Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 11:44 PM EDT

PDB ID	:	6QPG
Title	:	Influenza A virus Polymerase Heterotrimer A/nt/60/1968(H3N2) in complex with Nanobody NB8205
Authors	:	Fan, H.T.; Keown, J.R.; Fodor, E.; Grimes, J.M.
Deposited on	:	2019-02-13
Resolution	:	3.34 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:

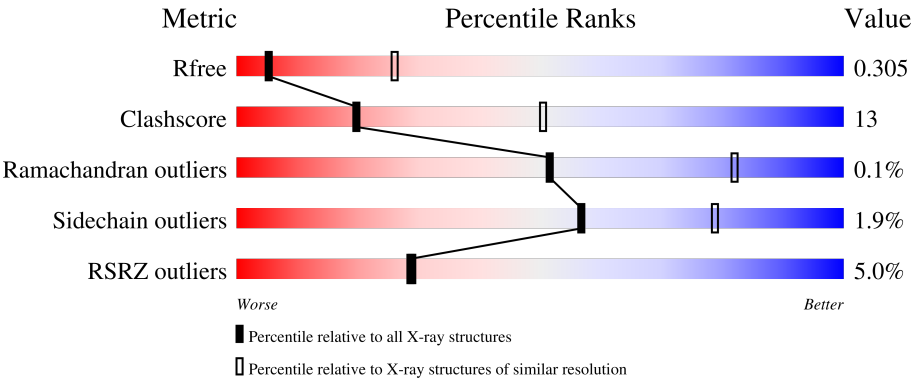
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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 <=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	716	3% 66% 30%
1	D	716	3% 69% 27%
1	G	716	4% 68% 28%
1	J	716	5% 69% 27%
2	B	757	2% 60% 27% 13%

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Mol	Chain	Length	Quality of chain
2	E	757	3% 62% 26% 12%
2	H	757	6% 60% 28% 12%
2	K	757	4% 61% 27% 12%
3	C	765	6% 67% 26% 6%
3	F	765	10% 65% 29% 5%
3	I	765	5% 65% 29% 5%
3	L	765	7% 64% 29% 5%
4	M	134	% 66% 23% 10%
4	N	134	3% 70% 20% 10%
4	O	134	4% 58% 32% 10%
4	P	134	3% 71% 19% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 70549 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	691	Total	C	N	O	S	0	0	0
			5621	3570	952	1059	40			
1	D	695	Total	C	N	O	S	0	0	0
			5652	3586	957	1069	40			
1	G	694	Total	C	N	O	S	0	0	0
			5644	3582	955	1067	40			
1	J	692	Total	C	N	O	S	0	0	0
			5631	3572	953	1066	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	656	Total	C	N	O	S	0	0	0
			5239	3305	903	991	40			
2	E	666	Total	C	N	O	S	0	0	0
			5326	3357	919	1008	42			
2	H	667	Total	C	N	O	S	0	0	0
			5327	3361	916	1009	41			
2	K	664	Total	C	N	O	S	0	0	0
			5303	3342	916	1004	41			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	577	LYS	GLU	conflict	UNP P03432
E	577	LYS	GLU	conflict	UNP P03432
H	577	LYS	GLU	conflict	UNP P03432
K	577	LYS	GLU	conflict	UNP P03432

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	717	Total	C	N	O	S	0	0	0
			5720	3596	1037	1047	40			
3	F	726	Total	C	N	O	S	0	0	0
			5786	3637	1045	1063	41			
3	I	728	Total	C	N	O	S	0	0	0
			5804	3648	1049	1066	41			
3	L	723	Total	C	N	O	S	0	0	0
			5764	3623	1043	1057	41			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLU	-	expression tag	UNP P03429
C	761	ASN	-	expression tag	UNP P03429
C	762	LEU	-	expression tag	UNP P03429
C	763	TYR	-	expression tag	UNP P03429
C	764	PHE	-	expression tag	UNP P03429
C	765	GLN	-	expression tag	UNP P03429
F	760	GLU	-	expression tag	UNP P03429
F	761	ASN	-	expression tag	UNP P03429
F	762	LEU	-	expression tag	UNP P03429
F	763	TYR	-	expression tag	UNP P03429
F	764	PHE	-	expression tag	UNP P03429
F	765	GLN	-	expression tag	UNP P03429
I	760	GLU	-	expression tag	UNP P03429
I	761	ASN	-	expression tag	UNP P03429
I	762	LEU	-	expression tag	UNP P03429
I	763	TYR	-	expression tag	UNP P03429
I	764	PHE	-	expression tag	UNP P03429
I	765	GLN	-	expression tag	UNP P03429
L	760	GLU	-	expression tag	UNP P03429
L	761	ASN	-	expression tag	UNP P03429
L	762	LEU	-	expression tag	UNP P03429
L	763	TYR	-	expression tag	UNP P03429
L	764	PHE	-	expression tag	UNP P03429
L	765	GLN	-	expression tag	UNP P03429

- Molecule 4 is a protein called Nanobody NB8205.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	121	Total	C	N	O	S	0	0	0
			933	581	164	182	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	121	Total	C	N	O	S	0	0	0
			933	581	164	182	6			
4	O	121	Total	C	N	O	S	0	0	0
			933	581	164	182	6			
4	P	121	Total	C	N	O	S	0	0	0
			933	581	164	182	6			

3 Residue-property plots (i)

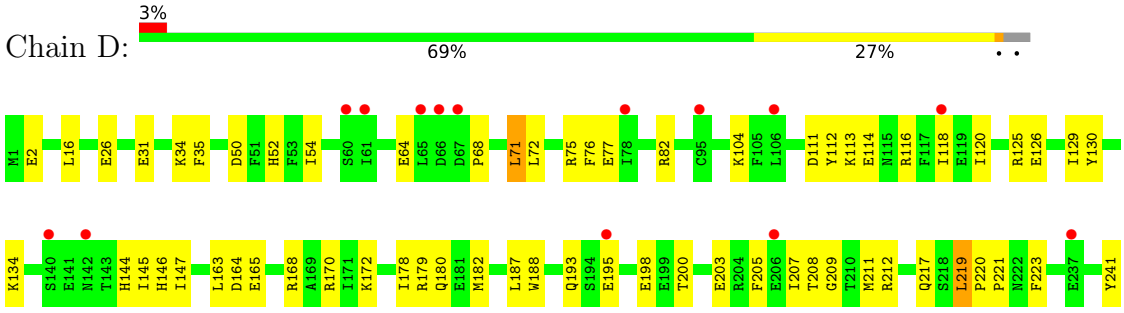
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

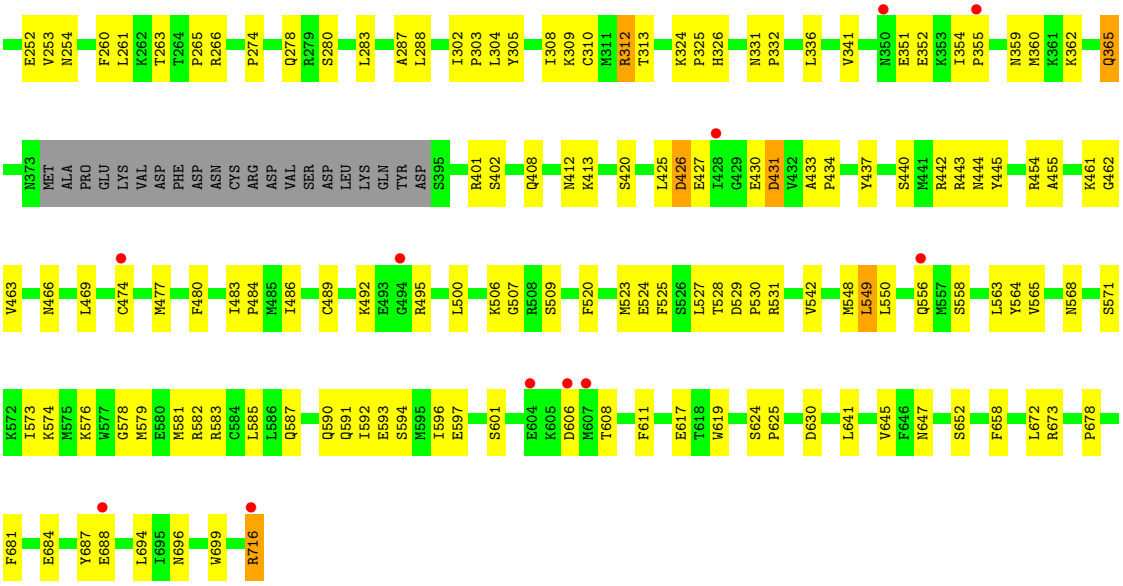
• Molecule 1: Polymerase acidic protein

Chain A:

• Molecule 1: Polymerase acidic protein

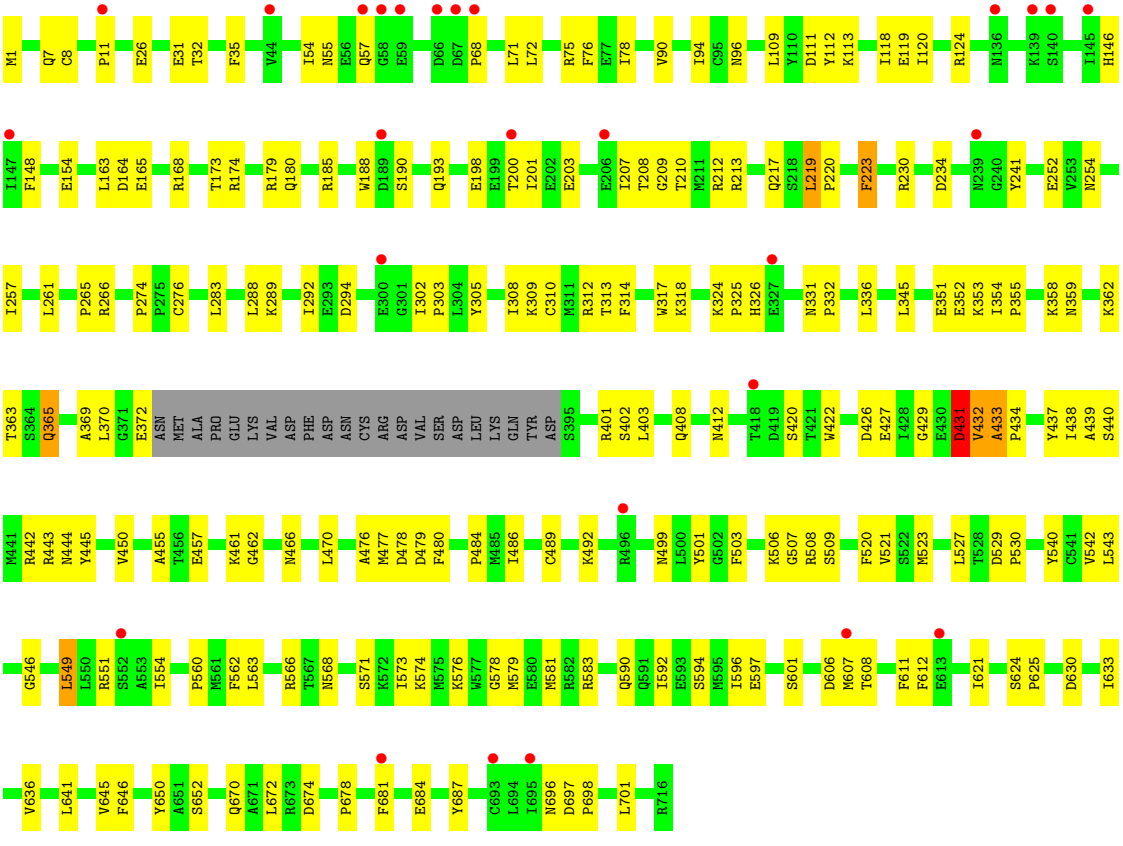
Chain D:





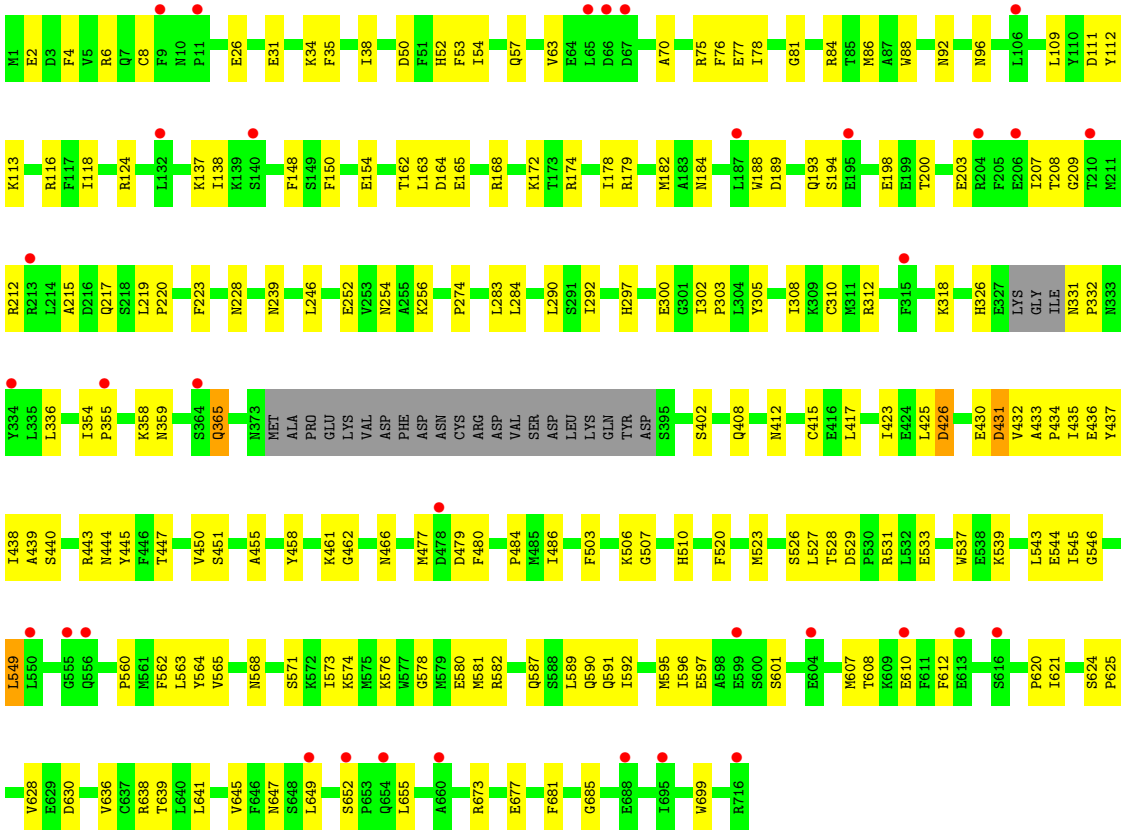
• Molecule 1: Polymerase acidic protein

Chain G:



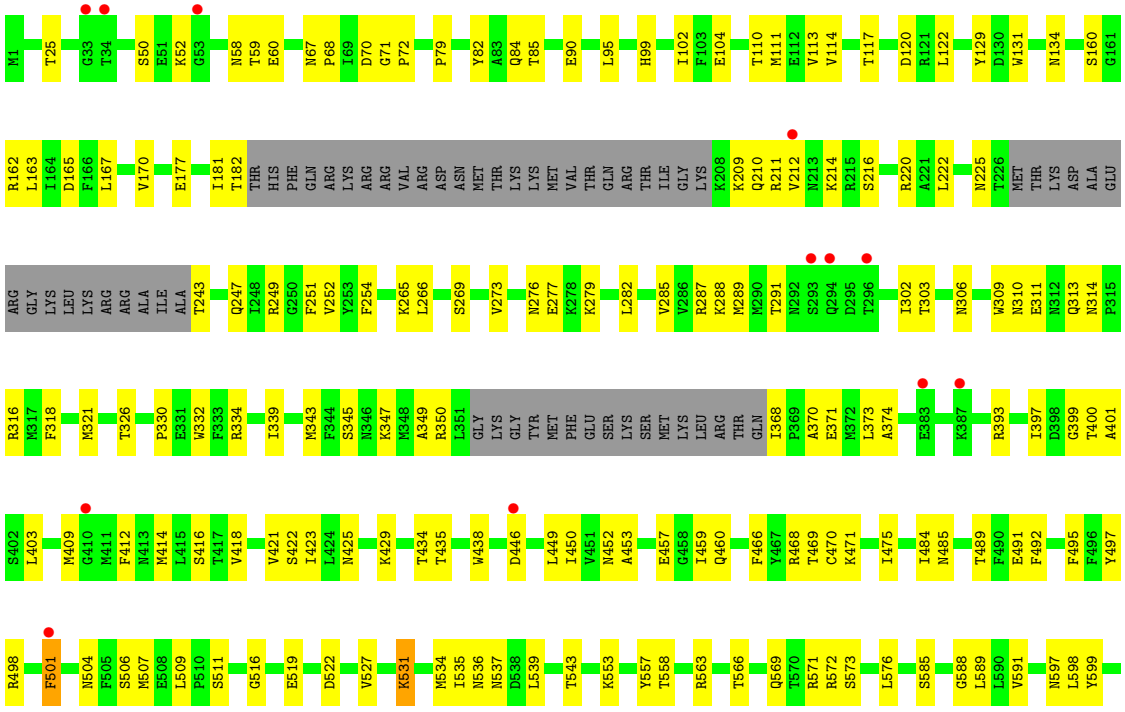
• Molecule 1: Polymerase acidic protein

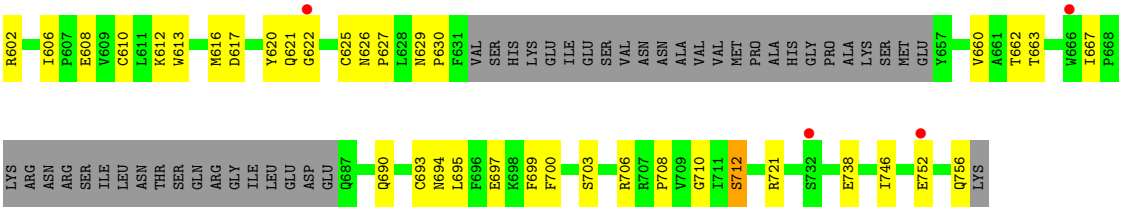
Chain J:



• Molecule 2: RNA-directed RNA polymerase catalytic subunit

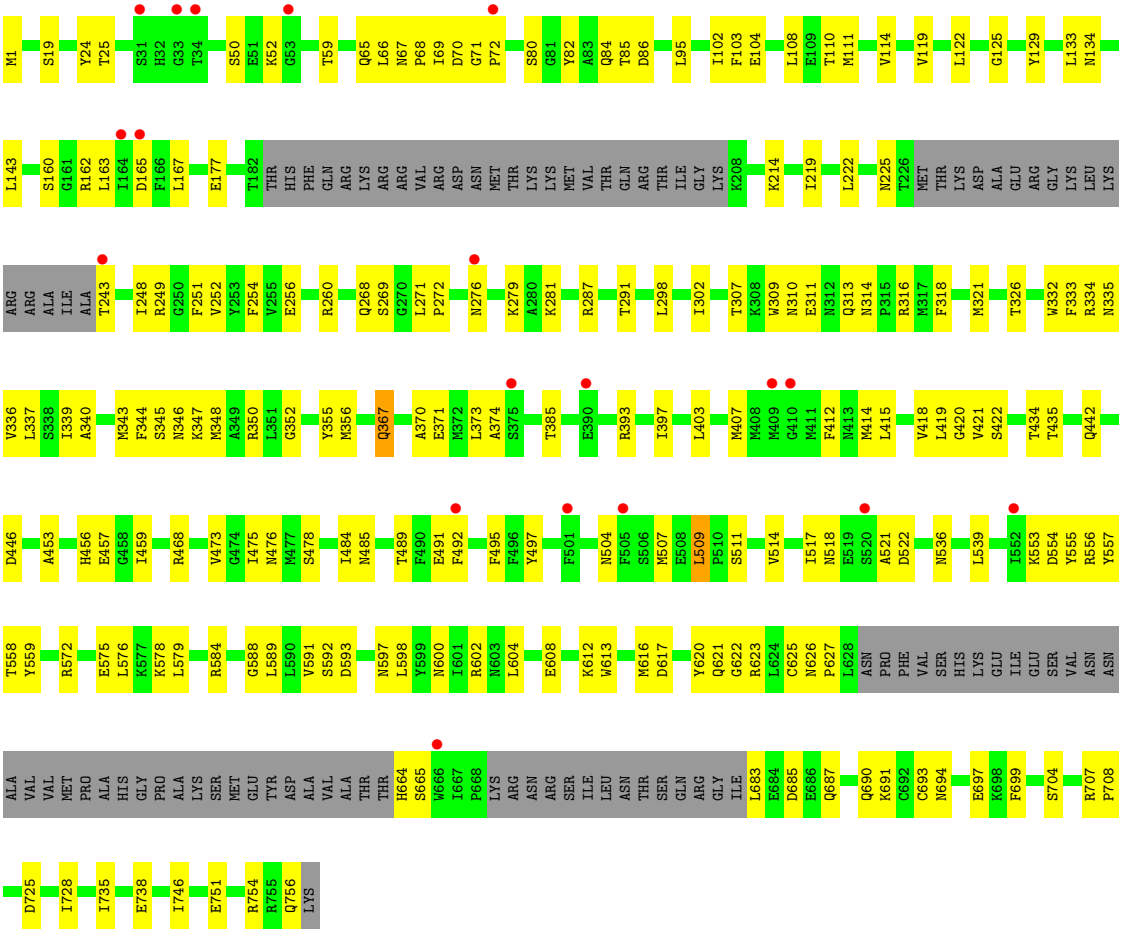
Chain B:





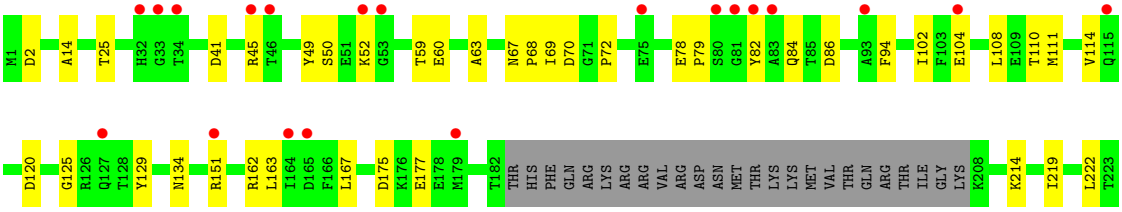
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

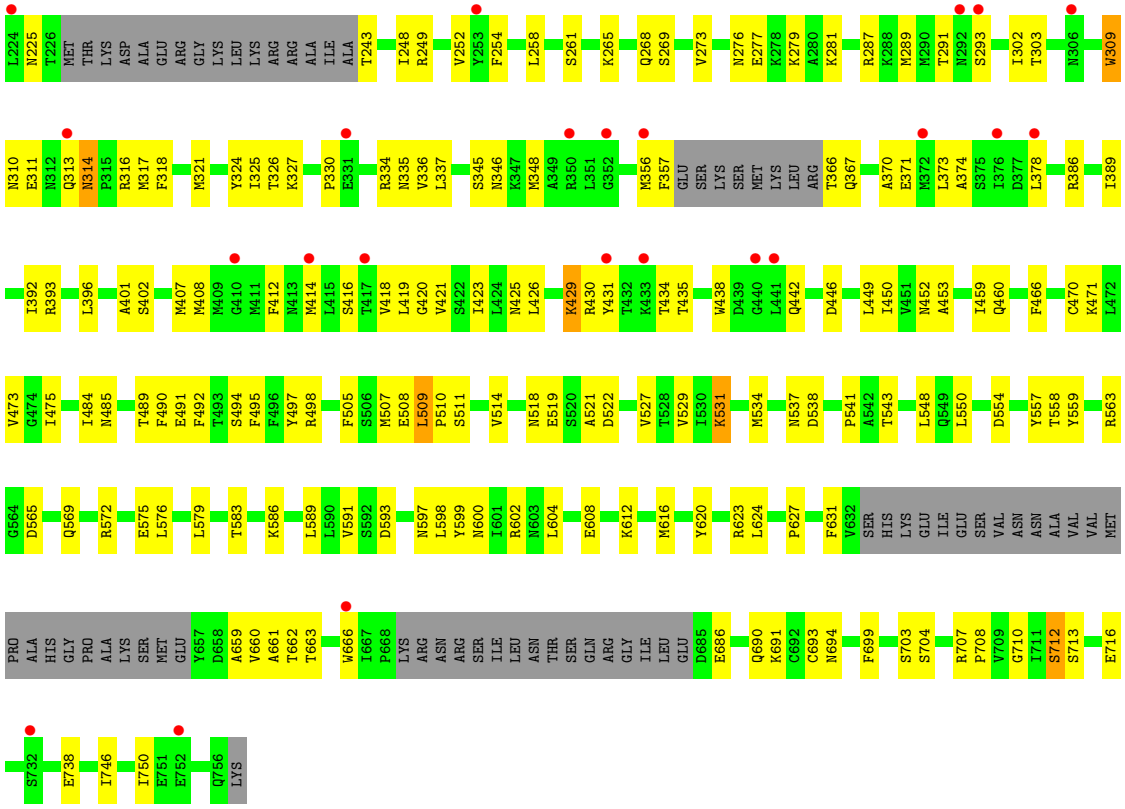
Chain E:



• Molecule 2: RNA-directed RNA polymerase catalytic subunit

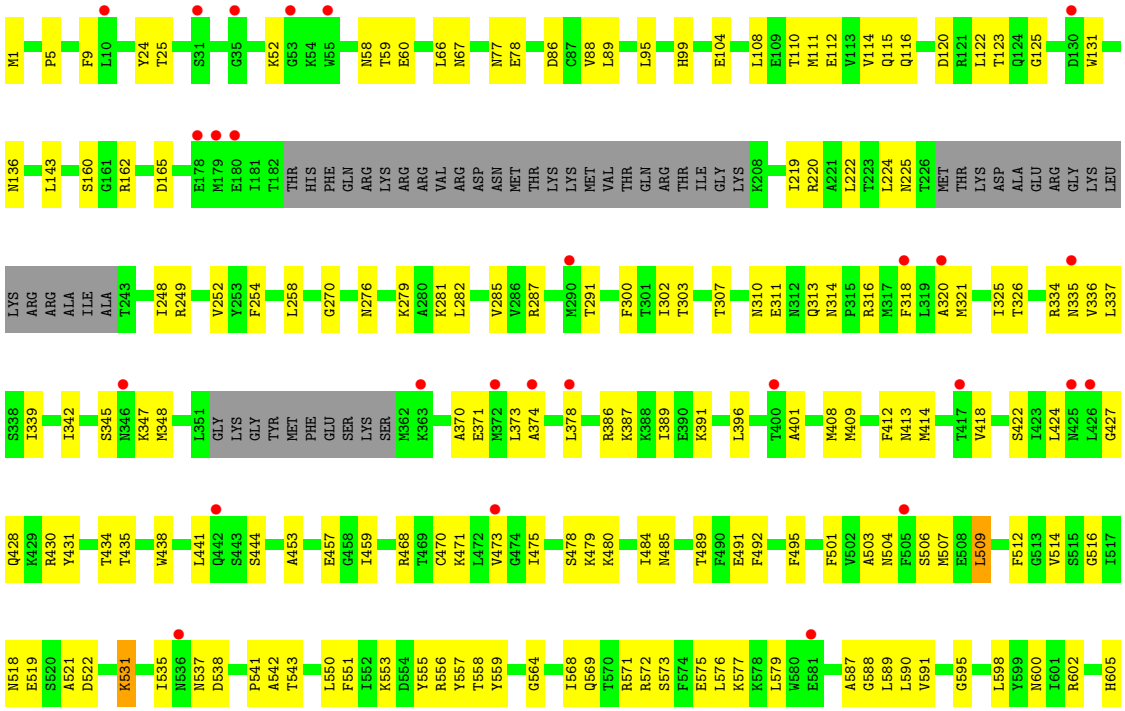
Chain H:

