Full wwPDB EM Validation Report ⓘ

Sep 2, 2024 – 02:13 PM JST

PDB ID	:	8ZC9
EMDB ID	:	EMD-39925
Title	:	The Cryo-EM structure of DSR2-Tail tube-NAD+ complex
Authors	:	Wang, R.; Xu, Q.; Wu, Z.; Li, J.; Yang, R.; Shi, Z.; Li, F.
Deposited on	:	2024-04-29
Resolution	:	3.14 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:

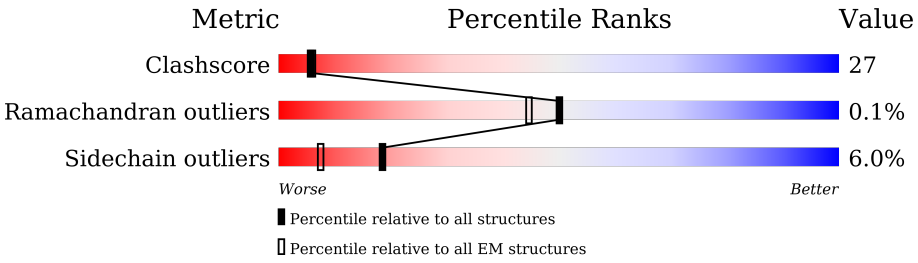
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.14 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	9% 51% 45%
1	B	1005	55% 39%
1	D	1005	17% 50% 45%
1	E	1005	49% 44%
2	C	264	5% 23% 28% 47%
2	F	264	22% 27% 25% 47%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35352 atoms, of which 104 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	B	971	Total	C	N	O	S	0	0
			8096	5240	1309	1516	31		
1	A	1000	Total	C	N	O	S	0	0
			8328	5388	1345	1563	32		
1	E	971	Total	C	N	O	S	0	0
			8096	5240	1309	1516	31		
1	D	1000	Total	C	N	O	S	0	0
			8328	5388	1345	1563	32		

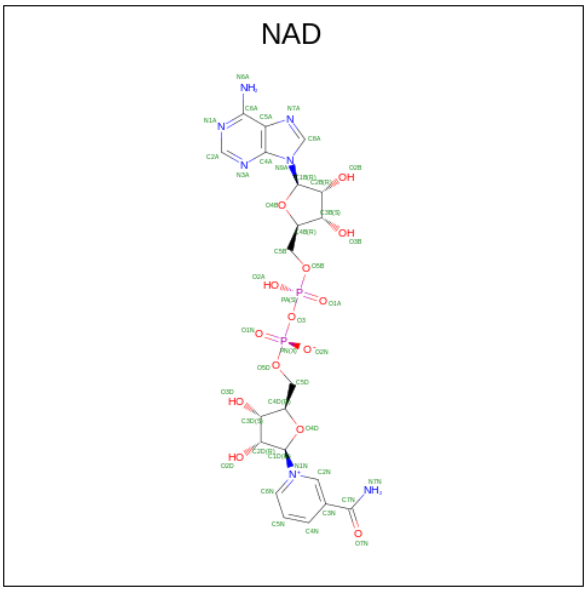
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	171	ALA	HIS	conflict	UNP D4G637
A	171	ALA	HIS	conflict	UNP D4G637
E	171	ALA	HIS	conflict	UNP D4G637
D	171	ALA	HIS	conflict	UNP D4G637

- Molecule 2 is a protein called tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	141	Total	C	N	O	S	0	0
			1112	705	178	225	4		
2	F	141	Total	C	N	O	S	0	0
			1112	705	178	225	4		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



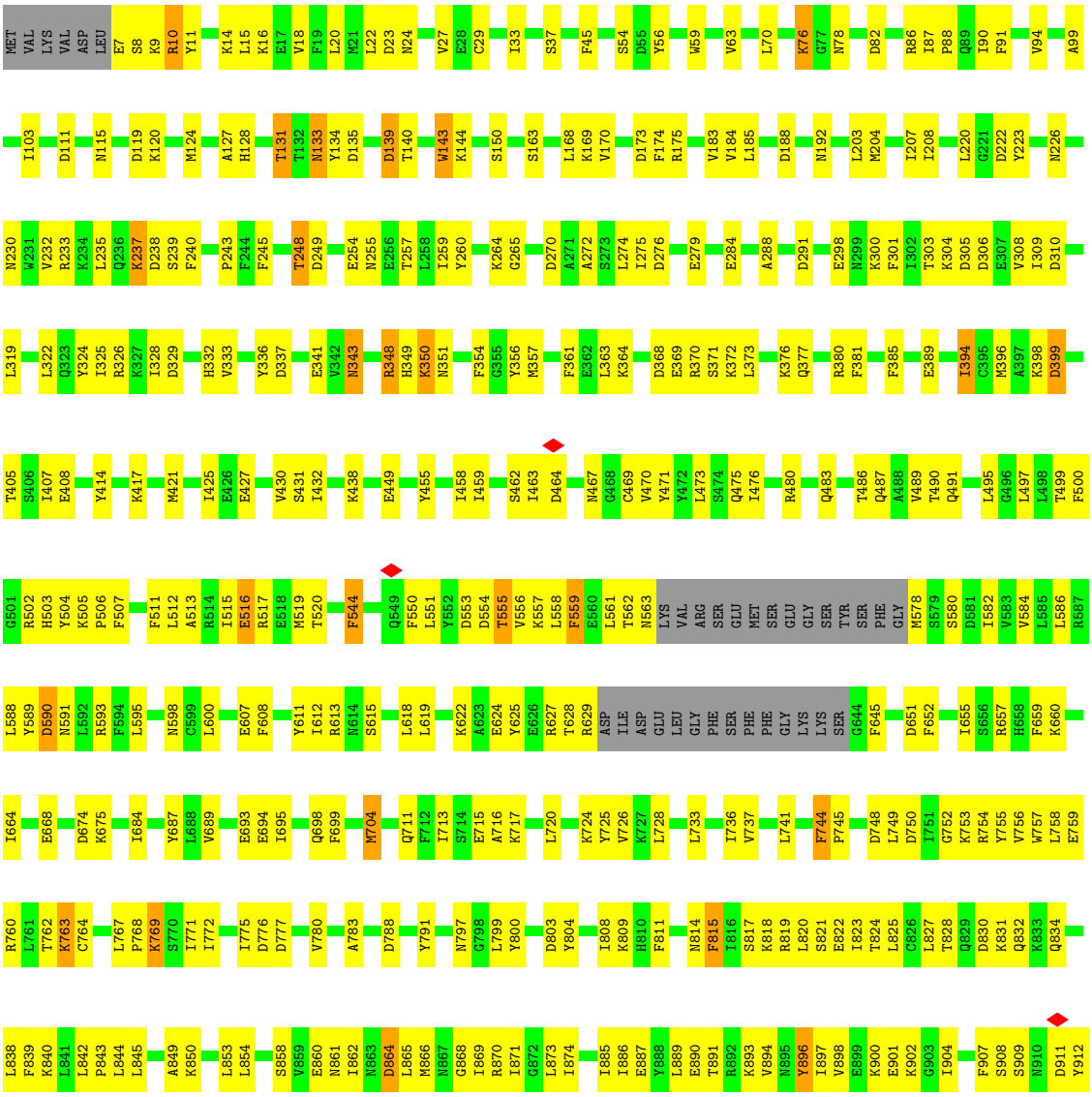
Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
3	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
3	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
3	D	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

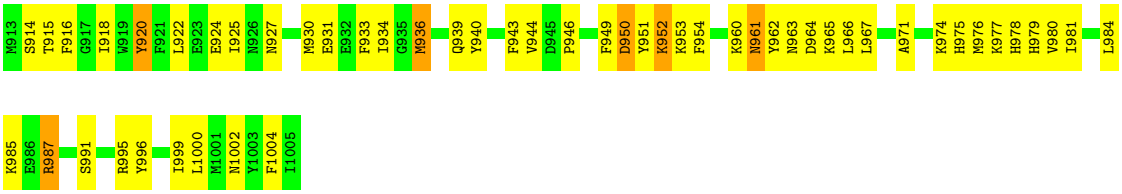
3 Residue-property plots (i)

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

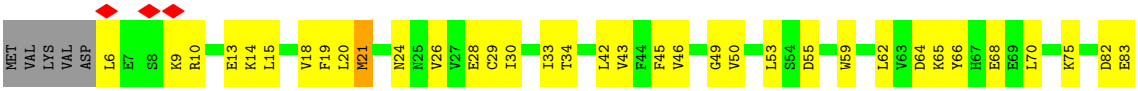
Chain B:

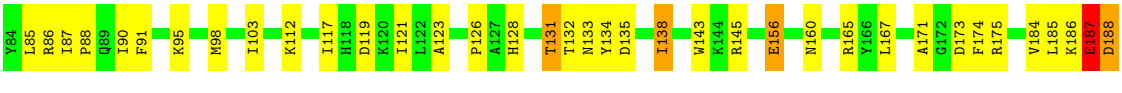


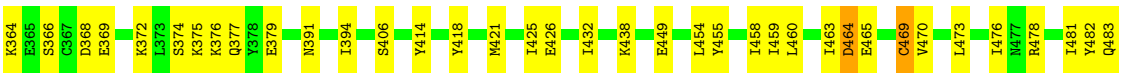


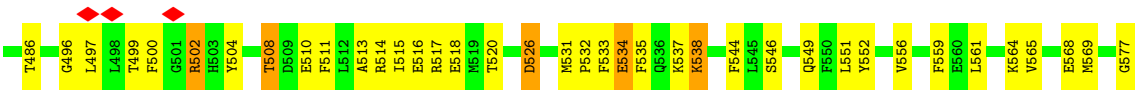
• Molecule 1: SIR2-like domain-containing protein

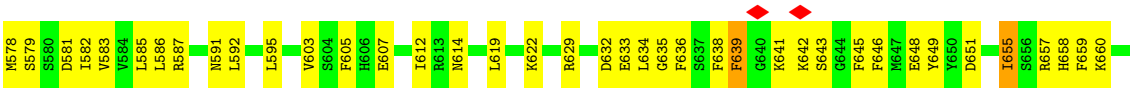
Chain A:

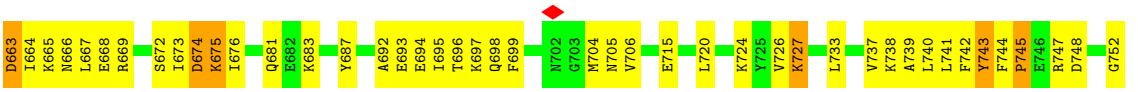


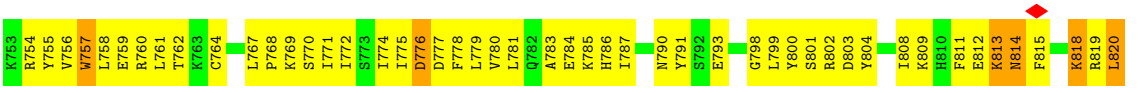


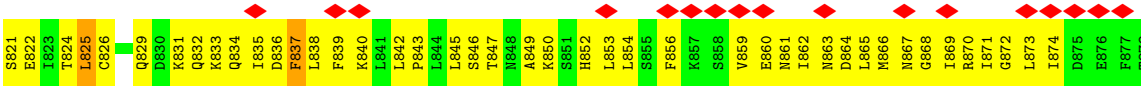


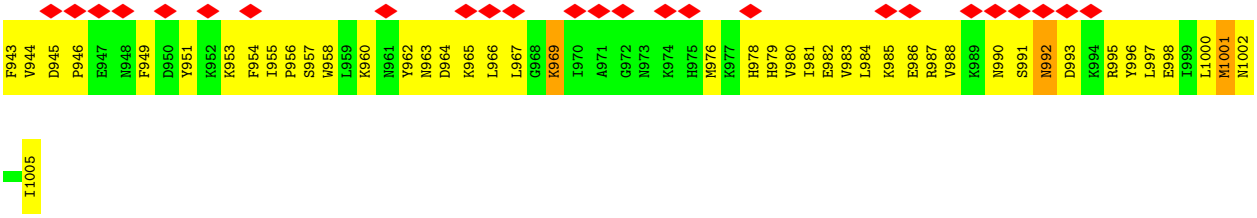






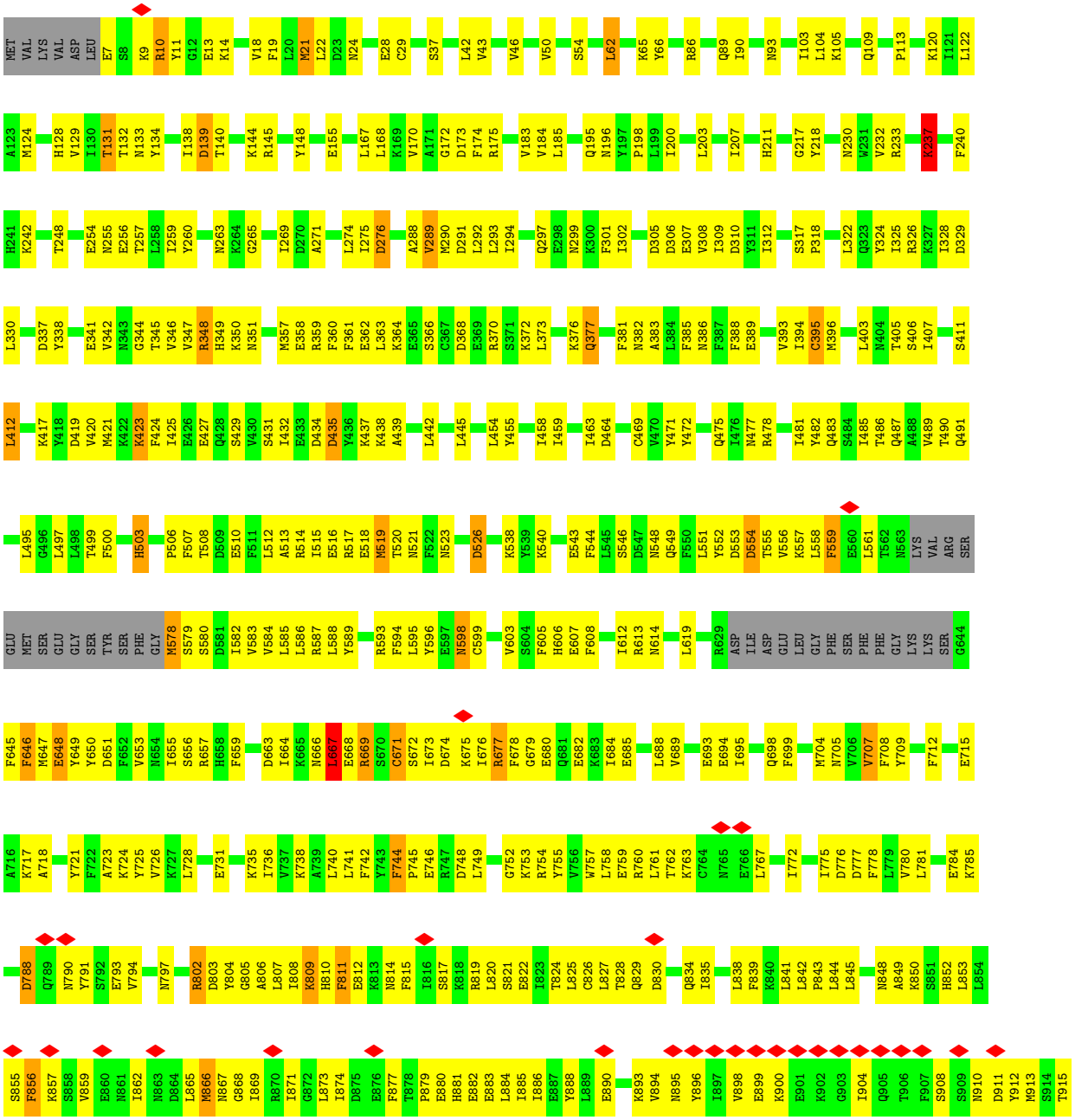


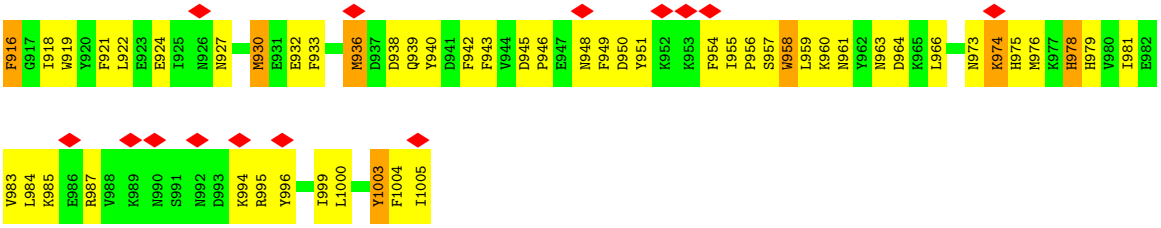




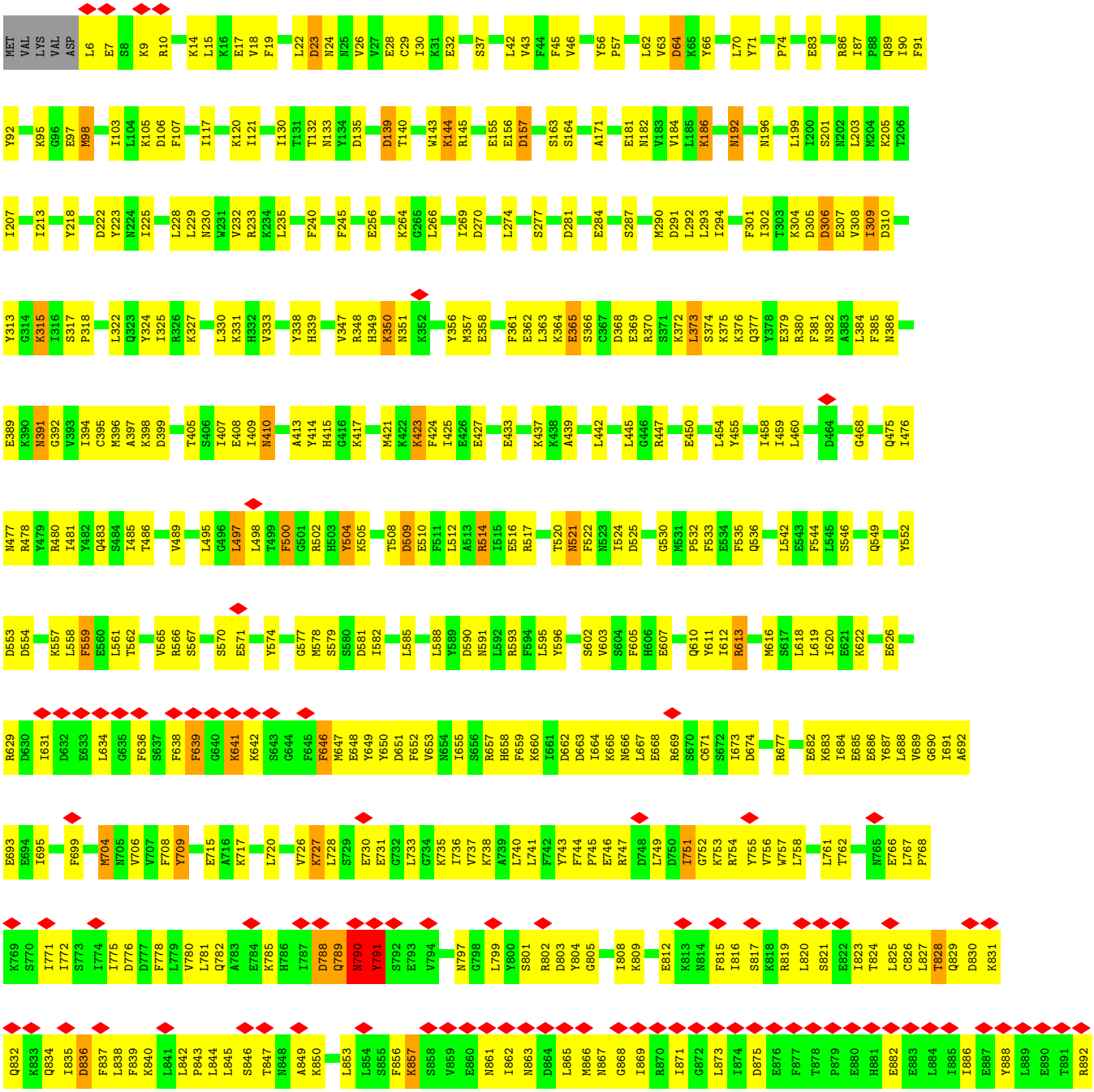
• Molecule 1: SIR2-like domain-containing protein

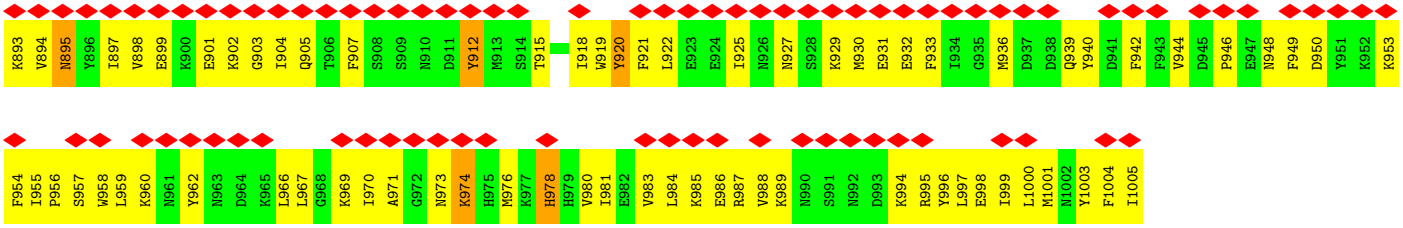
Chain E:





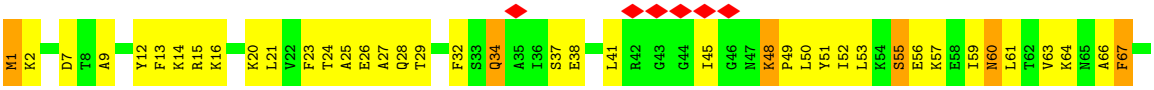
• Molecule 1: SIR2-like domain-containing protein

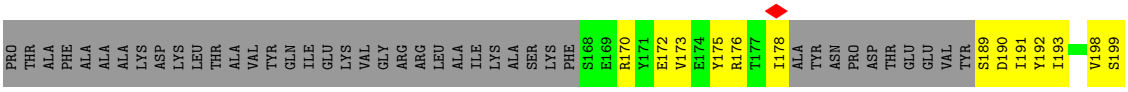


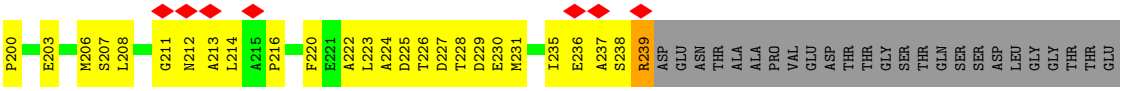


• Molecule 2: tail tube protein

Chain C:

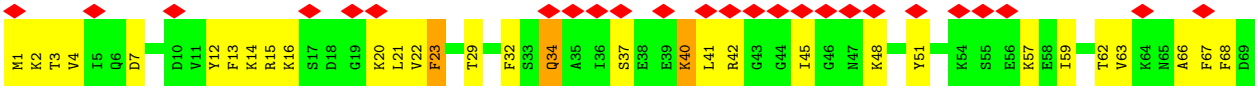


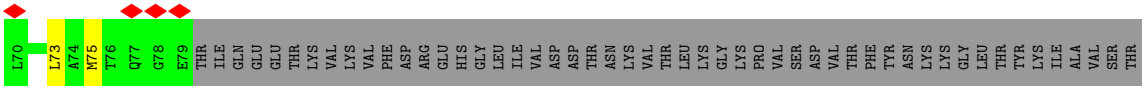


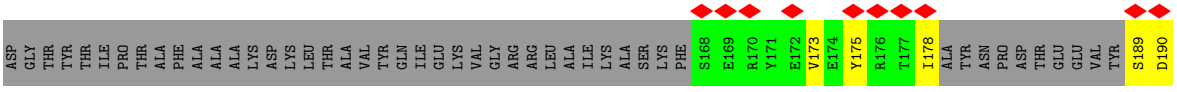


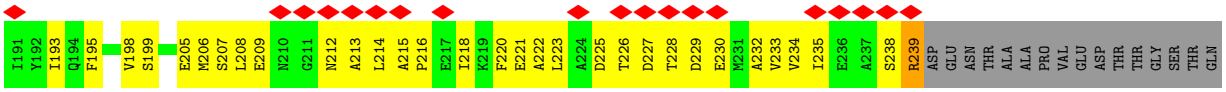
• Molecule 2: tail tube protein

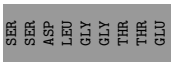
Chain F:











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57864	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.240	Depositor
Minimum map value	-0.321	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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	0.27	0/8521	0.49	3/11474 (0.0%)
1	B	0.26	0/8282	0.46	1/11155 (0.0%)
1	D	0.26	0/8521	0.46	1/11474 (0.0%)
1	E	0.25	0/8282	0.46	1/11155 (0.0%)
2	C	0.27	0/1128	0.54	0/1518
2	F	0.27	0/1128	0.51	0/1518
All	All	0.26	0/35862	0.47	6/48294 (0.0%)

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	B	0	2
1	D	0	4
1	E	0	1
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	745	PRO	N-CD-CG	-6.67	93.20	103.20
1	A	745	PRO	CA-N-CD	-6.51	102.39	111.50
1	D	836	ASP	CB-CG-OD2	6.08	123.78	118.30
1	E	667	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	769	LYS	CA-CB-CG	5.39	125.25	113.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	992	ASN	Peptide
1	B	237	LYS	Peptide
1	B	952	LYS	Peptide
1	D	349	HIS	Peptide
1	D	788	ASP	Peptide
1	D	790	ASN	Peptide
1	D	791	TYR	Peptide
1	E	237	LYS	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	8328	0	8168	456	0
1	B	8096	0	7944	351	0
1	D	8328	0	8168	547	0
1	E	8096	0	7944	454	0
2	C	1112	0	1090	85	0
2	F	1112	0	1090	72	0
3	A	44	26	26	0	0
3	B	44	26	26	0	0
3	D	44	26	26	0	0
3	E	44	26	26	0	0
All	All	35248	104	34508	1869	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 27.

