Full wwPDB EM Validation Report

Feb 27, 2025 – 05:51 PM JST

PDB ID	:	8YGP
EMDB ID	:	EMD-39259
Title	:	The tetramer Structure of DSR2-SPR with NAD
Authors	:	Gao, X.; Zhu, H.; Cui, S.
Deposited on	:	2024-02-26
Resolution	:	4.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

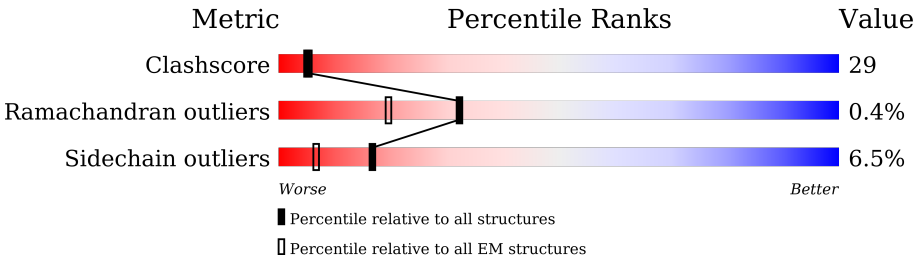
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1005	22% 51% 42%
1	B	1005	26% 54% 40%
1	E	1005	46% 46% 5%
1	F	1005	6% 44% 46% 7%
2	C	264	40% 36% 18% 43%
2	D	264	36% 31% 26% 43%
2	G	264	14% 28% 24% 5% 43%
2	H	264	18% 27% 27% 43%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37524 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		
1	B	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		
1	E	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		
1	F	983	Total	C	N	O	S	0	0
			8183	5292	1322	1538	31		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	HIS	engineered mutation	UNP D4G637
B	171	ALA	HIS	engineered mutation	UNP D4G637
E	171	ALA	HIS	engineered mutation	UNP D4G637
F	171	ALA	HIS	engineered mutation	UNP D4G637

- Molecule 2 is a protein called SPR.

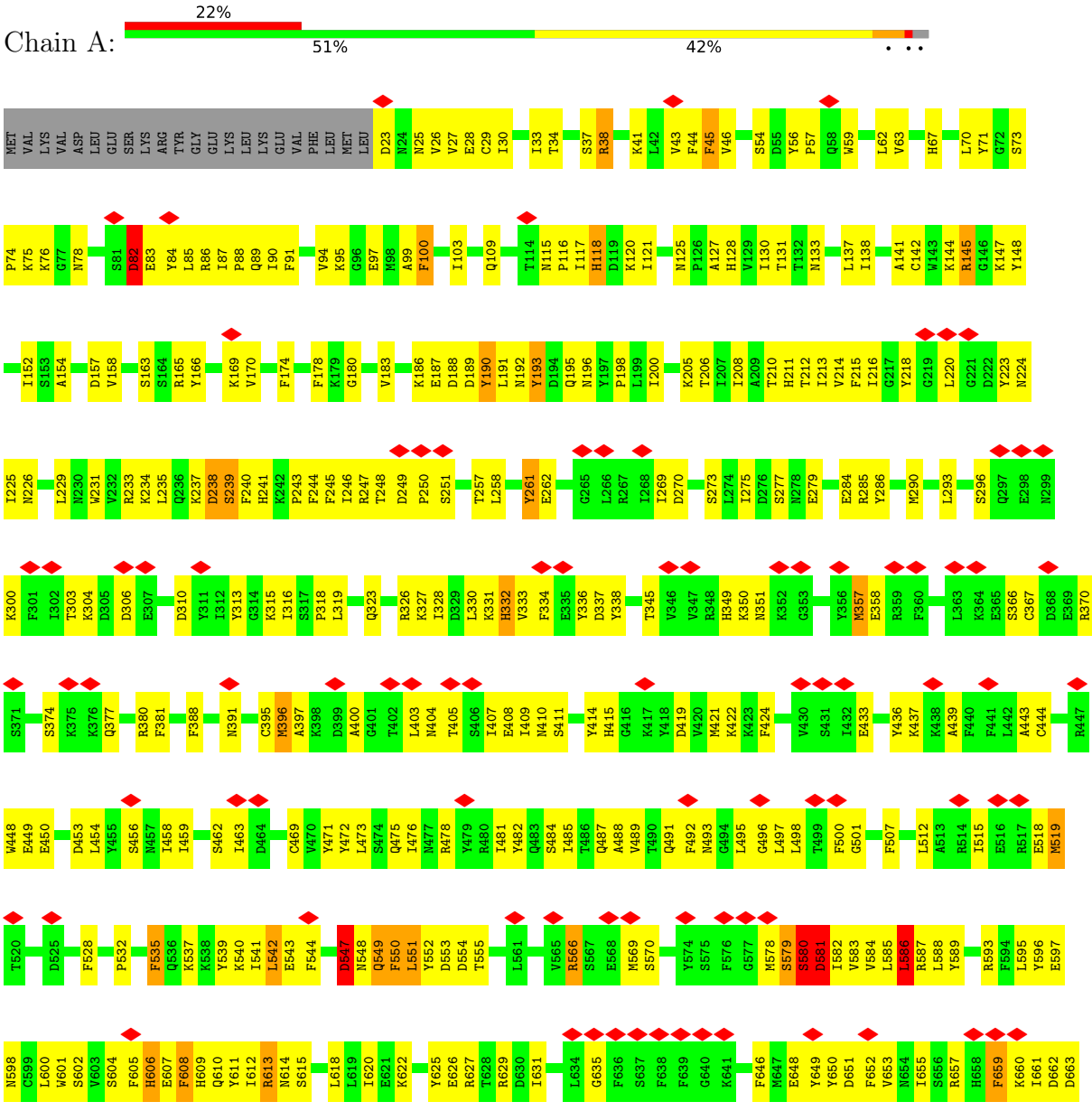
Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		
2	D	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		
2	G	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		
2	H	151	Total	C	N	O	S	0	0
			1198	758	189	247	4		

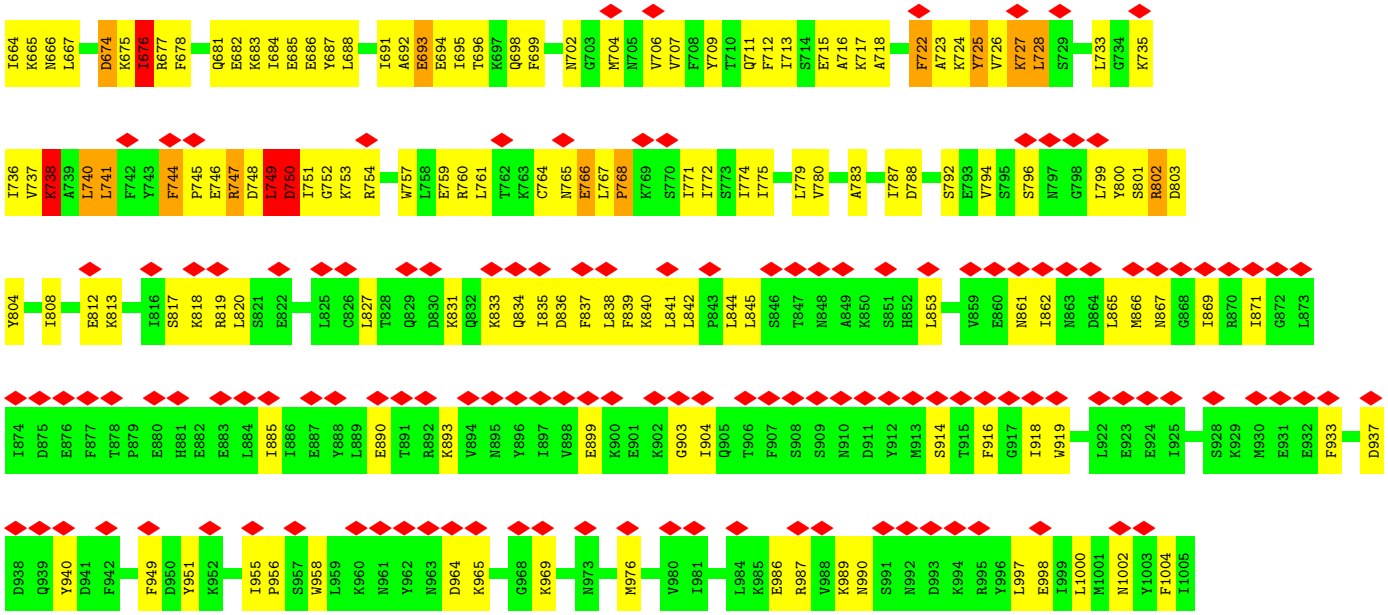
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: SIR2-like domain-containing protein

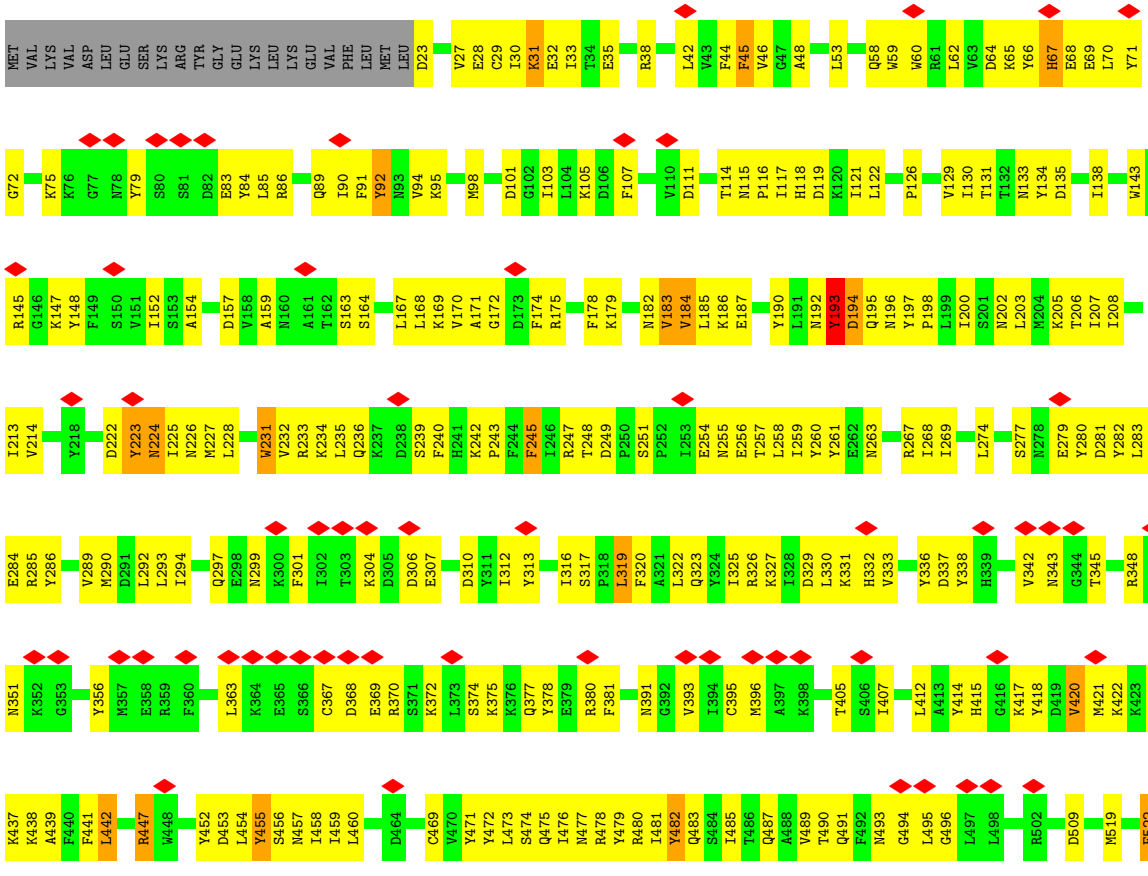
Chain A:

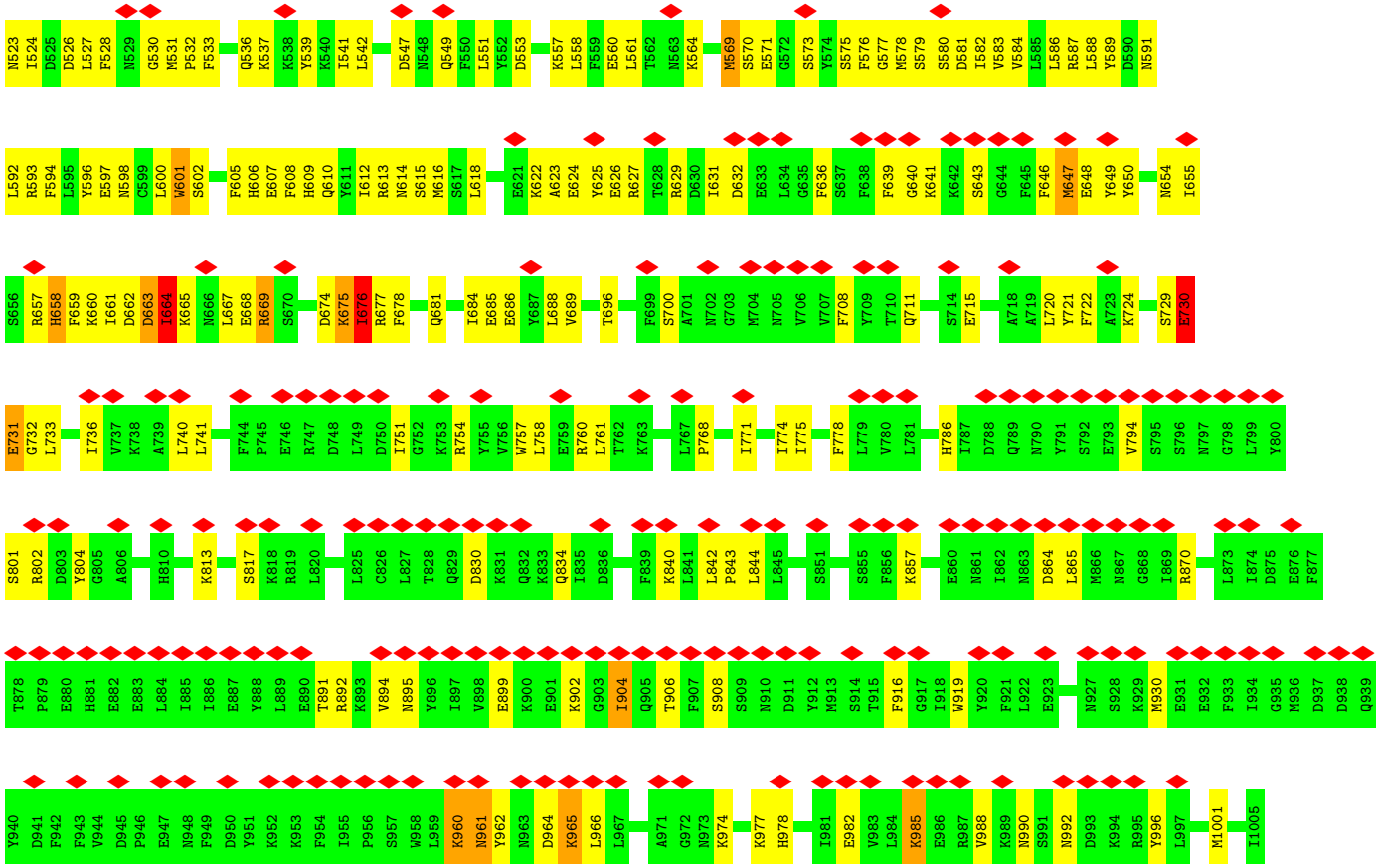




• Molecule 1: SIR2-like domain-containing protein

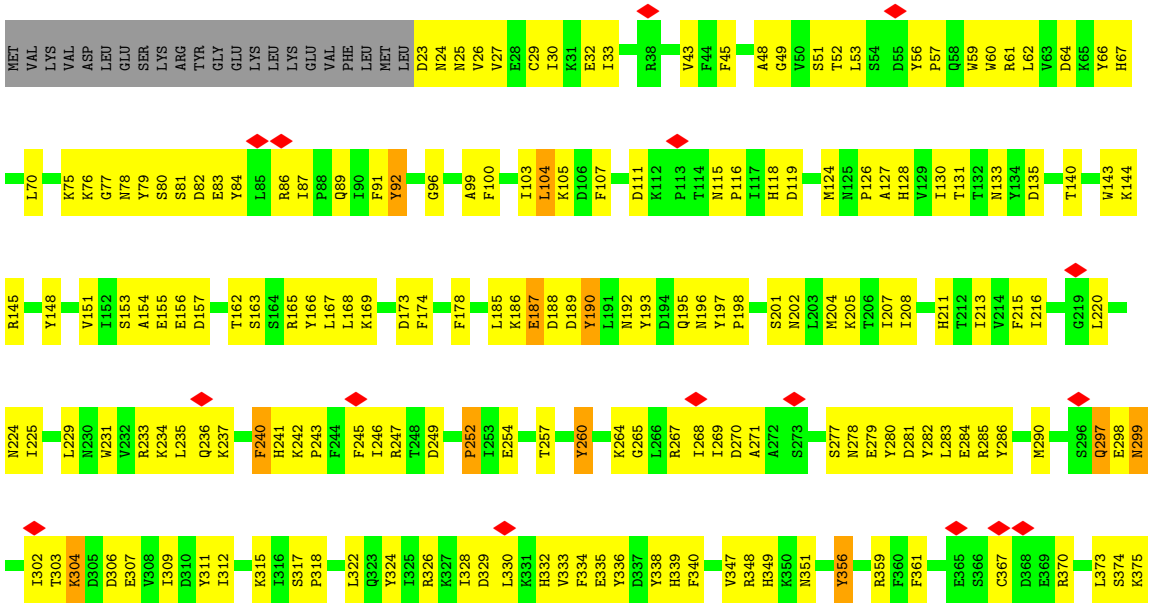
Chain B:

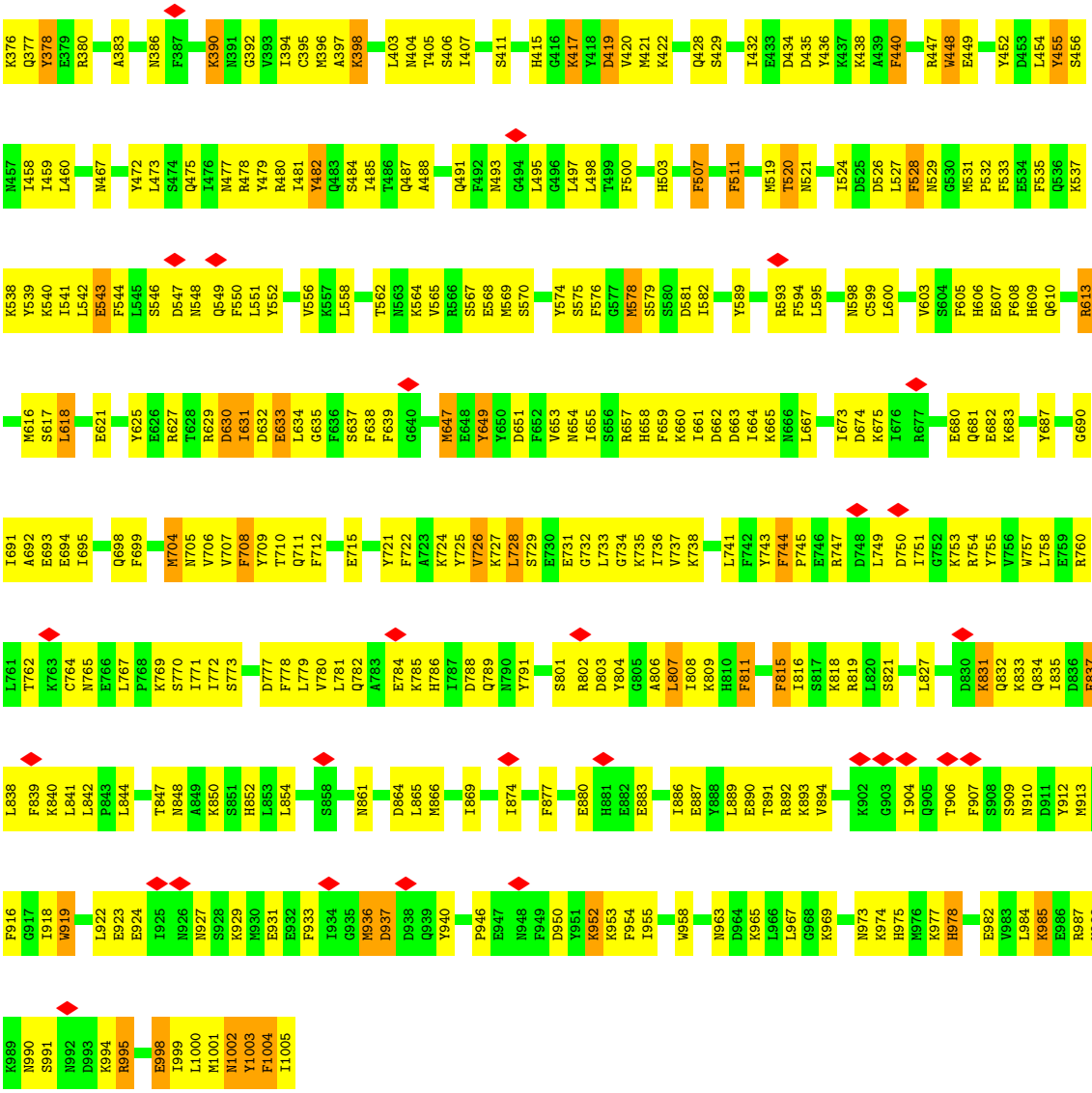




• Molecule 1: SIR2-like domain-containing protein

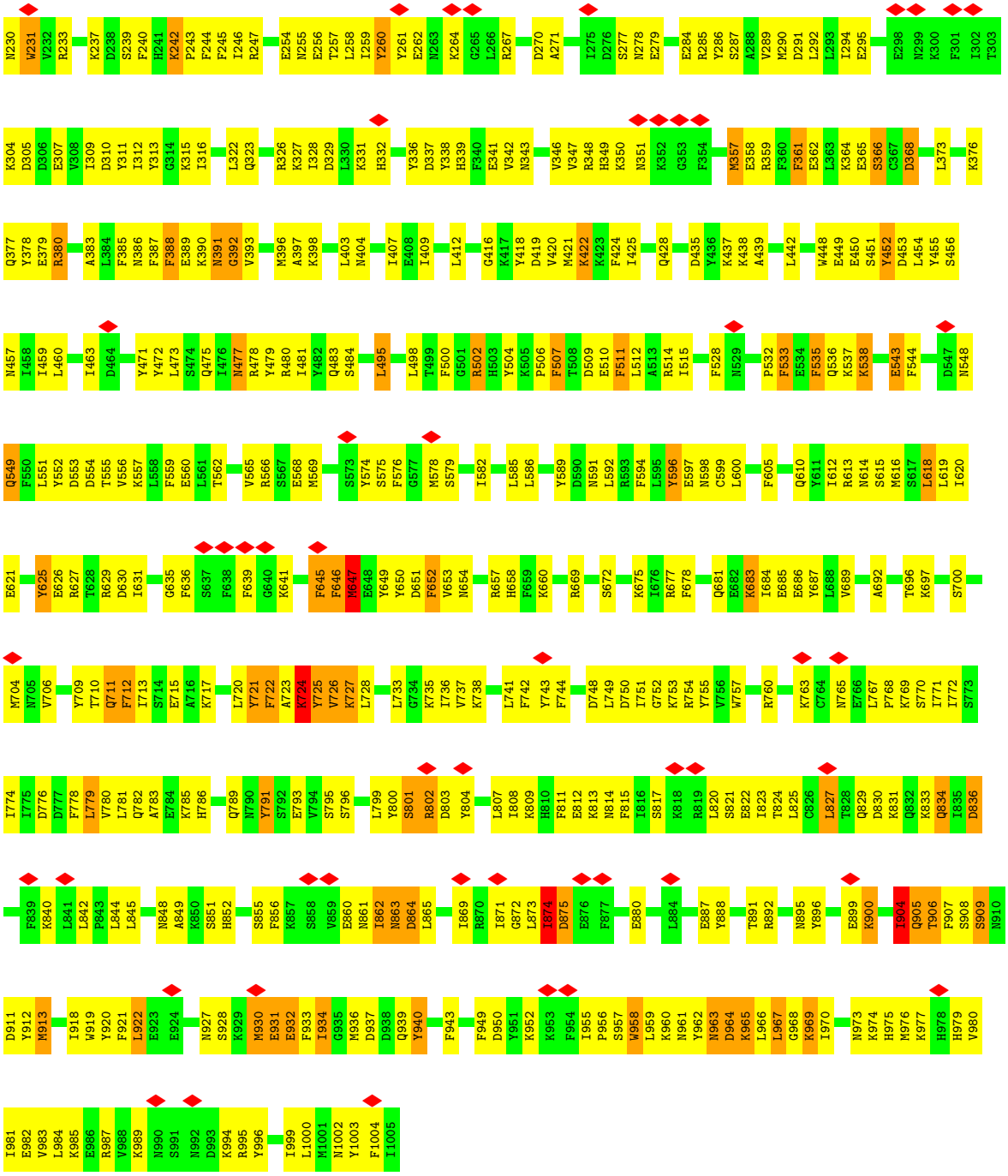
Chain E:





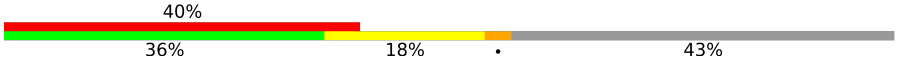
• Molecule 1: SIR2-like domain-containing protein

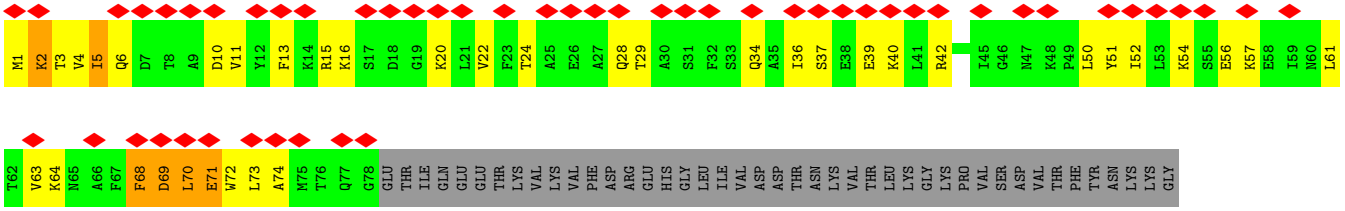
Chain F:

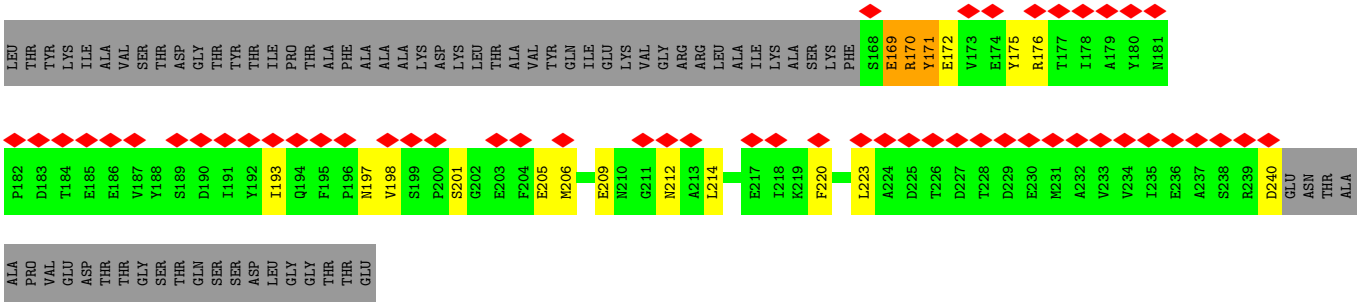


• Molecule 2: SPR

Chain C:

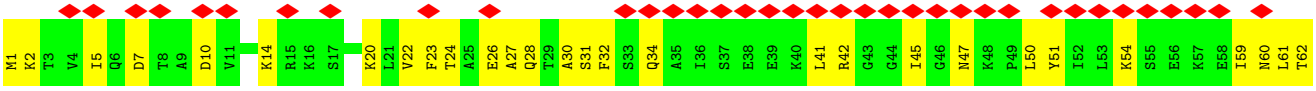


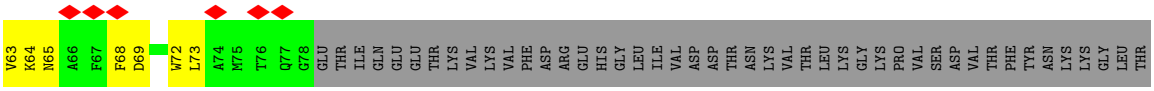


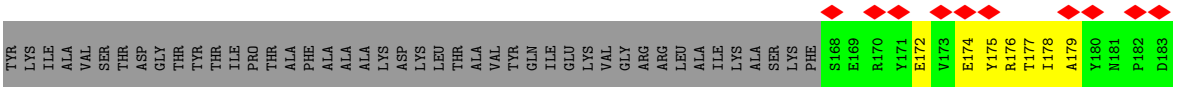


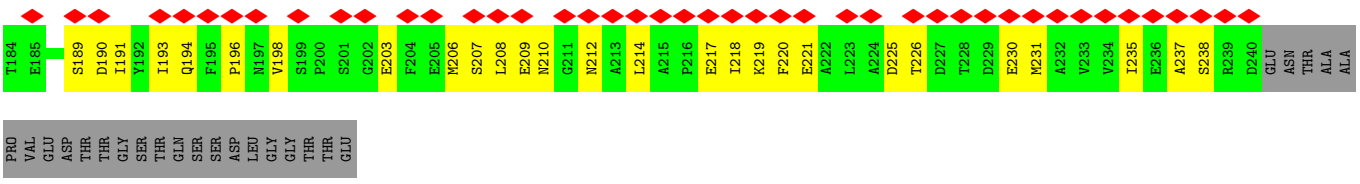
• Molecule 2: SPR

Chain D:



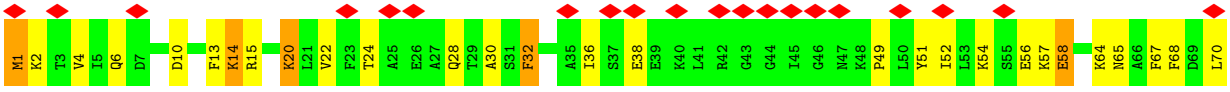


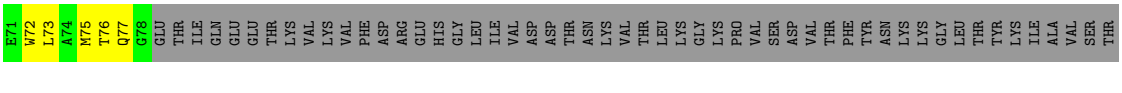


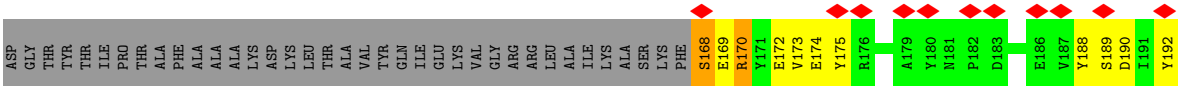


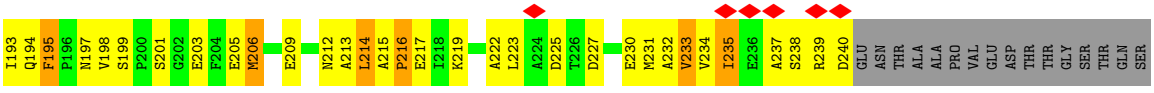
• Molecule 2: SPR

Chain G:

