:TYR:CZ	3:L:449:MET:HG3	2.56	0.40
1:A:444:ALA:O	1:A:448:GLU:HG2	2.22	0.40
3:C:755:SER:O	3:C:756:GLN:C	2.64	0.40
1:D:222:GLU:O	1:D:226:LYS:HB2	2.20	0.40
1:D:444:ALA:O	1:D:448:GLU:HG2	2.22	0.40
2:E:370:ILE:HD11	2:E:374:LYS:HB2	2.03	0.40
2:E:404:LEU:HA	2:E:405:PRO:HD3	1.95	0.40
2:H:370:ILE:HD12	2:H:370:ILE:HA	1.98	0.40
2:H:370:ILE:HD11	2:H:374:LYS:HB2	2.02	0.40
1:J:677:CYS:SG	1:J:678:LEU:CD1	3.09	0.40
3:L:445:TYR:O	3:L:448:VAL:HB	2.21	0.40

All (18) 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:E:215:LYS:CE	3:I:628:THR:OG1[3_554]	0.85	1.35
2:E:215:LYS:NZ	3:I:628:THR:OG1[3_554]	0.92	1.28
2:E:215:LYS:CE	3:I:628:THR:CB[3_554]	1.49	0.71
2:B:457:TRP:N	1:J:84:ASP:OD2[1_565]	1.72	0.48
2:B:54:VAL:CG2	3:F:282:MET:CG[1_655]	1.75	0.45
2:B:54:VAL:CG2	3:F:282:MET:CB[1_655]	1.75	0.45
2:B:362:LYS:CE	1:D:81:LYS:NZ[1_655]	1.75	0.45
3:F:650:GLN:CG	1:J:143:GLU:CB[1_465]	1.79	0.41
2:B:362:LYS:NZ	1:D:81:LYS:NZ[1_655]	1.92	0.28
3:F:648:PRO:O	1:J:99:GLU:OE2[1_465]	1.92	0.28
2:B:384:GLU:OE1	1:D:75:LEU:CG[1_655]	1.96	0.24
1:A:223:LEU:C	3:F:559:ASP:OD2[1_655]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:215:LYS:CD	3:I:628:THR:OG1[3_554]	2.05	0.15
3:F:647:ALA:CB	1:J:99:GLU:O[1_465]	2.11	0.09
1:D:363:GLU:CD	1:G:592:ASN:O[3_654]	2.12	0.08
1:D:363:GLU:OE1	1:G:592:ASN:N[3_654]	2.16	0.04
3:F:645:TYR:O	1:J:100:LYS:NZ[1_465]	2.17	0.03
3:F:650:GLN:CG	1:J:143:GLU:CG[1_465]	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	685/709 (97%)	631 (92%)	51 (7%)	3 (0%)	30	66
1	D	685/709 (97%)	634 (93%)	49 (7%)	2 (0%)	36	71
1	G	685/709 (97%)	635 (93%)	48 (7%)	2 (0%)	36	71
1	J	685/709 (97%)	633 (92%)	50 (7%)	2 (0%)	36	71
2	B	703/754 (93%)	670 (95%)	30 (4%)	3 (0%)	30	66
2	E	703/754 (93%)	669 (95%)	31 (4%)	3 (0%)	30	66
2	H	703/754 (93%)	670 (95%)	30 (4%)	3 (0%)	30	66
2	K	703/754 (93%)	669 (95%)	31 (4%)	3 (0%)	30	66
3	C	746/782 (95%)	679 (91%)	64 (9%)	3 (0%)	30	66
3	F	756/782 (97%)	683 (90%)	69 (9%)	4 (0%)	24	62
3	I	756/782 (97%)	685 (91%)	68 (9%)	3 (0%)	30	66
3	L	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	30	66
All	All	8566/8980 (95%)	7944 (93%)	588 (7%)	34 (0%)	30	66

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	503	VAL

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Mol	Chain	Res	Type
2	E	503	VAL
3	F	758	ALA
2	H	503	VAL
2	K	503	VAL
3	C	533	ILE
1	D	141	ASN
3	F	533	ILE
3	I	533	ILE
3	L	533	ILE
1	A	141	ASN
1	G	141	ASN
1	J	141	ASN
1	A	87	PRO
2	B	405	PRO
2	E	405	PRO
2	H	405	PRO
2	K	405	PRO
3	C	550	GLN
2	E	23	PRO
3	F	550	GLN
3	I	550	GLN
3	L	550	GLN
2	B	23	PRO
2	H	23	PRO
2	K	23	PRO
3	C	745	GLY
3	F	745	GLY
3	I	745	GLY
3	L	745	GLY
1	J	679	ILE
1	A	679	ILE
1	D	679	ILE
1	G	679	ILE

