



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 07:58 PM EDT

PDB ID : 5D9A
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.; Vornrhein, C.; Bricogne, G.; Stuart, D.I.; Grimes, J.M.; Fodor, E.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

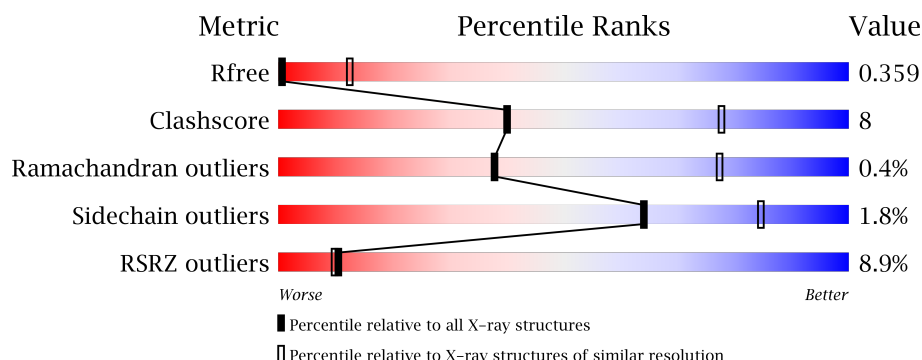
1 Overall quality at a glance

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}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	D	709	
1	G	709	
1	J	709	
2	B	754	

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Mol	Chain	Length	Quality of chain
2	E	754	<div><div></div><div>4%</div><div>81%</div><div>13%</div><div>6%</div></div>
2	H	754	<div><div></div><div>6%</div><div>80%</div><div>14%</div><div>6%</div></div>
2	K	754	<div><div></div><div>8%</div><div>83%</div><div>11%</div><div>6%</div></div>
3	C	782	<div><div></div><div>21%</div><div>86%</div><div>10%</div><div></div></div>
3	F	782	<div><div></div><div>6%</div><div>82%</div><div>15%</div><div></div></div>
3	I	782	<div><div></div><div>12%</div><div>84%</div><div>13%</div><div></div></div>
3	L	782	<div><div></div><div>17%</div><div>87%</div><div>10%</div><div></div></div>

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			

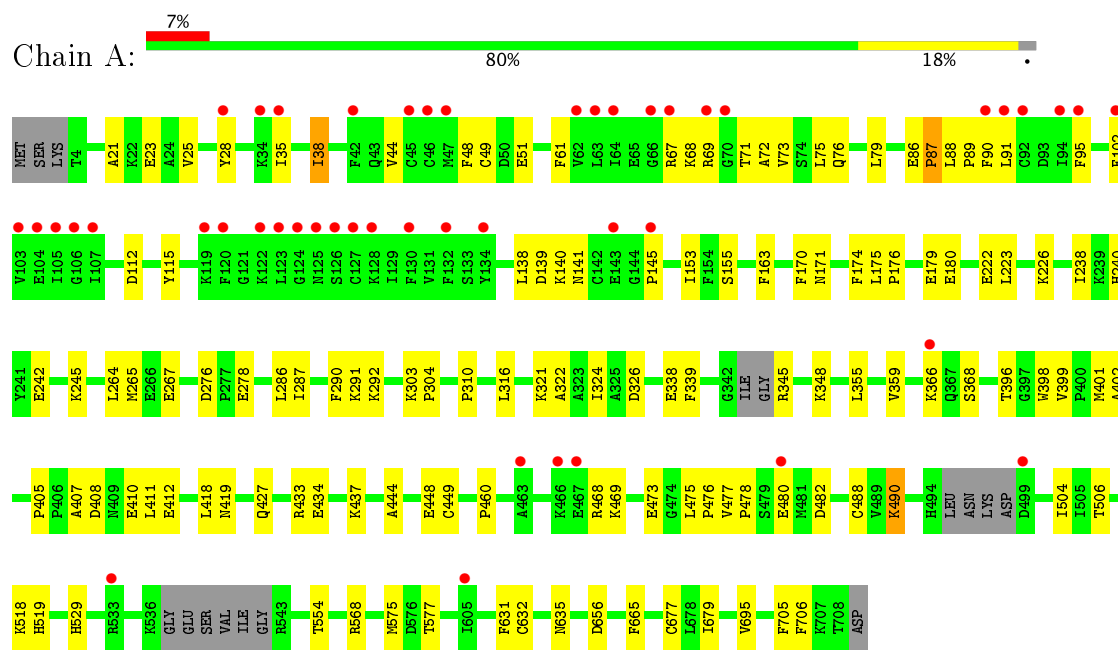
There are 32 discrepancies between the modelled and reference sequences:

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

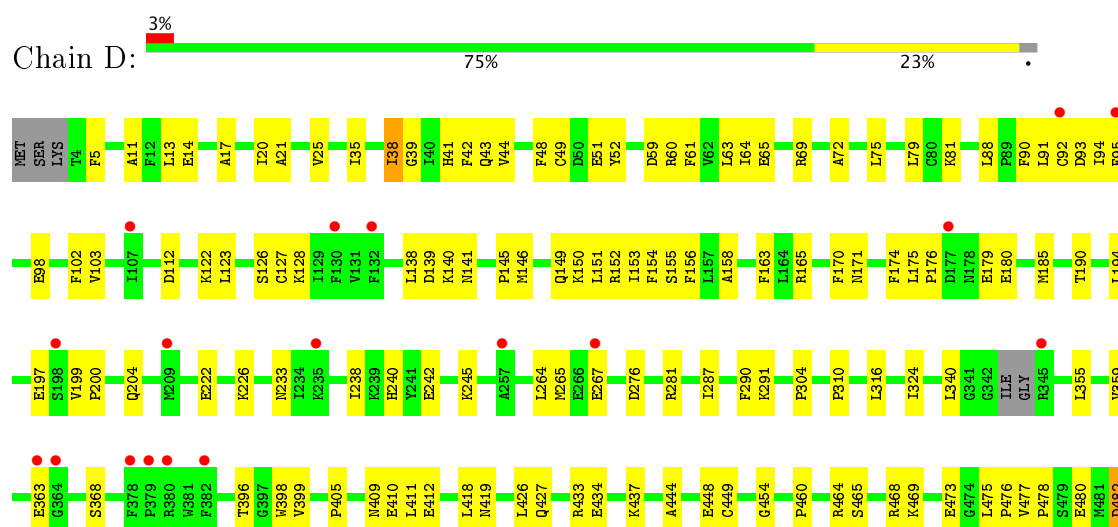
3 Residue-property plots [i](#)

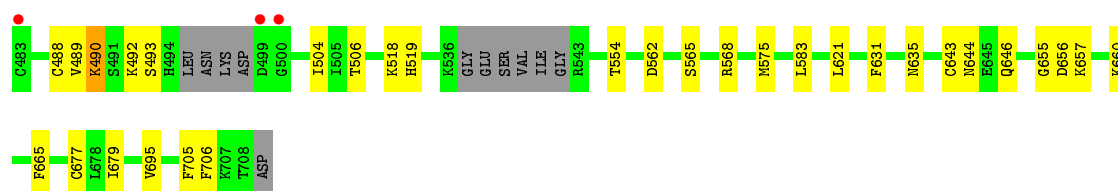
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Polymerase acidic protein