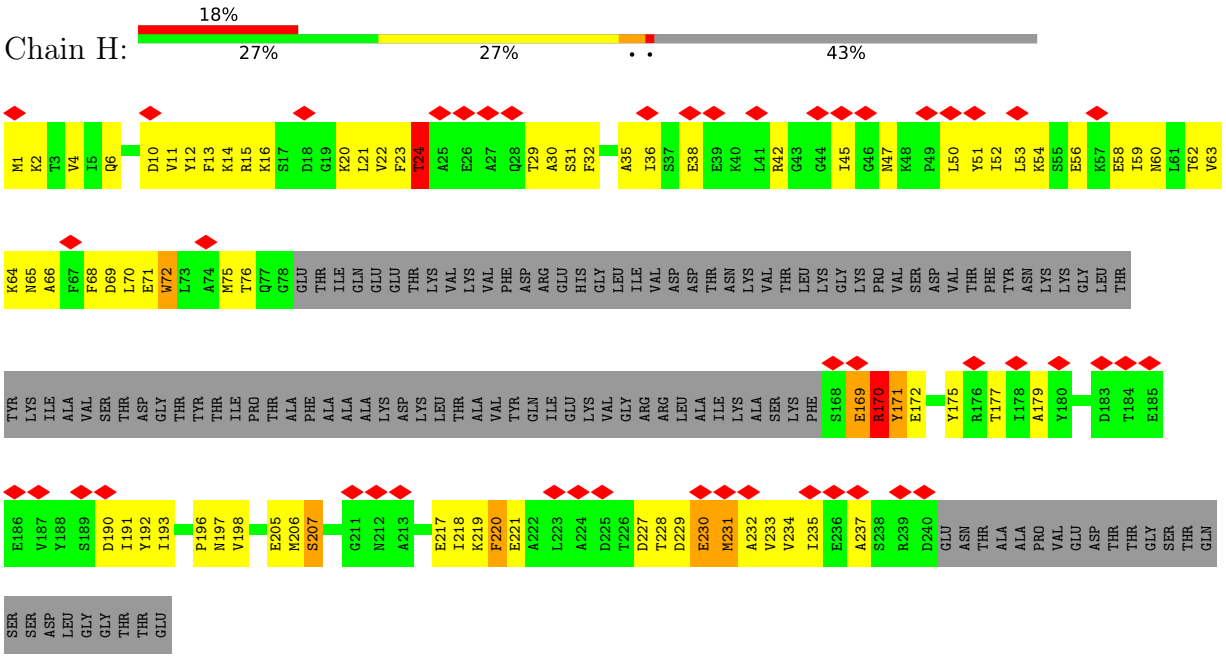








• Molecule 2: SPR



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.187	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	381.8, 381.8, 381.8	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

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	0.34	1/8374 (0.0%)	0.66	18/11280 (0.2%)
1	B	0.30	0/8374	0.68	20/11280 (0.2%)
1	E	0.34	0/8374	0.62	6/11280 (0.1%)
1	F	0.36	0/8374	0.74	26/11280 (0.2%)
2	C	0.30	0/1218	0.65	3/1645 (0.2%)
2	D	0.26	0/1218	0.55	0/1645
2	G	0.40	0/1218	0.65	0/1645
2	H	0.36	0/1218	0.93	7/1645 (0.4%)
All	All	0.33	1/38368 (0.0%)	0.68	80/51700 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
2	H	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	580	SER	C-O	-6.54	1.10	1.23

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	230	GLU	CB-CA-C	-15.48	79.43	110.40
1	F	964	ASP	N-CA-CB	-15.46	82.78	110.60
1	B	676	ILE	CB-CA-C	14.94	141.48	111.60
1	B	601	TRP	N-CA-C	14.44	149.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	630	ASP	N-CA-C	-14.12	72.89	111.00
2	H	24	THR	CB-CA-C	-13.88	74.12	111.60
1	A	738	LYS	N-CA-CB	-13.59	86.14	110.60
1	F	964	ASP	N-CA-C	13.31	146.95	111.00
1	B	602	SER	N-CA-CB	-13.06	90.91	110.50
1	A	737	VAL	N-CA-C	12.98	146.04	111.00
1	A	737	VAL	CB-CA-C	-12.60	87.47	111.40
1	F	647	MET	N-CA-CB	-12.57	87.97	110.60
1	F	392	GLY	N-CA-C	12.53	144.41	113.10
1	B	663	ASP	N-CA-C	12.13	143.74	111.00
2	H	230	GLU	N-CA-C	11.75	142.73	111.00
1	B	731	GLU	N-CA-C	-11.10	81.02	111.00
1	F	646	PHE	CB-CA-C	-10.60	89.21	110.40
1	B	676	ILE	N-CA-C	-10.54	82.54	111.00
1	B	601	TRP	CB-CA-C	-10.42	89.55	110.40
2	C	171	TYR	N-CA-C	-10.14	83.62	111.00
1	E	252	PRO	CA-N-CD	-10.09	97.38	111.50
2	H	231	MET	N-CA-CB	-10.04	92.53	110.60
1	F	875	ASP	N-CA-CB	-9.87	92.84	110.60
1	B	193	TYR	N-CA-C	9.76	137.36	111.00
1	B	182	ASN	N-CA-C	9.65	137.06	111.00
1	B	663	ASP	CB-CA-C	-9.58	91.24	110.40
1	A	749	LEU	N-CA-C	-9.57	85.16	111.00
1	F	801	SER	N-CA-C	-9.36	85.72	111.00
1	F	391	ASN	N-CA-C	-9.23	86.06	111.00
1	F	366	SER	N-CA-C	-9.00	86.69	111.00
1	B	194	ASP	N-CA-CB	8.58	126.04	110.60
1	A	579	SER	N-CA-C	-8.57	87.86	111.00
1	A	747	ARG	N-CA-C	-8.32	88.53	111.00
1	A	543	GLU	N-CA-CB	8.25	125.45	110.60
1	B	183	VAL	N-CA-C	-8.19	88.89	111.00
1	A	750	ASP	N-CA-C	7.66	131.67	111.00
1	F	722	PHE	CB-CA-C	-7.65	95.09	110.40
1	F	830	ASP	N-CA-C	7.52	131.31	111.00
1	A	586	LEU	CA-CB-CG	7.49	132.53	115.30
1	F	802	ARG	N-CA-C	-7.33	91.20	111.00
1	A	722	PHE	CB-CA-C	-7.14	96.12	110.40
1	F	549	GLN	N-CA-C	-7.13	91.75	111.00
1	B	664	ILE	N-CA-CB	-7.01	94.67	110.80
1	B	183	VAL	N-CA-CB	6.99	126.89	111.50
1	F	961	ASN	N-CA-C	-6.99	92.13	111.00
1	B	730	GLU	CB-CA-C	-6.96	96.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	547	ASP	N-CA-C	-6.92	92.33	111.00
1	B	664	ILE	N-CA-C	-6.85	92.51	111.00
1	F	366	SER	CB-CA-C	6.74	122.91	110.10
1	F	647	MET	N-CA-C	6.61	128.85	111.00
1	F	904	ILE	N-CA-C	-6.56	93.28	111.00
1	B	194	ASP	N-CA-C	-6.55	93.31	111.00
1	F	712	PHE	N-CA-CB	6.55	122.38	110.60
1	F	743	TYR	C-N-CA	-6.46	105.56	121.70
1	E	104	LEU	CA-CB-CG	6.41	130.04	115.30
1	E	693	GLU	CA-CB-CG	6.37	127.42	113.40
2	H	171	TYR	CB-CA-C	6.36	123.13	110.40
1	A	606	HIS	N-CA-C	6.26	127.89	111.00
2	C	68	PHE	N-CA-C	-6.17	94.36	111.00
1	F	618	LEU	CA-CB-CG	6.14	129.41	115.30
1	F	228	LEU	CB-CA-C	-6.06	98.68	110.20
2	H	24	THR	C-N-CA	6.04	136.81	121.70
2	C	171	TYR	CB-CA-C	6.02	122.44	110.40
1	F	963	ASN	N-CA-C	-5.99	94.83	111.00
1	F	724	LYS	N-CA-C	-5.93	94.98	111.00
1	E	520	THR	N-CA-C	-5.91	95.05	111.00
1	A	542	LEU	CB-CA-C	-5.90	98.98	110.20
1	A	543	GLU	N-CA-C	-5.90	95.06	111.00
1	E	521	ASN	N-CA-CB	-5.88	100.02	110.60
1	F	967	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	B	569	MET	CB-CG-SD	5.81	129.84	112.40
1	A	723	ALA	N-CA-C	-5.64	95.76	111.00
1	A	608	PHE	N-CA-C	-5.61	95.86	111.00
1	A	581	ASP	N-CA-C	-5.30	96.68	111.00
1	B	730	GLU	N-CA-C	-5.29	96.71	111.00
1	B	442	LEU	CA-CB-CG	5.28	127.44	115.30
1	F	779	LEU	CA-CB-CG	5.15	127.14	115.30
1	F	549	GLN	N-CA-CB	5.13	119.83	110.60
2	H	170	ARG	N-CA-C	-5.08	97.28	111.00
1	A	82	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	SER	Mainchain
1	E	297	GLN	Peptide
2	H	24	THR	Peptide

5.2 Too-close contacts (i)

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	8183	0	8010	484	0
1	B	8183	0	8010	406	0
1	E	8183	0	8010	502	0
1	F	8183	0	8010	552	0
2	C	1198	0	1159	65	0
2	D	1198	0	1159	74	0
2	G	1198	0	1159	96	0
2	H	1198	0	1159	109	0
All	All	37524	0	36676	2121	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 29.