All (1869) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:728:LEU:HD21	1:D:736:ILE:HD12	1.41	1.00
1:D:15:LEU:HD21	1:D:291:ASP:HB3	1.45	0.99
1:A:937:ASP:HB3	1:A:940:TYR:HB2	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:762:THR:HG22	1:D:767:LEU:HD21	1.46	0.98
1:D:980:VAL:HG13	1:D:984:LEU:HB2	1.47	0.94
1:A:681:GLN:HG2	1:A:726:VAL:HG13	1.50	0.94
1:A:50:VAL:HG11	1:A:117:ILE:HG21	1.49	0.93
1:A:825:LEU:HB3	1:A:849:ALA:HA	1.48	0.93
1:B:561:LEU:HD13	1:B:580:SER:HB2	1.52	0.92
1:D:812:GLU:HG2	1:D:815:PHE:HB2	1.52	0.92
1:A:218:TYR:HB3	1:A:225:ILE:HD11	1.52	0.91
1:D:960:LYS:HG2	1:D:995:ARG:HG2	1.53	0.90
1:A:352:LYS:HA	1:A:352:LYS:HE3	1.53	0.90
1:B:319:LEU:HD11	1:B:333:VAL:HG21	1.52	0.89
1:D:649:TYR:HA	1:D:684:ILE:HD11	1.55	0.88
1:D:648:GLU:HG3	2:F:2:LYS:HG2	1.54	0.88
1:A:30:ILE:HG23	1:A:293:LEU:HD23	1.54	0.87
2:C:192:TYR:HB2	2:C:235:ILE:HB	1.56	0.87
1:D:922:LEU:HD23	1:D:969:LYS:HD3	1.56	0.87
1:D:740:LEU:HG	1:D:741:LEU:HD22	1.54	0.87
1:A:934:ILE:HG23	1:A:941:ASP:HB3	1.55	0.87
1:D:476:ILE:HD11	1:D:546:SER:HB3	1.57	0.86
1:B:827:LEU:HD11	1:B:838:LEU:HD12	1.58	0.85
1:E:842:LEU:HB3	1:E:871:ILE:HD11	1.57	0.85
2:F:14:LYS:HG2	2:F:21:LEU:HA	1.58	0.85
2:C:189:SER:HA	2:C:239:ARG:HA	1.58	0.85
2:C:175:TYR:HB2	2:C:193:ILE:HB	1.58	0.84
1:A:772:ILE:HD11	1:A:808:ILE:HG23	1.59	0.84
1:D:950:ASP:HB3	1:D:953:LYS:HE3	1.60	0.84
2:C:199:SER:HB2	2:C:223:LEU:HD21	1.60	0.84
1:D:339:HIS:HB2	1:D:347:VAL:HG22	1.57	0.83
1:A:740:LEU:HD21	1:A:757:TRP:HB3	1.60	0.83
1:D:868:GLY:HA2	1:D:871:ILE:HG12	1.59	0.83
1:E:407:ILE:HG13	1:E:589:TYR:HB3	1.61	0.82
1:E:881:HIS:HA	1:E:884:LEU:HD12	1.60	0.82
1:E:749:LEU:HD12	1:E:753:LYS:HE3	1.60	0.81
1:B:904:ILE:HG12	2:C:235:ILE:HG12	1.63	0.81
1:E:922:LEU:HD21	1:E:966:LEU:HD11	1.63	0.80
1:E:742:PHE:HE1	1:E:778:PHE:HB2	1.46	0.80
1:A:256:GLU:HG2	1:D:70:LEU:HD22	1.64	0.80
1:A:995:ARG:HD2	1:A:998:GLU:HB2	1.65	0.79
1:D:781:LEU:HG	1:D:785:LYS:HE2	1.65	0.79
1:D:898:VAL:HG12	1:D:902:LYS:HE3	1.64	0.79
1:D:407:ILE:HD11	2:F:2:LYS:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:980:VAL:HA	1:D:984:LEU:HD13	1.64	0.78
1:A:922:LEU:HD12	1:A:965:LYS:HD3	1.66	0.78
1:E:672:SER:HB3	1:E:675:LYS:HD3	1.65	0.78
1:D:956:PRO:HD2	1:D:987:ARG:HG3	1.66	0.77
1:A:85:LEU:HB3	1:A:187:GLU:HB2	1.66	0.77
1:E:780:VAL:HG12	1:E:820:LEU:HD13	1.67	0.77
1:D:827:LEU:HD11	1:D:838:LEU:HD12	1.67	0.77
1:B:684:ILE:HG21	1:B:726:VAL:HG21	1.67	0.76
1:E:865:LEU:HD12	1:E:874:ILE:HD13	1.66	0.75
1:E:973:ASN:HB3	1:E:976:MET:HB2	1.67	0.75
2:F:178:ILE:HA	2:F:190:ASP:HA	1.68	0.75
1:E:29:CYS:HB3	1:E:269:ILE:HD11	1.69	0.75
1:D:377:GLN:HA	1:D:380:ARG:HD2	1.66	0.75
2:F:45:ILE:HG23	2:F:48:LYS:HB2	1.67	0.75
1:A:374:SER:HB3	1:A:377:GLN:HE21	1.50	0.75
1:D:626:GLU:HA	1:D:629:ARG:HD3	1.67	0.75
1:E:497:LEU:HD13	1:E:503:HIS:HB3	1.66	0.75
1:E:822:GLU:HA	1:E:825:LEU:HD23	1.69	0.74
1:A:138:ILE:HG22	1:A:167:LEU:HD11	1.69	0.74
1:A:904:ILE:HG23	1:A:906:THR:H	1.52	0.74
1:E:168:LEU:HD11	1:E:200:ILE:HG23	1.69	0.74
1:B:489:VAL:HG11	1:B:512:LEU:HD21	1.69	0.74
1:B:724:LYS:HD2	1:B:760:ARG:HB3	1.67	0.74
1:A:121:ILE:HD11	1:A:216:ILE:HD13	1.67	0.74
1:E:772:ILE:HD12	1:E:812:GLU:HG2	1.70	0.74
1:D:369:GLU:HA	1:D:372:LYS:HE2	1.69	0.74
1:D:478:ARG:HA	1:D:481:ILE:HG22	1.67	0.74
1:D:309:ILE:HD11	1:D:380:ARG:HB2	1.70	0.73
1:E:131:THR:OG1	1:E:133:ASN:OD1	2.06	0.73
1:D:306:ASP:OD1	1:D:306:ASP:N	2.20	0.73
2:F:68:PHE:HB2	2:F:73:LEU:HD11	1.69	0.73
1:E:299:ASN:HB3	1:E:302:ILE:HD12	1.71	0.73
1:D:869:ILE:HG12	1:D:875:ASP:HA	1.71	0.73
1:A:698:GLN:NE2	1:A:704:MET:SD	2.62	0.73
1:D:824:THR:HA	1:D:838:LEU:HD13	1.71	0.72
1:A:607:GLU:OE1	1:A:607:GLU:N	2.21	0.72
1:E:956:PRO:HB3	1:E:987:ARG:HD3	1.71	0.72
1:D:758:LEU:HD23	1:D:761:LEU:HD11	1.72	0.72
1:E:805:GLY:HA2	1:E:808:ILE:HD12	1.71	0.72
1:D:565:VAL:HG11	1:D:618:LEU:HD11	1.72	0.72
1:D:749:LEU:HG	1:D:754:ARG:HG2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:HD13	1:B:475:GLN:HG2	1.72	0.72
1:B:755:TYR:HD2	1:B:799:LEU:HD13	1.55	0.72
1:E:325:ILE:HD13	1:E:330:LEU:HD13	1.71	0.72
1:A:592:LEU:HD21	1:A:612:ILE:HD11	1.72	0.71
2:C:49:PRO:HB2	2:C:50:LEU:HD22	1.72	0.71
1:A:897:ILE:HA	1:A:900:LYS:HB3	1.71	0.71
1:E:22:LEU:HD22	1:E:274:LEU:HD22	1.70	0.71
1:D:514:ARG:HD2	1:D:517:ARG:HH12	1.55	0.71
1:B:843:PRO:HD3	1:B:871:ILE:HG23	1.73	0.71
1:A:915:THR:O	1:A:919:TRP:N	2.23	0.71
1:E:595:LEU:HB3	1:E:603:VAL:HG12	1.70	0.71
1:D:229:LEU:HD13	1:D:264:LYS:HE3	1.73	0.71
1:B:559:PHE:HD1	1:B:562:THR:HB	1.55	0.71
1:B:562:THR:HG23	1:B:618:LEU:HD13	1.73	0.71
1:A:824:THR:HG21	1:A:845:LEU:HD22	1.73	0.71
1:D:683:LYS:HA	1:D:686:GLU:HG3	1.73	0.70
1:E:930:MET:N	1:E:930:MET:SD	2.65	0.70
1:D:988:VAL:HG11	1:D:997:LEU:HD13	1.73	0.70
1:A:865:LEU:HA	1:A:869:ILE:HG12	1.72	0.70
1:D:304:LYS:HB2	1:D:307:GLU:HG3	1.74	0.70
1:D:439:ALA:HB2	1:D:454:LEU:HD23	1.73	0.70
1:E:432:ILE:HD11	1:E:458:ILE:HG23	1.71	0.70
1:E:124:MET:SD	1:E:297:GLN:NE2	2.65	0.70
1:E:435:ASP:N	1:E:435:ASP:OD1	2.24	0.69
1:E:385:PHE:O	1:E:389:GLU:HG3	1.92	0.69
1:D:980:VAL:HG22	1:D:984:LEU:HD13	1.74	0.69
1:B:562:THR:HG21	1:A:559:PHE:HE1	1.56	0.69
1:B:373:LEU:HD22	1:B:377:GLN:HB3	1.74	0.69
1:B:769:LYS:HA	1:B:772:ILE:HD13	1.73	0.69
1:D:373:LEU:HD23	1:D:374:SER:H	1.58	0.69
1:B:82:ASP:OD2	1:B:86:ARG:NH1	2.26	0.69
1:A:10:ARG:NH2	1:A:13:GLU:OE1	2.26	0.69
1:D:840:LYS:HA	1:D:871:ILE:HB	1.74	0.69
1:A:824:THR:HG22	1:A:838:LEU:HD12	1.75	0.69
1:A:82:ASP:OD2	1:A:86:ARG:NH1	2.27	0.68
1:B:886:ILE:HD11	1:B:927:ASN:HD21	1.59	0.68
1:A:899:GLU:HB3	1:A:904:ILE:HG22	1.76	0.68
1:A:945:ASP:HB2	1:A:949:PHE:HB2	1.75	0.68
1:A:960:LYS:HA	1:A:960:LYS:HE3	1.74	0.68
1:D:740:LEU:O	1:D:754:ARG:NH1	2.26	0.68
2:C:37:SER:HB3	2:C:41:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LYS:HB3	1:D:333:VAL:HG12	1.76	0.68
1:B:711:GLN:NE2	2:C:206:MET:SD	2.66	0.68
1:B:783:ALA:O	1:B:834:GLN:NE2	2.27	0.68
1:B:772:ILE:HG23	1:B:808:ILE:HG23	1.76	0.67
1:D:132:THR:OG1	1:D:218:TYR:OH	2.12	0.67
1:D:957:SER:HA	1:D:960:LYS:HE3	1.75	0.67
1:D:827:LEU:HD13	1:D:835:ILE:HA	1.77	0.67
1:A:919:TRP:HA	1:A:922:LEU:CD2	2.24	0.67
1:E:553:ASP:O	1:E:557:LYS:NZ	2.27	0.67
1:E:731:GLU:O	1:E:735:LYS:NZ	2.27	0.67
1:D:731:GLU:HG3	1:D:735:LYS:HE3	1.75	0.67
1:E:893:LYS:NZ	1:E:932:GLU:O	2.28	0.67
1:D:922:LEU:HD21	1:D:966:LEU:HB2	1.75	0.67
1:A:998:GLU:O	1:A:1002:ASN:ND2	2.28	0.67
1:B:248:THR:O	1:B:248:THR:OG1	2.12	0.67
1:B:559:PHE:O	1:B:563:ASN:ND2	2.27	0.67
1:E:439:ALA:HB2	1:E:454:LEU:HD23	1.76	0.67
1:E:842:LEU:HD13	1:E:873:LEU:HD11	1.75	0.67
1:D:869:ILE:HG23	1:D:875:ASP:HB3	1.77	0.66
1:E:132:THR:OG1	1:E:218:TYR:OH	2.09	0.66
1:E:668:GLU:HG2	1:E:673:ILE:HG21	1.77	0.66
1:B:414:TYR:O	1:B:657:ARG:NH2	2.29	0.66
1:E:1000:LEU:HD22	1:E:1004:PHE:HB2	1.75	0.66
2:F:13:PHE:HD1	2:F:173:VAL:HG22	1.60	0.66
1:B:984:LEU:HD11	1:B:999:ILE:HG13	1.76	0.66
1:E:259:ILE:O	1:E:263:ASN:ND2	2.29	0.66
1:D:755:TYR:HD2	1:D:799:LEU:HD13	1.59	0.66
1:E:843:PRO:HD3	1:E:871:ILE:HD11	1.78	0.66
1:E:383:ALA:HA	1:E:386:ASN:HD21	1.60	0.66
1:D:782:GLN:HB3	1:D:837:PHE:HZ	1.60	0.66
1:E:341:GLU:HB2	1:E:345:THR:HG22	1.77	0.66
1:D:930:MET:HA	1:D:933:PHE:HD2	1.61	0.66
1:A:790:ASN:OD1	1:A:791:TYR:N	2.29	0.66
1:E:429:SER:HB3	1:E:438:LYS:HE3	1.78	0.66
1:D:613:ARG:NH2	1:D:663:ASP:HB2	2.11	0.66
1:D:394:ILE:HD12	1:D:395:CYS:N	2.11	0.65
1:D:782:GLN:HA	1:D:785:LYS:HG2	1.78	0.65
1:B:497:LEU:HD11	1:B:503:HIS:HB2	1.78	0.65
1:B:809:LYS:NZ	1:B:814:ASN:O	2.28	0.65
1:A:865:LEU:HD22	1:A:869:ILE:HD13	1.77	0.65
1:E:808:ILE:HB	1:E:844:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:895:ASN:O	1:E:899:GLU:HG3	1.95	0.65
1:B:588:LEU:HD11	1:B:612:ILE:HD13	1.78	0.65
2:C:239:ARG:H	2:C:239:ARG:HD3	1.60	0.65
1:A:922:LEU:HD13	1:A:966:LEU:CD1	2.26	0.65
1:E:904:ILE:HG23	2:F:233:VAL:HG13	1.79	0.65
1:B:800:TYR:OH	2:C:224:ALA:O	2.14	0.65
1:A:303:THR:N	1:A:307:GLU:OE1	2.29	0.65
1:A:850:LYS:HA	1:A:853:LEU:HG	1.78	0.65
1:E:516:GLU:O	1:E:520:THR:OG1	2.05	0.65
1:E:842:LEU:CD1	1:E:873:LEU:HD11	2.27	0.65
1:A:635:GLY:HA2	1:A:638:PHE:HB3	1.77	0.65
1:E:698:GLN:HB3	1:E:704:MET:HB2	1.79	0.65
1:D:631:ILE:HG23	1:D:636:PHE:HB2	1.78	0.65
1:B:324:TYR:OH	1:B:590:ASP:OD1	2.12	0.65
1:B:940:TYR:O	1:B:944:VAL:HG23	1.97	0.65
1:B:432:ILE:HD11	1:B:458:ILE:HG23	1.78	0.64
1:E:589:TYR:OH	1:E:651:ASP:OD1	2.13	0.64
1:D:751:ILE:O	1:D:804:TYR:OH	2.15	0.64
1:B:310:ASP:OD1	1:B:380:ARG:NH1	2.30	0.64
1:B:950:ASP:CB	1:B:953:LYS:HD2	2.28	0.64
1:E:388:PHE:CD1	1:E:393:VAL:HG11	2.32	0.64
1:E:985:LYS:HE3	1:D:1005:ILE:HD13	1.79	0.64
2:F:37:SER:HB3	2:F:41:LEU:HD12	1.79	0.64
2:C:199:SER:CB	2:C:223:LEU:HD21	2.27	0.64
1:E:359:ARG:NH1	1:E:362:GLU:OE1	2.28	0.64
1:E:740:LEU:HD23	1:E:741:LEU:HD23	1.78	0.64
1:B:687:TYR:OH	1:B:715:GLU:OE2	2.13	0.64
2:C:238:SER:OG	2:C:239:ARG:NH1	2.30	0.64
1:B:763:LYS:HE3	1:B:764:CYS:HB3	1.80	0.64
1:E:842:LEU:HD21	1:E:850:LYS:HG2	1.79	0.64
1:D:775:ILE:HG22	1:D:808:ILE:HD11	1.79	0.64
1:D:823:ILE:HG22	1:D:838:LEU:HD11	1.79	0.64
1:B:133:ASN:OD1	1:B:133:ASN:N	2.29	0.64
1:A:55:ASP:O	1:A:112:LYS:NZ	2.30	0.64
1:D:497:LEU:HD12	1:D:498:LEU:H	1.62	0.64
1:B:364:LYS:NZ	1:B:394:ILE:O	2.29	0.64
1:B:487:GLN:HA	1:B:490:THR:HG22	1.80	0.64
1:E:412:LEU:HD11	1:E:420:VAL:HB	1.79	0.64
1:D:350:LYS:HG2	1:D:351:ASN:H	1.62	0.64
1:D:927:ASN:HB2	1:D:930:MET:HG2	1.80	0.64
1:D:347:VAL:HG12	1:D:397:ALA:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:HB2	1:B:329:ASP:OD1	1.97	0.63
1:A:894:VAL:O	1:A:898:VAL:HG23	1.98	0.63
1:A:655:ILE:O	1:A:659:PHE:HB2	1.97	0.63
1:A:824:THR:HB	1:A:849:ALA:HB1	1.80	0.63
1:D:410:ASN:OD1	1:D:410:ASN:N	2.31	0.63
1:D:985:LYS:O	1:D:989:LYS:HG3	1.98	0.63
2:F:238:SER:OG	2:F:239:ARG:NH1	2.31	0.63
1:B:995:ARG:O	1:B:999:ILE:HG23	1.98	0.63
1:A:304:LYS:HE3	1:A:306:ASP:HB2	1.80	0.63
1:B:767:LEU:HD22	1:B:772:ILE:CD1	2.29	0.63
1:A:511:PHE:O	1:A:515:ILE:HG23	1.98	0.63
1:E:11:TYR:OH	1:E:291:ASP:OD2	2.11	0.63
1:A:315:LYS:NZ	1:A:335:GLU:OE2	2.31	0.63
1:A:786:HIS:HB3	1:A:791:TYR:HD2	1.63	0.63
1:A:831:LYS:HG2	1:A:834:GLN:H	1.62	0.63
1:D:843:PRO:HD3	1:D:871:ILE:O	1.98	0.63
1:D:862:ILE:HG12	1:D:888:TYR:HB2	1.80	0.63
2:C:21:LEU:HD11	2:C:24:THR:HG22	1.80	0.63
1:E:549:GLN:HG2	1:E:552:TYR:HB2	1.80	0.63
1:A:327:LYS:NZ	1:A:391:ASN:O	2.31	0.63
1:A:845:LEU:HD13	1:A:853:LEU:HD22	1.81	0.63
1:E:459:ILE:HD13	1:E:475:GLN:HG2	1.78	0.63
1:E:709:TYR:OH	1:E:748:ASP:OD2	2.12	0.63
1:E:843:PRO:HD3	1:E:871:ILE:CD1	2.29	0.63
1:A:881:HIS:HD2	1:A:884:LEU:HD12	1.63	0.62
1:E:704:MET:HE2	1:E:709:TYR:HB2	1.80	0.62
1:A:674:ASP:N	1:A:674:ASP:OD1	2.32	0.62
1:A:834:GLN:HG3	1:A:838:LEU:HD23	1.82	0.62
1:D:824:THR:HG23	1:D:853:LEU:HD13	1.80	0.62
2:C:13:PHE:HD1	2:C:173:VAL:HG22	1.65	0.62
1:E:132:THR:HG22	1:E:170:VAL:HG22	1.81	0.62
1:B:655:ILE:O	1:B:659:PHE:HB2	1.99	0.62
1:A:587:ARG:O	1:A:591:ASN:ND2	2.32	0.62
1:E:22:LEU:HD11	1:E:292:LEU:HD21	1.81	0.62
1:B:922:LEU:HD21	1:B:965:LYS:HE3	1.82	0.62
1:E:388:PHE:O	1:E:393:VAL:HG12	2.00	0.62
1:D:930:MET:HA	1:D:933:PHE:CD2	2.34	0.62
1:D:524:ILE:HG13	1:D:546:SER:HB2	1.81	0.62
1:B:668:GLU:OE2	1:B:725:TYR:OH	2.17	0.62
1:B:960:LYS:O	1:B:995:ARG:NH2	2.32	0.62
1:E:105:LYS:O	1:E:109:GLN:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:794:VAL:CG1	2:F:223:LEU:HB3	2.30	0.62
1:B:865:LEU:O	1:B:869:ILE:HG12	2.00	0.62
1:D:339:HIS:HB2	1:D:347:VAL:CG2	2.30	0.62
1:A:842:LEU:HD21	1:A:873:LEU:HD22	1.82	0.61
1:D:394:ILE:HD12	1:D:395:CYS:H	1.64	0.61
1:A:962:TYR:CZ	1:A:966:LEU:HB3	2.34	0.61
1:E:497:LEU:CD1	1:E:503:HIS:HB3	2.31	0.61
1:E:695:ILE:HG13	1:E:712:PHE:HE2	1.64	0.61
1:A:257:THR:HG1	1:D:71:TYR:HH	1.48	0.61
1:B:607:GLU:OE1	1:B:607:GLU:N	2.33	0.61
1:E:655:ILE:O	1:E:659:PHE:HB2	2.00	0.61
1:E:809:LYS:HE3	1:E:814:ASN:HA	1.82	0.61
1:B:16:LYS:HD3	1:B:20:LEU:HD23	1.82	0.61
1:B:724:LYS:HE2	1:B:763:LYS:HE2	1.82	0.61
1:A:756:VAL:O	1:A:759:GLU:HG3	2.00	0.61
1:E:248:THR:HA	1:E:271:ALA:HB3	1.82	0.61
1:E:363:LEU:HD13	1:E:373:LEU:HD11	1.83	0.61
1:E:981:ILE:O	1:E:985:LYS:HG3	2.00	0.61
1:D:574:TYR:O	2:F:29:THR:OG1	2.11	0.61
1:D:684:ILE:HG21	1:D:726:VAL:HG21	1.83	0.61
1:E:605:PHE:CD2	2:F:208:LEU:HD12	2.36	0.61
1:B:120:LYS:NZ	1:B:291:ASP:OD1	2.34	0.61
1:E:666:ASN:ND2	1:D:567:SER:OG	2.34	0.61
1:E:822:GLU:HA	1:E:825:LEU:CD2	2.31	0.61
1:D:509:ASP:N	1:D:509:ASP:OD1	2.33	0.61
1:D:768:PRO:HD2	1:D:771:ILE:HG13	1.82	0.61
1:B:819:ARG:O	1:B:823:ILE:HG22	2.01	0.61
1:A:65:LYS:HG3	1:A:103:ILE:HD13	1.83	0.61
1:A:694:GLU:O	1:A:698:GLN:HG3	2.00	0.61
1:E:957:SER:O	1:E:961:ASN:ND2	2.34	0.61
1:D:305:ASP:HB3	1:D:373:LEU:HD11	1.81	0.61
1:A:786:HIS:CB	1:A:791:TYR:HB3	2.31	0.61
1:A:901:GLU:HB2	1:A:902:LYS:NZ	2.16	0.61
1:A:831:LYS:HG3	1:A:833:LYS:H	1.65	0.60
1:A:922:LEU:HG	1:A:924:GLU:HG2	1.81	0.60
1:D:752:GLY:HA2	1:D:799:LEU:HB2	1.81	0.60
1:D:976:MET:O	1:D:980:VAL:HG23	2.00	0.60
1:B:800:TYR:N	1:B:803:ASP:OD1	2.23	0.60
1:B:825:LEU:HD21	1:B:849:ALA:HA	1.83	0.60
1:E:677:ARG:HA	1:E:677:ARG:HE	1.66	0.60
1:D:827:LEU:HD21	1:D:834:GLN:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:ILE:O	1:D:901:GLU:HG3	2.01	0.60
1:E:598:ASN:N	1:E:598:ASN:OD1	2.34	0.60
1:D:758:LEU:HA	1:D:761:LEU:HG	1.82	0.60
1:D:988:VAL:HG13	1:D:997:LEU:HB2	1.83	0.60
1:B:511:PHE:O	1:B:515:ILE:HG23	2.02	0.60
1:B:724:LYS:HB2	1:B:760:ARG:HB3	1.83	0.60
1:A:777:ASP:O	1:A:781:LEU:HD23	2.01	0.60
1:B:950:ASP:HB2	1:B:953:LYS:HD2	1.84	0.60
1:A:85:LEU:HB3	1:A:187:GLU:CB	2.31	0.60
1:D:235:LEU:HD12	1:D:240:PHE:HB3	1.83	0.60
1:D:364:LYS:NZ	1:D:394:ILE:O	2.25	0.60
1:B:864:ASP:OD1	1:B:864:ASP:N	2.33	0.60
1:A:786:HIS:HA	1:A:791:TYR:HB3	1.84	0.60
1:E:705:ASN:HD21	1:E:707:VAL:HG23	1.66	0.60
2:F:48:LYS:HG3	2:F:51:TYR:OH	2.00	0.60
1:B:767:LEU:CD2	1:B:771:ILE:HB	2.30	0.60
1:B:963:ASN:N	2:C:51:TYR:OH	2.28	0.60
1:A:997:LEU:HD22	1:A:1000:LEU:HB3	1.82	0.60
1:E:1005:ILE:O	1:D:1004:PHE:HB3	2.01	0.60
1:B:140:THR:HG22	1:B:144:LYS:HE2	1.84	0.60
1:A:733:LEU:O	1:A:737:VAL:HG13	2.01	0.60
1:E:558:LEU:HD21	1:E:614:ASN:HB3	1.82	0.60
1:E:583:VAL:O	1:E:587:ARG:HG3	2.01	0.60
1:D:999:ILE:HG23	1:D:1003:TYR:CE2	2.37	0.60
1:B:854:LEU:HD21	1:B:873:LEU:HD21	1.84	0.60
1:B:907:PHE:CE2	1:A:633:GLU:HG3	2.37	0.60
1:D:43:VAL:HB	1:D:213:ILE:HD13	1.83	0.60
1:D:959:LEU:HD23	1:D:970:ILE:HG21	1.83	0.60
1:B:589:TYR:OH	1:B:651:ASP:OD1	2.18	0.59
1:B:931:GLU:O	1:B:934:ILE:HG12	2.01	0.59
1:A:916:PHE:O	1:A:925:ILE:HG13	2.01	0.59
2:C:176:ARG:HG3	2:C:176:ARG:HH11	1.66	0.59
1:E:455:TYR:O	1:E:459:ILE:HG13	2.00	0.59
1:B:255:ASN:O	1:B:259:ILE:HG13	2.02	0.59
1:E:828:THR:OG1	1:E:830:ASP:OD1	2.13	0.59
1:E:865:LEU:O	1:E:869:ILE:HG13	2.02	0.59
1:D:327:LYS:NZ	1:D:391:ASN:O	2.35	0.59
1:D:751:ILE:HA	1:D:754:ARG:HG3	1.82	0.59
1:B:487:GLN:O	1:B:491:GLN:HG3	2.02	0.59
1:A:738:LYS:HG3	1:A:742:PHE:HD2	1.66	0.59
1:A:937:ASP:OD2	1:A:939:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:GLU:O	2:C:63:VAL:HG13	2.02	0.59
1:E:412:LEU:CD1	1:E:421:MET:HG2	2.32	0.59
1:A:769:LYS:O	1:A:772:ILE:HG22	2.02	0.59
1:B:971:ALA:O	1:B:977:LYS:HD2	2.03	0.59
1:A:824:THR:HG22	1:A:838:LEU:CD1	2.33	0.59
1:D:866:MET:CE	1:D:915:THR:HG21	2.33	0.59
1:A:339:HIS:HB2	1:A:347:VAL:CG1	2.32	0.59
1:A:767:LEU:HD12	1:A:771:ILE:HB	1.84	0.59
1:E:741:LEU:HA	1:E:754:ARG:HD3	1.85	0.59
1:E:983:VAL:O	1:E:987:ARG:HG2	2.03	0.59
1:D:647:MET:HE2	1:D:651:ASP:HB3	1.83	0.59
1:B:933:PHE:O	1:B:934:ILE:HD13	2.02	0.59
1:E:526:ASP:OD1	1:E:526:ASP:N	2.36	0.59
1:D:978:HIS:O	1:D:981:ILE:HD13	2.02	0.59
1:B:949:PHE:HE2	1:B:954:PHE:HB2	1.67	0.59
1:A:455:TYR:O	1:A:459:ILE:HG13	2.03	0.59
1:A:800:TYR:N	1:A:803:ASP:OD2	2.36	0.59
1:D:738:LYS:HE2	1:D:743:TYR:HE2	1.66	0.59
1:A:98:MET:N	1:A:98:MET:SD	2.76	0.59
1:A:132:THR:HG23	1:A:171:ALA:HB2	1.85	0.59
1:A:956:PRO:HG3	1:A:983:VAL:CG2	2.33	0.59
1:E:230:ASN:O	1:E:233:ARG:HG2	2.03	0.59
1:D:308:VAL:HG13	1:D:356:TYR:HB2	1.84	0.59
1:D:655:ILE:HG13	1:D:659:PHE:CE1	2.38	0.59
1:A:987:ARG:HG2	1:A:996:TYR:CD1	2.38	0.58
1:D:382:ASN:O	1:D:386:ASN:ND2	2.36	0.58
1:D:585:LEU:HD12	1:D:619:LEU:HD13	1.84	0.58
2:F:239:ARG:H	2:F:239:ARG:HD3	1.66	0.58
1:A:26:VAL:O	1:A:30:ILE:HG12	2.03	0.58
1:E:129:VAL:HB	1:E:167:LEU:HD22	1.85	0.58
1:E:242:LYS:HB3	1:E:265:GLY:O	2.02	0.58
1:A:963:ASN:O	1:A:967:LEU:HG	2.03	0.58
1:E:767:LEU:HG	1:E:811:PHE:CZ	2.38	0.58
1:D:415:HIS:HB3	1:D:417:LYS:HE2	1.85	0.58
2:F:189:SER:HA	2:F:239:ARG:HA	1.84	0.58
1:A:874:ILE:HG21	1:A:881:HIS:CE1	2.38	0.58
2:C:213:ALA:O	2:C:216:PRO:HD3	2.04	0.58
1:E:981:ILE:HG23	1:E:985:LYS:NZ	2.18	0.58
1:D:181:GLU:HG3	1:D:182:ASN:OD1	2.02	0.58
1:D:425:ILE:HD13	1:D:442:LEU:HD13	1.85	0.58
1:D:565:VAL:CG1	1:D:618:LEU:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:LYS:HG2	1:B:399:ASP:OD1	2.04	0.58
1:B:949:PHE:CE2	1:B:954:PHE:HB2	2.38	0.58
1:E:607:GLU:OE1	1:E:607:GLU:N	2.36	0.58
1:A:418:TYR:HA	1:A:421:MET:HE3	1.85	0.58
1:A:770:SER:O	1:A:774:ILE:HG13	2.04	0.58
1:D:322:LEU:HD21	1:D:542:LEU:HD11	1.86	0.58
1:D:797:ASN:HB2	1:D:799:LEU:HG	1.86	0.58
1:D:899:GLU:HB3	1:D:904:ILE:O	2.04	0.58
1:A:62:LEU:HD11	1:A:103:ILE:HG22	1.85	0.58
1:A:775:ILE:CG2	1:A:808:ILE:HD11	2.33	0.58
1:E:973:ASN:OD1	1:E:975:HIS:ND1	2.37	0.58
1:E:985:LYS:HE3	1:D:1005:ILE:CD1	2.33	0.58
1:D:86:ARG:O	1:D:90:ILE:HG13	2.04	0.58
1:B:495:LEU:O	1:B:499:THR:HG23	2.04	0.58
1:B:550:PHE:O	1:B:551:LEU:HG	2.03	0.58
1:B:776:ASP:O	1:B:780:VAL:HG13	2.03	0.58
1:D:6:LEU:HB3	1:D:9:LYS:HB3	1.86	0.58
1:D:368:ASP:O	1:D:372:LYS:HG3	2.03	0.58
1:B:966:LEU:HB2	2:C:51:TYR:HE2	1.68	0.58
1:A:18:VAL:HA	1:A:21:MET:HE3	1.86	0.58
1:D:364:LYS:HB2	1:D:385:PHE:HE1	1.69	0.58
2:C:21:LEU:HD11	2:C:24:THR:CG2	2.34	0.58
1:D:842:LEU:HB3	1:D:871:ILE:O	2.03	0.58
1:E:684:ILE:HG21	1:E:726:VAL:HG11	1.86	0.57
2:C:16:LYS:HD3	2:C:172:GLU:OE1	2.04	0.57
2:C:175:TYR:HB2	2:C:193:ILE:CB	2.33	0.57
1:E:922:LEU:HD11	1:E:966:LEU:HD12	1.86	0.57
1:B:907:PHE:HE2	1:A:633:GLU:HG3	1.69	0.57
1:A:66:TYR:CE1	1:A:103:ILE:HD12	2.40	0.57
1:E:826:CYS:O	1:E:827:LEU:HD23	2.02	0.57
1:D:132:THR:HG1	1:D:218:TYR:HH	1.50	0.57
1:B:720:LEU:HD12	1:B:744:PHE:HE2	1.67	0.57
1:E:427:GLU:O	1:E:438:LYS:NZ	2.26	0.57
1:E:588:LEU:HD11	1:E:612:ILE:HD13	1.85	0.57
1:E:809:LYS:O	1:E:811:PHE:N	2.37	0.57
1:A:938:ASP:OD1	1:A:953:LYS:HD3	2.05	0.57
1:E:19:PHE:CD2	1:E:301:PHE:HB3	2.40	0.57
1:B:427:GLU:O	1:B:438:LYS:NZ	2.33	0.57
1:B:558:LEU:HD22	1:B:618:LEU:CD2	2.35	0.57
1:B:920:TYR:CD1	1:B:944:VAL:HG13	2.38	0.57
1:A:376:LYS:HA	1:A:379:GLU:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:684:ILE:CG2	1:E:726:VAL:HG11	2.35	0.57
1:D:424:PHE:HE2	1:D:437:LYS:HZ1	1.53	0.57
1:D:425:ILE:HD13	1:D:442:LEU:CD1	2.34	0.57
1:B:920:TYR:HA	1:B:925:ILE:HD11	1.86	0.57
1:B:984:LEU:HD22	1:B:1000:LEU:HB2	1.86	0.57
1:E:172:GLY:HA3	1:E:183:VAL:HA	1.87	0.57
1:E:974:LYS:HD2	1:E:975:HIS:N	2.19	0.57
1:D:613:ARG:CZ	1:D:663:ASP:HB2	2.35	0.57
1:D:667:LEU:O	1:D:671:CYS:HB2	2.04	0.57
1:B:421:MET:O	1:B:425:ILE:HG13	2.05	0.57
1:E:305:ASP:HB2	1:E:373:LEU:HD21	1.85	0.57
1:E:472:TYR:OH	1:E:546:SER:HB2	2.04	0.57
1:E:695:ILE:HG23	1:E:699:PHE:HD1	1.69	0.57
1:D:306:ASP:HA	1:D:309:ILE:HG22	1.85	0.57
1:B:619:LEU:HD23	1:B:645:PHE:CE2	2.40	0.57
1:A:564:LYS:O	1:A:568:GLU:HG3	2.04	0.57
1:A:893:LYS:HA	1:A:936:MET:CE	2.34	0.57
1:A:987:ARG:HG3	1:A:991:SER:O	2.05	0.57
1:A:988:VAL:HG13	1:A:992:ASN:OD1	2.05	0.57
1:D:62:LEU:HD21	1:D:107:PHE:HB3	1.87	0.57
1:D:83:GLU:HG2	1:D:86:ARG:HH22	1.68	0.57
1:D:840:LYS:HD3	1:D:871:ILE:HD12	1.85	0.57
1:B:399:ASP:OD1	1:B:399:ASP:N	2.37	0.56
1:B:909:SER:HB3	2:C:231:MET:CG	2.35	0.56
1:A:258:LEU:HD12	1:A:268:ILE:HD12	1.86	0.56
1:E:66:TYR:CE1	1:E:103:ILE:HD12	2.40	0.56
1:D:687:TYR:O	1:D:691:ILE:HD12	2.04	0.56
1:D:816:ILE:HD13	1:D:846:SER:HA	1.86	0.56
1:E:553:ASP:HA	1:D:552:TYR:OH	2.05	0.56
1:E:664:ILE:O	1:E:668:GLU:HG3	2.05	0.56
1:D:728:LEU:CD2	1:D:736:ILE:HD12	2.28	0.56
1:B:304:LYS:O	1:B:308:VAL:HG13	2.05	0.56
1:A:738:LYS:O	1:A:742:PHE:HB2	2.06	0.56
1:E:682:GLU:OE2	1:E:682:GLU:N	2.35	0.56
1:E:995:ARG:O	1:E:999:ILE:HG23	2.05	0.56
1:D:92:TYR:CG	1:D:186:LYS:HE3	2.40	0.56
1:D:157:ASP:N	1:D:157:ASP:OD1	2.38	0.56
1:D:324:TYR:OH	1:D:590:ASP:OD1	2.11	0.56
1:D:669:ARG:HA	1:D:994:LYS:HE3	1.85	0.56
1:D:687:TYR:CE2	1:D:691:ILE:HD11	2.40	0.56
1:D:776:ASP:O	1:D:780:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:LEU:HB3	1:A:869:ILE:HD11	1.87	0.56
1:D:817:SER:HB3	1:D:820:LEU:HB2	1.85	0.56
1:B:554:ASP:OD2	1:B:591:ASN:ND2	2.39	0.56
1:B:607:GLU:HB2	2:C:208:LEU:HD12	1.87	0.56
1:B:893:LYS:O	1:B:897:ILE:HG12	2.06	0.56
1:A:922:LEU:HD13	1:A:966:LEU:HD12	1.88	0.56
1:E:918:ILE:O	1:E:922:LEU:HD13	2.04	0.56
1:D:921:PHE:O	1:D:969:LYS:NZ	2.23	0.56
2:F:207:SER:HB3	2:F:212:ASN:OD1	2.06	0.56
1:B:243:PRO:HD2	1:B:265:GLY:O	2.04	0.56
1:E:62:LEU:HD11	1:E:104:LEU:HD23	1.88	0.56
1:E:904:ILE:HA	2:F:234:VAL:O	2.05	0.56
1:D:140:THR:O	1:D:144:LYS:HG2	2.05	0.56
1:D:413:ALA:HA	1:D:421:MET:CE	2.36	0.56