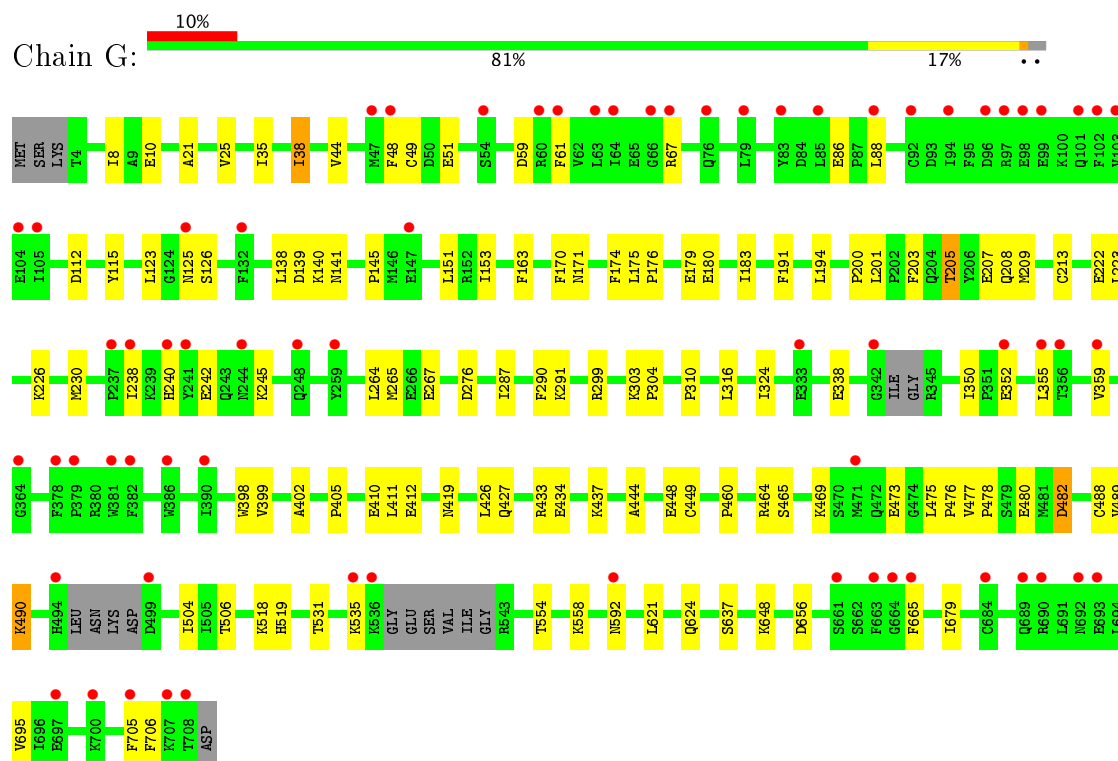


• Molecule 1: Polymerase acidic protein

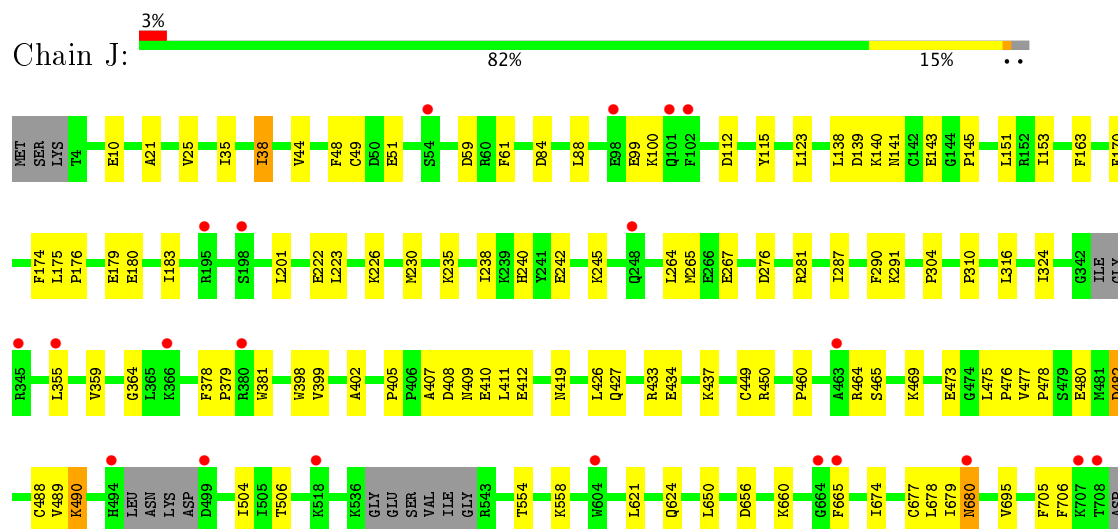




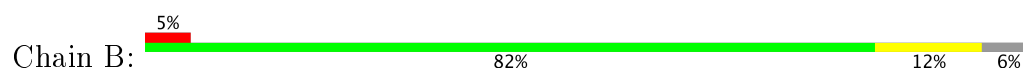
• Molecule 1: Polymerase acidic protein

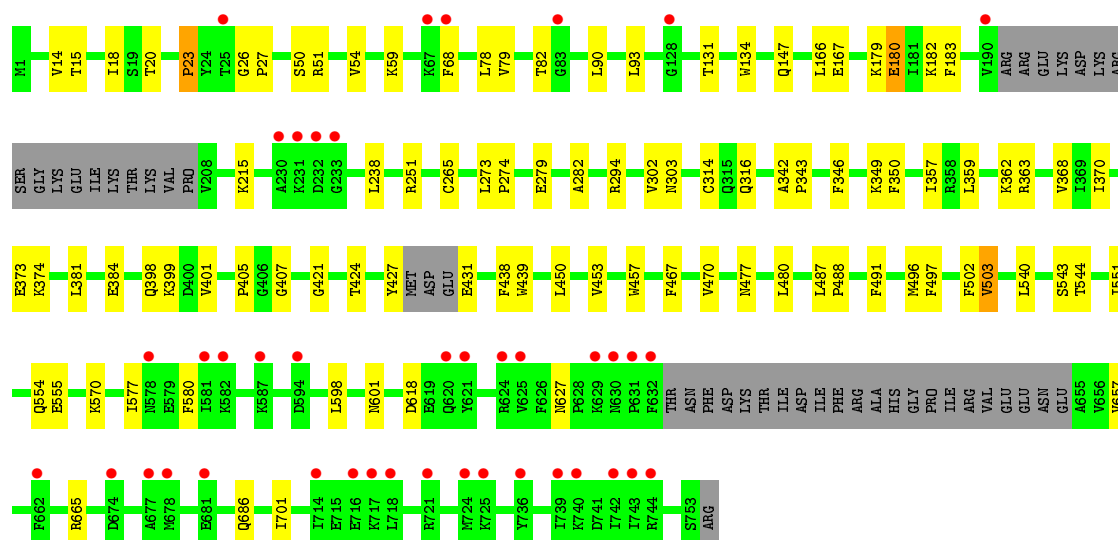


• Molecule 1: Polymerase acidic protein

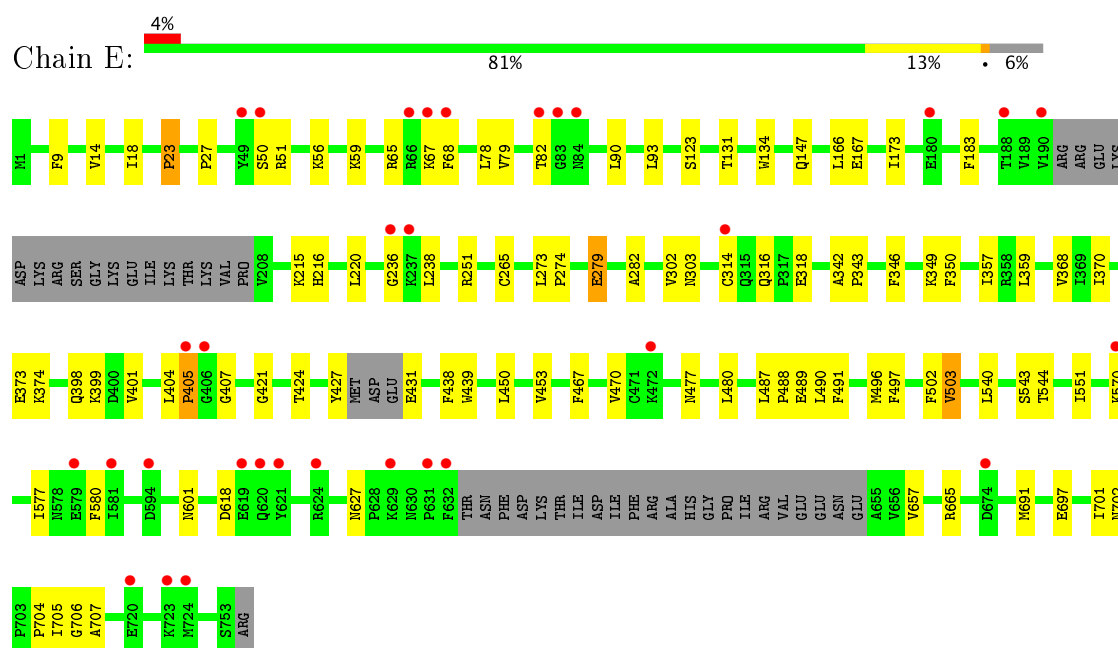


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

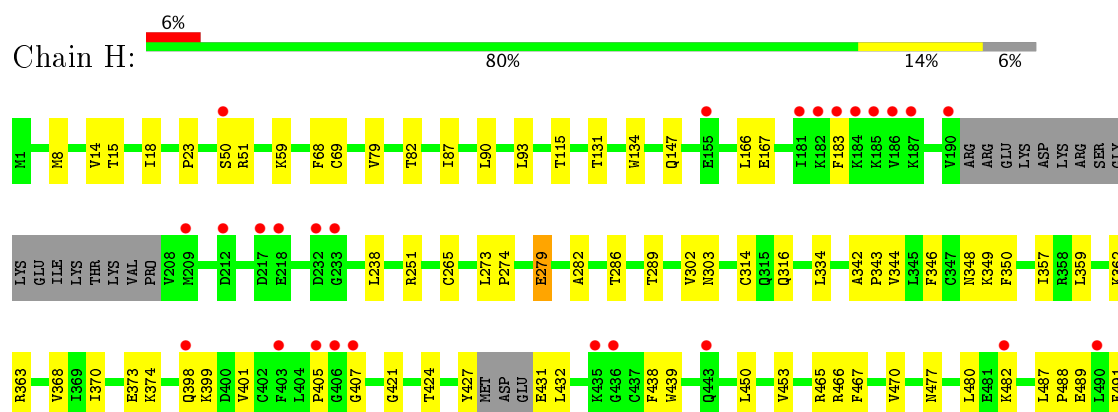


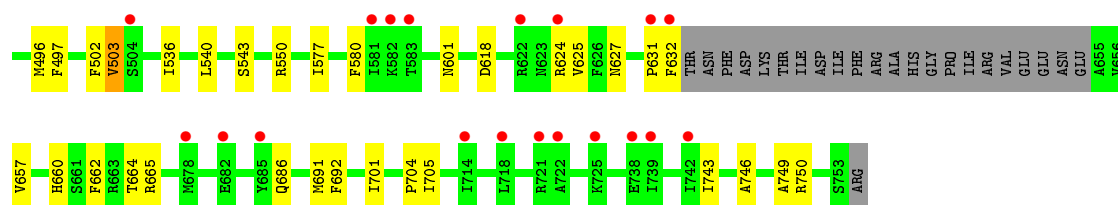


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

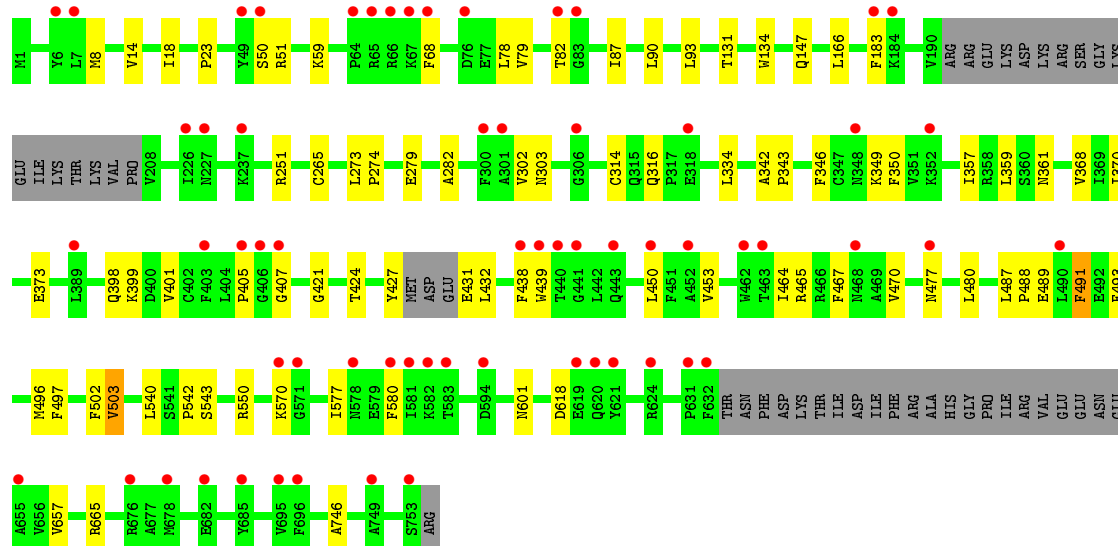
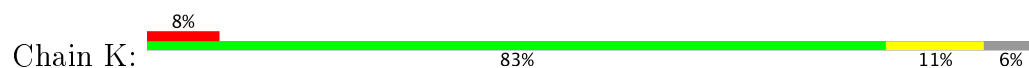