All (2121) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TYR:CD2	1:B:183:VAL:HG13	1.48	1.45
1:B:601:TRP:CD2	1:B:601:TRP:O	1.72	1.39
1:B:134:TYR:CD2	1:B:183:VAL:CG1	2.09	1.34
1:B:134:TYR:CE2	1:B:183:VAL:HG13	1.81	1.14
1:E:519:MET:SD	1:E:520:THR:O	2.04	1.14
1:B:601:TRP:O	1:B:601:TRP:CE3	2.01	1.14
1:A:405:THR:H	2:C:4:VAL:HB	1.16	1.10
2:H:23:PHE:H	2:H:69:ASP:HB2	1.18	1.09
1:B:601:TRP:O	1:B:601:TRP:CG	2.06	1.09
1:A:582:ILE:HA	1:A:585:LEU:HG	1.35	1.08
2:H:24:THR:O	2:H:65:ASN:ND2	1.89	1.06
1:F:963:ASN:O	1:F:967:LEU:HD21	1.56	1.03
2:H:13:PHE:HB3	2:H:171:TYR:HE2	1.23	1.00
1:B:193:TYR:O	1:B:193:TYR:HD1	1.45	0.98
1:B:134:TYR:CD2	1:B:183:VAL:HG11	1.97	0.97
1:F:908:SER:HA	2:G:231:MET:HB3	1.45	0.97
1:A:403:LEU:H	2:C:6:GLN:HE22	1.15	0.94
1:B:134:TYR:HD2	1:B:183:VAL:HG13	1.22	0.92
1:B:610:GLN:O	1:B:614:ASN:ND2	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:801:SER:O	1:F:840:LYS:HE3	1.70	0.91
1:A:549:GLN:CA	1:A:552:TYR:HB2	2.01	0.90
1:F:652:PHE:CZ	1:F:722:PHE:O	2.25	0.90
1:A:547:ASP:O	1:A:550:PHE:CE1	2.25	0.90
1:B:193:TYR:O	1:B:193:TYR:CD1	2.26	0.89
1:A:247:ARG:NH2	1:A:251:SER:O	2.04	0.89
1:F:963:ASN:O	1:F:967:LEU:CD2	2.20	0.88
1:B:134:TYR:HD2	1:B:183:VAL:CG1	1.71	0.87
1:A:547:ASP:O	1:A:550:PHE:HE1	1.57	0.87
2:C:16:LYS:HG3	2:C:170:ARG:HB2	1.57	0.87
1:E:629:ARG:CD	1:E:630:ASP:O	2.24	0.86
1:E:749:LEU:HG	1:E:753:LYS:HD3	1.57	0.86
1:F:223:TYR:O	1:F:227:MET:HB3	1.77	0.85
1:A:582:ILE:HA	1:A:585:LEU:CG	2.06	0.85
1:B:58:GLN:HG3	1:B:60:TRP:H	1.41	0.84
1:A:713:ILE:HG21	1:A:717:LYS:HB2	1.57	0.84
1:E:698:GLN:HG2	1:E:712:PHE:HE2	1.42	0.84
1:F:222:ASP:H	1:F:225:ILE:HG22	1.42	0.84
1:F:652:PHE:HZ	1:F:722:PHE:O	1.60	0.83
2:G:28:GLN:HB3	2:G:64:LYS:HD3	1.59	0.83
1:A:549:GLN:HA	1:A:552:TYR:HB2	1.60	0.83
1:B:576:PHE:HA	1:B:639:PHE:HB3	1.58	0.82
1:F:331:LYS:HZ1	1:F:338:TYR:H	1.26	0.82
1:A:682:GLU:O	1:A:686:GLU:HG2	1.80	0.82
1:E:629:ARG:HG3	1:E:631:ILE:HB	1.59	0.82
1:B:472:TYR:HE2	1:B:542:LEU:HG	1.42	0.82
1:A:580:SER:HB2	1:A:582:ILE:HG23	1.60	0.82
1:F:962:TYR:HD1	1:F:967:LEU:HD22	1.45	0.82
1:A:646:PHE:HB3	1:A:677:ARG:HE	1.43	0.81
1:E:242:LYS:NZ	1:E:265:GLY:O	2.13	0.81
1:B:612:ILE:HG21	1:B:654:ASN:HB3	1.62	0.81
1:A:489:VAL:O	1:A:493:ASN:ND2	2.13	0.80
1:A:580:SER:C	1:A:582:ILE:N	2.28	0.80
2:H:64:LYS:HG2	2:H:217:GLU:HB3	1.61	0.80
1:F:974:LYS:HA	1:F:977:LYS:HE3	1.64	0.79
1:F:338:TYR:HA	1:F:348:ARG:HA	1.62	0.79
1:B:193:TYR:CD1	1:B:193:TYR:C	2.55	0.79
1:B:213:ILE:HB	1:B:243:PRO:HB3	1.63	0.79
1:F:310:ASP:HA	1:F:380:ARG:HH12	1.46	0.79
2:H:22:VAL:CG1	2:H:171:TYR:OH	2.30	0.79
2:H:23:PHE:HE1	2:H:66:ALA:HB2	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:800:TYR:O	1:F:802:ARG:N	2.14	0.79
1:E:987:ARG:NH1	1:F:630:ASP:OD2	2.16	0.79
1:A:405:THR:N	2:C:4:VAL:HB	1.98	0.78
1:E:837:PHE:HA	1:E:840:LYS:HB3	1.65	0.78
1:F:553:ASP:OD1	1:F:554:ASP:N	2.17	0.77
1:A:316:ILE:HG23	1:A:319:LEU:HD22	1.66	0.77
1:A:582:ILE:CA	1:A:585:LEU:HG	2.14	0.77
1:E:647:MET:SD	1:E:647:MET:N	2.58	0.77
1:B:152:ILE:HG23	1:B:157:ASP:HB2	1.66	0.77
1:B:661:ILE:HG13	1:B:663:ASP:H	1.49	0.77
2:D:26:GLU:O	2:D:65:ASN:ND2	2.18	0.77
1:F:985:LYS:O	1:F:989:LYS:HB3	1.85	0.77
1:A:86:ARG:NH2	1:E:260:TYR:OH	2.18	0.76
1:F:909:SER:H	2:G:231:MET:CB	1.98	0.76
1:A:582:ILE:HG13	1:A:583:VAL:N	2.01	0.76
1:F:247:ARG:HB3	1:F:271:ALA:H	1.51	0.75
1:F:984:LEU:HB3	1:F:1000:LEU:HD12	1.66	0.75
2:G:20:LYS:HG2	2:G:72:TRP:CZ3	2.21	0.75
1:E:487:GLN:NE2	2:H:207:SER:H	1.85	0.75
1:E:605:PHE:HA	2:H:207:SER:HB2	1.67	0.75
1:A:771:ILE:HG12	1:A:775:ILE:HD11	1.67	0.75
1:F:551:LEU:O	1:F:555:THR:OG1	2.05	0.75
1:F:869:ILE:HD11	1:F:874:ILE:O	1.87	0.75
1:A:586:LEU:HA	1:A:589:TYR:HD2	1.52	0.74
1:E:487:GLN:HE22	2:H:207:SER:H	1.33	0.74
2:H:21:LEU:O	2:H:69:ASP:HB3	1.87	0.74
1:A:678:PHE:HB2	1:A:726:VAL:HA	1.68	0.74
1:F:85:LEU:O	1:F:89:GLN:NE2	2.20	0.74
1:F:41:LYS:HG2	1:F:211:HIS:HD2	1.52	0.74
1:E:543:GLU:O	1:E:546:SER:OG	2.05	0.74
1:F:800:TYR:C	1:F:802:ARG:H	1.89	0.74
1:E:706:VAL:HA	1:E:709:TYR:HB3	1.70	0.74
2:G:14:LYS:O	2:G:172:GLU:N	2.20	0.74
1:F:711:GLN:O	1:F:712:PHE:CD1	2.41	0.74
1:E:788:ASP:OD1	1:E:789:GLN:N	2.21	0.73
1:B:233:ARG:NH1	1:B:263:ASN:O	2.21	0.73
2:D:45:ILE:HG23	2:D:47:ASN:H	1.52	0.73
1:E:30:ILE:HA	1:E:33:ILE:HD12	1.69	0.73
1:A:580:SER:C	1:A:582:ILE:H	1.89	0.73
1:A:713:ILE:HG13	1:A:716:ALA:HB3	1.71	0.73
1:F:342:VAL:HG21	1:F:586:LEU:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:909:SER:H	2:G:231:MET:HB2	1.52	0.73
1:E:967:LEU:HD22	1:E:1004:PHE:HE1	1.52	0.73
1:F:1002:ASN:OD1	1:F:1003:TYR:N	2.21	0.73
1:B:640:GLY:O	1:B:641:LYS:HG3	1.89	0.72
1:B:584:VAL:O	1:B:588:LEU:HB2	1.89	0.72
2:C:212:ASN:ND2	2:C:214:LEU:O	2.22	0.72
1:A:331:LYS:HB2	1:A:541:ILE:HG12	1.72	0.72
1:A:570:SER:O	1:B:669:ARG:NH2	2.23	0.72
1:B:457:ASN:HA	1:B:460:LEU:HD12	1.71	0.72
1:A:759:GLU:HG3	2:D:41:LEU:HB3	1.72	0.72
1:E:487:GLN:NE2	2:H:205:GLU:OE2	2.22	0.72
1:F:341:GLU:OE1	1:F:343:ASN:ND2	2.22	0.72
1:A:548:ASN:HB2	2:D:210:ASN:HD21	1.53	0.72
1:F:970:ILE:O	1:F:973:ASN:ND2	2.23	0.72
1:B:685:GLU:OE1	1:B:732:GLY:N	2.22	0.72
1:E:304:LYS:HZ3	1:E:307:GLU:HB2	1.55	0.72
1:B:172:GLY:O	1:B:183:VAL:HG22	1.89	0.71
1:B:593:ARG:HA	1:B:596:TYR:HB2	1.72	0.71
1:A:606:HIS:HD2	2:D:208:LEU:HB3	1.55	0.71
1:A:751:ILE:HA	1:A:754:ARG:CG	2.19	0.71
1:A:753:LYS:HB3	1:A:757:TRP:CZ3	2.25	0.71
2:C:2:LYS:HD2	2:C:3:THR:HG22	1.72	0.71
1:F:574:TYR:N	2:H:32:PHE:O	2.20	0.71
1:F:887:GLU:OE2	1:F:891:THR:OG1	2.09	0.71
2:G:14:LYS:HA	2:G:20:LYS:HB3	1.72	0.71
1:A:332:HIS:HA	1:A:336:TYR:H	1.54	0.71
1:B:327:LYS:HA	1:B:327:LYS:HE3	1.72	0.71
1:B:661:ILE:O	1:B:665:LYS:HB3	1.90	0.71
1:E:674:ASP:OD1	1:E:725:TYR:OH	2.05	0.71
2:H:190:ASP:H	2:H:237:ALA:HB3	1.55	0.71
2:G:15:ARG:HG2	2:G:20:LYS:HG3	1.73	0.71
2:H:13:PHE:HB3	2:H:171:TYR:CE2	2.16	0.71
1:E:151:VAL:HA	1:E:167:LEU:HB3	1.71	0.71
1:F:575:SER:HA	2:H:31:SER:HA	1.72	0.70
1:B:145:ARG:HG3	1:B:147:LYS:HE2	1.72	0.70
1:B:588:LEU:HD21	1:B:615:SER:HB2	1.73	0.70
2:D:30:ALA:HA	2:D:63:VAL:HG12	1.73	0.70
1:E:370:ARG:NH1	1:E:370:ARG:O	2.25	0.70
1:A:842:LEU:HD12	1:A:845:LEU:HD12	1.72	0.70
1:E:473:LEU:HD22	1:E:600:LEU:HD21	1.73	0.70
1:E:631:ILE:HG13	1:E:632:ASP:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:339:HIS:N	1:F:347:VAL:O	2.24	0.70
1:F:801:SER:C	1:F:840:LYS:HE3	2.11	0.70
1:F:471:TYR:O	1:F:475:GLN:NE2	2.24	0.70
1:F:842:LEU:HA	1:F:845:LEU:HD12	1.73	0.70
1:B:477:ASN:O	1:B:481:ILE:HG12	1.91	0.70
1:A:482:TYR:HE2	1:A:519:MET:HB2	1.57	0.70
1:B:405:THR:O	2:D:1:MET:N	2.25	0.70
1:F:614:ASN:OD1	1:F:615:SER:N	2.24	0.70
2:H:24:THR:O	2:H:24:THR:OG1	1.94	0.70
1:A:154:ALA:N	1:A:157:ASP:OD2	2.24	0.70
1:F:453:ASP:O	1:F:456:SER:OG	2.06	0.70
2:G:168:SER:N	2:G:170:ARG:HE	1.88	0.70
1:B:575:SER:HB2	1:B:578:MET:HG2	1.73	0.69
1:E:277:SER:OG	1:E:285:ARG:NH2	2.25	0.69
2:H:23:PHE:H	2:H:69:ASP:CB	2.02	0.69
1:A:549:GLN:O	1:A:553:ASP:N	2.26	0.69
2:C:15:ARG:HD2	2:C:169:GLU:HB2	1.73	0.69
1:B:343:ASN:HA	1:B:586:LEU:HG	1.73	0.69
2:H:179:ALA:HB2	2:H:191:ILE:HD11	1.73	0.69
1:A:627:ARG:O	1:B:990:ASN:ND2	2.26	0.69
1:E:195:GLN:O	1:F:237:LYS:NZ	2.21	0.69
1:B:551:LEU:HD13	1:B:607:GLU:HB2	1.75	0.69
1:E:967:LEU:HD22	1:E:1004:PHE:CE1	2.28	0.69
1:A:551:LEU:O	1:A:555:THR:OG1	2.09	0.69
1:E:728:LEU:HD13	1:E:765:ASN:HB3	1.75	0.69
1:E:751:ILE:O	1:E:804:TYR:OH	2.09	0.69
1:F:261:TYR:HA	1:F:264:LYS:HG2	1.75	0.68
1:E:309:ILE:H	1:E:309:ILE:HD12	1.57	0.68
2:H:72:TRP:HA	2:H:72:TRP:CE3	2.29	0.68
1:A:74:PRO:O	1:A:76:LYS:NZ	2.26	0.68
1:E:395:CYS:SG	1:E:396:MET:N	2.67	0.68
1:A:659:PHE:CD2	1:A:664:ILE:HD11	2.29	0.68
1:A:676:ILE:HG23	1:A:677:ARG:N	2.08	0.68
1:A:831:LYS:HB3	1:A:834:GLN:HB3	1.76	0.68
1:B:561:LEU:HA	1:B:564:LYS:HB2	1.75	0.68
1:E:236:GLN:HB3	1:E:240:PHE:HB2	1.74	0.68
1:A:746:GLU:O	1:A:748:ASP:N	2.27	0.68
1:E:662:ASP:OD1	1:E:663:ASP:N	2.27	0.68
1:F:711:GLN:O	1:F:712:PHE:HD1	1.76	0.68
1:F:869:ILE:CD1	1:F:874:ILE:O	2.41	0.68
1:A:86:ARG:HD2	1:A:187:GLU:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:LYS:NZ	1:F:599:CYS:SG	2.62	0.68
1:A:681:GLN:O	1:A:685:GLU:HB2	1.94	0.68
1:A:622:LYS:O	1:A:626:GLU:HB2	1.94	0.68
1:B:115:ASN:H	1:B:118:HIS:CD2	2.12	0.68
1:E:252:PRO:HD2	1:E:252:PRO:O	1.94	0.67
1:E:493:ASN:HA	1:E:503:HIS:HE1	1.58	0.67
2:C:61:LEU:HB2	2:C:220:PHE:HB2	1.75	0.67
1:A:235:LEU:HD22	1:B:195:GLN:HA	1.76	0.67
1:A:707:VAL:O	1:A:711:GLN:NE2	2.27	0.67
1:A:606:HIS:CD2	2:D:208:LEU:HB3	2.29	0.67
1:B:646:PHE:HB3	1:B:677:ARG:NH1	2.09	0.67
1:B:724:LYS:HD2	1:B:761:LEU:HA	1.75	0.67
1:E:915:THR:HA	1:E:918:ILE:HG22	1.75	0.67
1:A:296:SER:HA	1:A:300:LYS:HD2	1.77	0.67
1:B:587:ARG:O	1:B:591:ASN:ND2	2.27	0.67
2:G:175:TYR:HB2	2:G:193:ILE:HB	1.77	0.67
2:C:170:ARG:HA	2:C:170:ARG:CZ	2.23	0.67
1:E:231:TRP:HA	1:E:234:LYS:HB2	1.77	0.67
1:E:247:ARG:HD3	1:E:249:ASP:H	1.58	0.67
1:E:616:MET:HG2	1:E:659:PHE:CZ	2.30	0.67
1:E:629:ARG:HD3	1:E:630:ASP:O	1.93	0.67
1:F:279:GLU:O	1:F:285:ARG:NH1	2.25	0.67
1:A:802:ARG:HB2	1:A:840:LYS:HB3	1.74	0.67
1:A:699:PHE:HB2	1:A:704:MET:HG3	1.76	0.67
1:B:118:HIS:HA	1:B:121:ILE:HG22	1.77	0.67
2:C:16:LYS:CG	2:C:170:ARG:HB2	2.25	0.67
1:E:567:SER:OG	1:E:568:GLU:OE1	2.10	0.67
1:E:605:PHE:O	1:E:609:HIS:ND1	2.24	0.67
1:F:304:LYS:HB2	1:F:307:GLU:HB2	1.77	0.67
1:F:849:ALA:HA	1:F:852:HIS:HE1	1.59	0.67
2:D:31:SER:N	2:D:62:THR:O	2.28	0.67
1:F:228:LEU:HD12	1:F:228:LEU:O	1.94	0.67
1:F:892:ARG:HA	1:F:895:ASN:HD22	1.59	0.67
1:A:463:ILE:HD13	1:B:143:TRP:HB3	1.76	0.66
1:E:937:ASP:OD1	1:E:940:TYR:N	2.22	0.66
1:A:582:ILE:O	1:A:586:LEU:N	2.23	0.66
1:B:593:ARG:O	1:B:597:GLU:N	2.28	0.66
1:E:302:ILE:HG23	1:E:307:GLU:HB3	1.77	0.66
1:E:374:SER:HB2	1:E:377:GLN:HG2	1.77	0.66
1:F:800:TYR:C	1:F:802:ARG:N	2.41	0.66
1:A:501:GLY:HA3	1:A:747:ARG:HH22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLU:C	1:A:609:HIS:N	2.41	0.66
1:A:751:ILE:HG23	1:A:799:LEU:HD22	1.75	0.66
1:B:482:TYR:HA	1:B:485:ILE:HD12	1.78	0.66
1:B:571:GLU:OE1	1:B:571:GLU:N	2.29	0.66
1:B:724:LYS:HZ2	1:B:760:ARG:HB3	1.59	0.66
2:C:70:LEU:HA	2:C:73:LEU:HB3	1.76	0.66
2:D:28:GLN:OE1	2:D:28:GLN:N	2.27	0.66
1:E:570:SER:O	1:F:669:ARG:NH2	2.28	0.66
1:A:549:GLN:HB2	1:A:552:TYR:HB2	1.78	0.66
1:A:780:VAL:HG11	1:A:819:ARG:HB2	1.78	0.66
2:H:45:ILE:HG23	2:H:47:ASN:H	1.61	0.66
1:A:676:ILE:HG23	1:A:677:ARG:H	1.61	0.66
1:F:605:PHE:HD2	2:G:209:GLU:HB2	1.60	0.66
1:A:75:LYS:NZ	1:A:78:ASN:O	2.28	0.66
1:F:753:LYS:HE2	1:F:757:TRP:CE2	2.30	0.66
1:B:242:LYS:O	1:B:267:ARG:NH2	2.29	0.66
2:H:54:LYS:NZ	2:H:56:GLU:OE2	2.29	0.66
1:E:404:ASN:HA	2:G:4:VAL:HG11	1.77	0.66
1:F:452:TYR:HE1	1:F:514:ARG:HH21	1.42	0.66
1:F:869:ILE:HG12	1:F:919:TRP:HZ2	1.60	0.66
1:E:80:SER:HA	1:E:84:TYR:HB2	1.78	0.65
1:F:783:ALA:HA	1:F:786:HIS:CD2	2.32	0.65
1:E:629:ARG:C	1:E:630:ASP:O	2.20	0.65
1:A:581:ASP:O	1:A:584:VAL:HB	1.96	0.65
1:A:433:GLU:OE1	1:A:437:LYS:NZ	2.30	0.65
1:A:648:GLU:HB3	1:A:651:ASP:HB2	1.79	0.65
1:B:729:SER:HB3	1:B:731:GLU:CD	2.16	0.65
2:C:22:VAL:HG12	2:C:69:ASP:OD1	1.97	0.65
1:F:930:MET:SD	1:F:931:GLU:N	2.70	0.65
1:B:569:MET:CE	1:B:570:SER:H	2.10	0.65
1:A:405:THR:HB	2:C:4:VAL:HG21	1.77	0.65
1:A:549:GLN:CB	1:A:552:TYR:HB2	2.27	0.65
1:A:698:GLN:O	1:A:702:ASN:N	2.24	0.65
1:F:331:LYS:HZ1	1:F:337:ASP:H	1.45	0.65
1:F:717:LYS:NZ	1:F:748:ASP:O	2.23	0.65
1:B:578:MET:HA	1:B:582:ILE:HG13	1.79	0.65
1:F:173:ASP:OD2	1:F:175:ARG:NE	2.28	0.65
2:H:11:VAL:HG13	2:H:175:TYR:HE1	1.61	0.65
1:E:755:TYR:CE2	1:E:803:ASP:HB3	2.31	0.65
2:H:22:VAL:HG13	2:H:171:TYR:OH	1.97	0.65
1:A:46:VAL:HG23	1:A:216:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:TYR:OH	1:E:651:ASP:OD1	2.12	0.65
1:E:606:HIS:NE2	2:H:205:GLU:O	2.30	0.65
1:F:25:ASN:OD1	1:F:26:VAL:N	2.30	0.65
1:F:91:PHE:HA	1:F:94:VAL:HG12	1.80	0.65
2:C:16:LYS:O	2:C:169:GLU:HG2	1.98	0.64
2:H:14:LYS:HB3	2:H:172:GLU:HG2	1.79	0.64
1:B:184:VAL:O	1:B:185:LEU:HD22	1.96	0.64
2:D:22:VAL:HB	2:D:72:TRP:HB2	1.78	0.64
1:E:127:ALA:O	1:E:128:HIS:ND1	2.30	0.64
1:E:711:GLN:NE2	1:E:715:GLU:OE2	2.30	0.64
1:A:82:ASP:OD1	1:A:83:GLU:N	2.30	0.64
1:A:235:LEU:HD11	1:B:198:PRO:HG3	1.77	0.64
1:E:29:CYS:SG	1:E:267:ARG:NH2	2.68	0.64
1:E:75:LYS:HG2	1:E:77:GLY:H	1.62	0.64
2:G:73:LEU:O	2:G:77:GLN:HB3	1.97	0.64
1:A:63:VAL:HG21	1:A:84:TYR:HD1	1.63	0.64
1:B:624:GLU:HB3	1:B:627:ARG:HH21	1.61	0.64
1:F:70:LEU:HD21	1:F:95:LYS:HE2	1.79	0.64
1:F:331:LYS:NZ	1:F:338:TYR:H	1.93	0.64
2:H:32:PHE:HE1	2:H:59:ILE:HG23	1.61	0.64
1:B:613:ARG:HA	1:B:659:PHE:CZ	2.32	0.64
1:E:440:PHE:CD2	1:E:599:CYS:HA	2.33	0.64
1:F:396:MET:SD	1:F:398:LYS:N	2.67	0.64
1:F:404:ASN:O	2:H:1:MET:N	2.24	0.64
1:F:495:LEU:HA	1:F:498:LEU:HD23	1.80	0.64
1:A:407:ILE:HB	2:C:2:LYS:HZ2	1.63	0.64
1:A:189:ASP:O	1:A:193:TYR:N	2.31	0.64
1:B:455:TYR:O	1:B:459:ILE:HG12	1.97	0.64
1:E:189:ASP:O	1:E:193:TYR:N	2.30	0.64
1:F:721:TYR:O	1:F:723:ALA:N	2.30	0.64
1:F:849:ALA:HA	1:F:852:HIS:CE1	2.32	0.64
1:E:82:ASP:OD1	1:E:83:GLU:N	2.31	0.64
1:E:616:MET:HG2	1:E:659:PHE:HZ	1.63	0.64
1:F:869:ILE:HA	1:F:874:ILE:H	1.63	0.64
1:A:141:ALA:HA	1:A:144:LYS:HZ2	1.61	0.64
1:A:223:TYR:O	1:A:226:ASN:N	2.29	0.64
1:A:659:PHE:HB3	1:A:718:ALA:HB3	1.79	0.64
1:B:609:HIS:HA	1:B:658:HIS:HB3	1.80	0.64
1:B:626:GLU:HA	1:B:629:ARG:HE	1.63	0.64
2:G:14:LYS:N	2:G:172:GLU:O	2.29	0.64
1:A:357:MET:HE3	1:A:357:MET:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:ARG:HA	2:G:170:ARG:O	1.97	0.63
1:A:411:SER:HB3	1:A:414:TYR:HB3	1.79	0.63
1:A:473:LEU:HD12	1:A:600:LEU:HD21	1.79	0.63
1:F:724:LYS:HB3	1:F:760:ARG:O	1.99	0.63
2:C:22:VAL:HG21	2:C:171:TYR:HE1	1.63	0.63
1:E:241:HIS:NE2	1:F:159:ALA:O	2.27	0.63
1:E:488:ALA:HA	1:E:491:GLN:HE21	1.63	0.63
1:F:339:HIS:HD2	1:F:349:HIS:HB3	1.63	0.63
1:F:975:HIS:ND1	1:F:976:MET:SD	2.70	0.63
1:A:583:VAL:O	1:A:586:LEU:HD12	1.98	0.63
1:E:190:TYR:OH	1:E:224:ASN:OD1	2.15	0.63
1:E:277:SER:OG	1:E:278:ASN:N	2.30	0.63
1:F:709:TYR:CD1	1:F:713:ILE:HG13	2.33	0.63
1:A:334:PHE:O	1:A:337:ASP:HB2	1.97	0.63
1:F:939:GLN:HG2	1:F:943:PHE:CZ	2.33	0.63
2:G:194:GLN:NE2	2:G:195:PHE:O	2.32	0.63
1:A:580:SER:C	1:A:583:VAL:H	2.02	0.63
1:A:614:ASN:OD1	1:A:615:SER:N	2.31	0.63
1:B:184:VAL:C	1:B:185:LEU:HD22	2.19	0.63
1:F:41:LYS:HZ2	1:F:211:HIS:HA	1.64	0.63
1:F:960:LYS:HD3	1:F:996:TYR:CE2	2.33	0.63
1:E:78:ASN:HB2	1:E:81:SER:HB3	1.81	0.63
1:F:722:PHE:HA	1:F:724:LYS:HE2	1.79	0.63
1:E:544:PHE:CZ	1:E:550:PHE:HB2	2.33	0.63
1:A:83:GLU:HA	1:A:86:ARG:HB2	1.80	0.62
1:B:29:CYS:O	1:B:33:ILE:HG12	1.98	0.62
1:E:396:MET:SD	1:E:397:ALA:N	2.72	0.62
1:E:606:HIS:HB3	1:E:610:GLN:NE2	2.14	0.62
1:F:780:VAL:HG11	1:F:820:LEU:HB3	1.81	0.62
2:G:189:SER:HB3	2:G:238:SER:HB3	1.81	0.62
1:A:728:LEU:HG	1:A:764:CYS:SG	2.38	0.62
1:A:802:ARG:HD2	1:A:840:LYS:HG2	1.80	0.62
1:B:247:ARG:HE	1:B:248:THR:H	1.45	0.62
1:E:680:GLU:O	1:E:680:GLU:OE2	2.15	0.62
1:F:960:LYS:HD2	1:F:962:TYR:CE2	2.34	0.62
2:C:170:ARG:O	2:C:172:GLU:N	2.32	0.62
1:E:674:ASP:HA	1:E:725:TYR:CE1	2.35	0.62
2:H:35:ALA:O	2:H:58:GLU:N	2.33	0.62
1:E:419:ASP:OD1	1:E:419:ASP:N	2.31	0.62
2:H:60:ASN:HA	2:H:219:LYS:HZ3	1.65	0.62
1:E:375:LYS:HA	1:E:378:TYR:HD1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:ILE:O	1:E:485:ILE:HG12	2.00	0.62
1:F:326:ARG:NH1	1:F:591:ASN:OD1	2.28	0.62
2:D:22:VAL:HG23	2:D:69:ASP:HB2	1.80	0.62
1:A:41:LYS:HD2	1:A:211:HIS:HA	1.82	0.62
1:A:582:ILE:O	1:A:583:VAL:C	2.36	0.62
1:B:90:ILE:HG12	1:F:260:TYR:HD2	1.65	0.62
2:C:22:VAL:HG21	2:C:171:TYR:CE1	2.35	0.62
1:E:731:GLU:HA	1:E:734:GLY:HA2	1.82	0.62
1:E:984:LEU:O	1:E:988:VAL:HG23	2.00	0.62
1:A:651:ASP:O	1:A:655:ILE:HG12	1.99	0.62
1:B:490:THR:HA	1:B:493:ASN:HB2	1.82	0.62
1:E:581:ASP:OD1	1:E:582:ILE:N	2.33	0.62
1:A:717:LYS:NZ	1:A:749:LEU:HB3	2.15	0.62
1:B:476:ILE:O	1:B:480:ARG:HG2	1.99	0.62
1:B:899:GLU:HA	1:B:904:ILE:HD12	1.82	0.62
1:F:979:HIS:HD1	1:F:980:VAL:HG23	1.64	0.62
1:B:569:MET:HE3	1:B:570:SER:H	1.65	0.62
1:F:724:LYS:HD2	1:F:725:TYR:CE1	2.35	0.62
1:A:662:ASP:HA	1:A:665:LYS:HE2	1.80	0.61
1:B:223:TYR:HA	1:B:226:ASN:ND2	2.15	0.61
1:F:627:ARG:NH1	1:F:672:SER:OG	2.31	0.61
2:G:192:TYR:HB2	2:G:235:ILE:HB	1.80	0.61
1:B:348:ARG:NH1	1:B:351:ASN:O	2.33	0.61
1:E:370:ARG:NH1	1:E:373:LEU:HD22	2.15	0.61
1:E:724:LYS:NZ	1:E:760:ARG:O	2.30	0.61
1:F:376:LYS:HZ1	1:F:380:ARG:HE	1.48	0.61
1:E:558:LEU:O	1:E:562:THR:HG23	2.00	0.61
1:F:228:LEU:O	1:F:228:LEU:CG	2.49	0.61
1:F:509:ASP:HA	1:F:512:LEU:HD12	1.81	0.61
1:F:683:LYS:HA	1:F:686:GLU:OE2	2.00	0.61
2:H:169:GLU:O	2:H:170:ARG:C	2.38	0.61
1:A:586:LEU:HA	1:A:589:TYR:CD2	2.35	0.61
1:A:956:PRO:O	1:A:987:ARG:NH1	2.34	0.61
1:F:627:ARG:HH21	1:F:675:LYS:HZ2	1.48	0.61
1:F:995:ARG:O	1:F:999:ILE:HG12	2.01	0.61
1:A:67:HIS:ND1	1:A:73:SER:O	2.34	0.61
1:A:147:LYS:HD3	1:B:530:GLY:HA3	1.82	0.61
1:B:646:PHE:HB3	1:B:677:ARG:HH12	1.66	0.61
1:E:140:THR:O	1:E:144:LYS:HE2	2.01	0.61
1:E:208:ILE:HA	1:E:213:ILE:HG13	1.82	0.61
1:F:686:GLU:HA	1:F:689:VAL:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:LYS:HG3	1:A:661:ILE:H	1.66	0.61
1:B:724:LYS:NZ	1:B:760:ARG:HB3	2.16	0.61
1:E:758:LEU:HD11	1:E:807:LEU:HD22	1.81	0.61
1:F:956:PRO:HG3	1:F:987:ARG:HD2	1.82	0.61
2:G:72:TRP:O	2:G:76:THR:HB	2.00	0.61
1:A:475:GLN:OE1	1:A:478:ARG:NH1	2.29	0.61
1:A:528:PHE:HE2	1:A:542:LEU:O	1.83	0.61
2:D:61:LEU:O	2:D:220:PHE:N	2.32	0.61
1:F:86:ARG:HG3	1:F:87:ILE:HD12	1.83	0.61
1:F:286:TYR:O	1:F:290:MET:HG2	2.00	0.61
1:F:439:ALA:HB2	1:F:454:LEU:HD22	1.83	0.61
1:F:936:MET:N	1:F:936:MET:SD	2.74	0.61
1:B:472:TYR:CE2	1:B:542:LEU:HG	2.32	0.61
2:D:203:GLU:OE1	2:D:203:GLU:N	2.26	0.61
1:E:205:LYS:HZ3	1:F:199:LEU:HD23	1.66	0.61
1:E:848:ASN:OD1	1:E:852:HIS:NE2	2.33	0.61
2:H:196:PRO:HG3	2:H:230:GLU:HA	1.82	0.61
1:A:34:THR:O	1:A:37:SER:OG	2.14	0.61
1:B:609:HIS:NE2	1:B:660:LYS:HG2	2.16	0.61
1:E:904:ILE:HG12	2:H:235:ILE:HG23	1.81	0.61
1:F:294:ILE:O	1:F:295:GLU:HG2	2.01	0.61
2:G:38:GLU:HA	2:G:54:LYS:HZ1	1.65	0.61
1:B:154:ALA:N	1:B:157:ASP:OD2	2.30	0.60
1:E:912:TYR:O	1:E:915:THR:OG1	2.15	0.60
1:F:962:TYR:CD1	1:F:967:LEU:HD22	2.31	0.60
1:A:94:VAL:HG13	1:A:95:LYS:HD3	1.81	0.60
1:A:238:ASP:OD1	1:A:238:ASP:N	2.32	0.60
1:E:1001:MET:HE2	1:F:985:LYS:HD3	1.83	0.60
1:B:452:TYR:HA	1:B:455:TYR:CD2	2.36	0.60
1:B:688:LEU:HD21	1:B:736:ILE:HD11	1.83	0.60
2:D:196:PRO:HG2	2:D:230:GLU:HA	1.83	0.60
1:E:56:TYR:CZ	1:E:135:ASP:HB3	2.36	0.60
1:F:504:TYR:HE2	1:F:706:VAL:HG21	1.67	0.60
1:F:960:LYS:O	1:F:962:TYR:N	2.33	0.60
1:A:751:ILE:HG13	1:A:754:ARG:HB2	1.83	0.60
1:A:808:ILE:HG13	1:A:844:LEU:HD11	1.83	0.60
1:B:42:LEU:HD12	1:B:44:PHE:HE1	1.67	0.60
1:B:663:ASP:O	1:B:667:LEU:HB2	2.01	0.60
1:E:375:LYS:HA	1:E:378:TYR:CD1	2.35	0.60
1:E:922:LEU:HD22	1:E:969:LYS:HE2	1.81	0.60
1:F:357:MET:SD	1:F:358:GLU:N	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:GLU:OE2	1:A:728:LEU:HA	2.01	0.60
1:B:647:MET:SD	1:B:647:MET:N	2.75	0.60
1:F:407:ILE:H	2:H:2:LYS:HB3	1.65	0.60
2:H:21:LEU:C	2:H:69:ASP:HB3	2.22	0.60
1:B:130:ILE:HD13	1:B:168:LEU:HB3	1.82	0.60
1:B:175:ARG:NH1	1:B:175:ARG:O	2.34	0.60
1:E:519:MET:O	1:E:520:THR:C	2.39	0.60
1:F:895:ASN:O	1:F:899:GLU:HB2	2.02	0.60
1:F:228:LEU:O	1:F:228:LEU:HG	2.01	0.60
1:F:987:ARG:HA	1:F:987:ARG:CZ	2.32	0.60
1:B:375:LYS:HA	1:B:378:TYR:HB2	1.84	0.60
1:E:192:ASN:O	1:E:196:ASN:N	2.31	0.60
1:B:794:VAL:HG22	2:C:223:LEU:HD12	1.84	0.60
1:E:683:LYS:HA	1:E:683:LYS:HE3	1.84	0.60
1:E:698:GLN:HG2	1:E:712:PHE:CE2	2.32	0.60
1:F:134:TYR:OH	1:F:184:VAL:O	2.20	0.60
1:A:374:SER:OG	1:A:377:GLN:OE1	2.19	0.59
1:A:491:GLN:OE1	1:A:491:GLN:N	2.31	0.59
1:A:812:GLU:CD	1:A:813:LYS:H	2.05	0.59
1:E:565:VAL:O	1:E:569:MET:HG2	2.01	0.59
1:E:245:PHE:HD2	1:E:268:ILE:HG23	1.66	0.59
1:A:25:ASN:HA	1:A:28:GLU:OE2	2.01	0.59
1:F:233:ARG:NE	1:F:264:LYS:HA	2.17	0.59
2:G:188:TYR:CD2	2:G:238:SER:HB2	2.37	0.59
1:A:239:SER:O	1:A:239:SER:OG	2.19	0.59
1:B:414:TYR:OH	1:B:650:TYR:O	2.20	0.59
1:F:357:MET:HE3	1:F:357:MET:H	1.67	0.59
2:H:22:VAL:HG12	2:H:171:TYR:OH	2.03	0.59
1:A:495:LEU:HD13	2:D:218:ILE:HD12	1.84	0.59
1:B:116:PRO:HA	1:B:119:ASP:OD2	2.01	0.59
1:F:796:SER:OG	2:G:222:ALA:O	2.20	0.59
1:F:809:LYS:HB2	1:F:844:LEU:HD11	1.84	0.59
1:E:990:ASN:HA	1:F:994:LYS:HE3	1.85	0.59
1:E:1001:MET:O	1:E:1002:ASN:HB2	2.02	0.59
1:F:86:ARG:NH1	1:F:87:ILE:HA	2.17	0.59
2:G:13:PHE:N	2:G:22:VAL:O	2.36	0.59
2:H:62:THR:OG1	2:H:218:ILE:O	2.16	0.59
1:B:659:PHE:HB3	1:B:662:ASP:HA	1.83	0.59
1:E:281:ASP:O	1:E:285:ARG:NH2	2.36	0.59
1:E:680:GLU:OE1	1:E:683:LYS:N	2.32	0.59
1:F:222:ASP:H	1:F:225:ILE:CG2	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:LYS:C	1:F:391:ASN:O	2.36	0.59
1:A:404:ASN:HA	2:C:4:VAL:O	2.02	0.59
1:E:629:ARG:HD2	1:E:630:ASP:O	2.03	0.59
1:F:170:VAL:HA	1:F:200:ILE:HD11	1.84	0.59
2:G:14:LYS:HA	2:G:20:LYS:HE3	1.84	0.59
1:E:978:HIS:O	1:E:982:GLU:HG2	2.02	0.59
1:F:891:THR:O	1:F:895:ASN:ND2	2.36	0.59
1:A:213:ILE:HB	1:A:243:PRO:HB3	1.84	0.59
1:A:548:ASN:CB	2:D:210:ASN:HD21	2.16	0.59
1:B:442:LEU:HB3	1:B:447:ARG:HH12	1.68	0.59
1:B:964:ASP:HB2	1:B:965:LYS:NZ	2.18	0.59
1:E:815:PHE:CG	1:E:815:PHE:O	2.56	0.59
1:F:81:SER:OG	1:F:82:ASP:N	2.35	0.59
1:A:607:GLU:O	1:A:608:PHE:C	2.39	0.58
2:G:65:ASN:CG	2:G:67:PHE:H	2.05	0.58
1:A:275:ILE:HG23	1:A:285:ARG:HH12	1.66	0.58
1:F:962:TYR:CE2	1:F:999:ILE:HG21	2.38	0.58
1:A:610:GLN:HA	1:A:613:ARG:HB3	1.85	0.58
1:A:794:VAL:HA	2:D:225:ASP:HA	1.85	0.58
1:B:46:VAL:HG11	1:B:138:ILE:HG21	1.84	0.58
1:B:247:ARG:HE	1:B:248:THR:N	2.01	0.58
2:C:28:GLN:HB3	2:C:64:LYS:HD2	1.85	0.58
1:F:817:SER:HB3	1:F:821:SER:HB3	1.85	0.58
1:A:54:SER:OG	1:A:115:ASN:ND2	2.30	0.58
1:A:367:CYS:SG	1:A:370:ARG:NH2	2.77	0.58
1:A:449:GLU:HG3	1:A:507:PHE:HE1	1.69	0.58
1:B:118:HIS:O	1:B:122:LEU:HG	2.03	0.58
1:B:134:TYR:CG	1:B:183:VAL:HG11	2.38	0.58
1:F:836:ASP:OD1	1:F:836:ASP:N	2.32	0.58
1:B:254:GLU:O	1:B:257:THR:OG1	2.19	0.58
1:B:407:ILE:HG12	2:D:2:LYS:HB3	1.85	0.58
2:D:190:ASP:H	2:D:237:ALA:HB3	1.69	0.58
1:F:53:LEU:HB3	1:F:115:ASN:HD22	1.68	0.58
1:F:776:ASP:O	1:F:780:VAL:HG22	2.04	0.58
1:A:1000:LEU:HA	1:A:1004:PHE:HB2	1.85	0.58
1:E:242:LYS:HG3	1:E:267:ARG:HD3	1.85	0.58
1:F:311:TYR:O	1:F:315:LYS:HG2	2.03	0.58
1:F:706:VAL:O	1:F:710:THR:HG23	2.04	0.58
1:F:852:HIS:O	1:F:855:SER:OG	2.22	0.58
2:G:4:VAL:O	2:G:6:GLN:HG3	2.02	0.58
1:A:631:ILE:HD12	1:A:635:GLY:HA3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:LEU:HD11	1:A:844:LEU:HD22	1.86	0.58
1:B:297:GLN:HE21	1:B:301:PHE:HZ	1.51	0.58
1:E:893:LYS:NZ	1:E:933:PHE:HA	2.19	0.58
1:F:812:GLU:OE1	1:F:813:LYS:N	2.34	0.58
1:A:606:HIS:O	1:A:609:HIS:CD2	2.57	0.58
1:E:549:GLN:HA	1:E:552:TYR:HD2	1.69	0.58
1:F:228:LEU:HA	1:F:231:TRP:HE3	1.67	0.58
1:E:32:GLU:OE1	1:E:267:ARG:NH2	2.36	0.58
1:F:548:ASN:HB3	2:G:209:GLU:OE2	2.02	0.58
2:D:175:TYR:HB2	2:D:193:ILE:HB	1.85	0.58
1:E:153:SER:OG	1:E:173:ASP:OD1	2.19	0.58
1:E:782:GLN:HA	1:E:785:LYS:HB2	1.86	0.58
1:E:801:SER:H	1:E:840:LYS:HZ1	1.50	0.58
1:A:783:ALA:HB1	1:A:838:LEU:HD12	1.86	0.57
2:C:69:ASP:OD1	2:C:69:ASP:N	2.37	0.57
1:E:48:ALA:O	1:E:51:SER:OG	2.22	0.57
1:E:277:SER:OG	1:E:284:GLU:OE2	2.16	0.57
1:E:279:GLU:HG2	1:E:280:TYR:H	1.68	0.57
1:E:744:PHE:HB3	1:E:749:LEU:HD22	1.86	0.57
1:F:119:ASP:HB2	1:F:120:LYS:HZ2	1.68	0.57
1:F:277:SER:OG	1:F:278:ASN:N	2.36	0.57
1:F:908:SER:CA	2:G:231:MET:HB3	2.27	0.57
1:A:26:VAL:O	1:A:30:ILE:HG22	2.03	0.57
1:A:148:TYR:HB3	1:B:532:PRO:HD3	1.85	0.57
1:B:131:THR:OG1	1:B:133:ASN:OD1	2.20	0.57
1:F:403:LEU:H	2:H:6:GLN:HB2	1.68	0.57
1:F:737:VAL:HG21	1:F:771:ILE:HD12	1.86	0.57
1:F:822:GLU:HA	1:F:825:LEU:HG	1.85	0.57
1:F:860:GLU:O	1:F:861:ASN:C	2.43	0.57
1:F:861:ASN:O	1:F:862:ILE:C	2.43	0.57
1:F:869:ILE:HD12	1:F:874:ILE:N	2.19	0.57
1:A:29:CYS:O	1:A:33:ILE:HG12	2.04	0.57
1:B:325:ILE:HG21	1:B:330:LEU:HD13	1.85	0.57
1:B:479:TYR:CE2	1:B:524:ILE:HD13	2.39	0.57
1:E:691:ILE:HA	1:E:694:GLU:OE2	2.05	0.57
1:F:24:ASN:OD1	1:F:25:ASN:N	2.38	0.57
1:F:582:ILE:HA	1:F:585:LEU:HD23	1.86	0.57
1:F:875:ASP:OD2	2:G:49:PRO:HD2	2.04	0.57
1:A:780:VAL:HG22	1:A:820:LEU:HD22	1.85	0.57
2:D:32:PHE:HD1	2:D:61:LEU:HD13	1.70	0.57
1:E:126:PRO:O	1:E:165:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:927:ASN:HD21	1:E:929:LYS:HD3	1.69	0.57
1:F:419:ASP:OD1	1:F:420:VAL:N	2.38	0.57
2:G:36:ILE:HG23	2:G:54:LYS:HD2	1.86	0.57
1:A:450:GLU:OE1	1:A:450:GLU:N	2.38	0.57
1:B:105:LYS:HA	1:B:178:PHE:HD2	1.69	0.57
1:E:186:LYS:HD2	1:E:188:ASP:H	1.69	0.57
1:E:242:LYS:HE2	1:E:242:LYS:HA	1.86	0.57
1:E:373:LEU:HD23	1:E:378:TYR:CD2	2.40	0.57
1:F:309:ILE:HA	1:F:312:ILE:HG12	1.87	0.57
1:B:187:GLU:HA	1:B:190:TYR:CD1	2.39	0.57
1:F:652:PHE:CE2	1:F:726:VAL:HG11	2.40	0.57
1:A:498:LEU:HD11	2:D:23:PHE:HE1	1.70	0.57
1:B:179:LYS:HD3	1:B:179:LYS:N	2.19	0.57
1:B:259:ILE:O	1:B:263:ASN:ND2	2.38	0.57
1:B:576:PHE:CE1	1:B:641:LYS:HB2	2.39	0.57
1:B:593:ARG:HG3	1:B:597:GLU:HB3	1.86	0.57
2:D:41:LEU:HD11	2:D:54:LYS:HE2	1.85	0.57
1:F:472:TYR:HD1	1:F:473:LEU:HD12	1.70	0.57
1:A:290:MET:O	1:A:293:LEU:HG	2.05	0.57
1:B:312:ILE:O	1:B:316:ILE:HG22	2.04	0.57
1:E:32:GLU:OE2	1:E:267:ARG:NH1	2.35	0.57
1:A:86:ARG:HH12	1:A:89:GLN:HB3	1.68	0.57
1:A:192:ASN:OD1	1:A:196:ASN:ND2	2.36	0.57
1:A:497:LEU:HD21	2:D:73:LEU:HD12	1.86	0.57
1:E:475:GLN:HA	1:E:478:ARG:HH12	1.70	0.57
1:E:762:THR:HG22	1:E:767:LEU:HD21	1.87	0.57
1:F:188:ASP:OD1	1:F:189:ASP:N	2.38	0.57
1:F:373:LEU:HB3	1:F:377:GLN:HB2	1.87	0.57
1:A:407:ILE:HB	2:C:2:LYS:NZ	2.19	0.57
1:A:717:LYS:HG3	1:A:757:TRP:CH2	2.40	0.57
1:F:627:ARG:HH21	1:F:675:LYS:NZ	2.02	0.57
1:F:753:LYS:HE2	1:F:757:TRP:NE1	2.20	0.57
1:F:768:PRO:HD2	1:F:771:ILE:HG12	1.86	0.57
1:A:663:ASP:HA	1:A:666:ASN:OD1	2.05	0.56
1:A:771:ILE:O	1:A:775:ILE:HD12	2.05	0.56
1:E:755:TYR:HE2	1:E:803:ASP:HB3	1.70	0.56
1:E:807:LEU:HD12	1:E:808:ILE:H	1.70	0.56
1:E:827:LEU:HB3	1:E:831:LYS:HD3	1.86	0.56
1:F:119:ASP:HB2	1:F:120:LYS:NZ	2.19	0.56
1:F:815:PHE:CZ	1:F:817:SER:HA	2.39	0.56
1:F:957:SER:HA	1:F:960:LYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:LEU:HD11	1:B:757:TRP:HE3	1.69	0.56
2:C:3:THR:OG1	2:C:5:ILE:HD11	2.05	0.56
1:F:247:ARG:NH1	1:F:270:ASP:OD1	2.34	0.56
1:A:367:CYS:HA	1:A:370:ARG:HE	1.69	0.56
1:A:549:GLN:HA	1:A:552:TYR:CB	2.33	0.56
1:A:580:SER:CB	1:A:582:ILE:HG12	2.35	0.56
1:A:613:ARG:HD3	1:A:663:ASP:HB3	1.86	0.56
1:B:439:ALA:HB2	1:B:454:LEU:HD22	1.86	0.56
2:D:179:ALA:O	2:D:189:SER:OG	2.24	0.56
1:E:475:GLN:HA	1:E:478:ARG:NH1	2.20	0.56
1:E:551:LEU:HG	1:E:607:GLU:HG2	1.87	0.56
1:E:681:GLN:NE2	1:E:682:GLU:OE1	2.38	0.56
1:F:755:TYR:CE2	1:F:803:ASP:HB3	2.41	0.56
1:F:863:ASN:HD21	1:F:865:LEU:HB2	1.71	0.56
2:C:13:PHE:HE2	2:C:24:THR:HG1	1.53	0.56
1:B:412:LEU:HD21	1:B:420:VAL:HG23	1.86	0.56
1:B:685:GLU:OE1	1:B:731:GLU:HB2	2.06	0.56
1:B:740:LEU:HD22	1:B:758:LEU:HD21	1.87	0.56
1:E:216:ILE:HD13	1:E:246:ILE:HD13	1.86	0.56
1:E:729:SER:OG	1:E:732:GLY:N	2.37	0.56
1:A:500:PHE:HA	1:A:747:ARG:HG3	1.88	0.56
1:B:475:GLN:HB3	1:B:527:LEU:HD11	1.88	0.56
1:E:174:PHE:HB3	1:E:178:PHE:CD1	2.41	0.56
1:F:559:PHE:O	1:F:562:THR:OG1	2.19	0.56
1:F:966:LEU:O	1:F:970:ILE:HG12	2.05	0.56
1:A:802:ARG:CB	1:A:840:LYS:HB3	2.36	0.56
1:E:89:GLN:HE21	1:E:187:GLU:HG3	1.71	0.56
1:F:75:LYS:NZ	1:F:83:GLU:HB3	2.20	0.56
1:F:592:LEU:O	1:F:596:TYR:HB2	2.06	0.56
1:F:822:GLU:OE1	1:F:822:GLU:N	2.34	0.56
1:A:491:GLN:O	1:A:496:GLY:N	2.38	0.56
1:A:800:TYR:HD1	2:D:226:THR:HG23	1.71	0.56
2:C:40:LYS:NZ	2:C:42:ARG:O	2.38	0.56
1:E:405:THR:O	2:G:1:MET:N	2.38	0.56
1:F:27:VAL:O	1:F:31:LYS:HG2	2.05	0.56
1:F:386:ASN:O	1:F:390:LYS:HB3	2.06	0.56
1:F:442:LEU:HD12	1:F:451:SER:HA	1.87	0.56
2:H:197:ASN:OD1	2:H:198:VAL:N	2.39	0.56
1:E:1000:LEU:HA	1:E:1004:PHE:CE2	2.40	0.56
1:F:532:PRO:O	1:F:536:GLN:NE2	2.29	0.56
1:F:722:PHE:HA	1:F:724:LYS:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD21	1:A:91:PHE:HA	1.87	0.56
1:E:616:MET:SD	1:E:617:SER:N	2.79	0.56
1:F:47:GLY:N	1:F:216:ILE:O	2.38	0.56
1:F:242:LYS:HE3	1:F:267:ARG:HG2	1.88	0.56
2:H:68:PHE:HD1	2:H:70:LEU:H	1.53	0.56
1:A:580:SER:O	1:A:583:VAL:HB	2.07	0.55
1:A:768:PRO:O	1:A:772:ILE:N	2.33	0.55
2:C:170:ARG:O	2:C:171:TYR:C	2.42	0.55
1:F:189:ASP:O	1:F:193:TYR:N	2.39	0.55
1:E:807:LEU:HD12	1:E:808:ILE:N	2.21	0.55
1:F:727:LYS:HE3	1:F:765:ASN:HB3	1.88	0.55
1:A:56:TYR:HD1	1:A:57:PRO:HD2	1.72	0.55
1:E:452:TYR:HA	1:E:455:TYR:CD2	2.42	0.55
1:E:931:GLU:OE1	1:E:931:GLU:N	2.39	0.55
1:A:117:ILE:HA	1:A:120:LYS:HD2	1.88	0.55
1:A:817:SER:OG	1:A:844:LEU:O	2.18	0.55
1:B:407:ILE:HB	2:D:2:LYS:HG2	1.89	0.55
1:F:610:GLN:OE1	1:F:613:ARG:NH2	2.39	0.55
1:A:327:LYS:HA	1:A:330:LEU:HG	1.88	0.55
1:A:752:GLY:HA2	1:A:799:LEU:HD13	1.87	0.55
1:E:53:LEU:HD11	1:E:286:TYR:CE2	2.41	0.55
1:F:741:LEU:HB3	1:F:778:PHE:CD2	2.42	0.55
1:F:760:ARG:HA	1:F:763:LYS:HG3	1.87	0.55
1:F:906:THR:O	2:G:232:ALA:HB3	2.06	0.55
2:G:168:SER:O	2:G:169:GLU:C	2.43	0.55
1:A:475:GLN:HA	1:A:478:ARG:NH1	2.22	0.55
1:B:659:PHE:HD2	1:B:662:ASP:HA	1.71	0.55
2:C:42:ARG:HD3	2:C:52:ILE:HD13	1.88	0.55
2:C:52:ILE:HD11	2:C:54:LYS:HG2	1.87	0.55
1:F:189:ASP:OD1	1:F:190:TYR:N	2.39	0.55
1:F:620:ILE:HA	1:F:645:PHE:HE2	1.71	0.55
1:A:247:ARG:HB2	1:A:270:ASP:HA	1.89	0.55
1:B:135:ASP:O	1:B:169:LYS:NZ	2.40	0.55
1:B:721:TYR:OH	1:B:760:ARG:NH2	2.39	0.55
1:E:284:GLU:HG2	1:E:285:ARG:N	2.21	0.55
1:E:304:LYS:HD2	1:E:307:GLU:H	1.72	0.55
1:F:285:ARG:O	1:F:289:VAL:HG22	2.06	0.55
1:F:366:SER:OG	1:F:368:ASP:OD1	2.25	0.55
1:F:376:LYS:HZ1	1:F:380:ARG:NE	2.04	0.55
2:G:65:ASN:OD1	2:G:67:PHE:N	2.35	0.55
2:H:15:ARG:HD3	2:H:20:LYS:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:LYS:HZ1	1:E:265:GLY:C	2.05	0.55
1:F:802:ARG:HB2	1:F:840:LYS:HA	1.89	0.55
1:F:904:ILE:HG22	2:G:235:ILE:H	1.70	0.55
1:A:70:LEU:HD23	1:A:95:LYS:HE3	1.89	0.55
1:A:316:ILE:HA	1:A:319:LEU:HD13	1.89	0.55
1:A:532:PRO:HB3	1:B:148:TYR:CZ	2.42	0.55
1:B:236:GLN:NE2	1:B:239:SER:O	2.40	0.55
1:B:282:TYR:H	1:B:285:ARG:CZ	2.20	0.55
1:B:481:ILE:O	1:B:485:ILE:HG13	2.07	0.55
2:C:175:TYR:N	2:C:193:ILE:O	2.40	0.55
1:E:145:ARG:O	1:E:145:ARG:NE	2.40	0.55
1:F:132:THR:HA	1:F:170:VAL:HG12	1.88	0.55
2:G:24:THR:HB	2:G:65:ASN:HD22	1.72	0.55
1:A:583:VAL:O	1:A:587:ARG:HG3	2.06	0.55
1:B:307:GLU:HA	1:B:310:ASP:HB2	1.89	0.55
1:B:434:ASP:O	1:B:438:LYS:HG3	2.06	0.55
1:E:396:MET:SD	1:E:398:LYS:HD2	2.47	0.55
1:F:228:LEU:O	1:F:228:LEU:CD1	2.55	0.55
1:A:116:PRO:HB2	1:A:120:LYS:HE3	1.89	0.54
1:A:454:LEU:O	1:A:458:ILE:HD12	2.06	0.54
1:A:750:ASP:OD2	1:A:751:ILE:HG22	2.06	0.54
1:E:406:SER:OG	1:E:407:ILE:N	2.40	0.54
1:E:916:PHE:HA	1:E:919:TRP:CZ3	2.42	0.54
1:F:116:PRO:O	1:F:120:LYS:NZ	2.32	0.54
1:F:696:THR:O	1:F:700:SER:CB	2.54	0.54
1:A:59:TRP:HZ3	1:A:62:LEU:HD23	1.72	0.54
1:A:547:ASP:HB2	1:A:549:GLN:OE1	2.08	0.54
1:A:580:SER:HB2	1:A:582:ILE:CG2	2.36	0.54
1:A:580:SER:HB2	1:A:582:ILE:HG12	1.88	0.54
1:E:632:ASP:CG	1:E:633:GLU:H	2.11	0.54
1:F:259:ILE:O	1:F:262:GLU:HG3	2.07	0.54
1:F:862:ILE:HD13	1:F:862:ILE:H	1.72	0.54
1:A:152:ILE:HG23	1:A:157:ASP:HB2	1.89	0.54
1:A:270:ASP:O	1:A:273:SER:OG	2.24	0.54
1:A:535:PHE:HE1	1:A:542:LEU:HD23	1.72	0.54