1:B:463:ILE:HG21	1:A:143:TRP:CD1	2.41	0.56
1:B:817:SER:OG	1:B:820:LEU:HB2	2.05	0.56
2:C:190:ASP:OD2	2:C:237:ALA:HB3	2.06	0.56
1:E:349:HIS:HB3	1:E:350:LYS:CE	2.36	0.56
1:E:685:GLU:O	1:E:689:VAL:HG23	2.05	0.56
1:E:723:ALA:HB3	1:E:761:LEU:HD21	1.87	0.56
1:E:775:ILE:HG22	1:E:808:ILE:HD11	1.86	0.56
1:E:825:LEU:O	1:E:852:HIS:NE2	2.38	0.56
1:E:868:GLY:HA2	1:E:871:ILE:HG22	1.86	0.56
1:B:337:ASP:HB3	1:B:351:ASN:HA	1.86	0.56
2:F:199:SER:HB2	2:F:223:LEU:HD11	1.88	0.56
1:B:325:ILE:HD12	1:B:325:ILE:O	2.05	0.56
1:A:846:SER:O	1:A:850:LYS:HG3	2.06	0.56
1:B:887:GLU:O	1:B:891:THR:HG22	2.06	0.56
2:C:189:SER:CA	2:C:239:ARG:HA	2.33	0.56
2:C:207:SER:HB3	2:C:212:ASN:ND2	2.21	0.56
1:E:559:PHE:HA	1:D:559:PHE:HE2	1.71	0.56
1:D:829:GLN:OE1	1:D:829:GLN:N	2.39	0.56
1:D:840:LYS:HA	1:D:871:ILE:CB	2.35	0.56
1:A:15:LEU:HD22	1:A:292:LEU:HD12	1.86	0.55
1:D:824:THR:CA	1:D:838:LEU:HD13	2.36	0.55
1:B:337:ASP:O	1:B:349:HIS:N	2.29	0.55
1:A:804:TYR:O	1:A:808:ILE:HG13	2.06	0.55
2:C:28:GLN:HG3	2:C:64:LYS:HD3	1.87	0.55
1:E:366:SER:O	1:E:370:ARG:NH2	2.39	0.55
1:D:761:LEU:HD12	1:D:762:THR:HG23	1.89	0.55
1:D:821:SER:O	1:D:825:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLU:HB2	1:B:257:THR:HG22	1.87	0.55
1:B:749:LEU:HD21	1:B:757:TRP:CE3	2.42	0.55
1:B:866:MET:HG3	1:B:912:TYR:CE1	2.41	0.55
1:A:860:GLU:HB2	1:A:863:ASN:HB2	1.89	0.55
2:C:23:PHE:HB2	2:C:67:PHE:O	2.07	0.55
1:E:326:ARG:HB2	1:E:329:ASP:OD1	2.07	0.55
1:D:652:PHE:HA	1:D:655:ILE:HG22	1.89	0.55
2:F:13:PHE:CD1	2:F:173:VAL:HG22	2.41	0.55
1:B:821:SER:O	1:B:825:LEU:HG	2.07	0.55
1:A:918:ILE:HG12	1:A:943:PHE:CE2	2.42	0.55
2:C:191:ILE:HG12	2:C:236:GLU:OE1	2.06	0.55
1:E:478:ARG:HG2	1:E:519:MET:HE1	1.88	0.55
1:E:808:ILE:O	1:E:812:GLU:HB3	2.07	0.55
1:E:943:PHE:O	1:E:946:PRO:HD3	2.06	0.55
1:D:500:PHE:HB2	1:D:502:ARG:HE	1.71	0.55
1:B:767:LEU:HD12	1:B:811:PHE:CD2	2.41	0.55
1:B:920:TYR:CE1	1:B:930:MET:HB2	2.41	0.55
1:A:668:GLU:OE2	1:A:760:ARG:NH2	2.31	0.55
1:A:739:ALA:O	1:A:744:PHE:HB2	2.06	0.55
1:A:838:LEU:HD12	1:A:845:LEU:HD11	1.89	0.55
1:A:893:LYS:HD2	1:A:933:PHE:HD1	1.72	0.55
2:C:34:GLN:CG	2:C:57:LYS:HG2	2.36	0.55
1:E:407:ILE:HG13	1:E:589:TYR:CB	2.33	0.55
1:E:868:GLY:HA2	1:E:871:ILE:CG2	2.37	0.55
1:E:973:ASN:CB	1:E:976:MET:HB2	2.34	0.55
1:D:651:ASP:OD1	2:F:2:LYS:HD2	2.07	0.55
1:D:766:GLU:OE1	1:D:766:GLU:N	2.39	0.55
1:D:809:LYS:HD3	1:D:844:LEU:HD23	1.88	0.55
1:D:845:LEU:HB3	1:D:849:ALA:CB	2.37	0.55
1:D:893:LYS:O	1:D:897:ILE:HG13	2.05	0.55
2:F:213:ALA:O	2:F:216:PRO:HD3	2.07	0.55
1:A:359:ARG:O	1:A:363:LEU:HG	2.07	0.55
1:A:784:GLU:O	1:A:787:ILE:HG12	2.07	0.55
2:C:12:TYR:HE1	2:C:176:ARG:HH11	1.53	0.55
1:D:652:PHE:CD2	1:D:684:ILE:HD12	2.42	0.55
1:B:974:LYS:HZ1	1:B:978:HIS:HB2	1.72	0.55
1:A:354:PHE:HZ	1:A:359:ARG:HG3	1.72	0.55
1:D:14:LYS:O	1:D:18:VAL:HG23	2.06	0.55
1:B:284:GLU:OE1	1:B:284:GLU:N	2.40	0.55
1:B:843:PRO:HD3	1:B:871:ILE:HD12	1.87	0.55
1:A:514:ARG:O	1:A:518:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:ILE:O	1:E:485:ILE:HG13	2.06	0.55
1:D:56:TYR:CZ	1:D:135:ASP:HB3	2.42	0.55
1:D:203:LEU:O	1:D:207:ILE:HG13	2.06	0.55
1:D:613:ARG:HH21	1:D:660:LYS:H	1.55	0.55
1:B:519:MET:HA	1:B:519:MET:CE	2.37	0.55
1:B:769:LYS:O	1:B:769:LYS:HD2	2.05	0.55
1:B:788:ASP:OD2	1:B:791:TYR:HB3	2.07	0.55
1:A:205:LYS:HD2	1:A:231:TRP:CE2	2.42	0.55
1:A:667:LEU:HD11	1:A:673:ILE:HD11	1.89	0.55
1:A:866:MET:HE2	1:A:870:ARG:HD2	1.89	0.55
1:E:437:LYS:HG2	1:E:599:CYS:SG	2.47	0.55
1:D:364:LYS:HB2	1:D:385:PHE:CE1	2.41	0.55
1:D:668:GLU:HG2	1:D:673:ILE:HG12	1.88	0.55
1:B:987:ARG:O	1:B:991:SER:HB3	2.07	0.55
1:E:37:SER:HB2	1:E:42:LEU:HD22	1.88	0.55
1:E:879:PRO:O	1:E:883:GLU:HG2	2.06	0.55
1:E:979:HIS:O	1:E:983:VAL:HG12	2.07	0.55
1:D:663:ASP:HA	1:D:666:ASN:HD21	1.72	0.55
2:F:175:TYR:HB2	2:F:193:ILE:HB	1.89	0.55
1:B:513:ALA:O	1:B:517:ARG:HG3	2.07	0.54
1:B:775:ILE:HG22	1:B:808:ILE:HD11	1.88	0.54
1:A:283:LEU:O	1:A:287:SER:OG	2.22	0.54
2:C:45:ILE:CG2	2:C:48:LYS:HB3	2.37	0.54
1:D:407:ILE:HD12	1:D:407:ILE:O	2.08	0.54
1:B:840:LYS:NZ	2:C:226:THR:HG21	2.22	0.54
1:B:894:VAL:O	1:B:898:VAL:HG23	2.07	0.54
1:A:133:ASN:HB3	1:A:135:ASP:OD1	2.07	0.54
1:A:406:SER:HB2	2:C:1:MET:HE1	1.89	0.54
1:A:783:ALA:HA	1:A:786:HIS:NE2	2.23	0.54
1:A:914:SER:O	1:A:918:ILE:N	2.30	0.54
1:E:7:GLU:N	1:E:10:ARG:HB3	2.22	0.54
1:E:124:MET:CE	1:E:293:LEU:HD23	2.38	0.54
1:D:132:THR:CG2	1:D:171:ALA:HB2	2.37	0.54
1:D:940:TYR:CE2	1:D:944:VAL:HG21	2.41	0.54
1:B:10:ARG:O	1:B:14:LYS:HG2	2.07	0.54
1:B:305:ASP:O	1:B:309:ILE:HG12	2.07	0.54
1:B:608:PHE:O	1:B:612:ILE:HG12	2.08	0.54
1:E:9:LYS:HD3	1:E:13:GLU:HG3	1.90	0.54
1:D:577:GLY:HA2	2:F:7:ASP:O	2.07	0.54
1:D:894:VAL:O	1:D:898:VAL:HG23	2.07	0.54
1:B:544:PHE:CE2	1:B:550:PHE:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:ASP:OD2	1:B:753:LYS:HE2	2.06	0.54
1:A:919:TRP:HB3	1:A:924:GLU:HB2	1.89	0.54
2:C:230:GLU:OE2	2:C:230:GLU:N	2.32	0.54
1:E:358:GLU:HG2	1:E:396:MET:CE	2.37	0.54
1:E:364:LYS:HA	1:E:370:ARG:NH1	2.22	0.54
1:D:361:PHE:O	1:D:364:LYS:HG2	2.06	0.54
1:B:962:TYR:HB2	1:B:967:LEU:HD21	1.90	0.54
1:A:962:TYR:CE2	1:A:966:LEU:HD23	2.42	0.54
1:E:674:ASP:N	1:E:674:ASP:OD1	2.39	0.54
1:E:721:TYR:O	1:E:760:ARG:NH2	2.38	0.54
1:D:641:LYS:HG2	1:D:641:LYS:O	2.06	0.54
1:D:997:LEU:HD11	1:D:1001:MET:HE1	1.89	0.54
2:F:23:PHE:HB2	2:F:67:PHE:O	2.08	0.54
2:F:40:LYS:H	2:F:40:LYS:HD2	1.72	0.54
1:B:850:LYS:O	1:B:854:LEU:HD12	2.08	0.54
1:E:132:THR:HG22	1:E:170:VAL:CG2	2.37	0.54
1:E:744:PHE:CD1	1:E:745:PRO:HD2	2.43	0.54
1:E:955:ILE:O	1:E:958:TRP:HB2	2.07	0.54
1:D:348:ARG:HE	1:D:351:ASN:ND2	2.05	0.54
1:D:476:ILE:CD1	1:D:546:SER:HB3	2.34	0.54
1:D:665:LYS:HD2	1:D:669:ARG:HH12	1.73	0.54
1:D:768:PRO:HD2	1:D:771:ILE:CG1	2.37	0.54
2:F:12:TYR:HB3	2:F:14:LYS:NZ	2.22	0.54
1:A:755:TYR:CD2	1:A:799:LEU:HD23	2.42	0.54
1:E:613:ARG:HA	1:E:659:PHE:CE1	2.42	0.54
1:E:896:TYR:O	1:E:900:LYS:HG2	2.06	0.54
1:D:308:VAL:HG13	1:D:356:TYR:CB	2.38	0.54
1:D:663:ASP:HA	1:D:666:ASN:ND2	2.22	0.54
1:B:127:ALA:O	1:B:128:HIS:ND1	2.41	0.54
1:A:203:LEU:O	1:A:207:ILE:HG13	2.08	0.54
1:A:325:ILE:HD11	1:A:330:LEU:HG	1.90	0.54
1:A:375:LYS:O	1:A:379:GLU:HG3	2.07	0.54
1:A:665:LYS:HG2	1:A:669:ARG:HH21	1.73	0.54
1:E:207:ILE:O	1:E:211:HIS:HB2	2.07	0.54
1:E:255:ASN:O	1:E:259:ILE:HG13	2.08	0.54
1:E:780:VAL:HG21	1:E:819:ARG:HE	1.72	0.54
1:D:790:ASN:O	1:D:790:ASN:ND2	2.36	0.54
1:B:230:ASN:O	1:B:233:ARG:HG2	2.08	0.54
1:A:699:PHE:CE1	1:A:745:PRO:HD3	2.42	0.54
1:A:752:GLY:O	1:A:756:VAL:HG23	2.08	0.54
2:C:48:LYS:HG3	2:C:49:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:595:LEU:HB3	1:E:603:VAL:CG1	2.37	0.54
1:E:922:LEU:HD21	1:E:966:LEU:CD1	2.35	0.54
1:D:424:PHE:HA	1:D:427:GLU:OE1	2.07	0.54
1:D:704:MET:HG3	1:D:708:PHE:HD2	1.72	0.54
1:D:755:TYR:CZ	1:D:803:ASP:HB3	2.43	0.54
1:D:898:VAL:CG1	1:D:902:LYS:HE3	2.37	0.54
1:B:886:ILE:HD11	1:B:927:ASN:ND2	2.21	0.54
1:A:738:LYS:HG3	1:A:742:PHE:CD2	2.43	0.54
2:C:60:ASN:O	2:C:61:LEU:HD23	2.06	0.54
1:E:183:VAL:HG23	1:E:185:LEU:HG	1.90	0.54
1:E:648:GLU:OE1	1:E:649:TYR:N	2.40	0.54
2:F:14:LYS:HA	2:F:22:VAL:HG23	1.90	0.54
1:A:414:TYR:O	1:A:657:ARG:NH2	2.24	0.53
1:A:998:GLU:HA	1:A:1001:MET:CE	2.38	0.53
1:E:405:THR:HG21	1:E:586:LEU:CD2	2.38	0.53
1:A:693:GLU:O	1:A:697:LYS:HG3	2.08	0.53
1:E:140:THR:O	1:E:144:LYS:HG3	2.07	0.53
1:D:574:TYR:CD1	1:D:639:PHE:HB2	2.43	0.53
2:F:37:SER:HB3	2:F:41:LEU:CD1	2.38	0.53
1:A:64:ASP:O	1:A:68:GLU:HG2	2.08	0.53
1:A:579:SER:O	1:A:583:VAL:HG23	2.08	0.53
1:D:667:LEU:HD23	1:D:673:ILE:HG21	1.90	0.53
1:D:967:LEU:HD22	1:D:1003:TYR:OH	2.08	0.53
1:B:624:GLU:O	1:B:628:THR:HG23	2.08	0.53
1:D:350:LYS:HD3	1:D:350:LYS:H	1.72	0.53
1:B:361:PHE:CD2	1:B:396:MET:HG2	2.43	0.53
1:B:755:TYR:CD2	1:B:799:LEU:HD13	2.40	0.53
1:A:70:LEU:CD2	1:A:95:LYS:HD3	2.38	0.53
1:A:531:MET:HB3	1:A:532:PRO:HD2	1.91	0.53
1:E:419:ASP:OD1	1:E:419:ASP:N	2.41	0.53
1:D:839:PHE:CE2	1:D:853:LEU:HG	2.43	0.53
1:B:974:LYS:NZ	1:B:974:LYS:O	2.38	0.53
1:A:132:THR:OG1	1:A:218:TYR:OH	2.25	0.53
1:A:207:ILE:O	1:A:211:HIS:HB2	2.08	0.53
2:C:28:GLN:CG	2:C:64:LYS:HD3	2.38	0.53
1:E:89:GLN:NE2	1:E:93:ASN:OD1	2.41	0.53
1:E:419:ASP:O	1:E:423:LYS:HE2	2.09	0.53
1:E:776:ASP:O	1:E:780:VAL:HG13	2.07	0.53
1:D:562:THR:OG1	1:D:618:LEU:HD22	2.07	0.53
1:A:777:ASP:OD1	1:A:819:ARG:NH1	2.42	0.53
1:E:383:ALA:HA	1:E:386:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:824:THR:O	1:E:827:LEU:HG	2.09	0.53
1:D:14:LYS:HA	1:D:17:GLU:OE2	2.09	0.53
2:F:199:SER:HB2	2:F:223:LEU:CD1	2.38	0.53
1:E:755:TYR:HB2	1:E:804:TYR:CE2	2.44	0.53
1:E:791:TYR:CE2	1:E:793:GLU:HB2	2.43	0.53
1:E:912:TYR:O	1:E:915:THR:N	2.41	0.53
1:D:19:PHE:CE2	1:D:301:PHE:HB3	2.44	0.53
1:D:414:TYR:HA	1:D:657:ARG:HH12	1.74	0.53
1:D:514:ARG:HD2	1:D:517:ARG:NH1	2.24	0.53
1:D:685:GLU:O	1:D:689:VAL:HG12	2.09	0.53
1:D:832:GLN:HE22	1:D:857:LYS:HE2	1.74	0.53
1:B:59:TRP:O	1:B:63:VAL:HG23	2.08	0.53
1:B:275:ILE:HD13	1:B:288:ALA:CB	2.39	0.53
1:B:976:MET:O	1:B:980:VAL:HG23	2.09	0.53
1:D:480:ARG:HD2	1:D:602:SER:OG	2.09	0.53
1:D:821:SER:HA	1:D:845:LEU:HD22	1.91	0.53
1:B:769:LYS:HA	1:B:772:ILE:CD1	2.38	0.53
1:A:43:VAL:HG22	1:A:128:HIS:HB2	1.90	0.53
1:A:225:ILE:HD13	1:A:245:PHE:HE1	1.73	0.53
1:A:930:MET:HA	1:A:933:PHE:CD2	2.44	0.53
2:C:49:PRO:O	2:C:50:LEU:HD13	2.09	0.53
1:D:652:PHE:O	1:D:655:ILE:HG22	2.09	0.53
1:B:555:THR:HB	1:A:556:VAL:HG21	1.90	0.52
1:A:87:ILE:HB	1:A:88:PRO:HD3	1.90	0.52
1:A:123:ALA:HB2	1:A:145:ARG:HH12	1.73	0.52
1:A:834:GLN:O	1:A:838:LEU:HD23	2.09	0.52
1:E:669:ARG:NH2	1:D:571:GLU:HG2	2.24	0.52
1:B:18:VAL:O	1:B:22:LEU:HG	2.09	0.52
1:B:660:LYS:HD3	2:C:203:GLU:OE2	2.09	0.52
1:B:828:THR:OG1	1:B:830:ASP:OD1	2.22	0.52
1:A:758:LEU:HD21	1:A:775:ILE:CD1	2.39	0.52
1:A:775:ILE:HG22	1:A:808:ILE:HD11	1.89	0.52
1:A:954:PHE:CE2	1:A:983:VAL:HG11	2.44	0.52
2:C:173:VAL:HG23	2:C:198:VAL:HG21	1.91	0.52
1:E:964:ASP:OD1	1:E:964:ASP:N	2.42	0.52
1:D:64:ASP:OD1	1:D:74:PRO:HB3	2.08	0.52
1:B:14:LYS:O	1:B:18:VAL:HG23	2.08	0.52
1:A:454:LEU:O	1:A:458:ILE:HG13	2.09	0.52
2:C:207:SER:HB2	2:C:211:GLY:HA2	1.91	0.52
1:E:62:LEU:HD22	1:E:66:TYR:CE2	2.44	0.52
1:E:688:LEU:HB3	1:E:736:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:694:GLU:O	1:E:698:GLN:HG2	2.09	0.52
1:E:772:ILE:HB	1:E:808:ILE:HG23	1.91	0.52
1:D:504:TYR:HB3	1:D:706:VAL:HG21	1.92	0.52
1:D:922:LEU:HD21	1:D:966:LEU:CB	2.38	0.52
1:B:752:GLY:O	1:B:756:VAL:HG23	2.09	0.52
1:B:984:LEU:HD21	1:B:996:TYR:O	2.10	0.52
1:A:787:ILE:HA	1:A:831:LYS:NZ	2.24	0.52
1:A:962:TYR:OH	1:A:966:LEU:HB3	2.09	0.52
1:E:987:ARG:NH1	1:E:987:ARG:HA	2.25	0.52
1:D:588:LEU:HD13	1:D:612:ILE:HG12	1.91	0.52
1:D:987:ARG:HB3	1:D:996:TYR:CD2	2.43	0.52
1:D:824:THR:CG2	1:D:853:LEU:HD13	2.40	0.52
1:B:858:SER:O	1:B:860:GLU:HG3	2.10	0.52
1:A:893:LYS:HD2	1:A:933:PHE:CD1	2.45	0.52
2:C:227:ASP:OD1	2:C:228:THR:HG23	2.10	0.52
1:D:959:LEU:H	1:D:959:LEU:HD12	1.74	0.52
1:D:984:LEU:HD12	1:D:984:LEU:H	1.74	0.52
1:B:664:ILE:O	1:B:668:GLU:HG3	2.10	0.52
1:B:755:TYR:HB2	1:B:804:TYR:CZ	2.45	0.52
1:A:366:SER:OG	1:A:369:GLU:HG3	2.09	0.52
1:A:755:TYR:HD2	1:A:799:LEU:HD23	1.74	0.52
1:A:916:PHE:HA	1:A:919:TRP:HE3	1.74	0.52
2:C:15:ARG:HG2	2:C:16:LYS:H	1.74	0.52
1:E:558:LEU:HG	1:D:559:PHE:CZ	2.45	0.52
1:E:728:LEU:HD13	1:E:736:ILE:HD12	1.90	0.52
1:E:939:GLN:HG2	1:E:943:PHE:CZ	2.44	0.52
1:D:277:SER:HB3	1:D:281:ASP:HB2	1.90	0.52
1:D:477:ASN:O	1:D:481:ILE:N	2.42	0.52
1:D:649:TYR:HD1	1:D:684:ILE:HD13	1.75	0.52
1:D:862:ILE:HB	1:D:865:LEU:HD12	1.90	0.52
2:F:195:PHE:CE1	2:F:232:ALA:HB2	2.44	0.52
1:A:585:LEU:HD13	1:A:619:LEU:HD13	1.90	0.52
1:E:305:ASP:OD1	1:E:306:ASP:N	2.43	0.52
1:E:669:ARG:O	1:E:669:ARG:HG2	2.10	0.52
1:D:520:THR:HG23	1:D:521:ASN:OD1	2.10	0.52
1:B:222:ASP:O	1:B:226:ASN:ND2	2.37	0.52
1:B:500:PHE:HB3	1:B:504:TYR:HE2	1.75	0.52
1:B:840:LYS:O	1:B:871:ILE:HD11	2.10	0.52
1:A:639:PHE:CD2	1:A:642:LYS:HG2	2.45	0.52
1:A:818:LYS:O	1:A:822:GLU:HG3	2.10	0.52
1:A:910:ASN:HB3	1:A:912:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:TYR:CZ	1:D:532:PRO:HG3	2.45	0.52
1:E:513:ALA:O	1:E:517:ARG:HG3	2.10	0.52
1:E:963:ASN:HB2	2:F:42:ARG:NH1	2.24	0.52
1:D:684:ILE:O	1:D:688:LEU:HG	2.10	0.52
1:D:826:CYS:O	1:D:831:LYS:NZ	2.37	0.52
1:B:364:LYS:HE3	1:B:385:PHE:HE1	1.75	0.52
1:B:368:ASP:O	1:B:371:SER:OG	2.16	0.52
1:B:767:LEU:HD22	1:B:772:ILE:HD12	1.92	0.52
1:B:819:ARG:NH1	1:B:819:ARG:HB2	2.24	0.52
1:A:476:ILE:HD11	1:A:546:SER:HB3	1.91	0.52
1:A:692:ALA:O	1:A:695:ILE:HG22	2.10	0.52
1:A:939:GLN:HB3	1:A:958:TRP:CD2	2.44	0.52
1:E:742:PHE:CE1	1:E:778:PHE:HB2	2.37	0.52
1:E:956:PRO:HB3	1:E:987:ARG:CD	2.39	0.52
1:D:433:GLU:OE1	1:D:433:GLU:N	2.40	0.52
1:D:478:ARG:O	1:D:481:ILE:HG22	2.10	0.52
1:D:828:THR:HB	1:D:830:ASP:OD1	2.09	0.52
1:D:994:LYS:O	1:D:998:GLU:HB2	2.10	0.52
1:A:847:THR:HA	1:A:850:LYS:HB2	1.92	0.51
1:D:15:LEU:HG	1:D:292:LEU:HD12	1.92	0.51
2:F:34:GLN:CG	2:F:57:LYS:HG2	2.40	0.51
1:B:558:LEU:HD22	1:B:618:LEU:HD23	1.92	0.51
1:A:83:GLU:O	1:A:87:ILE:HG12	2.10	0.51
1:A:338:TYR:CZ	1:A:357:MET:HB2	2.44	0.51
1:E:338:TYR:CE2	1:E:357:MET:HB2	2.45	0.51
1:E:649:TYR:O	1:E:653:VAL:HG23	2.09	0.51
1:E:794:VAL:HG12	2:F:223:LEU:HB3	1.93	0.51
1:D:730:GLU:O	1:D:771:ILE:HD11	2.11	0.51
1:B:37:SER:OG	1:B:124:MET:O	2.28	0.51
1:B:329:ASP:O	1:B:333:VAL:HG23	2.11	0.51
1:A:258:LEU:HG	1:A:262:GLU:OE1	2.11	0.51
1:A:785:LYS:O	1:A:785:LYS:HD2	2.10	0.51
1:A:893:LYS:HA	1:A:936:MET:HE3	1.93	0.51
1:E:361:PHE:HD1	1:E:364:LYS:HE2	1.74	0.51
1:E:613:ARG:NH1	1:E:659:PHE:HA	2.25	0.51
1:E:862:ILE:CD1	1:E:884:LEU:HB3	2.39	0.51
1:E:871:ILE:CG2	1:E:873:LEU:HD13	2.40	0.51
1:B:476:ILE:O	1:B:480:ARG:HG2	2.10	0.51
1:A:787:ILE:O	1:A:831:LYS:HE3	2.11	0.51
1:E:310:ASP:OD1	1:E:377:GLN:NE2	2.44	0.51
1:E:645:PHE:HE2	1:E:647:MET:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:648:GLU:HB2	1:E:680:GLU:OE1	2.10	0.51
1:E:699:PHE:CE1	1:E:745:PRO:HD3	2.46	0.51
1:E:752:GLY:HA3	1:E:797:ASN:OD1	2.10	0.51
1:D:439:ALA:CB	1:D:454:LEU:HD23	2.40	0.51
1:D:839:PHE:CE2	1:D:857:LYS:HE3	2.45	0.51
1:B:563:ASN:OD1	1:A:614:ASN:ND2	2.43	0.51
1:B:869:ILE:HD13	1:B:874:ILE:HB	1.93	0.51
1:A:482:TYR:O	1:A:486:THR:HG22	2.10	0.51
1:E:987:ARG:HA	1:E:987:ARG:CZ	2.40	0.51
1:D:892:ARG:O	1:D:895:ASN:ND2	2.43	0.51
1:B:768:PRO:O	1:B:769:LYS:HB3	2.11	0.51
1:A:737:VAL:O	1:A:741:LEU:HG	2.11	0.51
1:A:954:PHE:CZ	1:A:980:VAL:HG22	2.46	0.51
1:E:14:LYS:O	1:E:18:VAL:HG23	2.10	0.51
1:E:985:LYS:HE3	1:D:1005:ILE:HG21	1.91	0.51
1:B:455:TYR:O	1:B:459:ILE:HG13	2.11	0.51
1:A:793:GLU:OE2	1:A:801:SER:HB2	2.11	0.51
1:E:668:GLU:OE2	1:E:725:TYR:OH	2.15	0.51
1:D:9:LYS:HG3	1:D:10:ARG:NH1	2.26	0.51
1:D:230:ASN:HA	1:D:233:ARG:NH1	2.26	0.51
1:D:789:GLN:O	1:D:790:ASN:ND2	2.44	0.51
1:D:839:PHE:HA	1:D:853:LEU:HD21	1.93	0.51
1:A:50:VAL:HG12	1:A:53:LEU:CD1	2.41	0.51
1:A:863:ASN:O	1:A:867:ASN:ND2	2.35	0.51
1:A:873:LEU:O	1:A:874:ILE:HD13	2.11	0.51
1:A:874:ILE:HG21	1:A:881:HIS:HE1	1.75	0.51
2:C:37:SER:HB3	2:C:41:LEU:CD2	2.39	0.51
1:D:660:LYS:O	1:D:664:ILE:HG13	2.11	0.51
1:B:557:LYS:O	1:B:561:LEU:HG	2.11	0.51
1:B:985:LYS:HE3	1:A:1005:ILE:HD11	1.92	0.51
1:A:646:PHE:O	1:A:648:GLU:HG2	2.11	0.51
1:E:985:LYS:CE	1:D:1005:ILE:HG21	2.41	0.51
1:D:649:TYR:O	1:D:653:VAL:HG13	2.10	0.51
1:D:782:GLN:HA	1:D:785:LYS:CG	2.41	0.51
1:D:868:GLY:HA2	1:D:871:ILE:CG1	2.37	0.51
1:B:188:ASP:O	1:B:192:ASN:ND2	2.44	0.51
1:B:469:CYS:O	1:B:473:LEU:HG	2.11	0.51
1:B:483:GLN:O	1:B:487:GLN:HG3	2.10	0.51
1:A:698:GLN:HB3	1:A:704:MET:SD	2.51	0.51
1:A:865:LEU:CA	1:A:869:ILE:HG12	2.41	0.51
1:D:512:LEU:O	1:D:516:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:867:ASN:O	1:D:871:ILE:N	2.43	0.51
1:B:370:ARG:HD3	1:B:381:PHE:CE2	2.45	0.50
1:B:824:THR:HG21	1:B:849:ALA:HB1	1.92	0.50
1:A:980:VAL:O	1:A:984:LEU:HG	2.11	0.50
1:E:487:GLN:HA	1:E:490:THR:HG22	1.92	0.50
1:B:238:ASP:OD1	1:B:239:SER:N	2.40	0.50
1:A:245:PHE:HB3	1:A:268:ILE:HA	1.93	0.50
1:A:469:CYS:O	1:A:473:LEU:HG	2.11	0.50
1:E:139:ASP:N	1:E:139:ASP:OD1	2.44	0.50
1:E:195:GLN:HG2	1:E:196:ASN:OD1	2.11	0.50
1:D:685:GLU:OE2	1:D:728:LEU:HA	2.11	0.50
1:A:46:VAL:O	1:A:131:THR:HA	2.10	0.50
1:D:362:GLU:O	1:D:365:GLU:HG3	2.10	0.50
1:D:986:GLU:HA	1:D:989:LYS:HD2	1.93	0.50
1:B:417:LYS:O	1:B:421:MET:HG3	2.11	0.50
1:B:911:ASP:OD2	2:C:53:LEU:HD12	2.12	0.50
1:A:513:ALA:O	1:A:517:ARG:HG3	2.12	0.50
1:A:864:ASP:O	1:A:868:GLY:N	2.41	0.50
2:C:45:ILE:HG21	2:C:48:LYS:HD3	1.94	0.50
1:E:368:ASP:O	1:E:372:LYS:HG3	2.11	0.50
1:D:29:CYS:HB3	1:D:269:ILE:HD11	1.94	0.50
1:D:579:SER:HB2	1:D:581:ASP:OD1	2.11	0.50
1:D:809:LYS:HE2	1:D:843:PRO:HB3	1.93	0.50
1:A:740:LEU:O	1:A:754:ARG:HD3	2.12	0.50
1:E:370:ARG:HD3	1:E:381:PHE:CE2	2.47	0.50
1:E:411:SER:OG	1:E:596:TYR:HB3	2.10	0.50
1:E:671:CYS:SG	1:E:672:SER:N	2.84	0.50
1:D:447:ARG:HB3	1:D:450:GLU:OE1	2.12	0.50
1:D:588:LEU:CD1	1:D:612:ILE:HG12	2.42	0.50
1:D:812:GLU:HG2	1:D:815:PHE:CB	2.34	0.50
1:D:840:LYS:HD3	1:D:871:ILE:CD1	2.42	0.50
1:B:275:ILE:HD13	1:B:288:ALA:HB2	1.93	0.50
1:B:341:GLU:OE1	1:B:578:MET:HE1	2.12	0.50
1:B:556:VAL:HG21	1:A:552:TYR:CD2	2.47	0.50
1:A:758:LEU:O	1:A:762:THR:HG23	2.11	0.50
1:D:26:VAL:O	1:D:30:ILE:HG12	2.12	0.50
1:D:98:MET:N	1:D:98:MET:SD	2.85	0.50
1:D:500:PHE:O	1:D:502:ARG:HG3	2.12	0.50
1:D:847:THR:HG23	1:D:850:LYS:HE3	1.93	0.50
1:B:516:GLU:O	1:B:520:THR:OG1	2.26	0.50
1:B:777:ASP:O	1:B:780:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:815:PHE:CD2	1:E:844:LEU:HD23	2.47	0.50
1:D:652:PHE:CZ	1:D:688:LEU:HD21	2.46	0.50
1:D:866:MET:HE3	1:D:915:THR:HG21	1.93	0.50
2:F:34:GLN:HG2	2:F:57:LYS:HG2	1.93	0.50
1:B:553:ASP:HA	1:A:552:TYR:HH	1.76	0.50
1:A:308:VAL:HG21	1:A:354:PHE:HE2	1.77	0.50
1:A:833:LYS:HA	1:A:836:ASP:OD2	2.12	0.50
1:A:919:TRP:HD1	1:A:922:LEU:HD21	1.77	0.50
1:A:980:VAL:HA	1:A:983:VAL:HG12	1.94	0.50
1:E:704:MET:HE3	1:E:709:TYR:HA	1.94	0.50
1:E:705:ASN:OD1	1:E:708:PHE:N	2.34	0.50
1:E:755:TYR:HB2	1:E:804:TYR:HE2	1.76	0.50
1:E:842:LEU:CD2	1:E:850:LYS:HG2	2.41	0.50
1:E:945:ASP:OD2	1:E:948:ASN:HB2	2.12	0.50
1:D:489:VAL:HG13	1:D:505:LYS:HE3	1.94	0.50
1:B:717:LYS:HB3	1:B:757:TRP:HH2	1.77	0.50
1:A:288:ALA:O	1:A:292:LEU:HD13	2.12	0.50
1:E:54:SER:OG	1:E:113:PRO:O	2.17	0.50
1:E:337:ASP:HB3	1:E:350:LYS:C	2.33	0.50
1:E:804:TYR:O	1:E:808:ILE:HD12	2.11	0.50
1:E:996:TYR:O	1:E:999:ILE:HG12	2.11	0.50
1:D:967:LEU:HA	1:D:970:ILE:HB	1.93	0.50
2:F:227:ASP:OD1	2:F:228:THR:HG23	2.11	0.50
1:B:235:LEU:HD23	1:B:240:PHE:CD2	2.47	0.49
1:B:861:ASN:OD1	1:B:862:ILE:N	2.45	0.49
1:A:665:LYS:HG2	1:A:669:ARG:NH2	2.27	0.49
1:A:901:GLU:HB2	1:A:902:LYS:HZ3	1.77	0.49
1:E:755:TYR:CE1	1:E:807:LEU:HD23	2.47	0.49
1:E:785:LYS:HD3	1:E:791:TYR:CE1	2.47	0.49
1:E:893:LYS:NZ	1:E:933:PHE:HA	2.27	0.49
1:E:954:PHE:CE2	1:E:983:VAL:HG11	2.47	0.49
1:D:133:ASN:HB3	1:D:135:ASP:OD1	2.12	0.49
1:D:581:ASP:OD2	1:D:622:LYS:HG2	2.12	0.49
1:D:613:ARG:HH22	1:D:664:ILE:HG13	1.76	0.49
1:D:790:ASN:HD22	1:D:790:ASN:C	2.14	0.49
1:D:980:VAL:HG22	1:D:984:LEU:CD1	2.40	0.49
1:B:54:SER:OG	1:B:115:ASN:ND2	2.44	0.49
1:B:449:GLU:HG3	1:B:511:PHE:CZ	2.48	0.49
1:A:768:PRO:HB2	1:A:771:ILE:HG12	1.95	0.49
1:A:939:GLN:HA	1:A:942:PHE:HB3	1.93	0.49
1:E:122:LEU:HD12	1:E:145:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:866:MET:HG3	1:E:912:TYR:CE1	2.48	0.49
1:D:91:PHE:CE2	1:D:95:LYS:HG3	2.47	0.49
1:D:325:ILE:HD13	1:D:330:LEU:HG	1.94	0.49
1:D:421:MET:HB2	1:D:445:LEU:HD11	1.94	0.49
1:A:741:LEU:HB3	1:A:778:PHE:CD1	2.47	0.49
1:A:742:PHE:O	1:A:744:PHE:N	2.46	0.49
1:A:922:LEU:HB2	1:A:969:LYS:HZ2	1.76	0.49
1:A:928:SER:O	1:A:931:GLU:HG2	2.12	0.49
1:A:984:LEU:O	1:A:988:VAL:HG23	2.11	0.49
1:E:10:ARG:O	1:E:14:LYS:HG2	2.12	0.49
1:E:358:GLU:HG2	1:E:396:MET:HE1	1.93	0.49
1:E:862:ILE:HG13	1:E:888:TYR:HB2	1.93	0.49
1:D:756:VAL:HG22	1:D:799:LEU:CD1	2.42	0.49
1:B:775:ILE:CG2	1:B:808:ILE:HD11	2.42	0.49
1:A:132:THR:CG2	1:A:171:ALA:HB2	2.42	0.49
1:A:565:VAL:O	1:A:569:MET:HG3	2.12	0.49
1:A:664:ILE:O	1:A:668:GLU:HG3	2.12	0.49
1:A:847:THR:HA	1:A:850:LYS:HD2	1.93	0.49
1:E:669:ARG:HH22	1:D:571:GLU:HG2	1.77	0.49
2:F:23:PHE:CD1	2:F:66:ALA:HB1	2.48	0.49
1:B:562:THR:CG2	1:B:618:LEU:HD13	2.42	0.49
1:B:595:LEU:HD23	1:B:600:LEU:HD12	1.94	0.49
1:A:29:CYS:O	1:A:33:ILE:HG13	2.13	0.49
1:A:693:GLU:OE1	1:A:697:LYS:HD3	2.13	0.49
1:A:802:ARG:NH1	1:A:802:ARG:HB3	2.27	0.49
1:D:532:PRO:O	1:D:536:GLN:HG3	2.12	0.49
1:A:920:TYR:CD2	1:A:944:VAL:HG22	2.47	0.49
1:E:173:ASP:OD2	1:E:175:ARG:HG3	2.12	0.49
1:D:83:GLU:HG2	1:D:86:ARG:NH2	2.28	0.49
1:D:317:SER:OG	1:D:318:PRO:HD3	2.11	0.49
1:D:954:PHE:CE2	1:D:956:PRO:HA	2.48	0.49
2:F:15:ARG:HG2	2:F:16:LYS:H	1.77	0.49
2:F:63:VAL:HG22	2:F:218:ILE:HB	1.94	0.49
1:B:363:LEU:HD23	1:B:369:GLU:HB2	1.94	0.49
1:B:962:TYR:HB2	1:B:967:LEU:CD2	2.43	0.49
1:A:449:GLU:HG3	1:A:511:PHE:CE1	2.48	0.49
1:A:939:GLN:HB3	1:A:958:TRP:CE2	2.48	0.49
1:E:495:LEU:HG	1:E:499:THR:HG23	1.95	0.49