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

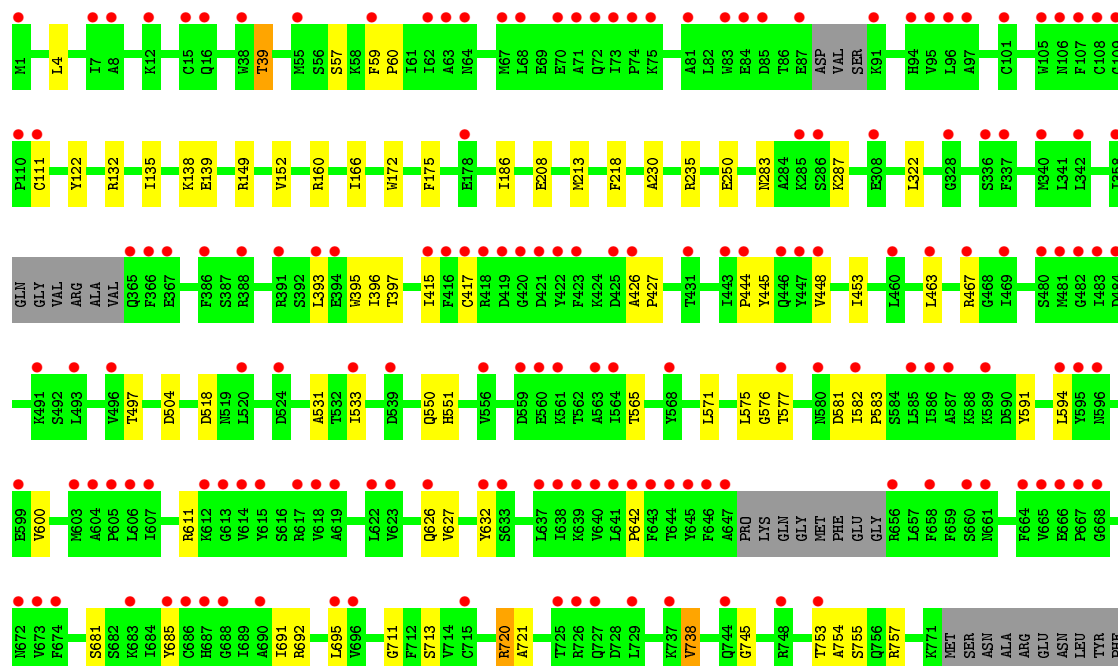
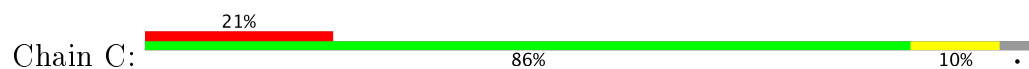




• Molecule 2: RNA-directed RNA polymerase catalytic subunit

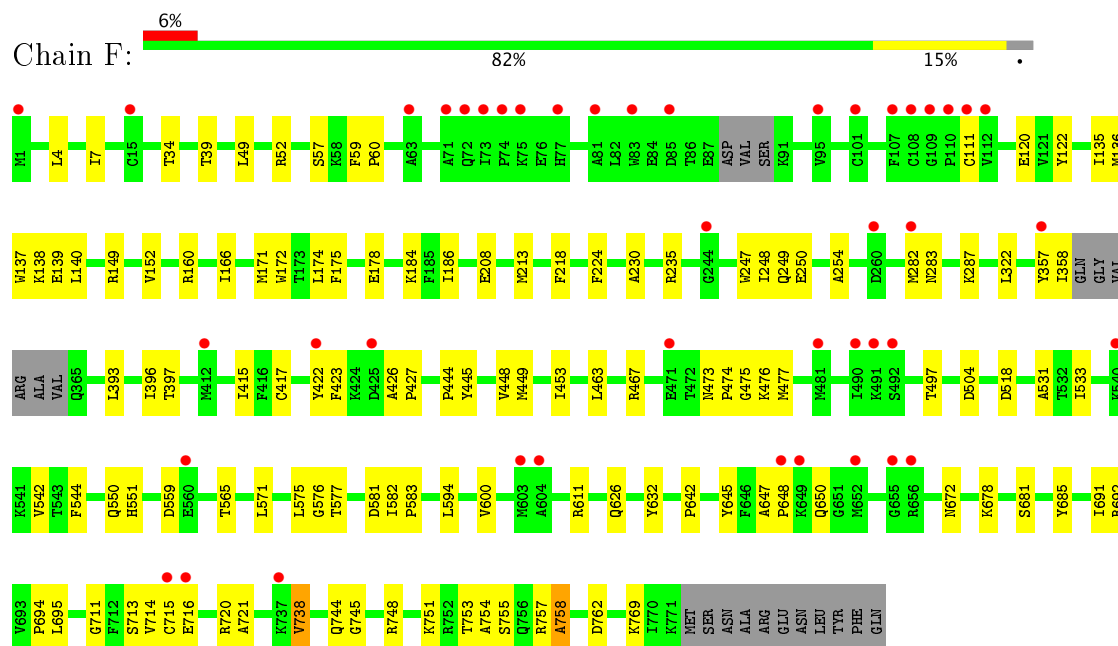


• Molecule 3: Polymerase basic protein 2



GLN

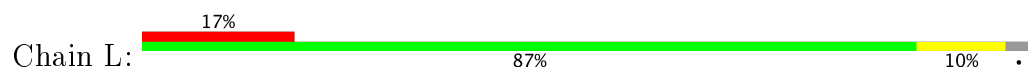
- Molecule 3: Polymerase basic protein 2

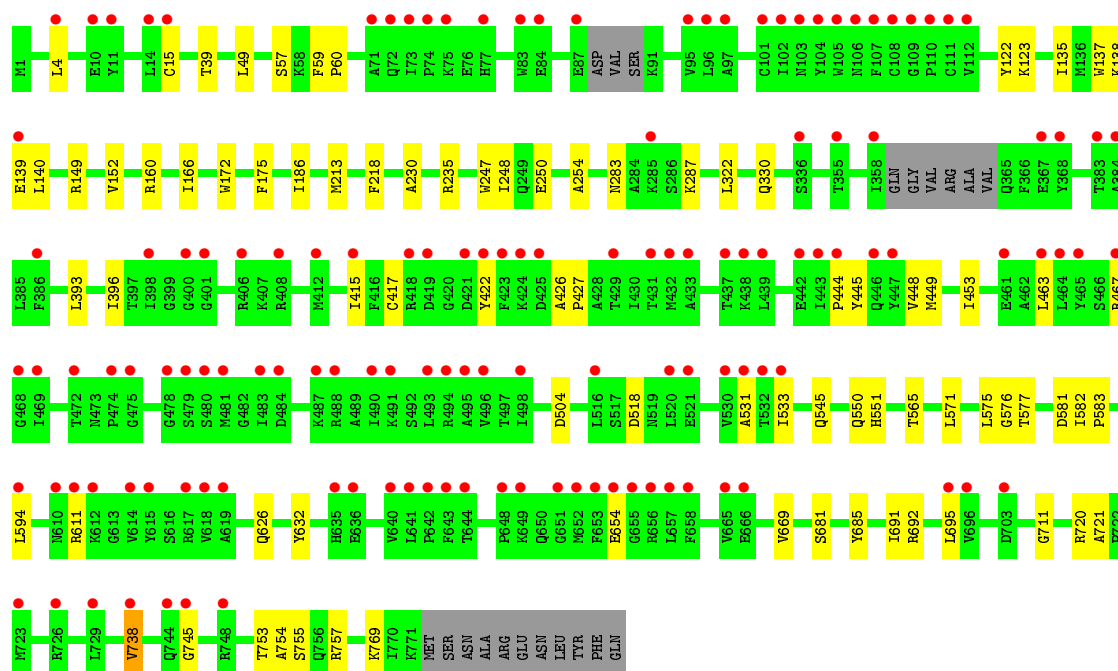


- Molecule 3: Polymerase basic protein 2



- 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	107.28 Å 217.50 Å 597.75 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 4.30 80.90 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-4.30) 98.9 (80.90-4.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 4.30 Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.316 , 0.368 0.311 , 0.359	Depositor DCC
R_{free} test set	4744 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	146.0	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 108.5	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	0.85	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	0.46	0/5746	0.65	0/7717
1	D	0.47	0/5746	0.66	0/7717
1	G	0.46	0/5746	0.64	0/7717
1	J	0.46	0/5746	0.64	0/7717
2	B	0.45	0/5749	0.65	1/7723 (0.0%)
2	E	0.44	0/5749	0.65	0/7723
2	H	0.44	0/5749	0.64	0/7723
2	K	0.43	0/5749	0.64	0/7723
3	C	0.45	0/6121	0.69	1/8236 (0.0%)
3	F	0.46	0/6185	0.69	0/8322
3	I	0.45	0/6185	0.68	1/8322 (0.0%)
3	L	0.44	0/6185	0.68	0/8322
All	All	0.45	0/70656	0.66	3/94962 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	720	ARG	NE-CZ-NH1	6.60	123.60	120.30
3	C	720	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	B	180	GLU	OE1-CD-OE2	-6.36	115.67	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5630	0	5632	144	1
1	D	5630	0	5632	192	5
1	G	5630	0	5632	167	2
1	J	5630	0	5632	116	6
2	B	5652	0	5749	122	6
2	E	5652	0	5749	104	3
2	H	5652	0	5749	129	0
2	K	5652	0	5749	77	0
3	C	6015	0	6124	54	0
3	F	6076	0	6183	171	8
3	I	6076	0	6183	119	3
3	L	6076	0	6183	80	0
All	All	69371	0	70197	1164	17

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 8.