1:B:304:LYS:HB3	1:B:307:GLU:HB2	1.88	0.54
1:E:690:GLY:O	1:E:694:GLU:HG3	2.07	0.54
1:F:278:ASN:O	1:F:285:ARG:NH2	2.40	0.54
1:F:291:ASP:HA	1:F:294:ILE:HD12	1.90	0.54
2:G:214:LEU:O	2:G:216:PRO:HD3	2.07	0.54
2:H:177:THR:O	2:H:191:ILE:N	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ILE:HD12	1:F:229:LEU:HD21	1.90	0.54
1:F:294:ILE:HG22	1:F:295:GLU:H	1.73	0.54
1:F:424:PHE:O	1:F:438:LYS:NZ	2.38	0.54
1:B:319:LEU:HB2	1:B:322:LEU:HD13	1.88	0.54
1:B:741:LEU:HD11	1:B:775:ILE:HG22	1.90	0.54
1:E:205:LYS:HD3	1:E:231:TRP:CH2	2.42	0.54
1:E:526:ASP:CG	1:E:529:ASN:H	2.11	0.54
1:F:793:GLU:OE1	1:F:799:LEU:HB3	2.07	0.54
1:F:937:ASP:OD1	1:F:940:TYR:N	2.39	0.54
1:B:224:ASN:O	1:B:228:LEU:HG	2.07	0.54
1:B:990:ASN:HB3	1:B:992:ASN:HD22	1.72	0.54
1:F:44:PHE:HZ	1:F:124:MET:HG3	1.72	0.54
1:F:327:LYS:HD3	1:F:392:GLY:HA3	1.90	0.54
1:B:786:HIS:O	1:B:834:GLN:NE2	2.41	0.54
1:E:531:MET:HE3	1:E:532:PRO:HD2	1.90	0.54
1:E:655:ILE:HG23	1:E:659:PHE:HE2	1.72	0.54
1:E:724:LYS:HZ2	1:E:764:CYS:HB2	1.72	0.54
1:F:57:PRO:HA	1:F:61:ARG:NH2	2.22	0.54
1:F:809:LYS:HZ3	1:F:814:ASN:HA	1.73	0.54
1:A:95:LYS:HD3	1:A:95:LYS:N	2.23	0.54
1:A:223:TYR:HB3	1:A:225:ILE:HG13	1.90	0.54
1:A:357:MET:H	1:A:357:MET:CE	2.21	0.54
1:E:500:PHE:HA	1:E:747:ARG:CZ	2.37	0.54
1:E:729:SER:N	1:E:732:GLY:HA3	2.23	0.54
1:B:53:LEU:HD13	1:B:117:ILE:HG13	1.90	0.54
1:F:230:ASN:N	1:F:230:ASN:OD1	2.40	0.54
1:A:366:SER:O	1:A:370:ARG:NE	2.41	0.54
1:A:652:PHE:CZ	1:A:687:TYR:HB3	2.43	0.54
1:A:989:LYS:HD2	1:B:1001:MET:SD	2.48	0.54
1:B:768:PRO:HD2	1:B:771:ILE:HD13	1.90	0.54
1:B:974:LYS:HA	1:B:977:LYS:HD3	1.90	0.54
2:D:34:GLN:HA	2:D:59:ILE:HD13	1.90	0.54
1:E:918:ILE:HG23	2:H:51:TYR:CD2	2.42	0.54
1:F:118:HIS:NE2	1:F:138:ILE:HA	2.23	0.54
1:F:213:ILE:HB	1:F:243:PRO:HB3	1.89	0.54
1:F:311:TYR:CZ	1:F:315:LYS:HE2	2.43	0.54
1:B:494:GLY:O	1:B:496:GLY:N	2.41	0.53
1:F:615:SER:HA	1:F:618:LEU:HD13	1.90	0.53
1:F:651:ASP:HA	1:F:654:ASN:HD21	1.71	0.53
1:F:681:GLN:HA	1:F:684:ILE:HD11	1.91	0.53
1:F:861:ASN:OD1	1:F:862:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ILE:HA	1:A:754:ARG:HG2	1.90	0.53
1:A:869:ILE:HG12	2:D:50:LEU:HD13	1.90	0.53
1:A:976:MET:SD	1:A:976:MET:N	2.81	0.53
2:C:39:GLU:HG2	2:C:40:LYS:H	1.74	0.53
1:E:312:ILE:HD11	1:E:356:TYR:CD2	2.43	0.53
1:E:579:SER:H	1:E:582:ILE:HD11	1.72	0.53
1:F:553:ASP:O	1:F:557:LYS:NZ	2.42	0.53
2:H:171:TYR:O	2:H:196:PRO:O	2.25	0.53
1:A:275:ILE:HG23	1:A:285:ARG:NH1	2.24	0.53
1:A:607:GLU:O	1:A:610:GLN:N	2.41	0.53
1:A:652:PHE:HZ	1:A:687:TYR:HB3	1.74	0.53
1:B:594:PHE:O	1:B:598:ASN:ND2	2.41	0.53
1:B:964:ASP:CG	1:B:966:LEU:HB2	2.28	0.53
1:E:57:PRO:HB3	1:E:107:PHE:HE1	1.73	0.53
1:E:270:ASP:OD1	1:E:271:ALA:N	2.41	0.53
1:F:358:GLU:HA	1:F:361:PHE:CE1	2.43	0.53
1:F:479:TYR:O	1:F:483:GLN:NE2	2.41	0.53
1:F:509:ASP:OD1	1:F:510:GLU:N	2.42	0.53
1:A:99:ALA:O	1:A:103:ILE:HG13	2.08	0.53
1:A:303:THR:OG1	1:A:304:LYS:N	2.42	0.53
1:A:388:PHE:HA	1:A:391:ASN:ND2	2.23	0.53
1:A:582:ILE:HA	1:A:585:LEU:CD1	2.38	0.53
1:B:65:LYS:HE2	1:B:103:ILE:HG23	1.90	0.53
2:H:60:ASN:HA	2:H:219:LYS:NZ	2.22	0.53
1:A:453:ASP:O	1:A:456:SER:OG	2.20	0.53
1:A:695:ILE:O	1:A:698:GLN:HB2	2.08	0.53
1:B:231:TRP:O	1:B:235:LEU:HG	2.09	0.53
1:E:326:ARG:HH21	1:E:594:PHE:HE2	1.56	0.53
1:F:187:GLU:HA	1:F:190:TYR:HD2	1.73	0.53
1:A:403:LEU:N	2:C:6:GLN:HE22	1.97	0.53
1:A:800:TYR:CD1	2:D:226:THR:HG23	2.43	0.53
1:F:89:GLN:HA	1:F:186:LYS:HE2	1.89	0.53
1:F:720:LEU:HB2	1:F:757:TRP:HZ3	1.73	0.53
2:H:171:TYR:C	2:H:172:GLU:OE1	2.47	0.53
1:E:606:HIS:O	1:E:609:HIS:N	2.42	0.53
1:E:687:TYR:CZ	1:E:691:ILE:HD11	2.43	0.53
1:F:41:LYS:HG2	1:F:211:HIS:CD2	2.39	0.53
1:A:41:LYS:O	1:A:212:THR:N	2.39	0.53
1:A:800:TYR:O	1:A:802:ARG:N	2.38	0.53
1:E:755:TYR:CD1	1:E:807:LEU:HD23	2.44	0.53
1:F:801:SER:H	1:F:840:LYS:HZ2	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:976:MET:HB3	1:F:979:HIS:CE1	2.44	0.53
1:E:595:LEU:HG	1:E:603:VAL:HG12	1.91	0.53
1:F:646:PHE:HD1	1:F:677:ARG:HB3	1.74	0.53
2:H:58:GLU:O	2:H:59:ILE:HD13	2.08	0.53
1:A:188:ASP:O	1:A:192:ASN:N	2.40	0.53
1:A:736:ILE:HG21	1:A:761:LEU:HD22	1.90	0.53
1:A:738:LYS:O	1:A:741:LEU:HD22	2.09	0.53
2:D:14:LYS:HG3	2:D:172:GLU:HB3	1.91	0.53
2:D:174:GLU:HG2	2:D:194:GLN:HB3	1.90	0.53
1:E:459:ILE:HD11	1:E:478:ARG:HH11	1.74	0.53
1:E:699:PHE:HD2	1:E:743:TYR:HB3	1.73	0.53
1:E:841:LEU:HD23	1:E:844:LEU:HD12	1.91	0.53
1:F:576:PHE:HB2	2:H:30:ALA:HB3	1.91	0.53
1:F:957:SER:CA	1:F:960:LYS:HB3	2.39	0.53
1:A:128:HIS:CE1	1:A:166:TYR:H	2.26	0.52
2:D:60:ASN:ND2	2:D:221:GLU:OE2	2.41	0.52
1:F:44:PHE:CZ	1:F:124:MET:HG3	2.44	0.52
2:H:71:GLU:O	2:H:72:TRP:HB2	2.08	0.52
1:A:403:LEU:H	2:C:6:GLN:NE2	1.96	0.52
1:B:631:ILE:HB	1:B:636:PHE:HD1	1.74	0.52
1:E:526:ASP:CG	1:E:528:PHE:H	2.11	0.52
1:F:627:ARG:NH2	1:F:675:LYS:HZ2	2.06	0.52
2:H:15:ARG:HD2	2:H:72:TRP:HE1	1.74	0.52
1:B:38:ARG:HA	1:B:38:ARG:NE	2.25	0.52
1:E:99:ALA:O	1:E:103:ILE:HG12	2.10	0.52
1:E:455:TYR:HA	1:E:458:ILE:HG12	1.90	0.52
1:E:755:TYR:CZ	1:E:807:LEU:HB3	2.45	0.52
1:E:801:SER:HB3	1:E:840:LYS:HZ3	1.74	0.52
1:F:105:LYS:HA	1:F:178:PHE:HD2	1.73	0.52
1:F:422:LYS:O	1:F:425:ILE:HG22	2.09	0.52
2:H:21:LEU:HB3	2:H:69:ASP:OD2	2.09	0.52
1:B:282:TYR:H	1:B:285:ARG:NH2	2.07	0.52
2:D:1:MET:N	2:D:1:MET:HE2	2.24	0.52
1:E:245:PHE:O	1:E:269:ILE:N	2.41	0.52
1:F:960:LYS:HA	1:F:962:TYR:CE2	2.45	0.52
1:A:128:HIS:HE1	1:A:165:ARG:HA	1.75	0.52
1:B:105:LYS:HD2	1:B:178:PHE:CD2	2.44	0.52
1:B:205:LYS:NZ	1:B:232:VAL:HG22	2.25	0.52
1:B:577:GLY:HA2	2:D:5:ILE:HG22	1.90	0.52
2:C:16:LYS:HE3	2:C:172:GLU:HG2	1.91	0.52
1:E:201:SER:HA	1:E:204:MET:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:540:LYS:HG3	1:E:541:ILE:N	2.25	0.52
1:F:733:LEU:HD12	1:F:771:ILE:HD11	1.91	0.52
1:F:801:SER:H	1:F:840:LYS:NZ	2.06	0.52
1:A:205:LYS:HB2	1:B:202:ASN:HD21	1.75	0.52
1:A:548:ASN:HA	1:A:550:PHE:CE1	2.44	0.52
1:A:779:LEU:HD13	1:A:841:LEU:HD22	1.90	0.52
1:B:842:LEU:HG	1:B:843:PRO:HD3	1.91	0.52
2:C:13:PHE:HZ	2:C:63:VAL:HG21	1.73	0.52
1:F:386:ASN:O	1:F:390:LYS:CB	2.57	0.52
1:F:646:PHE:CD1	1:F:677:ARG:HB3	2.45	0.52
1:A:469:CYS:HB2	1:A:539:TYR:CE2	2.45	0.52
1:A:606:HIS:O	1:A:609:HIS:HD2	1.92	0.52
1:B:134:TYR:CE2	1:B:183:VAL:CG1	2.67	0.52
1:B:640:GLY:O	1:B:641:LYS:CG	2.58	0.52
1:E:967:LEU:HD13	1:E:1003:TYR:HE2	1.75	0.52
1:E:982:GLU:OE1	1:E:985:LYS:NZ	2.23	0.52
1:F:535:PHE:HA	1:F:538:LYS:HZ2	1.75	0.52
1:A:488:ALA:HA	1:A:491:GLN:HE22	1.73	0.52
1:A:893:LYS:HD2	1:A:933:PHE:HE1	1.75	0.52
1:B:274:LEU:HD13	1:B:292:LEU:HG	1.91	0.52
1:B:573:SER:HA	2:D:31:SER:HA	1.91	0.52
2:D:50:LEU:HD23	2:D:51:TYR:H	1.75	0.52
1:E:533:PHE:O	1:E:537:LYS:HG2	2.09	0.52
1:E:657:ARG:HB3	1:E:658:HIS:ND1	2.25	0.52
1:F:376:LYS:NZ	1:F:379:GLU:OE2	2.41	0.52
1:B:475:GLN:HG3	1:B:478:ARG:HH12	1.75	0.52
1:E:26:VAL:O	1:E:30:ILE:HG12	2.09	0.52
1:E:376:LYS:HD2	1:E:380:ARG:HE	1.75	0.52
1:E:564:LYS:O	1:E:567:SER:OG	2.27	0.52
1:E:692:ALA:HB2	1:E:736:ILE:HG22	1.91	0.52
1:E:735:LYS:HA	1:E:738:LYS:HZ3	1.75	0.52
1:E:779:LEU:O	1:E:782:GLN:HG3	2.10	0.52
1:F:801:SER:HB3	1:F:840:LYS:HZ1	1.74	0.52
1:F:896:TYR:HB2	1:F:933:PHE:HE1	1.75	0.52
1:F:906:THR:CG2	2:G:233:VAL:HA	2.40	0.52
1:A:548:ASN:HD22	2:D:209:GLU:HB2	1.74	0.52
1:A:803:ASP:OD1	1:A:803:ASP:N	2.41	0.52
1:E:610:GLN:HB3	1:E:613:ARG:NH2	2.25	0.52
1:A:751:ILE:HG23	1:A:799:LEU:CD2	2.40	0.51
1:B:322:LEU:H	1:B:322:LEU:HD12	1.75	0.51
2:D:10:ASP:HA	2:D:26:GLU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:TYR:O	1:E:70:LEU:HD12	2.09	0.51
1:E:629:ARG:NH1	1:E:631:ILE:HD12	2.25	0.51
1:F:741:LEU:HB3	1:F:778:PHE:HD2	1.75	0.51
1:A:585:LEU:O	1:A:588:LEU:HB2	2.10	0.51
1:A:625:TYR:HA	1:B:992:ASN:ND2	2.25	0.51
2:D:225:ASP:H	2:D:230:GLU:HG3	1.75	0.51
1:E:815:PHE:HZ	1:E:844:LEU:HB3	1.75	0.51
1:F:921:PHE:HE2	1:F:970:ILE:HA	1.74	0.51
1:A:357:MET:SD	1:A:358:GLU:N	2.84	0.51
1:A:443:ALA:O	1:A:448:TRP:NE1	2.39	0.51
1:A:601:TRP:O	1:A:604:SER:OG	2.28	0.51
1:B:472:TYR:CE1	1:B:476:ILE:HD11	2.46	0.51
1:E:398:LYS:HD2	1:E:398:LYS:H	1.76	0.51
1:E:411:SER:O	1:E:415:HIS:ND1	2.41	0.51
1:E:479:TYR:CD2	1:E:524:ILE:HG12	2.44	0.51
2:H:35:ALA:HB3	2:H:58:GLU:HB3	1.91	0.51
1:A:549:GLN:HG3	1:B:549:GLN:HE22	1.76	0.51
1:B:48:ALA:HA	1:B:133:ASN:HD22	1.74	0.51
1:B:135:ASP:HA	1:B:174:PHE:HE2	1.74	0.51
1:B:472:TYR:HA	1:B:475:GLN:HE21	1.75	0.51
1:B:612:ILE:HG22	1:B:659:PHE:HE1	1.76	0.51
1:E:770:SER:O	1:E:773:SER:OG	2.26	0.51
1:E:403:LEU:O	2:G:6:GLN:NE2	2.44	0.51
1:E:456:SER:O	1:E:460:LEU:HD23	2.10	0.51
1:E:556:VAL:HG11	1:F:552:TYR:HE2	1.74	0.51
1:F:331:LYS:NZ	1:F:337:ASP:H	2.08	0.51
1:F:438:LYS:O	1:F:442:LEU:HG	2.11	0.51
2:G:72:TRP:O	2:G:76:THR:CB	2.57	0.51
1:A:528:PHE:CE2	1:A:542:LEU:O	2.62	0.51
1:B:64:ASP:O	1:B:68:GLU:HG2	2.10	0.51
1:B:66:TYR:CE1	1:B:103:ILE:HG21	2.46	0.51
1:B:802:ARG:HB3	1:B:840:LYS:HB3	1.93	0.51
1:B:985:LYS:HA	1:B:988:VAL:HG22	1.92	0.51
1:A:250:PRO:HB3	1:A:279:GLU:HA	1.91	0.51
1:A:620:ILE:HG13	1:A:667:LEU:HD21	1.93	0.51
1:A:986:GLU:OE2	1:A:990:ASN:ND2	2.42	0.51
1:B:614:ASN:O	1:B:618:LEU:HD22	2.11	0.51
1:B:90:ILE:HG12	1:F:260:TYR:CD2	2.45	0.51
1:B:919:TRP:HZ3	2:C:50:LEU:HG	1.75	0.51
1:E:155:GLU:HG2	1:E:197:TYR:HD1	1.75	0.51
1:F:242:LYS:HG2	1:F:267:ARG:CZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:ASN:O	1:F:460:LEU:HG	2.11	0.51
1:F:610:GLN:HA	1:F:613:ARG:NH2	2.26	0.51
1:A:241:HIS:NE2	1:B:159:ALA:HB1	2.26	0.51
1:B:255:ASN:HA	1:B:258:LEU:HG	1.93	0.51
1:E:174:PHE:HB3	1:E:178:PHE:CE1	2.46	0.51
1:E:333:VAL:HG23	1:E:541:ILE:HG13	1.92	0.51
1:E:422:LYS:HE2	1:E:422:LYS:HA	1.93	0.51
1:E:834:GLN:O	1:E:838:LEU:N	2.40	0.51
1:F:129:VAL:HB	1:F:167:LEU:HG	1.93	0.51
1:F:254:GLU:O	1:F:257:THR:OG1	2.27	0.51
1:F:477:ASN:O	1:F:481:ILE:HG22	2.10	0.51
2:G:189:SER:CB	2:G:238:SER:HB3	2.40	0.51
1:A:436:TYR:OH	1:A:598:ASN:O	2.18	0.51
1:A:459:ILE:HG13	1:A:471:TYR:CE2	2.46	0.51
1:B:491:GLN:O	1:B:495:LEU:HB2	2.10	0.51
2:D:176:ARG:NH1	2:D:178:ILE:HG13	2.26	0.51
1:E:487:GLN:HE22	2:H:207:SER:N	2.06	0.51
1:E:497:LEU:HB3	1:E:503:HIS:ND1	2.25	0.51
1:F:66:TYR:HB3	1:F:87:ILE:HG12	1.93	0.51
2:H:23:PHE:O	2:H:69:ASP:HB2	2.11	0.51
1:A:337:ASP:O	1:A:350:LYS:N	2.39	0.50
1:A:449:GLU:N	1:A:449:GLU:OE1	2.44	0.50
1:A:606:HIS:NE2	2:D:206:MET:HB3	2.25	0.50
1:A:767:LEU:N	1:A:768:PRO:HD3	2.26	0.50
1:B:115:ASN:OD1	1:B:118:HIS:NE2	2.45	0.50
1:B:203:LEU:O	1:B:207:ILE:HG22	2.11	0.50
1:B:469:CYS:HB3	1:B:539:TYR:CZ	2.46	0.50
1:E:128:HIS:HD1	1:E:166:TYR:H	1.59	0.50
1:E:680:GLU:O	1:E:680:GLU:CD	2.50	0.50
1:E:780:VAL:HG21	1:E:819:ARG:HH12	1.76	0.50
1:F:396:MET:SD	1:F:397:ALA:N	2.85	0.50
1:F:906:THR:HG22	2:G:234:VAL:H	1.76	0.50
2:H:175:TYR:HB2	2:H:193:ILE:HB	1.93	0.50
2:H:219:LYS:HD2	2:H:220:PHE:N	2.26	0.50
1:A:332:HIS:CE1	1:A:540:LYS:HD2	2.46	0.50
1:A:593:ARG:O	1:A:597:GLU:HG3	2.11	0.50
1:B:720:LEU:HD13	1:B:740:LEU:HD12	1.92	0.50
1:F:720:LEU:HD22	1:F:736:ILE:HD13	1.93	0.50
1:F:905:GLN:H	2:G:234:VAL:HG12	1.76	0.50
1:B:475:GLN:HG3	1:B:478:ARG:NH1	2.27	0.50
1:B:491:GLN:NE2	2:C:206:MET:HG2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:THR:O	1:F:533:PHE:HE2	1.95	0.50
1:E:339:HIS:N	1:E:347:VAL:O	2.34	0.50
1:E:946:PRO:HG2	1:E:975:HIS:NE2	2.27	0.50
1:F:89:GLN:CD	1:F:187:GLU:HG2	2.31	0.50
2:G:13:PHE:HD1	2:G:173:VAL:HG22	1.76	0.50
2:G:205:GLU:O	2:G:206:MET:C	2.46	0.50
1:E:326:ARG:HG2	1:E:329:ASP:OD2	2.11	0.50
1:E:479:TYR:CZ	1:E:524:ILE:HG21	2.47	0.50
1:F:30:ILE:HD11	1:F:292:LEU:HD11	1.92	0.50
1:A:840:LYS:HA	1:A:871:ILE:HG21	1.93	0.50
1:B:277:SER:HB2	1:B:281:ASP:OD2	2.11	0.50
1:E:205:LYS:NZ	1:F:199:LEU:HD23	2.26	0.50
1:E:635:GLY:HA2	1:E:638:PHE:CE2	2.46	0.50
1:F:71:TYR:HE1	1:F:86:ARG:HH21	1.58	0.50
1:F:101:ASP:HA	1:F:104:LEU:HG	1.93	0.50
1:A:692:ALA:O	1:A:695:ILE:HG12	2.12	0.50
1:B:23:ASP:O	1:B:27:VAL:HG12	2.12	0.50
1:B:135:ASP:HA	1:B:174:PHE:CE2	2.47	0.50
1:F:109:GLN:OE1	1:F:109:GLN:N	2.36	0.50
1:F:692:ALA:O	1:F:696:THR:HG23	2.11	0.50
1:F:931:GLU:H	1:F:931:GLU:CD	2.15	0.50
2:H:64:LYS:HA	2:H:217:GLU:HA	1.92	0.50
1:E:634:LEU:HG	1:F:905:GLN:OE1	2.12	0.50
1:F:472:TYR:HB2	1:F:535:PHE:CE2	2.46	0.50
1:F:724:LYS:HG2	1:F:760:ARG:HG3	1.94	0.50
2:G:188:TYR:O	2:G:238:SER:HA	2.11	0.50
1:A:566:ARG:HA	1:A:569:MET:HG3	1.93	0.50
1:A:885:ILE:HG12	1:A:916:PHE:HE1	1.77	0.50
1:B:59:TRP:HE3	1:B:62:LEU:HD12	1.77	0.50
1:B:581:ASP:CG	1:B:622:LYS:HD3	2.32	0.50
1:E:59:TRP:CD1	1:E:62:LEU:HD23	2.46	0.50
1:E:148:TYR:CE2	1:E:163:SER:HB3	2.47	0.50
1:E:154:ALA:N	1:E:157:ASP:OD2	2.24	0.50
1:E:576:PHE:HB2	2:G:30:ALA:HB3	1.94	0.50
1:F:905:GLN:H	2:G:234:VAL:CG1	2.24	0.50
1:F:913:MET:CE	1:F:913:MET:H	2.24	0.50
1:A:86:ARG:HH22	1:A:90:ILE:HD11	1.77	0.50
1:A:215:PHE:CE1	1:A:243:PRO:HB2	2.47	0.50
1:A:487:GLN:O	1:A:491:GLN:NE2	2.44	0.50
1:A:501:GLY:HA3	1:A:747:ARG:NH2	2.27	0.50
1:A:717:LYS:HZ2	1:A:749:LEU:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ILE:O	1:A:866:MET:HE3	2.12	0.50
1:B:607:GLU:HG3	1:B:608:PHE:HD1	1.77	0.50
1:E:909:SER:HB3	2:H:231:MET:HE3	1.92	0.50
1:F:649:TYR:HE1	1:F:687:TYR:HB2	1.77	0.50
1:F:812:GLU:CD	1:F:813:LYS:H	2.14	0.50
1:F:960:LYS:HZ1	1:F:999:ILE:HG13	1.77	0.50
1:B:44:PHE:CE2	1:B:126:PRO:HB3	2.47	0.49
1:B:472:TYR:O	1:B:476:ILE:HG12	2.12	0.49
1:B:557:LYS:HG3	1:B:587:ARG:HH12	1.77	0.49
1:B:729:SER:HB3	1:B:731:GLU:OE1	2.12	0.49
1:E:436:TYR:OH	1:E:598:ASN:O	2.30	0.49
1:E:635:GLY:O	1:E:638:PHE:N	2.45	0.49
1:E:680:GLU:CD	1:E:683:LYS:H	2.12	0.49
1:A:332:HIS:NE2	1:A:540:LYS:HB3	2.27	0.49
1:B:286:TYR:HA	1:B:289:VAL:HG12	1.93	0.49
1:B:661:ILE:HG13	1:B:663:ASP:N	2.23	0.49
1:E:417:LYS:HD3	1:E:420:VAL:HG22	1.95	0.49
1:E:791:TYR:O	1:E:833:LYS:NZ	2.43	0.49
1:F:128:HIS:CE1	1:F:165:ARG:HA	2.48	0.49
1:F:967:LEU:HA	1:F:970:ILE:HB	1.94	0.49
1:A:566:ARG:O	1:A:569:MET:HG3	2.12	0.49
1:B:94:VAL:HG21	1:F:256:GLU:HB2	1.93	0.49
1:E:850:LYS:O	1:E:854:LEU:HG	2.11	0.49
1:F:130:ILE:HD12	1:F:168:LEU:O	2.12	0.49
1:F:409:ILE:HG13	1:F:650:TYR:CZ	2.46	0.49
1:F:738:LYS:O	1:F:742:PHE:HB2	2.12	0.49
1:F:801:SER:O	1:F:840:LYS:CE	2.55	0.49
1:F:831:LYS:HB3	1:F:833:LYS:HG2	1.93	0.49
2:G:198:VAL:HG22	2:G:222:ALA:HA	1.93	0.49
1:A:713:ILE:CG2	1:A:717:LYS:H	2.26	0.49
1:B:688:LEU:HD23	1:B:732:GLY:CA	2.42	0.49
1:E:744:PHE:HD1	1:E:745:PRO:HD2	1.77	0.49
1:E:815:PHE:HE2	1:E:844:LEU:HA	1.77	0.49
1:E:936:MET:SD	1:E:936:MET:N	2.77	0.49
1:E:1004:PHE:HB2	1:E:1005:ILE:HD12	1.93	0.49
1:F:696:THR:O	1:F:700:SER:HB3	2.11	0.49
1:F:768:PRO:O	1:F:772:ILE:HG12	2.12	0.49
1:F:987:ARG:HA	1:F:987:ARG:NE	2.27	0.49
2:G:28:GLN:HB3	2:G:64:LYS:CD	2.38	0.49
1:B:134:TYR:CE2	1:B:171:ALA:HB1	2.48	0.49
1:E:488:ALA:HA	1:E:491:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:786:HIS:CD2	1:E:791:TYR:HB3	2.47	0.49
1:F:56:TYR:CD1	1:F:57:PRO:HD2	2.47	0.49
1:F:331:LYS:HD2	1:F:336:TYR:HA	1.93	0.49
1:F:533:PHE:O	1:F:537:LYS:HE2	2.13	0.49
2:H:14:LYS:NZ	2:H:21:LEU:HA	2.27	0.49
1:B:558:LEU:HD11	1:B:614:ASN:HB2	1.95	0.49
1:F:418:TYR:O	1:F:421:MET:HG3	2.12	0.49
2:H:229:ASP:O	2:H:230:GLU:HB2	2.11	0.49
1:A:472:TYR:O	1:A:476:ILE:HG22	2.11	0.49
1:B:990:ASN:HB3	1:B:992:ASN:ND2	2.28	0.49
2:C:10:ASP:HB2	2:C:176:ARG:HB3	1.94	0.49
2:C:70:LEU:HD13	2:C:74:ALA:HB2	1.95	0.49
1:E:547:ASP:OD1	1:E:547:ASP:N	2.41	0.49
1:E:809:LYS:HZ1	1:E:815:PHE:HD2	1.61	0.49
1:F:246:ILE:HG22	1:F:247:ARG:H	1.77	0.49
1:F:404:ASN:HA	2:H:4:VAL:O	2.13	0.49
1:F:769:LYS:HD2	1:F:769:LYS:O	2.12	0.49
2:H:192:TYR:HD2	2:H:235:ILE:HB	1.78	0.49
2:H:230:GLU:O	2:H:231:MET:CE	2.61	0.49
1:A:313:TYR:HA	1:A:380:ARG:HH21	1.77	0.49
1:A:614:ASN:O	1:A:618:LEU:HB2	2.12	0.49
1:A:839:PHE:HA	1:A:853:LEU:HD21	1.94	0.49
1:B:649:TYR:CD1	1:B:684:ILE:HG12	2.48	0.49
2:C:69:ASP:HB2	2:C:72:TRP:CD1	2.48	0.49
2:D:41:LEU:HD12	2:D:42:ARG:HG3	1.95	0.49
1:E:406:SER:HB2	2:G:2:LYS:HB2	1.95	0.49
1:F:388:PHE:CD1	1:F:393:VAL:HG13	2.47	0.49
1:B:453:ASP:O	1:B:456:SER:OG	2.19	0.49
1:E:89:GLN:HE22	1:E:188:ASP:H	1.60	0.49
1:E:706:VAL:CA	1:E:709:TYR:HB3	2.42	0.49
1:E:832:GLN:HA	1:E:835:ILE:HG12	1.94	0.49
1:A:408:GLU:HA	1:A:650:TYR:OH	2.13	0.49
1:A:607:GLU:OE1	1:A:610:GLN:HG2	2.12	0.49
1:B:299:ASN:OD1	1:B:299:ASN:N	2.42	0.49
1:B:631:ILE:HG21	1:B:636:PHE:HB3	1.95	0.49
2:D:208:LEU:HD11	2:D:212:ASN:HB3	1.95	0.49
1:E:286:TYR:O	1:E:290:MET:HG2	2.13	0.49
1:E:349:HIS:HE1	2:G:213:ALA:HA	1.77	0.49
1:E:396:MET:SD	1:E:398:LYS:N	2.85	0.49
1:E:803:ASP:HA	1:E:806:ALA:HB3	1.94	0.49
1:F:639:PHE:O	1:F:641:LYS:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:955:ILE:HG21	1:F:958:TRP:CE2	2.47	0.49
2:H:69:ASP:O	2:H:70:LEU:HB2	2.12	0.49
1:A:180:GLY:HA2	1:A:183:VAL:HG12	1.95	0.48
1:A:218:TYR:OH	1:A:224:ASN:N	2.34	0.48
1:A:655:ILE:HD12	1:A:659:PHE:CZ	2.47	0.48
1:A:899:GLU:O	1:A:903:GLY:N	2.46	0.48
1:B:249:ASP:OD2	1:B:251:SER:OG	2.24	0.48
1:E:551:LEU:HD11	1:E:608:PHE:HD1	1.78	0.48
1:E:705:ASN:O	1:E:708:PHE:N	2.45	0.48
1:F:965:LYS:C	1:F:967:LEU:N	2.61	0.48
1:A:433:GLU:O	1:A:437:LYS:HG2	2.13	0.48
1:B:231:TRP:HA	1:B:234:LYS:HD3	1.95	0.48
2:C:171:TYR:O	2:C:198:VAL:O	2.30	0.48
1:E:190:TYR:HA	1:E:193:TYR:HB2	1.94	0.48
1:E:629:ARG:CG	1:E:630:ASP:O	2.61	0.48
1:E:750:ASP:O	1:E:753:LYS:HG2	2.13	0.48
1:E:906:THR:HG22	2:H:233:VAL:HG13	1.94	0.48
2:G:14:LYS:CA	2:G:20:LYS:HE3	2.43	0.48
2:G:190:ASP:H	2:G:237:ALA:HB3	1.78	0.48
1:A:43:VAL:HG13	1:A:213:ILE:HD13	1.95	0.48
1:A:310:ASP:HA	1:A:313:TYR:HB3	1.94	0.48
1:A:550:PHE:O	1:A:551:LEU:C	2.45	0.48
1:A:615:SER:HA	1:A:618:LEU:HB2	1.96	0.48
1:B:44:PHE:CD2	1:B:126:PRO:HB3	2.49	0.48
1:B:553:ASP:OD1	1:B:553:ASP:N	2.47	0.48
1:F:724:LYS:HD2	1:F:725:TYR:CD1	2.48	0.48
2:G:192:TYR:HD2	2:G:235:ILE:HG21	1.78	0.48
2:H:16:LYS:HE2	2:H:170:ARG:HH21	1.78	0.48
1:A:277:SER:HB3	1:A:285:ARG:NH2	2.28	0.48
1:A:419:ASP:N	1:A:419:ASP:OD1	2.45	0.48
1:B:242:LYS:HB2	1:B:267:ARG:NH2	2.28	0.48
1:E:1000:LEU:HA	1:E:1004:PHE:HE2	1.79	0.48
1:F:449:GLU:HG3	1:F:450:GLU:OE1	2.13	0.48
1:F:579:SER:HB3	1:F:582:ILE:HG12	1.94	0.48
1:F:809:LYS:HZ3	1:F:815:PHE:H	1.61	0.48
1:A:163:SER:HA	1:B:533:PHE:CE1	2.48	0.48
1:A:205:LYS:CB	1:B:202:ASN:HD21	2.27	0.48
1:A:444:CYS:HA	1:A:601:TRP:HZ3	1.77	0.48
1:A:456:SER:HA	1:A:459:ILE:HG22	1.96	0.48
1:A:693:GLU:O	1:A:696:THR:OG1	2.24	0.48
1:B:111:ASP:OD1	1:B:111:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HB	1:B:167:LEU:HD13	1.95	0.48
1:B:632:ASP:OD1	1:B:632:ASP:N	2.40	0.48
1:E:481:ILE:O	1:E:484:SER:OG	2.21	0.48
1:E:630:ASP:HB3	1:F:956:PRO:HG3	1.95	0.48
1:A:733:LEU:O	1:A:736:ILE:HG22	2.13	0.48
1:A:787:ILE:HG22	1:A:788:ASP:H	1.78	0.48
1:E:163:SER:HA	1:F:533:PHE:CE2	2.49	0.48
1:E:767:LEU:HD12	1:E:811:PHE:HD2	1.78	0.48
1:F:79:TYR:HB3	1:F:84:TYR:CG	2.48	0.48
1:F:188:ASP:O	1:F:192:ASN:N	2.47	0.48
1:F:744:PHE:HB3	1:F:749:LEU:HD23	1.95	0.48
2:G:14:LYS:HG2	2:G:172:GLU:O	2.13	0.48
1:A:131:THR:HG22	1:A:133:ASN:H	1.79	0.48
1:A:512:LEU:HD13	1:A:515:ILE:HD11	1.95	0.48
1:A:688:LEU:O	1:A:691:ILE:HG13	2.14	0.48
1:B:92:TYR:HB3	1:B:186:LYS:HZ3	1.78	0.48
1:E:186:LYS:HE3	1:E:186:LYS:HB3	1.67	0.48
1:E:544:PHE:CE2	1:E:550:PHE:HB2	2.48	0.48
1:E:729:SER:O	1:E:733:LEU:N	2.36	0.48
1:F:982:GLU:O	1:F:985:LYS:HB2	2.13	0.48
1:A:86:ARG:NH2	1:E:260:TYR:CZ	2.82	0.48
1:A:131:THR:HB	1:A:169:LYS:HA	1.96	0.48
1:A:481:ILE:O	1:A:484:SER:OG	2.25	0.48
1:A:548:ASN:HD22	2:D:209:GLU:CB	2.26	0.48
1:B:130:ILE:HD11	1:B:170:VAL:HG22	1.95	0.48
2:D:206:MET:N	2:D:206:MET:SD	2.86	0.48
1:E:334:PHE:O	1:E:335:GLU:HG3	2.14	0.48
1:E:428:GLN:NE2	1:E:429:SER:O	2.46	0.48
1:E:493:ASN:HA	1:E:503:HIS:CE1	2.44	0.48
1:E:531:MET:CE	1:E:532:PRO:HD2	2.44	0.48
1:E:839:PHE:HA	1:E:842:LEU:HB2	1.95	0.48
1:F:331:LYS:O	1:F:331:LYS:HD3	2.14	0.48
1:F:511:PHE:O	1:F:515:ILE:HG12	2.14	0.48
2:H:20:LYS:HE2	2:H:71:GLU:OE2	2.13	0.48
2:H:172:GLU:HB3	2:H:196:PRO:O	2.14	0.48
1:B:688:LEU:HD23	1:B:732:GLY:HA2	1.96	0.48
1:F:848:ASN:O	1:F:852:HIS:ND1	2.45	0.48
1:F:957:SER:O	1:F:959:LEU:N	2.47	0.48
1:B:28:GLU:O	1:B:32:GLU:HG2	2.13	0.48
1:B:66:TYR:HE1	1:B:103:ILE:HG21	1.77	0.48
1:B:588:LEU:HD12	1:B:588:LEU:HA	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:MET:HB2	1:B:659:PHE:HZ	1.79	0.48
1:E:326:ARG:HD2	1:E:328:ILE:HD11	1.96	0.48
1:E:330:LEU:HB3	1:E:340:PHE:HE2	1.79	0.48
1:F:89:GLN:CD	1:F:89:GLN:H	2.17	0.48
1:F:905:GLN:C	2:G:234:VAL:HB	2.34	0.48
1:F:966:LEU:HD12	2:G:51:TYR:HB3	1.96	0.48
1:A:46:VAL:HG12	1:A:130:ILE:O	2.14	0.47
1:A:583:VAL:O	1:A:584:VAL:C	2.49	0.47
1:A:904:ILE:HG12	2:D:235:ILE:HG23	1.96	0.47
1:B:222:ASP:OD1	1:B:225:ILE:HG23	2.14	0.47
1:B:245:PHE:O	1:B:269:ILE:HD12	2.13	0.47
1:B:675:LYS:HD3	1:B:675:LYS:HA	1.36	0.47
1:B:741:LEU:HD22	1:B:778:PHE:CG	2.49	0.47
1:B:982:GLU:O	1:B:985:LYS:HG3	2.13	0.47
1:E:711:GLN:O	1:E:712:PHE:HD1	1.96	0.47
1:F:336:TYR:O	1:F:350:LYS:HE2	2.14	0.47
1:F:820:LEU:HA	1:F:823:ILE:HG12	1.96	0.47
2:G:38:GLU:CA	2:G:54:LYS:HZ1	2.27	0.47
2:G:197:ASN:HB2	2:G:230:GLU:CD	2.34	0.47
2:H:23:PHE:HE1	2:H:66:ALA:CB	2.23	0.47
2:H:52:ILE:HG13	2:H:53:LEU:H	1.79	0.47
2:H:230:GLU:O	2:H:231:MET:HE2	2.14	0.47
1:A:370:ARG:HD3	1:A:381:PHE:CZ	2.49	0.47
1:A:964:ASP:N	1:A:964:ASP:OD1	2.47	0.47
1:B:83:GLU:HA	1:B:86:ARG:HG2	1.96	0.47
1:B:114:THR:HB	1:B:118:HIS:HD2	1.79	0.47
1:B:377:GLN:O	1:B:380:ARG:HG2	2.14	0.47
1:B:626:GLU:HA	1:B:629:ARG:NE	2.27	0.47
1:E:59:TRP:CZ2	1:E:185:LEU:HG	2.49	0.47
1:F:134:TYR:CZ	1:F:183:VAL:HB	2.49	0.47
1:F:290:MET:O	1:F:294:ILE:HG13	2.13	0.47
1:F:906:THR:HB	2:G:233:VAL:CA	2.44	0.47
2:H:10:ASP:OD2	2:H:12:TYR:OH	2.30	0.47
1:A:206:THR:HG22	1:B:203:LEU:HD22	1.96	0.47
1:A:270:ASP:HB3	1:A:273:SER:HB3	1.95	0.47
1:A:736:ILE:HG21	1:A:761:LEU:CD2	2.44	0.47
1:B:257:THR:O	1:B:261:TYR:HD1	1.97	0.47
1:E:79:TYR:HA	1:E:83:GLU:CD	2.35	0.47
1:E:655:ILE:HG23	1:E:659:PHE:CE2	2.49	0.47
1:E:861:ASN:ND2	1:E:864:ASP:OD2	2.46	0.47
1:B:569:MET:HE3	1:B:571:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:MET:CA	1:B:582:ILE:HG13	2.44	0.47
1:E:215:PHE:HE2	1:E:243:PRO:HB2	1.80	0.47
1:E:927:ASN:ND2	1:E:929:LYS:HD3	2.30	0.47
2:G:36:ILE:HG23	2:G:54:LYS:HE2	1.97	0.47
2:H:36:ILE:HA	2:H:56:GLU:O	2.14	0.47
1:A:186:LYS:O	1:A:189:ASP:HB2	2.14	0.47
1:A:487:GLN:OE1	2:D:207:SER:N	2.47	0.47
1:A:606:HIS:CD2	2:D:206:MET:HB3	2.49	0.47
1:B:205:LYS:O	1:B:208:ILE:HG22	2.15	0.47
1:B:260:TYR:HA	1:B:263:ASN:HD21	1.79	0.47
1:B:322:LEU:HD21	1:B:542:LEU:HD22	1.95	0.47
1:B:367:CYS:SG	1:B:370:ARG:NH2	2.88	0.47
1:B:455:TYR:O	1:B:458:ILE:HG22	2.13	0.47
1:B:802:ARG:HD3	1:B:840:LYS:HD2	1.96	0.47
1:E:242:LYS:NZ	1:E:243:PRO:HD2	2.29	0.47
1:F:481:ILE:HD12	1:F:484:SER:OG	2.14	0.47
1:F:809:LYS:NZ	1:F:815:PHE:H	2.12	0.47
2:G:15:ARG:H	2:G:20:LYS:CB	2.27	0.47
2:H:64:LYS:CG	2:H:217:GLU:HB3	2.39	0.47
1:A:30:ILE:O	1:A:34:THR:HG23	2.15	0.47
1:A:206:THR:HG21	1:B:206:THR:OG1	2.15	0.47
1:A:345:THR:HB	1:A:397:ALA:N	2.29	0.47
1:A:488:ALA:HA	1:A:491:GLN:NE2	2.29	0.47
1:B:483:GLN:OE1	1:B:483:GLN:HA	2.15	0.47
1:E:207:ILE:HG22	1:E:213:ILE:HD11	1.96	0.47
2:H:63:VAL:HG22	2:H:220:PHE:CZ	2.49	0.47
1:A:85:LEU:O	1:A:187:GLU:HG2	2.15	0.47
1:A:247:ARG:HH12	1:A:249:ASP:N	2.13	0.47
1:A:337:ASP:HA	1:A:350:LYS:HB2	1.97	0.47
1:A:549:GLN:HA	1:A:552:TYR:CG	2.49	0.47
1:B:59:TRP:CE3	1:B:62:LEU:HD12	2.50	0.47
1:B:491:GLN:HE22	2:C:205:GLU:N	2.12	0.47
1:E:635:GLY:HA2	1:E:638:PHE:CD2	2.50	0.47
1:E:891:THR:O	1:E:894:VAL:HG22	2.15	0.47
1:F:174:PHE:HD2	1:F:178:PHE:HA	1.79	0.47
1:F:244:PHE:CD1	1:F:267:ARG:HB2	2.49	0.47
1:F:598:ASN:CG	1:F:600:LEU:HD13	2.34	0.47
1:F:744:PHE:HE1	1:F:748:ASP:HB3	1.79	0.47
1:F:770:SER:O	1:F:774:ILE:HG13	2.14	0.47
1:F:825:LEU:HB3	1:F:852:HIS:NE2	2.29	0.47
2:G:15:ARG:H	2:G:20:LYS:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:NE	1:A:537:LYS:HD3	2.30	0.47
1:A:220:LEU:HB3	1:A:223:TYR:OH	2.14	0.47
1:A:225:ILE:O	1:A:229:LEU:CB	2.63	0.47
1:B:31:LYS:O	1:B:35:GLU:HG3	2.14	0.47
1:B:114:THR:HB	1:B:118:HIS:CD2	2.50	0.47
1:E:49:GLY:O	1:E:52:THR:OG1	2.24	0.47
1:E:233:ARG:NE	1:E:264:LYS:O	2.37	0.47
1:E:526:ASP:OD2	1:E:529:ASN:N	2.48	0.47
1:E:535:PHE:CE2	1:E:539:TYR:HD2	2.32	0.47
1:E:629:ARG:CG	1:E:631:ILE:HB	2.38	0.47
1:E:721:TYR:HD1	1:E:757:TRP:CE2	2.32	0.47
1:F:118:HIS:NE2	1:F:138:ILE:HD13	2.30	0.47
1:F:376:LYS:NZ	1:F:380:ARG:HD3	2.30	0.47
1:F:565:VAL:O	1:F:568:GLU:HG3	2.15	0.47
1:F:649:TYR:HH	1:F:687:TYR:HD1	1.61	0.47
1:F:904:ILE:HG22	2:G:235:ILE:N	2.30	0.47
1:A:45:PHE:CE2	1:A:130:ILE:HG13	2.50	0.47
1:A:473:LEU:HA	1:A:476:ILE:HG22	1.97	0.47
1:A:606:HIS:CE1	2:D:206:MET:HB3	2.50	0.47
1:A:649:TYR:O	1:A:653:VAL:HG23	2.15	0.47
1:A:717:LYS:NZ	1:A:749:LEU:HD23	2.30	0.47
1:A:801:SER:HB3	1:A:837:PHE:HE1	1.79	0.47
1:E:111:ASP:N	1:E:111:ASP:OD1	2.42	0.47
1:E:370:ARG:HH12	1:E:373:LEU:HD22	1.80	0.47
1:F:312:ILE:HG13	1:F:313:TYR:N	2.30	0.47
2:H:38:GLU:HA	2:H:54:LYS:HZ1	1.79	0.47
1:A:235:LEU:HD13	1:B:195:GLN:O	2.14	0.47
1:A:422:LYS:HA	1:A:422:LYS:HD2	1.49	0.47
1:A:549:GLN:C	1:A:552:TYR:HB2	2.34	0.47
1:B:491:GLN:HE22	2:C:206:MET:H	1.63	0.47
2:C:34:GLN:HG2	2:C:57:LYS:HZ1	1.80	0.47
2:D:31:SER:O	2:D:61:LEU:HD12	2.15	0.47
1:E:681:GLN:NE2	1:E:682:GLU:HA	2.30	0.47
1:E:866:MET:HA	1:E:869:ILE:HG12	1.97	0.47
1:F:358:GLU:OE1	1:F:362:GLU:HG2	2.15	0.47
1:F:861:ASN:HB3	1:F:863:ASN:O	2.15	0.47
1:F:906:THR:HB	2:G:233:VAL:HA	1.96	0.47
2:G:170:ARG:NH1	2:G:199:SER:HB2	2.30	0.47
1:A:90:ILE:O	1:A:94:VAL:HG12	2.14	0.46
1:B:89:GLN:OE1	1:B:187:GLU:HG3	2.15	0.46
2:C:11:VAL:HG11	2:C:63:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:633:GLU:C	1:E:635:GLY:N	2.65	0.46
1:F:218:TYR:OH	1:F:224:ASN:ND2	2.48	0.46
1:F:751:ILE:HD13	1:F:754:ARG:NE	2.30	0.46
2:G:13:PHE:HD2	2:G:22:VAL:HG12	1.81	0.46
1:B:439:ALA:HB1	1:B:455:TYR:CE1	2.51	0.46
1:B:648:GLU:HB3	2:D:2:LYS:HZ1	1.79	0.46
1:E:448:TRP:CH2	1:E:707:VAL:HB	2.51	0.46
1:F:323:GLN:HE21	1:F:597:GLU:HG3	1.81	0.46
1:F:861:ASN:C	1:F:863:ASN:N	2.68	0.46
1:F:965:LYS:HE3	1:F:966:LEU:HG	1.98	0.46
1:B:313:TYR:HA	1:B:316:ILE:HG22	1.98	0.46
1:B:374:SER:OG	1:B:375:LYS:N	2.48	0.46
1:E:195:GLN:HA	1:E:198:PRO:HG3	1.97	0.46
1:E:699:PHE:CD2	1:E:743:TYR:HB3	2.50	0.46
1:F:75:LYS:HZ1	1:F:83:GLU:HB3	1.79	0.46
1:F:328:ILE:HG13	1:F:329:ASP:N	2.31	0.46
1:F:439:ALA:HB2	1:F:454:LEU:CD2	2.45	0.46
1:F:752:GLY:N	1:F:799:LEU:HD21	2.31	0.46
1:A:174:PHE:CD1	1:A:178:PHE:HA	2.51	0.46
1:A:608:PHE:CZ	1:A:612:ILE:HD11	2.51	0.46
1:B:62:LEU:HD13	1:B:66:TYR:CE2	2.51	0.46
1:B:664:ILE:HD13	1:B:722:PHE:HE2	1.81	0.46
1:E:202:ASN:CG	1:F:205:LYS:HE2	2.36	0.46
1:F:657:ARG:HA	1:F:715:GLU:CD	2.35	0.46
1:F:952:LYS:HE2	1:F:952:LYS:HA	1.97	0.46
1:F:960:LYS:HD2	1:F:962:TYR:HE2	1.80	0.46
1:B:290:MET:HA	1:B:293:LEU:HG	1.97	0.46
1:E:124:MET:HE3	1:E:124:MET:H	1.80	0.46
1:E:407:ILE:HD11	1:E:593:ARG:HB2	1.97	0.46
1:E:749:LEU:O	1:E:754:ARG:NH1	2.49	0.46
1:E:907:PHE:HD2	2:H:232:ALA:HB3	1.79	0.46
1:F:207:ILE:HA	1:F:210:THR:HG22	1.98	0.46
1:F:922:LEU:HA	1:F:969:LYS:HZ3	1.80	0.46
2:H:22:VAL:HG13	2:H:22:VAL:O	2.16	0.46
1:A:548:ASN:OD1	1:A:548:ASN:N	2.48	0.46
1:B:569:MET:SD	1:B:570:SER:OG	2.65	0.46
1:B:664:ILE:HB	1:B:722:PHE:CZ	2.51	0.46
1:B:685:GLU:OE2	1:B:688:LEU:HD23	2.15	0.46
1:B:817:SER:OG	1:B:844:LEU:O	2.30	0.46
1:E:455:TYR:CE2	1:E:481:ILE:HG21	2.51	0.46
1:E:550:PHE:H	1:E:550:PHE:HD1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:652:PHE:CE1	1:F:722:PHE:HD2	2.34	0.46
2:H:70:LEU:HD23	2:H:70:LEU:HA	1.75	0.46
1:A:491:GLN:HB2	1:A:495:LEU:HB3	1.98	0.46
1:A:712:PHE:CG	1:A:713:ILE:N	2.83	0.46
1:B:326:ARG:HB2	1:B:329:ASP:HB2	1.97	0.46
1:B:482:TYR:HE2	1:B:519:MET:HB2	1.80	0.46
1:B:643:SER:HB3	2:D:5:ILE:HG12	1.96	0.46
1:B:659:PHE:CD2	1:B:662:ASP:HA	2.50	0.46
1:E:367:CYS:O	1:E:370:ARG:HB2	2.16	0.46
1:E:449:GLU:HG3	1:E:511:PHE:CE2	2.51	0.46
1:E:737:VAL:HG21	1:E:771:ILE:HG23	1.96	0.46
1:F:187:GLU:HA	1:F:190:TYR:CD2	2.50	0.46
1:F:202:ASN:HA	1:F:205:LYS:HZ2	1.81	0.46
2:G:15:ARG:HG2	2:G:20:LYS:CG	2.43	0.46
2:G:225:ASP:OD2	2:G:227:ASP:HB3	2.16	0.46
2:H:192:TYR:HB2	2:H:235:ILE:HB	1.98	0.46
1:A:491:GLN:HB2	1:A:495:LEU:CB	2.46	0.46
1:A:549:GLN:HB2	1:A:552:TYR:CB	2.45	0.46
1:A:655:ILE:HG23	1:A:659:PHE:CE2	2.51	0.46
1:B:290:MET:O	1:B:294:ILE:HG12	2.15	0.46
1:E:202:ASN:ND2	1:F:205:LYS:HE2	2.30	0.46
1:E:434:ASP:O	1:E:438:LYS:HG2	2.16	0.46
1:E:456:SER:HA	1:E:459:ILE:HD12	1.97	0.46
1:E:475:GLN:CD	1:E:478:ARG:HH22	2.18	0.46
1:F:229:LEU:O	1:F:233:ARG:HG2	2.15	0.46
1:F:284:GLU:O	1:F:287:SER:OG	2.29	0.46
1:F:332:HIS:CE1	1:F:543:GLU:HG2	2.50	0.46
1:A:118:HIS:HE1	1:A:137:LEU:C	2.20	0.46
1:A:187:GLU:HA	1:A:190:TYR:CD2	2.51	0.46
1:B:62:LEU:HD23	1:B:107:PHE:CG	2.51	0.46
2:D:54:LYS:HB3	2:D:54:LYS:HE3	1.67	0.46
1:E:574:TYR:OH	1:E:629:ARG:NH1	2.47	0.46
1:F:612:ILE:HG21	1:F:658:HIS:ND1	2.30	0.46
1:F:712:PHE:O	1:F:713:ILE:C	2.50	0.46
1:F:728:LEU:HD12	1:F:728:LEU:HA	1.78	0.46
1:F:786:HIS:HA	1:F:791:TYR:HD2	1.80	0.46
1:A:188:ASP:O	1:A:192:ASN:ND2	2.49	0.46
1:A:581:ASP:HA	1:A:584:VAL:HG23	1.97	0.46
1:B:588:LEU:HD11	1:B:615:SER:CB	2.46	0.46
2:C:37:SER:N	2:C:56:GLU:OE2	2.49	0.46
1:E:781:LEU:O	1:E:784:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:506:PRO:HG2	1:F:507:PHE:CE2	2.51	0.46
1:F:776:ASP:HA	1:F:779:LEU:HG	1.97	0.46
1:A:336:TYR:O	1:A:349:HIS:ND1	2.49	0.45
1:A:750:ASP:CG	1:A:751:ILE:H	2.19	0.45
1:B:197:TYR:O	1:B:197:TYR:HD1	1.98	0.45
1:B:279:GLU:O	1:B:285:ARG:NH2	2.49	0.45
1:B:533:PHE:CD1	1:B:533:PHE:N	2.83	0.45
1:B:891:THR:HA	1:B:894:VAL:HG22	1.98	0.45
2:D:177:THR:OG1	2:D:191:ILE:HB	2.16	0.45
1:E:45:PHE:HE1	1:E:213:ILE:HD12	1.81	0.45
1:E:633:GLU:C	1:E:635:GLY:H	2.18	0.45
1:E:883:GLU:O	1:E:886:ILE:HG22	2.16	0.45
1:F:842:LEU:O	1:F:845:LEU:HB2	2.16	0.45
1:F:892:ARG:HA	1:F:895:ASN:ND2	2.29	0.45
1:F:963:ASN:ND2	2:G:52:ILE:HG22	2.30	0.45
2:G:197:ASN:HB3	2:G:223:LEU:O	2.15	0.45
1:A:649:TYR:CE1	1:A:683:LYS:HB3	2.51	0.45
1:A:655:ILE:HG23	1:A:659:PHE:CZ	2.51	0.45
1:B:573:SER:OG	2:D:31:SER:HB2	2.16	0.45
2:D:198:VAL:HG13	2:D:220:PHE:HB3	1.97	0.45
1:E:606:HIS:CE1	2:H:206:MET:HA	2.51	0.45
1:E:721:TYR:O	1:E:760:ARG:NH2	2.43	0.45
1:E:923:GLU:O	1:E:923:GLU:HG2	2.16	0.45
1:F:130:ILE:HD13	1:F:168:LEU:HD23	1.98	0.45
1:F:326:ARG:HD3	1:F:594:PHE:CD2	2.51	0.45
1:F:827:LEU:HG	1:F:834:GLN:NE2	2.31	0.45
1:F:932:GLU:H	1:F:932:GLU:HG2	1.34	0.45
1:A:145:ARG:CZ	1:A:147:LYS:HG2	2.46	0.45
1:A:674:ASP:OD1	1:A:724:LYS:HB3	2.17	0.45
1:E:205:LYS:HB2	1:E:231:TRP:HZ2	1.81	0.45
1:E:448:TRP:HB3	1:E:481:ILE:HD11	1.98	0.45
2:G:215:ALA:O	2:G:217:GLU:N	2.49	0.45
1:A:792:SER:HA	1:A:833:LYS:HD3	1.98	0.45
1:B:730:GLU:HG2	1:B:733:LEU:HD12	1.98	0.45
1:E:79:TYR:HA	1:E:83:GLU:OE1	2.15	0.45
1:F:53:LEU:O	1:F:115:ASN:ND2	2.49	0.45
1:F:59:TRP:CH2	1:F:185:LEU:HG	2.51	0.45
1:F:151:VAL:HG22	1:F:167:LEU:HB3	1.99	0.45
1:F:472:TYR:HB2	1:F:535:PHE:HE2	1.81	0.45
1:F:727:LYS:HA	1:F:727:LYS:HD2	1.34	0.45
1:F:861:ASN:CG	1:F:863:ASN:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:GLN:HA	1:A:478:ARG:HH12	1.80	0.45
1:A:657:ARG:HA	1:A:715:GLU:OE2	2.15	0.45
1:A:768:PRO:HA	1:A:772:ILE:HB	1.99	0.45