1:E:695:ILE:HG23	1:E:699:PHE:CD1	2.47	0.49
1:D:459:ILE:HD11	1:D:475:GLN:HA	1.94	0.49
1:D:869:ILE:HG23	1:D:875:ASP:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:948:ASN:N	1:D:948:ASN:OD1	2.46	0.49
1:B:23:ASP:O	1:B:27:VAL:HG23	2.13	0.49
1:B:674:ASP:OD1	1:B:674:ASP:N	2.44	0.49
1:B:977:LYS:HG3	1:B:1004:PHE:CE1	2.48	0.49
1:A:861:ASN:O	1:A:862:ILE:HD13	2.12	0.49
1:E:904:ILE:HG12	2:F:235:ILE:HG12	1.95	0.49
1:D:350:LYS:O	1:D:351:ASN:HB2	2.13	0.49
1:D:385:PHE:O	1:D:389:GLU:HG3	2.13	0.49
1:D:485:ILE:O	1:D:489:VAL:HG23	2.12	0.49
1:D:749:LEU:HD12	1:D:753:LYS:HB2	1.95	0.49
1:D:862:ILE:HG12	1:D:888:TYR:CB	2.43	0.49
1:B:305:ASP:HA	1:B:308:VAL:HG22	1.94	0.49
1:A:963:ASN:OD1	1:A:966:LEU:HD22	2.13	0.49
1:E:463:ILE:HD12	1:D:143:TRP:HD1	1.77	0.49
1:E:835:ILE:HG22	1:E:857:LYS:HD2	1.94	0.49
1:D:57:PRO:HG2	1:D:107:PHE:O	2.13	0.49
1:D:956:PRO:CG	1:D:984:LEU:HG	2.42	0.49
1:B:487:GLN:HA	1:B:490:THR:CG2	2.42	0.49
1:A:842:LEU:CD2	1:A:873:LEU:HD22	2.43	0.49
1:E:454:LEU:O	1:E:458:ILE:HG13	2.12	0.49
1:E:859:VAL:HG21	1:E:874:ILE:HD11	1.95	0.49
1:D:46:VAL:HG22	1:D:121:ILE:HD13	1.94	0.49
1:B:845:LEU:O	1:B:850:LYS:HE3	2.13	0.48
1:A:86:ARG:O	1:A:90:ILE:HG13	2.12	0.48
1:A:319:LEU:HD13	1:A:325:ILE:HD13	1.95	0.48
1:E:424:PHE:O	1:E:427:GLU:HG3	2.13	0.48
1:E:506:PRO:HG2	1:E:507:PHE:CD2	2.48	0.48
1:E:559:PHE:CZ	1:D:558:LEU:HD23	2.47	0.48
1:E:578:MET:HG2	1:E:582:ILE:CG2	2.43	0.48
1:E:780:VAL:HG21	1:E:819:ARG:HH21	1.78	0.48
1:E:904:ILE:CG2	2:F:233:VAL:HG13	2.43	0.48
2:F:59:ILE:HB	2:F:222:ALA:HB2	1.95	0.48
1:B:924:GLU:OE1	2:C:50:LEU:HA	2.13	0.48
1:A:577:GLY:HA2	2:C:7:ASP:O	2.13	0.48
1:A:920:TYR:HE2	1:A:930:MET:HB3	1.77	0.48
1:A:995:ARG:HD2	1:A:998:GLU:CB	2.39	0.48
1:A:1001:MET:SD	1:A:1002:ASN:N	2.87	0.48
1:E:483:GLN:O	1:E:487:GLN:HG3	2.14	0.48
1:D:815:PHE:CD2	1:D:844:LEU:HD22	2.48	0.48
2:F:13:PHE:HD2	2:F:22:VAL:HB	1.77	0.48
1:A:899:GLU:CB	1:A:904:ILE:HG22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:ARG:HH21	1:A:990:ASN:HB2	1.77	0.48
1:E:666:ASN:HA	1:E:669:ARG:NH1	2.29	0.48
1:E:805:GLY:HA2	1:E:808:ILE:CD1	2.42	0.48
1:E:841:LEU:O	1:E:845:LEU:HG	2.12	0.48
1:D:97:GLU:HB3	1:D:98:MET:HE1	1.95	0.48
1:D:863:ASN:HA	1:D:912:TYR:HE2	1.78	0.48
1:A:919:TRP:HA	1:A:922:LEU:HD23	1.95	0.48
1:E:790:ASN:OD1	1:E:790:ASN:N	2.46	0.48
1:D:132:THR:HG22	1:D:171:ALA:HB2	1.94	0.48
1:D:304:LYS:HE2	1:D:306:ASP:OD1	2.13	0.48
1:B:372:LYS:HD3	1:B:372:LYS:N	2.28	0.48
1:B:832:GLN:OE1	1:B:832:GLN:N	2.47	0.48
1:A:312:ILE:HD11	1:A:356:TYR:O	2.13	0.48
1:A:786:HIS:CA	1:A:791:TYR:HB3	2.42	0.48
1:A:837:PHE:O	1:A:840:LYS:HG3	2.12	0.48
1:E:148:TYR:HB3	1:D:530:GLY:O	2.13	0.48
1:D:407:ILE:HD11	2:F:2:LYS:H	1.78	0.48
1:A:15:LEU:HD22	1:A:292:LEU:CD1	2.43	0.48
1:A:673:ILE:CG2	1:A:676:ILE:HB	2.44	0.48
1:A:757:TRP:O	1:A:761:LEU:HD13	2.13	0.48
1:E:667:LEU:HD12	1:E:668:GLU:N	2.27	0.48
1:E:762:THR:HG22	1:E:811:PHE:CE2	2.48	0.48
1:D:376:LYS:HA	1:D:379:GLU:CD	2.34	0.48
1:D:788:ASP:O	1:D:790:ASN:N	2.46	0.48
1:D:827:LEU:HD21	1:D:834:GLN:CG	2.43	0.48
1:B:901:GLU:HB2	1:B:902:LYS:NZ	2.28	0.48
1:A:369:GLU:HA	1:A:372:LYS:HE3	1.95	0.48
1:A:922:LEU:HD12	1:A:965:LYS:CD	2.38	0.48
1:A:954:PHE:HE2	1:A:983:VAL:HG11	1.79	0.48
1:E:487:GLN:O	1:E:491:GLN:HG3	2.13	0.48
1:D:827:LEU:CD1	1:D:835:ILE:HA	2.42	0.48
1:B:16:LYS:NZ	1:B:301:PHE:HA	2.29	0.48
1:A:30:ILE:HG23	1:A:293:LEU:CD2	2.36	0.48
1:A:75:LYS:HE3	1:A:83:GLU:OE1	2.14	0.48
1:A:350:LYS:HG3	1:A:351:ASN:H	1.77	0.48
1:A:516:GLU:O	1:A:520:THR:OG1	2.27	0.48
1:A:724:LYS:O	1:A:764:CYS:HB2	2.13	0.48
1:A:964:ASP:O	1:A:967:LEU:HB2	2.12	0.48
1:E:825:LEU:HA	1:E:852:HIS:CD2	2.48	0.48
1:B:558:LEU:CD2	1:B:615:SER:HA	2.43	0.48
1:B:797:ASN:HB3	2:C:56:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ASN:HB3	1:A:912:TYR:CZ	2.48	0.48
2:C:173:VAL:CG2	2:C:198:VAL:HG21	2.43	0.48
2:C:178:ILE:HG23	2:C:189:SER:O	2.14	0.48
1:E:815:PHE:CE2	1:E:817:SER:HB2	2.48	0.48
1:E:984:LEU:HD11	1:E:1000:LEU:HG	1.95	0.48
1:D:376:LYS:HA	1:D:379:GLU:OE1	2.14	0.48
1:D:415:HIS:O	1:D:417:LYS:HG3	2.14	0.48
1:D:605:PHE:HB3	1:D:607:GLU:OE1	2.13	0.48
1:D:929:LYS:HA	1:D:932:GLU:OE2	2.14	0.48
1:D:959:LEU:HA	1:D:962:TYR:CD2	2.49	0.48
1:B:558:LEU:HD11	1:A:559:PHE:CE2	2.49	0.48
1:B:689:VAL:HG12	1:B:693:GLU:OE2	2.14	0.48
1:B:818:LYS:O	1:B:822:GLU:HG3	2.13	0.48
1:B:868:GLY:HA3	1:B:874:ILE:CD1	2.44	0.48
1:A:476:ILE:CD1	1:A:546:SER:HB3	2.43	0.48
1:A:634:LEU:HD11	2:C:32:PHE:CE2	2.49	0.48
1:E:346:VAL:HB	1:E:396:MET:SD	2.54	0.48
1:E:497:LEU:H	1:E:497:LEU:HD22	1.78	0.48
1:E:578:MET:HG2	1:E:582:ILE:HG23	1.96	0.48
1:E:978:HIS:O	1:E:981:ILE:HG22	2.14	0.48
1:D:839:PHE:CD2	1:D:853:LEU:HG	2.49	0.48
1:A:534:GLU:O	1:A:538:LYS:HD3	2.13	0.47
1:A:978:HIS:O	1:A:982:GLU:HG3	2.13	0.47
1:E:839:PHE:HB2	1:E:853:LEU:HD11	1.96	0.47
1:E:1000:LEU:HD22	1:E:1000:LEU:O	2.14	0.47
1:D:228:LEU:O	1:D:232:VAL:HG23	2.14	0.47
1:D:690:GLY:O	1:D:693:GLU:HG3	2.13	0.47
1:D:781:LEU:O	1:D:785:LYS:HG2	2.14	0.47
1:D:956:PRO:CD	1:D:987:ARG:HG3	2.38	0.47
1:B:203:LEU:O	1:B:207:ILE:HG13	2.15	0.47
1:B:405:THR:HG21	1:B:586:LEU:HD22	1.96	0.47
1:B:869:ILE:CD1	1:B:874:ILE:HB	2.43	0.47
1:A:49:GLY:HA3	1:A:217:GLY:CA	2.44	0.47
1:A:942:PHE:HA	1:A:949:PHE:CG	2.49	0.47
1:E:308:VAL:O	1:E:312:ILE:HB	2.15	0.47
1:E:911:ASP:O	1:E:915:THR:HG23	2.14	0.47
1:E:950:ASP:N	1:E:950:ASP:OD1	2.46	0.47
1:D:717:LYS:HG2	1:D:757:TRP:CH2	2.49	0.47
1:D:727:LYS:HE2	1:D:728:LEU:O	2.13	0.47
1:B:222:ASP:OD1	1:B:223:TYR:N	2.47	0.47
1:A:639:PHE:CG	1:A:642:LYS:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LYS:NZ	1:A:643:SER:O	2.44	0.47
1:A:920:TYR:CE2	1:A:944:VAL:HG13	2.50	0.47
1:E:1005:ILE:OXT	1:D:1005:ILE:HG12	2.14	0.47
1:D:306:ASP:HA	1:D:309:ILE:CG2	2.44	0.47
1:D:955:ILE:HG12	1:D:987:ARG:CZ	2.43	0.47
1:D:997:LEU:HD11	1:D:1001:MET:CE	2.45	0.47
1:B:741:LEU:HA	1:B:754:ARG:HD3	1.96	0.47
1:B:759:GLU:OE2	2:C:38:GLU:HG3	2.14	0.47
1:A:85:LEU:O	1:A:187:GLU:HB3	2.14	0.47
1:E:24:ASN:O	1:E:28:GLU:HG2	2.14	0.47
1:D:683:LYS:HA	1:D:686:GLU:CG	2.42	0.47
1:D:866:MET:HE2	1:D:915:THR:HG21	1.97	0.47
1:B:16:LYS:HZ3	1:B:301:PHE:HA	1.80	0.47
1:B:407:ILE:HG23	1:B:593:ARG:HD2	1.96	0.47
1:B:559:PHE:CD1	1:B:562:THR:HB	2.44	0.47
1:B:772:ILE:HG22	1:B:815:PHE:HE1	1.80	0.47
1:B:842:LEU:HB3	1:B:871:ILE:CG2	2.45	0.47
1:A:246:ILE:HG23	1:A:289:VAL:HG11	1.97	0.47
1:E:551:LEU:HD21	1:E:595:LEU:HD11	1.96	0.47
1:E:922:LEU:HD11	1:E:966:LEU:CD1	2.45	0.47
1:D:324:TYR:CE2	1:D:593:ARG:HD3	2.49	0.47
1:D:413:ALA:HA	1:D:421:MET:HE3	1.96	0.47
1:D:459:ILE:CD1	1:D:475:GLN:HG2	2.44	0.47
1:B:143:TRP:HE1	1:A:463:ILE:HG12	1.80	0.47
1:B:619:LEU:HD23	1:B:645:PHE:HE2	1.80	0.47
1:A:578:MET:HG2	1:A:583:VAL:CG2	2.44	0.47
1:A:579:SER:HB2	1:A:581:ASP:OD1	2.15	0.47
1:A:696:THR:HG23	1:A:743:TYR:CE1	2.50	0.47
1:A:820:LEU:HD12	1:A:821:SER:N	2.30	0.47
1:E:254:GLU:HB2	1:E:257:THR:HG22	1.95	0.47
1:E:302:ILE:HG23	1:E:307:GLU:OE1	2.15	0.47
1:E:364:LYS:HA	1:E:370:ARG:HH12	1.78	0.47
1:E:523:ASN:HB2	1:E:526:ASP:OD1	2.14	0.47
1:E:544:PHE:HZ	1:E:594:PHE:HE2	1.62	0.47
1:E:613:ARG:HD3	1:E:663:ASP:OD2	2.15	0.47
1:E:871:ILE:HG23	1:E:873:LEU:HD13	1.96	0.47
1:D:417:LYS:O	1:D:421:MET:HG3	2.14	0.47
1:D:634:LEU:HD21	2:F:32:PHE:CD2	2.50	0.47
1:D:647:MET:HE2	1:D:651:ASP:CB	2.44	0.47
1:D:780:VAL:HG11	1:D:819:ARG:NH2	2.30	0.47
2:F:40:LYS:HD2	2:F:40:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ASN:HD21	1:B:470:VAL:HB	1.79	0.47
1:B:733:LEU:O	1:B:737:VAL:HG23	2.15	0.47
1:B:758:LEU:O	1:B:762:THR:HG23	2.15	0.47
1:B:767:LEU:HD12	1:B:811:PHE:CG	2.49	0.47
1:B:915:THR:O	1:B:918:ILE:HG22	2.15	0.47
1:A:6:LEU:O	1:A:10:ARG:HG2	2.14	0.47
1:A:50:VAL:HG11	1:A:117:ILE:CG2	2.34	0.47
1:A:308:VAL:HG13	1:A:356:TYR:HB2	1.95	0.47
1:A:317:SER:OG	1:A:318:PRO:HD3	2.15	0.47
1:A:783:ALA:HA	1:A:786:HIS:CD2	2.50	0.47
1:A:786:HIS:HB3	1:A:791:TYR:CD2	2.47	0.47
1:A:984:LEU:HB3	1:A:1000:LEU:HD12	1.97	0.47
2:C:34:GLN:HG2	2:C:57:LYS:HG2	1.96	0.47
1:E:21:MET:CE	1:E:274:LEU:HA	2.45	0.47
1:E:43:VAL:HG22	1:E:128:HIS:H	1.80	0.47
1:E:173:ASP:OD1	1:E:174:PHE:N	2.46	0.47
1:E:657:ARG:HA	1:E:715:GLU:HG3	1.96	0.47
1:D:23:ASP:O	1:D:24:ASN:HB3	2.14	0.47
1:D:225:ILE:O	1:D:229:LEU:HG	2.13	0.47
1:D:688:LEU:HB3	1:D:736:ILE:HD11	1.97	0.47
1:D:824:THR:OG1	1:D:838:LEU:HD22	2.14	0.47
1:D:827:LEU:HD13	1:D:835:ILE:HG12	1.96	0.47
2:F:29:THR:HG22	2:F:62:THR:OG1	2.15	0.47
1:B:260:TYR:O	1:B:264:LYS:HG3	2.15	0.47
1:B:343:ASN:ND2	1:B:578:MET:SD	2.86	0.47
1:B:459:ILE:HG23	1:B:471:TYR:CE1	2.50	0.47
1:A:359:ARG:NH1	1:A:362:GLU:OE1	2.47	0.47
1:A:375:LYS:HA	1:A:375:LYS:HE2	1.97	0.47
1:E:361:PHE:O	1:E:364:LYS:HG2	2.14	0.47
1:E:763:LYS:HB3	2:F:40:LYS:NZ	2.29	0.47
1:D:28:GLU:O	1:D:32:GLU:HG3	2.15	0.47
1:D:92:TYR:HE1	1:D:97:GLU:HG3	1.80	0.47
1:D:761:LEU:HD12	1:D:762:THR:N	2.30	0.47
1:D:904:ILE:HG22	1:D:905:GLN:H	1.79	0.47
1:D:922:LEU:HD23	1:D:969:LYS:CD	2.36	0.47
2:F:189:SER:CA	2:F:239:ARG:HA	2.44	0.47
1:B:143:TRP:NE1	1:A:463:ILE:HG12	2.30	0.47
1:B:984:LEU:CD2	1:B:1000:LEU:HB2	2.44	0.47
1:A:421:MET:O	1:A:425:ILE:HG13	2.15	0.47
1:A:809:LYS:HA	1:A:812:GLU:O	2.15	0.47
1:A:881:HIS:HA	1:A:884:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:GLN:OE1	2:F:206:MET:HA	2.14	0.47
1:E:646:PHE:HE1	1:E:679:GLY:HA3	1.79	0.47
1:D:863:ASN:HA	1:D:912:TYR:CE2	2.49	0.47
1:D:956:PRO:O	1:D:960:LYS:HE3	2.14	0.47
1:B:9:LYS:H	1:B:10:ARG:NH1	2.12	0.47
1:B:270:ASP:O	1:B:274:LEU:HG	2.15	0.47
1:B:713:ILE:HG12	1:B:748:ASP:OD2	2.15	0.47
1:E:324:TYR:CE2	1:E:593:ARG:HD3	2.50	0.47
1:E:344:GLY:O	1:E:394:ILE:HD12	2.15	0.47
1:E:347:VAL:HG12	1:E:349:HIS:CD2	2.50	0.47
1:D:155:GLU:OE2	1:D:199:LEU:N	2.26	0.47
1:D:755:TYR:HB2	1:D:804:TYR:CZ	2.50	0.47
2:F:230:GLU:OE1	2:F:233:VAL:HG22	2.15	0.47
1:B:809:LYS:HE2	1:B:844:LEU:HG	1.97	0.46
1:A:271:ALA:HB2	1:A:289:VAL:HG21	1.97	0.46
1:E:852:HIS:O	1:E:855:SER:OG	2.21	0.46
1:E:859:VAL:HG11	1:E:874:ILE:HD11	1.97	0.46
1:E:949:PHE:CE2	1:E:951:TYR:HA	2.50	0.46
2:F:209:GLU:HB3	2:F:212:ASN:HB3	1.97	0.46
1:A:366:SER:OG	1:A:368:ASP:OD1	2.32	0.46
1:A:889:LEU:O	1:A:893:LYS:HB2	2.14	0.46
1:A:954:PHE:HA	1:A:958:TRP:CZ3	2.50	0.46
1:A:976:MET:O	1:A:980:VAL:HG23	2.15	0.46
1:E:919:TRP:HB3	1:E:924:GLU:HB2	1.97	0.46
1:D:738:LYS:HE2	1:D:743:TYR:CE2	2.48	0.46
1:D:767:LEU:HD13	1:D:775:ILE:HD12	1.98	0.46
1:D:805:GLY:O	1:D:809:LYS:HG2	2.16	0.46
1:D:816:ILE:HG21	1:D:846:SER:HB3	1.95	0.46
1:D:836:ASP:HA	1:D:839:PHE:HB2	1.96	0.46
1:D:966:LEU:O	1:D:969:LYS:HG2	2.16	0.46
1:A:50:VAL:HG13	1:A:286:TYR:CE2	2.51	0.46
1:A:242:LYS:HB3	1:A:265:GLY:O	2.16	0.46
1:A:605:PHE:HB3	1:A:607:GLU:OE1	2.15	0.46
1:A:776:ASP:HB2	1:A:815:PHE:CZ	2.50	0.46
1:E:120:LYS:HB3	1:E:290:MET:HG2	1.97	0.46
1:E:561:LEU:HD13	1:E:584:VAL:CG2	2.46	0.46
1:D:827:LEU:HB2	1:D:856:PHE:CE2	2.51	0.46
1:D:832:GLN:HA	1:D:835:ILE:HD12	1.96	0.46
1:B:168:LEU:HG	1:B:170:VAL:HG12	1.97	0.46
1:B:430:VAL:O	1:B:431:SER:OG	2.34	0.46
1:B:949:PHE:HB3	1:B:951:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:LYS:HA	1:A:936:MET:HE1	1.97	0.46
2:C:13:PHE:CZ	2:C:200:PRO:HG3	2.51	0.46
1:E:173:ASP:N	1:E:183:VAL:HG12	2.31	0.46
1:E:557:LYS:O	1:E:561:LEU:N	2.39	0.46
1:D:817:SER:N	1:D:844:LEU:O	2.43	0.46
1:D:867:ASN:O	1:D:871:ILE:HG23	2.16	0.46
1:D:981:ILE:HD12	1:D:1004:PHE:HZ	1.80	0.46
1:B:140:THR:O	1:B:144:LYS:HG3	2.15	0.46
1:B:908:SER:OG	2:C:229:ASP:HB2	2.15	0.46
1:A:24:ASN:O	1:A:28:GLU:HG3	2.15	0.46
1:A:478:ARG:HA	1:A:481:ILE:HG22	1.97	0.46
1:A:812:GLU:HG3	1:A:814:ASN:ND2	2.31	0.46
1:E:759:GLU:HA	1:E:762:THR:OG1	2.14	0.46
1:E:981:ILE:HG23	1:E:985:LYS:HZ1	1.79	0.46
1:D:66:TYR:CE1	1:D:103:ILE:HD12	2.51	0.46
1:D:439:ALA:CA	1:D:454:LEU:HD23	2.46	0.46
1:D:454:LEU:O	1:D:458:ILE:HG13	2.15	0.46
1:D:460:LEU:O	1:D:460:LEU:HD23	2.15	0.46
1:D:497:LEU:HD12	1:D:498:LEU:N	2.30	0.46
1:D:514:ARG:HA	1:D:517:ARG:HH11	1.80	0.46
1:D:687:TYR:OH	1:D:715:GLU:OE2	2.28	0.46
1:D:717:LYS:HG2	1:D:757:TRP:HH2	1.81	0.46
1:D:780:VAL:HG11	1:D:819:ARG:CZ	2.46	0.46
1:D:842:LEU:HD13	1:D:853:LEU:HD23	1.97	0.46
1:A:369:GLU:HA	1:A:372:LYS:CE	2.46	0.46
1:E:777:ASP:O	1:E:780:VAL:HG22	2.15	0.46
1:B:459:ILE:CD1	1:B:475:GLN:HG2	2.42	0.46
1:B:463:ILE:HD13	1:A:143:TRP:CD1	2.50	0.46
1:B:839:PHE:HA	1:B:853:LEU:HD21	1.97	0.46
1:B:842:LEU:HB3	1:B:871:ILE:HG21	1.97	0.46
2:C:176:ARG:HG3	2:C:176:ARG:NH1	2.31	0.46
1:E:318:PRO:HB3	1:E:538:LYS:HB3	1.96	0.46
1:E:342:VAL:HG11	1:E:587:ARG:HG2	1.98	0.46
1:E:506:PRO:HG2	1:E:507:PHE:CE2	2.51	0.46
1:E:619:LEU:HD11	1:E:645:PHE:CE2	2.50	0.46
1:E:886:ILE:O	1:E:890:GLU:HG2	2.16	0.46
1:D:313:TYR:HD1	1:D:384:LEU:HD11	1.81	0.46
1:D:868:GLY:CA	1:D:871:ILE:HG12	2.38	0.46
1:D:898:VAL:HA	1:D:901:GLU:OE1	2.16	0.46
1:A:663:ASP:N	1:A:663:ASP:OD1	2.46	0.46
1:E:361:PHE:CE1	1:E:395:CYS:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:916:PHE:HA	1:E:919:TRP:CE3	2.51	0.46
1:D:375:LYS:O	1:D:379:GLU:HG3	2.15	0.46
1:D:423:LYS:HB2	1:D:423:LYS:HE2	1.73	0.46
1:D:831:LYS:O	1:D:835:ILE:HG13	2.15	0.46
1:B:675:LYS:HB3	1:B:675:LYS:HE3	1.67	0.46
1:B:728:LEU:HD22	1:B:736:ILE:HD12	1.98	0.46
1:B:885:ILE:O	1:B:889:LEU:HD23	2.15	0.46
1:B:939:GLN:NE2	1:B:962:TYR:OH	2.48	0.46
1:A:14:LYS:O	1:A:18:VAL:HG23	2.16	0.46
1:A:248:THR:HA	1:A:271:ALA:HB3	1.98	0.46
1:A:549:GLN:HA	1:A:552:TYR:CB	2.46	0.46
1:A:829:GLN:OE1	1:A:829:GLN:N	2.36	0.46
1:E:124:MET:HE1	1:E:293:LEU:HD23	1.98	0.46
1:E:455:TYR:CE2	1:E:477:ASN:HB3	2.51	0.46
1:E:512:LEU:HA	1:E:515:ILE:HG12	1.98	0.46
1:E:673:ILE:HD12	1:E:676:ILE:HG13	1.97	0.46
1:D:631:ILE:H	1:D:631:ILE:HD12	1.81	0.46
1:D:847:THR:HG23	1:D:850:LYS:CE	2.46	0.46
1:D:882:GLU:O	1:D:886:ILE:HG12	2.16	0.46
1:D:920:TYR:HA	1:D:925:ILE:O	2.16	0.46
1:D:933:PHE:O	1:D:936:MET:HE2	2.16	0.46
1:B:376:LYS:O	1:B:380:ARG:HG3	2.16	0.46
1:B:749:LEU:HD11	1:B:757:TRP:CH2	2.51	0.46
1:B:889:LEU:HD21	1:B:916:PHE:CD2	2.50	0.46
1:B:911:ASP:OD1	1:B:911:ASP:N	2.39	0.46
1:A:338:TYR:CD1	1:A:348:ARG:HA	2.51	0.46
1:A:432:ILE:HD12	1:A:470:VAL:HG11	1.98	0.46
1:A:872:GLY:O	1:A:873:LEU:HB3	2.16	0.46
1:E:155:GLU:OE1	1:E:198:PRO:HD2	2.16	0.46
1:E:865:LEU:HD12	1:E:874:ILE:CD1	2.43	0.46
1:B:319:LEU:HD11	1:B:333:VAL:CG2	2.35	0.45
1:B:348:ARG:NH2	1:B:351:ASN:HB3	2.31	0.45
1:A:50:VAL:HG12	1:A:53:LEU:HD11	1.98	0.45
1:A:225:ILE:O	1:A:229:LEU:HG	2.16	0.45
1:A:831:LYS:CG	1:A:834:GLN:H	2.28	0.45
1:A:919:TRP:HA	1:A:922:LEU:HD21	1.97	0.45
1:E:50:VAL:HG23	1:E:217:GLY:HA3	1.98	0.45
1:D:350:LYS:CG	1:D:351:ASN:H	2.29	0.45
1:D:405:THR:O	2:F:3:THR:HA	2.17	0.45
1:E:459:ILE:HG23	1:E:471:TYR:CE1	2.51	0.45
1:E:664:ILE:HA	1:E:667:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:PHE:HB2	1:D:502:ARG:NE	2.31	0.45
1:B:173:ASP:OD1	1:B:174:PHE:N	2.49	0.45
1:B:369:GLU:HA	1:B:372:LYS:HE2	1.98	0.45
1:B:896:TYR:CE1	1:B:936:MET:HA	2.51	0.45
1:A:839:PHE:O	1:A:842:LEU:HB2	2.17	0.45
1:A:889:LEU:HD13	1:A:933:PHE:CE2	2.51	0.45
1:E:780:VAL:O	1:E:784:GLU:HG3	2.16	0.45
1:D:338:TYR:CZ	1:D:357:MET:HB2	2.51	0.45
1:D:652:PHE:CE2	1:D:684:ILE:HG23	2.52	0.45
1:D:886:ILE:HD12	1:D:929:LYS:HB2	1.98	0.45
1:D:920:TYR:HE2	1:D:944:VAL:HA	1.80	0.45
1:B:595:LEU:HD12	1:B:608:PHE:CE1	2.51	0.45
1:A:270:ASP:O	1:A:274:LEU:HD13	2.16	0.45
1:A:745:PRO:HB2	1:A:748:ASP:OD2	2.17	0.45
1:A:812:GLU:HG3	1:A:814:ASN:HD21	1.81	0.45
1:A:832:GLN:HA	1:A:835:ILE:HD12	1.97	0.45
1:A:840:LYS:HA	1:A:871:ILE:CD1	2.46	0.45
1:E:445:LEU:O	1:E:708:PHE:HB2	2.16	0.45
1:E:459:ILE:CD1	1:E:475:GLN:HG2	2.47	0.45
1:E:746:GLU:HA	1:E:749:LEU:O	2.16	0.45
1:D:744:PHE:HB3	1:D:754:ARG:NH1	2.32	0.45
2:F:190:ASP:OD1	2:F:190:ASP:N	2.50	0.45
1:B:131:THR:O	1:B:169:LYS:HA	2.16	0.45
1:A:173:ASP:OD2	1:A:175:ARG:HG3	2.16	0.45
1:A:201:SER:O	1:A:205:LYS:HG3	2.16	0.45
1:A:982:GLU:O	1:A:986:GLU:HG3	2.15	0.45
2:C:60:ASN:N	2:C:60:ASN:OD1	2.48	0.45
1:E:120:LYS:CB	1:E:290:MET:HG2	2.47	0.45
1:E:138:ILE:HG23	1:E:139:ASP:OD1	2.16	0.45
1:E:648:GLU:OE2	1:E:650:TYR:HB2	2.16	0.45
1:D:245:PHE:HD2	1:D:266:LEU:HD22	1.81	0.45
1:D:699:PHE:CB	1:D:743:TYR:HB3	2.47	0.45
1:B:987:ARG:CZ	1:B:991:SER:HB2	2.47	0.45
1:A:19:PHE:CE2	1:A:301:PHE:HB3	2.50	0.45
1:A:860:GLU:CB	1:A:863:ASN:HB2	2.47	0.45
1:A:880:GLU:O	1:A:884:LEU:HG	2.16	0.45
1:E:821:SER:HB2	1:E:849:ALA:CB	2.46	0.45
1:E:867:ASN:O	1:E:871:ILE:HG22	2.17	0.45
1:D:92:TYR:CD2	1:D:186:LYS:HE3	2.51	0.45
1:D:139:ASP:OD1	1:D:139:ASP:N	2.41	0.45
1:D:229:LEU:HD13	1:D:264:LYS:CE	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LYS:HB3	1:D:306:ASP:OD1	2.17	0.45
1:D:957:SER:HA	1:D:960:LYS:CE	2.46	0.45
1:A:70:LEU:HD22	1:D:256:GLU:HG2	1.98	0.45
1:A:406:SER:HB2	2:C:1:MET:CE	2.47	0.45
1:A:767:LEU:HB3	1:A:811:PHE:CE2	2.52	0.45
1:A:779:LEU:HD21	1:A:804:TYR:HB2	1.99	0.45
1:A:781:LEU:HA	1:A:784:GLU:OE1	2.17	0.45
1:E:482:TYR:CG	1:E:519:MET:HG3	2.52	0.45
1:E:963:ASN:HB3	1:E:966:LEU:CD2	2.47	0.45
1:D:338:TYR:CE1	1:D:357:MET:HB2	2.52	0.45
1:D:369:GLU:HA	1:D:372:LYS:CE	2.44	0.45
1:D:549:GLN:HA	1:D:552:TYR:HB2	1.98	0.45
1:D:613:ARG:HG2	1:D:660:LYS:HE2	1.99	0.45
1:D:869:ILE:HA	1:D:875:ASP:OD1	2.17	0.45
1:D:919:TRP:HB3	1:D:925:ILE:CD1	2.47	0.45
1:D:980:VAL:CA	1:D:984:LEU:HD13	2.42	0.45
1:B:699:PHE:CE2	1:B:745:PRO:HD3	2.52	0.45
1:B:772:ILE:HD12	1:B:772:ILE:H	1.82	0.45
1:B:825:LEU:CD2	1:B:849:ALA:HA	2.46	0.45
1:B:911:ASP:OD2	2:C:55:SER:OG	2.34	0.45
2:C:225:ASP:OD1	2:C:226:THR:N	2.48	0.45
1:E:37:SER:OG	1:E:124:MET:O	2.34	0.45
1:E:290:MET:O	1:E:294:ILE:HG13	2.16	0.45
1:E:788:ASP:HB3	1:E:790:ASN:OD1	2.17	0.45
1:D:898:VAL:O	1:D:902:LYS:HG3	2.16	0.45
1:B:99:ALA:O	1:B:103:ILE:HG12	2.17	0.45
1:B:204:MET:O	1:B:208:ILE:HG13	2.17	0.45
1:B:232:VAL:HG22	1:B:240:PHE:CZ	2.51	0.45
1:A:258:LEU:HD11	1:A:268:ILE:HB	1.99	0.45
1:A:533:PHE:CE2	1:A:537:LYS:HE2	2.52	0.45
1:A:720:LEU:O	1:A:761:LEU:HD11	2.17	0.45
1:A:922:LEU:HB2	1:A:969:LYS:NZ	2.32	0.45
1:A:951:TYR:HB3	1:A:979:HIS:CG	2.52	0.45
1:E:424:PHE:O	1:E:438:LYS:HE2	2.16	0.45
1:D:664:ILE:O	1:D:668:GLU:HB2	2.17	0.45
1:B:183:VAL:HG23	1:B:185:LEU:HG	1.98	0.45
1:B:695:ILE:HD11	1:B:716:ALA:HB1	1.99	0.45
1:A:339:HIS:HB2	1:A:347:VAL:HG13	1.98	0.45
1:A:869:ILE:HG22	1:A:874:ILE:HB	1.99	0.45
2:C:34:GLN:HG3	2:C:57:LYS:HE2	1.99	0.45
1:E:483:GLN:O	1:E:486:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:758:LEU:O	1:E:762:THR:OG1	2.35	0.45
1:E:910:ASN:HB3	1:E:912:TYR:CZ	2.52	0.45
1:D:63:VAL:HG13	1:D:87:ILE:HB	1.99	0.45
1:D:728:LEU:CD2	1:D:733:LEU:HD12	2.47	0.45
1:D:728:LEU:HD22	1:D:733:LEU:HD12	1.99	0.45
1:B:356:TYR:CD1	1:B:357:MET:HG2	2.52	0.44
1:A:186:LYS:O	1:A:188:ASP:N	2.50	0.44
1:A:342:VAL:HG12	1:A:586:LEU:HB3	1.99	0.44
1:A:786:HIS:HA	1:A:791:TYR:CB	2.47	0.44
1:A:853:LEU:HD12	1:A:854:LEU:HG	1.97	0.44
1:E:802:ARG:H	1:E:802:ARG:HD2	1.82	0.44
1:E:829:GLN:OE1	1:E:856:PHE:HB3	2.17	0.44
1:E:834:GLN:O	1:E:838:LEU:HD23	2.18	0.44
1:D:409:ILE:HG21	1:D:414:TYR:CG	2.52	0.44
2:F:14:LYS:CG	2:F:21:LEU:HA	2.40	0.44
1:B:150:SER:OG	1:B:163:SER:HB3	2.16	0.44
1:B:625:TYR:HE1	1:B:629:ARG:HD3	1.82	0.44
1:B:652:PHE:CE2	1:B:684:ILE:HG23	2.52	0.44
1:A:317:SER:HA	1:A:320:PHE:CE2	2.52	0.44
1:A:500:PHE:HB3	1:A:502:ARG:HH11	1.82	0.44
1:A:504:TYR:CD1	1:A:706:VAL:HG11	2.52	0.44
1:A:758:LEU:HD21	1:A:775:ILE:HD13	1.98	0.44
1:A:866:MET:HE1	1:A:870:ARG:HH11	1.81	0.44
1:E:821:SER:HB2	1:E:849:ALA:HB2	1.99	0.44
1:D:437:LYS:HB3	1:D:437:LYS:NZ	2.33	0.44
1:D:478:ARG:CA	1:D:481:ILE:HG22	2.42	0.44
1:B:303:THR:O	1:B:304:LYS:HG3	2.18	0.44
1:B:308:VAL:HG11	1:B:354:PHE:HE2	1.82	0.44
1:B:744:PHE:CD1	1:B:745:PRO:HD2	2.52	0.44
1:B:925:ILE:HD12	1:B:925:ILE:O	2.17	0.44
1:A:34:THR:HG23	1:A:297:GLN:HB3	1.99	0.44
1:A:49:GLY:HA3	1:A:217:GLY:HA3	2.00	0.44
1:A:70:LEU:HD23	1:A:95:LYS:HD3	1.99	0.44
1:A:786:HIS:HB3	1:A:791:TYR:HB3	1.98	0.44
2:C:230:GLU:HG2	2:C:230:GLU:O	2.18	0.44
1:E:46:VAL:O	1:E:131:THR:HA	2.17	0.44
1:E:237:LYS:HD2	1:E:237:LYS:C	2.38	0.44
1:D:290:MET:O	1:D:294:ILE:HG13	2.17	0.44
1:D:322:LEU:HD11	1:D:542:LEU:HD11	1.99	0.44
1:D:522:PHE:HE2	1:D:524:ILE:HD13	1.82	0.44
1:D:648:GLU:CG	2:F:2:LYS:HG2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ASP:HA	1:B:350:LYS:H	1.83	0.44
1:B:985:LYS:HB2	1:B:985:LYS:HE2	1.73	0.44
1:A:414:TYR:HA	1:A:657:ARG:HH12	1.83	0.44
1:E:46:VAL:HG13	1:E:50:VAL:HG21	2.00	0.44
1:E:325:ILE:HD12	1:E:325:ILE:O	2.18	0.44
1:E:582:ILE:O	1:E:586:LEU:HG	2.17	0.44
1:E:1000:LEU:CD2	1:E:1004:PHE:HB2	2.46	0.44
1:D:230:ASN:HA	1:D:233:ARG:HH11	1.83	0.44
1:D:301:PHE:O	1:D:302:ILE:HD13	2.18	0.44
1:D:634:LEU:HD11	2:F:32:PHE:CE2	2.53	0.44
1:D:893:LYS:HD2	1:D:933:PHE:HD1	1.83	0.44
1:D:950:ASP:CB	1:D:953:LYS:HE3	2.41	0.44
1:D:981:ILE:HD12	1:D:1004:PHE:CZ	2.53	0.44
1:A:888:TYR:OH	1:A:913:MET:HB3	2.17	0.44
1:E:382:ASN:O	1:E:386:ASN:ND2	2.50	0.44
1:E:669:ARG:HD3	1:D:570:SER:HB2	1.99	0.44
1:D:682:GLU:O	1:D:685:GLU:HB2	2.17	0.44
1:D:888:TYR:CZ	1:D:892:ARG:HG3	2.52	0.44
1:A:364:LYS:NZ	1:A:394:ILE:O	2.47	0.44