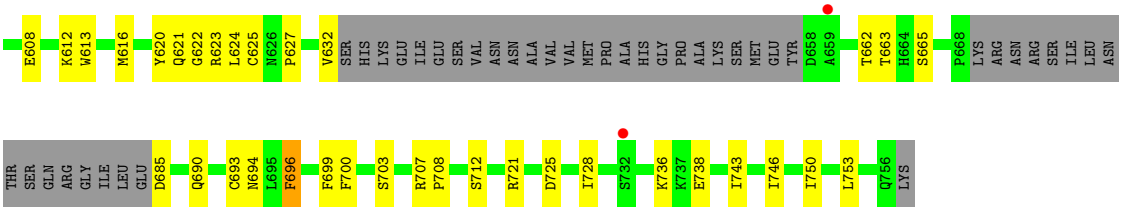




• Molecule 2: RNA-directed RNA polymerase catalytic subunit

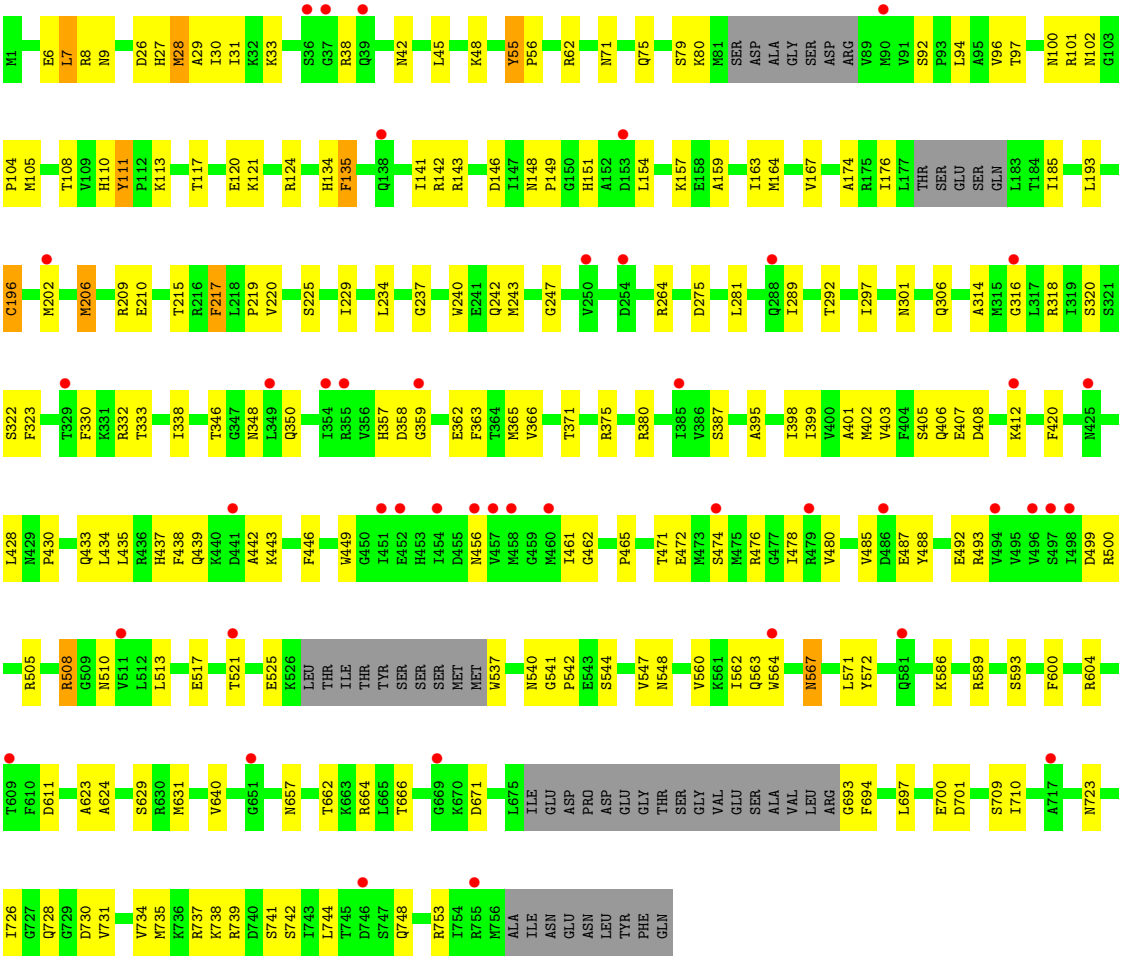
Chain K:





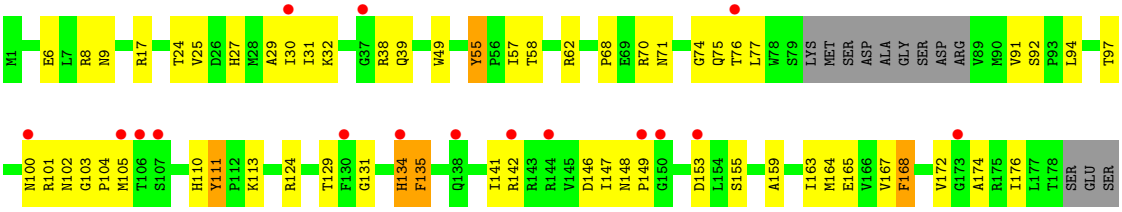
• Molecule 3: Polymerase basic protein 2

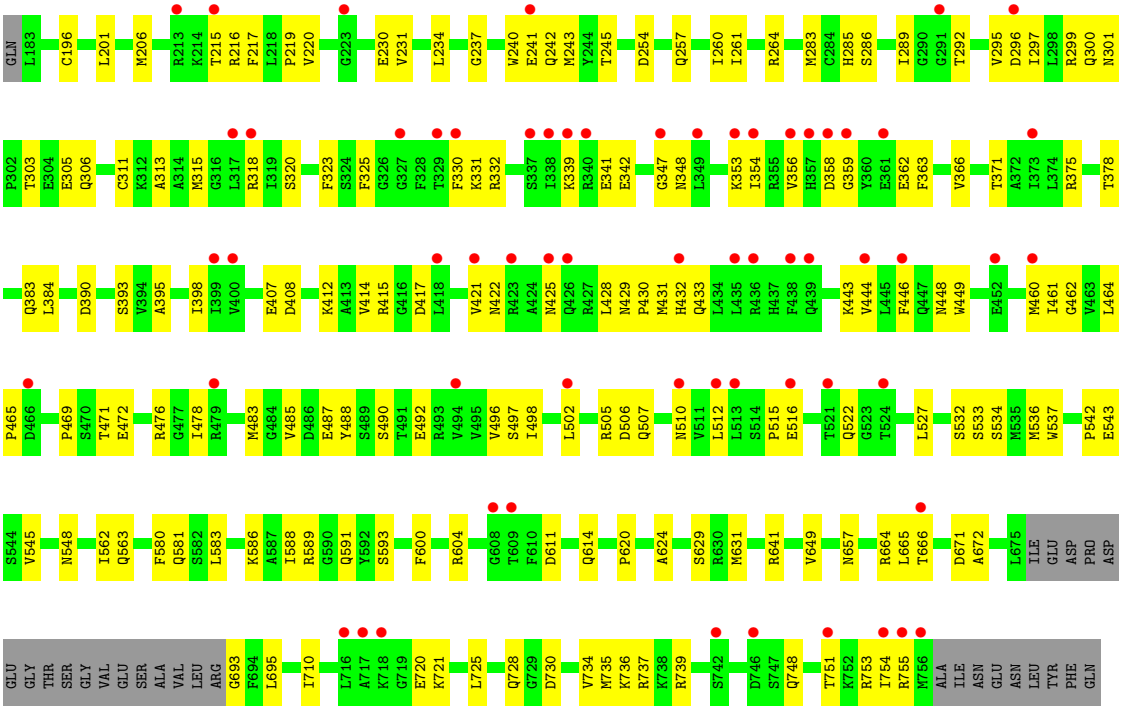
Chain C:



• Molecule 3: Polymerase basic protein 2

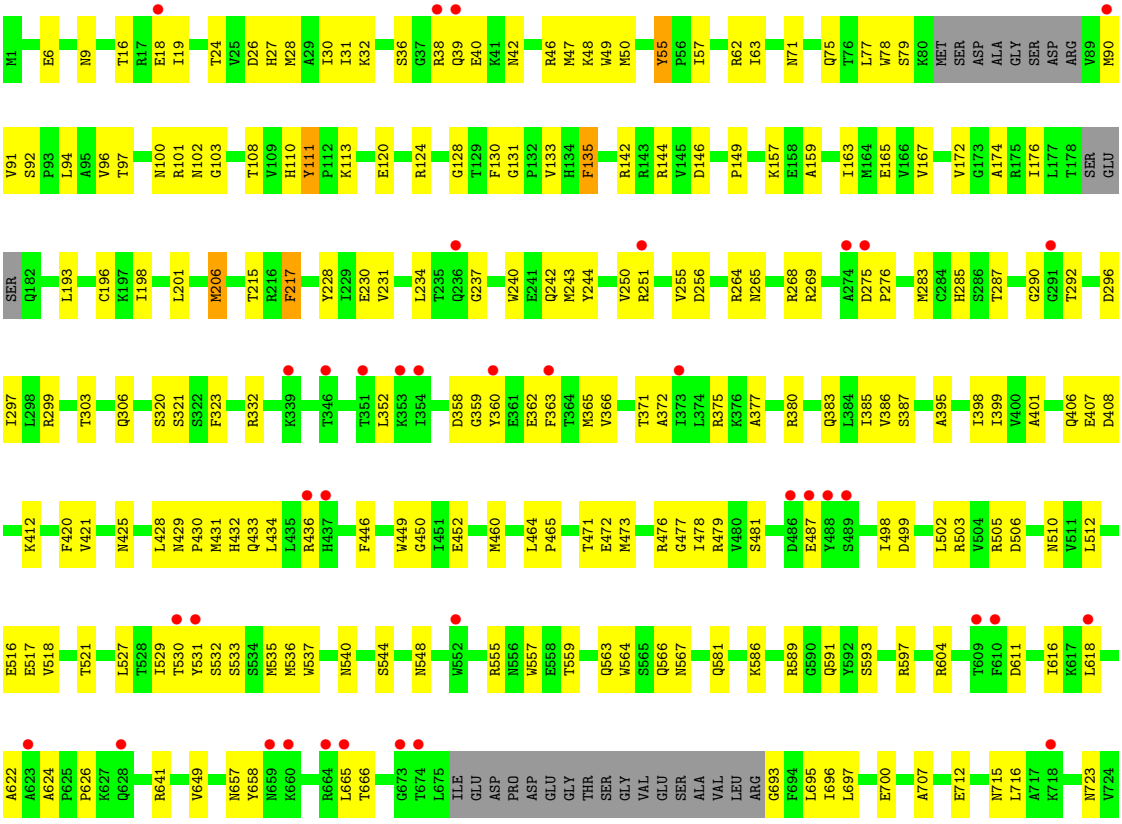
Chain F:

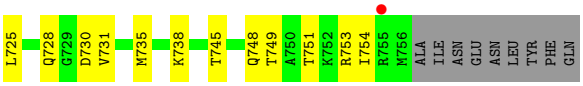




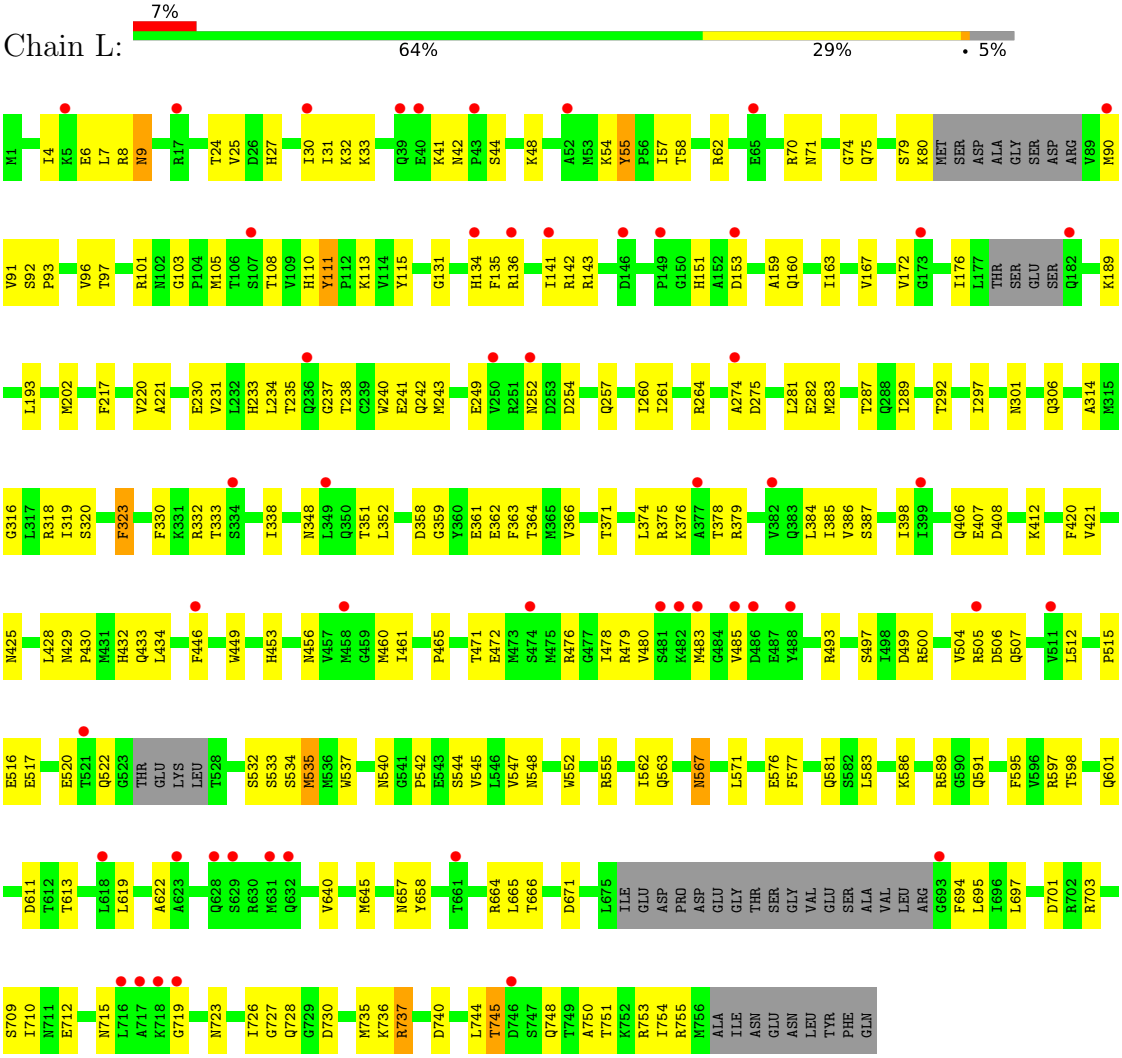
• Molecule 3: Polymerase basic protein 2

Chain I:





• Molecule 3: Polymerase basic protein 2



• Molecule 4: Nanobody NB8205

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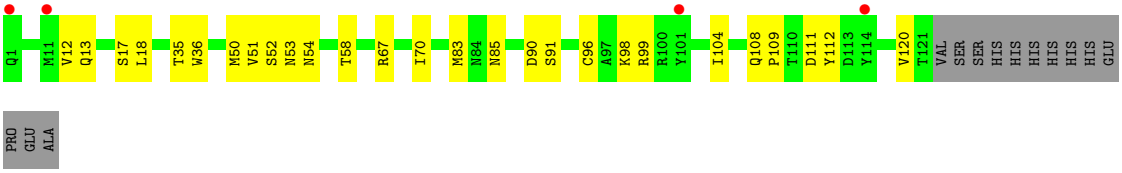
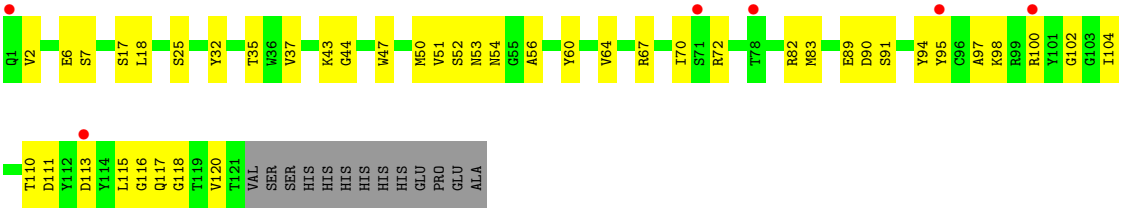
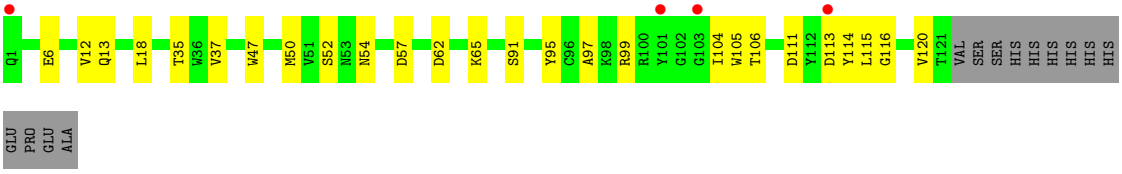


• Molecule 4: Nanobody NB8205



• Molecule 4: Nanobody NB8205



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	335.18Å 192.90Å 235.10Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	234.98 – 3.34 234.98 – 3.34	Depositor EDS
% Data completeness (in resolution range)	41.5 (234.98-3.34) 37.7 (234.98-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.251 , 0.305 0.251 , 0.305	Depositor DCC
R_{free} test set	4533 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 73.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.016 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.017 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.016 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	70549	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/5742	0.46	0/7740
1	D	0.25	0/5773	0.45	1/7783 (0.0%)
1	G	0.25	0/5765	0.46	0/7772
1	J	0.25	0/5751	0.45	0/7753
2	B	0.26	0/5343	0.46	0/7214
2	E	0.26	0/5430	0.45	0/7323
2	H	0.26	0/5433	0.45	0/7334
2	K	0.25	0/5406	0.46	0/7297
3	C	0.25	0/5812	0.47	0/7825
3	F	0.25	0/5880	0.47	0/7921
3	I	0.25	0/5898	0.48	0/7944
3	L	0.25	0/5857	0.48	0/7887
4	M	0.26	0/954	0.52	1/1293 (0.1%)
4	N	0.25	0/954	0.47	0/1293
4	O	0.26	0/954	0.48	0/1293
4	P	0.26	0/954	0.48	0/1293
All	All	0.25	0/71906	0.46	2/96965 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	71	LEU	CA-CB-CG	-6.02	101.45	115.30
4	M	115	LEU	CA-CB-CG	5.42	127.76	115.30