All (1164) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:575:LEU:HD13	3:I:582:ILE:CD1	1.88	1.03
3:I:547:VAL:HG13	3:I:688:GLY:HA2	1.35	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
3:L:692:ARG:NH2	3:L:755:SER:OG	1.91	1.01
1:A:407:ALA:HB1	1:A:412:GLU:CB	1.90	1.01
3:F:477:MET:HE1	1:G:88:LEU:CD1	1.89	1.01
1:A:355:LEU:CD1	1:A:366:LYS:NZ	2.24	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:576:GLY:HA2	3:F:583:PRO:HG3	1.42	0.98
3:F:575:LEU:HD13	3:F:582:ILE:CD1	1.92	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
3:F:477:MET:HE1	1:G:88:LEU:HD11	0.97	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
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:410:GLU:HB3	3:F:137:TRP:HB3	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:CYS:SG	1:D:102:PHE:HD2	1.93	0.90
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: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
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
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
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
2:H:363:ARG:HA	1:J:409:ASN:CG	1.97	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
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:H:363:ARG:C	1:J:409:ASN:ND2	2.31	0.83
2:E:18:ILE:HD12	2:E:497:PHE:CE1	2.13	0.83
3:F:358:ILE:C	3:F:423:PHE:O	2.04	0.83
2:B:182:LYS:HZ1	1:G:205:THR:HG23	1.43	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:O	3:I:554:LEU:HD12	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:90:PHE:CE2	1:D:122:LYS:HB3	2.14	0.81
2:B:363:ARG:CD	3:F:139:GLU:OE2	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:410:GLU:HG2	3:F:137:TRP:CD2	2.22	0.74
1:D:44:VAL:HG13	1:D:153:ILE:HD11	1.70	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
1:A:89:PRO:HG2	1:A:90:PHE:CD1	2.24	0.73
1:D:52:TYR:CD2	1:D:146:MET:HE3	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:410:GLU:OE1	1:G:411:LEU:CB	2.37	0.72
1:G:350:ILE:HB	2:H:368:VAL:HG22	1.69	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
3:F:477:MET:CE	1:G:88:LEU:CD1	2.57	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
1:J:680:ASN:HD22	1:J:680:ASN:H	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:D:52:TYR:CD1	1:D:146:MET:HE1	2.25	0.71
2:K:487:LEU:HD23	2:K:488:PRO:CD	2.20	0.71
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
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:138:LEU:HD11	1:A:140:LYS:HE3	1.73	0.69
3:F:358:ILE:CA	3:F:423:PHE:C	2.57	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
3:C:692:ARG:HH22	3:C:755:SER:CB	2.06	0.69
3:F:575:LEU:CD1	3:F:582:ILE:CD1	2.61	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:155:SER:HB3	3:F:713:SER:OG	1.95	0.66
1:D:69:ARG:CD	1:D:91:LEU:HD11	2.25	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
1:A:304:PRO:HG3	1:A:310:PRO:HB3	1.77	0.65
1:A:67:ARG:HD3	1:A:71:THR:CG2	2.26	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
3:F:475:GLY:C	1:G:86:GLU:HG3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:575:LEU:HD12	3:L:582:ILE:HD12	1.79	0.64
3:F:358:ILE:HA	3:F:423:PHE:C	2.18	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
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
2:E:14:VAL:O	2:E:18:ILE:HG23	1.98	0.63
1:D:368:SER:HB2	2:E:359:LEU:HD23	1.81	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:102:PHE:O	1:D:128:LYS:N	2.26	0.62
1:D:64:ILE:N	1:D:93:ASP:O	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:554:LEU:HD13	3:I:557:LEU:H	1.65	0.61
1:D:52:TYR:CG	1:D:146:MET:HE1	2.34	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
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
2:B:180:GLU:CB	1:G:203:PHE:HE1	2.13	0.61
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:D:52:TYR:CG	1:D:146:MET:CE	2.84	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
1:A:171:ASN:ND2	2:B:167:GLU:OE2	2.35	0.60
1:A:396:THR:HG21	1:A:468:ARG:CG	2.31	0.59
1:A:73:VAL:CA	1:A:91:LEU:HD11	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:410:GLU:OE1	1:D:411:LEU:N	2.35	0.59
1:D:48:PHE:HA	1:D:149:GLN:HE21	1.66	0.59
2:E:303:ASN:ND2	2:E:488:PRO:O	2.34	0.59
1:A:476:PRO:O	1:A:477:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HG	1:A:95:PHE:CZ	2.37	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
2:B:180:GLU:CD	2:B:215:LYS:HD3	2.17	0.59
3:F:358:ILE:C	3:F:423:PHE:C	2.61	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:199:VAL:O	2:E:67:LYS:HD2	2.03	0.59
1:D:52:TYR:HE2	1:D:149:GLN:OE1	1.86	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
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
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
1:J:464:ARG:HG2	1:J:482:ASP:HB3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:487:LEU:CD2	2:E:488:PRO:CD	2.81	0.57
2:E:50:SER:HB3	2:E:68:PHE:CD1	2.38	0.57
1:A:176:PRO:HA	1:A:180:GLU:HB3	1.85	0.57
1:A:72:ALA:O	1:A:91:LEU:CD2	2.50	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:410:GLU:CD	1:D:411:LEU:N	2.58	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
1:J:410:GLU:CD	1:J:411:LEU:N	2.59	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:G:410:GLU:CD	1:G:411:LEU:N	2.59	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
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
1:A:322:ALA:HA	3:F:544:PHE:CG	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:686:GLN:CD	3:I:39:THR:OG1	2.45	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:90:PHE:CZ	1:D:122:LYS:CB	2.76	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
2:E:123:SER:HB3	3:F:34:THR:HG22	1.88	0.55
1:D:575:MET:CG	2:E:544:THR:HA	2.36	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
3:F:575:LEU:HD12	3:F:582:ILE:HD12	1.79	0.54
2:B:179:LYS:CB	1:G:203:PHE:HZ	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:52:TYR:CE2	1:D:146:MET:HE3	2.41	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
1:D:69:ARG:HE	1:D:91:LEU:CD2	2.20	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:487:LEU:C	2:K:487:LEU:HD23	2.29	0.53
2:K:496:MET:HA	2:K:503:VAL:HG21	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:E:487:LEU:C	2:E:487:LEU:HD23	2.29	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:G:203:PHE:HB3	1:G:208:GLN:HB2	1.89	0.53
1:J:449:CYS:SG	1:J:490:LYS:NZ	2.81	0.53
1:J:412:GLU:OE1	2:K:601:ASN:ND2	2.42	0.53
2:E:496:MET:HA	2:E:503:VAL:HG21	1.90	0.53
3:I:554:LEU:C	3:I:554:LEU:HD12	2.29	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
2:B:182:LYS:HZ3	1:G:205:THR:HG23	1.68	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: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
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:476:PRO:O	1:A:477:VAL:CG2	2.57	0.52
1:A:86:GLU:O	1:A:88:LEU:HD22	2.10	0.52
1:D:69:ARG:NH1	1:D:91:LEU:CD1	2.62	0.52
2:E:421:GLY:O	2:E:424:THR:OG1	2.24	0.52
2:B:363:ARG:CZ	3:F:139:GLU:OE2	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:398:TRP:CG	1:G:433:ARG:HA	2.45	0.52
1:G:200:PRO:CB	2:H:69:CYS:HB2	2.40	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:678:LEU:N	1:J:678:LEU:CD1	2.73	0.51
1:A:449:CYS:SG	1:A:490:LYS:NZ	2.82	0.51
1:D:13:LEU:HD21	1:D:39:GLY:O	2.11	0.51
1:D:449:CYS:SG	1:D:490:LYS:NZ	2.82	0.51
1:D:197:GLU:O	2:E:65:ARG:NH1	2.43	0.51
2:H:373:GLU:HA	2:H:399:LYS:O	2.10	0.51
1:G:624:GLN:NE2	2:H:8:MET:SD	2.80	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:469:LYS:HD3	1:J:475:LEU:CD1	2.40	0.51
1:J:59:ASP:OD2	3:L:769:LYS:NZ	2.44	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:398:GLN:HG3	2:E:399:LYS:H	1.76	0.50
2:E:18:ILE:HD13	2:E:497:PHE:CD1	2.38	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
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
2:E:282:ALA:CB	3:F:149:ARG:HD3	2.40	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:B:421:GLY:O	2:B:424:THR:OG1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:230:ALA:HB1	3:C:235:ARG:HD2	1.94	0.49
3:L:230:ALA:HB1	3:L:235:ARG:HD2	1.95	0.49
3:L:57:SER:HB2	3:L:60:PRO:HG3	1.94	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
2:H:686:GLN:CD	3:I:39:THR:HG1	2.16	0.49
3:L:138:LYS:HE2	3:L:140:LEU:CD1	2.43	0.49
1:D:405:PRO:HG2	2:E:601:ASN:ND2	2.28	0.49
1:D:165:ARG:HD3	2:E:706:GLY:CA	2.42	0.49
3:I:575:LEU:HD12	3:I:582:ILE:HD12	1.77	0.49
3:C:565:THR:HG22	3:C:685:TYR:HB3	1.95	0.49
3:C:57:SER:HB2	3:C:60:PRO:HG3	1.94	0.49
2:H:487:LEU:C	2:H:487:LEU:HD23	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:180:GLU:HG3	1:G:203:PHE:CD1	2.47	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:477:VAL:CG1	1:G:478:PRO:CD	2.92	0.48
1:G:240:HIS:NE2	1:G:656:ASP:OD2	2.47	0.48
2:H:282:ALA:HB3	3:I:149:ARG:HD3	1.96	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:J:183:ILE:HD13	2:K:334:LEU:HD13	1.94	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:473:GLU:OE2	1:A:475:LEU:HD21	2.14	0.48
1:A:469:LYS:CD	1:A:475:LEU:HD13	2.40	0.48
1:A:67:ARG:HG2	1:A:71:THR:HB	1.94	0.48
2:B:359:LEU:HB2	2:B:368:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:473:GLU:OE2	1:J:475:LEU:HD21	2.14	0.48
1:A:115:TYR:CZ	1:A:175:LEU:HD12	2.48	0.48
1:A:112:ASP:HB2	1:A:139:ASP:HB2	1.95	0.48
1:A:632:CYS:HA	2:B:26:GLY:HA3	1.95	0.48
1:D:52:TYR:CD2	1:D:146:MET:CE	2.96	0.48
1:D:69:ARG:NH2	1:D:91:LEU:CD1	2.70	0.48
3:F:139:GLU:O	3:F:140:LEU:HG	2.14	0.48
1:D:583:LEU:HD13	3:F:247:TRP:CZ2	2.49	0.48
3:F:475:GLY:C	1:G:86:GLU:CG	2.81	0.48
1:G:535:LYS:NZ	3:L:654:GLU:HG2	2.29	0.48
3:F:474:PRO:HG3	1:G:126:SER:C	2.33	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:203:PHE:HB3	1:G:208:GLN:CB	2.44	0.48
1:G:191:PHE:CE1	2:H:344:VAL:HG21	2.49	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
3:L:138:LYS:HD3	3:L:250:GLU:CG	2.44	0.47
1:J:151:LEU:HD13	3:L:753:THR:OG1	2.14	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:477:VAL:CG1	1:D:478:PRO:CD	2.92	0.47