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	618/631 (98%)	604 (98%)	14 (2%)	44	64
1	D	618/631 (98%)	603 (98%)	15 (2%)	43	63
1	G	618/631 (98%)	604 (98%)	14 (2%)	44	64
1	J	618/631 (98%)	602 (97%)	16 (3%)	40	60
2	B	629/669 (94%)	612 (97%)	17 (3%)	39	60
2	E	629/669 (94%)	612 (97%)	17 (3%)	39	60
2	H	629/669 (94%)	611 (97%)	18 (3%)	37	58
2	K	629/669 (94%)	611 (97%)	18 (3%)	37	58
3	C	663/686 (97%)	648 (98%)	15 (2%)	44	64
3	F	669/686 (98%)	655 (98%)	14 (2%)	47	65
3	I	669/686 (98%)	655 (98%)	14 (2%)	47	65
3	L	669/686 (98%)	655 (98%)	14 (2%)	47	65
All	All	7658/7944 (96%)	7472 (98%)	186 (2%)	43	63

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	170	PHE
1	A	192	LEU
1	A	205	THR
1	A	305	LEU
1	A	355	LEU
1	A	390	ILE
1	A	412	GLU
1	A	490	LYS
1	A	506	THR
1	A	554	THR
1	A	621	LEU
1	A	625	LEU
1	A	673	LYS
2	B	147	GLN
2	B	166	LEU
2	B	263	LYS
2	B	273	LEU
2	B	279	GLU
2	B	302	VAL
2	B	341	VAL
2	B	412	MET

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Mol	Chain	Res	Type
2	B	478	MET
2	B	491	PHE
2	B	492	GLU
2	B	502	PHE
2	B	540	LEU
2	B	657	VAL
2	B	665	ARG
2	B	705	ILE
2	B	717	LYS
3	C	4	LEU
3	C	39	THR
3	C	129	LEU
3	C	135	ILE
3	C	139	GLU
3	C	152	VAL
3	C	160	ARG
3	C	227	VAL
3	C	393	LEU
3	C	450	MET
3	C	582	ILE
3	C	594	LEU
3	C	695	LEU
3	C	720	ARG
3	C	738	VAL
1	D	38	ILE
1	D	170	PHE
1	D	192	LEU
1	D	205	THR
1	D	305	LEU
1	D	355	LEU
1	D	390	ILE
1	D	419	ASN
1	D	482	ASP
1	D	490	LYS
1	D	506	THR
1	D	554	THR
1	D	621	LEU
1	D	625	LEU
1	D	673	LYS
2	E	147	GLN
2	E	166	LEU
2	E	263	LYS

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Mol	Chain	Res	Type
2	E	273	LEU
2	E	279	GLU
2	E	302	VAL
2	E	341	VAL
2	E	412	MET
2	E	478	MET
2	E	491	PHE
2	E	492	GLU
2	E	502	PHE
2	E	540	LEU
2	E	657	VAL
2	E	665	ARG
2	E	705	ILE
2	E	717	LYS
3	F	4	LEU
3	F	39	THR
3	F	129	LEU
3	F	135	ILE
3	F	152	VAL
3	F	160	ARG
3	F	227	VAL
3	F	393	LEU
3	F	450	MET
3	F	582	ILE
3	F	594	LEU
3	F	695	LEU
3	F	720	ARG
3	F	738	VAL
1	G	38	ILE
1	G	170	PHE
1	G	192	LEU
1	G	205	THR
1	G	305	LEU
1	G	355	LEU
1	G	390	ILE
1	G	482	ASP
1	G	490	LYS
1	G	506	THR
1	G	554	THR
1	G	621	LEU
1	G	625	LEU
1	G	673	LYS

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Mol	Chain	Res	Type
2	H	147	GLN
2	H	166	LEU
2	H	214	ILE
2	H	263	LYS
2	H	273	LEU
2	H	279	GLU
2	H	302	VAL
2	H	341	VAL
2	H	412	MET
2	H	478	MET
2	H	491	PHE
2	H	492	GLU
2	H	502	PHE
2	H	540	LEU
2	H	657	VAL
2	H	665	ARG
2	H	705	ILE
2	H	717	LYS
3	I	4	LEU
3	I	129	LEU
3	I	135	ILE
3	I	139	GLU
3	I	152	VAL
3	I	160	ARG
3	I	227	VAL
3	I	393	LEU
3	I	450	MET
3	I	582	ILE
3	I	594	LEU
3	I	695	LEU
3	I	720	ARG
3	I	738	VAL
1	J	38	ILE
1	J	170	PHE
1	J	192	LEU
1	J	205	THR
1	J	305	LEU
1	J	355	LEU
1	J	390	ILE
1	J	482	ASP
1	J	490	LYS
1	J	506	THR