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	5621	0	5563	161	0
1	D	5652	0	5583	146	0
1	G	5644	0	5577	152	0
1	J	5631	0	5555	144	0
2	B	5239	0	5190	155	0
2	E	5326	0	5286	167	0
2	H	5327	0	5270	175	0
2	K	5303	0	5261	166	0
3	C	5720	0	5867	147	0
3	F	5786	0	5931	188	0
3	I	5804	0	5952	174	0
3	L	5764	0	5907	174	0
4	M	933	0	893	22	0
4	N	933	0	893	18	0
4	O	933	0	893	34	0
4	P	933	0	893	16	0
All	All	70549	0	70514	1784	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1784) 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)
3:I:290:GLY:H	3:I:529:ILE:HG12	1.32	0.95
3:F:134:HIS:HE1	3:F:241:GLU:HG2	1.35	0.91
2:B:667:ILE:HG13	3:C:56:PRO:O	1.71	0.90
1:A:714:ALA:O	1:A:716:ARG:NH1	2.07	0.88
1:A:353:LYS:HB3	1:G:353:LYS:HB3	1.57	0.87
3:L:264:ARG:HH12	3:L:520:GLU:HG2	1.44	0.83
2:E:177:GLU:HA	2:E:214:LYS:HB2	1.62	0.82
3:F:134:HIS:HE1	3:F:241:GLU:CG	1.92	0.81
1:J:432:VAL:HG21	2:K:602:ARG:HD3	1.62	0.81
3:F:134:HIS:CE1	3:F:241:GLU:HG2	2.16	0.81
3:F:283:MET:HG2	3:F:533:SER:HB2	1.63	0.80
2:H:623:ARG:HD3	3:I:103:GLY:H	1.45	0.80
3:C:275:ASP:HA	3:C:500:ARG:HH11	1.45	0.80
1:A:26:GLU:HG3	1:A:31:GLU:HG3	1.63	0.79
3:F:542:PRO:HB3	3:F:583:LEU:HD21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:ASN:HD21	3:L:275:ASP:HB3	1.45	0.79
3:L:534:SER:HB3	3:L:576:GLU:HA	1.65	0.78
1:A:219:LEU:HD22	1:A:223:PHE:HB2	1.65	0.78
3:I:275:ASP:H	1:J:96:ASN:HD21	1.29	0.78
2:E:453:ALA:HB3	2:E:459:ILE:HG12	1.64	0.77
3:F:286:SER:HB2	3:F:532:SER:HB2	1.63	0.77
3:C:176:ILE:HG13	3:C:693:GLY:HA3	1.65	0.77
2:B:302:ILE:HG22	2:B:484:ILE:HG23	1.67	0.76
1:A:356:ARG:NH2	1:G:351:GLU:O	2.19	0.76
1:G:266:ARG:NH1	1:G:684:GLU:OE2	2.18	0.76
2:E:309:TRP:CZ3	2:E:475:ILE:HG12	2.20	0.76
1:A:560:PRO:HB2	1:A:562:PHE:HE1	1.51	0.75
3:L:701:ASP:O	3:L:723:ASN:ND2	2.19	0.75
3:C:701:ASP:O	3:C:723:ASN:ND2	2.19	0.75
3:F:323:PHE:HB3	3:F:330:PHE:HB2	1.69	0.75
1:D:408:GLN:HE21	1:D:412:ASN:HD21	1.34	0.75
1:G:560:PRO:HB2	1:G:562:PHE:HE1	1.52	0.75
4:M:37:VAL:O	4:M:95:TYR:HB2	1.86	0.75
2:B:269:SER:HB2	2:B:421:VAL:HG21	1.68	0.74
4:P:37:VAL:O	4:P:95:TYR:HB2	1.87	0.74
2:B:453:ALA:HB3	2:B:459:ILE:HG12	1.68	0.74
2:B:708:PRO:HB3	3:C:728:GLN:HG3	1.69	0.74
1:G:219:LEU:HD22	1:G:223:PHE:HB2	1.70	0.73
2:K:302:ILE:HG22	2:K:484:ILE:HG23	1.71	0.73
2:E:302:ILE:HG22	2:E:484:ILE:HG23	1.70	0.73
1:G:408:GLN:HE21	1:G:412:ASN:HD21	1.36	0.73
1:D:219:LEU:HD22	1:D:223:PHE:HB2	1.68	0.73
1:G:266:ARG:O	1:G:687:TYR:OH	2.06	0.73
2:K:120:ASP:HB3	3:L:33:LYS:HD2	1.70	0.73
2:B:485:ASN:ND2	2:B:489:THR:O	2.21	0.73
3:F:147:ILE:HD11	3:F:216:ARG:HE	1.53	0.73
3:F:176:ILE:HG13	3:F:693:GLY:HA3	1.69	0.73
1:G:583:ARG:HH22	2:H:511:SER:HA	1.53	0.73
2:H:518:ASN:HA	2:H:666:TRP:CH2	2.24	0.72
1:J:2:GLU:OE1	3:L:318:ARG:NH2	2.22	0.72
3:F:581:GLN:HG2	3:F:589:ARG:HD3	1.69	0.72
2:K:316:ARG:NH2	2:K:345:SER:OG	2.23	0.72
2:B:397:ILE:O	2:B:397:ILE:HD12	1.88	0.72
2:H:356:MET:HA	2:H:367:GLN:HA	1.71	0.72
1:G:302:ILE:HD12	1:G:303:PRO:HD2	1.71	0.72
1:J:86:MET:SD	3:L:755:ARG:NH1	2.62	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:626:ASN:ND2	3:F:104:PRO:O	2.22	0.72
3:C:323:PHE:HB3	3:C:330:PHE:HB2	1.72	0.71
2:B:99:HIS:NE2	3:C:333:THR:O	2.23	0.71
3:F:422:ASN:ND2	3:F:516:GLU:OE2	2.23	0.71
1:G:578:GLY:HA2	1:G:581:MET:HG3	1.72	0.71
1:D:221:PRO:HD3	2:E:69:ILE:HG23	1.71	0.71
2:E:397:ILE:O	2:E:397:ILE:HD12	1.89	0.71
1:G:408:GLN:O	1:G:412:ASN:ND2	2.21	0.71
1:G:420:SER:HB3	1:G:489:CYS:HB2	1.71	0.71
3:I:420:PHE:O	3:I:433:GLN:NE2	2.23	0.71
4:O:115:LEU:HD22	4:O:116:GLY:H	1.54	0.71
1:G:370:LEU:HD13	1:G:507:GLY:HA2	1.72	0.71
3:I:697:LEU:HD11	3:I:735:MET:HB2	1.71	0.71
1:G:672:LEU:HD23	1:G:678:PRO:HD2	1.72	0.71
2:B:489:THR:HA	2:B:497:TYR:O	1.91	0.71
3:I:165:GLU:HG2	3:I:172:VAL:HG21	1.73	0.71
1:J:576:LYS:NZ	3:L:42:ASN:OD1	2.22	0.70
2:E:281:LYS:HE3	3:F:142:ARG:HH12	1.57	0.70
1:A:359:ASN:ND2	1:A:479:ASP:OD2	2.24	0.70
1:D:302:ILE:HD12	1:D:303:PRO:HD2	1.72	0.70
2:E:473:VAL:HG23	2:E:475:ILE:HG13	1.72	0.70
3:C:55:TYR:HD1	3:C:92:SER:HB2	1.55	0.70
2:E:492:PHE:O	2:E:495:PHE:HB2	1.92	0.69
2:E:370:ALA:HA	2:E:373:LEU:HD13	1.74	0.69
3:C:366:VAL:HA	3:C:371:THR:HG22	1.74	0.69
2:H:219:ILE:HG23	2:H:348:MET:HG3	1.75	0.69
3:F:147:ILE:O	3:F:148:ASN:ND2	2.25	0.69
2:H:291:THR:OG1	3:I:383:GLN:OE1	2.08	0.69
1:D:278:GLN:OE1	1:D:280:SER:OG	2.11	0.69
2:K:485:ASN:ND2	2:K:489:THR:O	2.24	0.69
1:A:606:ASP:HB2	3:C:135:PHE:CG	2.28	0.69
1:D:573:ILE:HA	1:D:576:LYS:HG2	1.75	0.69
2:H:302:ILE:HG22	2:H:484:ILE:HG23	1.73	0.69
2:K:88:VAL:HG22	2:K:473:VAL:HG12	1.75	0.69
3:F:55:TYR:HD1	3:F:92:SER:HB2	1.58	0.69
2:H:378:LEU:HD23	2:H:386:ARG:HG3	1.74	0.69
1:G:26:GLU:HG3	1:G:31:GLU:HG3	1.75	0.68
3:L:420:PHE:O	3:L:433:GLN:NE2	2.26	0.68
1:A:578:GLY:HA2	1:A:581:MET:HG3	1.75	0.68
1:A:283:LEU:O	1:A:461:LYS:NZ	2.25	0.68
2:E:316:ARG:NH2	2:E:345:SER:OG	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:GLN:HE21	1:G:203:GLU:HG3	1.59	0.68
2:H:426:LEU:HA	2:H:431:TYR:HD2	1.58	0.68
3:I:398:ILE:HD11	3:I:478:ILE:HD11	1.74	0.68
3:I:593:SER:HB2	3:I:624:ALA:HB3	1.74	0.68
1:J:8:CYS:O	1:J:174:ARG:NH2	2.25	0.68
2:E:309:TRP:HZ3	2:E:475:ILE:HG12	1.59	0.68
1:A:408:GLN:HE21	1:A:412:ASN:HD21	1.39	0.68
2:B:519:GLU:HG2	2:B:662:THR:HG22	1.76	0.67
2:E:572:ARG:HA	3:F:94:LEU:HD12	1.75	0.67
2:K:620:TYR:O	2:K:624:LEU:HB2	1.93	0.67
3:L:398:ILE:HD11	3:L:478:ILE:HD11	1.76	0.67
2:E:225:ASN:O	2:E:243:THR:N	2.27	0.67
3:F:614:GLN:NE2	3:F:649:VAL:O	2.28	0.67
3:C:117:THR:OG1	3:C:209:ARG:NH1	2.28	0.67
1:J:523:MET:HB3	1:J:563:LEU:HD11	1.77	0.67
1:A:523:MET:HB3	1:A:563:LEU:HD11	1.76	0.67
2:H:453:ALA:HB3	2:H:459:ILE:HG12	1.75	0.67
2:K:623:ARG:HD3	3:L:103:GLY:H	1.58	0.67
2:K:509:LEU:HD23	2:K:509:LEU:H	1.60	0.67
2:H:593:ASP:OD2	3:I:100:ASN:ND2	2.28	0.67
1:A:573:ILE:HA	1:A:576:LYS:HG2	1.77	0.66
2:E:313:GLN:HB3	2:E:318:PHE:HE2	1.60	0.66
3:F:588:ILE:HD12	3:F:588:ILE:N	2.09	0.66
1:J:408:GLN:O	1:J:412:ASN:ND2	2.26	0.66
2:H:374:ALA:O	2:H:393:ARG:NH2	2.28	0.66
1:J:292:ILE:HD11	1:J:310:CYS:SG	2.35	0.66
2:K:326:THR:HB	2:K:334:ARG:HG2	1.74	0.66
2:E:613:TRP:O	2:E:621:GLN:NE2	2.28	0.66
2:B:287:ARG:O	2:B:291:THR:OG1	2.14	0.66
1:D:266:ARG:NH1	1:D:684:GLU:OE2	2.28	0.66
3:L:141:ILE:HB	3:L:220:VAL:O	1.94	0.66
1:A:408:GLN:O	1:A:412:ASN:ND2	2.24	0.66
2:B:309:TRP:HZ2	2:B:416:SER:HB3	1.59	0.66
2:E:608:GLU:OE2	2:E:612:LYS:NZ	2.29	0.66
1:A:302:ILE:HD12	1:A:303:PRO:HD2	1.78	0.66
2:E:326:THR:HB	2:E:334:ARG:HG2	1.77	0.66
2:E:489:THR:HA	2:E:497:TYR:O	1.94	0.66
1:A:551:ARG:NE	4:O:89:GLU:OE1	2.28	0.66
1:G:198:GLU:HG2	1:G:200:THR:HG22	1.77	0.66
3:L:563:GLN:HG2	3:L:571:LEU:HB2	1.78	0.66
3:L:712:GLU:HB2	3:L:715:ASN:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:HB3	1:A:75:ARG:HE	1.61	0.66
3:F:242:GLN:NE2	3:F:243:MET:O	2.29	0.66
2:H:310:ASN:ND2	2:H:407:MET:O	2.29	0.65
3:I:657:ASN:HB3	3:I:666:THR:HB	1.78	0.65
2:B:599:TYR:OH	2:B:606:ILE:O	2.12	0.65
3:C:71:ASN:ND2	3:C:75:GLN:OE1	2.29	0.65
3:F:71:ASN:ND2	3:F:75:GLN:OE1	2.30	0.65
2:K:613:TRP:O	2:K:621:GLN:NE2	2.29	0.65
1:A:67:ASP:OD2	1:A:69:ASN:ND2	2.29	0.65
2:E:420:GLY:HA3	2:E:442:GLN:HG2	1.77	0.65
3:L:697:LEU:HD11	3:L:735:MET:HB2	1.79	0.65
1:D:408:GLN:O	1:D:412:ASN:ND2	2.25	0.65
1:G:75:ARG:NH1	1:G:111:ASP:OD2	2.30	0.65
2:H:608:GLU:OE2	2:H:612:LYS:NZ	2.25	0.65
1:J:523:MET:HG2	1:J:565:VAL:HG22	1.78	0.65
2:K:99:HIS:NE2	3:L:333:THR:O	2.30	0.65
3:C:593:SER:HB2	3:C:624:ALA:HB3	1.79	0.65
2:K:690:GLN:O	2:K:694:ASN:ND2	2.26	0.65
2:K:712:SER:OG	3:L:730:ASP:HB3	1.97	0.65
3:L:71:ASN:ND2	3:L:75:GLN:OE1	2.29	0.65
2:E:593:ASP:OD2	3:F:100:ASN:ND2	2.30	0.65
3:F:142:ARG:HB3	3:F:217:PHE:HE1	1.62	0.65
1:J:573:ILE:HA	1:J:576:LYS:HG2	1.78	0.65
2:B:95:LEU:HD12	2:B:422:SER:HB3	1.77	0.64
1:J:435:ILE:HD11	3:L:234:LEU:HD23	1.78	0.64
2:K:122:LEU:HD11	2:K:249:ARG:HB3	1.79	0.64
2:K:564:GLY:HA2	2:K:577:LYS:HG2	1.79	0.64
3:C:387:SER:HB3	3:C:485:VAL:HG23	1.78	0.64
3:I:429:ASN:OD1	3:I:432:HIS:ND1	2.30	0.64
2:K:282:LEU:HB2	2:K:501:PHE:HZ	1.63	0.64
4:O:52:SER:O	4:O:72:ARG:NH1	2.29	0.64
3:I:366:VAL:HA	3:I:371:THR:HG22	1.80	0.64
3:F:593:SER:HB2	3:F:624:ALA:HB3	1.79	0.64
1:G:363:THR:HB	1:G:365:GLN:OE1	1.97	0.64
4:M:115:LEU:HD22	4:M:116:GLY:H	1.62	0.64
3:F:545:VAL:HG11	3:F:583:LEU:HD22	1.80	0.64
3:C:700:GLU:HB2	3:C:731:VAL:HB	1.78	0.64
1:J:326:HIS:O	1:J:326:HIS:ND1	2.29	0.64
2:K:78:GLU:O	2:K:471:LYS:NZ	2.31	0.64
3:L:535:MET:N	3:L:535:MET:SD	2.71	0.64
3:C:697:LEU:HD11	3:C:735:MET:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:588:ILE:HD12	3:F:588:ILE:H	1.62	0.64
3:F:296:ASP:OD1	3:F:299:ARG:NH1	2.31	0.64
2:H:279:LYS:NZ	2:H:538:ASP:OD2	2.24	0.64
3:I:700:GLU:HB2	3:I:731:VAL:HB	1.79	0.64
1:J:283:LEU:O	1:J:461:LYS:NZ	2.31	0.64
1:A:2:GLU:OE1	3:C:318:ARG:NH2	2.23	0.63
2:B:690:GLN:O	2:B:694:ASN:ND2	2.26	0.63
1:J:450:VAL:HG13	1:J:641:LEU:HD22	1.79	0.63
2:K:576:LEU:HD12	3:L:97:THR:HG21	1.80	0.63
3:L:429:ASN:OD1	3:L:432:HIS:ND1	2.31	0.63
3:L:581:GLN:HG2	3:L:589:ARG:HD3	1.80	0.63
1:A:193:GLN:NE2	1:A:203:GLU:OE2	2.32	0.63
1:A:455:ALA:HB1	1:A:645:VAL:HG21	1.79	0.63
3:I:506:ASP:OD1	3:I:510:ASN:N	2.27	0.63
3:C:572:TYR:HB3	3:C:623:ALA:HA	1.79	0.63
1:J:203:GLU:OE2	2:K:162:ARG:NH2	2.30	0.63
2:B:752:GLU:O	2:B:756:GLN:NE2	2.32	0.63
2:E:291:THR:O	3:F:383:GLN:NE2	2.32	0.63
3:F:543:GLU:OE2	3:F:641:ARG:NE	2.30	0.63
1:G:455:ALA:HB1	1:G:645:VAL:HG21	1.80	0.63
1:D:118:ILE:HG12	1:D:144:HIS:HB3	1.81	0.63
3:F:55:TYR:OH	3:F:76:THR:HB	1.98	0.63
3:L:362:GLU:HG3	3:L:375:ARG:HG2	1.80	0.63
1:A:193:GLN:OE1	1:A:193:GLN:N	2.32	0.63
1:A:590:GLN:HB3	2:B:543:THR:HG21	1.79	0.63
1:J:300:GLU:HB2	2:K:571:ARG:HH21	1.64	0.63
3:L:499:ASP:OD2	3:L:505:ARG:NH2	2.31	0.63
1:G:462:GLY:O	1:G:466:ASN:ND2	2.30	0.63
2:K:453:ALA:HB3	2:K:459:ILE:HG12	1.80	0.63
3:F:443:LYS:HA	3:F:446:PHE:HD2	1.64	0.62
3:I:532:SER:O	3:I:555:ARG:NH1	2.31	0.62
1:A:116:ARG:NH1	1:A:162:THR:OG1	2.32	0.62
2:E:665:SER:OG	3:F:58:THR:O	2.16	0.62
3:F:358:ASP:OD1	3:F:359:GLY:N	2.32	0.62
2:H:309:TRP:HZ2	2:H:416:SER:HB3	1.65	0.62
1:J:318:LYS:NZ	1:J:544:GLU:OE2	2.31	0.62
2:B:282:LEU:HB2	2:B:501:PHE:HZ	1.64	0.62
2:B:371:GLU:OE1	2:B:371:GLU:N	2.32	0.62
2:E:509:LEU:HD23	2:E:509:LEU:H	1.64	0.62
1:G:365:GLN:CD	1:G:365:GLN:H	2.02	0.62
2:H:326:THR:HB	2:H:334:ARG:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:572:ARG:HA	3:I:94:LEU:HD12	1.81	0.62
2:B:746:ILE:HG23	3:C:8:ARG:HD3	1.82	0.62
1:G:427:GLU:HA	4:O:56:ALA:HB1	1.80	0.62
2:H:509:LEU:HD23	2:H:509:LEU:H	1.64	0.62
2:K:222:LEU:HB3	2:K:347:LYS:HA	1.82	0.62
3:L:597:ARG:NH2	3:L:622:ALA:O	2.30	0.62
1:A:75:ARG:NH1	1:A:111:ASP:OD2	2.32	0.62
1:G:429:GLY:O	4:O:54:ASN:ND2	2.33	0.62
1:A:674:ASP:OD2	2:B:498:ARG:NH2	2.32	0.62
3:F:407:GLU:OE1	3:F:476:ARG:NH2	2.25	0.62
1:G:442:ARG:HE	1:G:608:THR:HG23	1.65	0.62
2:H:660:VAL:HG23	2:H:661:ALA:H	1.64	0.62
1:J:647:ASN:OD1	1:J:699:TRP:NE1	2.29	0.62
2:B:700:PHE:O	2:B:703:SER:OG	2.16	0.62
3:F:341:GLU:HA	3:F:354:ILE:O	2.00	0.62
3:F:586:LYS:HG2	3:F:589:ARG:HH21	1.64	0.62
1:G:173:THR:OG1	3:I:696:ILE:N	2.28	0.62
1:G:530:PRO:HG3	1:G:542:VAL:HG11	1.82	0.62
3:I:296:ASP:OD1	3:I:299:ARG:NH1	2.31	0.62
1:A:198:GLU:HG2	1:A:200:THR:HG22	1.82	0.62
1:G:606:ASP:HB2	3:I:135:PHE:CG	2.35	0.62
4:P:115:LEU:HD22	4:P:116:GLY:H	1.64	0.62
1:G:573:ILE:HA	1:G:576:LYS:HG2	1.82	0.62
3:I:124:ARG:HH12	3:I:149:PRO:HG3	1.65	0.62
1:J:189:ASP:HA	2:K:162:ARG:HH12	1.65	0.62
1:D:31:GLU:OE1	1:D:200:THR:OG1	2.18	0.62
2:H:485:ASN:ND2	2:H:489:THR:O	2.28	0.61
1:D:198:GLU:HG2	1:D:200:THR:HG22	1.82	0.61
1:J:198:GLU:HG2	1:J:200:THR:HG22	1.81	0.61
1:G:432:VAL:HG21	2:H:602:ARG:HD3	1.81	0.61
1:G:506:LYS:NZ	1:G:507:GLY:O	2.28	0.61
1:J:193:GLN:OE1	1:J:193:GLN:N	2.33	0.61
3:C:358:ASP:OD1	3:C:359:GLY:N	2.33	0.61
1:D:506:LYS:NZ	1:D:507:GLY:O	2.28	0.61
3:F:165:GLU:HG2	3:F:172:VAL:HG21	1.83	0.61
2:H:129:TYR:OH	2:H:134:ASN:OD1	2.13	0.61
2:H:507:MET:SD	2:H:537:ASN:ND2	2.73	0.61
1:A:506:LYS:NZ	1:A:507:GLY:O	2.29	0.61
1:D:77:GLU:OE2	3:F:753:ARG:NH2	2.34	0.61
2:E:276:ASN:O	2:E:279:LYS:HB2	2.00	0.61
2:H:313:GLN:HB3	2:H:318:PHE:HE2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:666:TRP:NE1	3:I:47:MET:SD	2.74	0.61
2:K:370:ALA:HA	2:K:373:LEU:HD13	1.83	0.61
2:E:108:LEU:HA	2:E:111:MET:HE2	1.82	0.61
3:I:176:ILE:HG13	3:I:693:GLY:HA3	1.83	0.61
1:J:219:LEU:HD23	1:J:223:PHE:HB2	1.82	0.61
2:K:279:LYS:HE3	2:K:503:ALA:HB2	1.81	0.61
2:E:287:ARG:NH1	3:F:460:MET:SD	2.73	0.61
1:G:11:PRO:HG2	3:I:285:HIS:NE2	2.16	0.61
1:G:324:LYS:NZ	1:G:325:PRO:O	2.28	0.61
2:H:225:ASN:O	2:H:243:THR:N	2.34	0.61
2:H:289:MET:HB3	2:H:452:ASN:HD21	1.66	0.61
3:I:250:VAL:HG12	3:I:251:ARG:H	1.65	0.61
1:J:77:GLU:OE2	3:L:753:ARG:NH2	2.33	0.61
2:K:131:TRP:O	2:K:220:ARG:NH1	2.34	0.61
2:K:492:PHE:O	2:K:495:PHE:HB2	2.01	0.61
2:E:485:ASN:ND2	2:E:489:THR:O	2.25	0.60
2:H:311:GLU:N	2:H:311:GLU:OE1	2.33	0.60
3:I:618:LEU:HD21	3:I:649:VAL:HG12	1.81	0.60
3:I:142:ARG:HB3	3:I:217:PHE:HE1	1.66	0.60
3:L:358:ASP:OD1	3:L:359:GLY:N	2.34	0.60
1:D:193:GLN:OE1	1:D:193:GLN:N	2.33	0.60
3:I:751:THR:HA	3:I:754:ILE:HG22	1.83	0.60
2:K:591:VAL:HG23	2:K:612:LYS:HZ1	1.66	0.60
1:A:543:LEU:HD12	1:A:563:LEU:HD23	1.84	0.60
3:F:657:ASN:HB3	3:F:666:THR:HB	1.83	0.60
1:G:234:ASP:OD1	2:H:334:ARG:NH2	2.35	0.60
3:L:260:ILE:O	3:L:264:ARG:HG2	2.02	0.60
2:B:313:GLN:HB3	2:B:318:PHE:HE2	1.67	0.60
2:B:370:ALA:HA	2:B:373:LEU:HD13	1.83	0.60
2:B:572:ARG:NH2	3:C:97:THR:OG1	2.29	0.60
2:B:708:PRO:HA	3:C:728:GLN:HE21	1.66	0.60
3:C:242:GLN:NE2	3:C:243:MET:O	2.35	0.60
1:D:484:PRO:HB2	1:D:486:ILE:HG13	1.84	0.60
1:A:326:HIS:O	1:A:326:HIS:ND1	2.32	0.60
2:E:95:LEU:HD12	2:E:422:SER:HB3	1.83	0.60
2:E:514:VAL:HG11	2:E:558:THR:HG21	1.84	0.60
1:A:529:ASP:HB3	1:A:531:ARG:HG2	1.82	0.60
1:D:120:ILE:HA	1:D:146:HIS:O	2.02	0.60
2:K:662:THR:HG23	3:L:96:VAL:HG11	1.83	0.60
1:A:33:ASN:HD22	1:A:193:GLN:HG2	1.66	0.60
1:J:359:ASN:ND2	1:J:479:ASP:OD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:647:ASN:OD1	1:D:699:TRP:NE1	2.32	0.60
2:E:708:PRO:HB3	3:F:728:GLN:HG3	1.83	0.60
1:J:652:SER:N	2:K:24:TYR:OH	2.33	0.60
1:A:68:PRO:HB3	1:A:72:LEU:HG	1.84	0.59
2:B:706:ARG:HH11	3:C:164:MET:HG3	1.67	0.59
2:E:685:ASP:OD2	2:E:687:GLN:HB2	2.02	0.59
1:G:438:ILE:HG23	1:G:608:THR:HG21	1.83	0.59
1:J:26:GLU:HG3	1:J:31:GLU:HG3	1.82	0.59
3:L:361:GLU:OE1	3:L:376:LYS:NZ	2.32	0.59
1:D:427:GLU:O	2:E:597:ASN:ND2	2.35	0.59
1:G:68:PRO:HB3	1:G:72:LEU:HD13	1.84	0.59
3:I:533:SER:O	3:I:537:TRP:NE1	2.36	0.59
3:L:289:ILE:O	3:L:292:THR:OG1	2.19	0.59
3:C:662:THR:HG22	3:C:664:ARG:HG3	1.83	0.59
1:G:193:GLN:OE1	1:G:193:GLN:N	2.36	0.59
1:J:148:PHE:HE1	1:J:154:GLU:HG3	1.67	0.59
2:K:588:GLY:HA3	2:K:616:MET:HA	1.84	0.59
1:J:300:GLU:HB2	2:K:571:ARG:NH2	2.18	0.59
2:K:572:ARG:NH2	3:L:97:THR:OG1	2.33	0.59
3:L:153:ASP:OD2	3:L:301:ASN:ND2	2.34	0.59
2:E:517:ILE:N	2:E:522:ASP:OD2	2.31	0.59
3:F:542:PRO:O	3:F:545:VAL:HG12	2.02	0.59
2:H:370:ALA:HA	2:H:373:LEU:HD13	1.85	0.59
4:M:100:ARG:NH2	4:M:110:THR:OG1	2.36	0.59
1:A:170:ARG:HE	3:C:741:SER:HB3	1.67	0.59
3:C:289:ILE:O	3:C:292:THR:OG1	2.21	0.59
3:C:560:VAL:HG13	3:C:571:LEU:HD11	1.83	0.59
2:B:662:THR:HG23	3:C:96:VAL:HG11	1.85	0.59
2:E:125:GLY:HA3	2:E:249:ARG:HH21	1.67	0.59
1:J:302:ILE:HD12	1:J:303:PRO:HD2	1.84	0.59
3:L:338:ILE:HG23	3:L:358:ASP:HB3	1.85	0.59
1:A:484:PRO:HB2	1:A:486:ILE:HG13	1.85	0.59
2:H:423:ILE:HD13	2:H:475:ILE:HD12	1.84	0.59
3:I:446:PHE:HB3	3:I:465:PRO:HB3	1.84	0.59
3:C:657:ASN:HB3	3:C:666:THR:HB	1.83	0.59
2:E:691:LYS:NZ	3:F:6:GLU:OE2	2.35	0.59
1:G:351:GLU:OE2	1:G:358:LYS:NZ	2.36	0.59
2:K:608:GLU:OE2	2:K:612:LYS:NZ	2.32	0.59
3:F:297:ILE:O	3:F:301:ASN:N	2.36	0.58
2:K:556:ARG:NH2	2:K:595:GLY:O	2.36	0.58
3:C:135:PHE:CE2	3:C:240:TRP:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:287:ARG:NH1	3:I:460:MET:SD	2.75	0.58
2:K:612:LYS:O	2:K:616:MET:HG3	2.02	0.58
2:B:310:ASN:ND2	2:B:409:MET:HA	2.18	0.58
2:E:756:GLN:O	3:F:17:ARG:NH1	2.36	0.58
3:C:742:SER:HB3	3:C:744:LEU:HG	1.84	0.58
1:G:326:HIS:O	1:G:326:HIS:ND1	2.33	0.58