1:D:155:SER:HA	3:F:714:VAL:HG23	1.96	0.47
1:G:151:LEU:HA	3:I:714:VAL:O	2.15	0.47
1:G:477:VAL:CG1	1:G:478:PRO:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:115:TYR:CZ	1:J:175:LEU:HD12	2.49	0.47
1:J:677:CYS:C	1:J:678:LEU:HD12	2.34	0.47
1:A:238:ILE:HG21	1:A:665:PHE:HA	1.96	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
3:F:474:PRO:HD3	1:G:125:ASN:C	2.35	0.47
2:B:180:GLU:OE2	2:B:215:LYS:HE2	2.14	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
1:A:477:VAL:CG1	1:A:478:PRO:N	2.77	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: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: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: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
1:D:233:ASN:CG	2:E:78:LEU:HD12	2.35	0.46
2:E:697:GLU:N	3:F:178:GLU:OE2	2.49	0.46
3:F:754:ALA:O	3:F:755:SER:C	2.50	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:E:14:VAL:HG12	2:E:18:ILE:HG22	1.96	0.46
1:D:635:ASN:ND2	2:E:27:PRO:O	2.48	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
1:A:401:MET:CE	2:B:551:ILE:HD11	2.44	0.46
2:B:439:TRP:HB2	2:B:450:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:469:LYS:HD3	1:G:475:LEU:CD1	2.40	0.46
1:G:238:ILE:HG21	1:G:665:PHE:HA	1.96	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
3:I:283:ASN:O	3:I:287:LYS:NZ	2.46	0.46
2:H:289:THR:HG21	3:I:499:GLN:OE1	2.16	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
1:G:242:GLU:OE1	1:G:242:GLU:N	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
1:A:88:LEU:C	1:A:90:PHE:N	2.66	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:287:ILE:HA	1:J:290:PHE:HB2	1.98	0.46
1:J:201:LEU:HD21	2:K:87:ILE:HD11	1.98	0.46
3:L:393:LEU:HD22	3:L:396:ILE:HD11	1.98	0.45
1:D:190:THR:HG21	2:E:216:HIS:CE1	2.50	0.45
1:D:14:GLU:HG2	1:D:43:GLN:NE2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:59:PHE:N	3:C:60:PRO:HD3	2.32	0.45
1:A:529:HIS:NE2	3:F:678:LYS:CE	2.79	0.45
1:G:209:MET:SD	1:G:209:MET:C	2.94	0.45
1:A:23:GLU:OE1	1:A:68:LYS:CD	2.63	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:OE1	1:J:242:GLU:N	2.49	0.45
3:L:59:PHE:N	3:L:60:PRO:HD3	2.32	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:N	1:A:242:GLU:OE1	2.50	0.45
1:A:469:LYS:HB2	1:A:475:LEU:CD1	2.47	0.45
1:A:418:LEU:HB3	2:B:543:SER:OG	2.17	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:469:LYS:HB2	1:G:475:LEU:CD1	2.47	0.45
1:G:8:ILE:HD11	2:H:115:THR:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:453:ILE:HG12	3:F:463:LEU:HD22	1.98	0.44
3:I:692:ARG:CZ	3:I:755:SER:OG	2.61	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:F:477:MET:CE	1:G:126:SER:OG	2.65	0.44
1:A:577:THR:HG21	2:B:20:THR:CG2	2.47	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: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: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
1:G:338:GLU:HG2	3:L:254:ALA:CB	2.48	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
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
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:355:LEU:HD13	1:G:359:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:GLU:HG3	2:H:370:ILE:CD1	2.47	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
1:G:488:CYS:SG	1:G:504:ILE:HD11	2.57	0.43
1:G:49:CYS:HB2	1:G:61:PHE:HB2	2.00	0.43
3:I:393:LEU:HD21	3:I:467:ARG:CZ	2.48	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
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: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:A:286:LEU:CD1	1:A:482:ASP:OD2	2.60	0.43
1:D:51:GLU:N	1:D:51:GLU:OE1	2.51	0.43
2:E:427:TYR:CD2	2:E:431:GLU:HB2	2.53	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
2:B:363:ARG:NH2	3:F:139:GLU:CD	2.67	0.43
3:C:393:LEU:HD22	3:C:396:ILE:HD11	1.99	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
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: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
3:F:172:TRP:CD1	3:F:186:ILE:HD11	2.54	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:G:303:LYS:CE	3:L:123:LYS:HD3	2.49	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:131:THR:HG21	2:E:251:ARG:HD2	2.00	0.43
2:E:68:PHE:O	2:E:68:PHE:CD1	2.72	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
2:E:705:ILE:H	3:F:744:GLN:HB2	1.84	0.43
2:H:265:CYS:HB3	2:H:274:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:705:ILE:O	3:I:744:GLN:HB2	2.18	0.43
1:J:265:MET:HG2	1:J:434:GLU:HG2	2.00	0.43
1:J:49:CYS:HB2	1:J:61:PHE:HB2	2.00	0.43
1:A:399:VAL:HB	1:A:427:GLN:HE22	1.84	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:467:PHE:O	2:B:470:VAL:HG12	2.18	0.43
2:B:79:VAL:HB	2:B:480:LEU:HD11	2.01	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
3:F:139:GLU:OE1	3:F:139:GLU:N	2.51	0.43
1:G:410:GLU:HG2	3:I:137:TRP:HB3	1.99	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
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
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
1:D:52:TYR:HE2	1:D:149:GLN:CD	2.23	0.42
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:399:VAL:HB	1:G:427:GLN:HE22	1.84	0.42
1:G:226:LYS:HD2	2:H:466:ARG:NE	2.34	0.42
2:H:632:PHE:CE1	3:I:102:ILE:HG23	2.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:ALA:HA	1:D:42:PHE:CE2	2.55	0.42
1:D:454:GLY:H	1:D:492:LYS:HD2	1.85	0.42
1:D:52:TYR:CD1	1:D:146:MET:CE	3.01	0.42
3:F:426:ALA:N	3:F:427:PRO:HD3	2.34	0.42
3:F:551:HIS:ND1	3:F:551:HIS:O	2.53	0.42
3:F:474:PRO:CB	1:G:126:SER:O	2.67	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
2:B:179:LYS:C	1:G:203:PHE:HE1	2.22	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:265:MET:HG2	1:G:434:GLU:HG2	2.02	0.42
1:G:25:VAL:HG21	1:G:35:ILE:HG22	2.02	0.42
2:K:487:LEU:HD23	2:K:489:GLU:N	2.33	0.42
1:D:102:PHE:HB3	1:D:127:CYS:SG	2.59	0.42
1:D:20:ILE:HD13	1:D:42:PHE:CZ	2.55	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
2:K:282:ALA:HB3	3:L:149:ARG:HD3	2.01	0.42
1:A:25:VAL:HG21	1:A:35:ILE:HG22	2.02	0.42
1:A:408:ASP:OD2	3:C:132:ARG:NH2	2.53	0.42
1:A:87:PRO:O	1:A:89:PRO:N	2.53	0.42
1:D:469:LYS:HB2	1:D:475:LEU:CD1	2.48	0.42
3:F:283:ASN:O	3:F:287:LYS:NZ	2.45	0.42
3:F:477:MET:HE1	1:G:126:SER:OG	2.20	0.42
2:B:179:LYS:HB3	1:G:203:PHE:HZ	1.84	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
3:L:283:ASN:O	3:L:287:LYS:NZ	2.46	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:551:HIS:ND1	3:I:551:HIS:O	2.53	0.42
3:I:549:PHE:CZ	3:I:569:GLU:OE1	2.73	0.42
1:J:25:VAL:HG21	1:J:35:ILE:HG22	2.02	0.42
2:K:68:PHE:O	2:K:68:PHE:CD1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:HD3	1:A:71:THR:HG21	2.02	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: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: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:746:ALA:HB1	3:L:15:CYS:SG	2.60	0.42
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:140:LYS:HE2	1:G:145:PRO:HD2	2.01	0.41
1:G:59:ASP:OD2	3:I:769:LYS:NZ	2.52	0.41
1:A:88:LEU:CD2	1:A:102:PHE:CZ	3.01	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
1:A:345:ARG:NH1	3:F:136:MET:HB3	2.35	0.41
3:F:445:TYR:O	3:F:448:VAL:HB	2.20	0.41
1:J:245:LYS:HA	1:J:706:PHE:CB	2.51	0.41
3:L:551:HIS:ND1	3:L:551:HIS:O	2.53	0.41
1:D:245:LYS:HA	1:D:706:PHE:CB	2.50	0.41
1:D:25:VAL:HG21	1:D:35:ILE:HG22	2.03	0.41
1:D:426:LEU:HD21	1:D:621:LEU:HD22	2.02	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:577:ILE:HA	2:B:580:PHE:HB3	2.02	0.41
2:B:51:ARG:HH12	2:B:78:LEU:HA	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:ND1	3:C:551:HIS:O	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
1:G:316:LEU:HD21	1:G:489:VAL:HG21	2.02	0.41
1:G:183:ILE:CD1	2:H:334:LEU:HD22	2.50	0.41
1:J:378:PHE:HA	1:J:379:PRO:HD3	1.97	0.41
1:J:680:ASN:N	1:J:680:ASN:ND2	2.65	0.41
2:K:542:PRO:HD3	3:L:247:TRP:CE2	2.56	0.41
2:K:51:ARG:HH12	2:K:78:LEU:HA	1.86	0.41
2:B:18:ILE:HD13	2:B:497:PHE:CD2	2.55	0.41
3:C:397:THR:HA	3:C:497:THR:O	2.21	0.41
1:D:197:GLU:O	2:E:65:ARG:CZ	2.69	0.41
1:D:565:SER:CB	3:F:52:ARG:HH22	2.34	0.41
2:E:279:GLU:HB2	3:F:224:PHE:CE2	2.56	0.41
1:D:410:GLU:HB2	3:F:249:GLN:OE1	2.21	0.41
3:F:358:ILE:N	3:F:423:PHE:HB3	2.34	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
2:B:294:ARG:HG3	3:C:395:TRP:CH2	2.55	0.41
3:C:600:VAL:HG13	3:C:642:PRO:HA	2.02	0.41
1:D:643:CYS:HA	1:D:646:GLN:HB3	2.03	0.41
1:G:412:GLU:CD	1:G:412:GLU:N	2.73	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
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
1:G:245:LYS:HA	1:G:706:PHE:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:316:LEU:HD22	1:A:339:PHE:CE2	2.57	0.40
1:A:155:SER:HB3	3:C:713:SER:OG	2.21	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
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 (17) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:215:LYS:NZ	3:I:628:THR:OG1[3_554]	0.92	1.28
2:B:457:TRP:N	1:J:84:ASP:OD2[1_565]	1.72	0.48
2:B:362:LYS:CE	1:D:81:LYS:NZ[1_655]	1.75	0.45
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
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
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	38	77
1	D	685/709 (97%)	634 (93%)	49 (7%)	2 (0%)	44	81
1	G	685/709 (97%)	635 (93%)	48 (7%)	2 (0%)	44	81
1	J	685/709 (97%)	633 (92%)	50 (7%)	2 (0%)	44	81
2	B	703/754 (93%)	670 (95%)	30 (4%)	3 (0%)	38	77
2	E	703/754 (93%)	669 (95%)	31 (4%)	3 (0%)	38	77
2	H	703/754 (93%)	670 (95%)	30 (4%)	3 (0%)	38	77
2	K	703/754 (93%)	669 (95%)	31 (4%)	3 (0%)	38	77
3	C	746/782 (95%)	679 (91%)	64 (9%)	3 (0%)	38	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	756/782 (97%)	683 (90%)	69 (9%)	4 (0%)	32	74
3	I	756/782 (97%)	685 (91%)	68 (9%)	3 (0%)	38	77
3	L	756/782 (97%)	686 (91%)	67 (9%)	3 (0%)	38	77
All	All	8566/8980 (95%)	7944 (93%)	588 (7%)	34 (0%)	38	77