1:B:289:VAL:O	1:B:293:LEU:HG	2.16	0.45
1:B:316:ILE:CD1	1:B:319:LEU:HD11	2.46	0.45
1:B:741:LEU:HD12	1:B:774:ILE:HG22	1.97	0.45
1:E:417:LYS:HD2	1:E:417:LYS:O	2.17	0.45
1:E:651:ASP:HA	1:E:654:ASN:HD21	1.81	0.45
1:E:664:ILE:O	1:E:667:LEU:HG	2.16	0.45
1:F:210:THR:HG23	1:F:211:HIS:ND1	2.31	0.45
1:F:566:ARG:O	1:F:569:MET:HB3	2.16	0.45
1:F:956:PRO:O	1:F:960:LYS:HG2	2.15	0.45
1:A:246:ILE:HA	1:A:269:ILE:HG23	1.99	0.45
1:B:660:LYS:HD3	1:B:660:LYS:HA	1.76	0.45
1:B:751:ILE:HD13	1:B:754:ARG:HH21	1.81	0.45
1:E:749:LEU:HB3	1:E:754:ARG:CZ	2.47	0.45
1:F:227:MET:SD	1:F:228:LEU:N	2.90	0.45
1:F:425:ILE:HD11	1:F:442:LEU:HD23	1.98	0.45
1:F:958:TRP:N	1:F:958:TRP:CD1	2.84	0.45
1:F:979:HIS:O	1:F:983:VAL:HG23	2.17	0.45
1:A:409:ILE:HD13	1:A:414:TYR:CE1	2.52	0.45
1:B:170:VAL:HG12	1:B:200:ILE:HG22	1.99	0.45
1:B:331:LYS:HE3	1:B:336:TYR:HE1	1.82	0.45
1:E:208:ILE:HA	1:E:213:ILE:CG1	2.46	0.45
1:E:297:GLN:O	1:E:299:ASN:N	2.50	0.45
1:E:482:TYR:C	1:E:482:TYR:CD1	2.90	0.45
1:E:767:LEU:HB2	1:E:811:PHE:CE2	2.52	0.45
1:E:847:THR:HA	1:E:850:LYS:HE3	1.99	0.45
1:F:59:TRP:O	1:F:63:VAL:HG23	2.16	0.45
1:F:79:TYR:HB3	1:F:84:TYR:HA	1.99	0.45
1:F:376:LYS:HZ1	1:F:380:ARG:CD	2.30	0.45
1:F:976:MET:HB3	1:F:979:HIS:NE2	2.32	0.45
1:A:117:ILE:HG13	1:A:120:LYS:HZ3	1.82	0.45
1:A:388:PHE:HA	1:A:391:ASN:HD21	1.80	0.45
1:B:240:PHE:CZ	1:B:243:PRO:HD3	2.52	0.45
1:B:342:VAL:HG12	1:B:586:LEU:HB3	1.98	0.45
1:B:442:LEU:HB3	1:B:447:ARG:HH22	1.82	0.45
1:B:489:VAL:O	1:B:493:ASN:N	2.48	0.45
1:B:965:LYS:H	1:B:965:LYS:HG3	1.55	0.45
1:E:195:GLN:HE22	1:F:237:LYS:HE3	1.82	0.45
1:E:877:PHE:HE2	1:E:924:GLU:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:ARG:HB2	1:F:329:ASP:HB2	1.99	0.45
1:F:338:TYR:HE1	1:F:351:ASN:HB2	1.81	0.45
1:F:502:ARG:O	1:F:502:ARG:HD3	2.17	0.45
1:F:749:LEU:HD11	1:F:754:ARG:HG3	1.99	0.45
1:F:904:ILE:HG22	2:G:235:ILE:HA	1.99	0.45
1:F:955:ILE:HD13	1:F:958:TRP:NE1	2.31	0.45
1:A:23:ASP:O	1:A:27:VAL:HG23	2.17	0.45
1:E:43:VAL:HG22	1:E:128:HIS:H	1.81	0.45
1:E:186:LYS:NZ	1:E:188:ASP:HB2	2.31	0.45
1:E:500:PHE:HD1	1:E:747:ARG:HH22	1.64	0.45
1:E:726:VAL:HG22	1:E:727:LYS:H	1.82	0.45
1:F:342:VAL:HG22	1:F:586:LEU:HD13	1.98	0.45
1:F:681:GLN:O	1:F:685:GLU:HG3	2.17	0.45
1:F:932:GLU:O	1:F:934:ILE:HG12	2.17	0.45
1:F:962:TYR:HH	1:F:1004:PHE:HZ	1.63	0.45
1:F:979:HIS:ND1	1:F:980:VAL:HG23	2.31	0.45
1:A:547:ASP:O	1:A:550:PHE:CD1	2.69	0.45
1:A:772:ILE:HA	1:A:775:ILE:HD12	1.99	0.45
1:B:964:ASP:HB2	1:B:965:LYS:HZ3	1.80	0.45
1:E:124:MET:N	1:E:124:MET:SD	2.90	0.45
1:E:163:SER:OG	1:E:165:ARG:O	2.35	0.45
1:E:815:PHE:CE2	1:E:844:LEU:HA	2.52	0.45
1:E:818:LYS:HA	1:E:821:SER:HB2	1.99	0.45
1:E:865:LEU:HD23	1:E:865:LEU:HA	1.83	0.45
1:F:279:GLU:HA	1:F:285:ARG:HH22	1.82	0.45
1:F:909:SER:HB3	2:G:231:MET:HG2	1.98	0.45
1:A:87:ILE:HA	1:A:90:ILE:HG12	1.98	0.44
1:A:231:TRP:HA	1:A:234:LYS:HE2	1.99	0.44
1:A:257:THR:HA	1:E:86:ARG:HH22	1.83	0.44
1:B:152:ILE:HB	1:B:168:LEU:HD12	1.99	0.44
1:B:222:ASP:O	1:B:225:ILE:HG12	2.17	0.44
1:B:223:TYR:HA	1:B:226:ASN:HD21	1.82	0.44
1:E:61:ARG:NH1	1:E:64:ASP:HB2	2.32	0.44
1:E:105:LYS:CE	1:E:178:PHE:HB2	2.47	0.44
1:E:324:TYR:HA	1:E:390:LYS:HZ3	1.81	0.44
1:E:422:LYS:NZ	1:E:447:ARG:HH22	2.15	0.44
1:E:495:LEU:O	1:E:498:LEU:HG	2.17	0.44
1:E:973:ASN:O	1:E:977:LYS:HB2	2.17	0.44
1:F:294:ILE:HG22	1:F:295:GLU:N	2.32	0.44
2:G:20:LYS:HA	2:G:72:TRP:CH2	2.52	0.44
1:A:229:LEU:O	1:A:233:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:HIS:O	1:B:70:LEU:HB2	2.17	0.44
1:B:661:ILE:O	1:B:665:LYS:CB	2.64	0.44
1:F:963:ASN:O	1:F:967:LEU:HD23	2.11	0.44
1:F:965:LYS:O	1:F:968:GLY:N	2.50	0.44
2:H:72:TRP:HA	2:H:72:TRP:HE3	1.74	0.44
1:A:44:PHE:CE2	1:A:121:ILE:HD12	2.53	0.44
1:A:86:ARG:NH2	1:A:90:ILE:HD11	2.31	0.44
1:A:193:TYR:O	1:A:193:TYR:HD1	2.00	0.44
1:A:469:CYS:O	1:A:473:LEU:HD23	2.17	0.44
1:A:537:LYS:HA	1:A:537:LYS:HD2	1.76	0.44
1:A:620:ILE:HG21	1:A:667:LEU:HD21	1.99	0.44
1:A:794:VAL:HG12	1:A:796:SER:H	1.83	0.44
1:A:836:ASP:O	1:A:839:PHE:HB3	2.18	0.44
1:B:317:SER:HA	1:B:320:PHE:CZ	2.53	0.44
1:E:143:TRP:CE2	1:F:463:ILE:HG22	2.52	0.44
1:E:1001:MET:HG3	1:F:985:LYS:HE3	1.99	0.44
1:F:322:LEU:HD12	1:F:323:GLN:H	1.82	0.44
1:F:650:TYR:O	1:F:654:ASN:ND2	2.51	0.44
1:F:912:TYR:H	1:F:913:MET:HE1	1.81	0.44
2:H:42:ARG:NH1	2:H:52:ILE:HD13	2.32	0.44
1:B:169:LYS:HE2	1:B:172:GLY:O	2.17	0.44
1:B:368:ASP:N	1:B:368:ASP:OD1	2.49	0.44
1:B:639:PHE:C	1:B:641:LYS:H	2.21	0.44
1:B:892:ARG:HA	1:B:895:ASN:HD21	1.82	0.44
2:C:240:ASP:N	2:C:240:ASP:OD1	2.50	0.44
1:F:32:GLU:O	1:F:35:GLU:HG3	2.18	0.44
1:F:119:ASP:OD1	1:F:119:ASP:N	2.50	0.44
2:H:205:GLU:HG3	2:H:207:SER:OG	2.18	0.44
2:H:228:THR:HG22	2:H:229:ASP:CG	2.38	0.44
1:A:827:LEU:HD13	1:A:835:ILE:HG22	1.99	0.44
1:A:914:SER:O	1:A:918:ILE:HG13	2.17	0.44
1:A:955:ILE:HD12	1:A:958:TRP:HZ2	1.81	0.44
1:B:245:PHE:O	1:B:268:ILE:HD12	2.17	0.44
2:C:11:VAL:HB	2:C:24:THR:HB	1.99	0.44
2:C:15:ARG:HE	2:C:20:LYS:HE2	1.83	0.44
1:E:283:LEU:O	1:E:283:LEU:HD12	2.18	0.44
1:E:312:ILE:HD13	1:E:312:ILE:HA	1.78	0.44
1:E:333:VAL:HA	1:E:540:LYS:HD3	1.99	0.44
1:E:549:GLN:HA	1:E:552:TYR:CD2	2.51	0.44
1:F:725:TYR:CD1	1:F:725:TYR:N	2.84	0.44
1:F:789:GLN:HG3	1:F:831:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:975:HIS:HD1	1:F:976:MET:CG	2.30	0.44
1:A:685:GLU:OE1	1:A:685:GLU:N	2.51	0.44
1:A:727:LYS:HB2	1:A:727:LYS:HZ2	1.82	0.44
1:B:169:LYS:HG2	1:B:172:GLY:H	1.83	0.44
1:B:412:LEU:HA	1:B:415:HIS:CD2	2.52	0.44
1:B:475:GLN:HA	1:B:478:ARG:CZ	2.47	0.44
1:B:607:GLU:HG3	1:B:608:PHE:N	2.32	0.44
1:B:664:ILE:HG23	1:B:668:GLU:HG2	1.99	0.44
1:E:45:PHE:HA	1:E:130:ILE:O	2.18	0.44
1:E:629:ARG:HH11	1:E:631:ILE:HD12	1.83	0.44
1:E:725:TYR:O	1:E:726:VAL:HG12	2.17	0.44
1:E:963:ASN:ND2	1:E:965:LYS:HB3	2.32	0.44
1:E:974:LYS:O	1:E:974:LYS:HD3	2.17	0.44
1:F:104:LEU:HD13	1:F:174:PHE:HE2	1.82	0.44
1:F:205:LYS:O	1:F:208:ILE:HG22	2.18	0.44
1:A:147:LYS:NZ	1:B:526:ASP:O	2.51	0.44
1:A:605:PHE:O	1:A:609:HIS:NE2	2.51	0.44
1:A:751:ILE:O	1:A:752:GLY:C	2.53	0.44
1:B:197:TYR:O	1:B:197:TYR:CD1	2.71	0.44
1:B:363:LEU:HD23	1:B:369:GLU:HB3	1.99	0.44
1:B:593:ARG:HA	1:B:596:TYR:CB	2.46	0.44
1:B:864:ASP:OD1	1:B:865:LEU:N	2.50	0.44
1:E:61:ARG:HH12	1:E:64:ASP:HB2	1.83	0.44
1:E:156:GLU:OE1	1:F:239:SER:HB3	2.18	0.44
1:E:995:ARG:O	1:E:999:ILE:HB	2.17	0.44
1:F:224:ASN:O	1:F:228:LEU:HB3	2.16	0.44
1:F:316:ILE:HD12	1:F:316:ILE:HA	1.85	0.44
1:F:827:LEU:HD13	1:F:827:LEU:HA	1.81	0.44
1:F:940:TYR:HA	1:F:943:PHE:CD2	2.53	0.44
1:A:174:PHE:CE1	1:A:178:PHE:HA	2.53	0.44
1:A:225:ILE:O	1:A:229:LEU:HB2	2.18	0.44
1:A:439:ALA:HB2	1:A:454:LEU:HD23	2.00	0.44
1:A:580:SER:O	1:A:583:VAL:N	2.46	0.44
1:A:919:TRP:HE1	2:D:51:TYR:HB2	1.81	0.44
1:B:135:ASP:OD1	1:B:135:ASP:N	2.42	0.44
1:B:348:ARG:HG3	1:B:351:ASN:HB3	1.99	0.44
1:B:417:LYS:C	1:B:421:MET:HE3	2.38	0.44
2:D:20:LYS:HA	2:D:72:TRP:CE2	2.52	0.44
1:E:115:ASN:HB2	1:E:116:PRO:HD2	1.99	0.44
1:E:589:TYR:HE2	2:G:2:LYS:HZ1	1.65	0.44
1:E:994:LYS:NZ	1:F:989:LYS:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLN:HG3	1:F:61:ARG:NH1	2.33	0.44
1:F:735:LYS:HD2	1:F:735:LYS:HA	1.82	0.44
1:A:290:MET:SD	1:A:293:LEU:HD21	2.58	0.44
2:C:201:SER:O	2:C:201:SER:OG	2.33	0.44
1:E:359:ARG:NH1	1:E:359:ARG:HA	2.33	0.44
1:E:861:ASN:C	1:E:861:ASN:OD1	2.56	0.44
1:E:950:ASP:HB3	1:E:953:LYS:HZ3	1.83	0.44
1:F:326:ARG:NH1	1:F:591:ASN:HA	2.33	0.44
1:F:407:ILE:H	2:H:2:LYS:CB	2.30	0.44
1:F:616:MET:HE2	1:F:616:MET:HB3	1.83	0.44
1:F:918:ILE:O	1:F:922:LEU:HB2	2.18	0.44
1:F:927:ASN:OD1	1:F:928:SER:N	2.51	0.44
1:F:939:GLN:HG3	1:F:958:TRP:HB3	1.99	0.44
1:F:956:PRO:HB2	1:F:996:TYR:OH	2.18	0.44
1:F:981:ILE:HG23	1:F:982:GLU:OE1	2.18	0.44
1:A:44:PHE:CD2	1:A:121:ILE:HG23	2.53	0.43
1:A:85:LEU:O	1:A:88:PRO:HG2	2.18	0.43
1:A:152:ILE:HG21	1:A:158:VAL:HG23	2.00	0.43
1:A:315:LYS:O	1:A:318:PRO:HD2	2.18	0.43
1:A:395:CYS:SG	1:A:396:MET:N	2.91	0.43
1:A:404:ASN:OD1	2:C:5:ILE:HA	2.17	0.43
1:A:772:ILE:HA	1:A:772:ILE:HD12	1.83	0.43
1:B:333:VAL:HG23	1:B:541:ILE:HD12	2.00	0.43
1:B:583:VAL:O	1:B:587:ARG:HG2	2.18	0.43
1:E:51:SER:OG	1:E:133:ASN:OD1	2.21	0.43
1:E:83:GLU:O	1:E:87:ILE:HG12	2.18	0.43
1:E:404:ASN:HB3	2:G:1:MET:HA	2.00	0.43
1:E:480:ARG:HG3	1:E:605:PHE:CZ	2.53	0.43
1:E:531:MET:HE3	1:F:148:TYR:CD2	2.52	0.43
1:E:673:ILE:HG23	1:E:725:TYR:CE2	2.52	0.43
1:F:89:GLN:HA	1:F:186:LYS:CE	2.47	0.43
1:F:821:SER:O	1:F:824:THR:OG1	2.27	0.43
1:A:662:ASP:OD1	1:A:663:ASP:N	2.51	0.43
1:A:764:CYS:O	1:A:765:ASN:ND2	2.51	0.43
1:B:134:TYR:CZ	1:B:171:ALA:HB1	2.53	0.43
1:B:312:ILE:HD13	1:B:312:ILE:HA	1.85	0.43
1:B:345:THR:HA	1:B:395:CYS:O	2.18	0.43
1:E:76:LYS:HE2	1:E:76:LYS:HA	1.99	0.43
1:E:507:PHE:N	1:E:507:PHE:CD1	2.83	0.43
1:E:544:PHE:CE1	1:E:550:PHE:HB2	2.53	0.43
1:E:706:VAL:O	1:E:710:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:VAL:HA	1:F:30:ILE:HD12	2.00	0.43
1:F:60:TRP:CZ3	1:F:61:ARG:HG2	2.53	0.43
1:F:994:LYS:HD3	1:F:994:LYS:HA	1.72	0.43
2:H:29:THR:HG23	2:H:64:LYS:HZ2	1.83	0.43
1:A:706:VAL:HA	1:A:709:TYR:HD2	1.84	0.43
1:A:722:PHE:CZ	1:A:725:TYR:HD2	2.36	0.43
1:B:916:PHE:HA	1:B:919:TRP:HD1	1.83	0.43
2:C:70:LEU:HD23	2:C:73:LEU:HD23	2.00	0.43
2:D:24:THR:N	2:D:68:PHE:HA	2.33	0.43
1:E:755:TYR:CE1	1:E:807:LEU:HB3	2.52	0.43
1:E:965:LYS:HA	1:E:965:LYS:HD2	1.90	0.43
1:F:322:LEU:HD11	1:F:598:ASN:HB3	1.99	0.43
1:F:724:LYS:HD3	1:F:760:ARG:CZ	2.48	0.43
2:G:65:ASN:O	2:G:216:PRO:HD2	2.18	0.43
1:A:548:ASN:CB	2:D:210:ASN:ND2	2.79	0.43
1:A:688:LEU:HD11	1:A:736:ILE:HD13	2.00	0.43
1:B:45:PHE:HB2	1:B:214:VAL:O	2.19	0.43
1:B:69:GLU:HB2	1:B:91:PHE:HE1	1.84	0.43
1:B:326:ARG:NH1	1:B:329:ASP:OD2	2.51	0.43
1:B:978:HIS:NE2	1:B:982:GLU:OE2	2.51	0.43
1:E:254:GLU:H	1:E:254:GLU:CD	2.21	0.43
1:E:893:LYS:HZ3	1:E:933:PHE:HA	1.84	0.43
1:F:357:MET:HG2	1:F:361:PHE:CZ	2.53	0.43
1:F:569:MET:CE	1:F:621:GLU:HB3	2.48	0.43
1:F:657:ARG:HG2	1:F:715:GLU:CD	2.39	0.43
1:A:97:GLU:HA	1:A:100:PHE:HB2	2.00	0.43
1:A:261:TYR:HD1	1:A:261:TYR:HA	1.68	0.43
1:A:955:ILE:HB	1:A:958:TRP:CE2	2.54	0.43
1:B:231:TRP:CE2	1:B:235:LEU:HD11	2.54	0.43
1:B:256:GLU:O	1:B:259:ILE:HG22	2.18	0.43
1:B:369:GLU:HA	1:B:372:LYS:HD3	2.01	0.43
1:B:575:SER:O	1:B:579:SER:OG	2.22	0.43
1:B:577:GLY:N	2:D:7:ASP:OD1	2.47	0.43
1:B:646:PHE:HB3	1:B:677:ARG:CZ	2.49	0.43
2:D:1:MET:HE2	2:D:1:MET:H1	1.84	0.43
1:E:282:TYR:O	1:E:283:LEU:HB3	2.18	0.43
1:E:315:LYS:HD2	1:E:315:LYS:HA	1.77	0.43
1:E:528:PHE:O	1:E:531:MET:HB2	2.18	0.43
1:E:987:ARG:O	1:E:991:SER:HB3	2.18	0.43
1:F:94:VAL:HG13	1:F:95:LYS:HG2	2.00	0.43
1:F:412:LEU:O	1:F:416:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:911:ASP:HA	1:F:913:MET:HE1	2.01	0.43
1:A:206:THR:O	1:A:210:THR:HG23	2.19	0.43
1:A:326:ARG:NH1	1:A:328:ILE:HB	2.33	0.43
1:A:421:MET:HA	1:A:424:PHE:HB3	2.01	0.43
1:B:304:LYS:HE3	1:B:306:ASP:HB2	1.99	0.43
1:B:964:ASP:C	1:B:966:LEU:N	2.72	0.43
1:E:247:ARG:O	1:E:271:ALA:N	2.52	0.43
1:E:373:LEU:HD12	1:E:373:LEU:HA	1.72	0.43
1:E:479:TYR:CG	1:E:524:ILE:HG12	2.54	0.43
1:E:1000:LEU:HD12	1:E:1004:PHE:HD2	1.84	0.43
1:F:376:LYS:O	1:F:379:GLU:HG3	2.17	0.43
1:F:620:ILE:O	1:F:620:ILE:HG13	2.18	0.43
1:F:751:ILE:HA	1:F:754:ARG:HE	1.83	0.43
1:F:815:PHE:HD2	1:F:844:LEU:HD23	1.84	0.43
1:F:960:LYS:NZ	1:F:999:ILE:HG13	2.33	0.43
1:A:304:LYS:HE2	1:A:306:ASP:HB2	2.00	0.43
1:A:717:LYS:HG3	1:A:757:TRP:HH2	1.84	0.43
1:A:751:ILE:HA	1:A:754:ARG:CB	2.48	0.43
1:A:766:GLU:HB2	1:A:768:PRO:HD3	2.00	0.43
1:A:774:ILE:HD12	1:A:774:ILE:N	2.34	0.43
1:B:42:LEU:HB3	1:B:44:PHE:CE1	2.53	0.43
1:B:118:HIS:HA	1:B:121:ILE:CG2	2.46	0.43
1:B:661:ILE:HA	1:B:665:LYS:CE	2.48	0.43
1:B:696:THR:O	1:B:700:SER:CB	2.67	0.43
2:D:32:PHE:CD1	2:D:61:LEU:HD13	2.53	0.43
1:E:569:MET:HE2	1:E:569:MET:HA	2.00	0.43
1:E:657:ARG:HB3	1:E:658:HIS:CE1	2.54	0.43
1:E:892:ARG:HD2	1:E:892:ARG:HA	1.70	0.43
1:F:136:ASN:O	1:F:140:THR:HG23	2.19	0.43
1:F:827:LEU:HG	1:F:834:GLN:HE21	1.84	0.43
1:A:473:LEU:HD12	1:A:600:LEU:CD2	2.47	0.43
1:A:515:ILE:O	1:A:518:GLU:HG3	2.19	0.43
1:A:998:GLU:O	1:A:1002:ASN:HB2	2.19	0.43
1:B:522:PHE:CD1	1:B:522:PHE:C	2.92	0.43
1:B:608:PHE:O	1:B:612:ILE:HG13	2.19	0.43
1:E:886:ILE:HD12	1:E:886:ILE:HA	1.85	0.43
1:E:1002:ASN:O	1:E:1003:TYR:C	2.57	0.43
1:F:29:CYS:SG	1:F:244:PHE:HE1	2.42	0.43
1:F:89:GLN:HB3	1:F:186:LYS:HZ3	1.82	0.43
1:A:237:LYS:HB2	1:A:238:ASP:OD1	2.18	0.43
1:A:458:ILE:O	1:A:462:SER:OG	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HG12	1:B:442:LEU:HD23	2.01	0.43
1:B:589:TYR:HA	1:B:592:LEU:HB3	1.99	0.43
2:C:5:ILE:O	2:C:6:GLN:HB3	2.18	0.43
1:E:100:PHE:O	1:E:104:LEU:HG	2.19	0.43
1:E:317:SER:OG	1:E:318:PRO:HD3	2.18	0.43
1:E:627:ARG:CZ	1:E:675:LYS:HB3	2.48	0.43
1:E:767:LEU:HB2	1:E:811:PHE:HE2	1.82	0.43
1:F:224:ASN:OD1	1:F:225:ILE:N	2.52	0.43
1:F:549:GLN:O	1:F:552:TYR:N	2.51	0.43
1:F:627:ARG:HE	1:F:675:LYS:HZ2	1.67	0.43
1:F:631:ILE:HG21	1:F:635:GLY:HA3	2.00	0.43
1:F:672:SER:OG	1:F:672:SER:O	2.36	0.43
1:A:396:MET:O	1:A:400:ALA:N	2.52	0.43
1:A:661:ILE:HD11	2:D:219:LYS:NZ	2.33	0.43
1:B:79:TYR:HB3	1:B:83:GLU:HB2	2.00	0.43
1:B:661:ILE:HA	1:B:665:LYS:HE3	2.00	0.43
1:B:675:LYS:C	1:B:676:ILE:HG12	2.39	0.43
1:E:148:TYR:CD2	1:F:532:PRO:HG3	2.54	0.43
1:E:435:ASP:HA	1:E:438:LYS:HE2	2.01	0.43
1:E:807:LEU:HD12	1:E:808:ILE:HG22	2.01	0.43
1:F:41:LYS:NZ	1:F:211:HIS:HA	2.31	0.43
1:F:950:ASP:OD1	1:F:950:ASP:O	2.37	0.43
1:A:225:ILE:HG13	1:A:226:ASN:N	2.33	0.42
1:A:551:LEU:HA	1:A:554:ASP:OD2	2.18	0.42
1:A:626:GLU:OE2	1:A:629:ARG:HD2	2.18	0.42
1:A:802:ARG:CZ	1:A:867:ASN:HA	2.49	0.42
1:A:866:MET:HA	1:A:869:ILE:HG22	2.00	0.42
1:B:85:LEU:O	1:B:187:GLU:HB3	2.19	0.42
1:B:254:GLU:OE1	1:B:254:GLU:N	2.52	0.42
1:B:438:LYS:HA	1:B:441:PHE:HD1	1.83	0.42
1:B:902:LYS:HB3	1:B:904:ILE:HD11	2.00	0.42
1:E:487:GLN:HG2	1:E:491:GLN:NE2	2.34	0.42
1:E:578:MET:H	1:E:578:MET:CE	2.32	0.42
1:E:801:SER:HB3	1:E:840:LYS:NZ	2.34	0.42
1:E:880:GLU:HA	1:E:883:GLU:OE1	2.19	0.42
1:F:851:SER:OG	1:F:852:HIS:N	2.50	0.42
2:G:72:TRP:N	2:G:72:TRP:CD1	2.87	0.42
2:G:212:ASN:C	2:G:214:LEU:N	2.72	0.42
1:A:170:VAL:HA	1:A:200:ILE:HD11	2.01	0.42
1:A:660:LYS:O	1:A:664:ILE:HD13	2.18	0.42
1:B:105:LYS:HE3	1:B:105:LYS:HB3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ILE:HB	1:E:243:PRO:HB3	2.01	0.42
1:E:220:LEU:HD21	1:E:247:ARG:HH22	1.84	0.42
1:E:322:LEU:HD13	1:E:322:LEU:HA	1.86	0.42
1:E:605:PHE:HA	2:H:207:SER:CB	2.42	0.42
1:E:695:ILE:HB	1:E:699:PHE:CE2	2.54	0.42
1:E:724:LYS:NZ	1:E:764:CYS:HB2	2.33	0.42
1:E:869:ILE:HD12	2:H:50:LEU:HG	2.01	0.42
1:F:346:VAL:H	1:F:396:MET:HA	1.83	0.42
1:F:802:ARG:HE	1:F:840:LYS:HA	1.85	0.42
1:F:921:PHE:CE2	1:F:970:ILE:HD13	2.54	0.42
2:H:22:VAL:HA	2:H:69:ASP:H	1.84	0.42
1:A:87:ILE:N	1:A:88:PRO:HD2	2.34	0.42
1:A:578:MET:HG3	1:A:578:MET:O	2.19	0.42
1:B:533:PHE:N	1:B:533:PHE:HD1	2.17	0.42
1:E:24:ASN:OD1	1:E:25:ASN:N	2.52	0.42
1:E:53:LEU:HD11	1:E:286:TYR:HE2	1.81	0.42
1:F:216:ILE:HG22	1:F:246:ILE:HG13	2.01	0.42
2:H:21:LEU:O	2:H:71:GLU:HB3	2.19	0.42
2:H:63:VAL:HG22	2:H:220:PHE:HZ	1.83	0.42
1:A:214:VAL:HG12	1:A:244:PHE:HD2	1.85	0.42
1:A:215:PHE:HB2	1:A:245:PHE:HD1	1.82	0.42
1:A:286:TYR:N	1:A:286:TYR:CD1	2.87	0.42
1:A:581:ASP:O	1:A:585:LEU:N	2.39	0.42
1:B:27:VAL:HA	1:B:30:ILE:HG22	2.01	0.42
1:B:606:HIS:ND1	1:B:609:HIS:HB3	2.35	0.42
1:E:130:ILE:HA	1:E:168:LEU:O	2.19	0.42
1:E:233:ARG:HH21	1:E:264:LYS:C	2.23	0.42
1:F:626:GLU:HG2	1:F:629:ARG:NH2	2.35	0.42
2:H:192:TYR:O	2:H:234:VAL:HA	2.20	0.42
1:A:248:THR:HB	1:A:286:TYR:CZ	2.54	0.42
1:A:659:PHE:HD2	1:A:718:ALA:HB1	1.85	0.42
1:A:744:PHE:HD1	1:A:745:PRO:HD2	1.84	0.42
1:B:75:LYS:HB3	1:B:79:TYR:CZ	2.54	0.42
1:E:304:LYS:CD	1:E:307:GLU:H	2.32	0.42
1:E:326:ARG:HD2	1:E:328:ILE:CD1	2.49	0.42
1:E:556:VAL:HG11	1:F:552:TYR:CE2	2.53	0.42
1:E:687:TYR:O	1:E:691:ILE:HG12	2.19	0.42
1:E:801:SER:OG	1:E:841:LEU:HD11	2.20	0.42
1:F:117:ILE:HD12	1:F:290:MET:SD	2.60	0.42
1:F:376:LYS:HZ1	1:F:380:ARG:HD3	1.84	0.42
1:F:697:LYS:HE2	1:F:697:LYS:HB2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:965:LYS:HZ2	2:G:49:PRO:HA	1.84	0.42
1:A:128:HIS:CE1	1:A:165:ARG:HA	2.54	0.42
1:A:473:LEU:HA	1:A:476:ILE:CG2	2.49	0.42
1:B:438:LYS:O	1:B:442:LEU:HG	2.19	0.42
1:B:547:ASP:N	1:B:547:ASP:OD1	2.49	0.42
2:D:27:ALA:HB1	2:D:64:LYS:H	1.85	0.42
1:E:131:THR:HG22	1:E:169:LYS:HB2	2.01	0.42
1:E:477:ASN:O	1:E:481:ILE:HG22	2.18	0.42
1:E:955:ILE:HB	1:E:958:TRP:CE2	2.55	0.42
1:F:66:TYR:CB	1:F:87:ILE:HG12	2.50	0.42
1:F:255:ASN:O	1:F:258:LEU:HG	2.19	0.42
1:F:289:VAL:HG23	1:F:290:MET:CE	2.50	0.42
1:F:724:LYS:HD3	1:F:760:ARG:NH2	2.35	0.42
2:H:227:ASP:O	2:H:228:THR:OG1	2.25	0.42
1:A:585:LEU:HA	1:A:588:LEU:HB2	2.02	0.42
1:A:694:GLU:CD	1:A:694:GLU:H	2.23	0.42
1:A:750:ASP:O	1:A:753:LYS:HB2	2.20	0.42
1:A:949:PHE:CE2	1:A:951:TYR:HA	2.54	0.42
1:B:69:GLU:N	1:B:69:GLU:OE1	2.52	0.42
1:B:247:ARG:HD3	1:B:249:ASP:HB2	2.02	0.42
1:E:454:LEU:O	1:E:458:ILE:HG23	2.19	0.42
1:E:606:HIS:CE1	2:H:205:GLU:O	2.73	0.42
1:E:613:ARG:O	1:E:616:MET:HG3	2.20	0.42
1:E:660:LYS:HD2	1:E:661:ILE:HG22	2.00	0.42
1:E:869:ILE:HG22	1:E:874:ILE:HB	2.02	0.42
1:E:916:PHE:HA	1:E:919:TRP:CE3	2.55	0.42
1:F:984:LEU:HD22	1:F:1000:LEU:HB2	2.02	0.42
2:G:170:ARG:HB3	2:G:172:GLU:OE2	2.19	0.42
2:H:15:ARG:HB2	2:H:171:TYR:CE1	2.55	0.42
1:A:208:ILE:HD13	1:A:213:ILE:HG13	2.01	0.42
1:A:345:THR:HG22	1:A:395:CYS:O	2.20	0.42
1:A:757:TRP:HA	1:A:760:ARG:HB2	2.00	0.42
1:A:937:ASP:HB3	1:A:940:TYR:HB2	2.01	0.42
1:B:231:TRP:NE1	1:B:235:LEU:HD11	2.34	0.42
1:B:664:ILE:HG13	1:B:668:GLU:OE1	2.20	0.42
1:B:830:ASP:OD1	1:B:830:ASP:N	2.52	0.42
1:B:870:ARG:HA	2:C:51:TYR:CZ	2.55	0.42
2:D:189:SER:HA	2:D:238:SER:HB3	2.01	0.42
1:E:304:LYS:HD2	1:E:306:ASP:N	2.35	0.42
1:E:375:LYS:HD3	1:E:375:LYS:C	2.40	0.42
1:E:574:TYR:HD2	2:G:32:PHE:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:618:LEU:O	1:E:621:GLU:HB2	2.20	0.42
1:F:44:PHE:HD1	1:F:214:VAL:HB	1.84	0.42
1:F:305:ASP:O	1:F:309:ILE:HG12	2.19	0.42
1:A:676:ILE:CG2	1:A:677:ARG:N	2.78	0.42
1:A:747:ARG:HD3	1:A:747:ARG:HA	1.66	0.42
1:B:708:PHE:HA	1:B:711:GLN:HG2	2.02	0.42
2:C:70:LEU:HD22	2:C:74:ALA:N	2.35	0.42
1:E:130:ILE:HD12	1:E:168:LEU:HB3	2.02	0.42
1:E:279:GLU:OE1	1:E:279:GLU:N	2.45	0.42
1:E:606:HIS:CD2	2:H:206:MET:O	2.73	0.42
1:F:186:LYS:HZ2	1:F:188:ASP:H	1.66	0.42
1:F:245:PHE:N	1:F:267:ARG:O	2.51	0.42
1:F:409:ILE:HG13	1:F:650:TYR:CE2	2.55	0.42
1:F:657:ARG:NH1	1:F:715:GLU:OE1	2.53	0.42
1:F:782:GLN:OE1	1:F:785:LYS:HD2	2.20	0.42
1:A:91:PHE:CE2	1:A:103:ILE:HD12	2.54	0.42
1:A:481:ILE:O	1:A:485:ILE:HG13	2.20	0.42
1:A:606:HIS:HA	2:D:206:MET:O	2.19	0.42
1:A:772:ILE:HD12	1:A:775:ILE:HD13	2.02	0.42
1:B:391:ASN:ND2	1:B:393:VAL:HG23	2.34	0.42
1:B:418:TYR:O	1:B:422:LYS:HG3	2.20	0.42
1:B:473:LEU:HD21	1:B:542:LEU:HD21	2.00	0.42
1:B:560:GLU:OE1	1:B:564:LYS:HD2	2.20	0.42
1:B:655:ILE:O	1:B:659:PHE:HB2	2.19	0.42
1:B:892:ARG:HH21	1:B:908:SER:HB2	1.83	0.42
2:C:36:ILE:HA	2:C:56:GLU:O	2.20	0.42
1:E:432:ILE:H	1:E:432:ILE:HG12	1.64	0.42
1:E:660:LYS:N	1:E:663:ASP:OD2	2.45	0.42
1:E:801:SER:CB	1:E:841:LEU:HD11	2.50	0.42
1:F:71:TYR:O	1:F:73:SER:N	2.53	0.42
1:F:118:HIS:HE1	1:F:137:LEU:C	2.23	0.42
1:F:185:LEU:HD12	1:F:185:LEU:HA	1.88	0.42
1:F:871:ILE:HG13	1:F:872:GLY:N	2.35	0.42
2:H:23:PHE:CE1	2:H:66:ALA:HB2	2.37	0.42
2:H:192:TYR:CD2	2:H:235:ILE:HB	2.55	0.42
1:A:117:ILE:O	1:A:121:ILE:HG12	2.19	0.41
1:A:258:LEU:O	1:A:262:GLU:HG3	2.20	0.41
1:A:607:GLU:OE1	1:A:607:GLU:HA	2.19	0.41
1:A:699:PHE:CB	1:A:704:MET:HG3	2.48	0.41
1:A:709:TYR:O	1:A:712:PHE:HB2	2.20	0.41
1:A:861:ASN:O	1:A:865:LEU:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:LEU:O	1:A:1000:LEU:HG	2.19	0.41
1:B:147:LYS:N	1:B:147:LYS:HD3	2.33	0.41
1:B:471:TYR:O	1:B:474:SER:OG	2.31	0.41
1:E:115:ASN:OD1	1:E:118:HIS:ND1	2.53	0.41
1:E:627:ARG:NH1	1:E:675:LYS:HB3	2.35	0.41
1:E:629:ARG:O	1:E:630:ASP:C	2.52	0.41
1:E:704:MET:HA	1:E:704:MET:CE	2.49	0.41
1:E:755:TYR:CE1	1:E:807:LEU:HD23	2.54	0.41
1:E:834:GLN:HA	1:E:837:PHE:HB3	2.01	0.41
1:E:919:TRP:O	1:E:924:GLU:HB2	2.20	0.41
1:F:68:GLU:OE1	1:F:74:PRO:HD3	2.20	0.41
1:F:385:PHE:CE1	1:F:389:GLU:HG3	2.55	0.41
1:F:647:MET:SD	1:F:678:PHE:HD1	2.43	0.41
1:F:795:SER:OG	1:F:799:LEU:HG	2.20	0.41
2:H:170:ARG:O	2:H:171:TYR:HB2	2.19	0.41
1:A:195:GLN:HG2	1:A:196:ASN:N	2.34	0.41
1:A:198:PRO:HG3	1:B:235:LEU:HD22	2.02	0.41
1:A:367:CYS:HA	1:A:370:ARG:NE	2.35	0.41
1:A:746:GLU:O	1:A:747:ARG:C	2.52	0.41
1:B:332:HIS:HB2	1:B:541:ILE:HG13	2.02	0.41
1:B:407:ILE:HD12	1:B:589:TYR:CB	2.50	0.41
1:B:509:ASP:N	1:B:509:ASP:OD1	2.53	0.41
2:D:178:ILE:HG12	2:D:190:ASP:OD1	2.20	0.41
1:E:92:TYR:HA	1:E:96:GLY:O	2.19	0.41
1:E:472:TYR:CD2	1:E:542:LEU:HG	2.55	0.41
1:E:491:GLN:O	1:E:495:LEU:HD23	2.20	0.41
1:E:801:SER:HB3	1:E:841:LEU:HD11	2.01	0.41
1:E:946:PRO:HG2	1:E:975:HIS:CE1	2.55	0.41
1:F:43:VAL:HG12	1:F:212:THR:O	2.19	0.41
1:F:256:GLU:HA	1:F:259:ILE:HG12	2.02	0.41
1:F:569:MET:SD	1:F:625:TYR:HD2	2.44	0.41
2:H:66:ALA:HB3	2:H:218:ILE:HD11	2.03	0.41
1:A:338:TYR:HE1	1:A:351:ASN:HB2	1.84	0.41
1:A:411:SER:HB2	1:A:415:HIS:CE1	2.54	0.41
1:A:582:ILE:O	1:A:585:LEU:N	2.52	0.41
1:B:657:ARG:HA	1:B:715:GLU:HG3	2.01	0.41
1:B:857:LYS:HA	1:B:857:LYS:HD3	1.83	0.41
1:B:960:LYS:HD3	1:B:996:TYR:CE1	2.55	0.41
1:E:674:ASP:HA	1:E:725:TYR:CZ	2.54	0.41
1:E:816:ILE:HG22	1:E:818:LYS:HG2	2.02	0.41
1:E:887:GLU:O	1:E:890:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:889:LEU:HB3	1:E:933:PHE:CE2	2.55	0.41
1:F:615:SER:O	1:F:619:LEU:HG	2.21	0.41
1:F:653:VAL:HG22	1:F:687:TYR:CE1	2.56	0.41
1:F:677:ARG:HG2	1:F:678:PHE:H	1.85	0.41
1:F:821:SER:O	1:F:825:LEU:HG	2.19	0.41
1:A:208:ILE:HA	1:A:213:ILE:HD11	2.02	0.41
1:A:332:HIS:O	1:A:333:VAL:C	2.57	0.41
1:A:675:LYS:O	1:A:678:PHE:HB3	2.20	0.41
1:A:740:LEU:O	1:A:741:LEU:C	2.56	0.41
1:A:890:GLU:O	1:A:893:LYS:HG2	2.20	0.41
1:B:48:ALA:HA	1:B:133:ASN:HB3	2.02	0.41
1:B:283:LEU:HD12	1:B:284:GLU:HG3	2.01	0.41
1:B:286:TYR:O	1:B:289:VAL:HG12	2.20	0.41
1:B:420:VAL:HB	1:B:424:PHE:CZ	2.55	0.41
1:E:124:MET:H	1:E:124:MET:CE	2.33	0.41
1:E:705:ASN:O	1:E:705:ASN:OD1	2.38	0.41
1:E:708:PHE:CD1	1:E:711:GLN:HB3	2.55	0.41
1:E:1002:ASN:N	1:E:1005:ILE:OXT	2.50	0.41
1:F:41:LYS:NZ	1:F:210:THR:O	2.53	0.41
1:F:383:ALA:O	1:F:386:ASN:HB2	2.20	0.41
1:F:435:ASP:O	1:F:438:LYS:HB2	2.20	0.41
1:F:660:LYS:HE2	2:G:203:GLU:OE2	2.20	0.41
1:F:804:TYR:O	1:F:808:ILE:HD12	2.21	0.41
1:F:845:LEU:HD13	1:F:849:ALA:HB1	2.03	0.41
2:G:14:LYS:NZ	2:G:174:GLU:HB2	2.35	0.41
1:A:71:TYR:HH	1:E:257:THR:HG1	1.65	0.41
1:A:652:PHE:CD1	1:A:684:ILE:HG23	2.55	0.41
1:B:33:ILE:HG12	1:B:33:ILE:H	1.72	0.41
1:B:222:ASP:CG	1:B:225:ILE:HG23	2.40	0.41
1:B:813:LYS:HE2	1:B:813:LYS:HB2	1.93	0.41
2:C:70:LEU:O	2:C:71:GLU:C	2.58	0.41
1:E:661:ILE:HG13	1:E:665:LYS:HZ3	1.85	0.41
1:E:741:LEU:HD12	1:E:778:PHE:CG	2.56	0.41
1:E:769:LYS:HA	1:E:772:ILE:HD13	2.02	0.41
1:E:777:ASP:OD1	1:E:819:ARG:NH2	2.53	0.41
1:F:362:GLU:O	1:F:365:GLU:HG2	2.20	0.41
2:G:15:ARG:N	2:G:20:LYS:HE3	2.35	0.41
2:H:14:LYS:HZ1	2:H:21:LEU:HD13	1.85	0.41
1:A:85:LEU:HB2	1:A:187:GLU:OE2	2.20	0.41
1:A:235:LEU:O	1:A:237:LYS:HG2	2.20	0.41
1:A:326:ARG:HA	1:A:593:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASN:OD1	2:C:5:ILE:HG23	2.21	0.41
1:A:607:GLU:HB3	1:A:610:GLN:HB2	2.02	0.41
1:A:713:ILE:HG23	1:A:717:LYS:H	1.86	0.41
1:A:885:ILE:HG12	1:A:916:PHE:CE1	2.55	0.41
1:B:31:LYS:HD2	1:B:31:LYS:C	2.41	0.41
1:B:337:ASP:OD1	1:B:338:TYR:N	2.54	0.41
1:B:437:LYS:O	1:B:441:PHE:CD1	2.74	0.41
1:B:801:SER:HA	1:B:804:TYR:CD2	2.55	0.41
1:F:449:GLU:CB	1:F:511:PHE:HE2	2.34	0.41
1:F:799:LEU:HA	1:F:799:LEU:HD23	1.58	0.41
1:F:869:ILE:HD12	1:F:874:ILE:O	2.17	0.41
1:A:86:ARG:NH1	1:A:89:GLN:HB3	2.33	0.41
1:A:198:PRO:HG2	1:B:235:LEU:HD13	2.02	0.41
1:A:277:SER:HB3	1:A:285:ARG:HH21	1.86	0.41
1:A:284:GLU:OE1	1:A:285:ARG:NH2	2.53	0.41
1:A:750:ASP:CG	1:A:796:SER:CB	2.89	0.41
1:B:205:LYS:HZ2	1:B:232:VAL:HG22	1.86	0.41
1:B:479:TYR:CE2	1:B:524:ILE:HG21	2.56	0.41
1:B:961:ASN:OD1	1:B:961:ASN:N	2.52	0.41
1:E:23:ASP:O	1:E:27:VAL:HG23	2.20	0.41
1:E:552:TYR:CE1	1:F:556:VAL:HG11	2.56	0.41
1:E:952:LYS:HB2	1:E:952:LYS:HE3	1.77	0.41
1:F:131:THR:O	1:F:169:LYS:HA	2.20	0.41
1:F:173:ASP:N	1:F:173:ASP:OD1	2.53	0.41
1:F:376:LYS:HA	1:F:376:LYS:HD2	1.93	0.41
1:F:802:ARG:HB2	1:F:840:LYS:CA	2.50	0.41
2:G:214:LEU:HA	2:G:214:LEU:HD13	1.59	0.41
1:A:323:GLN:HB2	1:A:597:GLU:OE1	2.21	0.41
1:B:95:LYS:HA	1:B:95:LYS:HD2	1.65	0.41
1:B:148:TYR:HE2	1:B:163:SER:HB2	1.85	0.41
1:B:729:SER:O	1:B:731:GLU:N	2.54	0.41
2:C:70:LEU:HD23	2:C:73:LEU:HB3	2.03	0.41
1:E:116:PRO:HA	1:E:119:ASP:OD2	2.20	0.41
1:E:163:SER:HA	1:F:533:PHE:CZ	2.55	0.41
1:E:661:ILE:HA	1:E:664:ILE:HD12	2.03	0.41
1:E:692:ALA:O	1:E:695:ILE:HG12	2.21	0.41
1:E:954:PHE:HB2	1:E:958:TRP:HZ3	1.86	0.41
1:F:80:SER:O	1:F:83:GLU:N	2.54	0.41
1:F:455:TYR:OH	1:F:477:ASN:OD1	2.23	0.41
1:F:723:ALA:O	1:F:726:VAL:HG22	2.21	0.41
1:A:127:ALA:O	1:A:128:HIS:ND1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:O	1:A:319:LEU:HB2	2.20	0.41
1:A:331:LYS:O	1:A:332:HIS:C	2.59	0.41
1:A:549:GLN:O	1:A:552:TYR:HB2	2.20	0.41
1:A:583:VAL:HA	1:A:586:LEU:CD1	2.51	0.41
1:A:655:ILE:HG21	1:A:722:PHE:CE1	2.56	0.41
1:A:674:ASP:OD1	1:A:724:LYS:NZ	2.49	0.41
1:B:245:PHE:N	1:B:267:ARG:O	2.54	0.41
1:B:536:GLN:HG2	1:B:537:LYS:N	2.36	0.41
2:C:170:ARG:NE	2:C:197:ASN:OD1	2.54	0.41
1:E:235:LEU:CG	1:E:236:GLN:H	2.34	0.41
1:E:304:LYS:NZ	1:E:307:GLU:HB2	2.31	0.41
1:E:324:TYR:HA	1:E:390:LYS:NZ	2.35	0.41
1:E:383:ALA:HA	1:E:386:ASN:HD21	1.86	0.41
1:E:540:LYS:HE2	1:E:540:LYS:HB2	1.92	0.41
1:E:606:HIS:HB3	1:E:610:GLN:HE21	1.85	0.41
1:E:963:ASN:O	1:E:967:LEU:N	2.46	0.41
1:F:37:SER:HB3	1:F:42:LEU:HD22	2.03	0.41
1:F:197:TYR:HD1	1:F:197:TYR:HA	1.81	0.41
1:F:478:ARG:HA	1:F:481:ILE:HG22	2.03	0.41
1:F:578:MET:HG2	1:F:582:ILE:HD11	2.03	0.41
1:F:614:ASN:O	1:F:618:LEU:HD12	2.21	0.41
1:F:696:THR:O	1:F:700:SER:OG	2.30	0.41
1:F:706:VAL:O	1:F:709:TYR:N	2.54	0.41
1:F:956:PRO:HB3	1:F:987:ARG:HG3	2.03	0.41
1:F:965:LYS:O	1:F:966:LEU:C	2.57	0.41
2:G:15:ARG:HG2	2:G:20:LYS:HB2	2.03	0.41
2:H:32:PHE:CE1	2:H:59:ILE:HG23	2.49	0.41
2:H:75:MET:O	2:H:76:THR:OG1	2.38	0.41
1:A:487:GLN:CD	2:D:207:SER:H	2.24	0.41
1:A:735:LYS:HD3	1:A:735:LYS:HA	1.80	0.41
1:B:192:ASN:HB3	1:B:196:ASN:OD1	2.20	0.41
1:B:414:TYR:OH	1:B:654:ASN:ND2	2.54	0.41
1:B:960:LYS:O	1:B:961:ASN:C	2.58	0.41
2:D:64:LYS:HB2	2:D:217:GLU:HA	2.02	0.41
1:E:105:LYS:HD3	1:E:178:PHE:HB2	2.03	0.41
1:E:754:ARG:HB2	1:E:804:TYR:OH	2.21	0.41
1:E:954:PHE:HB2	1:E:958:TRP:CZ3	2.55	0.41
1:F:95:LYS:HD3	1:F:95:LYS:HA	1.94	0.41
2:G:56:GLU:OE2	2:G:58:GLU:N	2.52	0.41
2:G:56:GLU:OE2	2:G:57:LYS:N	2.54	0.41
1:A:85:LEU:HD13	1:A:190:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASP:HA	1:A:191:LEU:HB3	2.03	0.40
1:A:596:TYR:N	1:A:596:TYR:CD1	2.89	0.40
1:A:802:ARG:CB	1:A:840:LYS:CB	2.99	0.40
1:B:79:TYR:HB2	1:B:84:TYR:CZ	2.56	0.40
1:B:280:TYR:HA	1:B:282:TYR:CZ	2.56	0.40
1:B:412:LEU:HA	1:B:415:HIS:HD2	1.85	0.40
1:B:491:GLN:NE2	2:C:206:MET:H	2.19	0.40
1:B:598:ASN:OD1	1:B:600:LEU:N	2.54	0.40
2:C:29:THR:OG1	2:C:64:LYS:HE3	2.21	0.40
1:E:448:TRP:HZ3	1:E:707:VAL:HG21	1.86	0.40
1:E:544:PHE:O	1:E:550:PHE:HB3	2.20	0.40
1:E:632:ASP:CG	1:F:955:ILE:HD11	2.41	0.40
1:F:359:ARG:HA	1:F:362:GLU:HB2	2.02	0.40
1:F:407:ILE:O	1:F:650:TYR:HE2	2.05	0.40
1:F:448:TRP:HB3	1:F:481:ILE:HD11	2.03	0.40
1:F:750:ASP:OD1	1:F:753:LYS:HB3	2.21	0.40
1:F:755:TYR:HE1	1:F:807:LEU:HD23	1.86	0.40
1:F:776:ASP:HB3	1:F:820:LEU:HD22	2.04	0.40
2:G:240:ASP:N	2:G:240:ASP:OD1	2.51	0.40
2:H:11:VAL:HG13	2:H:175:TYR:CE1	2.49	0.40
2:H:175:TYR:HD1	2:H:175:TYR:HA	1.75	0.40
2:H:177:THR:OG1	2:H:191:ILE:HB	2.22	0.40
1:A:487:GLN:HG3	2:D:207:SER:H	1.86	0.40
1:A:605:PHE:HD1	1:A:605:PHE:HA	1.78	0.40
1:A:717:LYS:HZ3	1:A:749:LEU:HD23	1.86	0.40
1:A:780:VAL:HG13	1:A:820:LEU:HB3	2.02	0.40
1:B:98:MET:HA	1:B:101:ASP:OD2	2.21	0.40
1:B:442:LEU:HB3	1:B:447:ARG:NH1	2.34	0.40
1:B:685:GLU:O	1:B:689:VAL:HG13	2.20	0.40
2:C:61:LEU:HD23	2:C:175:TYR:CZ	2.56	0.40
2:D:23:PHE:CZ	2:D:220:PHE:HZ	2.39	0.40
1:E:235:LEU:HD23	1:F:198:PRO:HG2	2.02	0.40
1:E:242:LYS:HZ3	1:E:243:PRO:HD2	1.84	0.40
1:E:375:LYS:HD3	1:E:376:LYS:N	2.36	0.40
1:E:415:HIS:HA	1:E:649:TYR:OH	2.20	0.40
1:E:475:GLN:HB2	1:E:527:LEU:HD21	2.03	0.40
1:F:452:TYR:OH	1:F:514:ARG:NE	2.55	0.40
1:F:459:ILE:HA	1:F:459:ILE:HD12	1.77	0.40
1:F:869:ILE:HG12	1:F:919:TRP:CZ2	2.49	0.40
1:F:873:LEU:O	1:F:874:ILE:C	2.60	0.40
1:F:888:TYR:CZ	1:F:912:TYR:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:900:LYS:HE2	1:F:900:LYS:HB2	1.90	0.40
2:G:68:PHE:O	2:G:68:PHE:CG	2.75	0.40
2:G:201:SER:O	2:G:219:LYS:HB2	2.21	0.40
2:H:177:THR:OG1	2:H:191:ILE:O	2.32	0.40
1:A:118:HIS:HE1	1:A:138:ILE:N	2.19	0.40
1:A:733:LEU:HD23	1:A:761:LEU:HD23	2.03	0.40
1:A:804:TYR:O	1:A:808:ILE:HG12	2.21	0.40
1:B:483:GLN:NE2	2:C:209:GLU:O	2.54	0.40
1:B:622:LYS:HG3	1:B:623:ALA:N	2.36	0.40
1:B:681:GLN:HE21	1:B:684:ILE:N	2.20	0.40
2:C:4:VAL:O	2:C:4:VAL:HG12	2.21	0.40
1:E:225:ILE:O	1:E:229:LEU:HD13	2.22	0.40
1:E:332:HIS:ND1	1:E:336:TYR:HE1	2.18	0.40
1:E:452:TYR:CE1	1:E:478:ARG:HG3	2.56	0.40
1:F:364:LYS:HD2	1:F:364:LYS:HA	1.61	0.40
1:F:589:TYR:OH	1:F:651:ASP:OD1	2.38	0.40
1:F:767:LEU:HD13	1:F:811:PHE:CD1	2.57	0.40
1:F:862:ILE:H	1:F:862:ILE:CD1	2.28	0.40
2:H:218:ILE:HG13	2:H:220:PHE:CE1	2.56	0.40
1:A:223:TYR:HB2	1:A:226:ASN:HB3	2.03	0.40
1:A:257:THR:HG23	1:E:86:ARG:HH22	1.86	0.40
1:A:783:ALA:HB2	1:A:841:LEU:HD12	2.02	0.40
1:B:616:MET:HA	1:B:616:MET:HE3	2.02	0.40
1:B:675:LYS:NZ	1:B:678:PHE:HZ	2.19	0.40
1:B:754:ARG:O	1:B:758:LEU:HG	2.21	0.40
1:E:186:LYS:HD2	1:E:188:ASP:N	2.35	0.40
1:E:338:TYR:CD2	1:E:348:ARG:HA	2.56	0.40
1:E:538:LYS:HB3	1:E:538:LYS:HE2	1.80	0.40
1:E:660:LYS:O	1:E:663:ASP:N	2.53	0.40
1:E:802:ARG:H	1:E:840:LYS:HE2	1.87	0.40
1:E:890:GLU:O	1:E:894:VAL:HG13	2.21	0.40
1:F:70:LEU:HA	1:F:70:LEU:HD23	1.71	0.40
1:F:880:GLU:CD	1:F:880:GLU:H	2.24	0.40
2:G:14:LYS:HB3	2:G:20:LYS:O	2.21	0.40
2:H:23:PHE:CG	2:H:24:THR:N	2.89	0.40
1:A:109:GLN:O	1:A:109:GLN:HG2	2.21	0.40
1:A:491:GLN:O	1:A:495:LEU:N	2.55	0.40
1:A:595:LEU:HD12	1:A:602:SER:HB2	2.03	0.40
1:A:969:LYS:HA	1:A:969:LYS:HD3	1.83	0.40
1:B:610:GLN:HG3	1:B:613:ARG:HH21	1.87	0.40
1:B:640:GLY:C	1:B:641:LYS:HG3	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:ILE:HA	1:B:665:LYS:HD2	2.03	0.40
1:E:392:GLY:O	1:E:394:ILE:HG12	2.22	0.40
1:E:634:LEU:O	1:E:637:SER:OG	2.33	0.40
1:E:649:TYR:O	1:E:653:VAL:HG12	2.21	0.40
1:E:811:PHE:HD1	1:E:811:PHE:HA	1.75	0.40
1:E:998:GLU:OE2	1:E:999:ILE:HG13	2.21	0.40
1:F:605:PHE:CD2	2:G:209:GLU:HB2	2.49	0.40
1:F:616:MET:HA	1:F:619:LEU:HD12	2.03	0.40
1:F:720:LEU:HB2	1:F:757:TRP:CZ3	2.56	0.40
1:F:793:GLU:OE2	1:F:799:LEU:HD13	2.21	0.40
1:F:906:THR:O	1:F:907:PHE:C	2.59	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 PDB entries followed by that with respect to all EM entries.