1:A:215:ALA:HB1	1:A:226:LEU:HD13	1.84	0.58
2:H:303:THR:HG21	2:H:491:GLU:HB3	1.85	0.58
1:J:455:ALA:HB1	1:J:645:VAL:HG21	1.83	0.58
3:I:275:ASP:HB2	1:J:92:ASN:HB3	1.86	0.58
2:K:427:GLY:HA3	2:K:438:TRP:CE2	2.39	0.58
3:L:461:ILE:HG13	3:L:480:VAL:HG13	1.84	0.58
1:A:462:GLY:O	1:A:466:ASN:ND2	2.31	0.58
3:C:159:ALA:O	3:C:163:ILE:HG12	2.03	0.58
2:H:548:LEU:HD11	2:H:599:TYR:HB3	1.86	0.58
1:D:26:GLU:HG3	1:D:31:GLU:HG3	1.85	0.57
2:E:50:SER:HB3	2:E:68:PRO:HG3	1.84	0.57
2:E:371:GLU:OE1	2:E:371:GLU:N	2.34	0.57
3:F:70:ARG:NH1	3:F:74:GLY:O	2.37	0.57
1:G:54:ILE:HG12	1:G:75:ARG:HB2	1.86	0.57
1:G:336:LEU:HB3	1:G:365:GLN:HG2	1.86	0.57
3:I:358:ASP:OD1	3:I:359:GLY:N	2.36	0.57
1:D:208:THR:HG22	1:D:209:GLY:H	1.69	0.57
3:I:237:GLY:HA3	3:I:240:TRP:CE2	2.38	0.57
1:J:297:HIS:HB3	2:K:568:ILE:HA	1.85	0.57
1:J:484:PRO:HB2	1:J:486:ILE:HG13	1.86	0.57
3:L:151:HIS:H	3:L:252:ASN:ND2	2.02	0.57
1:A:185:ARG:HH21	3:C:157:LYS:HE2	1.69	0.57
1:D:288:LEU:HD22	1:D:527:LEU:HD11	1.86	0.57
3:F:721:LYS:HA	3:F:734:VAL:O	2.03	0.57
1:G:1:MET:HG2	1:G:32:THR:HB	1.86	0.57
2:K:518:ASN:HD21	2:K:663:THR:HA	1.69	0.57
1:A:73:LYS:HE3	1:A:112:TYR:HE2	1.70	0.57
1:D:430:GLU:O	4:N:53:ASN:ND2	2.34	0.57
1:J:78:ILE:HA	1:J:109:LEU:HD12	1.86	0.57
4:O:67:ARG:NH1	4:O:90:ASP:OD2	2.36	0.57
1:D:578:GLY:HA2	1:D:581:MET:HG3	1.85	0.57
3:I:55:TYR:HD1	3:I:92:SER:HB2	1.70	0.57
2:B:302:ILE:HG12	2:B:449:LEU:HB3	1.87	0.57
3:L:249:GLU:N	3:L:249:GLU:OE1	2.37	0.57
3:L:471:THR:OG1	3:L:472:GLU:OE1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:532:SER:OG	3:L:555:ARG:NH1	2.35	0.57
3:F:664:ARG:NH2	3:F:671:ASP:OD2	2.38	0.57
1:G:597:GLU:O	1:G:601:SER:N	2.37	0.57
2:K:589:LEU:HA	2:K:620:TYR:HE2	1.69	0.57
3:C:154:LEU:HD11	3:C:185:ILE:HD12	1.86	0.57
2:K:276:ASN:O	2:K:279:LYS:HB2	2.05	0.57
1:A:208:THR:HG22	1:A:209:GLY:H	1.70	0.57
1:A:434:PRO:HB2	1:A:435:ILE:HD12	1.87	0.57
2:B:371:GLU:HG3	2:B:399:GLY:HA3	1.87	0.57
2:E:602:ARG:HA	3:F:234:LEU:HD12	1.87	0.57
1:G:427:GLU:O	2:H:597:ASN:ND2	2.37	0.57
2:K:434:THR:HG22	2:K:435:THR:H	1.69	0.57
1:A:522:SER:O	1:A:565:VAL:HA	2.05	0.56
3:C:398:ILE:HD11	3:C:478:ILE:HD11	1.86	0.56
2:E:397:ILE:HD12	2:E:397:ILE:C	2.25	0.56
2:E:746:ILE:HG23	3:F:8:ARG:HD3	1.87	0.56
2:E:260:ARG:HG3	2:E:414:MET:CE	2.35	0.56
2:E:623:ARG:HD3	3:F:103:GLY:H	1.70	0.56
3:F:261:ILE:HG23	3:F:522:GLN:HG3	1.87	0.56
1:J:246:LEU:O	2:K:468:ARG:NH2	2.38	0.56
3:L:57:ILE:O	3:L:91:VAL:N	2.38	0.56
1:A:432:VAL:HG11	2:B:602:ARG:HD3	1.87	0.56
3:C:499:ASP:HB3	3:C:505:ARG:HH12	1.70	0.56
3:C:544:SER:HA	3:C:547:VAL:HG22	1.86	0.56
1:D:495:ARG:NH1	4:N:85:ASN:HB2	2.21	0.56
1:G:276:CYS:HB2	1:G:698:PRO:HG3	1.88	0.56
1:G:359:ASN:ND2	1:G:479:ASP:OD2	2.39	0.56
2:H:518:ASN:HB3	2:H:521:ALA:HB3	1.86	0.56
3:I:408:ASP:O	3:I:412:LYS:HG2	2.06	0.56
3:I:586:LYS:HG2	3:I:589:ARG:NH2	2.20	0.56
3:L:374:LEU:HB2	3:L:384:LEU:HD13	1.87	0.56
4:M:95:TYR:CE1	4:M:115:LEU:HD11	2.40	0.56
1:A:220:PRO:HG2	1:A:223:PHE:HE2	1.70	0.56
2:K:374:ALA:HB2	2:K:396:LEU:HD11	1.86	0.56
4:M:51:VAL:HG23	4:M:58:THR:HG22	1.87	0.56
1:A:338:TRP:NE1	1:A:545:ILE:HD11	2.20	0.56
2:B:70:ASP:HB3	2:B:85:THR:H	1.71	0.56
2:B:318:PHE:HA	2:B:321:MET:HG2	1.88	0.56
2:E:70:ASP:HA	2:E:84:GLN:HA	1.88	0.56
2:K:110:THR:O	2:K:114:VAL:HG13	2.05	0.56
2:K:579:LEU:HD21	3:L:101:ARG:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:51:VAL:HB	4:O:70:ILE:HD13	1.87	0.56
1:J:326:HIS:CE1	1:J:539:LYS:HA	2.40	0.56
3:L:237:GLY:HA3	3:L:240:TRP:CE2	2.40	0.56
3:L:537:TRP:HH2	3:L:552:TRP:HB2	1.71	0.56
2:B:160:SER:OG	2:B:165:ASP:OD2	2.19	0.56
1:D:114:GLU:HB2	1:D:116:ARG:HG2	1.87	0.56
1:D:583:ARG:HD3	2:E:25:THR:HG21	1.88	0.56
1:G:492:LYS:HE2	4:O:82:ARG:HH22	1.70	0.56
2:H:318:PHE:HA	2:H:321:MET:HG2	1.87	0.56
3:I:71:ASN:ND2	3:I:75:GLN:OE1	2.37	0.56
3:L:497:SER:OG	3:L:505:ARG:O	2.24	0.56
1:A:449:GLU:O	1:A:638:ARG:NH2	2.39	0.56
1:D:125:ARG:HG2	1:D:126:GLU:H	1.69	0.56
3:I:230:GLU:HG3	3:I:231:VAL:HG13	1.86	0.56
2:K:700:PHE:O	2:K:703:SER:OG	2.22	0.56
3:L:385:ILE:HG23	3:L:460:MET:HE1	1.88	0.56
4:P:99:ARG:HH12	4:P:104:ILE:HA	1.71	0.56
2:B:102:ILE:HD11	2:B:265:LYS:HB2	1.87	0.56
2:B:397:ILE:HD12	2:B:397:ILE:C	2.27	0.56
3:L:748:GLN:OE1	3:L:748:GLN:N	2.39	0.56
4:O:52:SER:HA	4:O:104:ILE:HD11	1.88	0.56
1:A:673:ARG:HG2	1:A:716:ARG:NH2	2.21	0.56
3:I:276:PRO:HB2	3:I:502:LEU:HG	1.86	0.56
1:J:208:THR:HG22	1:J:209:GLY:H	1.70	0.56
2:K:224:LEU:HD23	2:K:408:MET:HG3	1.87	0.56
3:L:55:TYR:HD1	3:L:92:SER:HB2	1.70	0.56
1:G:148:PHE:HE1	1:G:154:GLU:HG3	1.71	0.55
1:G:208:THR:HG22	1:G:209:GLY:H	1.71	0.55
1:G:576:LYS:HA	1:G:579:MET:HG2	1.87	0.55
2:B:423:ILE:HD11	2:B:469:THR:HB	1.88	0.55
3:C:27:HIS:O	3:C:30:ILE:HG12	2.06	0.55
3:C:206:MET:HA	3:C:206:MET:HE3	1.88	0.55
1:D:606:ASP:HB2	3:F:135:PHE:CG	2.41	0.55
3:F:331:LYS:HE2	3:F:490:SER:H	1.71	0.55
3:I:131:GLY:H	3:I:242:GLN:NE2	2.04	0.55
3:I:296:ASP:HA	3:I:299:ARG:HD2	1.88	0.55
1:J:528:THR:O	1:J:564:TYR:OH	2.17	0.55
2:E:355:TYR:HE2	2:E:385:THR:HG21	1.71	0.55
3:F:27:HIS:O	3:F:30:ILE:HG12	2.07	0.55
3:F:488:TYR:HE1	3:F:490:SER:HB2	1.72	0.55
2:H:712:SER:OG	3:I:730:ASP:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:THR:O	1:A:564:TYR:OH	2.18	0.55
1:D:442:ARG:NH1	1:D:593:GLU:OE2	2.39	0.55
1:G:203:GLU:HG2	2:H:162:ARG:HH21	1.71	0.55
3:I:77:LEU:HD12	3:I:78:TRP:CD1	2.41	0.55
2:B:602:ARG:HA	3:C:234:LEU:HD12	1.89	0.55
1:A:120:ILE:HA	1:A:146:HIS:O	2.07	0.55
1:A:170:ARG:NH1	3:C:739:ARG:HB3	2.20	0.55
2:E:347:LYS:NZ	2:E:403:LEU:O	2.40	0.55
3:F:289:ILE:O	3:F:292:THR:OG1	2.21	0.55
3:F:444:VAL:O	3:F:448:ASN:HB2	2.06	0.55
2:H:620:TYR:O	2:H:624:LEU:HB2	2.06	0.55
1:J:590:GLN:HB3	2:K:543:THR:HG21	1.88	0.55
1:G:120:ILE:HA	1:G:146:HIS:O	2.06	0.55
2:H:589:LEU:HA	2:H:620:TYR:CE2	2.42	0.55
3:I:406:GLN:NE2	3:I:431:MET:SD	2.78	0.55
3:C:586:LYS:HG2	3:C:589:ARG:HH21	1.70	0.55
3:F:408:ASP:O	3:F:412:LYS:HG2	2.07	0.55
3:I:242:GLN:NE2	3:I:243:MET:O	2.40	0.55
3:I:275:ASP:N	1:J:96:ASN:HD21	2.02	0.55
1:J:50:ASP:O	1:J:52:HIS:ND1	2.40	0.55
3:F:57:ILE:O	3:F:91:VAL:N	2.40	0.55
2:H:281:LYS:HE3	3:I:142:ARG:HH12	1.70	0.55
2:H:371:GLU:OE1	2:H:371:GLU:N	2.36	0.55
1:J:580:GLU:HG2	2:K:512:PHE:HE1	1.70	0.55
2:K:371:GLU:OE1	2:K:371:GLU:N	2.37	0.55
2:K:504:ASN:HA	2:K:507:MET:HB2	1.87	0.55
3:C:135:PHE:CZ	3:C:240:TRP:HB3	2.42	0.55
1:D:413:LYS:HZ1	1:D:454:ARG:HH21	1.55	0.55
1:G:439:ALA:HB2	2:H:541:PRO:HB2	1.89	0.55
1:J:433:ALA:HB3	1:J:436:GLU:HG3	1.88	0.55
4:O:91:SER:OG	4:O:120:VAL:HG13	2.06	0.55
1:D:261:LEU:O	1:D:265:PRO:HD3	2.07	0.54
2:E:287:ARG:O	2:E:291:THR:OG1	2.22	0.54
3:F:124:ARG:HH22	3:F:149:PRO:HB2	1.72	0.54
3:F:748:GLN:OE1	3:F:748:GLN:N	2.40	0.54
1:G:230:ARG:NH1	2:H:335:ASN:OD1	2.40	0.54
2:H:269:SER:HB2	2:H:421:VAL:HG21	1.89	0.54
2:K:632:VAL:HG12	2:K:663:THR:HB	1.89	0.54
3:L:737:ARG:NH1	3:L:740:ASP:OD1	2.33	0.54
1:G:241:TYR:CD2	2:H:86:ASP:HB2	2.42	0.54
1:G:583:ARG:NH2	2:H:511:SER:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:576:LEU:HD12	3:C:97:THR:HG21	1.89	0.54
3:C:338:ILE:HG23	3:C:358:ASP:HB3	1.89	0.54
1:D:220:PRO:HG2	1:D:223:PHE:HE2	1.71	0.54
1:D:266:ARG:O	1:D:687:TYR:OH	2.16	0.54
2:H:602:ARG:HA	3:I:234:LEU:HD12	1.89	0.54
1:G:289:LYS:HB3	1:G:499:ASN:HD22	1.72	0.54
1:G:431:ASP:HB3	1:G:437:TYR:CE1	2.42	0.54
3:I:101:ARG:NE	3:I:102:ASN:OD1	2.27	0.54
3:I:146:ASP:HA	3:I:215:THR:HA	1.90	0.54
1:J:408:GLN:HE21	1:J:412:ASN:HD21	1.54	0.54
1:J:673:ARG:NH2	2:K:9:PHE:O	2.40	0.54
1:J:408:GLN:HE21	1:J:412:ASN:ND2	2.06	0.54
4:N:91:SER:OG	4:N:120:VAL:HG13	2.07	0.54
1:A:554:ILE:HA	4:O:43:LYS:HD3	1.89	0.54
2:B:70:ASP:HA	2:B:84:GLN:HA	1.89	0.54
1:D:50:ASP:O	1:D:52:HIS:ND1	2.39	0.54
1:D:125:ARG:HB2	1:D:195:GLU:HG3	1.90	0.54
3:F:533:SER:OG	3:F:536:MET:N	2.39	0.54
1:G:478:ASP:O	1:G:508:ARG:NH1	2.41	0.54
3:I:387:SER:HB3	3:I:481:SER:HB3	1.89	0.54
1:A:530:PRO:HG3	1:A:542:VAL:HG11	1.90	0.54
2:B:326:THR:HB	2:B:334:ARG:HG2	1.88	0.54
2:B:434:THR:HG22	2:B:435:THR:H	1.71	0.54
1:D:134:LYS:HB3	1:D:145:ILE:HD13	1.89	0.54
3:F:206:MET:HA	3:F:206:MET:HE3	1.88	0.54
1:G:408:GLN:HE21	1:G:412:ASN:ND2	2.03	0.54
2:H:514:VAL:HG11	2:H:558:THR:HG21	1.90	0.54
2:B:181:ILE:HB	2:B:211:ARG:HG3	1.90	0.54
1:D:16:LEU:HD21	3:F:754:ILE:HG12	1.90	0.54
1:D:326:HIS:O	1:D:326:HIS:ND1	2.38	0.54
2:H:423:ILE:HG21	2:H:473:VAL:HG21	1.88	0.54
2:H:434:THR:HG22	2:H:435:THR:H	1.72	0.54
1:J:529:ASP:HB3	1:J:531:ARG:HG2	1.89	0.54
1:A:408:GLN:HE21	1:A:412:ASN:ND2	2.05	0.54
1:A:440:SER:OG	4:M:54:ASN:OD1	2.18	0.54
3:C:420:PHE:O	3:C:433:GLN:NE2	2.41	0.54
1:D:408:GLN:HE21	1:D:412:ASN:ND2	2.04	0.54
3:F:131:GLY:H	3:F:242:GLN:HE22	1.56	0.54
2:H:627:PRO:HB3	3:I:198:ILE:HG23	1.90	0.54
3:I:372:ALA:HB2	3:I:386:VAL:HG13	1.89	0.54
2:B:569:GLN:HG3	2:B:573:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:540:ASN:OD1	3:C:541:GLY:N	2.36	0.54
1:D:681:PHE:CE1	2:E:484:ILE:HD11	2.42	0.54
1:G:549:LEU:HD23	1:G:549:LEU:H	1.73	0.54
3:I:517:GLU:N	3:I:517:GLU:OE1	2.41	0.54
2:K:587:ALA:HB2	4:P:105:TRP:HB2	1.90	0.54
2:K:721:ARG:NH2	3:L:709:SER:OG	2.40	0.54
1:A:266:ARG:O	1:A:687:TYR:OH	2.16	0.53
1:A:520:PHE:CE1	1:A:568:ASN:HB3	2.43	0.53
3:C:408:ASP:O	3:C:412:LYS:HG2	2.08	0.53
1:D:274:PRO:O	1:D:402:SER:N	2.37	0.53
2:E:260:ARG:HG3	2:E:414:MET:HE1	1.89	0.53
1:A:125:ARG:HG2	1:A:126:GLU:H	1.72	0.53
1:A:253:VAL:O	2:B:468:ARG:HD3	2.07	0.53
1:A:549:LEU:HD23	1:A:549:LEU:H	1.73	0.53
3:C:142:ARG:HB2	3:C:487:GLU:O	2.08	0.53
1:J:305:TYR:O	1:J:308:ILE:HG13	2.07	0.53
3:L:136:ARG:HD2	3:L:483:MET:HE3	1.88	0.53
3:L:366:VAL:HA	3:L:371:THR:HG22	1.90	0.53
1:D:263:THR:HG23	1:D:716:ARG:NH1	2.23	0.53
1:D:455:ALA:HB1	1:D:645:VAL:HG21	1.89	0.53
1:G:210:THR:HG21	2:H:175:ASP:HA	1.90	0.53
1:D:168:ARG:HG2	1:D:172:LYS:HE3	1.90	0.53
2:H:583:THR:O	2:H:586:LYS:NZ	2.33	0.53
2:H:627:PRO:HD3	3:I:108:THR:HG21	1.89	0.53
2:H:704:SER:HB2	3:I:201:LEU:HD21	1.91	0.53
3:L:697:LEU:HD21	3:L:735:MET:HB2	1.89	0.53
3:C:544:SER:O	3:C:548:ASN:HB2	2.08	0.53
3:C:748:GLN:OE1	3:C:748:GLN:N	2.41	0.53
1:D:241:TYR:HD2	2:E:86:ASP:HB2	1.74	0.53
3:F:589:ARG:HG2	3:F:624:ALA:HB2	1.90	0.53
2:K:258:LEU:HD21	2:K:325:ILE:HG21	1.90	0.53
3:L:242:GLN:NE2	3:L:243:MET:O	2.41	0.53
3:L:274:ALA:O	3:L:500:ARG:NH2	2.41	0.53
1:A:212:ARG:HH12	1:A:227:GLU:HG2	1.74	0.53
1:A:258:GLU:OE2	1:A:683:LEU:N	2.39	0.53
1:A:492:LYS:HE2	4:M:82:ARG:HH12	1.73	0.53
3:I:27:HIS:O	3:I:30:ILE:HG12	2.09	0.53
4:O:7:SER:HA	4:O:117:GLN:HE21	1.74	0.53
1:A:523:MET:HG2	1:A:565:VAL:HG22	1.91	0.53
1:D:520:PHE:CE1	1:D:568:ASN:HB3	2.43	0.53
2:E:219:ILE:HG23	2:E:348:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:GLU:OE2	1:G:168:ARG:HD2	2.09	0.53
2:H:558:THR:HG23	3:I:48:LYS:HG2	1.90	0.53
2:H:712:SER:OG	2:H:716:GLU:OE1	2.22	0.53
2:K:310:ASN:ND2	2:K:409:MET:HA	2.24	0.53
1:A:443:ARG:HH12	4:M:54:ASN:HB3	1.73	0.53
1:D:64:GLU:HG3	3:F:739:ARG:HD3	1.91	0.53
1:D:68:PRO:HB2	1:D:72:LEU:HG	1.90	0.53
2:E:707:ARG:HG2	3:F:29:ALA:HB2	1.90	0.53
1:G:431:ASP:HB3	1:G:437:TYR:HE1	1.73	0.53
3:I:135:PHE:CZ	3:I:240:TRP:HB3	2.44	0.53
2:K:470:CYS:HB3	2:K:475:ILE:O	2.09	0.53
3:L:27:HIS:O	3:L:30:ILE:HG12	2.08	0.53
4:O:37:VAL:HG22	4:O:47:TRP:HA	1.90	0.53
2:B:131:TRP:O	2:B:220:ARG:NH1	2.42	0.53
2:E:65:GLN:NE2	2:E:346:ASN:OD1	2.42	0.53
2:H:357:PHE:O	2:H:366:THR:N	2.41	0.53
2:H:518:ASN:OD1	2:H:663:THR:HA	2.08	0.53
1:D:684:GLU:O	1:D:688:GLU:HG2	2.08	0.53
2:E:434:THR:HG22	2:E:435:THR:H	1.74	0.53
3:F:55:TYR:CD1	3:F:92:SER:HB2	2.42	0.53
3:F:146:ASP:HA	3:F:215:THR:HA	1.91	0.53
3:F:428:LEU:HD22	3:F:516:GLU:HG2	1.91	0.53
4:M:35:THR:HG22	4:M:50:MET:HG2	1.90	0.53
2:B:70:ASP:OD2	2:B:85:THR:OG1	2.27	0.52
1:D:401:ARG:HH11	1:D:696:ASN:HB2	1.74	0.52
4:O:6:GLU:HG2	4:O:116:GLY:HA3	1.91	0.52
1:A:635:LYS:O	1:A:639:THR:OG1	2.22	0.52
2:E:133:LEU:HD11	2:E:683:LEU:HD22	1.91	0.52
2:E:690:GLN:O	2:E:694:ASN:ND2	2.34	0.52
1:G:310:CYS:O	1:G:313:THR:OG1	2.24	0.52
4:N:51:VAL:HG23	4:N:58:THR:HG22	1.91	0.52
1:D:203:GLU:OE2	2:E:162:ARG:NH2	2.43	0.52
1:D:530:PRO:HG3	1:D:542:VAL:HG11	1.91	0.52
1:G:403:LEU:HD12	1:G:701:LEU:HB3	1.91	0.52
3:I:290:GLY:N	3:I:529:ILE:HG12	2.13	0.52
3:L:108:THR:HA	3:L:110:HIS:HD2	1.75	0.52
1:A:274:PRO:O	1:A:402:SER:N	2.43	0.52
1:A:457:GLU:OE2	1:A:501:TYR:OH	2.27	0.52
2:B:627:PRO:HD3	3:C:108:THR:HG21	1.92	0.52
3:C:55:TYR:CD1	3:C:92:SER:HB2	2.39	0.52
1:D:463:VAL:HG11	1:D:582:ARG:HH22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:560:PRO:HB2	1:G:562:PHE:CE1	2.40	0.52
3:I:255:VAL:HA	3:I:527:LEU:HD11	1.92	0.52
1:J:290:LEU:HD23	1:J:310:CYS:HB3	1.92	0.52
2:K:335:ASN:O	2:K:339:ILE:HG12	2.08	0.52
3:L:387:SER:OG	3:L:485:VAL:N	2.40	0.52
2:B:710:GLY:N	3:C:26:ASP:OD1	2.34	0.52
3:C:142:ARG:HB3	3:C:217:PHE:HE1	1.75	0.52
3:I:395:ALA:O	3:I:398:ILE:HG22	2.09	0.52
2:K:387:LYS:HG2	2:K:391:LYS:HE2	1.91	0.52
2:K:708:PRO:HA	3:L:728:GLN:HE21	1.75	0.52
4:O:2:VAL:HA	4:O:25:SER:O	2.09	0.52
1:A:150:PHE:HB3	1:A:179:ARG:HB2	1.91	0.52
2:B:695:LEU:HD21	3:C:7:LEU:HG	1.92	0.52
2:E:70:ASP:HB3	2:E:85:THR:H	1.75	0.52
1:G:484:PRO:HB2	1:G:486:ILE:HG13	1.91	0.52
3:I:658:TYR:HB2	3:I:665:LEU:HD13	1.92	0.52
4:P:35:THR:HG22	4:P:50:MET:HG2	1.92	0.52
1:A:78:ILE:HA	1:A:109:LEU:HD12	1.91	0.52
3:C:380:ARG:HA	3:C:407:GLU:HG2	1.92	0.52
2:E:518:ASN:HB3	2:E:521:ALA:HB3	1.92	0.52
2:E:554:ASP:O	2:E:558:THR:OG1	2.25	0.52
3:F:371:THR:OG1	3:F:487:GLU:OE2	2.23	0.52
3:F:506:ASP:HB3	3:F:510:ASN:OD1	2.10	0.52
2:H:50:SER:HB3	2:H:68:PRO:HG3	1.92	0.52
1:J:359:ASN:HA	1:J:480:PHE:O	2.10	0.52
3:L:657:ASN:HB3	3:L:666:THR:HB	1.90	0.52
4:M:2:VAL:HA	4:M:25:SER:O	2.10	0.52
1:G:294:ASP:OD1	1:G:294:ASP:N	2.42	0.52
2:H:420:GLY:HA3	2:H:442:GLN:HG2	1.92	0.52
2:H:470:CYS:HB3	2:H:475:ILE:O	2.09	0.52
3:I:131:GLY:H	3:I:242:GLN:HE22	1.57	0.52
1:J:284:LEU:HB3	1:J:458:TYR:CZ	2.45	0.52
3:C:446:PHE:HB3	3:C:465:PRO:HB3	1.92	0.52
3:I:120:GLU:HB3	3:I:124:ARG:NH2	2.25	0.52
3:I:283:MET:O	3:I:533:SER:OG	2.28	0.52
2:K:538:ASP:N	2:K:538:ASP:OD1	2.43	0.52
1:A:305:TYR:O	1:A:308:ILE:HG13	2.10	0.52
2:B:225:ASN:O	2:B:243:THR:N	2.43	0.52
2:B:572:ARG:HA	3:C:94:LEU:HD12	1.92	0.52
1:G:220:PRO:HG2	1:G:223:PHE:HE2	1.74	0.52
3:I:265:ASN:OD1	3:I:268:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:269:ARG:NH2	3:I:535:MET:O	2.43	0.52
2:B:339:ILE:O	2:B:343:MET:HG3	2.09	0.51
3:F:131:GLY:H	3:F:242:GLN:NE2	2.08	0.51
2:H:94:PHE:HB3	2:H:431:TYR:CZ	2.45	0.51
3:I:163:ILE:O	3:I:167:VAL:HG12	2.11	0.51
4:N:67:ARG:NH1	4:N:90:ASP:OD2	2.32	0.51
1:A:583:ARG:HD3	2:B:25:THR:HG21	1.92	0.51
1:D:624:SER:HB3	2:E:1:MET:HA	1.91	0.51
1:G:652:SER:OG	1:G:697:ASP:OD2	2.26	0.51
2:B:613:TRP:O	2:B:621:GLN:NE2	2.44	0.51
3:C:163:ILE:O	3:C:167:VAL:HG12	2.10	0.51
3:C:237:GLY:HA3	3:C:240:TRP:CE2	2.46	0.51
2:E:576:LEU:HD12	3:F:97:THR:HG21	1.92	0.51
2:B:303:THR:HG21	2:B:491:GLU:HB3	1.91	0.51
3:C:281:LEU:HD21	3:C:314:ALA:HB1	1.92	0.51
1:G:257:ILE:HD13	2:H:460:GLN:HG3	1.91	0.51
1:G:274:PRO:O	1:G:402:SER:N	2.43	0.51
3:I:428:LEU:HD22	3:I:516:GLU:HG2	1.92	0.51
2:K:123:THR:HG22	2:K:143:LEU:HD13	1.93	0.51
1:G:305:TYR:O	1:G:308:ILE:HG13	2.10	0.51
3:I:144:ARG:HG2	3:I:217:PHE:HB2	1.92	0.51
1:J:75:ARG:NH1	1:J:111:ASP:OD2	2.43	0.51
1:J:76:PHE:HE1	1:J:118:ILE:HD12	1.75	0.51
1:J:439:ALA:HB2	2:K:541:PRO:HB2	1.91	0.51
2:K:685:ASP:N	2:K:685:ASP:OD1	2.41	0.51
3:L:408:ASP:HB3	3:L:412:LYS:NZ	2.26	0.51
3:L:446:PHE:HB3	3:L:465:PRO:HB3	1.91	0.51
4:O:95:TYR:HA	4:O:115:LEU:HD21	1.93	0.51
3:C:332:ARG:HA	3:C:363:PHE:HD1	1.74	0.51
3:F:296:ASP:HA	3:F:299:ARG:HD2	1.93	0.51
3:F:754:ILE:HG23	3:F:755:ARG:HG2	1.92	0.51
2:H:125:GLY:HA3	2:H:249:ARG:HH21	1.75	0.51
1:J:655:LEU:HD22	1:J:699:TRP:HD1	1.75	0.51
2:B:313:GLN:HB3	2:B:318:PHE:CE2	2.45	0.51
2:E:374:ALA:O	2:E:393:ARG:NH2	2.39	0.51
2:K:303:THR:HG21	2:K:491:GLU:HB3	1.93	0.51
2:K:743:ILE:HG12	3:L:4:ILE:HG21	1.92	0.51
1:A:33:ASN:ND2	1:A:202:GLU:OE2	2.43	0.51
1:A:592:ILE:O	1:A:596:ILE:HG13	2.09	0.51
2:B:608:GLU:OE2	2:B:612:LYS:NZ	2.39	0.51
3:C:357:HIS:ND1	3:C:406:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:371:THR:HG21	3:C:487:GLU:HG3	1.92	0.51