1:A:834:GLN:HG3	1:A:838:LEU:CD2	2.46	0.44
1:A:919:TRP:CB	1:A:924:GLU:HB2	2.47	0.44
2:C:178:ILE:HA	2:C:190:ASP:HA	1.98	0.44
1:E:357:MET:HA	1:E:360:PHE:HB3	2.00	0.44
1:E:486:THR:HA	1:E:489:VAL:HG12	1.99	0.44
1:D:235:LEU:HD12	1:D:240:PHE:CD1	2.53	0.44
1:D:350:LYS:HD3	1:D:350:LYS:N	2.33	0.44
1:D:616:MET:HE3	1:D:651:ASP:HA	2.00	0.44
1:D:758:LEU:HA	1:D:761:LEU:CG	2.46	0.44
1:B:29:CYS:O	1:B:33:ILE:HG13	2.17	0.44
1:B:70:LEU:HG	1:B:91:PHE:HD1	1.81	0.44
1:B:87:ILE:HB	1:B:88:PRO:HD3	2.00	0.44
1:B:943:PHE:O	1:B:946:PRO:HD3	2.18	0.44
1:A:809:LYS:HE2	1:A:813:LYS:HA	1.99	0.44
2:C:20:LYS:HZ3	2:C:71:GLU:HG2	1.83	0.44
1:E:645:PHE:CE2	1:E:647:MET:HG2	2.53	0.44
1:E:780:VAL:CG2	1:E:819:ARG:HH21	2.30	0.44
1:E:894:VAL:O	1:E:898:VAL:HG23	2.18	0.44
1:E:963:ASN:H	1:E:966:LEU:HD23	1.82	0.44
1:D:6:LEU:HG	1:D:9:LYS:H	1.81	0.44
1:D:758:LEU:O	1:D:761:LEU:HG	2.18	0.44
1:D:919:TRP:HB3	1:D:925:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:973:ASN:ND2	1:D:976:MET:SD	2.91	0.44
1:B:173:ASP:CG	1:B:175:ARG:HG3	2.38	0.44
1:B:336:TYR:O	1:B:349:HIS:HB3	2.18	0.44
1:B:556:VAL:HG21	1:A:552:TYR:CG	2.53	0.44
1:B:694:GLU:O	1:B:698:GLN:HG2	2.17	0.44
1:A:673:ILE:HG23	1:A:676:ILE:HB	1.99	0.44
1:A:998:GLU:HA	1:A:1001:MET:HE1	1.99	0.44
2:C:9:ALA:HB3	2:C:27:ALA:HB3	2.00	0.44
1:E:619:LEU:HD11	1:E:645:PHE:CZ	2.53	0.44
1:E:755:TYR:CE1	1:E:803:ASP:HB3	2.53	0.44
1:D:442:LEU:HD21	1:D:450:GLU:HB2	2.00	0.44
1:D:974:LYS:HD2	1:D:974:LYS:O	2.18	0.44
1:B:920:TYR:CE1	1:B:944:VAL:HG13	2.53	0.44
1:A:733:LEU:O	1:A:733:LEU:HD22	2.18	0.44
1:A:808:ILE:O	1:A:812:GLU:N	2.49	0.44
1:A:821:SER:O	1:A:824:THR:OG1	2.30	0.44
1:E:664:ILE:O	1:E:667:LEU:HD12	2.17	0.44
1:E:781:LEU:HA	1:E:784:GLU:OE2	2.17	0.44
1:E:809:LYS:O	1:E:812:GLU:N	2.42	0.44
1:E:999:ILE:HA	1:E:1003:TYR:CE1	2.53	0.44
1:D:755:TYR:CD2	1:D:799:LEU:HB3	2.53	0.44
1:D:866:MET:HB2	1:D:919:TRP:CH2	2.53	0.44
1:B:467:ASN:ND2	1:B:470:VAL:HB	2.33	0.43
1:B:694:GLU:OE2	1:B:698:GLN:NE2	2.51	0.43
1:A:727:LYS:HE3	1:A:764:CYS:SG	2.58	0.43
1:A:896:TYR:CD2	1:A:936:MET:HB2	2.53	0.43
1:E:306:ASP:HB3	1:E:377:GLN:OE1	2.18	0.43
1:E:767:LEU:H	1:E:767:LEU:HD12	1.82	0.43
1:E:933:PHE:HB3	1:E:936:MET:CE	2.48	0.43
1:D:117:ILE:O	1:D:121:ILE:HG13	2.17	0.43
1:D:363:LEU:O	1:D:370:ARG:HG3	2.18	0.43
2:F:12:TYR:HB3	2:F:14:LYS:HZ1	1.83	0.43
1:B:580:SER:OG	1:B:622:LYS:HE3	2.18	0.43
1:A:634:LEU:HD11	2:C:32:PHE:CZ	2.53	0.43
1:A:837:PHE:HA	1:A:840:LYS:HG2	2.00	0.43
1:A:881:HIS:CD2	1:A:884:LEU:HD12	2.48	0.43
1:A:924:GLU:O	1:A:925:ILE:HG12	2.18	0.43
2:C:23:PHE:HZ	2:C:220:PHE:HZ	1.63	0.43
1:E:148:TYR:CE2	1:D:532:PRO:HG3	2.53	0.43
1:E:330:LEU:HD12	1:E:330:LEU:HA	1.88	0.43
1:E:942:PHE:O	1:E:946:PRO:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:549:GLN:OE1	1:D:552:TYR:HB3	2.18	0.43
1:D:922:LEU:HD21	1:D:966:LEU:HA	1.99	0.43
1:A:59:TRP:HZ3	1:A:62:LEU:HD23	1.84	0.43
1:A:126:PRO:O	1:A:165:ARG:NH1	2.51	0.43
1:A:780:VAL:HG21	1:A:819:ARG:HH21	1.83	0.43
1:E:809:LYS:HZ2	1:E:844:LEU:HG	1.83	0.43
1:E:960:LYS:HE3	1:E:996:TYR:CE1	2.53	0.43
1:D:235:LEU:CD1	1:D:240:PHE:HB3	2.48	0.43
1:D:634:LEU:HD23	1:D:634:LEU:H	1.83	0.43
1:D:899:GLU:OE1	1:D:905:GLN:HA	2.18	0.43
1:D:930:MET:HG3	1:D:931:GLU:N	2.32	0.43
1:B:486:THR:O	1:B:490:THR:HG22	2.18	0.43
1:B:767:LEU:HD21	1:B:771:ILE:HB	2.00	0.43
1:E:554:ASP:HA	1:E:587:ARG:HH22	1.82	0.43
1:E:554:ASP:HA	1:E:587:ARG:NH2	2.33	0.43
1:E:656:SER:O	1:E:718:ALA:HB3	2.19	0.43
1:E:667:LEU:HD12	1:E:668:GLU:HG3	2.01	0.43
1:E:954:PHE:HZ	1:E:959:LEU:HD21	1.83	0.43
1:D:222:ASP:OD1	1:D:223:TYR:N	2.51	0.43
1:D:652:PHE:CD2	1:D:684:ILE:HG23	2.53	0.43
1:D:692:ALA:O	1:D:695:ILE:HG22	2.17	0.43
1:B:364:LYS:HE3	1:B:385:PHE:CE1	2.51	0.43
1:A:70:LEU:HD21	1:A:95:LYS:HD3	1.99	0.43
1:A:478:ARG:O	1:A:481:ILE:HG22	2.18	0.43
1:A:649:TYR:CD2	1:A:683:LYS:HE2	2.53	0.43
1:A:727:LYS:HE3	1:A:727:LYS:HA	2.00	0.43
1:A:915:THR:HA	1:A:918:ILE:HB	1.98	0.43
1:E:184:VAL:O	1:E:185:LEU:HD23	2.19	0.43
1:E:275:ILE:HD13	1:E:288:ALA:HB2	2.00	0.43
1:E:388:PHE:HD1	1:E:393:VAL:HG11	1.79	0.43
1:E:794:VAL:HG11	2:F:223:LEU:HB3	1.99	0.43
1:D:768:PRO:O	1:D:772:ILE:HG13	2.19	0.43
2:F:59:ILE:HB	2:F:222:ALA:CB	2.48	0.43
1:A:230:ASN:HA	1:A:233:ARG:NH1	2.33	0.43
1:A:309:ILE:HD11	1:A:363:LEU:HD12	2.00	0.43
1:A:997:LEU:O	1:A:997:LEU:HD13	2.19	0.43
1:E:606:HIS:HB2	2:F:205:GLU:OE1	2.17	0.43
1:E:677:ARG:HA	1:E:677:ARG:NE	2.34	0.43
1:D:483:GLN:HA	1:D:486:THR:CG2	2.47	0.43
1:D:939:GLN:HA	1:D:958:TRP:CZ3	2.53	0.43
1:B:220:LEU:HD12	1:B:220:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:TYR:O	1:B:900:LYS:HG2	2.18	0.43
1:A:496:GLY:HA2	1:A:499:THR:HB	2.01	0.43
1:A:581:ASP:OD2	1:A:622:LYS:HG2	2.18	0.43
1:A:634:LEU:HD23	1:A:634:LEU:H	1.84	0.43
1:A:663:ASP:HA	1:A:666:ASN:OD1	2.18	0.43
1:A:672:SER:HB3	1:A:674:ASP:OD1	2.18	0.43
1:A:861:ASN:OD1	1:A:888:TYR:HB2	2.18	0.43
2:C:23:PHE:CD2	2:C:66:ALA:HB1	2.53	0.43
1:E:431:SER:O	1:E:434:ASP:N	2.43	0.43
1:E:549:GLN:HG2	1:E:552:TYR:CB	2.47	0.43
1:D:245:PHE:CD2	1:D:266:LEU:HD22	2.54	0.43
1:D:370:ARG:HD3	1:D:381:PHE:CE1	2.54	0.43
1:D:733:LEU:O	1:D:737:VAL:HG23	2.17	0.43
1:B:558:LEU:HD23	1:B:615:SER:HA	2.01	0.43
1:B:613:ARG:HA	1:B:659:PHE:CE1	2.54	0.43
1:B:776:ASP:HB2	1:B:815:PHE:HZ	1.83	0.43
1:B:911:ASP:HB2	1:B:914:SER:OG	2.18	0.43
1:A:156:GLU:H	1:A:156:GLU:HG3	1.50	0.43
1:A:425:ILE:HA	1:A:438:LYS:HG3	2.00	0.43
1:A:482:TYR:HD1	1:A:515:ILE:HD12	1.84	0.43
1:A:500:PHE:HB3	1:A:502:ARG:NH1	2.34	0.43
1:A:885:ILE:O	1:A:889:LEU:HG	2.19	0.43
1:E:317:SER:HB3	1:E:318:PRO:HD3	2.01	0.43
1:E:677:ARG:HE	1:E:678:PHE:H	1.66	0.43
1:E:755:TYR:HE1	1:E:807:LEU:HD23	1.84	0.43
1:D:717:LYS:HA	1:D:757:TRP:HH2	1.83	0.43
1:D:918:ILE:O	1:D:922:LEU:N	2.47	0.43
1:D:986:GLU:HA	1:D:989:LYS:CD	2.48	0.43
1:B:298:GLU:OE1	1:B:300:LYS:HE3	2.19	0.43
1:B:698:GLN:HG3	1:B:704:MET:SD	2.58	0.43
1:B:893:LYS:HE3	1:B:933:PHE:HD1	1.84	0.43
1:A:549:GLN:HA	1:A:552:TYR:HB2	2.00	0.43
1:A:776:ASP:HB2	1:A:815:PHE:CE1	2.53	0.43
2:C:21:LEU:HD23	2:C:21:LEU:O	2.18	0.43
1:E:21:MET:HE3	1:E:274:LEU:HA	2.01	0.43
1:E:393:VAL:O	1:E:393:VAL:HG13	2.19	0.43
1:D:120:LYS:HD2	1:D:294:ILE:HD12	2.00	0.43
1:A:91:PHE:CE2	1:A:95:LYS:HG3	2.54	0.43
1:A:138:ILE:CG2	1:A:167:LEU:HD11	2.42	0.43
2:C:59:ILE:HB	2:C:222:ALA:HB3	2.01	0.43
1:E:425:ILE:HD13	1:E:442:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:579:SER:O	1:E:583:VAL:HG12	2.19	0.43
1:E:930:MET:HB3	1:E:940:TYR:OH	2.19	0.43
1:D:270:ASP:O	1:D:274:LEU:HD13	2.19	0.43
1:D:284:GLU:HA	1:D:287:SER:OG	2.19	0.43
1:D:828:THR:HG22	1:D:829:GLN:H	1.83	0.43
1:D:861:ASN:OD1	1:D:863:ASN:HB2	2.19	0.43
1:D:946:PRO:HB3	1:D:973:ASN:HD21	1.84	0.43
2:F:225:ASP:OD1	2:F:226:THR:N	2.46	0.43
1:B:940:TYR:CE2	1:B:944:VAL:HG21	2.54	0.42
1:A:882:GLU:O	1:A:886:ILE:HG12	2.18	0.42
1:A:987:ARG:HA	1:A:987:ARG:NE	2.34	0.42
1:E:203:LEU:O	1:E:207:ILE:HG13	2.19	0.42
1:E:548:ASN:ND2	2:F:209:GLU:HG3	2.34	0.42
1:D:6:LEU:HD12	1:D:7:GLU:H	1.84	0.42
1:D:649:TYR:HA	1:D:684:ILE:CD1	2.36	0.42
1:D:728:LEU:HB3	1:D:733:LEU:HD13	2.01	0.42
1:A:257:THR:OG1	1:D:71:TYR:OH	2.27	0.42
1:A:270:ASP:HB3	1:A:273:SER:OG	2.18	0.42
1:A:755:TYR:HB2	1:A:804:TYR:CZ	2.54	0.42
1:D:737:VAL:HG22	1:D:761:LEU:CD2	2.50	0.42
1:D:853:LEU:HD12	1:D:853:LEU:HA	1.88	0.42
1:B:343:ASN:HD21	1:B:578:MET:CG	2.32	0.42
1:B:348:ARG:HH22	1:B:351:ASN:HB3	1.84	0.42
1:B:607:GLU:OE2	2:C:208:LEU:HB2	2.19	0.42
1:B:961:ASN:OD1	1:B:961:ASN:N	2.52	0.42
1:E:554:ASP:OD1	1:E:554:ASP:N	2.52	0.42
1:E:802:ARG:HD2	1:E:802:ARG:N	2.33	0.42
1:D:63:VAL:CG1	1:D:87:ILE:HD12	2.49	0.42
1:D:171:ALA:O	1:D:184:VAL:N	2.51	0.42
1:D:305:ASP:HB3	1:D:373:LEU:CD1	2.47	0.42
1:D:567:SER:O	1:D:571:GLU:HG3	2.18	0.42
1:D:574:TYR:CD1	1:D:638:PHE:HB3	2.54	0.42
1:D:744:PHE:CD1	1:D:745:PRO:HD2	2.55	0.42
1:D:940:TYR:O	1:D:944:VAL:HG23	2.19	0.42
2:F:14:LYS:HA	2:F:22:VAL:H	1.83	0.42
2:F:23:PHE:HZ	2:F:220:PHE:HZ	1.66	0.42
1:B:76:LYS:HD3	1:B:76:LYS:N	2.34	0.42
1:B:503:HIS:HE1	1:B:505:LYS:HD3	1.85	0.42
1:B:544:PHE:HE2	1:B:551:LEU:H	1.66	0.42
1:B:558:LEU:HD11	1:A:559:PHE:CZ	2.54	0.42
1:B:561:LEU:HD12	1:B:584:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:VAL:CG1	1:B:619:LEU:HD11	2.49	0.42
1:B:819:ARG:HB2	1:B:819:ARG:HH11	1.82	0.42
1:A:171:ALA:O	1:A:184:VAL:HG22	2.19	0.42
1:E:242:LYS:HE3	1:E:265:GLY:HA2	2.01	0.42
1:E:349:HIS:HB3	1:E:350:LYS:HE3	2.01	0.42
1:D:37:SER:HB2	1:D:42:LEU:HD22	2.00	0.42
1:D:407:ILE:HD11	2:F:2:LYS:CB	2.43	0.42
1:D:596:TYR:CE2	1:D:603:VAL:HG21	2.55	0.42
2:F:59:ILE:HD12	2:F:222:ALA:CB	2.50	0.42
1:B:70:LEU:HD22	1:E:256:GLU:HG2	2.02	0.42
1:B:319:LEU:CD1	1:B:333:VAL:HG21	2.38	0.42
1:E:29:CYS:CB	1:E:269:ILE:HD11	2.44	0.42
1:D:313:TYR:CZ	1:D:317:SER:HB3	2.55	0.42
1:D:408:GLU:HG3	2:F:1:MET:SD	2.58	0.42
1:D:591:ASN:O	1:D:595:LEU:HG	2.19	0.42
1:D:613:ARG:NH2	1:D:660:LYS:H	2.18	0.42
1:D:683:LYS:HA	1:D:686:GLU:OE2	2.20	0.42
1:D:704:MET:N	1:D:704:MET:SD	2.92	0.42
1:B:15:LEU:HD11	1:B:291:ASP:HB3	2.00	0.42
1:B:720:LEU:HD12	1:B:744:PHE:CE2	2.52	0.42
1:B:842:LEU:CD1	1:B:850:LYS:HG2	2.49	0.42
1:B:842:LEU:HD11	1:B:850:LYS:HG2	2.00	0.42
1:B:977:LYS:O	1:B:981:ILE:HG22	2.19	0.42
1:A:937:ASP:HB3	1:A:940:TYR:CB	2.32	0.42
1:E:412:LEU:HD13	1:E:421:MET:HG2	2.00	0.42
1:E:464:ASP:OD1	1:E:464:ASP:N	2.53	0.42
1:E:559:PHE:HD1	1:D:559:PHE:CE2	2.37	0.42
1:E:880:GLU:O	1:E:884:LEU:HD12	2.20	0.42
1:E:913:MET:HA	1:E:916:PHE:CD2	2.54	0.42
1:D:6:LEU:HB3	1:D:9:LYS:CB	2.48	0.42
1:D:145:ARG:HE	1:D:145:ARG:HB3	1.70	0.42
1:D:398:LYS:HG3	1:D:399:ASP:OD1	2.20	0.42
1:D:720:LEU:HB2	1:D:757:TRP:CZ3	2.54	0.42
1:B:56:TYR:CZ	1:B:135:ASP:HB3	2.54	0.42
1:B:562:THR:HG21	1:A:559:PHE:CE1	2.45	0.42
1:B:627:ARG:NH1	1:B:628:THR:HG22	2.34	0.42
1:A:230:ASN:HA	1:A:233:ARG:HH12	1.85	0.42
1:A:836:ASP:O	1:A:840:LYS:HG2	2.20	0.42
2:C:63:VAL:HG21	2:C:220:PHE:CE2	2.55	0.42
1:E:324:TYR:CZ	1:E:593:ARG:HD3	2.55	0.42
1:E:975:HIS:CE1	1:E:976:MET:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LYS:HD3	1:D:339:HIS:CD2	2.53	0.42
1:D:840:LYS:HA	1:D:871:ILE:CG2	2.49	0.42
1:D:899:GLU:O	1:D:903:GLY:N	2.42	0.42
1:D:980:VAL:HG22	1:D:984:LEU:HD22	2.02	0.42
1:B:220:LEU:HD13	1:B:245:PHE:CE2	2.54	0.42
1:B:755:TYR:HB2	1:B:804:TYR:CE1	2.55	0.42
1:B:870:ARG:HG3	2:C:52:ILE:HG21	2.02	0.42
1:A:962:TYR:HE1	1:A:967:LEU:HD23	1.85	0.42
2:C:49:PRO:C	2:C:50:LEU:HD13	2.40	0.42
1:E:9:LYS:CD	1:E:13:GLU:HG3	2.50	0.42
1:E:65:LYS:HG3	1:E:103:ILE:HD13	2.02	0.42
1:E:689:VAL:O	1:E:693:GLU:HG3	2.19	0.42
1:D:562:THR:HA	1:D:618:LEU:CD2	2.49	0.42
1:D:662:ASP:O	1:D:666:ASN:ND2	2.53	0.42
1:B:184:VAL:HG23	1:B:184:VAL:O	2.18	0.42
1:B:949:PHE:O	1:B:951:TYR:HD1	2.03	0.42
1:A:42:LEU:HD11	1:A:214:VAL:HG21	2.00	0.42
1:A:225:ILE:HD13	1:A:245:PHE:CE1	2.54	0.42
1:A:483:GLN:HA	1:A:486:THR:HG22	2.01	0.42
1:A:675:LYS:HE2	1:A:675:LYS:H	1.85	0.42
1:A:843:PRO:HG3	1:A:871:ILE:O	2.20	0.42
1:A:893:LYS:NZ	1:A:933:PHE:HA	2.35	0.42
1:A:955:ILE:HG22	1:A:957:SER:H	1.85	0.42
1:E:421:MET:O	1:E:425:ILE:HG13	2.19	0.42
1:E:717:LYS:HD2	1:E:757:TRP:HH2	1.85	0.42
1:E:806:ALA:O	1:E:809:LYS:HB2	2.20	0.42
1:E:865:LEU:CD1	1:E:874:ILE:HD13	2.45	0.42
1:D:310:ASP:OD1	1:D:380:ARG:NH1	2.53	0.42
1:D:622:LYS:HG3	1:D:626:GLU:OE2	2.19	0.42
1:D:674:ASP:OD1	1:D:674:ASP:N	2.53	0.42
1:D:867:ASN:O	1:D:871:ILE:HG12	2.19	0.42
1:B:249:ASP:O	1:B:272:ALA:HB2	2.20	0.42
1:A:173:ASP:OD1	1:A:174:PHE:N	2.53	0.42
1:A:508:THR:OG1	1:A:510:GLU:HG3	2.20	0.42
1:A:582:ILE:HG12	1:A:645:PHE:CE1	2.55	0.42
1:E:124:MET:HE2	1:E:293:LEU:HD23	2.01	0.42
1:E:289:VAL:O	1:E:293:LEU:HD13	2.20	0.42
1:D:407:ILE:HD13	1:D:650:TYR:HD2	1.84	0.42
1:D:558:LEU:HD22	1:D:611:TYR:CE1	2.55	0.42
1:D:930:MET:HB2	1:D:940:TYR:OH	2.20	0.42
1:B:90:ILE:O	1:B:94:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:PRO:HG2	1:B:507:PHE:CD2	2.55	0.41
1:A:551:LEU:HD13	1:A:551:LEU:HA	1.90	0.41
1:A:937:ASP:OD2	1:A:940:TYR:N	2.53	0.41
1:E:86:ARG:O	1:E:90:ILE:HG13	2.20	0.41
1:E:322:LEU:HD21	1:E:469:CYS:SG	2.60	0.41
1:E:425:ILE:HD13	1:E:442:LEU:CD2	2.50	0.41
1:E:585:LEU:HG	1:E:589:TYR:CE2	2.56	0.41
1:E:918:ILE:HG13	1:E:943:PHE:CE2	2.55	0.41
1:E:927:ASN:O	1:E:930:MET:HE1	2.20	0.41
1:D:163:SER:OG	1:D:164:SER:N	2.52	0.41
1:D:557:LYS:HE3	1:D:561:LEU:HG	2.01	0.41
1:D:665:LYS:HB3	1:D:665:LYS:HE3	1.73	0.41
1:D:983:VAL:O	1:D:987:ARG:HG2	2.20	0.41
1:B:405:THR:HG21	1:B:586:LEU:HD13	2.02	0.41
1:B:551:LEU:HD12	1:B:551:LEU:O	2.20	0.41
1:A:59:TRP:CZ3	1:A:62:LEU:HD23	2.55	0.41
1:A:531:MET:HE2	1:A:535:PHE:CD2	2.55	0.41
1:A:905:GLN:HA	1:A:907:PHE:CE2	2.55	0.41
1:A:946:PRO:O	1:A:951:TYR:OH	2.29	0.41
1:A:957:SER:HA	1:A:960:LYS:HG2	2.02	0.41
1:E:18:VAL:HG12	1:E:22:LEU:HD21	2.01	0.41
1:E:232:VAL:HG13	1:E:240:PHE:CZ	2.55	0.41
1:E:276:ASP:OD2	1:E:276:ASP:N	2.50	0.41
1:E:432:ILE:HA	1:E:435:ASP:CG	2.39	0.41
1:E:724:LYS:HB3	1:E:760:ARG:HB3	2.01	0.41
1:E:776:ASP:HB2	1:E:815:PHE:CZ	2.56	0.41
1:E:797:ASN:OD1	1:E:797:ASN:N	2.50	0.41
1:D:89:GLN:OE1	1:D:186:LYS:HG3	2.19	0.41
1:D:325:ILE:O	1:D:325:ILE:HD12	2.19	0.41
1:D:616:MET:CE	1:D:651:ASP:HA	2.51	0.41
1:D:753:LYS:HA	1:D:756:VAL:HG23	2.00	0.41
1:D:980:VAL:CG2	1:D:984:LEU:HD13	2.48	0.41
2:F:45:ILE:HG23	2:F:48:LYS:CB	2.45	0.41
1:A:460:LEU:O	1:A:463:ILE:HG13	2.19	0.41
1:A:942:PHE:HA	1:A:949:PHE:CD2	2.55	0.41
1:E:349:HIS:HB3	1:E:350:LYS:HD2	2.02	0.41
1:E:561:LEU:HB3	1:E:580:SER:HB2	2.03	0.41
1:E:994:LYS:HA	1:E:994:LYS:HE2	2.02	0.41
1:D:495:LEU:O	1:D:495:LEU:HD13	2.20	0.41
1:D:801:SER:HA	1:D:804:TYR:HD2	1.85	0.41
1:D:942:PHE:HB2	1:D:949:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1000:LEU:O	1:D:1004:PHE:HB2	2.20	0.41
1:B:7:GLU:O	1:B:11:TYR:HB2	2.20	0.41
1:B:562:THR:OG1	1:B:618:LEU:HD22	2.21	0.41
1:B:582:ILE:O	1:B:586:LEU:HG	2.20	0.41
1:A:256:GLU:HG2	1:D:70:LEU:CD2	2.42	0.41
1:A:561:LEU:O	1:A:565:VAL:HG23	2.21	0.41
2:C:25:ALA:HB2	2:C:66:ALA:HA	2.02	0.41
1:E:309:ILE:HB	1:E:377:GLN:HG3	2.02	0.41
1:E:338:TYR:HA	1:E:348:ARG:HA	2.02	0.41
1:E:877:PHE:HB3	1:E:882:GLU:OE2	2.20	0.41
1:D:132:THR:HG23	1:D:171:ALA:HB2	2.02	0.41
1:D:660:LYS:HD3	1:D:660:LYS:N	2.36	0.41
1:D:828:THR:O	1:D:835:ILE:HD11	2.21	0.41
1:D:962:TYR:HB2	1:D:967:LEU:HD21	2.02	0.41
1:D:980:VAL:HG13	1:D:984:LEU:CB	2.34	0.41
1:B:23:ASP:OD1	1:B:24:ASN:N	2.53	0.41
1:B:90:ILE:HG12	1:E:260:TYR:CD2	2.56	0.41
1:B:964:ASP:N	1:B:964:ASP:OD1	2.53	0.41
1:A:660:LYS:HA	1:A:660:LYS:HD3	1.91	0.41
2:C:16:LYS:HB2	2:C:170:ARG:O	2.20	0.41
1:E:305:ASP:O	1:E:308:VAL:HG22	2.20	0.41
1:E:555:THR:O	1:E:558:LEU:HB3	2.20	0.41
1:E:677:ARG:NE	1:E:678:PHE:H	2.19	0.41
1:E:868:GLY:CA	1:E:871:ILE:HG22	2.51	0.41
1:D:478:ARG:HA	1:D:481:ILE:CG2	2.44	0.41
1:D:650:TYR:O	1:D:653:VAL:HG22	2.20	0.41
1:D:746:GLU:HA	1:D:754:ARG:HH21	1.86	0.41
1:B:558:LEU:HD22	1:B:618:LEU:HD22	2.03	0.41
1:B:625:TYR:CE1	1:B:629:ARG:HD3	2.56	0.41
1:B:920:TYR:HA	1:B:925:ILE:CD1	2.50	0.41
1:A:352:LYS:HE3	1:A:352:LYS:CA	2.38	0.41
1:A:845:LEU:HD13	1:A:853:LEU:CD2	2.48	0.41
1:A:893:LYS:O	1:A:897:ILE:HG13	2.20	0.41
2:C:14:LYS:HE2	2:C:14:LYS:HB3	1.90	0.41
2:C:224:ALA:HB2	2:C:231:MET:SD	2.60	0.41
1:E:9:LYS:HD3	1:E:9:LYS:O	2.21	0.41
1:E:558:LEU:HG	1:D:559:PHE:CE1	2.56	0.41
1:D:45:PHE:HA	1:D:130:ILE:O	2.20	0.41
1:D:455:TYR:CE2	1:D:477:ASN:HB3	2.56	0.41
1:D:582:ILE:HG23	2:F:4:VAL:HG11	2.03	0.41
1:D:802:ARG:HG2	1:D:803:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:973:ASN:HB3	1:D:976:MET:HB2	2.03	0.41
1:B:555:THR:O	1:B:558:LEU:HB3	2.20	0.41
1:A:220:LEU:HG	1:A:245:PHE:CE2	2.56	0.41
1:A:924:GLU:C	1:A:925:ILE:HG12	2.41	0.41
2:C:207:SER:HB2	2:C:211:GLY:CA	2.51	0.41
1:E:514:ARG:O	1:E:518:GLU:HG3	2.21	0.41
1:D:481:ILE:HD12	1:D:481:ILE:HA	1.88	0.41
1:D:581:ASP:OD1	1:D:582:ILE:N	2.53	0.41
1:B:933:PHE:C	1:B:934:ILE:HD13	2.41	0.41
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.89	0.41
1:A:208:ILE:HG12	1:A:213:ILE:HG13	2.03	0.41
1:A:578:MET:HG2	1:A:583:VAL:HG22	2.02	0.41
1:A:767:LEU:CD1	1:A:771:ILE:HB	2.51	0.41
1:A:853:LEU:CD1	1:A:854:LEU:HG	2.51	0.41
1:E:595:LEU:HD12	1:E:608:PHE:CE1	2.56	0.41
1:E:908:SER:OG	2:F:229:ASP:HB2	2.21	0.41
1:D:682:GLU:O	1:D:686:GLU:HG3	2.21	0.41
1:D:687:TYR:CD2	1:D:691:ILE:HD11	2.54	0.41
1:D:936:MET:HE3	1:D:936:MET:HB2	1.78	0.41
1:D:955:ILE:HG12	1:D:987:ARG:NH2	2.36	0.41
1:D:971:ALA:HB2	1:D:1003:TYR:CD1	2.56	0.41
1:B:139:ASP:OD1	1:B:139:ASP:N	2.53	0.41
1:B:235:LEU:HD23	1:B:240:PHE:CE2	2.55	0.41
1:B:328:ILE:O	1:B:332:HIS:ND1	2.47	0.41
1:B:588:LEU:HD12	1:B:611:TYR:CZ	2.56	0.41
1:A:464:ASP:OD1	1:A:464:ASP:N	2.26	0.41
1:A:981:ILE:O	1:A:985:LYS:HG3	2.20	0.41
1:E:348:ARG:HH12	1:E:351:ASN:HB3	1.86	0.41
1:E:540:LYS:NZ	1:E:543:GLU:OE1	2.54	0.41
1:E:938:ASP:OD1	1:E:938:ASP:N	2.54	0.41
1:D:30:ILE:HD12	1:D:293:LEU:HD23	2.02	0.41
1:D:455:TYR:OH	1:D:477:ASN:ND2	2.54	0.41
1:D:566:ARG:HD3	1:D:566:ARG:HA	1.71	0.41
1:D:842:LEU:HD23	1:D:873:LEU:N	2.36	0.41
1:B:8:SER:C	1:B:9:LYS:HD3	2.41	0.41
1:A:612:ILE:HD12	1:A:658:HIS:CD2	2.56	0.41
1:A:632:ASP:OD1	1:A:633:GLU:N	2.54	0.41
1:A:798:GLY:C	1:A:799:LEU:HD12	2.41	0.41
1:A:859:VAL:HA	1:A:864:ASP:HB2	2.03	0.41
1:E:866:MET:SD	1:E:869:ILE:HD12	2.61	0.41
1:D:358:GLU:HG3	1:D:396:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:737:VAL:HG22	1:D:761:LEU:HD22	2.03	0.41
1:D:832:GLN:O	1:D:835:ILE:HB	2.21	0.41
2:F:205:GLU:OE2	2:F:215:ALA:HB2	2.20	0.41
1:B:370:ARG:HA	1:B:373:LEU:HD12	2.02	0.40
1:B:462:SER:O	1:B:471:TYR:HB2	2.21	0.40
1:A:772:ILE:CD1	1:A:808:ILE:HG23	2.40	0.40
1:A:904:ILE:CG2	1:A:906:THR:HG23	2.51	0.40
1:A:939:GLN:O	1:A:942:PHE:HB3	2.21	0.40
2:C:1:MET:HB2	2:C:1:MET:HE2	1.91	0.40
1:E:405:THR:HG21	1:E:586:LEU:HD21	2.02	0.40
1:D:23:ASP:OD2	1:D:23:ASP:N	2.54	0.40
1:D:105:LYS:HE2	1:D:105:LYS:HB3	1.82	0.40
1:D:327:LYS:HZ1	1:D:392:GLY:HA3	1.86	0.40
1:D:620:ILE:HD11	1:D:647:MET:SD	2.61	0.40
1:D:646:PHE:O	1:D:648:GLU:HG2	2.21	0.40
1:D:830:ASP:OD1	1:D:831:LYS:HG3	2.21	0.40
1:B:584:VAL:HG11	1:B:619:LEU:HD11	2.02	0.40
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.83	0.40
1:A:354:PHE:CZ	1:A:359:ARG:HG3	2.55	0.40
1:A:687:TYR:OH	1:A:715:GLU:OE2	2.32	0.40
1:A:904:ILE:HG12	1:A:905:GLN:H	1.84	0.40
2:C:25:ALA:HB3	2:C:63:VAL:CG1	2.51	0.40
1:E:348:ARG:NH1	1:E:351:ASN:HB3	2.35	0.40
1:E:885:ILE:HG23	1:E:916:PHE:CD1	2.57	0.40
1:D:642:LYS:HD2	1:D:642:LYS:HA	1.86	0.40
1:B:260:TYR:CD2	1:E:90:ILE:HG12	2.57	0.40
1:B:322:LEU:HD22	1:B:598:ASN:ND2	2.37	0.40
1:B:459:ILE:HD11	1:B:475:GLN:HA	2.04	0.40
1:B:804:TYR:O	1:B:808:ILE:HG13	2.21	0.40
1:A:10:ARG:NH1	1:A:10:ARG:HA	2.37	0.40
1:A:595:LEU:HB3	1:A:603:VAL:HB	2.02	0.40
1:E:292:LEU:HD12	1:E:292:LEU:HA	1.96	0.40
1:E:507:PHE:HB3	1:E:512:LEU:HD21	2.03	0.40
1:E:556:VAL:HB	1:D:552:TYR:CE1	2.57	0.40
1:E:820:LEU:HG	1:E:845:LEU:CD2	2.51	0.40
1:D:192:ASN:O	1:D:196:ASN:HB2	2.21	0.40
1:D:752:GLY:O	1:D:756:VAL:HG23	2.21	0.40
1:D:995:ARG:HD2	1:D:995:ARG:HA	1.91	0.40
1:A:651:ASP:OD1	2:C:2:LYS:HD2	2.22	0.40
1:A:822:GLU:O	1:A:826:CYS:HB3	2.21	0.40
1:E:403:LEU:O	1:E:403:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:SER:O	1:E:407:ILE:HD13	2.22	0.40
1:E:694:GLU:OE2	1:E:698:GLN:NE2	2.55	0.40
1:E:820:LEU:HG	1:E:845:LEU:HD21	2.03	0.40
1:D:46:VAL:CG2	1:D:121:ILE:HD13	2.51	0.40
1:D:688:LEU:HB3	1:D:736:ILE:CD1	2.51	0.40
1:D:704:MET:CE	1:D:709:TYR:HB2	2.52	0.40
1:D:767:LEU:HD13	1:D:775:ILE:CD1	2.51	0.40
1:B:652:PHE:CD2	1:B:684:ILE:HG23	2.56	0.40
1:A:260:TYR:CD2	1:D:90:ILE:HG12	2.56	0.40
1:A:316:ILE:HD11	1:A:334:PHE:CZ	2.56	0.40
1:A:585:LEU:HD22	1:A:645:PHE:CE1	2.56	0.40
1:A:902:LYS:HB2	1:A:902:LYS:HE2	1.88	0.40
1:E:338:TYR:OH	1:E:358:GLU:HG3	2.21	0.40
1:E:781:LEU:HA	1:E:784:GLU:CD	2.42	0.40
1:D:22:LEU:HD13	1:D:26:VAL:HB	2.02	0.40
1:D:192:ASN:O	1:D:196:ASN:ND2	2.40	0.40
1:D:201:SER:OG	1:D:205:LYS:HE2	2.21	0.40
1:D:366:SER:OG	1:D:369:GLU:HG3	2.22	0.40
1:D:468:GLY:HA3	1:D:535:PHE:CE2	2.56	0.40
1:D:574:TYR:CE1	1:D:639:PHE:HB2	2.56	0.40
1:D:799:LEU:HA	1:D:803:ASP:CG	2.42	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	998/1005 (99%)	930 (93%)	67 (7%)	1 (0%)	48 77
1	B	965/1005 (96%)	919 (95%)	45 (5%)	1 (0%)	48 77
1	D	998/1005 (99%)	942 (94%)	53 (5%)	3 (0%)	37 65
1	E	965/1005 (96%)	924 (96%)	40 (4%)	1 (0%)	48 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	135/264 (51%)	123 (91%)	12 (9%)	0	100 100
2	F	135/264 (51%)	124 (92%)	11 (8%)	0	100 100
All	All	4196/4548 (92%)	3962 (94%)	228 (5%)	6 (0%)	50 77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	810	HIS
1	B	952	LYS
1	A	187	GLU
1	D	789	GLN
1	D	791	TYR
1	D	186	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	917/922 (100%)	858 (94%)	59 (6%)	14 38
1	B	891/922 (97%)	845 (95%)	46 (5%)	19 45
1	D	917/922 (100%)	861 (94%)	56 (6%)	15 40
1	E	891/922 (97%)	838 (94%)	53 (6%)	16 41
2	C	120/225 (53%)	111 (92%)	9 (8%)	11 33
2	F	120/225 (53%)	111 (92%)	9 (8%)	11 33
All	All	3856/4138 (93%)	3624 (94%)	232 (6%)	18 40