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Mol	Chain	Res	Type
1	J	554	THR
1	J	621	LEU
1	J	625	LEU
1	J	673	LYS
1	J	678	LEU
1	J	680	ASN
2	K	147	GLN
2	K	166	LEU
2	K	214	ILE
2	K	263	LYS
2	K	273	LEU
2	K	279	GLU
2	K	302	VAL
2	K	341	VAL
2	K	412	MET
2	K	478	MET
2	K	491	PHE
2	K	492	GLU
2	K	502	PHE
2	K	540	LEU
2	K	657	VAL
2	K	665	ARG
2	K	705	ILE
2	K	717	LYS
3	L	4	LEU
3	L	39	THR
3	L	129	LEU
3	L	135	ILE
3	L	152	VAL
3	L	160	ARG
3	L	227	VAL
3	L	393	LEU
3	L	450	MET
3	L	582	ILE
3	L	594	LEU
3	L	695	LEU
3	L	720	ARG
3	L	738	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	208	GLN
1	A	248	GLN
1	A	261	HIS
1	A	315	ASN
1	A	334	ASN
1	A	336	HIS
1	A	519	HIS
1	A	615	GLN
1	A	627	GLN
1	A	644	ASN
2	B	121	HIS
2	B	303	ASN
2	B	316	GLN
2	B	477	ASN
2	B	627	ASN
2	B	660	HIS
3	C	155	GLN
3	C	240	HIS
3	C	261	GLN
3	C	550	GLN
3	C	631	HIS
1	D	41	HIS
1	D	204	GLN
1	D	208	GLN
1	D	248	GLN
1	D	261	HIS
1	D	315	ASN
1	D	336	HIS
1	D	519	HIS
1	D	615	GLN
1	D	644	ASN
1	D	646	GLN
2	E	121	HIS
2	E	170	ASN
2	E	216	HIS
2	E	303	ASN
2	E	316	GLN
2	E	477	ASN
2	E	627	ASN
2	E	660	HIS
3	F	148	GLN
3	F	155	GLN

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Mol	Chain	Res	Type
3	F	261	GLN
3	F	451	ASN
3	F	550	GLN
3	F	631	HIS
3	F	727	GLN
3	F	766	ASN
1	G	31	HIS
1	G	208	GLN
1	G	248	GLN
1	G	261	HIS
1	G	312	HIS
1	G	315	ASN
1	G	336	HIS
1	G	519	HIS
1	G	615	GLN
1	G	628	GLN
1	G	644	ASN
2	H	121	HIS
2	H	303	ASN
2	H	316	GLN
2	H	477	ASN
2	H	554	GLN
2	H	627	ASN
2	H	660	HIS
3	I	155	GLN
3	I	261	GLN
3	I	330	GLN
3	I	550	GLN
3	I	631	HIS
3	I	727	GLN
3	I	766	ASN
1	J	31	HIS
1	J	208	GLN
1	J	248	GLN
1	J	261	HIS
1	J	306	GLN
1	J	315	ASN
1	J	336	HIS
1	J	519	HIS
1	J	615	GLN
1	J	638	GLN
1	J	644	ASN

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Mol	Chain	Res	Type
1	J	680	ASN
2	K	303	ASN
2	K	316	GLN
2	K	477	ASN
2	K	554	GLN
2	K	627	ASN
3	L	155	GLN
3	L	451	ASN
3	L	545	GLN
3	L	550	GLN
3	L	631	HIS
3	L	670	ASN
3	L	764	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](#)

There are no ligands in this entry.