1:D:597:GLU:O	1:D:601:SER:N	2.44	0.51
2:E:625:CYS:HB2	3:F:111:TYR:CZ	2.46	0.51
3:F:155:SER:HB3	3:F:300:GLN:HB3	1.92	0.51
3:L:55:TYR:CD1	3:L:92:SER:HB2	2.46	0.51
3:L:297:ILE:O	3:L:301:ASN:N	2.42	0.51
1:A:179:ARG:HG2	1:A:188:TRP:CZ3	2.46	0.51
2:B:310:ASN:HD21	2:B:409:MET:HA	1.75	0.51
3:C:362:GLU:HG3	3:C:375:ARG:HG2	1.93	0.51
2:E:457:GLU:OE1	2:E:457:GLU:N	2.43	0.51
2:E:579:LEU:HG	3:F:101:ARG:HG3	1.93	0.51
3:F:101:ARG:NE	3:F:102:ASN:OD1	2.24	0.51
1:G:78:ILE:HA	1:G:109:LEU:HD12	1.93	0.51
2:H:600:ASN:O	2:H:604:LEU:HG	2.11	0.51
1:J:34:LYS:HD2	1:J:200:THR:HB	1.93	0.51
4:P:115:LEU:HD13	4:P:116:GLY:N	2.26	0.51
3:C:499:ASP:OD2	3:C:505:ARG:NH2	2.44	0.51
1:D:443:ARG:HG3	1:D:444:ASN:N	2.26	0.51
1:G:674:ASP:OD2	2:H:498:ARG:NH2	2.40	0.51
1:J:549:LEU:HD23	1:J:549:LEU:H	1.76	0.51
3:L:730:ASP:OD1	3:L:730:ASP:N	2.37	0.51
3:C:471:THR:OG1	3:C:472:GLU:OE1	2.24	0.50
2:H:110:THR:O	2:H:114:VAL:HG13	2.11	0.50
2:H:519:GLU:HB2	2:H:662:THR:HG22	1.92	0.50
3:I:564:TRP:O	3:I:604:ARG:NH2	2.36	0.50
1:A:292:ILE:HD11	1:A:310:CYS:SG	2.50	0.50
2:E:318:PHE:HA	2:E:321:MET:HG2	1.92	0.50
3:F:449:TRP:HE1	3:F:476:ARG:HB3	1.77	0.50
1:G:554:ILE:HA	4:M:43:LYS:HD3	1.94	0.50
2:K:252:VAL:HG23	2:K:412:PHE:CE1	2.46	0.50
3:L:283:MET:O	3:L:287:THR:OG1	2.24	0.50
4:N:51:VAL:HB	4:N:70:ILE:HD13	1.93	0.50
4:O:6:GLU:HG3	4:O:117:GLN:H	1.76	0.50
1:D:587:GLN:HG2	1:D:591:GLN:NE2	2.26	0.50
2:E:589:LEU:HA	2:E:620:TYR:CE2	2.46	0.50
3:I:57:ILE:O	3:I:91:VAL:N	2.43	0.50
1:J:431:ASP:HB3	1:J:437:TYR:CE1	2.47	0.50
1:J:597:GLU:O	1:J:601:SER:N	2.43	0.50
2:K:378:LEU:HD11	2:K:389:ILE:HG21	1.94	0.50
1:D:351:GLU:O	1:D:352:GLU:HG2	2.12	0.50
3:I:377:ALA:HB3	3:I:380:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:116:ARG:NH1	1:J:162:THR:OG1	2.44	0.50
2:K:558:THR:HG23	3:L:48:LYS:HG2	1.93	0.50
3:L:571:LEU:HD21	3:L:619:LEU:HD21	1.92	0.50
3:L:591:GLN:OE1	3:L:591:GLN:N	2.39	0.50
4:M:37:VAL:HG22	4:M:47:TRP:HA	1.93	0.50
1:A:589:LEU:O	1:A:593:GLU:N	2.31	0.50
2:B:95:LEU:HA	2:B:425:ASN:HD21	1.76	0.50
2:B:311:GLU:OE1	2:B:311:GLU:N	2.44	0.50
2:B:693:CYS:SG	3:C:31:ILE:HG23	2.51	0.50
1:D:125:ARG:HH11	1:D:195:GLU:HG2	1.77	0.50
1:D:433:ALA:HA	1:D:437:TYR:CE2	2.47	0.50
2:H:589:LEU:HA	2:H:620:TYR:HE2	1.77	0.50
2:H:708:PRO:HB3	3:I:728:GLN:HG3	1.94	0.50
2:K:311:GLU:N	2:K:311:GLU:OE1	2.45	0.50
3:L:254:ASP:HA	3:L:257:GLN:HG2	1.93	0.50
4:N:17:SER:HA	4:N:83:MET:O	2.11	0.50
1:A:24:TYR:OH	1:A:84:ARG:NH1	2.45	0.50
3:I:611:ASP:OD1	3:I:611:ASP:N	2.45	0.50
1:J:84:ARG:HE	1:J:88:TRP:HE1	1.58	0.50
2:K:428:GLN:HE21	2:K:431:TYR:HE2	1.58	0.50
1:A:217:GLN:HE22	2:B:58:ASN:HA	1.77	0.50
1:A:672:LEU:HD12	1:A:716:ARG:HH21	1.77	0.50
1:D:2:GLU:CD	3:F:318:ARG:HH21	2.14	0.50
1:D:111:ASP:OD1	1:D:113:LYS:N	2.45	0.50
2:E:104:GLU:OE1	2:E:104:GLU:N	2.44	0.50
3:F:488:TYR:CE1	3:F:490:SER:HB2	2.46	0.50
3:F:527:LEU:HD23	3:F:527:LEU:H	1.77	0.50
1:G:612:PHE:HA	1:G:633:ILE:HD13	1.93	0.50
2:H:575:GLU:OE2	3:I:101:ARG:NH1	2.45	0.50
1:J:207:ILE:HG22	1:J:212:ARG:HB2	1.93	0.50
2:K:396:LEU:HA	2:K:401:ALA:HA	1.94	0.50
2:B:591:VAL:HG23	2:B:612:LYS:HZ1	1.75	0.50
2:B:625:CYS:HB3	3:C:111:TYR:CZ	2.46	0.50
3:C:611:ASP:OD1	3:C:611:ASP:N	2.45	0.50
2:H:59:THR:OG1	2:H:60:GLU:OE1	2.29	0.50
2:H:519:GLU:HG2	2:H:559:TYR:CE2	2.46	0.50
3:I:430:PRO:O	3:I:434:LEU:HG	2.11	0.50
3:I:471:THR:OG1	3:I:472:GLU:OE1	2.25	0.50
3:I:730:ASP:OD1	3:I:730:ASP:N	2.42	0.50
1:D:252:GLU:O	1:D:254:ASN:ND2	2.45	0.50
2:E:122:LEU:HD11	2:E:249:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:514:VAL:HG21	2:E:559:TYR:HE1	1.77	0.50
3:F:498:ILE:HD11	3:F:502:LEU:HA	1.94	0.50
3:F:586:LYS:HG2	3:F:589:ARG:NH2	2.27	0.50
1:J:444:ASN:OD1	1:J:445:TYR:N	2.44	0.50
1:J:624:SER:HB3	2:K:1:MET:HA	1.93	0.50
1:J:624:SER:OG	1:J:625:PRO:HD3	2.12	0.50
1:A:681:PHE:CZ	2:B:484:ILE:HD11	2.47	0.49
1:D:592:ILE:O	1:D:596:ILE:HG13	2.12	0.49
3:F:471:THR:OG1	3:F:472:GLU:OE1	2.23	0.49
1:G:154:GLU:OE2	1:G:168:ARG:NH1	2.45	0.49
2:K:136:ASN:OD1	2:K:225:ASN:ND2	2.45	0.49
4:N:98:LYS:O	4:N:111:ASP:OD1	2.30	0.49
1:A:280:SER:HB3	1:A:650:TYR:CZ	2.47	0.49
1:A:435:ILE:HD11	3:C:242:GLN:HB2	1.93	0.49
1:D:341:VAL:HG22	1:D:360:MET:HE3	1.94	0.49
1:D:420:SER:HB3	1:D:489:CYS:HB2	1.94	0.49
3:I:559:THR:O	3:I:563:GLN:HB2	2.11	0.49
2:K:378:LEU:HD23	2:K:386:ARG:HG3	1.94	0.49
3:L:408:ASP:O	3:L:412:LYS:HG2	2.12	0.49
4:N:35:THR:HG22	4:N:50:MET:HG2	1.94	0.49
4:P:62:ASP:HA	4:P:65:LYS:HE2	1.92	0.49
1:A:420:SER:HB2	1:A:422:TRP:NE1	2.27	0.49
3:C:141:ILE:HB	3:C:220:VAL:O	2.13	0.49
1:D:82:ARG:NH1	3:F:753:ARG:O	2.36	0.49
1:D:283:LEU:O	1:D:461:LYS:NZ	2.45	0.49
2:E:225:ASN:HD21	2:E:350:ARG:HH21	1.60	0.49
1:G:630:ASP:OD1	1:G:630:ASP:N	2.45	0.49
2:H:598:LEU:HD23	2:H:598:LEU:H	1.78	0.49
3:I:377:ALA:N	3:I:380:ARG:O	2.40	0.49
2:K:310:ASN:HD21	2:K:409:MET:HA	1.77	0.49
2:B:110:THR:O	2:B:114:VAL:HG13	2.12	0.49
1:D:523:MET:HG2	1:D:565:VAL:HG22	1.93	0.49
1:D:549:LEU:HD23	1:D:549:LEU:H	1.76	0.49
3:F:320:SER:HA	3:F:492:GLU:O	2.11	0.49
2:H:492:PHE:O	2:H:495:PHE:HB2	2.13	0.49
3:I:748:GLN:OE1	3:I:748:GLN:N	2.45	0.49
2:K:569:GLN:HG3	2:K:573:SER:HB2	1.94	0.49
1:D:52:HIS:O	1:D:75:ARG:HB3	2.13	0.49
2:E:598:LEU:HD23	2:E:598:LEU:H	1.76	0.49
3:F:325:PHE:CZ	3:F:431:MET:HB3	2.47	0.49
3:L:6:GLU:HA	3:L:9:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:430:PRO:O	3:L:434:LEU:HG	2.12	0.49
4:P:52:SER:HB3	4:P:57:ASP:HB3	1.94	0.49
1:A:318:LYS:H	1:A:546:GLY:HA2	1.78	0.49
1:A:362:LYS:HA	1:A:480:PHE:HE2	1.77	0.49
1:A:624:SER:OG	1:A:625:PRO:HD3	2.12	0.49
1:D:624:SER:OG	1:D:625:PRO:HD3	2.13	0.49
3:F:332:ARG:HA	3:F:363:PHE:HD1	1.78	0.49
1:G:7:GLN:OE1	1:G:185:ARG:NH2	2.46	0.49
2:H:666:TRP:H	2:H:666:TRP:HE3	1.59	0.49
1:J:430:GLU:O	2:K:600:ASN:ND2	2.44	0.49
2:K:313:GLN:HB3	2:K:318:PHE:HE2	1.77	0.49
2:B:122:LEU:HD11	2:B:249:ARG:HB3	1.95	0.49
3:C:449:TRP:NE1	3:C:476:ARG:HB3	2.28	0.49
1:D:469:LEU:HA	1:D:483:ILE:HD13	1.94	0.49
3:F:664:ARG:NE	3:F:671:ASP:OD1	2.36	0.49
2:H:52:LYS:HG2	2:H:82:TYR:CZ	2.47	0.49
2:H:691:LYS:NZ	3:I:6:GLU:OE2	2.44	0.49
3:I:503:ARG:HH12	3:I:505:ARG:HH22	1.60	0.49
3:C:694:PHE:CB	3:C:734:VAL:HG13	2.43	0.49
1:D:305:TYR:O	1:D:308:ILE:HG13	2.13	0.49
2:E:110:THR:O	2:E:114:VAL:HG13	2.13	0.49
2:E:491:GLU:HG2	2:E:492:PHE:N	2.27	0.49
3:F:398:ILE:HD11	3:F:478:ILE:HD11	1.95	0.49
2:K:516:GLY:N	2:K:522:ASP:OD1	2.46	0.49
3:C:151:HIS:HB3	3:C:210:GLU:O	2.13	0.49
3:C:395:ALA:O	3:C:398:ILE:HG22	2.13	0.49
1:D:630:ASP:N	1:D:630:ASP:OD1	2.44	0.49
2:E:591:VAL:HG23	2:E:612:LYS:HZ1	1.77	0.49
3:F:134:HIS:CE1	3:F:241:GLU:HB3	2.47	0.49
4:O:32:TYR:CG	4:O:98:LYS:HE3	2.47	0.49
1:A:130:TYR:HE1	1:A:197:GLY:HA2	1.78	0.49
1:A:168:ARG:O	1:A:172:LYS:HG3	2.13	0.49
1:A:426:ASP:OD1	2:B:553:LYS:HB2	2.13	0.49
2:B:225:ASN:ND2	2:B:350:ARG:HD3	2.28	0.49
3:C:430:PRO:O	3:C:434:LEU:HG	2.12	0.49
3:C:456:ASN:HB2	3:C:471:THR:O	2.13	0.49
1:D:427:GLU:OE1	2:E:556:ARG:NH2	2.41	0.49
1:G:324:LYS:HD2	1:G:325:PRO:HD2	1.95	0.49
2:H:396:LEU:HA	2:H:401:ALA:HA	1.94	0.49
1:J:581:MET:HE1	1:J:649:LEU:HG	1.95	0.49
2:K:693:CYS:SG	3:L:31:ILE:HG23	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:387:SER:HB3	3:L:485:VAL:HG23	1.94	0.49
2:B:598:LEU:HD23	2:B:598:LEU:H	1.78	0.48
2:B:612:LYS:O	2:B:616:MET:HG3	2.13	0.48
1:D:548:MET:O	1:D:558:SER:HA	2.13	0.48
1:D:576:LYS:HA	1:D:579:MET:HG2	1.94	0.48
3:F:359:GLY:H	3:F:378:THR:HB	1.78	0.48
1:G:543:LEU:HD12	1:G:563:LEU:HD23	1.95	0.48
1:J:440:SER:OG	4:P:54:ASN:OD1	2.20	0.48
3:L:544:SER:O	3:L:548:ASN:ND2	2.46	0.48
4:O:115:LEU:HD22	4:O:116:GLY:N	2.26	0.48
1:G:551:ARG:NH2	4:M:46:GLU:OE1	2.45	0.48
3:L:151:HIS:H	3:L:252:ASN:HD21	1.59	0.48
2:B:113:VAL:O	2:B:117:THR:OG1	2.29	0.48
2:B:316:ARG:NH2	2:B:345:SER:OG	2.47	0.48
2:E:307:THR:N	2:E:478:SER:HB2	2.28	0.48
1:J:137:LYS:HB3	1:J:138:ILE:HD12	1.94	0.48
1:J:520:PHE:CE1	1:J:568:ASN:HB3	2.48	0.48
1:A:180:GLN:NE2	3:C:174:ALA:H	2.10	0.48
2:B:120:ASP:HB3	3:C:33:LYS:HD2	1.95	0.48
2:B:222:LEU:HB3	2:B:347:LYS:HA	1.95	0.48
3:C:146:ASP:HA	3:C:215:THR:HA	1.94	0.48
2:E:693:CYS:SG	3:F:31:ILE:HG23	2.54	0.48
2:E:697:GLU:OE2	3:F:32:LYS:NZ	2.39	0.48
2:H:252:VAL:HG23	2:H:412:PHE:CE1	2.48	0.48
1:J:408:GLN:HG3	1:J:412:ASN:HD21	1.78	0.48
4:P:6:GLU:N	4:P:6:GLU:OE2	2.47	0.48
3:C:6:GLU:HA	3:C:9:ASN:OD1	2.13	0.48
1:D:111:ASP:OD1	1:D:112:TYR:N	2.46	0.48
2:E:704:SER:HB2	3:F:201:LEU:HD21	1.95	0.48
3:F:254:ASP:HA	3:F:257:GLN:HG2	1.96	0.48
2:H:268:GLN:HB2	2:H:421:VAL:HG13	1.95	0.48
2:H:389:ILE:HA	2:H:392:ILE:HG22	1.94	0.48
2:H:693:CYS:SG	3:I:31:ILE:HG23	2.53	0.48
3:I:398:ILE:HD11	3:I:478:ILE:CD1	2.43	0.48
3:I:450:GLY:O	3:I:476:ARG:N	2.47	0.48
2:K:491:GLU:HG2	2:K:492:PHE:N	2.27	0.48
2:B:302:ILE:O	2:B:302:ILE:HG13	2.13	0.48
1:J:432:VAL:HG23	1:J:433:ALA:H	1.77	0.48
3:L:517:GLU:N	3:L:517:GLU:OE2	2.45	0.48
1:A:205:PHE:H	2:B:332:TRP:HB2	1.79	0.48
3:F:362:GLU:HG3	3:F:375:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:415:ARG:HG3	3:F:444:VAL:HG11	1.95	0.48
2:H:276:ASN:O	2:H:279:LYS:HB2	2.14	0.48
2:H:310:ASN:HD21	2:H:408:MET:HA	1.77	0.48
3:I:111:TYR:O	3:I:113:LYS:N	2.42	0.48
2:K:531:LYS:O	2:K:535:ILE:HG12	2.13	0.48
3:L:701:ASP:OD2	3:L:703:ARG:HB2	2.14	0.48
4:O:97:ALA:HB1	4:O:111:ASP:CG	2.34	0.48
1:D:324:LYS:NZ	1:D:325:PRO:O	2.32	0.48
3:I:332:ARG:HA	3:I:363:PHE:HD1	1.77	0.48
3:I:530:THR:OG1	3:I:531:TYR:N	2.46	0.48
3:L:189:LYS:O	3:L:193:LEU:HG	2.14	0.48
1:A:407:ILE:HG23	1:A:702:LEU:HD22	1.96	0.48
1:A:422:TRP:CE2	1:A:457:GLU:HB2	2.49	0.48
2:B:266:LEU:HD13	2:B:421:VAL:HG11	1.96	0.48
3:C:28:MET:HG3	3:C:29:ALA:N	2.28	0.48
2:E:588:GLY:HA2	2:E:612:LYS:HB3	1.94	0.48
3:F:129:THR:O	3:F:245:THR:OG1	2.31	0.48
2:H:63:ALA:HB1	2:H:402:SER:HB3	1.96	0.48
1:J:434:PRO:O	1:J:437:TYR:HB2	2.14	0.48
4:P:91:SER:OG	4:P:120:VAL:HG13	2.14	0.48
3:C:567:ASN:O	3:C:567:ASN:ND2	2.42	0.48
2:E:160:SER:OG	2:E:165:ASP:OD2	2.22	0.48
3:F:141:ILE:HB	3:F:220:VAL:O	2.13	0.48
1:G:624:SER:OG	1:G:625:PRO:HD3	2.14	0.48
3:I:6:GLU:HA	3:I:9:ASN:OD1	2.13	0.48
3:I:398:ILE:HD12	3:I:398:ILE:HA	1.61	0.48
1:J:34:LYS:HB2	1:J:200:THR:HA	1.96	0.48
2:K:285:VAL:HG21	2:K:441:LEU:HD11	1.96	0.48
3:L:750:ALA:O	3:L:754:ILE:N	2.32	0.48
1:A:54:ILE:HD11	1:A:75:ARG:HD3	1.96	0.47
2:B:457:GLU:OE1	2:B:457:GLU:N	2.46	0.47
1:D:130:TYR:HB3	1:D:147:ILE:HD13	1.95	0.47
2:E:622:GLY:HA3	3:F:105:MET:SD	2.53	0.47
3:F:506:ASP:OD1	3:F:507:GLN:N	2.46	0.47
1:G:432:VAL:HG11	2:H:602:ARG:HD3	1.95	0.47
3:I:268:ARG:NH1	3:I:521:THR:OG1	2.47	0.47
3:I:452:GLU:OE2	3:I:479:ARG:NH1	2.28	0.47
3:I:626:PRO:HG2	1:J:57:GLN:HG3	1.95	0.47
2:K:738:GLU:OE1	2:K:738:GLU:N	2.47	0.47
3:L:141:ILE:HD13	3:L:221:ALA:HA	1.96	0.47
3:L:230:GLU:HG3	3:L:231:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:421:VAL:HG12	3:L:425:ASN:HA	1.95	0.47
2:E:504:ASN:HA	2:E:507:MET:HB2	1.96	0.47
3:F:347:GLY:H	3:F:414:VAL:HB	1.79	0.47
1:J:81:GLY:C	3:L:754:ILE:HD11	2.35	0.47
4:M:12:VAL:HG22	4:M:13:GLN:H	1.79	0.47
1:A:678:PRO:HA	2:B:485:ASN:HA	1.95	0.47
2:E:555:TYR:OH	2:E:592:SER:HB3	2.13	0.47
1:G:681:PHE:CZ	2:H:484:ILE:HD11	2.50	0.47
2:H:111:MET:HA	2:H:114:VAL:HG22	1.96	0.47
2:H:293:SER:HB2	3:I:452:GLU:HB2	1.95	0.47
1:J:252:GLU:O	1:J:254:ASN:ND2	2.47	0.47
2:K:519:GLU:HG2	2:K:559:TYR:CE2	2.49	0.47
3:L:111:TYR:O	3:L:113:LYS:N	2.41	0.47
2:B:374:ALA:O	2:B:393:ARG:NH2	2.38	0.47
1:D:528:THR:O	1:D:564:TYR:OH	2.27	0.47
1:D:571:SER:H	1:D:574:LYS:HB2	1.80	0.47
3:I:55:TYR:CD1	3:I:92:SER:HB2	2.48	0.47
1:J:477:MET:HG2	1:J:510:HIS:ND1	2.29	0.47
2:K:287:ARG:O	2:K:291:THR:OG1	2.32	0.47
2:K:605:HIS:HB3	3:L:233:HIS:HE1	1.79	0.47
3:L:710:ILE:HD11	3:L:726:ILE:HA	1.97	0.47
2:H:489:THR:HA	2:H:497:TYR:O	2.15	0.47
2:H:710:GLY:N	3:I:26:ASP:OD1	2.34	0.47
3:I:365:MET:HE1	3:I:401:ALA:HB2	1.97	0.47
3:I:375:ARG:HD3	3:I:383:GLN:HE21	1.79	0.47
3:I:597:ARG:NH2	3:I:622:ALA:O	2.42	0.47
2:K:77:ASN:ND2	2:K:479:LYS:HD2	2.30	0.47
4:O:94:TYR:H	4:O:118:GLY:HA3	1.78	0.47
2:B:71:GLY:O	2:B:84:GLN:NE2	2.46	0.47
2:B:210:GLN:O	2:B:211:ARG:NE	2.46	0.47
2:E:119:VAL:HG12	2:E:143:LEU:HD11	1.97	0.47
2:E:129:TYR:OH	2:E:134:ASN:OD1	2.25	0.47
2:E:623:ARG:NE	3:F:102:ASN:HA	2.29	0.47
3:F:237:GLY:HA3	3:F:240:TRP:CE2	2.49	0.47
3:L:408:ASP:HB3	3:L:412:LYS:HZ1	1.79	0.47
3:L:534:SER:CB	3:L:576:GLU:HA	2.39	0.47
4:O:95:TYR:CD1	4:O:115:LEU:HD21	2.50	0.47
1:A:154:GLU:OE2	1:A:168:ARG:NH1	2.48	0.47
1:A:283:LEU:HD12	1:A:524:GLU:HB2	1.97	0.47
2:B:59:THR:OG1	2:B:60:GLU:OE1	2.19	0.47
2:B:285:VAL:O	2:B:289:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:PHE:O	2:B:495:PHE:HB2	2.14	0.47
2:B:558:THR:HG23	3:C:48:LYS:HG2	1.97	0.47
1:D:263:THR:HG23	1:D:716:ARG:HH11	1.80	0.47
1:D:305:TYR:O	1:D:309:LYS:HG2	2.15	0.47
2:E:374:ALA:HA	2:E:393:ARG:HE	1.79	0.47
1:G:76:PHE:HE1	1:G:118:ILE:HD12	1.79	0.47
4:M:67:ARG:NH1	4:M:90:ASP:OD2	2.38	0.47
4:O:100:ARG:NH2	4:O:110:THR:OG1	2.47	0.47
3:F:665:LEU:HB3	3:F:672:ALA:O	2.14	0.47
1:G:55:ASN:HA	1:G:71:LEU:HD11	1.97	0.47
3:I:269:ARG:HG2	3:I:536:MET:HB3	1.96	0.47
1:J:560:PRO:HB2	1:J:562:PHE:CE1	2.50	0.47
2:E:575:GLU:OE2	3:F:101:ARG:NH1	2.48	0.47
3:F:331:LYS:HE2	3:F:490:SER:N	2.28	0.47
3:F:384:LEU:HB3	3:F:478:ILE:HD12	1.97	0.47
2:H:50:SER:HA	2:H:82:TYR:CE1	2.50	0.47
2:H:612:LYS:O	2:H:616:MET:HG3	2.15	0.47
3:I:79:SER:HB3	3:I:90:MET:HB2	1.96	0.47
1:J:587:GLN:HG2	1:J:591:GLN:NE2	2.30	0.47
2:K:746:ILE:HG23	3:L:8:ARG:HD2	1.97	0.47
3:L:398:ILE:HD12	3:L:398:ILE:HA	1.77	0.47
4:N:50:MET:SD	4:N:109:PRO:HB3	2.55	0.47
4:N:52:SER:HB3	4:N:104:ILE:HD11	1.97	0.47
1:A:144:HIS:CE1	1:A:160:ASP:HB3	2.49	0.47
1:A:422:TRP:CZ3	1:A:489:CYS:HB3	2.50	0.47
2:B:285:VAL:HA	2:B:288:LYS:HB2	1.96	0.47
3:C:79:SER:OG	3:C:80:LYS:N	2.48	0.47
3:C:120:GLU:HB3	3:C:124:ARG:NH2	2.29	0.47
3:C:402:MET:O	3:C:405:SER:OG	2.26	0.47
2:E:276:ASN:HB2	3:F:219:PRO:HG3	1.96	0.47
2:E:339:ILE:O	2:E:343:MET:HG3	2.15	0.47
2:H:554:ASP:O	2:H:558:THR:OG1	2.21	0.47
1:J:254:ASN:OD1	1:J:256:LYS:HB2	2.14	0.47
1:J:425:LEU:HD22	1:J:447:THR:HG21	1.96	0.47
2:K:665:SER:OG	3:L:58:THR:O	2.15	0.47
3:L:506:ASP:OD1	3:L:507:GLN:N	2.45	0.47
2:B:531:LYS:O	2:B:535:ILE:HG12	2.16	0.46
1:D:590:GLN:HG3	1:D:591:GLN:N	2.30	0.46
2:E:708:PRO:HA	3:F:728:GLN:HE21	1.80	0.46
3:F:264:ARG:HE	3:F:305:GLU:CD	2.19	0.46
3:F:580:PHE:CE2	3:F:620:PRO:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:571:SER:H	1:G:574:LYS:HB2	1.80	0.46
2:H:519:GLU:HG2	2:H:559:TYR:HE2	1.80	0.46
3:I:591:GLN:OE1	3:I:591:GLN:N	2.39	0.46
1:J:148:PHE:CE1	1:J:154:GLU:HG3	2.49	0.46
1:J:484:PRO:HA	1:J:503:PHE:HD1	1.80	0.46
3:C:42:ASN:HB3	3:C:45:LEU:HB2	1.97	0.46
3:C:371:THR:HG21	3:C:487:GLU:CG	2.45	0.46
2:H:631:PHE:CE2	3:I:96:VAL:HG22	2.50	0.46
3:I:206:MET:HE3	3:I:206:MET:HA	1.96	0.46
3:I:452:GLU:CD	3:I:477:GLY:H	2.18	0.46
1:J:506:LYS:NZ	1:J:507:GLY:O	2.35	0.46
1:J:677:GLU:HG3	2:K:300:PHE:HZ	1.80	0.46
2:K:746:ILE:O	2:K:750:ILE:HG13	2.16	0.46
3:C:403:VAL:HG21	3:C:435:LEU:HA	1.96	0.46
3:C:694:PHE:HB3	3:C:734:VAL:HG13	1.97	0.46
1:D:68:PRO:HB3	1:D:71:LEU:O	2.15	0.46
1:D:283:LEU:HD12	1:D:524:GLU:HB2	1.97	0.46
1:G:646:PHE:O	1:G:650:TYR:HB2	2.15	0.46
2:B:309:TRP:CZ2	2:B:416:SER:HB3	2.47	0.46
2:B:507:MET:CE	2:B:539:LEU:HB3	2.46	0.46
3:C:478:ILE:HD12	3:C:478:ILE:HA	1.74	0.46
2:E:256:GLU:OE1	2:E:414:MET:HB2	2.15	0.46
3:F:395:ALA:O	3:F:398:ILE:HG22	2.15	0.46
1:G:111:ASP:OD1	1:G:113:LYS:N	2.49	0.46
1:G:470:LEU:HG	3:I:49:TRP:HZ2	1.80	0.46
2:H:108:LEU:O	2:H:111:MET:HG2	2.15	0.46
3:I:557:TRP:CZ3	3:I:616:ILE:HD11	2.51	0.46
3:L:611:ASP:OD1	3:L:611:ASP:N	2.46	0.46
2:B:163:LEU:O	2:B:167:LEU:HG	2.16	0.46
2:B:504:ASN:HA	2:B:507:MET:HB2	1.98	0.46
3:C:101:ARG:NE	3:C:102:ASN:OD1	2.30	0.46
3:C:517:GLU:OE1	3:C:517:GLU:N	2.49	0.46
3:I:159:ALA:O	3:I:163:ILE:HG12	2.16	0.46
3:I:753:ARG:HD2	3:I:753:ARG:HA	1.70	0.46
1:J:111:ASP:OD1	1:J:112:TYR:N	2.49	0.46
3:L:323:PHE:HB3	3:L:330:PHE:HB2	1.96	0.46
3:C:318:ARG:HB3	3:C:493:ARG:HB3	1.97	0.46
3:F:164:MET:SD	3:F:168:PHE:HE1	2.38	0.46
3:F:562:ILE:HD12	3:F:563:GLN:N	2.31	0.46
1:G:624:SER:HB3	2:H:2:ASP:H	1.80	0.46