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	ARG
1	B	45	PHE
1	B	76	LYS
1	B	78	ASN

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Mol	Chain	Res	Type
1	B	111	ASP
1	B	119	ASP
1	B	131	THR
1	B	133	ASN
1	B	134	TYR
1	B	139	ASP
1	B	143	TRP
1	B	237	LYS
1	B	248	THR
1	B	276	ASP
1	B	279	GLU
1	B	306	ASP
1	B	343	ASN
1	B	348	ARG
1	B	350	LYS
1	B	389	GLU
1	B	394	ILE
1	B	399	ASP
1	B	408	GLU
1	B	464	ASP
1	B	502	ARG
1	B	516	GLU
1	B	544	PHE
1	B	555	THR
1	B	559	PHE
1	B	590	ASP
1	B	704	MET
1	B	744	PHE
1	B	763	LYS
1	B	815	PHE
1	B	831	LYS
1	B	864	ASP
1	B	890	GLU
1	B	896	TYR
1	B	920	TYR
1	B	936	MET
1	B	950	ASP
1	B	961	ASN
1	B	975	HIS
1	B	979	HIS
1	B	987	ARG
1	B	1002	ASN

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Mol	Chain	Res	Type
1	A	9	LYS
1	A	21	MET
1	A	45	PHE
1	A	119	ASP
1	A	131	THR
1	A	134	TYR
1	A	138	ILE
1	A	156	GLU
1	A	160	ASN
1	A	185	LEU
1	A	187	GLU
1	A	188	ASP
1	A	192	ASN
1	A	202	ASN
1	A	232	VAL
1	A	237	LYS
1	A	238	ASP
1	A	315	LYS
1	A	325	ILE
1	A	351	ASN
1	A	359	ARG
1	A	426	GLU
1	A	464	ASP
1	A	465	GLU
1	A	469	CYS
1	A	497	LEU
1	A	502	ARG
1	A	508	THR
1	A	526	ASP
1	A	534	GLU
1	A	538	LYS
1	A	544	PHE
1	A	629	ARG
1	A	636	PHE
1	A	639	PHE
1	A	655	ILE
1	A	663	ASP
1	A	674	ASP
1	A	675	LYS
1	A	705	ASN
1	A	727	LYS
1	A	743	TYR