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	693/709 (97%)	0.06	8 (1%) 76 61	66, 164, 326, 490	0
1	D	693/709 (97%)	0.12	11 (1%) 70 55	72, 156, 252, 382	0
1	G	693/709 (97%)	0.08	5 (0%) 84 71	90, 180, 290, 407	0
1	J	693/709 (97%)	0.06	4 (0%) 85 73	105, 181, 273, 414	0
2	B	711/754 (94%)	0.06	7 (0%) 79 64	70, 147, 290, 437	0
2	E	711/754 (94%)	0.04	5 (0%) 84 71	71, 143, 270, 490	0
2	H	711/754 (94%)	0.07	9 (1%) 75 59	82, 170, 287, 498	0
2	K	711/754 (94%)	-0.00	3 (0%) 88 77	83, 173, 284, 424	0
3	C	754/782 (96%)	0.19	12 (1%) 70 55	99, 240, 349, 416	0
3	F	762/782 (97%)	0.44	35 (4%) 37 33	87, 174, 295, 481	0
3	I	762/782 (97%)	0.20	11 (1%) 73 58	95, 224, 337, 500	0
3	L	762/782 (97%)	0.16	12 (1%) 70 55	108, 226, 332, 476	0
All	All	8656/8980 (96%)	0.13	122 (1%) 73 58	66, 181, 315, 500	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	695	LEU	7.4
3	I	102	ILE	5.2
3	F	695	LEU	5.1
3	C	286	SER	4.8
3	F	434	ASP	4.8
1	G	355	LEU	4.7
2	H	504	SER	4.5
3	F	564	ILE	4.4
3	F	696	VAL	3.9
3	F	603	MET	3.7
1	J	509	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
3	F	200	PHE	3.7
3	I	682	SER	3.7
3	F	729	LEU	3.6
1	A	202	PRO	3.5
3	L	729	LEU	3.5
3	L	55	MET	3.5
2	E	378	TYR	3.5
2	K	237	LYS	3.4
3	F	604	ALA	3.4
1	A	366	LYS	3.4
3	C	200	PHE	3.4
1	A	132	PHE	3.4
3	F	640	VAL	3.3
1	D	161	ALA	3.1
3	L	345	ILE	3.1
3	F	439	LEU	3.0
3	F	323	CYS	3.0
3	I	640	VAL	3.0
3	F	571	LEU	2.9
2	H	442	LEU	2.9
1	A	358	ASP	2.9
1	J	664	GLY	2.8
3	L	707	ALA	2.8
1	G	76	GLN	2.8
3	F	685	TYR	2.8
2	H	626	PHE	2.7
3	I	26	VAL	2.7
1	D	132	PHE	2.7
2	H	513	PHE	2.7
3	F	429	THR	2.7
3	I	573	LYS	2.7
3	I	311	LEU	2.7
3	F	755	SER	2.7
3	L	586	ILE	2.6
2	K	655	ALA	2.6
3	F	652	MET	2.6
3	C	270	CYS	2.6
2	H	722	ALA	2.6
1	D	664	GLY	2.5
3	F	655	GLY	2.5
2	H	739	ILE	2.5
1	A	327	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	55	MET	2.5
3	I	326	ALA	2.5
2	E	19	SER	2.5
1	J	366	LYS	2.5
3	C	308	GLU	2.5
3	F	7	ILE	2.5
3	F	658	PHE	2.4
3	F	550	GLN	2.4
1	D	130	PHE	2.4
1	A	487	ILE	2.4
3	F	26	VAL	2.4
3	I	279	ALA	2.4
2	B	581	ILE	2.4
1	D	366	LYS	2.3
3	F	274	CYS	2.3
3	F	244	GLY	2.3
3	F	280	SER	2.3
1	D	46	CYS	2.3
3	F	358	ILE	2.3
3	F	149	ARG	2.3
3	L	634	LEU	2.3
3	L	696	VAL	2.3
1	D	698	ALA	2.3
3	F	418	ARG	2.3
3	I	571	LEU	2.3
2	E	166	LEU	2.3
3	F	560	GLU	2.3
2	B	515	THR	2.3
2	B	734	SER	2.3
2	B	242	ALA	2.3
2	B	280	LYS	2.3
2	H	449	VAL	2.3
3	C	149	ARG	2.2
1	G	284	GLU	2.2
1	D	651	MET	2.2
3	L	101	CYS	2.2
3	C	255	GLY	2.2
3	F	563	ALA	2.2
3	C	178	GLU	2.2
1	A	664	GLY	2.2
3	L	638	ILE	2.2
2	E	10	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	637	LEU	2.2
3	C	447	TYR	2.2
2	K	661	SER	2.1
3	I	756	GLN	2.1
1	J	98	GLU	2.1
2	B	490	LEU	2.1
2	B	378	TYR	2.1
2	H	572	GLY	2.1
1	A	355	LEU	2.1
1	D	705	PHE	2.1
1	D	483	CYS	2.1
1	G	169	MET	2.1
3	F	447	TYR	2.1
1	D	355	LEU	2.1
3	C	520	LEU	2.1
3	C	707	ALA	2.1
3	I	103	ASN	2.1
3	L	755	SER	2.1
3	C	697	VAL	2.1
3	F	498	ILE	2.0
1	G	342	GLY	2.0
3	F	303	GLU	2.0
3	L	344	LYS	2.0
3	F	357	TYR	2.0
3	F	163	THR	2.0
2	E	753	SER	2.0
2	H	451	PHE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.