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	503	VAL
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

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Mol	Chain	Res	Type
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%)	610 (99%)	8 (1%)	73	87
1	D	618/631 (98%)	610 (99%)	8 (1%)	73	87
1	G	618/631 (98%)	608 (98%)	10 (2%)	68	86
1	J	618/631 (98%)	608 (98%)	10 (2%)	68	86
2	B	629/669 (94%)	617 (98%)	12 (2%)	62	83
2	E	629/669 (94%)	617 (98%)	12 (2%)	62	83
2	H	629/669 (94%)	617 (98%)	12 (2%)	62	83
2	K	629/669 (94%)	617 (98%)	12 (2%)	62	83
3	C	663/686 (97%)	649 (98%)	14 (2%)	59	81
3	F	669/686 (98%)	656 (98%)	13 (2%)	62	83
3	I	669/686 (98%)	656 (98%)	13 (2%)	62	83
3	L	669/686 (98%)	656 (98%)	13 (2%)	62	83
All	All	7658/7944 (96%)	7521 (98%)	137 (2%)	64	84

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	48	PHE
1	A	163	PHE
1	A	170	PHE
1	A	276	ASP
1	A	490	LYS
1	A	506	THR
1	A	554	THR
2	B	59	LYS

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Mol	Chain	Res	Type
2	B	147	GLN
2	B	166	LEU
2	B	273	LEU
2	B	279	GLU
2	B	302	VAL
2	B	491	PHE
2	B	502	PHE
2	B	540	LEU
2	B	618	ASP
2	B	657	VAL
2	B	665	ARG
3	C	4	LEU
3	C	39	THR
3	C	135	ILE
3	C	139	GLU
3	C	152	VAL
3	C	160	ARG
3	C	175	PHE
3	C	504	ASP
3	C	518	ASP
3	C	594	LEU
3	C	611	ARG
3	C	695	LEU
3	C	720	ARG
3	C	738	VAL
1	D	38	ILE
1	D	163	PHE
1	D	170	PHE
1	D	276	ASP
1	D	482	ASP
1	D	490	LYS
1	D	506	THR
1	D	554	THR
2	E	59	LYS
2	E	147	GLN
2	E	166	LEU
2	E	273	LEU
2	E	279	GLU
2	E	302	VAL
2	E	491	PHE
2	E	502	PHE
2	E	540	LEU

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Mol	Chain	Res	Type
2	E	618	ASP
2	E	657	VAL
2	E	665	ARG
3	F	4	LEU
3	F	39	THR
3	F	135	ILE
3	F	152	VAL
3	F	160	ARG
3	F	175	PHE
3	F	504	ASP
3	F	518	ASP
3	F	594	LEU
3	F	611	ARG
3	F	695	LEU
3	F	720	ARG
3	F	738	VAL
1	G	38	ILE
1	G	48	PHE
1	G	163	PHE
1	G	170	PHE
1	G	205	THR
1	G	276	ASP
1	G	482	ASP
1	G	490	LYS
1	G	506	THR
1	G	554	THR
2	H	59	LYS
2	H	147	GLN
2	H	166	LEU
2	H	273	LEU
2	H	279	GLU
2	H	302	VAL
2	H	491	PHE
2	H	502	PHE
2	H	540	LEU
2	H	618	ASP
2	H	657	VAL
2	H	665	ARG
3	I	4	LEU
3	I	135	ILE
3	I	139	GLU
3	I	152	VAL

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Mol	Chain	Res	Type
3	I	160	ARG
3	I	175	PHE
3	I	504	ASP
3	I	518	ASP
3	I	594	LEU
3	I	611	ARG
3	I	695	LEU
3	I	720	ARG
3	I	738	VAL
1	J	38	ILE
1	J	48	PHE
1	J	163	PHE
1	J	170	PHE
1	J	276	ASP
1	J	482	ASP
1	J	490	LYS
1	J	506	THR
1	J	554	THR
1	J	680	ASN
2	K	59	LYS
2	K	147	GLN
2	K	166	LEU
2	K	273	LEU
2	K	279	GLU
2	K	302	VAL
2	K	491	PHE
2	K	502	PHE
2	K	540	LEU
2	K	618	ASP
2	K	657	VAL
2	K	665	ARG
3	L	4	LEU
3	L	39	THR
3	L	135	ILE
3	L	152	VAL
3	L	160	ARG
3	L	175	PHE
3	L	504	ASP
3	L	518	ASP
3	L	594	LEU
3	L	611	ARG
3	L	695	LEU

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Mol	Chain	Res	Type
3	L	720	ARG
3	L	738	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	519	HIS
1	A	644	ASN
2	B	303	ASN
2	B	316	GLN
2	B	477	ASN
2	B	627	ASN
3	C	550	GLN
1	D	41	HIS
1	D	204	GLN
1	D	519	HIS
1	D	644	ASN
2	E	303	ASN
2	E	316	GLN
2	E	477	ASN
2	E	627	ASN
2	E	660	HIS
2	E	686	GLN
3	F	550	GLN
1	G	31	HIS
1	G	208	GLN
1	G	312	HIS
1	G	519	HIS
1	G	628	GLN
2	H	303	ASN
2	H	316	GLN
2	H	477	ASN
2	H	627	ASN
2	H	660	HIS
3	I	330	GLN
3	I	550	GLN
1	J	31	HIS
1	J	409	ASN
1	J	519	HIS
1	J	680	ASN
2	K	303	ASN

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Mol	Chain	Res	Type
2	K	316	GLN
2	K	477	ASN
2	K	627	ASN
3	L	545	GLN
3	L	550	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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%)	0.36	47 (6%)	18	15	66, 164, 326, 490	0
1	D	693/709 (97%)	0.14	21 (3%)	51	41	72, 156, 252, 382	0
1	G	693/709 (97%)	0.42	68 (9%)	8	8	90, 180, 290, 407	0
1	J	693/709 (97%)	0.18	21 (3%)	51	41	105, 181, 273, 414	0
2	B	711/754 (94%)	0.20	41 (5%)	24	20	70, 147, 290, 437	0
2	E	711/754 (94%)	0.21	32 (4%)	34	28	71, 143, 270, 490	0
2	H	711/754 (94%)	0.33	45 (6%)	21	17	82, 170, 287, 498	0
2	K	711/754 (94%)	0.49	63 (8%)	10	10	83, 173, 284, 424	0
3	C	754/782 (96%)	1.00	164 (21%)	1	3	99, 240, 349, 416	0
3	F	762/782 (97%)	0.30	44 (5%)	24	20	87, 174, 295, 481	0
3	I	762/782 (97%)	0.67	90 (11%)	5	7	95, 224, 337, 500	0
3	L	762/782 (97%)	0.85	135 (17%)	2	4	108, 226, 332, 476	0
All	All	8656/8980 (96%)	0.44	771 (8%)	10	10	66, 181, 315, 500	0