2:H:25:THR:O	2:H:508:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:231:VAL:HG21	3:I:244:TYR:HE2	1.81	0.46
3:I:449:TRP:CD1	3:I:476:ARG:HB3	2.50	0.46
1:J:545:ILE:HD12	1:J:545:ILE:HA	1.82	0.46
4:N:99:ARG:HH12	4:N:104:ILE:HA	1.80	0.46
2:B:712:SER:OG	3:C:730:ASP:HB3	2.16	0.46
3:C:124:ARG:NH2	3:C:149:PRO:HB2	2.31	0.46
3:C:461:ILE:HG13	3:C:480:VAL:HB	1.98	0.46
1:D:178:ILE:O	1:D:182:MET:HG2	2.15	0.46
1:D:413:LYS:NZ	1:D:454:ARG:HH21	2.14	0.46
2:H:309:TRP:CZ2	2:H:416:SER:HB3	2.46	0.46
2:H:713:SER:HA	3:I:24:THR:HA	1.97	0.46
2:K:736:LYS:HB2	2:K:738:GLU:HG2	1.96	0.46
3:L:55:TYR:O	3:L:90:MET:HB3	2.16	0.46
3:L:163:ILE:O	3:L:167:VAL:HG12	2.15	0.46
4:N:18:LEU:HD12	4:N:18:LEU:HA	1.84	0.46
4:O:35:THR:HG22	4:O:50:MET:HG2	1.98	0.46
3:C:318:ARG:NH1	3:C:493:ARG:O	2.48	0.46
2:E:248:ILE:HG21	2:E:344:PHE:CE1	2.51	0.46
2:E:522:ASP:OD2	2:E:559:TYR:OH	2.34	0.46
3:F:129:THR:OG1	3:F:245:THR:OG1	2.24	0.46
1:G:440:SER:HA	1:G:443:ARG:HG2	1.98	0.46
1:J:220:PRO:HG2	1:J:223:PHE:HE2	1.80	0.46
2:B:104:GLU:OE1	2:B:104:GLU:N	2.49	0.46
3:C:264:ARG:NH1	3:C:521:THR:O	2.49	0.46
3:C:297:ILE:O	3:C:301:ASN:N	2.49	0.46
1:D:179:ARG:HG2	1:D:188:TRP:CZ3	2.51	0.46
1:D:324:LYS:HB3	1:D:542:VAL:HG23	1.98	0.46
1:D:442:ARG:HE	1:D:608:THR:HG23	1.81	0.46
1:G:57:GLN:HG2	3:L:601:GLN:OE1	2.15	0.46
1:G:520:PHE:CE1	1:G:568:ASN:HB3	2.51	0.46
2:H:449:LEU:HD22	2:H:466:PHE:CD2	2.51	0.46
3:I:283:MET:O	3:I:287:THR:OG1	2.32	0.46
1:J:423:ILE:HG12	1:J:451:SER:HB2	1.98	0.46
1:J:578:GLY:HA2	1:J:581:MET:HG3	1.98	0.46
3:L:544:SER:OG	3:L:548:ASN:ND2	2.49	0.46
1:A:673:ARG:HG2	1:A:716:ARG:HH22	1.81	0.46
2:E:260:ARG:HA	2:E:414:MET:CE	2.46	0.46
3:F:159:ALA:O	3:F:163:ILE:HG12	2.16	0.46
1:J:607:MET:HG2	1:J:610:GLU:HB2	1.98	0.46
2:K:696:PHE:HZ	3:L:25:VAL:HG13	1.80	0.46
4:M:52:SER:HA	4:M:104:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASP:OD1	1:A:112:TYR:N	2.49	0.45
1:A:242:ILE:HG12	2:B:90:GLU:OE2	2.16	0.45
3:F:515:PRO:O	3:F:516:GLU:HB2	2.16	0.45
1:G:96:ASN:HD21	3:L:275:ASP:CB	2.23	0.45
2:H:519:GLU:CB	2:H:662:THR:HG22	2.46	0.45
3:I:478:ILE:HD12	3:I:478:ILE:HA	1.69	0.45
2:K:125:GLY:HA3	2:K:249:ARG:HH21	1.80	0.45
2:K:413:ASN:HB3	2:K:444:SER:OG	2.16	0.45
3:L:386:VAL:HG21	3:L:398:ILE:HD13	1.97	0.45
1:A:584:CYS:O	1:A:588:SER:OG	2.24	0.45
2:B:397:ILE:O	2:B:400:THR:OG1	2.30	0.45
3:C:111:TYR:O	3:C:113:LYS:N	2.43	0.45
1:D:221:PRO:HD3	2:E:69:ILE:CG2	2.43	0.45
1:D:444:ASN:OD1	1:D:445:TYR:N	2.49	0.45
1:D:617:GLU:HB3	1:D:619:TRP:CZ3	2.51	0.45
2:E:114:VAL:HG12	2:E:254:PHE:CE1	2.51	0.45
1:G:576:LYS:NZ	3:I:42:ASN:OD1	2.38	0.45
2:H:491:GLU:HG2	2:H:492:PHE:N	2.30	0.45
3:I:46:ARG:O	3:I:50:MET:HG3	2.16	0.45
3:I:362:GLU:HG3	3:I:375:ARG:HG2	1.98	0.45
1:A:429:GLY:HA2	2:B:598:LEU:HA	1.99	0.45
2:B:177:GLU:HA	2:B:214:LYS:HB2	1.97	0.45
1:D:170:ARG:HA	3:F:695:LEU:HD22	1.99	0.45
2:E:95:LEU:HD12	2:E:422:SER:CB	2.46	0.45
2:H:703:SER:HB2	3:I:28:MET:SD	2.56	0.45
2:K:219:ILE:HG23	2:K:348:MET:HG3	1.98	0.45
3:L:70:ARG:NH1	3:L:74:GLY:O	2.50	0.45
3:L:449:TRP:HE1	3:L:476:ARG:HB3	1.81	0.45
4:N:36:TRP:CZ3	4:N:96:CYS:HB2	2.51	0.45
4:O:60:TYR:HB3	4:O:64:VAL:HG23	1.98	0.45
1:A:261:LEU:O	1:A:265:PRO:HD3	2.17	0.45
1:A:324:LYS:HD2	1:A:325:PRO:HD2	1.99	0.45
2:B:470:CYS:HB3	2:B:475:ILE:O	2.16	0.45
1:D:34:LYS:HB2	1:D:200:THR:HA	1.97	0.45
2:E:222:LEU:HB3	2:E:347:LYS:HA	1.98	0.45
2:E:600:ASN:O	2:E:604:LEU:HG	2.17	0.45
3:F:497:SER:OG	3:F:505:ARG:O	2.30	0.45
2:H:78:GLU:O	2:H:471:LYS:NZ	2.50	0.45
2:K:457:GLU:N	2:K:457:GLU:OE1	2.49	0.45
3:L:640:VAL:CG2	3:L:645:MET:HG3	2.46	0.45
1:A:422:TRP:CE3	1:A:489:CYS:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:MET:HA	2:B:114:VAL:HG22	1.98	0.45
2:B:276:ASN:O	2:B:279:LYS:HB2	2.17	0.45
2:B:588:GLY:HA3	2:B:616:MET:HA	1.98	0.45
1:D:336:LEU:HD23	1:D:365:GLN:HG2	1.99	0.45
1:D:425:LEU:HD12	1:D:425:LEU:HA	1.82	0.45
2:E:622:GLY:O	2:E:626:ASN:ND2	2.50	0.45
3:F:506:ASP:HB2	3:F:512:LEU:HD11	1.99	0.45
1:G:164:ASP:OD1	1:G:165:GLU:N	2.48	0.45
1:G:444:ASN:OD1	1:G:445:TYR:N	2.49	0.45
1:G:457:GLU:OE2	1:G:501:TYR:OH	2.28	0.45
2:H:336:VAL:HG12	2:H:337:LEU:HD23	1.97	0.45
2:H:620:TYR:HE1	3:I:100:ASN:ND2	2.15	0.45
2:K:108:LEU:HA	2:K:111:MET:HE2	1.98	0.45
2:K:575:GLU:OE2	3:L:101:ARG:NH1	2.49	0.45
3:L:658:TYR:HB2	3:L:665:LEU:HD13	1.97	0.45
3:L:664:ARG:NH2	3:L:671:ASP:OD2	2.49	0.45
1:A:180:GLN:HE22	3:C:174:ALA:H	1.63	0.45
3:C:346:THR:HG23	3:C:350:GLN:O	2.16	0.45
1:D:462:GLY:O	1:D:466:ASN:ND2	2.39	0.45
1:D:463:VAL:HG11	1:D:582:ARG:NH2	2.31	0.45
1:D:652:SER:O	2:E:24:TYR:OH	2.34	0.45
2:E:356:MET:HA	2:E:367:GLN:HA	1.97	0.45
3:F:260:ILE:O	3:F:264:ARG:HG2	2.17	0.45
3:F:629:SER:HB2	3:F:631:MET:HG2	1.98	0.45
1:G:207:ILE:HG22	1:G:212:ARG:HB2	1.98	0.45
1:G:422:TRP:CE2	1:G:457:GLU:HB2	2.52	0.45
1:G:476:ALA:HB3	1:G:506:LYS:HE2	1.99	0.45
1:J:254:ASN:O	2:K:77:ASN:ND2	2.50	0.45
2:K:160:SER:OG	2:K:165:ASP:OD2	2.22	0.45
2:K:598:LEU:HD23	2:K:598:LEU:H	1.81	0.45
3:L:694:PHE:HB3	3:L:735:MET:O	2.17	0.45
3:L:754:ILE:HD12	3:L:754:ILE:HA	1.77	0.45
1:A:575:MET:O	1:A:579:MET:HG3	2.17	0.45
3:F:311:CYS:O	3:F:315:MET:HG2	2.16	0.45
1:G:318:LYS:H	1:G:546:GLY:HA2	1.81	0.45
1:A:53:PHE:CE2	1:A:63:VAL:HG21	2.52	0.45
1:A:130:TYR:CE1	1:A:197:GLY:HA2	2.52	0.45
2:B:626:ASN:ND2	3:C:104:PRO:O	2.50	0.45
3:C:398:ILE:HD12	3:C:398:ILE:HA	1.70	0.45
3:F:415:ARG:HG3	3:F:444:VAL:HG21	1.98	0.45
3:F:753:ARG:HD2	3:F:753:ARG:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:ARG:O	1:G:217:GLN:HG3	2.17	0.45
2:K:519:GLU:O	2:K:555:TYR:OH	2.27	0.45
1:A:314:PHE:HD2	1:A:317:TRP:CZ2	2.35	0.45
2:B:52:LYS:HG3	2:B:72:PRO:HD2	1.99	0.45
2:B:449:LEU:HG	2:B:450:ILE:N	2.32	0.45
3:F:339:LYS:O	3:F:356:VAL:N	2.50	0.45
1:G:283:LEU:O	1:G:461:LYS:NZ	2.49	0.45
1:G:292:ILE:HD11	1:G:310:CYS:SG	2.57	0.45
2:H:316:ARG:NH2	2:H:345:SER:OG	2.50	0.45
3:L:384:LEU:HB3	3:L:478:ILE:HD12	1.98	0.45
3:L:478:ILE:O	3:L:479:ARG:NH1	2.41	0.45
4:O:6:GLU:CG	4:O:117:GLN:H	2.30	0.45
4:O:17:SER:HA	4:O:83:MET:O	2.17	0.45
1:A:318:LYS:NZ	1:A:544:GLU:OE2	2.49	0.45
1:A:444:ASN:OD1	1:A:445:TYR:N	2.49	0.45
3:C:542:PRO:HB2	3:C:640:VAL:HG12	1.98	0.45
1:D:163:LEU:HA	1:D:163:LEU:HD23	1.72	0.45
2:E:52:LYS:HG2	2:E:82:TYR:CZ	2.52	0.45
1:G:252:GLU:O	1:G:254:ASN:ND2	2.50	0.45
2:H:531:LYS:HA	2:H:534:MET:HE3	1.98	0.45
2:H:746:ILE:O	2:H:750:ILE:HG13	2.17	0.45
3:I:472:GLU:HG2	3:I:473:MET:HG3	1.97	0.45
1:J:6:ARG:HD3	3:L:316:GLY:O	2.17	0.45
2:K:248:ILE:H	2:K:248:ILE:HG13	1.60	0.45
2:K:506:SER:HB3	2:K:537:ASN:OD1	2.17	0.45
2:K:514:VAL:O	3:L:44:SER:HB3	2.17	0.45
4:P:37:VAL:HG22	4:P:47:TRP:HA	1.99	0.45
1:A:276:CYS:HB2	1:A:698:PRO:HG3	1.99	0.44
3:C:141:ILE:HG21	3:C:143:ARG:NH2	2.32	0.44
3:C:142:ARG:HB3	3:C:217:PHE:CE1	2.52	0.44
1:D:104:LYS:HD2	1:D:104:LYS:HA	1.75	0.44
3:I:96:VAL:O	3:I:100:ASN:HB2	2.17	0.44
3:I:386:VAL:HG21	3:I:398:ILE:HD13	1.99	0.44
2:K:514:VAL:HA	2:K:551:PHE:HE1	1.81	0.44
3:L:719:GLY:HA2	3:L:736:LYS:HD3	1.98	0.44
4:O:115:LEU:HD13	4:O:116:GLY:N	2.32	0.44
1:A:209:GLY:C	1:A:211:MET:H	2.20	0.44
1:A:310:CYS:O	1:A:313:THR:OG1	2.25	0.44
2:B:449:LEU:HD22	2:B:466:PHE:CD2	2.53	0.44
1:D:362:LYS:HG3	1:D:480:PHE:CE2	2.52	0.44
3:F:461:ILE:HD12	3:F:469:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:16:THR:HA	3:I:19:ILE:HG22	1.98	0.44
1:J:305:TYR:N	1:J:305:TYR:CD1	2.83	0.44
2:K:572:ARG:CZ	3:L:93:PRO:HB2	2.48	0.44
4:O:37:VAL:O	4:O:95:TYR:N	2.50	0.44
2:E:335:ASN:O	2:E:339:ILE:HG12	2.18	0.44
1:G:369:ALA:HB1	1:G:521:VAL:HG21	1.99	0.44
2:H:68:PRO:HG2	2:H:314:ASN:HD21	1.81	0.44
2:H:414:MET:O	2:H:418:VAL:HG23	2.18	0.44
2:H:494:SER:HB2	2:H:505:PHE:HD1	1.83	0.44
2:H:659:ALA:HB1	2:H:663:THR:HB	1.99	0.44
2:K:627:PRO:HD3	3:L:108:THR:HG21	1.99	0.44
2:K:750:ILE:HA	2:K:753:LEU:HD12	2.00	0.44
4:O:43:LYS:HG3	4:O:44:GLY:O	2.18	0.44
1:A:331:ASN:N	1:A:332:PRO:HD2	2.31	0.44
2:B:289:MET:O	2:B:452:ASN:ND2	2.51	0.44
2:B:516:GLY:N	2:B:522:ASP:OD1	2.49	0.44
3:F:478:ILE:HD12	3:F:478:ILE:HA	1.76	0.44
2:H:430:ARG:CZ	3:I:360:TYR:HB3	2.46	0.44
2:H:538:ASP:N	2:H:538:ASP:OD1	2.50	0.44
2:K:503:ALA:HB3	2:K:538:ASP:OD1	2.18	0.44
3:L:318:ARG:HB3	3:L:493:ARG:HB3	1.98	0.44
3:L:534:SER:HB3	3:L:576:GLU:HG3	1.99	0.44
1:A:73:LYS:HD2	1:A:73:LYS:HA	1.73	0.44
1:A:583:ARG:NH2	2:B:511:SER:HA	2.33	0.44
2:B:252:VAL:HG23	2:B:412:PHE:CE1	2.53	0.44
2:B:330:PRO:HB2	2:B:332:TRP:CD1	2.53	0.44
1:G:213:ARG:HD3	2:H:60:GLU:CD	2.38	0.44
1:G:621:ILE:HG21	1:G:636:VAL:HG22	1.98	0.44
2:H:438:TRP:CG	2:H:449:LEU:HD11	2.53	0.44
2:H:686:GLU:HG3	3:I:36:SER:OG	2.18	0.44
3:I:264:ARG:HD3	3:I:518:VAL:CG2	2.48	0.44
3:I:464:LEU:HB3	3:I:465:PRO:HD2	1.99	0.44
1:J:168:ARG:O	1:J:172:LYS:HG3	2.17	0.44
3:L:540:ASN:HD21	3:L:544:SER:HB3	1.82	0.44
1:A:530:PRO:HG3	1:A:542:VAL:HG21	1.99	0.44
2:B:610:CYS:HA	2:B:613:TRP:HB2	1.98	0.44
2:E:252:VAL:HG23	2:E:412:PHE:CE1	2.52	0.44
3:I:193:LEU:HA	3:I:196:CYS:SG	2.57	0.44
1:J:571:SER:H	1:J:574:LYS:HB2	1.83	0.44
2:K:518:ASN:HB3	2:K:521:ALA:HB3	2.00	0.44
3:L:478:ILE:HD12	3:L:478:ILE:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:563:GLN:HB3	3:L:571:LEU:HD12	1.98	0.44
2:B:438:TRP:HB2	2:B:449:LEU:HD11	2.00	0.44
2:B:485:ASN:N	2:B:485:ASN:OD1	2.50	0.44
1:D:54:ILE:HD11	1:D:113:LYS:HG2	2.00	0.44
1:D:207:ILE:HG22	1:D:212:ARG:HB2	1.98	0.44
1:D:529:ASP:HB3	1:D:531:ARG:HG2	2.00	0.44
2:E:66:LEU:HD23	2:E:66:LEU:HA	1.87	0.44
1:J:54:ILE:HD11	1:J:75:ARG:HD3	2.00	0.44
2:K:52:LYS:HD3	2:K:52:LYS:HA	1.84	0.44
2:K:473:VAL:HG23	2:K:475:ILE:HG13	1.99	0.44
3:L:753:ARG:HA	3:L:753:ARG:HD2	1.81	0.44
1:A:630:ASP:OD1	1:A:630:ASP:N	2.44	0.44
3:F:135:PHE:CZ	3:F:240:TRP:HB3	2.53	0.44
3:F:230:GLU:HG3	3:F:231:VAL:HG13	2.00	0.44
3:F:398:ILE:HD12	3:F:398:ILE:HA	1.74	0.44
1:G:54:ILE:HD11	1:G:75:ARG:HD3	2.00	0.44
1:G:111:ASP:OD1	1:G:112:TYR:N	2.50	0.44
1:G:288:LEU:HD22	1:G:527:LEU:HD11	1.99	0.44
1:J:178:ILE:O	1:J:182:MET:HG2	2.18	0.44
2:K:112:GLU:HG2	2:K:116:GLN:HE22	1.81	0.44
1:A:408:GLN:HG3	1:A:412:ASN:ND2	2.32	0.44
3:C:55:TYR:HA	3:C:92:SER:HA	2.00	0.44
3:C:121:LYS:HA	3:C:124:ARG:HD2	2.00	0.44
3:C:710:ILE:HD11	3:C:726:ILE:HA	2.00	0.44
1:D:304:LEU:O	1:D:308:ILE:HG23	2.18	0.44
1:D:309:LYS:HB3	1:D:309:LYS:HE2	1.76	0.44
1:G:523:MET:HB3	1:G:563:LEU:HD11	2.00	0.44
2:H:49:TYR:CE1	2:H:79:PRO:HG2	2.53	0.44
2:H:302:ILE:O	2:H:302:ILE:HG13	2.18	0.44
3:I:385:ILE:HG23	3:I:460:MET:HE1	2.00	0.44
3:I:566:GLN:HG2	3:I:567:ASN:ND2	2.32	0.44
1:J:217:GLN:HE22	2:K:58:ASN:HA	1.82	0.44
3:L:332:ARG:HA	3:L:363:PHE:HD1	1.82	0.44
3:L:428:LEU:HB2	3:L:433:GLN:HG2	1.99	0.44
4:P:18:LEU:HD12	4:P:18:LEU:HA	1.82	0.44
4:P:106:THR:O	4:P:106:THR:OG1	2.34	0.44
1:A:537:TRP:HB3	1:A:540:TYR:HB2	2.00	0.43
2:B:52:LYS:HD3	2:B:52:LYS:HA	1.88	0.43
1:D:260:PHE:CZ	1:D:265:PRO:HG3	2.52	0.43
2:E:80:SER:N	2:E:476:ASN:OD1	2.31	0.43
2:E:735:ILE:HD12	2:E:735:ILE:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:264:ARG:HD3	3:I:518:VAL:HG22	2.00	0.43
1:J:179:ARG:HG2	1:J:188:TRP:CZ3	2.52	0.43
1:J:215:ALA:HA	2:K:342:ILE:HD13	2.00	0.43
1:J:408:GLN:HG3	1:J:412:ASN:ND2	2.33	0.43
2:K:270:GLY:HA2	2:K:281:LYS:NZ	2.33	0.43
4:M:18:LEU:HD12	4:M:18:LEU:HA	1.81	0.43
4:N:52:SER:CB	4:N:104:ILE:HD11	2.48	0.43
2:B:129:TYR:OH	2:B:134:ASN:OD1	2.27	0.43
2:B:697:GLU:HA	2:B:703:SER:OG	2.19	0.43
2:E:50:SER:HA	2:E:82:TYR:CE1	2.53	0.43
3:F:24:THR:OG1	3:F:25:VAL:N	2.51	0.43
3:F:313:ALA:CB	3:F:496:VAL:HG21	2.48	0.43
2:H:527:VAL:HG11	2:H:599:TYR:CD2	2.53	0.43
1:J:354:ILE:HA	1:J:355:PRO:HD3	1.84	0.43
1:J:438:ILE:HG23	1:J:608:THR:HG21	2.00	0.43
1:J:630:ASP:OD1	1:J:630:ASP:N	2.47	0.43
2:K:104:GLU:OE1	2:K:104:GLU:N	2.50	0.43
3:L:281:LEU:HD21	3:L:314:ALA:HB1	1.99	0.43
3:C:537:TRP:CZ3	3:C:548:ASN:HB3	2.53	0.43
3:C:664:ARG:NE	3:C:671:ASP:OD1	2.45	0.43
2:E:52:LYS:HG3	2:E:72:PRO:HD2	2.00	0.43
3:F:751:THR:HA	3:F:754:ILE:HG22	2.00	0.43
1:G:193:GLN:HB3	1:G:201:ILE:O	2.19	0.43
1:G:331:ASN:N	1:G:332:PRO:HD2	2.33	0.43
2:H:86:ASP:N	2:H:86:ASP:OD1	2.50	0.43
3:I:39:GLN:H	3:I:39:GLN:CD	2.22	0.43
3:I:540:ASN:HB2	3:I:544:SER:CB	2.48	0.43
1:J:592:ILE:O	1:J:596:ILE:HG13	2.18	0.43
4:M:106:THR:O	4:M:106:THR:OG1	2.35	0.43
2:B:114:VAL:HG12	2:B:254:PHE:CD1	2.53	0.43
2:B:368:ILE:HD12	2:B:368:ILE:O	2.19	0.43
2:B:534:MET:HE2	2:B:534:MET:HB2	1.85	0.43
1:D:523:MET:HB3	1:D:563:LEU:HD11	2.00	0.43
2:E:313:GLN:HB2	2:E:407:MET:HG2	2.00	0.43
2:E:589:LEU:HA	2:E:620:TYR:HE2	1.82	0.43
2:E:625:CYS:HB2	3:F:111:TYR:CE1	2.52	0.43
2:H:576:LEU:HD12	3:I:97:THR:HG21	1.99	0.43
3:I:395:ALA:O	3:I:399:ILE:HG12	2.17	0.43
2:K:302:ILE:O	2:K:302:ILE:HG13	2.16	0.43
3:L:141:ILE:HG21	3:L:143:ARG:NH2	2.34	0.43
3:L:159:ALA:O	3:L:163:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:176:ILE:HG13	3:L:694:PHE:H	1.83	0.43
1:A:359:ASN:HA	1:A:480:PHE:O	2.19	0.43
1:A:672:LEU:HD12	1:A:716:ARG:NH2	2.33	0.43
3:C:428:LEU:HB2	3:C:433:GLN:HG2	2.01	0.43
1:D:253:VAL:O	2:E:468:ARG:HD3	2.18	0.43
3:F:6:GLU:HA	3:F:9:ASN:OD1	2.19	0.43
1:G:354:ILE:HA	1:G:355:PRO:HD3	1.80	0.43
2:H:104:GLU:OE1	2:H:104:GLU:N	2.51	0.43
2:H:177:GLU:HA	2:H:214:LYS:HB2	2.00	0.43
2:H:449:LEU:HG	2:H:450:ILE:N	2.32	0.43
2:K:89:LEU:HD21	2:K:320:ALA:HB1	2.00	0.43
2:K:605:HIS:HD2	3:L:233:HIS:NE2	2.16	0.43
3:L:456:ASN:ND2	3:L:456:ASN:O	2.51	0.43
1:A:309:LYS:HA	1:A:312:ARG:HB2	2.01	0.43
2:B:589:LEU:HA	2:B:620:TYR:CE2	2.54	0.43
1:G:372:GLU:OE2	1:G:508:ARG:HD2	2.19	0.43
3:I:712:GLU:O	3:I:716:LEU:N	2.52	0.43
2:K:746:ILE:HG12	3:L:8:ARG:HH11	1.84	0.43
3:L:428:LEU:HB2	3:L:433:GLN:HE21	1.84	0.43
3:L:595:PHE:O	3:L:598:THR:HG22	2.18	0.43
2:B:52:LYS:HG2	2:B:82:TYR:CZ	2.53	0.43
2:B:347:LYS:NZ	2:B:403:LEU:O	2.40	0.43
1:D:205:PHE:H	2:E:332:TRP:HB2	1.82	0.43
1:D:431:ASP:OD1	4:N:54:ASN:ND2	2.51	0.43
2:E:291:THR:OG1	3:F:383:GLN:NE2	2.51	0.43
3:F:134:HIS:HE1	3:F:241:GLU:CB	2.32	0.43
3:F:167:VAL:HG13	3:F:168:PHE:CD2	2.54	0.43
1:G:163:LEU:HA	1:G:163:LEU:HD23	1.77	0.43
1:G:179:ARG:HG2	1:G:188:TRP:CZ3	2.54	0.43
1:G:431:ASP:HB2	4:O:53:ASN:HB2	2.00	0.43
2:H:248:ILE:H	2:H:248:ILE:HG13	1.62	0.43
2:H:330:PRO:O	2:H:334:ARG:HG3	2.18	0.43
3:I:142:ARG:HB2	3:I:487:GLU:O	2.18	0.43
1:J:274:PRO:O	1:J:402:SER:N	2.47	0.43
2:K:59:THR:OG1	2:K:60:GLU:OE1	2.37	0.43
2:K:318:PHE:HA	2:K:321:MET:HG2	2.00	0.43
2:K:703:SER:HA	2:K:708:PRO:HG3	2.01	0.43
3:L:282:GLU:OE1	3:L:533:SER:OG	2.37	0.43
3:L:542:PRO:HB2	3:L:583:LEU:HD21	2.01	0.43
2:B:273:VAL:HB	2:B:277:GLU:HG3	2.00	0.43
2:B:589:LEU:HA	2:B:620:TYR:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:LEU:O	1:G:265:PRO:HD3	2.19	0.43
2:H:579:LEU:HG	3:I:101:ARG:HG3	2.00	0.43
3:I:712:GLU:HA	3:I:715:ASN:HB2	2.00	0.43
1:A:309:LYS:HB3	1:A:309:LYS:HE2	1.80	0.43
1:A:401:ARG:NH1	1:A:696:ASN:HD22	2.17	0.43
2:B:738:GLU:OE1	2:B:738:GLU:N	2.48	0.43
2:E:252:VAL:HG23	2:E:412:PHE:HE1	1.84	0.43
2:E:336:VAL:HG12	2:E:337:LEU:HD23	2.01	0.43
3:F:111:TYR:O	3:F:113:LYS:N	2.41	0.43
3:F:730:ASP:OD1	3:F:730:ASP:N	2.37	0.43
1:G:8:CYS:O	1:G:174:ARG:NH2	2.52	0.43
1:G:592:ILE:O	1:G:596:ILE:HG13	2.19	0.43
2:H:163:LEU:O	2:H:167:LEU:HG	2.18	0.43
3:L:540:ASN:HD21	3:L:544:SER:CB	2.31	0.43
1:A:148:PHE:CE1	1:A:154:GLU:HB2	2.53	0.43
2:B:629:ASN:HA	2:B:630:PRO:HD3	1.85	0.43
3:C:365:MET:HE1	3:C:401:ALA:HB2	2.01	0.43
3:C:395:ALA:O	3:C:399:ILE:HG12	2.19	0.43
3:C:403:VAL:HG11	3:C:435:LEU:HB2	2.01	0.43
3:C:435:LEU:O	3:C:439:GLN:HG3	2.19	0.43
1:D:590:GLN:O	1:D:594:SER:N	2.34	0.43
3:F:348:ASN:ND2	3:F:417:ASP:HA	2.34	0.43
2:H:261:SER:O	2:H:265:LYS:NZ	2.36	0.43
1:J:443:ARG:HB3	2:K:542:ALA:HB1	2.00	0.43
1:J:591:GLN:O	1:J:595:MET:HG3	2.18	0.43
3:L:24:THR:OG1	3:L:25:VAL:N	2.52	0.43
4:M:43:LYS:HG3	4:M:44:GLY:O	2.19	0.43
1:A:178:ILE:O	1:A:182:MET:HG2	2.19	0.42
1:A:298:GLU:HG3	1:A:488:LYS:NZ	2.34	0.42
2:B:306:ASN:HB3	2:B:309:TRP:HB2	2.00	0.42
2:B:349:ALA:HB3	2:B:401:ALA:HB3	2.01	0.42
2:B:622:GLY:HA3	3:C:105:MET:SD	2.59	0.42
1:D:34:LYS:HD2	1:D:200:THR:HB	2.01	0.42
1:D:658:PHE:CD1	1:D:694:LEU:HD11	2.54	0.42
2:E:584:ARG:NH2	2:E:617:ASP:HB3	2.34	0.42
3:F:313:ALA:HB1	3:F:496:VAL:HG21	2.00	0.42