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	981/1005 (98%)	883 (90%)	95 (10%)	3 (0%)	37	72
1	B	981/1005 (98%)	908 (93%)	71 (7%)	2 (0%)	44	78
1	E	981/1005 (98%)	867 (88%)	108 (11%)	6 (1%)	22	59
1	F	981/1005 (98%)	848 (86%)	129 (13%)	4 (0%)	30	67
2	C	147/264 (56%)	122 (83%)	25 (17%)	0	100	100
2	D	147/264 (56%)	111 (76%)	35 (24%)	1 (1%)	19	56
2	G	147/264 (56%)	116 (79%)	30 (20%)	1 (1%)	19	56
2	H	147/264 (56%)	109 (74%)	38 (26%)	0	100	100
All	All	4512/5076 (89%)	3964 (88%)	531 (12%)	17 (0%)	32	67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	PRO
1	E	298	GLU
1	E	726	VAL
1	F	864	ASP
1	A	676	ILE
1	B	72	GLY
1	B	580	SER
1	E	978	HIS
1	E	1002	ASN
1	F	934	ILE
1	F	958	TRP
1	E	299	ASN
1	F	874	ILE
1	A	332	HIS
2	G	216	PRO
2	D	214	LEU
1	E	237	LYS

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 PDB entries followed by that with respect to all EM entries.