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Mol	Chain	Res	Type
1	A	747	ARG
1	A	757	TRP
1	A	776	ASP
1	A	813	LYS
1	A	814	ASN
1	A	818	LYS
1	A	820	LEU
1	A	825	LEU
1	A	837	PHE
1	A	852	HIS
1	A	856	PHE
1	A	907	PHE
1	A	913	MET
1	A	920	TYR
1	A	969	LYS
1	A	993	ASP
1	A	1001	MET
2	C	1	MET
2	C	29	THR
2	C	34	GLN
2	C	48	LYS
2	C	55	SER
2	C	60	ASN
2	C	67	PHE
2	C	214	LEU
2	C	239	ARG
1	E	10	ARG
1	E	21	MET
1	E	62	LEU
1	E	131	THR
1	E	134	TYR
1	E	139	ASP
1	E	237	LYS
1	E	276	ASP
1	E	289	VAL
1	E	328	ILE
1	E	348	ARG
1	E	376	LYS
1	E	377	GLN
1	E	395	CYS
1	E	412	LEU
1	E	417	LYS

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Mol	Chain	Res	Type
1	E	423	LYS
1	E	435	ASP
1	E	500	PHE
1	E	503	HIS
1	E	508	THR
1	E	510	GLU
1	E	519	MET
1	E	521	ASN
1	E	526	ASP
1	E	554	ASP
1	E	559	PHE
1	E	578	MET
1	E	598	ASN
1	E	646	PHE
1	E	648	GLU
1	E	667	LEU
1	E	669	ARG
1	E	671	CYS
1	E	677	ARG
1	E	707	VAL
1	E	738	LYS
1	E	744	PHE
1	E	788	ASP
1	E	802	ARG
1	E	809	LYS
1	E	811	PHE
1	E	848	ASN
1	E	856	PHE
1	E	866	MET
1	E	916	PHE
1	E	921	PHE
1	E	930	MET
1	E	936	MET
1	E	958	TRP
1	E	974	LYS
1	E	978	HIS
1	E	1003	TYR
1	D	23	ASP
1	D	64	ASP
1	D	98	MET
1	D	106	ASP
1	D	139	ASP

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Mol	Chain	Res	Type
1	D	144	LYS
1	D	156	GLU
1	D	157	ASP
1	D	192	ASN
1	D	306	ASP
1	D	309	ILE
1	D	315	LYS
1	D	350	LYS
1	D	365	GLU
1	D	373	LEU
1	D	391	ASN
1	D	410	ASN
1	D	423	LYS
1	D	497	LEU
1	D	500	PHE
1	D	504	TYR
1	D	508	THR
1	D	509	ASP
1	D	510	GLU
1	D	514	ARG
1	D	521	ASN
1	D	525	ASP
1	D	533	PHE
1	D	544	PHE
1	D	553	ASP
1	D	554	ASP
1	D	559	PHE
1	D	578	MET
1	D	610	GLN
1	D	613	ARG
1	D	639	PHE
1	D	641	LYS
1	D	646	PHE
1	D	658	HIS
1	D	677	ARG
1	D	704	MET
1	D	709	TYR
1	D	727	LYS
1	D	747	ARG
1	D	751	ILE
1	D	778	PHE
1	D	790	ASN

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Mol	Chain	Res	Type
1	D	791	TYR
1	D	828	THR
1	D	857	LYS
1	D	895	ASN
1	D	907	PHE
1	D	912	TYR
1	D	920	TYR
1	D	974	LYS
1	D	978	HIS
2	F	20	LYS
2	F	23	PHE
2	F	34	GLN
2	F	40	LYS
2	F	75	MET
2	F	198	VAL
2	F	214	LEU
2	F	221	GLU
2	F	239	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	961	ASN
1	A	377	GLN
1	A	487	GLN
1	A	881	HIS
1	A	1002	ASN
2	C	34	GLN
2	C	212	ASN
1	E	263	ASN
1	E	297	GLN
1	E	666	ASN
1	D	339	HIS
1	D	349	HIS
1	D	386	ASN

5.3.3 RNA

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	B	1101	-	42,48,48	5.17	18 (42%)	50,73,73	2.24	13 (26%)
3	NAD	A	1101	-	42,48,48	5.17	18 (42%)	50,73,73	2.20	12 (24%)
3	NAD	D	1101	-	42,48,48	5.22	18 (42%)	50,73,73	2.32	12 (24%)
3	NAD	E	1101	-	42,48,48	5.15	18 (42%)	50,73,73	2.20	12 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	1101	-	-	8/26/62/62	0/5/5/5
3	NAD	A	1101	-	-	5/26/62/62	0/5/5/5
3	NAD	D	1101	-	-	4/26/62/62	0/5/5/5
3	NAD	E	1101	-	-	4/26/62/62	0/5/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1101	NAD	C2B-C1B	-17.05	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	NAD	C2B-C1B	-16.50	1.28	1.53
3	B	1101	NAD	C2B-C1B	-16.50	1.28	1.53
3	E	1101	NAD	C2B-C1B	-16.19	1.29	1.53
3	E	1101	NAD	C2D-C1D	-16.06	1.29	1.53
3	A	1101	NAD	C2D-C1D	-16.06	1.29	1.53
3	D	1101	NAD	C2D-C1D	-16.03	1.29	1.53
3	B	1101	NAD	C2D-C1D	-15.95	1.29	1.53
3	A	1101	NAD	O4B-C1B	11.46	1.57	1.41
3	D	1101	NAD	O4B-C1B	11.45	1.57	1.41
3	E	1101	NAD	O4B-C1B	11.42	1.57	1.41
3	B	1101	NAD	O4B-C1B	11.17	1.56	1.41
3	E	1101	NAD	C3B-C4B	-9.84	1.27	1.53
3	D	1101	NAD	C3B-C4B	-9.83	1.27	1.53
3	B	1101	NAD	O4D-C1D	9.74	1.54	1.41
3	B	1101	NAD	C3B-C4B	-9.70	1.28	1.53
3	A	1101	NAD	C3B-C4B	-9.66	1.28	1.53
3	A	1101	NAD	O4D-C1D	9.55	1.54	1.41
3	E	1101	NAD	O4D-C1D	9.48	1.54	1.41
3	D	1101	NAD	O4D-C1D	9.42	1.54	1.41
3	B	1101	NAD	C3D-C4D	-9.32	1.29	1.53
3	A	1101	NAD	C3D-C4D	-9.22	1.29	1.53
3	D	1101	NAD	C3D-C4D	-9.21	1.29	1.53
3	E	1101	NAD	C3D-C4D	-9.16	1.29	1.53
3	B	1101	NAD	C2B-C3B	5.48	1.68	1.53
3	D	1101	NAD	O4B-C4B	5.48	1.57	1.45
3	A	1101	NAD	O4B-C4B	5.47	1.57	1.45
3	E	1101	NAD	C2B-C3B	5.42	1.68	1.53
3	B	1101	NAD	O4B-C4B	5.38	1.57	1.45
3	A	1101	NAD	C2B-C3B	5.32	1.67	1.53
3	D	1101	NAD	C2B-C3B	5.26	1.67	1.53
3	E	1101	NAD	O4B-C4B	5.23	1.56	1.45
3	E	1101	NAD	O4D-C4D	4.47	1.55	1.45
3	A	1101	NAD	O4D-C4D	4.47	1.55	1.45
3	B	1101	NAD	O4D-C4D	4.46	1.55	1.45
3	D	1101	NAD	O4D-C4D	4.34	1.54	1.45
3	D	1101	NAD	C2D-C3D	4.05	1.64	1.53
3	B	1101	NAD	C2D-C3D	4.01	1.64	1.53
3	A	1101	NAD	C2D-C3D	3.95	1.64	1.53
3	B	1101	NAD	C3N-C7N	3.94	1.56	1.50
3	D	1101	NAD	C3N-C7N	3.90	1.56	1.50
3	E	1101	NAD	C2D-C3D	3.89	1.64	1.53
3	A	1101	NAD	C3N-C7N	3.88	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1101	NAD	C3N-C7N	3.75	1.56	1.50
3	B	1101	NAD	C7N-N7N	3.71	1.40	1.33
3	D	1101	NAD	C7N-N7N	3.69	1.40	1.33
3	A	1101	NAD	C7N-N7N	3.68	1.40	1.33
3	E	1101	NAD	C7N-N7N	3.66	1.40	1.33
3	D	1101	NAD	O2D-C2D	3.37	1.50	1.43
3	A	1101	NAD	O2D-C2D	3.36	1.50	1.43
3	B	1101	NAD	O2D-C2D	3.35	1.50	1.43
3	E	1101	NAD	O2D-C2D	3.35	1.50	1.43
3	B	1101	NAD	C6A-N6A	2.99	1.44	1.34
3	D	1101	NAD	C6A-N6A	2.99	1.44	1.34
3	A	1101	NAD	C6A-N6A	2.99	1.44	1.34
3	E	1101	NAD	C6A-N6A	2.99	1.44	1.34
3	A	1101	NAD	C5A-C4A	-2.40	1.34	1.40
3	D	1101	NAD	C5A-C4A	-2.39	1.34	1.40
3	E	1101	NAD	C5A-C4A	-2.38	1.34	1.40
3	B	1101	NAD	C5A-C4A	-2.34	1.34	1.40
3	B	1101	NAD	C4N-C3N	-2.34	1.35	1.39
3	E	1101	NAD	C4N-C3N	-2.33	1.35	1.39
3	D	1101	NAD	C4N-C3N	-2.24	1.35	1.39
3	D	1101	NAD	C2N-C3N	2.23	1.42	1.39
3	E	1101	NAD	C5B-C4B	2.18	1.58	1.51
3	A	1101	NAD	C4N-C3N	-2.15	1.35	1.39
3	E	1101	NAD	C2N-C3N	2.13	1.42	1.39
3	B	1101	NAD	C2N-C3N	2.10	1.42	1.39
3	B	1101	NAD	C5B-C4B	2.07	1.58	1.51
3	A	1101	NAD	C2N-C3N	2.06	1.42	1.39
3	A	1101	NAD	C5B-C4B	2.04	1.58	1.51
3	D	1101	NAD	C5B-C4B	2.02	1.57	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1101	NAD	C5A-C6A-N6A	7.97	132.46	120.35
3	D	1101	NAD	C5A-C6A-N6A	7.89	132.35	120.35
3	A	1101	NAD	C5A-C6A-N6A	7.82	132.24	120.35
3	B	1101	NAD	C5A-C6A-N6A	7.82	132.23	120.35
3	D	1101	NAD	C1B-N9A-C4A	-7.45	113.56	126.64
3	A	1101	NAD	C1B-N9A-C4A	-6.73	114.82	126.64
3	E	1101	NAD	C1B-N9A-C4A	-6.66	114.95	126.64
3	B	1101	NAD	C1B-N9A-C4A	-6.42	115.37	126.64
3	D	1101	NAD	N3A-C2A-N1A	-5.57	119.98	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	NAD	N3A-C2A-N1A	-5.51	120.06	128.68
3	B	1101	NAD	N3A-C2A-N1A	-5.42	120.21	128.68
3	E	1101	NAD	N3A-C2A-N1A	-5.36	120.29	128.68
3	D	1101	NAD	N6A-C6A-N1A	-5.35	107.46	118.57
3	E	1101	NAD	N6A-C6A-N1A	-5.31	107.54	118.57
3	A	1101	NAD	N6A-C6A-N1A	-5.25	107.68	118.57
3	B	1101	NAD	N6A-C6A-N1A	-5.21	107.76	118.57
3	B	1101	NAD	C3D-C2D-C1D	4.65	107.98	100.98
3	D	1101	NAD	C3D-C2D-C1D	4.47	107.71	100.98
3	D	1101	NAD	C3B-C2B-C1B	3.81	106.72	100.98
3	E	1101	NAD	C3B-C2B-C1B	3.59	106.39	100.98
3	A	1101	NAD	C3D-C2D-C1D	3.36	106.03	100.98
3	A	1101	NAD	C3N-C7N-N7N	3.16	121.54	117.75
3	A	1101	NAD	C3B-C2B-C1B	3.11	105.66	100.98
3	B	1101	NAD	C3N-C7N-N7N	3.09	121.46	117.75
3	B	1101	NAD	C6N-N1N-C2N	-3.08	119.16	121.97
3	D	1101	NAD	C3N-C7N-N7N	2.96	121.30	117.75
3	A	1101	NAD	C6N-N1N-C2N	-2.90	119.33	121.97
3	E	1101	NAD	PN-O3-PA	-2.89	122.92	132.83
3	E	1101	NAD	C6N-N1N-C2N	-2.87	119.36	121.97
3	D	1101	NAD	C2D-C3D-C4D	2.85	108.18	102.64
3	B	1101	NAD	O4B-C1B-C2B	-2.84	102.78	106.93
3	B	1101	NAD	C3B-C2B-C1B	2.83	105.25	100.98
3	E	1101	NAD	C3D-C2D-C1D	2.74	105.10	100.98
3	E	1101	NAD	C3N-C7N-N7N	2.59	120.86	117.75
3	A	1101	NAD	C2D-C3D-C4D	2.58	107.66	102.64
3	D	1101	NAD	PN-O3-PA	-2.56	124.06	132.83
3	B	1101	NAD	O7N-C7N-N7N	-2.55	118.95	122.58
3	D	1101	NAD	C6N-N1N-C2N	-2.54	119.66	121.97
3	B	1101	NAD	PN-O3-PA	-2.49	124.28	132.83
3	A	1101	NAD	PN-O3-PA	-2.47	124.36	132.83
3	D	1101	NAD	O7N-C7N-N7N	-2.46	119.08	122.58
3	E	1101	NAD	C2D-C3D-C4D	2.46	107.43	102.64
3	A	1101	NAD	O7N-C7N-N7N	-2.46	119.08	122.58
3	A	1101	NAD	C2B-C3B-C4B	2.39	107.29	102.64
3	D	1101	NAD	C2B-C3B-C4B	2.35	107.20	102.64
3	B	1101	NAD	C2D-C3D-C4D	2.17	106.86	102.64
3	E	1101	NAD	O7N-C7N-N7N	-2.16	119.50	122.58
3	B	1101	NAD	C2B-C3B-C4B	2.03	106.58	102.64
3	E	1101	NAD	O4B-C4B-C3B	-2.01	101.13	105.11

There are no chirality outliers.

All (21) torsion outliers are listed below:

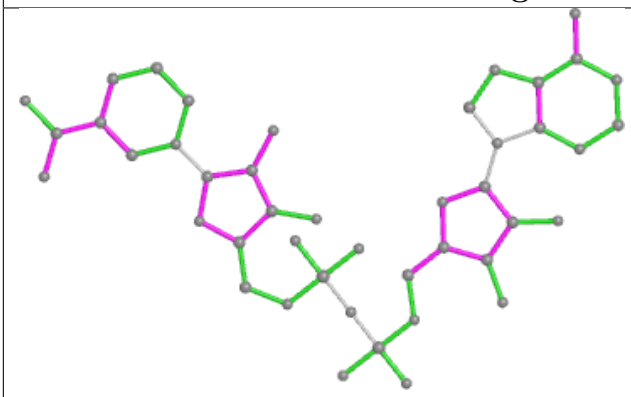
Mol	Chain	Res	Type	Atoms
3	B	1101	NAD	C5B-O5B-PA-O1A
3	B	1101	NAD	C5B-O5B-PA-O2A
3	B	1101	NAD	O4D-C1D-N1N-C2N
3	A	1101	NAD	O4B-C4B-C5B-O5B
3	A	1101	NAD	PA-O3-PN-O5D
3	A	1101	NAD	C5D-O5D-PN-O1N
3	E	1101	NAD	PN-O3-PA-O5B
3	D	1101	NAD	C5B-O5B-PA-O1A
3	A	1101	NAD	C3B-C4B-C5B-O5B
3	B	1101	NAD	O4D-C4D-C5D-O5D
3	B	1101	NAD	PN-O3-PA-O5B
3	A	1101	NAD	PN-O3-PA-O5B
3	D	1101	NAD	PA-O3-PN-O5D
3	D	1101	NAD	C5B-O5B-PA-O3
3	E	1101	NAD	PA-O3-PN-O2N
3	E	1101	NAD	C4B-C5B-O5B-PA
3	D	1101	NAD	O4B-C4B-C5B-O5B
3	B	1101	NAD	C3D-C4D-C5D-O5D
3	B	1101	NAD	C4B-C5B-O5B-PA
3	B	1101	NAD	C5B-O5B-PA-O3
3	E	1101	NAD	C5B-O5B-PA-O1A

There are no ring outliers.

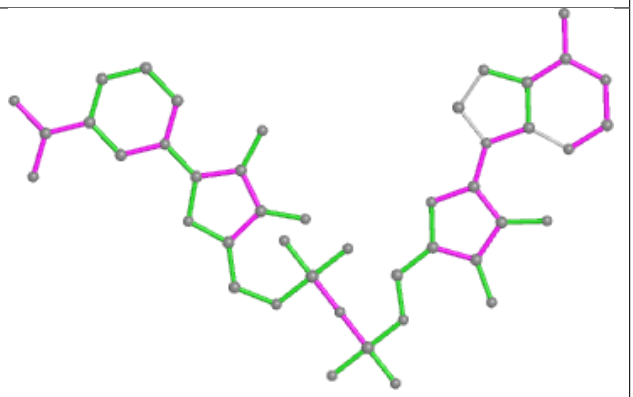
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