2:H:41:ASP:O	2:H:45:ARG:HG3	2.19	0.42
2:H:324:TYR:O	2:H:327:LYS:HB2	2.18	0.42
3:I:499:ASP:OD2	3:I:503:ARG:HB2	2.18	0.42
2:K:249:ARG:HA	2:K:252:VAL:HG12	2.00	0.42
2:E:251:PHE:HB2	2:E:340:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:68:PRO:O	3:F:77:LEU:HD11	2.19	0.42
3:F:428:LEU:HB2	3:F:433:GLN:HE21	1.84	0.42
3:F:591:GLN:OE1	3:F:591:GLN:N	2.42	0.42
1:G:124:ARG:NH2	1:G:190:SER:OG	2.52	0.42
1:G:590:GLN:O	1:G:594:SER:N	2.37	0.42
2:H:52:LYS:HG3	2:H:72:PRO:HD2	2.00	0.42
2:H:623:ARG:NE	3:I:102:ASN:HA	2.34	0.42
2:H:708:PRO:HA	3:I:728:GLN:HE21	1.85	0.42
3:I:745:THR:O	3:I:749:THR:HG23	2.19	0.42
3:L:358:ASP:HA	3:L:378:THR:HB	2.01	0.42
1:A:296:SER:N	1:A:496:ARG:HH11	2.17	0.42
2:B:50:SER:HB3	2:B:68:PRO:HG3	2.01	0.42
2:B:506:SER:HB3	2:B:537:ASN:OD1	2.19	0.42
3:C:508:ARG:HH12	3:C:510:ASN:CG	2.23	0.42
1:D:354:ILE:HA	1:D:355:PRO:HD3	1.81	0.42
3:F:421:VAL:HG12	3:F:425:ASN:HA	2.00	0.42
3:F:429:ASN:HB2	3:F:430:PRO:HD2	2.01	0.42
2:H:510:PRO:HG3	2:H:529:VAL:HG12	2.01	0.42
1:J:124:ARG:HD3	1:J:194:SER:HB3	2.02	0.42
1:J:336:LEU:HD23	1:J:365:GLN:HG2	2.01	0.42
1:J:589:LEU:HD23	2:K:543:THR:HA	2.01	0.42
1:J:685:GLY:HA3	2:K:480:LYS:HG2	1.99	0.42
2:K:249:ARG:O	2:K:252:VAL:HG12	2.18	0.42
3:L:407:GLU:OE1	3:L:476:ARG:NH2	2.52	0.42
1:A:130:TYR:HD2	1:A:147:ILE:HD13	1.84	0.42
1:D:477:MET:HA	1:D:509:SER:OG	2.20	0.42
1:D:492:LYS:HD2	1:D:492:LYS:HA	1.83	0.42
2:E:287:ARG:HH22	3:F:485:VAL:HA	1.85	0.42
2:E:612:LYS:O	2:E:616:MET:HG3	2.19	0.42
3:F:502:LEU:O	3:F:515:PRO:HD3	2.19	0.42
3:I:287:THR:OG1	3:I:533:SER:OG	2.24	0.42
2:K:414:MET:O	2:K:418:VAL:HG23	2.20	0.42
1:A:354:ILE:HA	1:A:355:PRO:HD3	1.82	0.42
2:B:563:ARG:HD3	2:B:566:THR:HG23	2.01	0.42
2:E:19:SER:HB3	2:E:504:ASN:ND2	2.34	0.42
3:F:142:ARG:HB2	3:F:487:GLU:O	2.20	0.42
3:F:384:LEU:HD23	3:F:478:ILE:HD11	2.02	0.42
3:F:390:ASP:HB2	3:F:393:SER:OG	2.20	0.42
1:G:193:GLN:HE21	1:G:203:GLU:CG	2.31	0.42
1:G:314:PHE:HD2	1:G:317:TRP:CZ2	2.38	0.42
1:G:607:MET:HE3	1:G:607:MET:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:ASP:OD2	3:I:30:ILE:HA	2.18	0.42
3:I:436:ARG:NH2	3:I:516:GLU:O	2.52	0.42
1:J:318:LYS:H	1:J:546:GLY:HA2	1.85	0.42
1:J:331:ASN:N	1:J:332:PRO:HD2	2.35	0.42
1:J:620:PRO:HB3	1:J:628:VAL:HG13	2.01	0.42
2:K:95:LEU:HD12	2:K:422:SER:CB	2.50	0.42
2:K:114:VAL:HG12	2:K:254:PHE:CD1	2.54	0.42
2:K:625:CYS:HB3	3:L:111:TYR:CZ	2.54	0.42
4:M:22:CYS:HB3	4:M:79:LEU:HB3	2.02	0.42
1:A:420:SER:HB3	1:A:489:CYS:HB2	2.01	0.42
1:A:428:ILE:HA	2:B:597:ASN:ND2	2.34	0.42
2:B:527:VAL:HG11	2:B:599:TYR:CD2	2.54	0.42
2:B:585:SER:HB3	2:B:617:ASP:OD1	2.20	0.42
3:C:462:GLY:HA3	3:C:474:SER:HB3	2.02	0.42
2:E:271:LEU:N	2:E:272:PRO:HD2	2.35	0.42
3:L:333:THR:OG1	3:L:364:THR:HG23	2.20	0.42
1:A:438:ILE:HG23	1:A:608:THR:HG21	2.02	0.42
2:B:182:THR:C	2:B:209:LYS:HD2	2.40	0.42
2:B:660:VAL:O	2:B:663:THR:OG1	2.23	0.42
3:C:500:ARG:CZ	3:C:500:ARG:HB3	2.48	0.42
1:D:434:PRO:HB3	3:F:242:GLN:OE1	2.20	0.42
2:E:248:ILE:H	2:E:248:ILE:HG13	1.65	0.42
2:E:310:ASN:ND2	2:E:407:MET:HG3	2.35	0.42
2:E:350:ARG:NH2	2:E:352:GLY:HA2	2.34	0.42
2:H:485:ASN:N	2:H:485:ASN:OD1	2.53	0.42
1:J:445:TYR:HD2	1:J:612:PHE:CD2	2.38	0.42
1:J:639:THR:HG22	2:K:5:PRO:HB3	2.01	0.42
2:K:86:ASP:OD1	2:K:86:ASP:N	2.53	0.42
2:K:518:ASN:ND2	2:K:663:THR:HA	2.34	0.42
3:L:504:VAL:O	3:L:512:LEU:N	2.45	0.42
3:L:751:THR:HA	3:L:754:ILE:HG22	2.02	0.42
4:M:36:TRP:CZ3	4:M:96:CYS:HB2	2.54	0.42
1:A:144:HIS:CE1	1:A:157:THR:HB	2.55	0.42
3:C:193:LEU:HA	3:C:196:CYS:SG	2.60	0.42
1:D:164:ASP:OD1	1:D:165:GLU:N	2.46	0.42
3:F:153:ASP:OD2	3:F:301:ASN:ND2	2.52	0.42
3:F:611:ASP:OD1	3:F:611:ASP:N	2.43	0.42
1:G:292:ILE:HD13	1:G:309:LYS:HG3	2.02	0.42
3:L:235:THR:O	3:L:241:GLU:HA	2.20	0.42
3:L:351:THR:O	3:L:352:LEU:HD12	2.20	0.42
2:B:79:PRO:HA	2:B:471:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:MET:O	2:B:418:VAL:HG23	2.20	0.42
3:F:129:THR:HG1	3:F:245:THR:HG1	1.62	0.42
2:H:738:GLU:OE1	2:H:738:GLU:N	2.50	0.42
1:J:426:ASP:OD1	2:K:553:LYS:HB2	2.20	0.42
1:J:431:ASP:HB3	1:J:437:TYR:CD1	2.55	0.42
3:L:142:ARG:HB3	3:L:217:PHE:HE1	1.83	0.42
3:L:379:ARG:HG2	3:L:406:GLN:O	2.20	0.42
4:M:108:GLN:OE1	4:M:108:GLN:N	2.52	0.42
1:A:119:GLU:OE1	1:A:145:ILE:HG23	2.20	0.42
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.76	0.42
3:C:600:PHE:O	3:C:604:ARG:HG3	2.19	0.42
3:C:738:LYS:HD3	3:C:738:LYS:HA	1.89	0.42
1:D:54:ILE:HD13	1:D:54:ILE:HA	1.90	0.42
1:D:75:ARG:HG3	1:D:76:PHE:CD2	2.55	0.42
1:D:217:GLN:OE1	2:E:59:THR:HG23	2.20	0.42
1:D:310:CYS:O	1:D:313:THR:OG1	2.29	0.42
2:E:664:HIS:HD2	3:F:57:ILE:HG13	1.84	0.42
1:G:345:LEU:HD11	1:G:503:PHE:HE2	1.85	0.42
1:G:433:ALA:HB2	3:I:130:PHE:CG	2.55	0.42
2:H:151:ARG:HH21	3:I:18:GLU:HG3	1.85	0.42
2:H:316:ARG:H	2:H:316:ARG:HG2	1.56	0.42
3:I:292:THR:OG1	3:I:297:ILE:HD11	2.20	0.42
3:I:421:VAL:HG12	3:I:425:ASN:HA	2.01	0.42
1:J:164:ASP:OD1	1:J:165:GLU:N	2.51	0.42
1:J:417:LEU:HD13	1:J:638:ARG:HD3	2.02	0.42
1:J:681:PHE:HB2	2:K:479:LYS:O	2.19	0.42
3:L:562:ILE:HD12	3:L:563:GLN:N	2.33	0.42
1:A:242:ILE:O	1:A:246:LEU:HG	2.19	0.41
1:A:583:ARG:HH22	2:B:511:SER:HA	1.85	0.41
2:B:162:ARG:H	2:B:162:ARG:HG2	1.74	0.41
3:C:148:ASN:HB3	3:C:151:HIS:CE1	2.55	0.41
3:C:420:PHE:CE2	3:C:437:HIS:HB2	2.55	0.41
2:E:70:ASP:OD2	2:E:85:THR:OG1	2.36	0.41
2:E:311:GLU:OE1	2:E:311:GLU:N	2.50	0.41
3:F:163:ILE:O	3:F:167:VAL:HG12	2.20	0.41
1:G:434:PRO:HB2	3:I:133:VAL:CG2	2.50	0.41
2:H:114:VAL:HG12	2:H:254:PHE:CE1	2.55	0.41
2:H:249:ARG:O	2:H:252:VAL:HG12	2.20	0.41
2:H:438:TRP:HB2	2:H:449:LEU:HD11	2.02	0.41
2:H:514:VAL:HG21	2:H:559:TYR:HE1	1.85	0.41
2:H:693:CYS:SG	3:I:32:LYS:HA	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:63:ILE:H	3:I:63:ILE:HG13	1.65	0.41
3:I:135:PHE:CE1	3:I:240:TRP:HB3	2.55	0.41
1:J:53:PHE:CE2	1:J:63:VAL:HG11	2.55	0.41
1:J:163:LEU:HD23	1:J:163:LEU:HA	1.76	0.41
1:J:462:GLY:O	1:J:466:ASN:ND2	2.42	0.41
1:J:543:LEU:HD12	1:J:563:LEU:HD23	2.02	0.41
2:K:590:LEU:HD23	2:K:612:LYS:HD2	2.01	0.41
3:L:131:GLY:H	3:L:242:GLN:NE2	2.18	0.41
3:L:319:ILE:HD12	3:L:320:SER:O	2.20	0.41
3:L:744:LEU:HB2	3:L:745:THR:H	1.76	0.41
1:A:124:ARG:HD3	1:A:194:SER:HB3	2.02	0.41
1:A:312:ARG:HG3	2:H:569:GLN:OE1	2.19	0.41
2:B:276:ASN:HB2	3:C:219:PRO:HG3	2.01	0.41
3:C:753:ARG:HA	3:C:753:ARG:HD2	1.73	0.41
1:D:474:CYS:HB2	3:F:49:TRP:CH2	2.55	0.41
1:G:180:GLN:NE2	3:I:174:ALA:H	2.18	0.41
1:G:352:GLU:HG3	1:G:353:LYS:HG3	2.01	0.41
1:G:450:VAL:HG13	1:G:641:LEU:HD22	2.02	0.41
1:G:477:MET:HA	1:G:509:SER:OG	2.19	0.41
2:H:690:GLN:O	2:H:694:ASN:ND2	2.39	0.41
1:J:189:ASP:HA	2:K:162:ARG:NH1	2.31	0.41
3:L:544:SER:HA	3:L:547:VAL:HG22	2.02	0.41
3:L:567:ASN:O	3:L:567:ASN:ND2	2.51	0.41
1:A:166:GLU:OE2	3:C:738:LYS:HB2	2.20	0.41
1:A:261:LEU:O	1:A:264:THR:OG1	2.35	0.41
2:B:212:VAL:HB	2:B:216:SER:HB3	2.02	0.41
3:C:225:SER:O	3:C:229:ILE:HG12	2.20	0.41
3:C:562:ILE:HD12	3:C:563:GLN:N	2.34	0.41
3:C:629:SER:HB2	3:C:631:MET:HG2	2.02	0.41
1:D:431:ASP:OD2	1:D:440:SER:OG	2.37	0.41
3:F:506:ASP:HB2	3:F:512:LEU:CD1	2.50	0.41
1:G:185:ARG:HE	3:I:157:LYS:HE2	1.84	0.41
3:I:120:GLU:HB3	3:I:124:ARG:CZ	2.51	0.41
3:I:707:ALA:HA	3:I:723:ASN:OD1	2.20	0.41
2:K:424:LEU:HA	2:K:438:TRP:HE1	1.85	0.41
3:L:542:PRO:HA	3:L:545:VAL:HG23	2.01	0.41
1:A:6:ARG:HD3	3:C:316:GLY:O	2.20	0.41
1:D:359:ASN:HA	1:D:480:PHE:O	2.21	0.41
2:E:738:GLU:OE1	2:E:738:GLU:N	2.51	0.41
3:F:39:GLN:H	3:F:39:GLN:CD	2.23	0.41
3:F:134:HIS:CE1	3:F:241:GLU:CG	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:285:HIS:ND1	3:F:295:VAL:HG11	2.35	0.41
3:F:301:ASN:OD1	3:F:303:THR:OG1	2.21	0.41
3:F:366:VAL:HA	3:F:371:THR:HG22	2.02	0.41
1:G:540:TYR:CD2	1:G:566:ARG:HB3	2.55	0.41
3:I:128:GLY:HA3	3:I:244:TYR:HE1	1.86	0.41
3:I:320:SER:OG	3:I:321:SER:N	2.53	0.41
3:L:54:LYS:H	3:L:54:LYS:HG2	1.55	0.41
3:L:261:ILE:HG12	3:L:522:GLN:HE21	1.86	0.41
1:A:589:LEU:HD23	2:B:543:THR:HA	2.02	0.41
2:B:249:ARG:O	2:B:252:VAL:HG12	2.20	0.41
1:D:583:ARG:NH2	2:E:511:SER:HA	2.36	0.41
3:F:735:MET:HG2	3:F:736:LYS:H	1.86	0.41
2:H:429:LYS:HG3	2:H:430:ARG:NH2	2.36	0.41
2:H:707:ARG:HA	2:H:708:PRO:HD3	1.94	0.41
2:K:485:ASN:OD1	2:K:485:ASN:N	2.53	0.41
2:K:708:PRO:HB3	3:L:728:GLN:HG3	2.01	0.41
3:L:515:PRO:O	3:L:517:GLU:N	2.53	0.41
4:N:12:VAL:HG22	4:N:13:GLN:H	1.85	0.41
1:A:257:ILE:HD13	2:B:460:GLN:HG3	2.02	0.41
2:B:170:VAL:HG11	2:B:247:GLN:HB3	2.02	0.41
2:E:260:ARG:HA	2:E:414:MET:HE1	2.02	0.41
2:E:298:LEU:HD12	2:E:456:HIS:N	2.36	0.41
2:E:664:HIS:CD2	3:F:57:ILE:HG13	2.56	0.41
3:F:172:VAL:HG12	3:F:710:ILE:HD13	2.02	0.41
2:H:70:ASP:HA	2:H:84:GLN:HA	2.02	0.41
2:H:268:GLN:NE2	2:H:425:ASN:OD1	2.34	0.41
2:H:273:VAL:HB	2:H:277:GLU:HG3	2.02	0.41
1:J:75:ARG:HG3	1:J:76:PHE:CD2	2.56	0.41
2:K:111:MET:O	2:K:114:VAL:HG22	2.20	0.41
2:K:579:LEU:HD23	2:K:579:LEU:HA	1.86	0.41
2:K:622:GLY:HA3	3:L:105:MET:SD	2.61	0.41
2:K:693:CYS:HB3	3:L:32:LYS:HD3	2.02	0.41
2:K:696:PHE:CZ	3:L:25:VAL:HG13	2.56	0.41
1:A:596:ILE:O	1:A:600:SER:OG	2.19	0.41
2:B:571:ARG:HE	2:B:571:ARG:HB2	1.63	0.41
3:C:438:PHE:O	3:C:442:ALA:HB2	2.19	0.41
1:D:182:MET:O	1:D:187:LEU:N	2.43	0.41
1:D:585:LEU:HD23	1:D:641:LEU:HD13	2.01	0.41
3:F:134:HIS:CE1	3:F:241:GLU:CB	3.03	0.41
3:F:342:GLU:O	3:F:353:LYS:HA	2.21	0.41
3:F:464:LEU:HB3	3:F:465:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:313:GLN:HB3	2:H:318:PHE:CE2	2.51	0.41
3:I:449:TRP:NE1	3:I:476:ARG:HB3	2.36	0.41
1:J:113:LYS:HE3	1:J:113:LYS:HB3	1.93	0.41
1:J:150:PHE:HB3	1:J:179:ARG:HB2	2.02	0.41
1:J:533:GLU:O	1:J:537:TRP:NE1	2.54	0.41
2:K:95:LEU:HD12	2:K:422:SER:HB3	2.03	0.41
2:K:111:MET:O	2:K:115:GLN:HG3	2.21	0.41
3:L:79:SER:OG	3:L:80:LYS:N	2.52	0.41
4:O:37:VAL:O	4:O:95:TYR:HB2	2.20	0.41
1:A:290:LEU:HB2	1:A:500:LEU:HB3	2.02	0.41
3:C:320:SER:HA	3:C:492:GLU:O	2.20	0.41
1:D:180:GLN:NE2	3:F:174:ALA:H	2.19	0.41
1:D:672:LEU:HD23	1:D:678:PRO:HD2	2.02	0.41
2:E:415:LEU:HD12	2:E:418:VAL:HB	2.03	0.41
3:F:110:HIS:CE1	3:F:196:CYS:HB3	2.56	0.41
1:G:529:ASP:HA	1:G:562:PHE:CE2	2.56	0.41
1:A:590:GLN:HG3	1:A:591:GLN:N	2.36	0.41
2:B:721:ARG:NH2	3:C:709:SER:OG	2.48	0.41
3:C:739:ARG:HD3	3:C:739:ARG:HA	1.93	0.41
1:D:125:ARG:HE	1:D:129:ILE:HB	1.86	0.41
1:D:426:ASP:OD1	2:E:553:LYS:HB2	2.20	0.41
1:D:550:LEU:O	1:D:556:GLN:HA	2.21	0.41
2:E:316:ARG:H	2:E:316:ARG:HG2	1.54	0.41
2:E:419:LEU:O	2:E:422:SER:OG	2.24	0.41
2:E:491:GLU:HA	2:E:495:PHE:O	2.21	0.41
2:E:578:LYS:HE3	2:E:578:LYS:HB3	1.96	0.41
2:E:751:GLU:O	2:E:754:ARG:HG2	2.21	0.41
1:G:90:VAL:O	1:G:94:ILE:HG12	2.20	0.41
1:G:193:GLN:O	1:G:201:ILE:HG12	2.21	0.41
1:G:362:LYS:HA	1:G:480:PHE:HE2	1.85	0.41
1:G:401:ARG:HH11	1:G:696:ASN:HB2	1.85	0.41
1:G:408:GLN:HG3	1:G:412:ASN:HD21	1.85	0.41
2:H:518:ASN:O	2:H:522:ASP:HB2	2.20	0.41
3:I:256:ASP:OD2	3:I:303:THR:OG1	2.39	0.41
3:I:407:GLU:OE1	3:I:476:ARG:NH2	2.54	0.41
3:I:581:GLN:HG2	3:I:589:ARG:HD3	2.01	0.41
3:I:738:LYS:HE2	3:I:738:LYS:HB3	1.88	0.41
1:J:526:SER:OG	1:J:527:LEU:N	2.54	0.41
2:K:25:THR:HG23	2:K:509:LEU:HD21	2.02	0.41
2:K:336:VAL:HG12	2:K:337:LEU:HD23	2.02	0.41
1:A:323:VAL:HG11	1:A:531:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:SER:OG	1:A:527:LEU:N	2.53	0.41
1:D:209:GLY:C	1:D:211:MET:H	2.24	0.41
2:E:86:ASP:OD1	2:E:86:ASP:N	2.53	0.41
2:E:268:GLN:HB2	2:E:421:VAL:HG13	2.02	0.41
2:E:269:SER:HB2	2:E:421:VAL:HG21	2.03	0.41
2:E:507:MET:CE	2:E:539:LEU:HB3	2.51	0.41
2:E:572:ARG:NH2	3:F:97:THR:OG1	2.42	0.41
1:G:670:GLN:HG2	2:H:14:ALA:H	1.85	0.41
2:H:102:ILE:HD11	2:H:265:LYS:HB2	2.02	0.41
2:H:303:THR:OG1	2:H:490:PHE:HB2	2.21	0.41
2:H:550:LEU:HD23	2:H:550:LEU:HA	1.86	0.41
2:H:591:VAL:HG23	2:H:612:LYS:HZ1	1.86	0.41
2:H:604:LEU:HD23	2:H:604:LEU:HA	1.88	0.41
3:I:421:VAL:HG11	3:I:425:ASN:OD1	2.21	0.41
1:J:228:ASN:OD1	1:J:228:ASN:N	2.54	0.41
1:J:425:LEU:CD2	1:J:447:THR:HG21	2.51	0.41
3:L:41:LYS:HE3	3:L:41:LYS:HB3	1.92	0.41
4:O:18:LEU:HD12	4:O:18:LEU:HA	1.92	0.41
1:A:33:ASN:ND2	1:A:193:GLN:HG2	2.34	0.40
2:B:120:ASP:OD2	3:C:30:ILE:HA	2.21	0.40
3:C:142:ARG:HH21	3:C:488:TYR:HB2	1.86	0.40
1:D:168:ARG:O	1:D:172:LYS:HG3	2.20	0.40
1:D:287:ALA:HA	1:D:525:PHE:O	2.21	0.40
1:D:310:CYS:SG	1:D:500:LEU:HB2	2.62	0.40
2:E:52:LYS:HD3	2:E:52:LYS:HA	1.83	0.40
2:E:302:ILE:O	2:E:302:ILE:HG13	2.20	0.40
2:E:485:ASN:OD1	2:E:485:ASN:N	2.54	0.40
3:F:142:ARG:HB3	3:F:217:PHE:CE1	2.50	0.40
3:F:462:GLY:O	3:F:469:PRO:HA	2.21	0.40
1:G:590:GLN:HB3	2:H:543:THR:HG21	2.03	0.40
2:H:258:LEU:HD21	2:H:325:ILE:HG21	2.02	0.40
2:H:419:LEU:O	2:H:423:ILE:HG23	2.21	0.40
3:I:321:SER:O	3:I:512:LEU:HD22	2.21	0.40
1:J:582:ARG:HE	2:K:550:LEU:HD21	1.85	0.40
2:K:66:LEU:HD23	2:K:66:LEU:HA	1.88	0.40
2:K:538:ASP:OD2	3:L:238:THR:HG22	2.20	0.40
2:K:738:GLU:CD	2:K:738:GLU:H	2.20	0.40
3:L:611:ASP:HB2	3:L:613:THR:HG22	2.03	0.40
4:P:12:VAL:HG22	4:P:13:GLN:H	1.85	0.40
1:A:111:ASP:OD1	1:A:113:LYS:N	2.54	0.40
3:C:560:VAL:O	3:C:564:TRP:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:GLY:O	2:E:84:GLN:NE2	2.45	0.40
2:E:225:ASN:ND2	2:E:350:ARG:HD3	2.36	0.40
3:F:754:ILE:HD12	3:F:754:ILE:HA	1.80	0.40
3:I:498:ILE:HD11	3:I:502:LEU:HA	2.02	0.40
1:J:358:LYS:HD2	1:J:358:LYS:HA	1.75	0.40
1:J:621:ILE:HG21	1:J:636:VAL:HG22	2.03	0.40
2:K:707:ARG:HA	2:K:708:PRO:HD3	1.95	0.40
1:A:571:SER:H	1:A:574:LYS:HB2	1.87	0.40
2:B:167:LEU:HD22	2:B:251:PHE:CZ	2.57	0.40
3:C:449:TRP:CD1	3:C:476:ARG:HB3	2.56	0.40
2:E:102:ILE:HG23	2:E:103:PHE:CD1	2.56	0.40
2:E:225:ASN:ND2	2:E:350:ARG:HH21	2.18	0.40
2:E:626:ASN:HA	2:E:627:PRO:HD3	1.97	0.40
2:H:222:LEU:HD13	2:H:346:ASN:O	2.21	0.40
1:J:34:LYS:HE2	1:J:38:ILE:HD11	2.04	0.40
1:J:587:GLN:C	1:J:591:GLN:HE21	2.21	0.40
3:L:160:GLN:HA	3:L:163:ILE:HG12	2.02	0.40
3:L:577:PHE:O	3:L:581:GLN:N	2.30	0.40
1:A:73:LYS:HE3	1:A:112:TYR:CE2	2.54	0.40
1:A:323:VAL:CG1	1:A:531:ARG:HH21	2.35	0.40
3:C:443:LYS:HA	3:C:446:PHE:HD2	1.87	0.40
1:D:309:LYS:HA	1:D:312:ARG:HB2	2.04	0.40
1:D:495:ARG:HH11	4:N:85:ASN:HB2	1.86	0.40
2:E:163:LEU:O	2:E:167:LEU:HG	2.21	0.40
2:E:222:LEU:HD13	2:E:346:ASN:O	2.21	0.40
2:E:725:ASP:HA	2:E:728:ILE:HG12	2.04	0.40
3:F:147:ILE:HD11	3:F:216:ARG:NE	2.29	0.40
3:F:412:LYS:O	3:F:415:ARG:NH1	2.43	0.40
3:F:600:PHE:O	3:F:604:ARG:HG3	2.21	0.40
1:G:408:GLN:HG3	1:G:412:ASN:ND2	2.36	0.40
3:I:352:LEU:HD23	3:I:352:LEU:HA	1.93	0.40
2:K:307:THR:H	2:K:478:SER:HB2	1.86	0.40
2:K:725:ASP:HA	2:K:728:ILE:HG12	2.04	0.40
3:L:586:LYS:HG2	3:L:589:ARG:NH2	2.37	0.40
1:A:597:GLU:O	1:A:601:SER:N	2.54	0.40
1:D:331:ASN:N	1:D:332:PRO:HD2	2.36	0.40
2:E:111:MET:HG2	2:E:333:PHE:CD1	2.57	0.40
3:F:534:SER:HA	3:F:537:TRP:CD2	2.56	0.40
2:H:69:ILE:HD13	2:H:317:MET:HB2	2.03	0.40
2:H:563:ARG:HG3	2:H:565:ASP:H	1.87	0.40
3:I:110:HIS:CE1	3:I:196:CYS:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:415:CYS:SG	1:J:639:THR:HA	2.61	0.40
1:J:440:SER:HA	1:J:443:ARG:HG2	2.03	0.40
3:L:115:TYR:OH	3:L:202:MET:SD	2.80	0.40
3:L:172:VAL:O	3:L:727:GLY:HA2	2.22	0.40
4:O:53:ASN:ND2	4:O:102:GLY:O	2.54	0.40
4:P:97:ALA:HB1	4:P:111:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	687/716 (96%)	638 (93%)	49 (7%)	0	100	100
1	D	691/716 (96%)	638 (92%)	53 (8%)	0	100	100
1	G	690/716 (96%)	633 (92%)	54 (8%)	3 (0%)	34	68
1	J	686/716 (96%)	629 (92%)	56 (8%)	1 (0%)	51	82
2	B	644/757 (85%)	600 (93%)	43 (7%)	1 (0%)	47	78
2	E	656/757 (87%)	616 (94%)	40 (6%)	0	100	100
2	H	655/757 (86%)	608 (93%)	46 (7%)	1 (0%)	47	78
2	K	652/757 (86%)	607 (93%)	45 (7%)	0	100	100
3	C	707/765 (92%)	644 (91%)	61 (9%)	2 (0%)	41	72
3	F	718/765 (94%)	655 (91%)	63 (9%)	0	100	100
3	I	720/765 (94%)	660 (92%)	60 (8%)	0	100	100
3	L	713/765 (93%)	644 (90%)	67 (9%)	2 (0%)	41	72
4	M	119/134 (89%)	115 (97%)	4 (3%)	0	100	100
4	N	119/134 (89%)	114 (96%)	5 (4%)	0	100	100
4	O	119/134 (89%)	116 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	P	119/134 (89%)	114 (96%)	5 (4%)	0	100 100
All	All	8695/9488 (92%)	8031 (92%)	654 (8%)	10 (0%)	51 82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	431	ASP
3	L	516	GLU
2	B	429	LYS
1	J	70	ALA
3	L	745	THR
3	C	322	SER
2	H	429	LYS
3	C	247	GLY
1	G	433	ALA
1	G	432	VAL