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	901/922 (98%)	852 (95%)	49 (5%)	18 40
1	B	901/922 (98%)	854 (95%)	47 (5%)	19 41
1	E	901/922 (98%)	839 (93%)	62 (7%)	13 33
1	F	901/922 (98%)	825 (92%)	76 (8%)	9 28
2	C	130/225 (58%)	121 (93%)	9 (7%)	13 33
2	D	130/225 (58%)	129 (99%)	1 (1%)	79 85
2	G	130/225 (58%)	114 (88%)	16 (12%)	4 16
2	H	130/225 (58%)	124 (95%)	6 (5%)	23 45
All	All	4124/4588 (90%)	3858 (94%)	266 (6%)	17 35

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	45	PHE
1	A	82	ASP
1	A	100	PHE
1	A	118	HIS
1	A	125	ASN
1	A	142	CYS
1	A	145	ARG
1	A	190	TYR
1	A	193	TYR
1	A	238	ASP
1	A	239	SER
1	A	240	PHE
1	A	261	TYR
1	A	357	MET
1	A	396	MET
1	A	410	ASN
1	A	492	PHE
1	A	519	MET
1	A	535	PHE
1	A	544	PHE
1	A	547	ASP
1	A	549	GLN
1	A	550	PHE
1	A	551	LEU
1	A	566	ARG
1	A	579	SER
1	A	580	SER
1	A	581	ASP
1	A	586	LEU
1	A	611	TYR
1	A	613	ARG
1	A	659	PHE
1	A	674	ASP
1	A	676	ILE
1	A	693	GLU
1	A	725	TYR
1	A	727	LYS
1	A	728	LEU
1	A	738	LYS
1	A	740	LEU
1	A	741	LEU
1	A	744	PHE

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Mol	Chain	Res	Type
1	A	749	LEU
1	A	750	ASP
1	A	766	GLU
1	A	802	ARG
1	A	818	LYS
1	A	965	LYS
1	B	31	LYS
1	B	45	PHE
1	B	67	HIS
1	B	71	TYR
1	B	92	TYR
1	B	164	SER
1	B	184	VAL
1	B	193	TYR
1	B	194	ASP
1	B	223	TYR
1	B	224	ASN
1	B	227	MET
1	B	231	TRP
1	B	245	PHE
1	B	319	LEU
1	B	323	GLN
1	B	356	TYR
1	B	381	PHE
1	B	396	MET
1	B	420	VAL
1	B	447	ARG
1	B	455	TYR
1	B	482	TYR
1	B	487	GLN
1	B	522	PHE
1	B	523	ASN
1	B	528	PHE
1	B	531	MET
1	B	605	PHE
1	B	625	TYR
1	B	647	MET
1	B	658	HIS
1	B	664	ILE
1	B	669	ARG
1	B	674	ASP
1	B	675	LYS

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Mol	Chain	Res	Type
1	B	676	ILE
1	B	686	GLU
1	B	730	GLU
1	B	904	ILE
1	B	906	THR
1	B	930	MET
1	B	960	LYS
1	B	961	ASN
1	B	962	TYR
1	B	965	LYS
1	B	985	LYS
2	C	1	MET
2	C	2	LYS
2	C	5	ILE
2	C	68	PHE
2	C	69	ASP
2	C	70	LEU
2	C	71	GLU
2	C	169	GLU
2	C	170	ARG
2	D	231	MET
1	E	60	TRP
1	E	67	HIS
1	E	91	PHE
1	E	92	TYR
1	E	187	GLU
1	E	190	TYR
1	E	211	HIS
1	E	240	PHE
1	E	260	TYR
1	E	303	THR
1	E	304	LYS
1	E	311	TYR
1	E	351	ASN
1	E	356	TYR
1	E	361	PHE
1	E	378	TYR
1	E	390	LYS
1	E	398	LYS
1	E	417	LYS
1	E	419	ASP
1	E	421	MET

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Mol	Chain	Res	Type
1	E	440	PHE
1	E	448	TRP
1	E	455	TYR
1	E	467	ASN
1	E	482	TYR
1	E	507	PHE
1	E	511	PHE
1	E	528	PHE
1	E	543	GLU
1	E	548	ASN
1	E	575	SER
1	E	578	MET
1	E	613	ARG
1	E	618	LEU
1	E	625	TYR
1	E	631	ILE
1	E	633	GLU
1	E	639	PHE
1	E	647	MET
1	E	649	TYR
1	E	704	MET
1	E	708	PHE
1	E	722	PHE
1	E	728	LEU
1	E	744	PHE
1	E	807	LEU
1	E	811	PHE
1	E	815	PHE
1	E	831	LYS
1	E	837	PHE
1	E	910	ASN
1	E	913	MET
1	E	919	TRP
1	E	936	MET
1	E	937	ASP
1	E	952	LYS
1	E	985	LYS
1	E	995	ARG
1	E	998	GLU
1	E	1003	TYR
1	E	1004	PHE
1	F	84	TYR

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Mol	Chain	Res	Type
1	F	119	ASP
1	F	145	ARG
1	F	166	TYR
1	F	193	TYR
1	F	218	TYR
1	F	222	ASP
1	F	231	TRP
1	F	240	PHE
1	F	242	LYS
1	F	260	TYR
1	F	357	MET
1	F	361	PHE
1	F	368	ASP
1	F	378	TYR
1	F	380	ARG
1	F	387	PHE
1	F	388	PHE
1	F	422	LYS
1	F	428	GLN
1	F	452	TYR
1	F	477	ASN
1	F	480	ARG
1	F	495	LEU
1	F	500	PHE
1	F	502	ARG
1	F	507	PHE
1	F	511	PHE
1	F	528	PHE
1	F	533	PHE
1	F	535	PHE
1	F	538	LYS
1	F	543	GLU
1	F	544	PHE
1	F	560	GLU
1	F	596	TYR
1	F	625	TYR
1	F	636	PHE
1	F	645	PHE
1	F	647	MET
1	F	652	PHE
1	F	683	LYS
1	F	704	MET

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Mol	Chain	Res	Type
1	F	711	GLN
1	F	721	TYR
1	F	724	LYS
1	F	725	TYR
1	F	726	VAL
1	F	727	LYS
1	F	781	LEU
1	F	791	TYR
1	F	827	LEU
1	F	829	GLN
1	F	834	GLN
1	F	836	ASP
1	F	856	PHE
1	F	862	ILE
1	F	863	ASN
1	F	864	ASP
1	F	874	ILE
1	F	900	LYS
1	F	904	ILE
1	F	905	GLN
1	F	906	THR
1	F	909	SER
1	F	913	MET
1	F	920	TYR
1	F	922	LEU
1	F	930	MET
1	F	931	GLU
1	F	932	GLU
1	F	940	TYR
1	F	949	PHE
1	F	964	ASP
1	F	965	LYS
1	F	969	LYS
2	G	1	MET
2	G	10	ASP
2	G	14	LYS
2	G	20	LYS
2	G	32	PHE
2	G	58	GLU
2	G	70	LEU
2	G	75	MET
2	G	168	SER

Continued on next page...

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Mol	Chain	Res	Type
2	G	170	ARG
2	G	195	PHE
2	G	206	MET
2	G	214	LEU
2	G	233	VAL
2	G	235	ILE
2	G	239	ARG
2	H	72	TRP
2	H	169	GLU
2	H	170	ARG
2	H	207	SER
2	H	220	PHE
2	H	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	493	ASN
1	A	548	ASN
1	A	609	HIS
1	A	610	GLN
1	A	711	GLN
1	A	765	ASN
1	B	118	HIS
1	B	236	GLN
1	B	263	ASN
1	B	391	ASN
1	B	491	GLN
1	B	521	ASN
1	B	654	ASN
1	B	939	GLN
1	B	963	ASN
1	B	992	ASN
2	C	6	GLN
1	E	89	GLN
1	E	297	GLN
1	E	349	HIS
1	E	428	GLN
1	E	487	GLN
1	E	491	GLN
1	E	610	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	E	681	GLN
1	E	1002	ASN
1	F	115	ASN
1	F	202	ASN
1	F	211	HIS
1	F	339	HIS
1	F	654	ASN
1	F	863	ASN
1	F	895	ASN
1	F	973	ASN
2	G	6	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

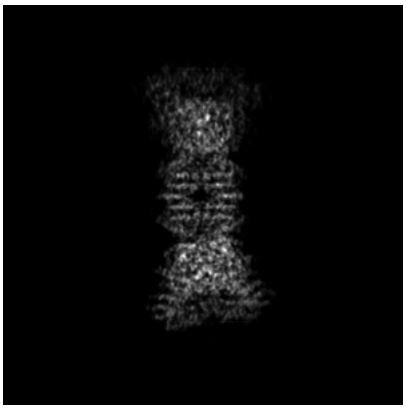
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39259. These allow visual inspection of the internal detail of the map and identification of artifacts.