All (771) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	95	VAL	16.6
3	C	665	VAL	10.7
3	L	656	ARG	10.6
3	I	96	LEU	9.9
3	L	655	GLY	9.6
3	I	422	TYR	7.4
3	C	446	GLN	7.1
3	F	491	LYS	7.1
3	C	687	HIS	7.0
1	A	63	LEU	6.7
3	C	695	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
3	C	425	ASP	6.6
3	C	63	ALA	6.6
3	L	107	PHE	6.5
3	C	643	PHE	6.4
3	C	640	VAL	6.3
3	C	83	TRP	6.1
2	H	738	GLU	6.0
3	L	469	ILE	5.9
3	C	72	GLN	5.8
3	L	488	ARG	5.8
2	E	67	LYS	5.7
3	L	424	LYS	5.7
2	H	184	LYS	5.6
3	I	433	ALA	5.6
1	G	707	LYS	5.5
3	C	605	PRO	5.5
3	I	446	GLN	5.5
3	C	603	MET	5.5
3	I	429	THR	5.4
1	J	499	ASP	5.4
3	L	431	THR	5.4
1	J	708	THR	5.4
3	C	110	PRO	5.4
3	L	73	ILE	5.3
3	C	696	VAL	5.3
3	C	686	CYS	5.3
3	L	83	TRP	5.2
3	I	106	ASN	5.2
3	C	71	ALA	5.1
1	G	499	ASP	5.1
3	L	696	VAL	5.1
3	C	447	TYR	5.1
3	C	422	TYR	5.1
3	C	639	LYS	5.1
3	C	418	ARG	5.0
3	L	703	ASP	5.0
3	C	685	TYR	5.0
3	C	606	LEU	4.9
3	L	654	GLU	4.9
2	H	632	PHE	4.9
3	F	737	LYS	4.9
3	L	443	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
3	C	286	SER	4.8
3	I	94	HIS	4.8
2	K	405	PRO	4.7
3	I	467	ARG	4.7
3	C	358	ILE	4.7
1	A	130	PHE	4.7
1	A	102	PHE	4.7
1	A	119	LYS	4.7
3	L	532	THR	4.7
3	C	726	ARG	4.6
3	I	415	ILE	4.6
2	E	629	LYS	4.6
3	I	418	ARG	4.6
1	A	95	PHE	4.6
3	I	365	GLN	4.6
1	A	123	LEU	4.5
3	L	72	GLN	4.5
3	C	645	TYR	4.5
1	A	69	ARG	4.5
3	L	648	PRO	4.5
1	G	60	ARG	4.5
3	I	102	ILE	4.5
3	C	67	MET	4.5
3	C	642	PRO	4.5
2	B	233	GLY	4.5
3	L	615	TYR	4.5
3	I	447	TYR	4.4
2	K	440	THR	4.4
3	I	434	ASP	4.4
3	I	72	GLN	4.4
3	C	106	ASN	4.4
3	I	110	PRO	4.4
1	A	92	CYS	4.4
2	H	682	GLU	4.4
3	C	391	ARG	4.4
3	L	11	TYR	4.4
3	F	85	ASP	4.4
3	C	96	LEU	4.4
1	D	499	ASP	4.3
3	L	358	ILE	4.3
2	B	67	LYS	4.3
3	L	442	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
3	F	110	PRO	4.3
3	L	468	GLY	4.3
3	I	279	ALA	4.3
3	L	531	ALA	4.3
3	I	703	ASP	4.2
3	C	587	ALA	4.2
3	L	611	ARG	4.2
2	K	67	LYS	4.2
3	L	429	THR	4.2
3	I	443	ILE	4.2
1	G	102	PHE	4.2
2	H	739	ILE	4.2
1	G	98	GLU	4.2
3	C	365	GLN	4.1
3	I	367	GLU	4.1
3	L	444	PRO	4.1
3	C	586	ILE	4.1
2	H	742	ILE	4.1
1	J	664	GLY	4.1
3	L	111	CYS	4.1
3	L	491	LYS	4.1
3	C	178	GLU	4.1
3	L	418	ARG	4.1
3	L	643	PHE	4.1
3	F	95	VAL	4.0
1	A	62	VAL	4.0
3	I	148	GLN	4.0
3	L	521	GLU	4.0
3	L	425	ASP	4.0
3	L	464	LEU	4.0
3	I	22	GLN	4.0
3	C	95	VAL	3.9
3	C	491	LYS	3.9
1	A	28	TYR	3.9
3	C	520	LEU	3.9
2	K	441	GLY	3.9
3	C	421	ASP	3.9
3	I	450	MET	3.9
2	K	406	GLY	3.9
3	C	618	VAL	3.9
3	L	479	SER	3.9
3	L	618	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	67	ARG	3.9
1	G	693	GLU	3.9
2	H	187	LYS	3.9
3	L	657	LEU	3.9
3	C	564	ILE	3.9
3	I	431	THR	3.9
2	B	581	ILE	3.9
3	C	15	CYS	3.9
3	L	110	PRO	3.8
3	C	285	LYS	3.8
3	C	467	ARG	3.8
3	C	560	GLU	3.8
1	J	494	HIS	3.8
3	C	617	ARG	3.8
1	G	94	ILE	3.8
3	L	483	ILE	3.8
1	A	103	VAL	3.8
2	B	736	TYR	3.8
1	G	356	THR	3.8
3	F	648	PRO	3.8
3	I	465	TYR	3.8
1	G	76	GLN	3.8
2	H	183	PHE	3.8
2	K	624	ARG	3.8
3	I	469	ILE	3.8
3	C	328	GLY	3.8
1	A	104	GLU	3.8
3	C	607	ILE	3.8
3	C	1	MET	3.7
2	K	318	GLU	3.7
3	C	109	GLY	3.7
1	A	64	ILE	3.7
3	F	715	CYS	3.7
3	L	642	PRO	3.7
3	C	415	ILE	3.7
2	B	578	ASN	3.7
1	G	125	ASN	3.7
3	I	63	ALA	3.7
3	L	487	LYS	3.7
3	I	425	ASP	3.7
2	B	739	ILE	3.7
2	K	300	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
3	L	641	LEU	3.7
1	G	83	TYR	3.7
3	L	666	GLU	3.7
3	C	594	LEU	3.7
3	F	357	TYR	3.6
3	C	666	GLU	3.6
3	I	77	HIS	3.6
1	A	125	ASN	3.6
3	I	444	PRO	3.6
2	K	83	GLY	3.6
1	G	147	GLU	3.6
1	G	61	PHE	3.6
1	G	535	LYS	3.6
3	C	623	VAL	3.6
3	C	493	LEU	3.6
2	E	68	PHE	3.5
3	I	449	MET	3.5
3	C	614	VAL	3.5
2	H	405	PRO	3.5
3	C	64	ASN	3.5
3	C	108	CYS	3.5
3	L	400	GLY	3.5
3	L	493	LEU	3.5
1	A	105	ILE	3.5
2	B	742	ILE	3.5
3	I	445	TYR	3.5
3	L	71	ALA	3.5
3	L	105	TRP	3.5
3	C	448	VAL	3.5
3	F	425	ASP	3.5
3	C	626	GLN	3.5
3	C	647	ALA	3.5
3	L	355	THR	3.5
2	B	624	ARG	3.5
3	C	737	LYS	3.5
3	L	112	VAL	3.5
3	C	619	ALA	3.5
3	C	604	ALA	3.4
3	I	93	ASP	3.4
2	H	583	THR	3.4
2	K	594	ASP	3.4
3	C	667	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	678	MET	3.4
3	F	560	GLU	3.4
3	L	415	ILE	3.4
1	D	130	PHE	3.4
1	J	707	LYS	3.4
3	L	533	ILE	3.4
2	K	620	GLN	3.4
3	C	482	GLY	3.4
3	C	641	LEU	3.4
3	L	432	MET	3.3
3	I	419	ASP	3.3
2	K	82	THR	3.3
2	B	190	VAL	3.3
3	I	483	ILE	3.3
2	E	674	ASP	3.3
2	K	582	LYS	3.3
1	G	97	ARG	3.3
2	H	721	ARG	3.3
1	A	132	PHE	3.3
3	C	483	ILE	3.3
1	A	94	ILE	3.3
3	F	655	GLY	3.3
2	B	677	ALA	3.3
1	G	708	THR	3.3
1	G	705	PHE	3.3
2	K	685	TYR	3.3
3	L	640	VAL	3.3
3	L	75	LYS	3.3
3	C	423	PHE	3.3
2	B	717	LYS	3.3
3	I	14	LEU	3.3
3	F	83	TRP	3.3
3	I	556	VAL	3.2
1	A	66	GLY	3.2
3	L	95	VAL	3.2
1	G	355	LEU	3.2
3	C	419	ASP	3.2
3	F	101	CYS	3.2
3	C	444	PRO	3.2
2	E	83	GLY	3.2
3	I	430	ILE	3.2
2	K	50	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	644	THR	3.2
3	C	81	ALA	3.2
1	G	96	ASP	3.2
3	F	72	GLN	3.2
3	C	481	MET	3.2
2	B	231	LYS	3.2
3	C	658	PHE	3.2
1	G	333	GLU	3.2
3	F	15	CYS	3.2
1	G	342	GLY	3.2
3	I	366	PHE	3.2
2	E	621	TYR	3.2
2	B	630	ASN	3.2
3	L	87	GLU	3.2
2	K	621	TYR	3.2
1	A	127	CYS	3.1
2	K	439	TRP	3.1
2	K	227	ASN	3.1
2	B	230	ALA	3.1
3	L	729	LEU	3.1
1	G	592	ASN	3.1
1	J	248	GLN	3.1
2	H	186	VAL	3.1
3	L	108	CYS	3.1
3	L	109	GLY	3.1
3	L	494	ARG	3.1
1	J	198	SER	3.1
3	C	38	TRP	3.1
1	A	467	GLU	3.1
1	G	241	TYR	3.1
1	J	98	GLU	3.1
2	B	68	PHE	3.1
1	G	47	MET	3.1
3	C	596	ASN	3.1
3	C	646	PHE	3.1
3	L	104	TYR	3.1
3	L	619	ALA	3.1
3	L	610	ASN	3.1
1	J	665	PHE	3.1
3	L	106	ASN	3.1
2	H	504	SER	3.1
3	C	480	SER	3.1