5.3.2 Protein sidechains (i)

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	620/644 (96%)	606 (98%)	14 (2%)	50 75
1	D	624/644 (97%)	614 (98%)	10 (2%)	62 81
1	G	623/644 (97%)	613 (98%)	10 (2%)	62 81
1	J	622/644 (97%)	613 (99%)	9 (1%)	67 83
2	B	580/669 (87%)	570 (98%)	10 (2%)	60 80
2	E	590/669 (88%)	582 (99%)	8 (1%)	67 83
2	H	589/669 (88%)	580 (98%)	9 (2%)	65 82
2	K	588/669 (88%)	580 (99%)	8 (1%)	67 83
3	C	634/676 (94%)	613 (97%)	21 (3%)	38 68
3	F	643/676 (95%)	629 (98%)	14 (2%)	52 76
3	I	645/676 (95%)	630 (98%)	15 (2%)	50 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	640/676 (95%)	625 (98%)	15 (2%)	50 75
4	M	99/111 (89%)	98 (99%)	1 (1%)	76 87
4	N	99/111 (89%)	97 (98%)	2 (2%)	55 78
4	O	99/111 (89%)	98 (99%)	1 (1%)	76 87
4	P	99/111 (89%)	97 (98%)	2 (2%)	55 78
All	All	7794/8400 (93%)	7645 (98%)	149 (2%)	57 79

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	35	PHE
1	A	74	HIS
1	A	219	LEU
1	A	223	PHE
1	A	239	ASN
1	A	312	ARG
1	A	346	GLN
1	A	426	ASP
1	A	443	ARG
1	A	469	LEU
1	A	549	LEU
1	A	611	PHE
1	A	688	GLU
2	B	67	ASN
2	B	314	ASN
2	B	446	ASP
2	B	501	PHE
2	B	509	LEU
2	B	531	LYS
2	B	536	ASN
2	B	557	TYR
2	B	699	PHE
2	B	712	SER
3	C	7	LEU
3	C	28	MET
3	C	38	ARG
3	C	55	TYR
3	C	62	ARG
3	C	100	ASN

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Mol	Chain	Res	Type
3	C	110	HIS
3	C	111	TYR
3	C	134	HIS
3	C	135	PHE
3	C	196	CYS
3	C	202	MET
3	C	206	MET
3	C	217	PHE
3	C	306	GLN
3	C	348	ASN
3	C	508	ARG
3	C	513	LEU
3	C	525	GLU
3	C	567	ASN
3	C	737	ARG
1	D	35	PHE
1	D	219	LEU
1	D	312	ARG
1	D	365	GLN
1	D	426	ASP
1	D	431	ASP
1	D	549	LEU
1	D	611	PHE
1	D	673	ARG
1	D	716	ARG
2	E	67	ASN
2	E	314	ASN
2	E	367	GLN
2	E	446	ASP
2	E	509	LEU
2	E	536	ASN
2	E	557	TYR
2	E	699	PHE
3	F	38	ARG
3	F	55	TYR
3	F	62	ARG
3	F	111	TYR
3	F	134	HIS
3	F	135	PHE
3	F	168	PHE
3	F	306	GLN
3	F	432	HIS

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Mol	Chain	Res	Type
3	F	483	MET
3	F	548	ASN
3	F	720	GLU
3	F	725	LEU
3	F	737	ARG
1	G	35	PHE
1	G	119	GLU
1	G	219	LEU
1	G	223	PHE
1	G	312	ARG
1	G	365	GLN
1	G	426	ASP
1	G	431	ASP
1	G	549	LEU
1	G	611	PHE
2	H	67	ASN
2	H	309	TRP
2	H	314	ASN
2	H	446	ASP
2	H	509	LEU
2	H	531	LYS
2	H	557	TYR
2	H	699	PHE
2	H	712	SER
3	I	38	ARG
3	I	40	GLU
3	I	55	TYR
3	I	62	ARG
3	I	111	TYR
3	I	135	PHE
3	I	206	MET
3	I	217	PHE
3	I	228	TYR
3	I	306	GLN
3	I	323	PHE
3	I	548	ASN
3	I	641	ARG
3	I	695	LEU
3	I	725	LEU
1	J	4	PHE
1	J	35	PHE
1	J	184	ASN

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Mol	Chain	Res	Type
1	J	239	ASN
1	J	312	ARG
1	J	365	GLN
1	J	426	ASP
1	J	431	ASP
1	J	549	LEU
2	K	67	ASN
2	K	314	ASN
2	K	430	ARG
2	K	509	LEU
2	K	531	LYS
2	K	557	TYR
2	K	696	PHE
2	K	699	PHE
3	L	7	LEU
3	L	9	ASN
3	L	55	TYR
3	L	62	ARG
3	L	111	TYR
3	L	134	HIS
3	L	135	PHE
3	L	306	GLN
3	L	323	PHE
3	L	348	ASN
3	L	453	HIS
3	L	535	MET
3	L	567	ASN
3	L	695	LEU
3	L	737	ARG
4	M	114	TYR
4	N	108	GLN
4	N	112	TYR
4	O	113	ASP
4	P	113	ASP
4	P	114	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	69	ASN
1	A	412	ASN

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Mol	Chain	Res	Type
1	A	510	HIS
2	B	310	ASN
2	B	605	HIS
3	C	252	ASN
1	D	408	GLN
2	E	605	HIS
3	F	100	ASN
3	F	134	HIS
3	F	233	HIS
3	F	614	GLN
1	G	96	ASN
1	G	412	ASN
3	I	100	ASN
3	I	242	GLN
3	I	567	ASN
1	J	408	GLN
1	J	587	GLN
2	K	605	HIS
3	L	110	HIS
3	L	252	ASN
3	L	522	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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, 95^{th} 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	691/716 (96%)	0.52	20 (2%) 51 51	23, 62, 108, 163	0
1	D	695/716 (97%)	0.58	25 (3%) 42 41	37, 74, 119, 183	0
1	G	694/716 (96%)	0.59	27 (3%) 39 38	24, 72, 114, 173	0
1	J	692/716 (96%)	0.64	34 (4%) 29 29	39, 81, 124, 177	0
2	B	656/757 (86%)	0.50	16 (2%) 59 57	24, 61, 102, 159	0
2	E	666/757 (87%)	0.54	19 (2%) 51 51	32, 71, 108, 191	0
2	H	667/757 (88%)	0.68	43 (6%) 19 20	28, 75, 115, 151	0
2	K	664/757 (87%)	0.63	29 (4%) 34 35	35, 81, 116, 169	0
3	C	717/765 (93%)	0.62	44 (6%) 21 22	33, 79, 128, 168	0
3	F	726/765 (94%)	0.88	79 (10%) 5 5	38, 91, 144, 186	0
3	I	728/765 (95%)	0.63	39 (5%) 25 26	34, 77, 120, 159	0
3	L	723/765 (94%)	0.70	52 (7%) 15 16	32, 82, 127, 183	0
4	M	121/134 (90%)	0.39	1 (0%) 86 87	38, 63, 111, 130	0
4	N	121/134 (90%)	0.62	4 (3%) 46 45	54, 88, 126, 142	0
4	O	121/134 (90%)	0.51	6 (4%) 28 29	34, 66, 101, 132	0
4	P	121/134 (90%)	0.72	4 (3%) 46 45	56, 86, 118, 145	0
All	All	8803/9488 (92%)	0.62	442 (5%) 28 29	23, 76, 123, 191	0

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	717	ALA	7.9
1	D	65	LEU	7.1
3	F	717	ALA	6.6
2	E	31	SER	6.6
2	H	33	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	716	ARG	6.3
2	H	352	GLY	6.1
3	F	754	ILE	5.7
3	F	436	ARG	5.7
3	L	250	VAL	5.6
1	D	66	ASP	5.6
3	F	149	PRO	5.5
3	F	337	SER	5.2
1	J	604	GLU	5.1
3	L	521	THR	5.1
1	D	604	GLU	5.1
3	L	716	LEU	5.1
2	B	293	SER	5.0
3	I	486	ASP	5.0
2	E	375	SER	4.9
3	L	65	GLU	4.9
2	K	35	GLY	4.8
3	L	182	GLN	4.7
2	K	290	MET	4.6
3	F	432	HIS	4.6
1	G	58	GLY	4.5
1	G	140	SER	4.5
2	K	320	ALA	4.4
3	F	400	VAL	4.4
3	L	153	ASP	4.4
1	D	142	ASN	4.4
3	F	291	GLY	4.4
3	F	446	PHE	4.2
4	O	113	ASP	4.2
3	F	354	ILE	4.2
1	J	716	ARG	4.2
2	H	179	MET	4.2
2	E	410	GLY	4.2
3	F	746	ASP	4.1
2	H	82	TYR	4.1
3	C	39	GLN	4.1
2	K	31	SER	4.1
2	K	346	ASN	4.1
1	D	140	SER	4.1
3	L	746	ASP	4.1
1	J	206	GLU	4.1
3	I	489	SER	4.0

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Mol	Chain	Res	Type	RSRZ
3	F	150	GLY	4.0
3	F	353	LYS	4.0
3	C	36	SER	4.0
3	L	628	GLN	3.9
4	P	1	GLN	3.8
3	C	451	ILE	3.8
2	H	80	SER	3.8
1	J	140	SER	3.8
3	F	340	ARG	3.8
1	G	206	GLU	3.8
1	A	550	LEU	3.8
3	C	153	ASP	3.8
3	F	105	MET	3.8
3	L	39	GLN	3.8
3	F	153	ASP	3.7
1	J	610	GLU	3.7
2	B	294	GLN	3.7
3	L	481	SER	3.7
3	F	524	THR	3.7
3	C	460	MET	3.7
3	F	37	GLY	3.7
3	F	452	GLU	3.7
1	A	101	GLU	3.6
3	F	609	THR	3.6
3	L	149	PRO	3.6
3	F	751	THR	3.6
3	C	316	GLY	3.6
2	H	292	ASN	3.6
3	C	458	MET	3.6
3	F	318	ARG	3.6
3	I	275	ASP	3.6
3	L	618	LEU	3.6
2	H	81	GLY	3.5
2	H	378	LEU	3.5
2	H	410	GLY	3.5
3	L	488	TYR	3.5
3	C	329	THR	3.5
2	H	83	ALA	3.5
3	F	134	HIS	3.5
3	L	134	HIS	3.5
3	F	358	ASP	3.4
2	K	732	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	313	GLN	3.4
3	F	421	VAL	3.4
3	L	107	SER	3.4
2	H	372	MET	3.4
3	C	474	SER	3.4
1	J	550	LEU	3.3
3	L	632	GLN	3.3
2	K	374	ALA	3.3
2	E	505	PHE	3.3
2	B	383	GLU	3.3
2	H	331	GLU	3.3
3	C	288	GLN	3.3
2	H	440	GLY	3.3
3	C	755	ARG	3.3
2	K	178	GLU	3.3
1	A	206	GLU	3.2
3	C	717	ALA	3.2
2	H	356	MET	3.2
3	I	339	LYS	3.2
1	A	557	MET	3.2
3	F	338	ILE	3.2
3	C	456	ASN	3.2
2	E	520	SER	3.2
3	F	144	ARG	3.2
2	H	46	THR	3.2
2	K	659	ALA	3.2
3	L	40	GLU	3.2
3	L	483	MET	3.1
4	N	11	MET	3.1
1	J	66	ASP	3.1
2	K	130	ASP	3.1
2	H	104	GLU	3.1
3	F	327	GLY	3.1
3	C	581	GLN	3.1
1	G	136	ASN	3.1
3	C	452	GLU	3.1
3	F	339	LYS	3.1
3	L	474	SER	3.1
2	H	293	SER	3.1
3	L	623	ALA	3.1
3	F	666	THR	3.1
2	H	350	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	460	MET	3.0
2	B	53	GLY	3.0
1	A	239	ASN	3.0
3	F	215	THR	3.0
1	J	616	SER	3.0
3	F	439	GLN	3.0
3	I	610	PHE	3.0
2	H	732	SER	3.0
3	C	479	ARG	3.0
1	G	57	GLN	3.0
1	G	200	THR	3.0
1	G	496	ARG	3.0
1	G	607	MET	3.0
2	E	666	TRP	2.9
1	J	695	ILE	2.9
3	F	512	LEU	2.9
1	G	239	ASN	2.9
2	K	372	MET	2.9
3	F	142	ARG	2.9
3	F	756	MET	2.9
3	I	90	MET	2.9
3	L	486	ASP	2.9
3	L	511	VAL	2.9
1	G	327	GLU	2.9
3	F	349	LEU	2.9
2	H	53	GLY	2.9
4	P	113	ASP	2.9
1	D	350	ASN	2.9
1	J	652	SER	2.9
3	C	521	THR	2.9
3	C	669	GLY	2.9
3	C	441	ASP	2.9
3	I	354	ILE	2.9
3	F	317	LEU	2.9
3	F	347	GLY	2.9
3	F	138	GLN	2.8
3	F	423	ARG	2.8
3	F	130	PHE	2.8
1	J	195	GLU	2.8
1	G	418	THR	2.8
1	J	213	ARG	2.8
2	E	53	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	496	VAL	2.8
1	A	100	ALA	2.8
2	B	622	GLY	2.8
1	D	67	ASP	2.8
3	F	399	ILE	2.8
2	E	33	GLY	2.8
3	C	138	GLN	2.8
2	B	752	GLU	2.8
3	C	412	LYS	2.8
3	I	351	THR	2.8
3	I	360	TYR	2.8
2	E	501	PHE	2.8
1	G	145	ILE	2.8
1	G	552	SER	2.8
2	E	409	MET	2.8
3	I	660	LYS	2.8
1	J	649	LEU	2.7
2	B	501	PHE	2.7
3	C	511	VAL	2.7
3	C	254	ASP	2.7
2	K	505	PHE	2.7
3	L	252	ASN	2.7
3	I	673	GLY	2.7
2	K	473	VAL	2.7
2	B	666	TRP	2.7
3	F	330	PHE	2.7
3	I	291	GLY	2.7
3	F	521	THR	2.7
3	L	5	LYS	2.7
3	C	349	LEU	2.7
1	J	334	TYR	2.7
3	I	437	HIS	2.7
1	J	210	THR	2.7
4	O	1	GLN	2.7
1	J	613	GLU	2.7
3	F	513	LEU	2.6
1	A	66	ASP	2.6
3	I	665	LEU	2.6
1	G	300	GLU	2.6
3	I	531	TYR	2.6
3	C	746	ASP	2.6
2	H	34	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	K	442	GLN	2.6
3	F	329	THR	2.6
1	D	716	ARG	2.6
3	I	436	ARG	2.6
2	H	93	ALA	2.6
1	D	606	ASP	2.6
1	J	478	ASP	2.6
3	F	716	LEU	2.6
3	L	718	LYS	2.6
1	D	206	GLU	2.6
2	K	180	GLU	2.6
4	N	1	GLN	2.6
2	H	376	ILE	2.6
3	F	435	LEU	2.6
3	C	359	GLY	2.6
2	H	414	MET	2.6
2	E	164	ILE	2.6
3	I	353	LYS	2.6
3	L	693	GLY	2.6
1	D	95	CYS	2.6
1	A	67	ASP	2.5
1	J	187	LEU	2.5
3	F	296	ASP	2.5
2	H	75	GLU	2.5
2	E	276	ASN	2.5
2	K	335	ASN	2.5
1	A	65	LEU	2.5
4	O	71	SER	2.5
1	D	355	PRO	2.5
3	L	505	ARG	2.5
1	A	350	ASN	2.5
3	I	674	THR	2.5
3	L	482	LYS	2.5
3	C	486	ASP	2.5
1	A	125	ARG	2.5
2	H	417	THR	2.5
2	E	165	ASP	2.5
1	J	106	LEU	2.5
3	C	355	ARG	2.5
3	I	39	GLN	2.5
2	H	666	TRP	2.5
1	G	11	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	53	PHE	2.5
3	L	629	SER	2.5
3	F	425	ASN	2.5
3	L	458	MET	2.5
3	C	37	GLY	2.5
2	E	552	ILE	2.5
1	D	494	GLY	2.4
2	E	243	THR	2.4
2	K	536	ASN	2.4
3	L	719	GLY	2.4
3	L	90	MET	2.4
3	F	223	GLY	2.4
4	P	103	GLY	2.4
3	F	173	GLY	2.4
2	K	363	LYS	2.4
3	F	30	ILE	2.4
3	F	418	LEU	2.4
3	F	466	ASP	2.4
1	J	204	ARG	2.4
2	K	378	LEU	2.4
2	B	410	GLY	2.4
3	F	494	VAL	2.4
3	I	488	TYR	2.4
3	I	664	ARG	2.4
2	K	417	THR	2.4
3	C	250	VAL	2.4
3	F	608	GLY	2.4
1	J	65	LEU	2.4
4	N	101	TYR	2.4
3	I	552	TRP	2.4
3	C	457	VAL	2.4
2	K	581	GLU	2.4
1	A	294	ASP	2.3
2	H	151	ARG	2.3
2	H	752	GLU	2.3
1	D	474	CYS	2.3
2	H	32	HIS	2.3
3	L	661	THR	2.3
2	B	33	GLY	2.3
3	F	356	VAL	2.3
1	J	9	PHE	2.3
1	J	688	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	61	ILE	2.3
1	G	147	ILE	2.3
4	N	114	TYR	2.3
2	B	732	SER	2.3
3	F	361	GLU	2.3
1	J	556	GLN	2.3
3	I	373	ILE	2.3
1	G	44	VAL	2.3
1	D	106	LEU	2.3
1	G	67	ASP	2.3
1	G	189	ASP	2.3
3	L	349	LEU	2.3
1	D	60	SER	2.3
2	H	306	ASN	2.3
1	D	607	MET	2.3
3	C	90	MET	2.3
3	C	497	SER	2.3
3	L	30	ILE	2.3
3	I	251	ARG	2.3
3	F	357	HIS	2.3
3	I	628	GLN	2.3
2	B	212	VAL	2.3
4	M	112	TYR	2.3
3	L	485	VAL	2.3
3	C	454	ILE	2.3
3	F	502	LEU	2.2
3	L	146	ASP	2.2
1	J	555	GLY	2.2
3	L	136	ARG	2.2
2	B	387	LYS	2.2
1	J	315	PHE	2.2
4	O	78	THR	2.2
3	L	382	VAL	2.2
4	P	101	TYR	2.2
2	E	72	PRO	2.2
2	K	318	PHE	2.2
1	A	430	GLU	2.2
1	D	237	GLU	2.2
2	E	34	THR	2.2
2	K	53	GLY	2.2
3	I	236	GLN	2.2
2	K	426	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	354	ILE	2.2
1	D	195	GLU	2.2
2	H	52	LYS	2.2
2	H	433	LYS	2.2
2	K	425	ASN	2.2
3	L	43	PRO	2.2
1	G	693	CYS	2.2
2	K	179	MET	2.2
3	I	363	PHE	2.2
1	A	25	GLY	2.2
2	H	165	ASP	2.2
3	F	755	ARG	2.2
1	G	695	ILE	2.2
3	C	494	VAL	2.2
3	I	755	ARG	2.2
2	K	400	THR	2.2
3	F	438	PHE	2.2
2	H	441	LEU	2.2
3	I	618	LEU	2.2
3	L	377	ALA	2.2
3	C	609	THR	2.2
3	F	479	ARG	2.2
3	I	38	ARG	2.2
1	J	11	PRO	2.2
1	J	599	GLU	2.2
3	C	202	MET	2.2
3	C	564	TRP	2.1
1	D	556	GLN	2.1
3	F	107	SER	2.1
2	B	446	ASP	2.1
3	F	444	VAL	2.1
3	L	141	ILE	2.1
3	I	718	LYS	2.1
3	C	425	ASN	2.1
2	H	253	TYR	2.1
2	H	127	GLN	2.1
1	G	68	PRO	2.1
3	I	18	GLU	2.1
3	C	651	GLY	2.1
2	E	390	GLU	2.1
1	J	132	LEU	2.1
2	B	34	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	492	PHE	2.1
3	F	76	THR	2.1
3	F	510	ASN	2.1
1	J	654	GLN	2.1
1	J	660	ALA	2.1
1	G	613	GLU	2.1
3	I	487	GLU	2.1
1	D	118	ILE	2.1
3	F	359	GLY	2.1
3	F	742	SER	2.1
4	O	100	ARG	2.1
1	D	78	ILE	2.1
3	L	399	ILE	2.1
2	K	10	LEU	2.1
3	L	631	MET	2.1
1	G	681	PHE	2.1
2	H	431	TYR	2.1
1	G	59	GLU	2.1
3	F	516	GLU	2.1
1	D	428	ILE	2.1
3	F	373	ILE	2.1
3	F	106	THR	2.1
3	L	274	ALA	2.1
1	A	400	LEU	2.1
3	L	173	GLY	2.1
1	A	238	PRO	2.1
3	L	52	ALA	2.1
3	C	385	ILE	2.1
2	B	296	THR	2.1
3	I	609	THR	2.1
1	D	688	GLU	2.1
3	F	241	GLU	2.1
2	H	164	ILE	2.1
1	J	67	ASP	2.1
2	H	224	LEU	2.1
3	I	623	ALA	2.1
3	C	498	ILE	2.1
3	L	236	GLN	2.0
3	L	446	PHE	2.0
3	F	213	ARG	2.0
3	L	17	ARG	2.0
3	F	100	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	530	THR	2.0
1	G	66	ASP	2.0
1	J	364	SER	2.0
2	H	45	ARG	2.0
3	L	334	SER	2.0
1	A	180	GLN	2.0
2	H	115	GLN	2.0
4	O	95	TYR	2.0
3	I	346	THR	2.0
3	I	659	ASN	2.0
2	K	55	TRP	2.0
1	A	78	ILE	2.0
3	F	426	GLN	2.0
3	F	718	LYS	2.0
3	I	274	ALA	2.0
1	J	355	PRO	2.0
1	G	139	LYS	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 monosaccharides 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.