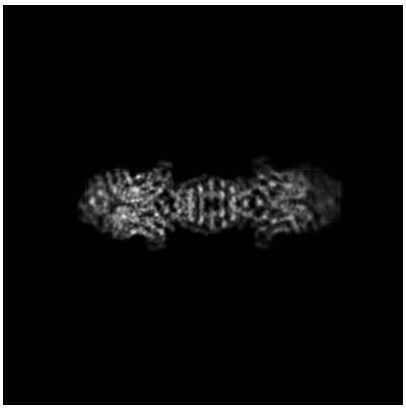
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

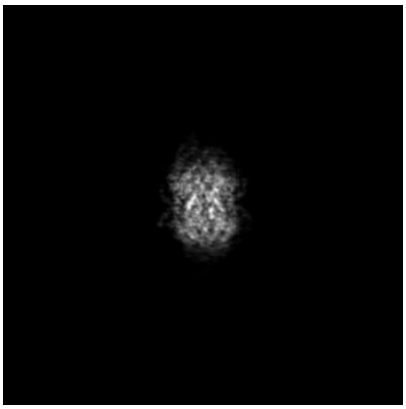
6.1.1 Primary map



X

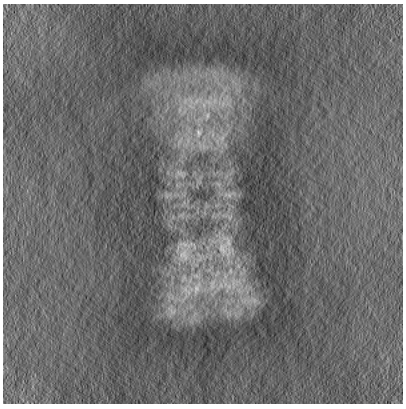


Y

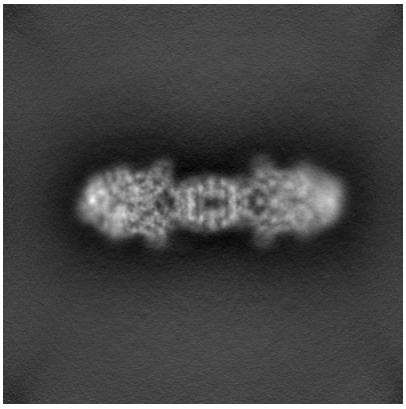


Z

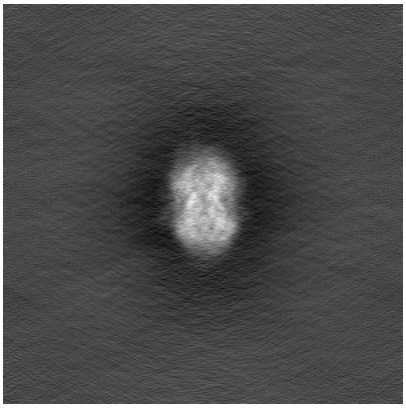
6.1.2 Raw map



X



Y



Z

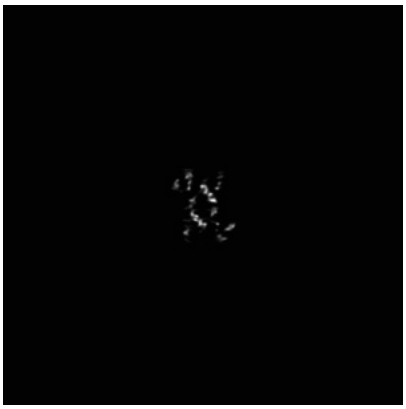
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

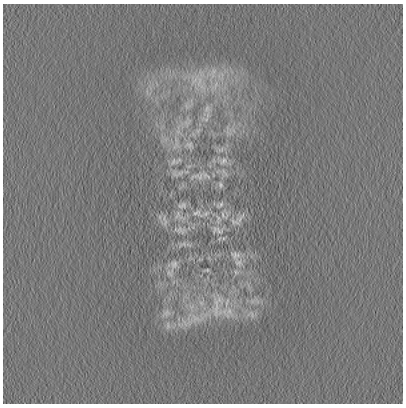
X Index: 230

Y Index: 230

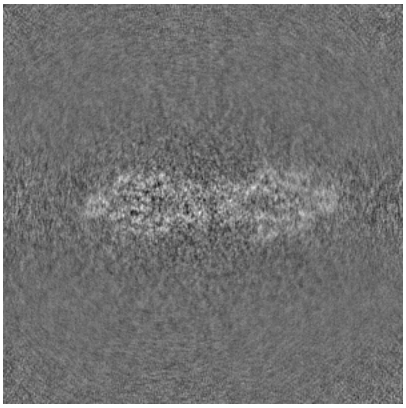


Z Index: 230

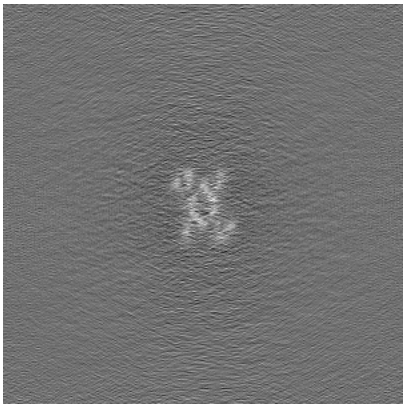
6.2.2 Raw map



X Index: 230



Y Index: 230



Z Index: 230

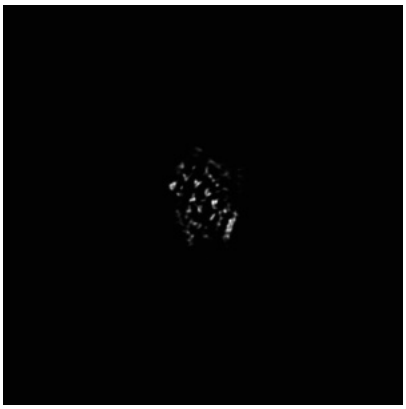
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

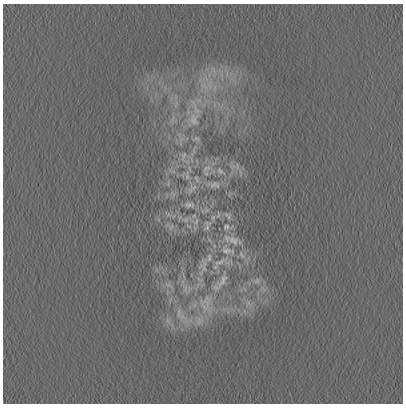
X Index: 245

Y Index: 225

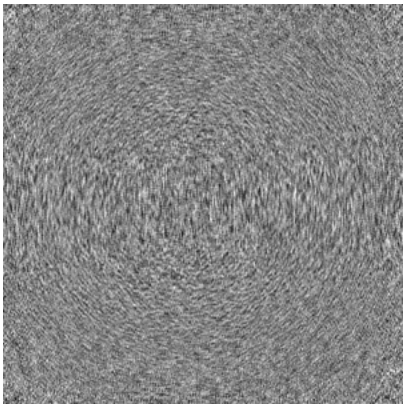


Z Index: 144

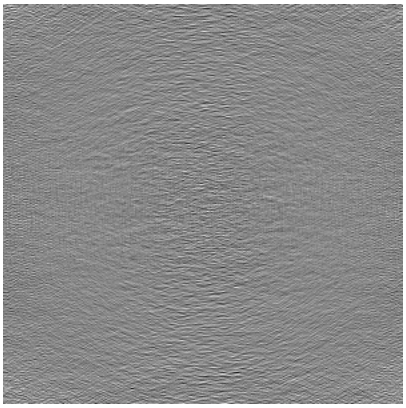
6.3.2 Raw map



X Index: 223



Y Index: 0

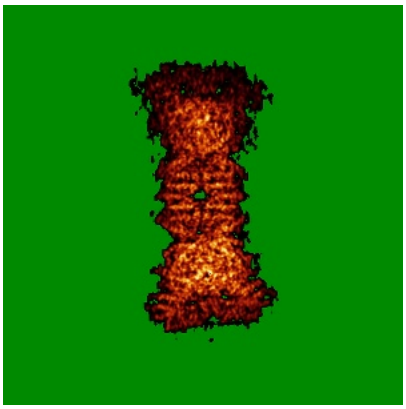


Z Index: 0

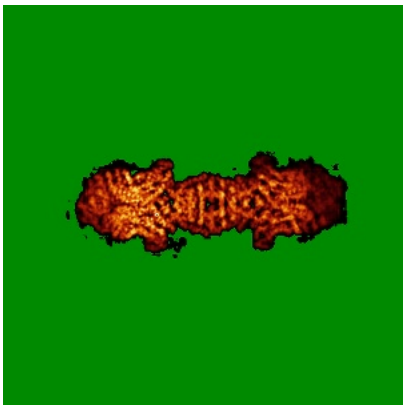
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

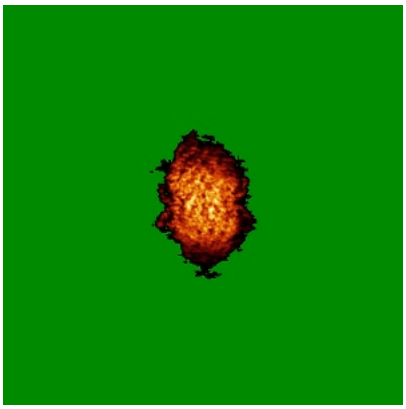
6.4.1 Primary map



X

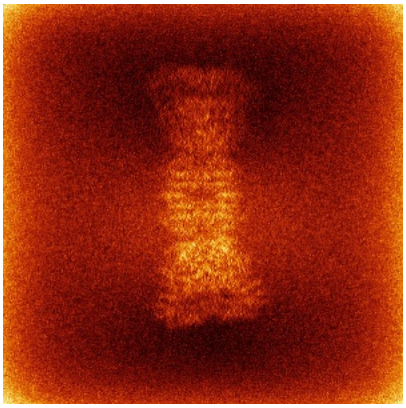


Y

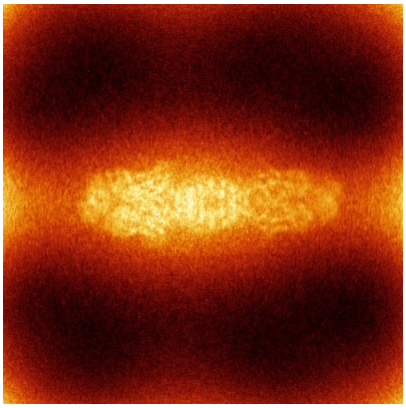


Z

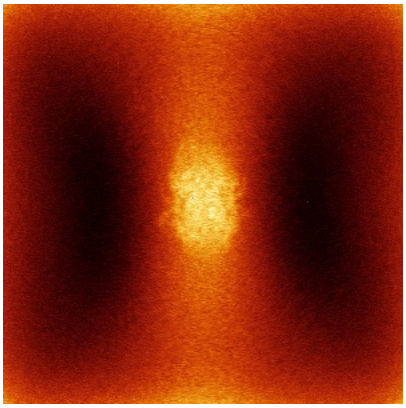
6.4.2 Raw map



X



Y



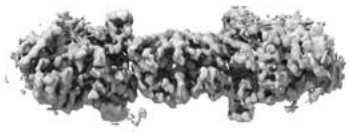
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

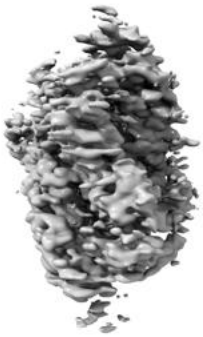
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



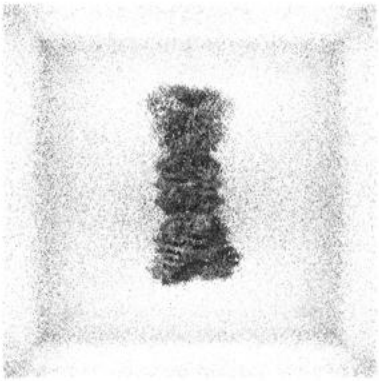
Y



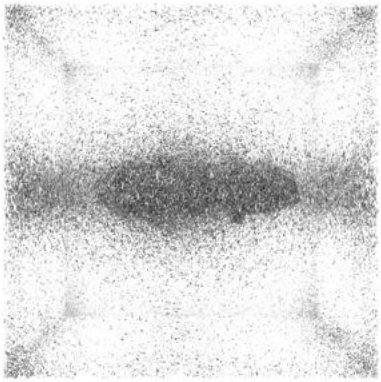
Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

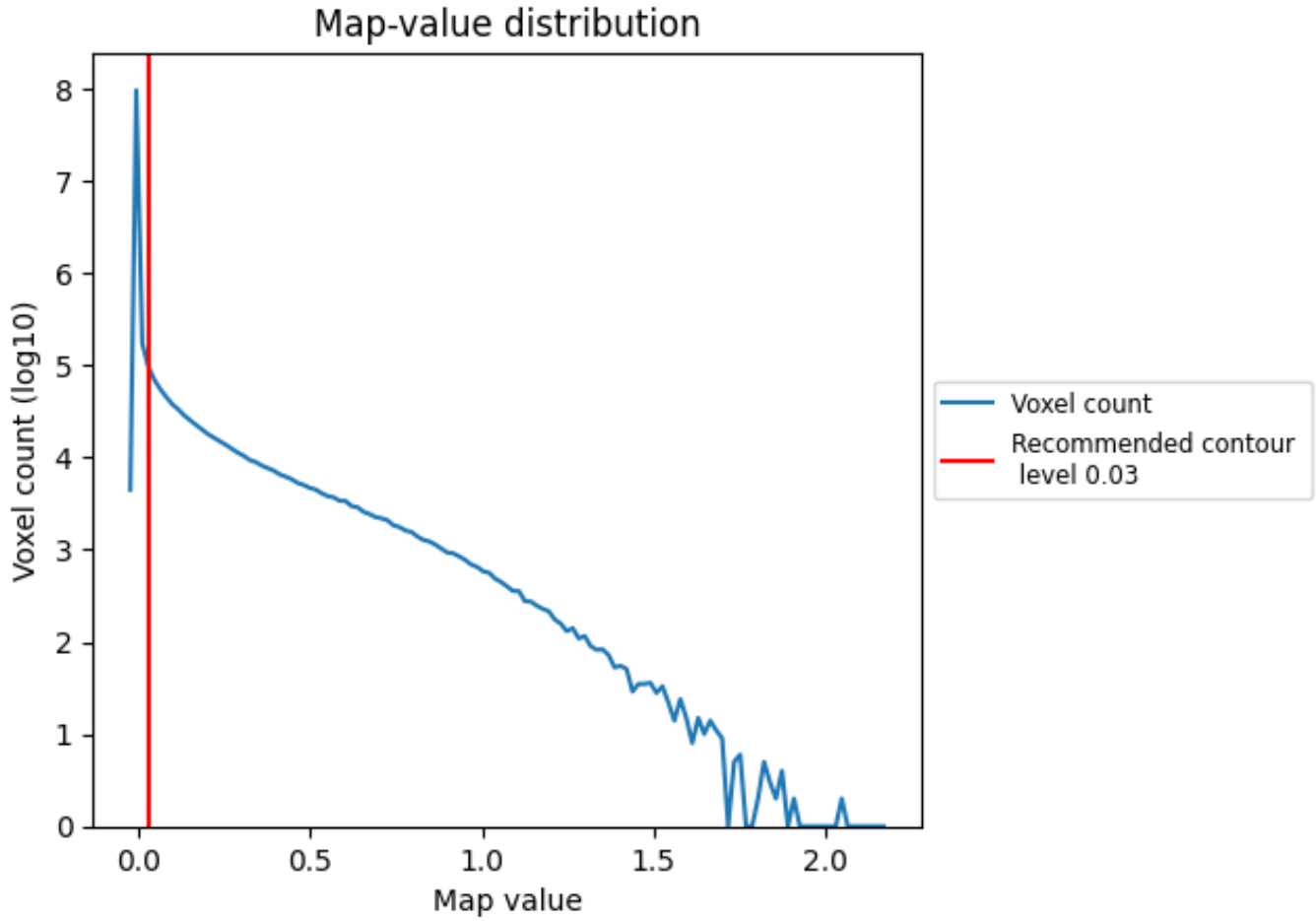
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

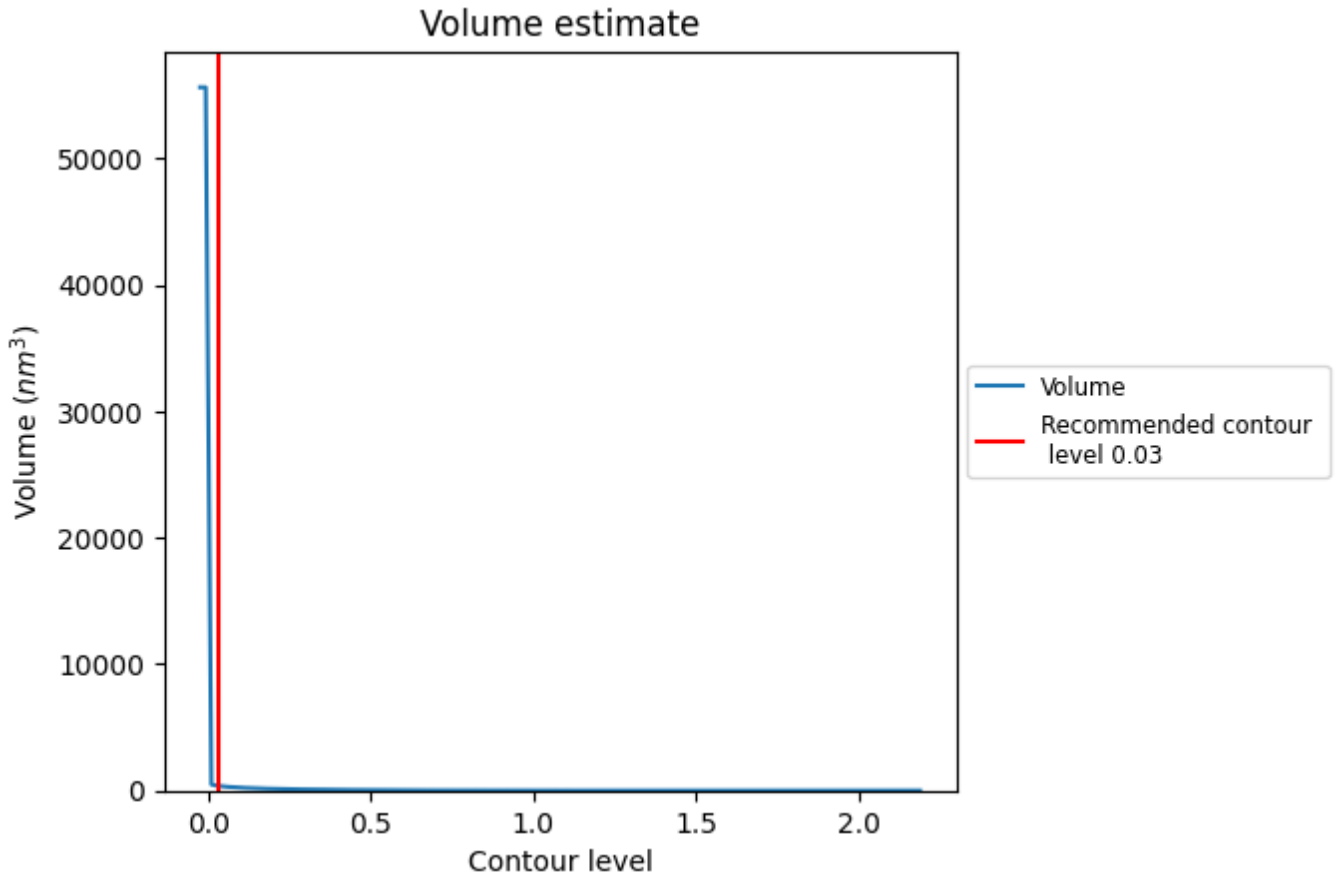
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

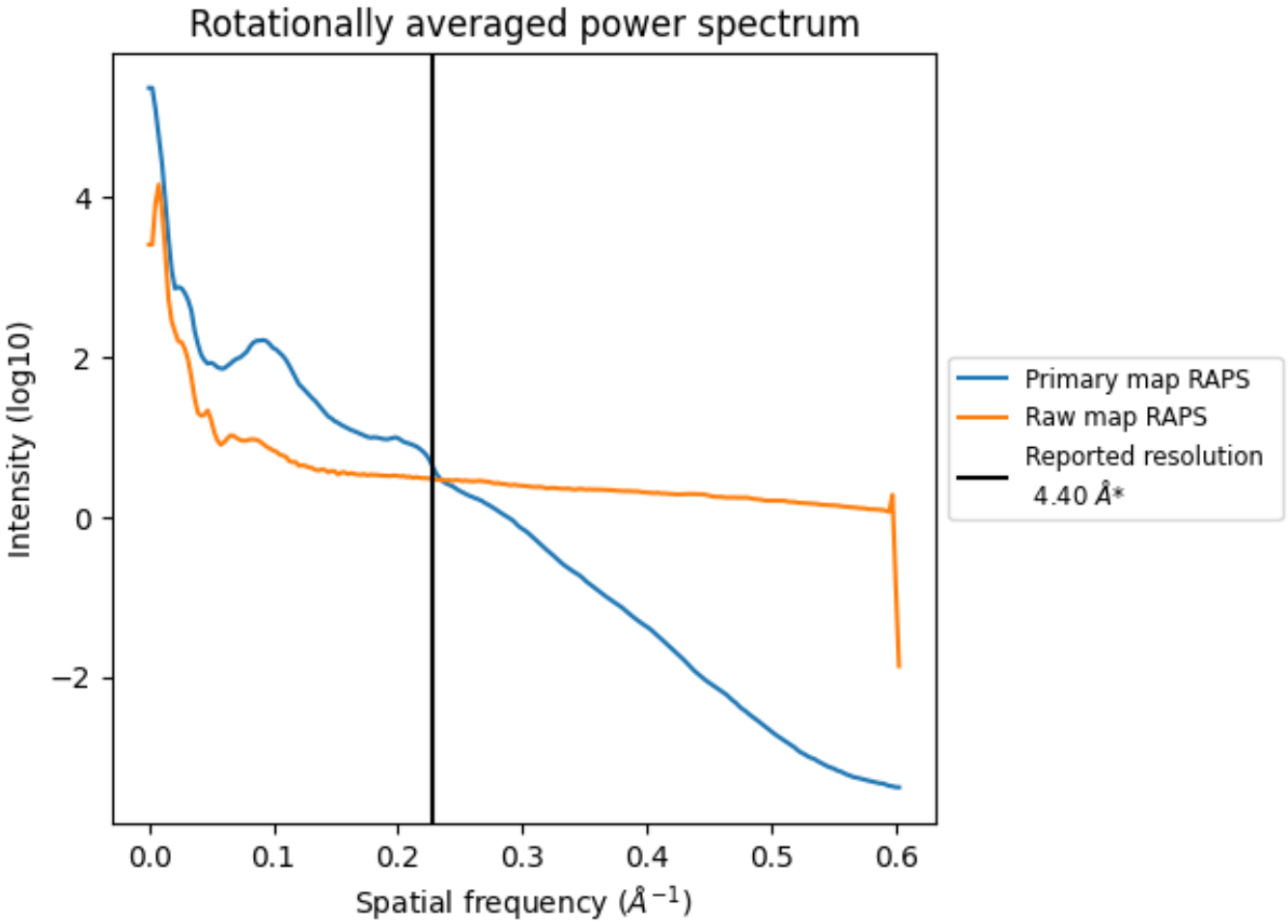
7.2 Volume estimate



The volume at the recommended contour level is 376 nm^3; this corresponds to an approximate mass of 340 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

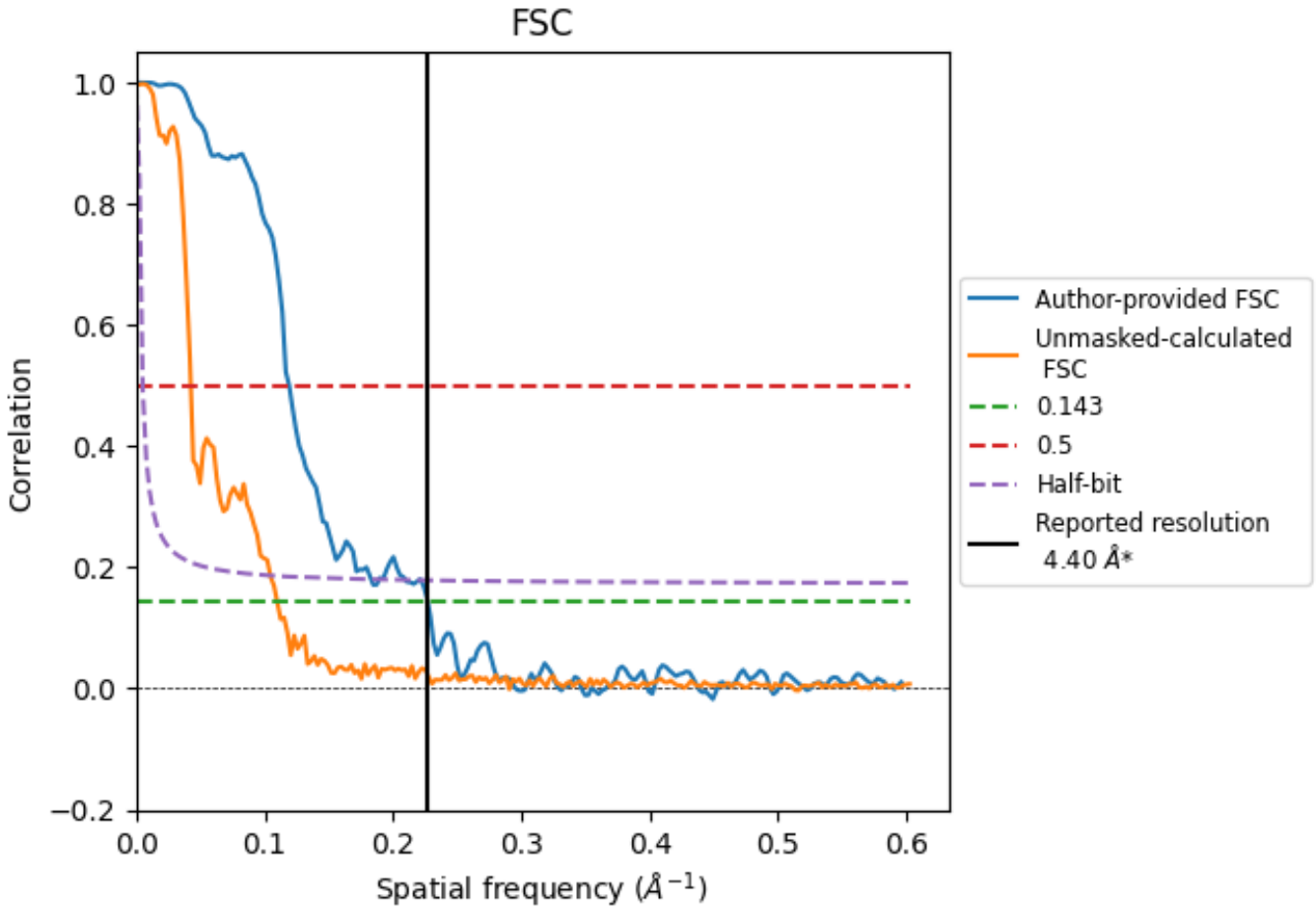


*Reported resolution corresponds to spatial frequency of 0.227 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

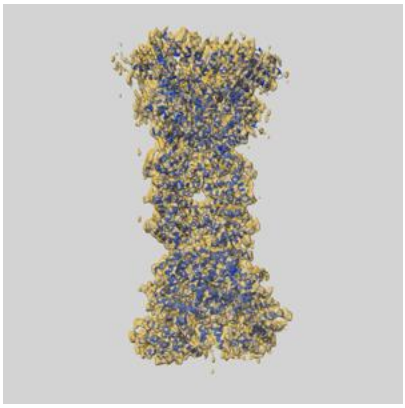
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	8.39	5.46
Unmasked-calculated*	9.11	23.47	9.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.11 differs from the reported value 4.4 by more than 10 %

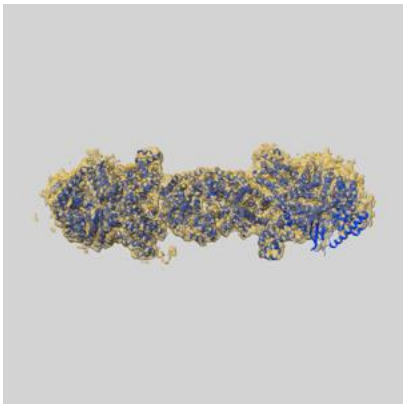
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39259 and PDB model 8YGP. Per-residue inclusion information can be found in section 3 on page 4.

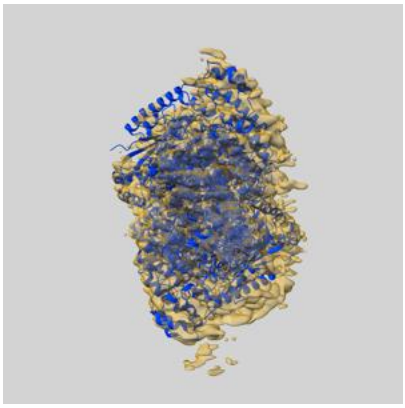
9.1 Map-model overlay



X



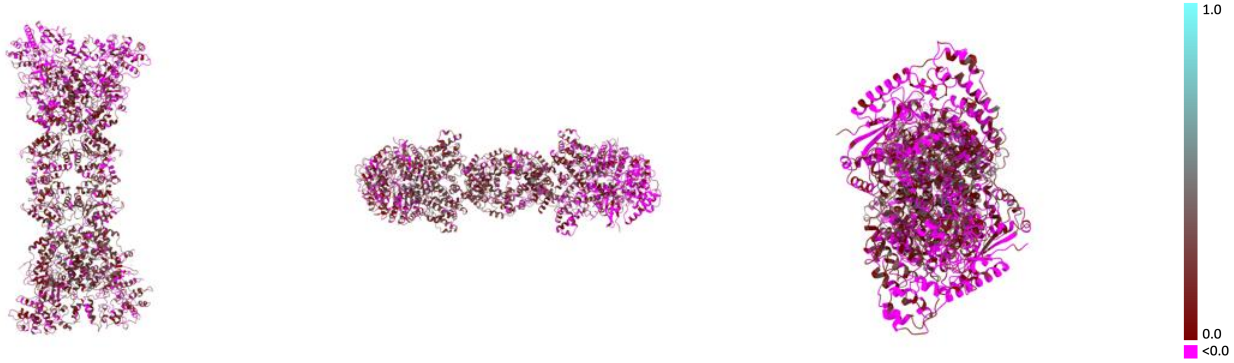
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

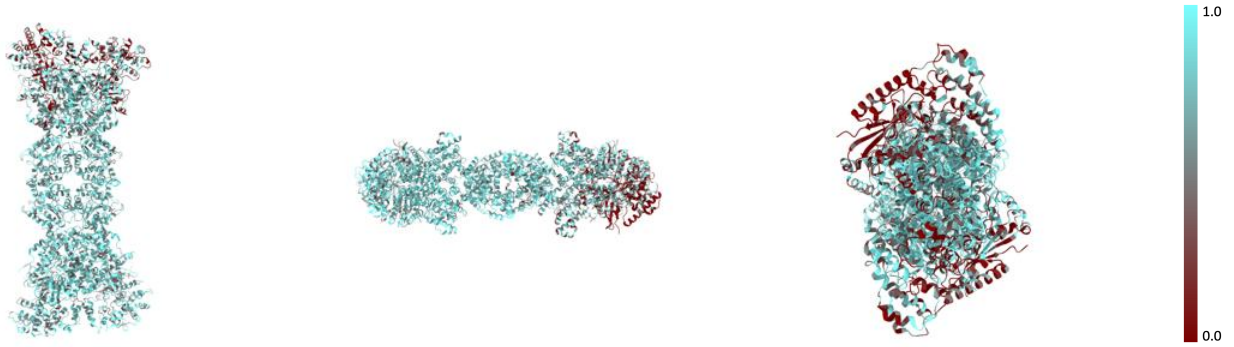
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

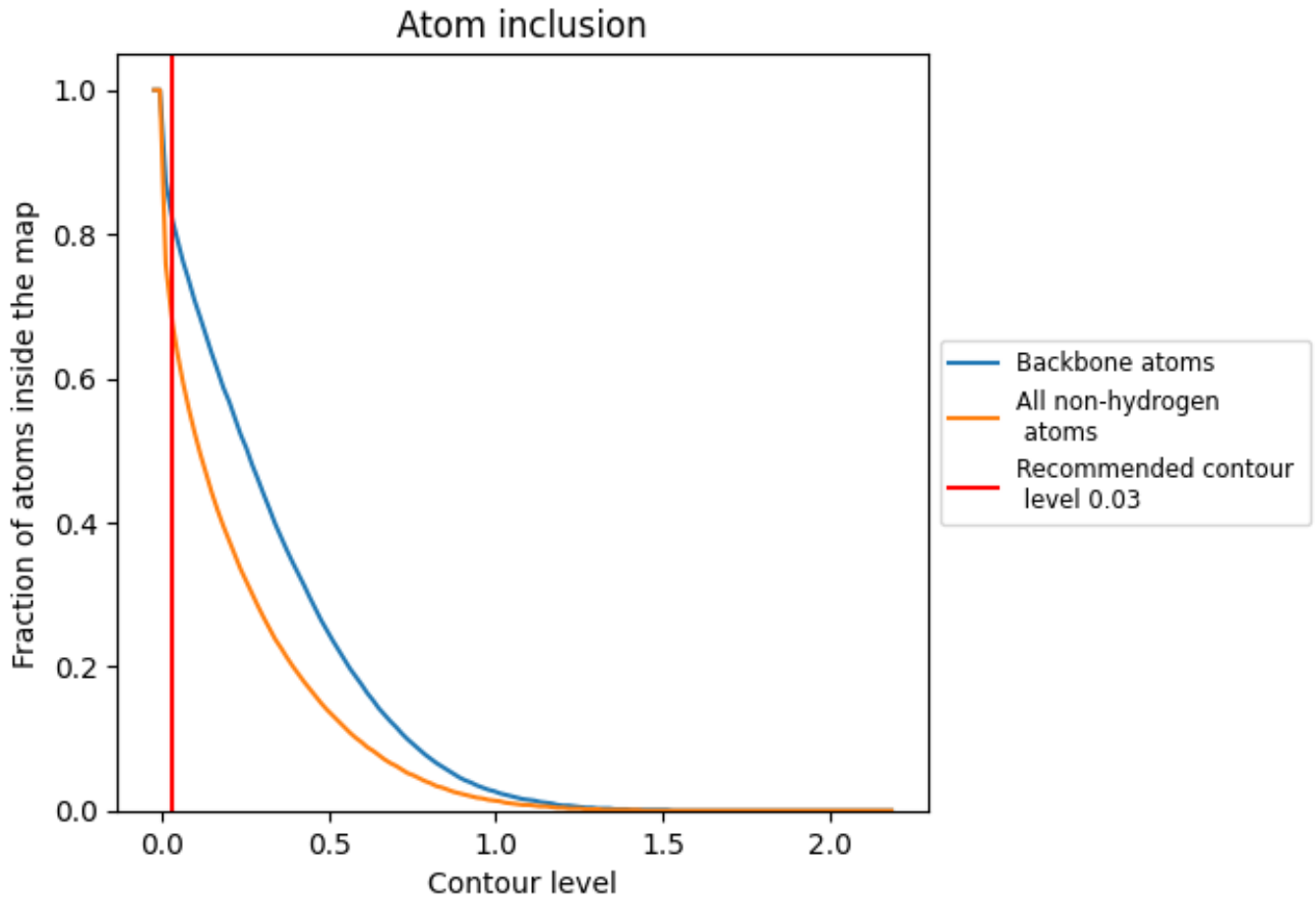
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6760	0.1320
A	0.6410	0.0940
B	0.6190	0.0910
C	0.2820	-0.0230
D	0.3460	-0.0400
E	0.7880	0.2000
F	0.7840	0.1980
G	0.6330	0.1260
H	0.5710	0.0810