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Mol	Chain	Res	Type	RSRZ
3	I	488	ARG	3.1
3	L	644	THR	3.1
3	L	612	LYS	3.1
1	A	126	SER	3.1
2	K	68	PHE	3.1
3	L	383	THR	3.1
3	F	604	ALA	3.1
1	A	107	ILE	3.0
1	J	366	LYS	3.0
3	I	83	TRP	3.0
3	L	101	CYS	3.0
2	H	685	TYR	3.0
3	C	85	ASP	3.0
2	H	631	PRO	3.0
1	D	380	ARG	3.0
3	C	688	GLY	3.0
3	F	77	HIS	3.0
1	A	128	LYS	3.0
3	F	63	ALA	3.0
3	L	475	GLY	3.0
3	C	672	ASN	3.0
3	I	414	MET	3.0
3	F	71	ALA	3.0
2	H	406	GLY	3.0
1	A	143	GLU	3.0
3	F	492	SER	3.0
3	C	367	GLU	3.0
2	K	64	PRO	3.0
3	C	420	GLY	3.0
1	D	483	CYS	3.0
1	D	379	PRO	3.0
2	B	582	LYS	3.0
2	B	629	LYS	3.0
3	C	577	THR	3.0
2	H	233	GLY	3.0
3	C	388	ARG	3.0
3	C	568	TYR	3.0
3	I	81	ALA	3.0
1	A	34	LYS	3.0
3	C	556	VAL	3.0
3	I	105	TRP	3.0
3	I	464	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	91	LYS	2.9
3	C	683	LYS	2.9
3	C	633	SER	2.9
3	L	96	LEU	2.9
3	L	398	ILE	2.9
1	G	101	GLN	2.9
2	K	348	ASN	2.9
1	A	35	ILE	2.9
3	F	73	ILE	2.9
3	I	529	ILE	2.9
2	K	682	GLU	2.9
3	L	446	GLN	2.9
3	C	68	LEU	2.9
3	C	660	SER	2.9
2	K	571	GLY	2.9
3	I	92	ARG	2.9
3	C	97	ALA	2.9
1	A	145	PRO	2.9
3	F	107	PHE	2.9
2	E	720	GLU	2.9
3	C	12	LYS	2.9
3	L	463	LEU	2.9
3	I	71	ALA	2.9
1	G	238	ILE	2.9
3	L	653	PHE	2.9
3	L	97	ALA	2.9
3	I	643	PHE	2.9
2	H	722	ALA	2.9
2	H	185	LYS	2.9
2	K	237	LYS	2.9
1	G	92	CYS	2.9
1	J	518	LYS	2.9
3	L	433	ALA	2.9
1	D	500	GLY	2.9
2	E	406	GLY	2.9
3	I	603	MET	2.8
2	E	405	PRO	2.8
3	C	416	PHE	2.8
3	C	8	ALA	2.8
2	E	620	GLN	2.8
3	L	77	HIS	2.8
3	L	386	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	66	GLY	2.8
1	J	463	ALA	2.8
3	C	393	LEU	2.8
3	L	423	PHE	2.8
1	G	364	GLY	2.8
3	L	520	LEU	2.8
3	I	454	GLN	2.8
3	L	695	LEU	2.8
2	B	232	ASP	2.8
2	K	407	GLY	2.8
3	I	15	CYS	2.8
3	L	438	LYS	2.8
2	K	450	LEU	2.8
2	H	182	LYS	2.8
3	I	687	HIS	2.8
2	E	180	GLU	2.8
1	G	665	PHE	2.8
3	L	652	MET	2.8
1	A	47	MET	2.8
1	A	67	ARG	2.8
1	A	463	ALA	2.8
2	K	583	THR	2.8
3	L	490	ILE	2.8
3	L	649	LYS	2.8
3	C	615	TYR	2.8
3	C	463	LEU	2.8
3	F	282	MET	2.8
1	J	101	GLN	2.8
3	C	496	VAL	2.8
3	C	613	GLY	2.8
1	G	661	SER	2.8
3	L	367	GLU	2.8
3	C	336	SER	2.7
2	B	631	PRO	2.7
1	A	106	GLY	2.7
3	C	105	TRP	2.7
2	H	678	MET	2.7
1	A	122	LYS	2.7
2	H	490	LEU	2.7
3	C	7	ILE	2.7
3	F	111	CYS	2.7
2	K	468	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	45	CYS	2.7
2	H	217	ASP	2.7
3	L	530	VAL	2.7
3	C	585	LEU	2.7
2	B	621	TYR	2.7
3	F	422	TYR	2.7
3	F	652	MET	2.7
3	C	84	GLU	2.7
3	C	661	ASN	2.7
3	L	84	GLU	2.7
3	L	723	MET	2.7
1	G	64	ILE	2.7
2	K	7	LEU	2.7
3	C	70	GLU	2.7
1	G	664	GLY	2.7
3	L	465	TYR	2.7
2	E	472	LYS	2.7
2	H	482	LYS	2.7
2	B	594	ASP	2.7
2	E	570	LYS	2.7
3	C	73	ILE	2.7
3	C	727	GLN	2.7
3	C	725	THR	2.7
1	A	466	LYS	2.7
1	G	105	ILE	2.7
2	E	624	ARG	2.7
3	C	394	GLU	2.7
2	K	6	TYR	2.6
3	C	111	CYS	2.6
3	C	664	PHE	2.6
3	C	94	HIS	2.6
2	K	301	ALA	2.6
3	I	766	ASN	2.6
3	C	748	ARG	2.6
3	F	108	CYS	2.6
3	I	278	ASN	2.6
3	L	498	ILE	2.6
3	I	386	PHE	2.6
2	B	740	LYS	2.6
3	C	612	LYS	2.6
3	I	682	SER	2.6
1	G	378	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	594	ASP	2.6
2	K	477	ASN	2.6
3	L	480	SER	2.6
3	C	484	ASP	2.6
3	C	563	ALA	2.6
3	C	744	GLN	2.6
3	F	490	ILE	2.6
3	L	496	VAL	2.6
3	L	726	ARG	2.6
3	C	75	LYS	2.6
3	F	112	VAL	2.6
3	I	683	LYS	2.6
2	K	678	MET	2.6
3	L	478	GLY	2.6
2	K	655	ALA	2.6
3	I	38	TRP	2.6
3	L	419	ASP	2.6
2	K	438	PHE	2.6
3	L	744	GLN	2.6
2	E	237	LYS	2.6
1	D	364	GLY	2.6
3	C	632	TYR	2.6
1	D	257	ALA	2.6
1	G	352	GLU	2.6
2	K	631	PRO	2.6
3	I	411	ALA	2.6
2	E	581	ILE	2.6
2	K	490	LEU	2.6
2	B	625	VAL	2.5
3	I	336	SER	2.5
1	A	91	LEU	2.5
1	G	88	LEU	2.5
1	G	104	GLU	2.5
2	K	580	PHE	2.5
2	B	620	GLN	2.5
3	L	422	TYR	2.5
2	K	578	ASN	2.5
2	H	718	LEU	2.5
2	H	725	LYS	2.5
1	D	267	GLU	2.5
2	B	681	GLU	2.5
3	L	516	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	49	TYR	2.5
3	F	471	GLU	2.5
3	L	484	ASP	2.5
1	G	244	ASN	2.5
2	H	435	LYS	2.5
2	K	403	PHE	2.5
1	A	42	PHE	2.5
2	K	570	LYS	2.5
3	I	424	LYS	2.5
3	L	4	LEU	2.5
2	K	66	ARG	2.5
3	I	397	THR	2.5
3	L	412	MET	2.5
3	L	495	ALA	2.5
1	G	99	GLU	2.5
3	L	658	PHE	2.5
2	E	188	THR	2.5
3	L	614	VAL	2.5
2	E	82	THR	2.5
3	C	366	PHE	2.5
2	K	184	LYS	2.5
3	C	16	GLN	2.5
3	L	467	ARG	2.5
1	G	382	PHE	2.5
3	I	412	MET	2.5
3	I	481	MET	2.5
2	B	716	GLU	2.5
3	F	75	LYS	2.5
2	B	743	ILE	2.4
2	K	65	ARG	2.4
2	H	155	GLU	2.4
3	L	103	ASN	2.4
1	J	195	ARG	2.4
2	E	66	ARG	2.4
3	L	472	THR	2.4
3	C	342	LEU	2.4
1	J	102	PHE	2.4
3	F	109	GLY	2.4
3	L	636	GLU	2.4
3	C	673	VAL	2.4
3	C	417	CYS	2.4
3	I	533	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	I	557	LEU	2.4
3	C	674	PHE	2.4
1	A	533	ARG	2.4
2	E	314	CYS	2.4
3	F	716	GLU	2.4
3	I	260	ASP	2.4
3	I	337	PHE	2.4
2	E	632	PHE	2.4
2	B	674	ASP	2.4
2	H	209	MET	2.4
3	F	481	MET	2.4
3	I	75	LYS	2.4
1	A	90	PHE	2.4
1	J	380	ARG	2.4
2	H	398	GLN	2.4
3	C	337	PHE	2.4
1	G	248	GLN	2.4
1	D	382	PHE	2.4
2	H	181	ILE	2.4
2	B	587	LYS	2.4
3	C	107	PHE	2.4
3	C	559	ASP	2.4
3	C	638	ILE	2.4
2	E	50	SER	2.4
2	K	696	PHE	2.4
1	A	70	GLY	2.4
1	A	480	GLU	2.4
3	C	443	ILE	2.3
1	G	471	MET	2.3
1	G	48	PHE	2.3
2	B	632	PHE	2.3
3	C	340	MET	2.3
3	L	437	THR	2.3
2	B	724	MET	2.3
3	C	599	GLU	2.3
3	L	384	ALA	2.3
1	G	689	GLN	2.3
2	K	183	PHE	2.3
3	I	396	ILE	2.3
2	B	83	GLY	2.3
2	H	436	GLY	2.3
2	K	443	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	381	TRP	2.3
3	I	64	ASN	2.3
3	C	524	ASP	2.3
2	B	721	ARG	2.3
1	A	120	PHE	2.3
1	G	79	LEU	2.3
3	L	738	VAL	2.3
1	A	366	LYS	2.3
1	G	536	LYS	2.3
1	G	103	VAL	2.3
1	D	363	GLU	2.3
3	L	139	GLU	2.3
3	I	673	VAL	2.3
3	I	87	GLU	2.3
1	D	95	PHE	2.3
2	K	463	THR	2.3
1	A	124	GLY	2.3
3	C	426	ALA	2.3
3	F	74	PRO	2.3
3	L	408	ARG	2.3
2	E	49	TYR	2.3
3	L	665	VAL	2.3
1	J	355	LEU	2.3
3	C	431	THR	2.3
1	D	378	PHE	2.3
3	I	513	HIS	2.3
3	C	622	LEU	2.3
3	C	589	LYS	2.3
1	A	499	ASP	2.3
3	L	439	LEU	2.3
3	F	1	MET	2.3
3	L	617	ARG	2.3
2	E	190	VAL	2.2
2	H	582	LYS	2.2
3	C	595	TYR	2.2
1	G	494	HIS	2.2
3	L	15	CYS	2.2
1	D	209	MET	2.2
2	B	128	GLY	2.2
3	C	460	LEU	2.2
3	L	447	TYR	2.2
2	B	662	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	81	ALA	2.2
1	G	85	LEU	2.2
3	I	82	LEU	2.2
1	A	46	CYS	2.2
3	L	635	HIS	2.2
1	G	690	ARG	2.2
2	E	236	GLY	2.2
3	F	244	GLY	2.2
3	I	421	ASP	2.2
2	K	632	PHE	2.2
3	F	260	ASP	2.2
2	K	676	ARG	2.2
3	C	308	GLU	2.2
3	L	406	ARG	2.2
3	C	690	ALA	2.2
3	I	91	LYS	2.2
3	C	62	ILE	2.2
3	F	412	MET	2.2
3	I	1	MET	2.2
1	D	132	PHE	2.2
1	G	684	CYS	2.2
1	J	54	SER	2.2
3	C	55	MET	2.2
3	F	656	ARG	2.2
3	C	539	ASP	2.2
1	G	240	HIS	2.2
2	H	714	ILE	2.2
3	L	285	LYS	2.2
1	J	604	TRP	2.2
2	E	724	MET	2.2
3	L	748	ARG	2.2
1	G	692	ASN	2.2
1	D	235	LYS	2.2
3	L	745	GLY	2.2
2	B	714	ILE	2.2
1	G	700	LYS	2.2
2	B	718	LEU	2.2
2	E	723	LYS	2.2
1	G	379	PRO	2.2
2	K	76	ASP	2.2
3	C	469	ILE	2.2
3	F	603	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	352	LYS	2.2
3	C	637	LEU	2.2
3	L	594	LEU	2.2
1	J	680	ASN	2.2
3	I	610	ASN	2.2
1	J	345	ARG	2.1
3	I	607	ILE	2.2
3	C	74	PRO	2.1
2	K	452	ALA	2.1
2	K	462	TRP	2.1
3	C	582	ILE	2.1
2	H	232	ASP	2.1
2	K	581	ILE	2.1
3	L	481	MET	2.1
3	C	533	ILE	2.1
2	H	581	ILE	2.1
3	L	651	GLY	2.1
2	K	749	ALA	2.1
3	C	101	CYS	2.1
3	C	668	GLY	2.1
3	L	474	PRO	2.1
2	K	753	SER	2.1
3	L	14	LEU	2.1
1	G	697	GLU	2.1
1	A	605	ILE	2.1
1	G	259	TYR	2.1
3	C	87	GLU	2.1
3	C	561	LYS	2.1
3	L	368	TYR	2.1
3	C	386	PHE	2.1
1	D	198	SER	2.1
3	C	715	CYS	2.1
2	H	212	ASP	2.1
3	I	612	LYS	2.1
1	G	386	TRP	2.1
2	E	84	ASN	2.1
2	H	190	VAL	2.1
2	E	631	PRO	2.1
2	H	50	SER	2.1
3	I	608	ARG	2.1
1	D	177	ASP	2.1
2	K	619	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	359	VAL	2.1
3	C	753	THR	2.1
1	G	663	PHE	2.1
3	I	11	TYR	2.1
2	E	579	GLU	2.1
2	K	306	GLY	2.1
3	I	461	GLU	2.1
1	D	107	ILE	2.1
2	B	744	ARG	2.1
2	H	403	PHE	2.1
1	G	63	LEU	2.1
1	G	132	PHE	2.1
1	G	390	ILE	2.1
2	K	226	ILE	2.1
1	G	54	SER	2.1
2	H	407	GLY	2.1
2	B	725	LYS	2.1
3	I	640	VAL	2.1
2	H	218	GLU	2.1
3	C	656	ARG	2.0
3	F	649	LYS	2.0
2	E	619	GLU	2.0
3	C	580	ASN	2.0
3	L	10	GLU	2.0
3	C	729	LEU	2.0
1	D	92	CYS	2.0
1	G	237	PRO	2.0
3	I	548	SER	2.0
3	L	401	GLY	2.0
2	H	622	ARG	2.0
2	H	443	GLN	2.0
3	L	74	PRO	2.0
3	L	336	SER	2.0
3	I	535	ASP	2.0
3	I	340	MET	2.0
3	C	59	PHE	2.0
3	F	540	LYS	2.0
1	A	134	TYR	2.0
2	K	389	LEU	2.0
3	L	421	ASP	2.0
2	K	695	VAL	2.0
3	L	102	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	345	ARG	2.0
3	L	461	GLU	2.0
2	B	25	THR	2.0
2	H	624	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.