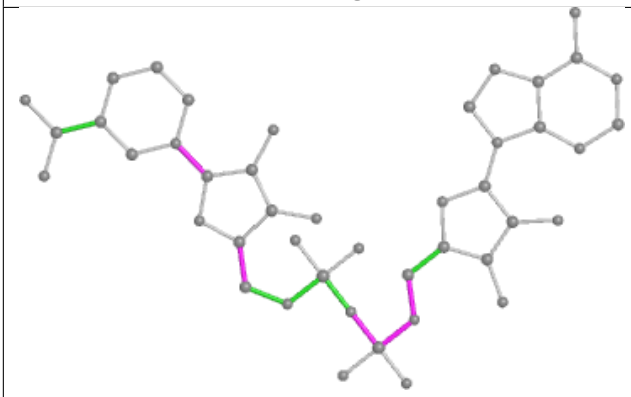
Ligand NAD B 1101



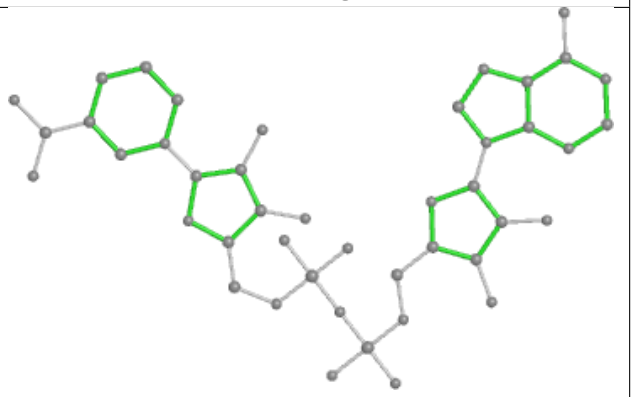
Bond lengths



Bond angles

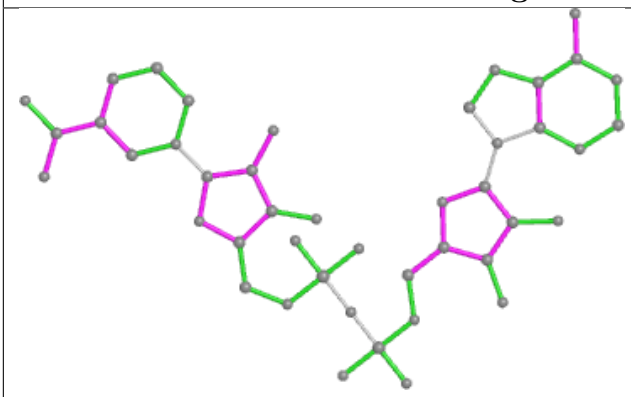


Torsions

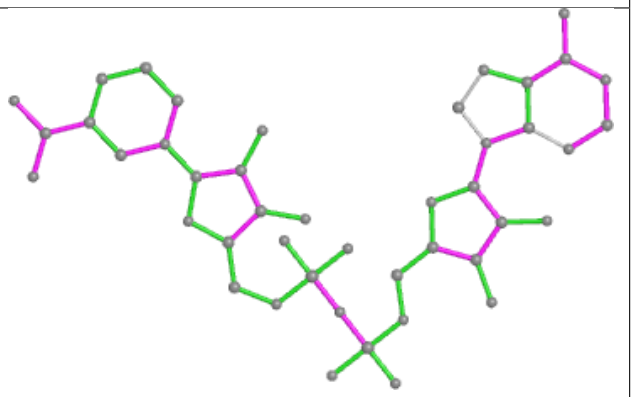


Rings

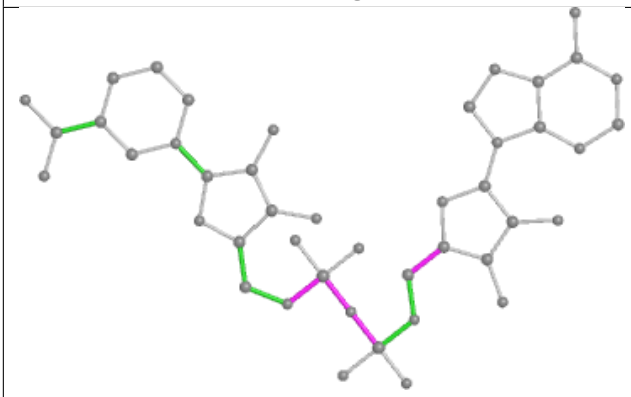
Ligand NAD A 1101



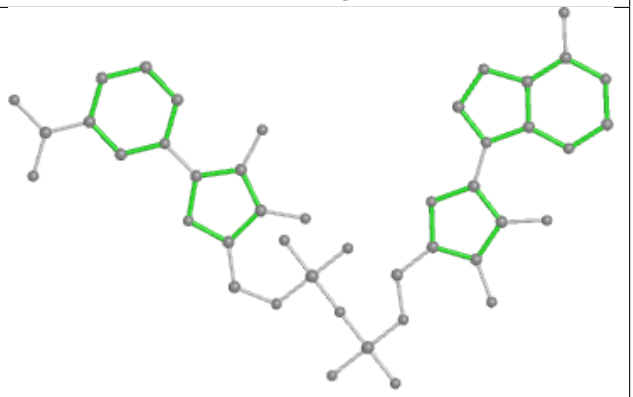
Bond lengths



Bond angles

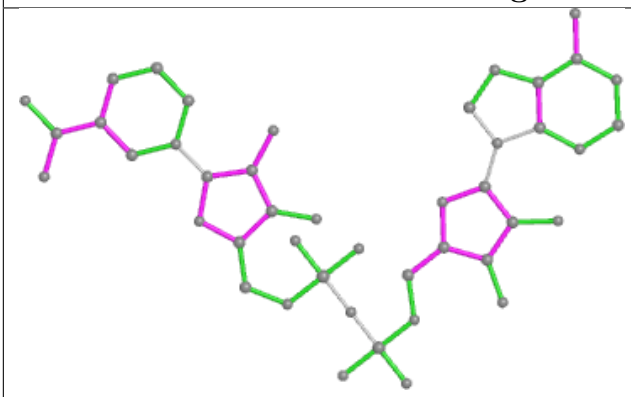


Torsions

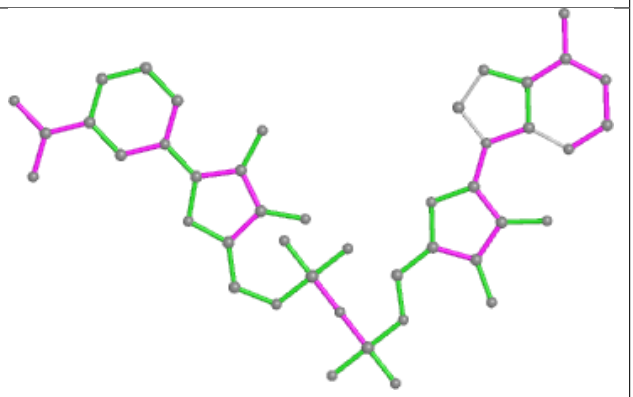


Rings

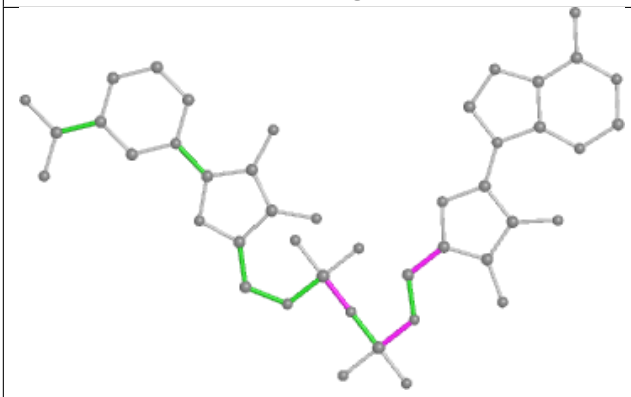
Ligand NAD D 1101



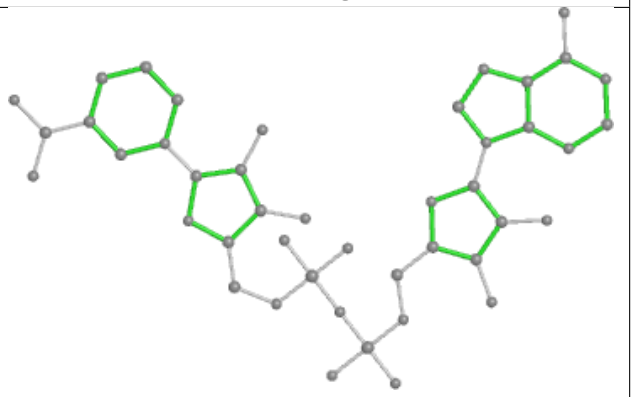
Bond lengths



Bond angles

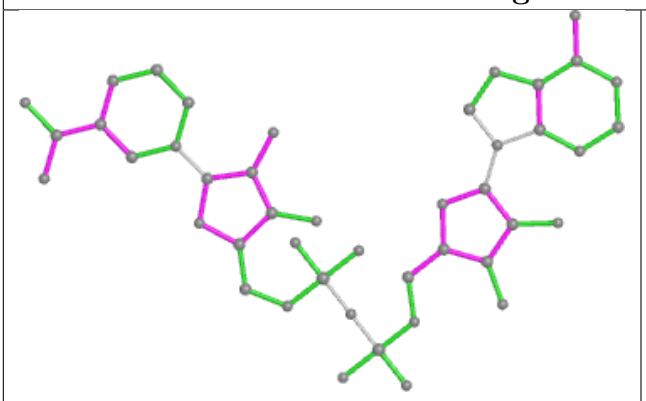


Torsions

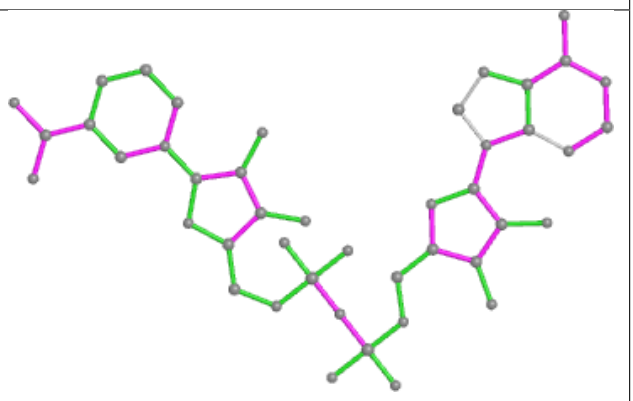


Rings

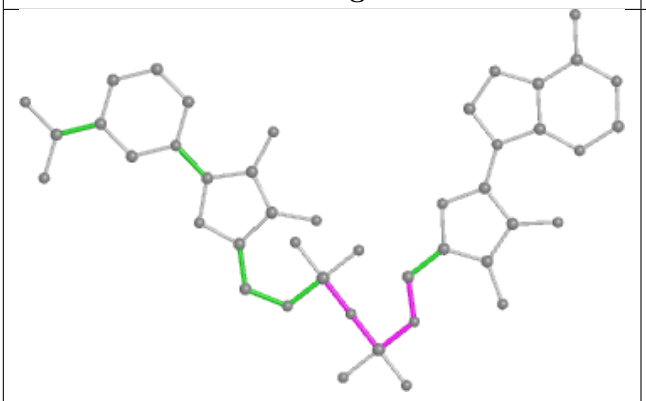
Ligand NAD E 1101



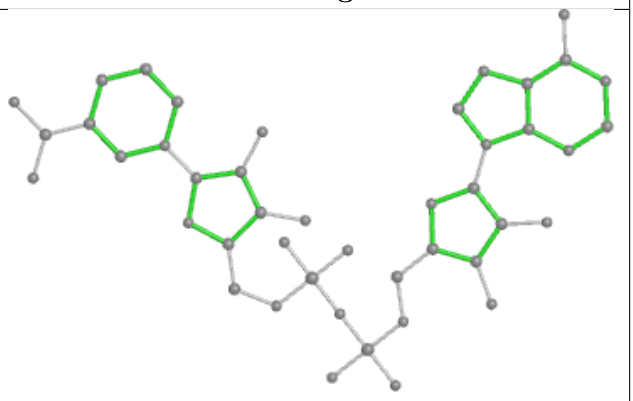
Bond lengths



Bond angles



Torsions



Rings

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.

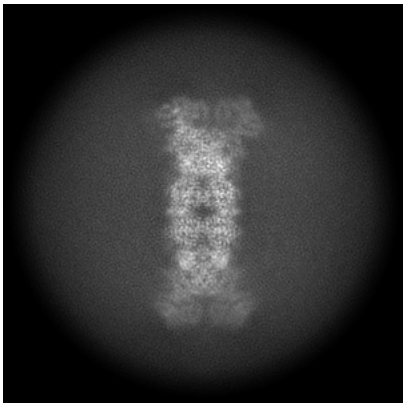
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39925. These allow visual inspection of the internal detail of the map and identification of artifacts.

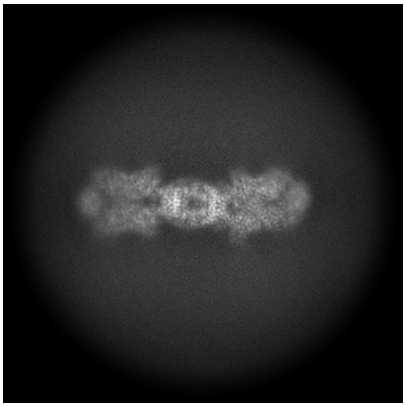
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

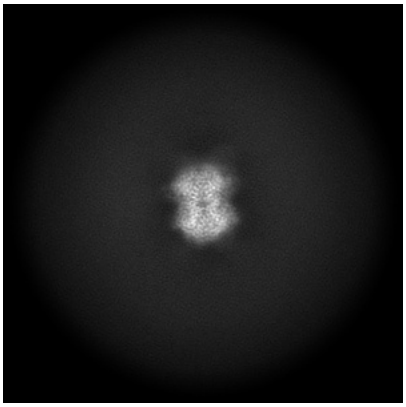
6.1.1 Primary map



X



Y

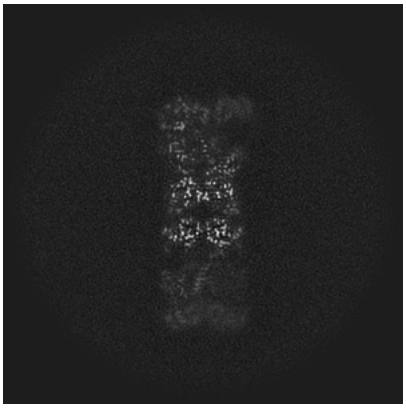


Z

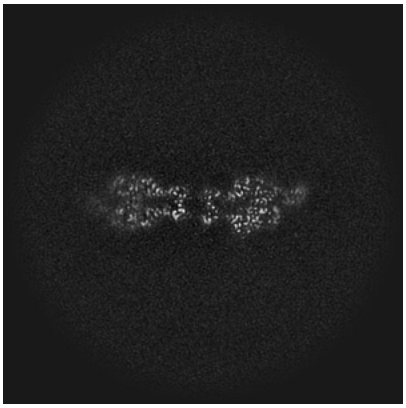
The images above show the map projected in three orthogonal directions.

6.2 Central slices

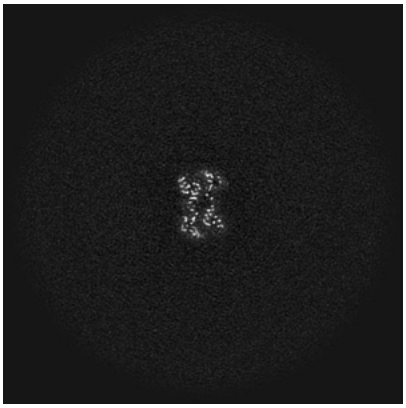
6.2.1 Primary map



X Index: 180



Y Index: 180

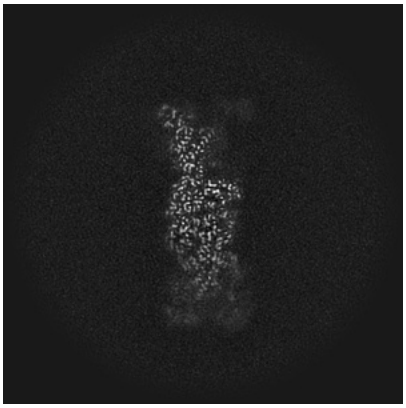


Z Index: 180

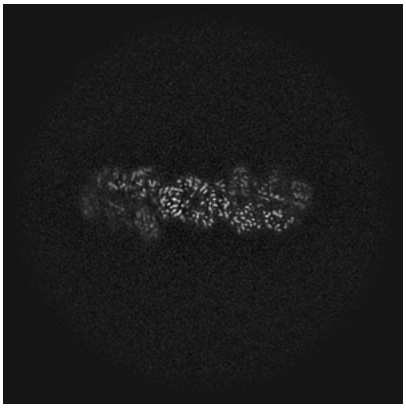
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

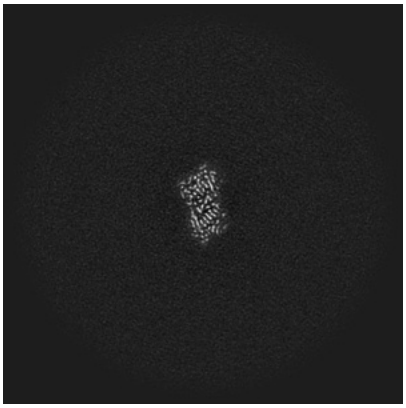
6.3.1 Primary map



X Index: 171



Y Index: 164

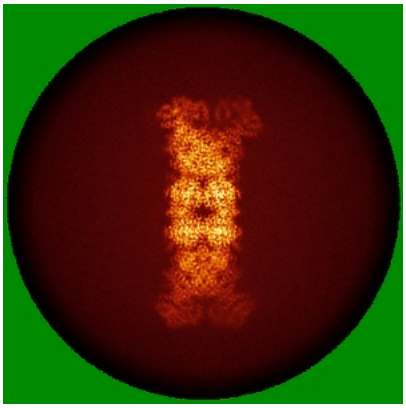


Z Index: 155

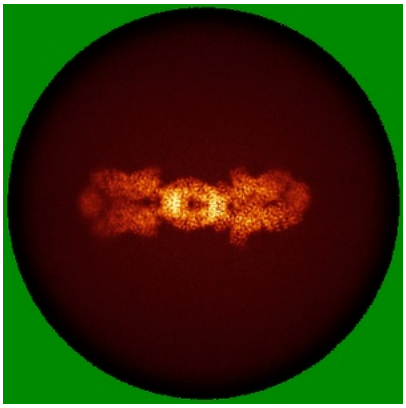
The images above show the largest variance slices of the map in three orthogonal directions.

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

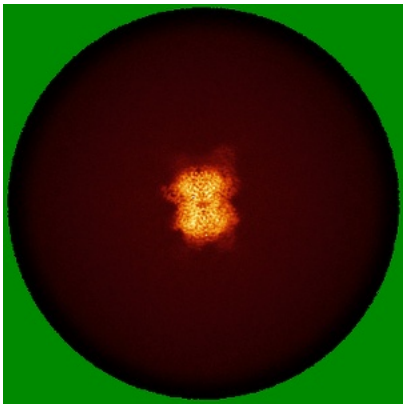
6.4.1 Primary map



X



Y

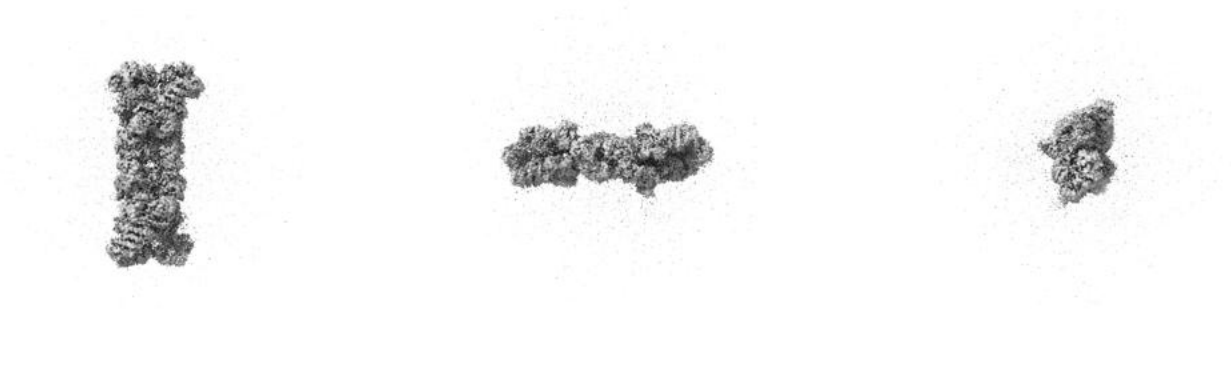


Z

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 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

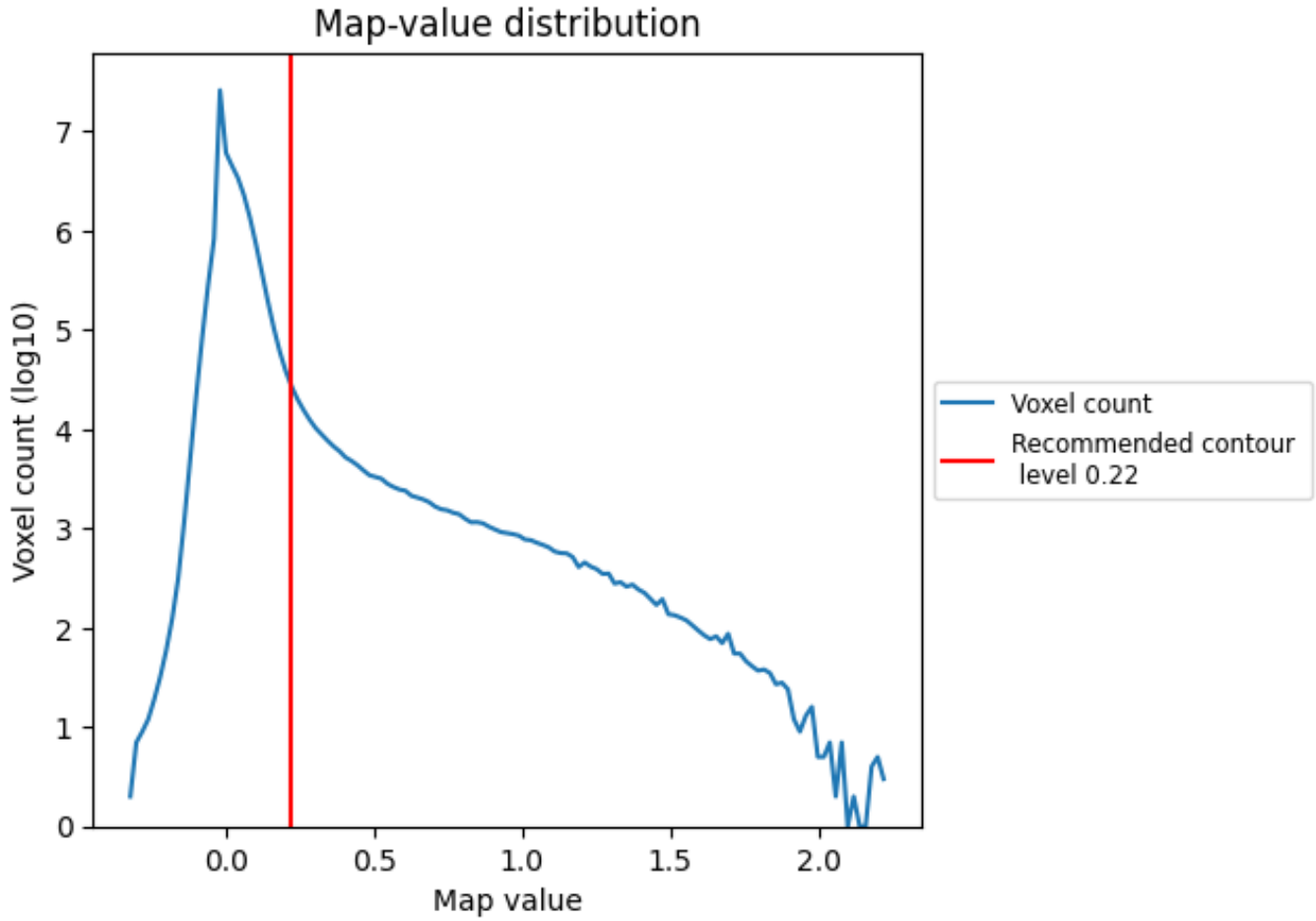
6.6 Mask visualisation (i)

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

7 Map analysis

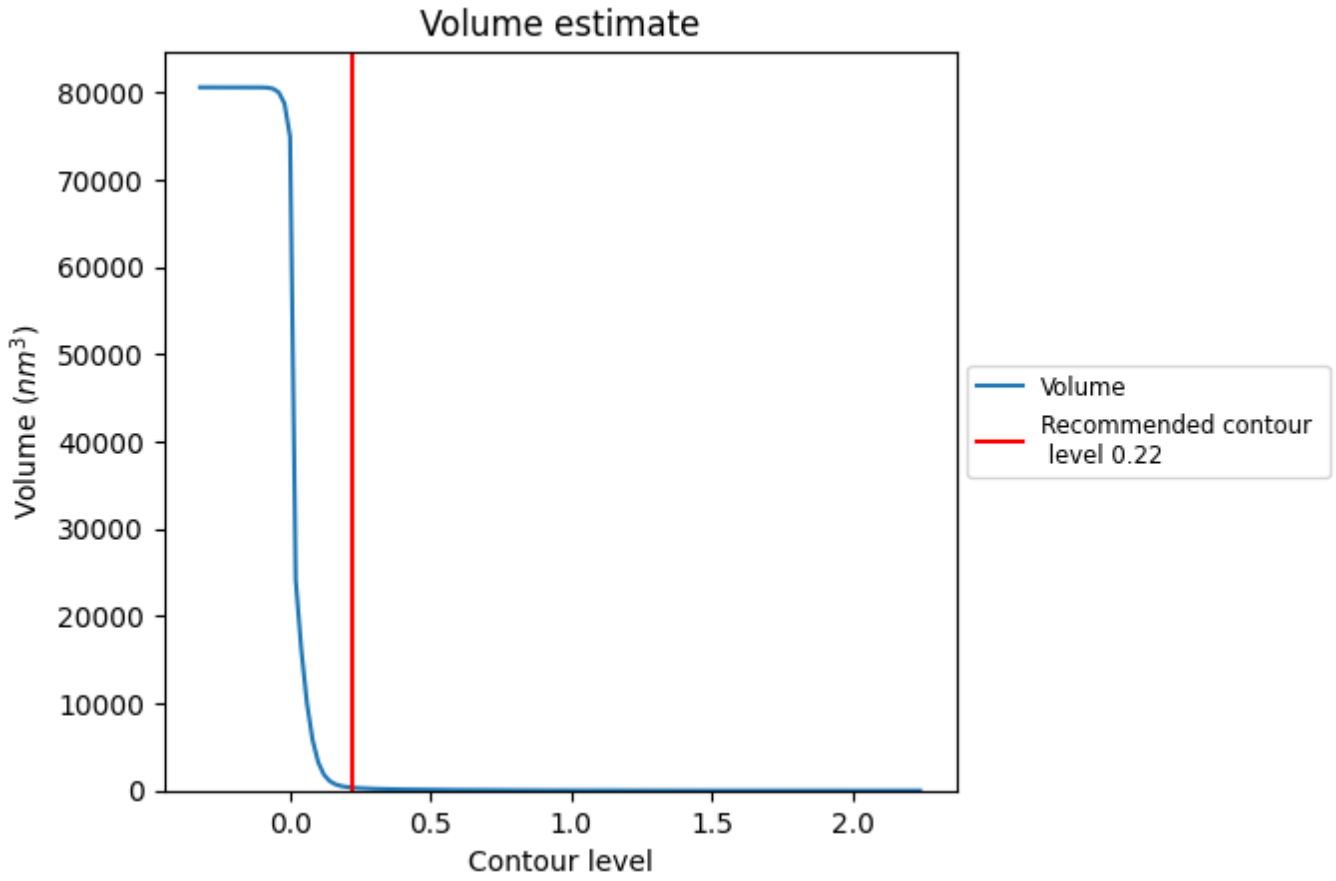
This section contains the results of statistical analysis of the map.

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.

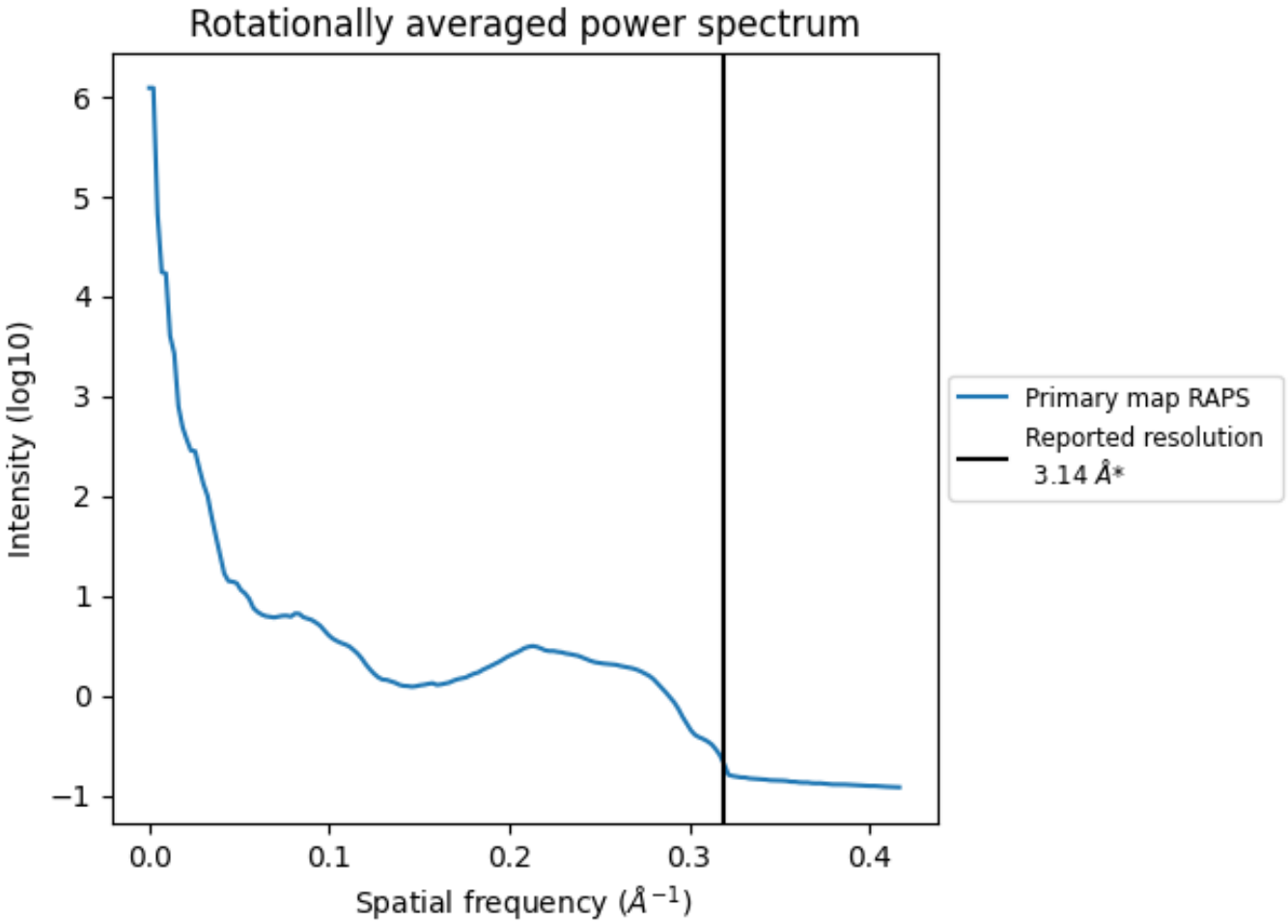
7.2 Volume estimate



The volume at the recommended contour level is 339 nm^3; this corresponds to an approximate mass of 307 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 0.318 $Å^{-1}$

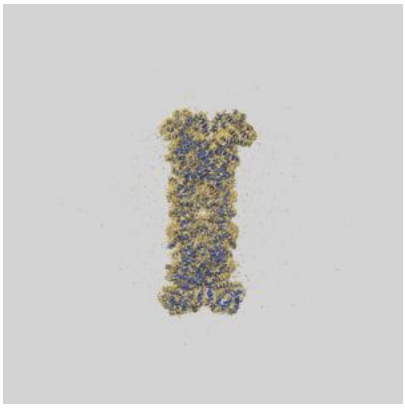
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

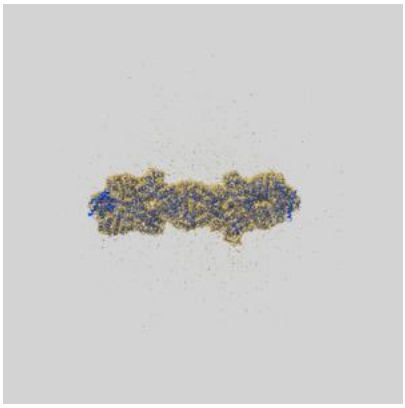
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39925 and PDB model 8ZC9. Per-residue inclusion information can be found in section 3 on page 5.

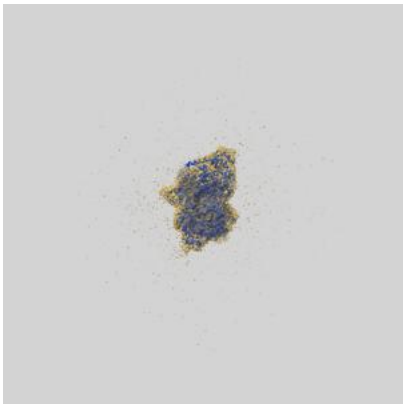
9.1 Map-model overlay



X



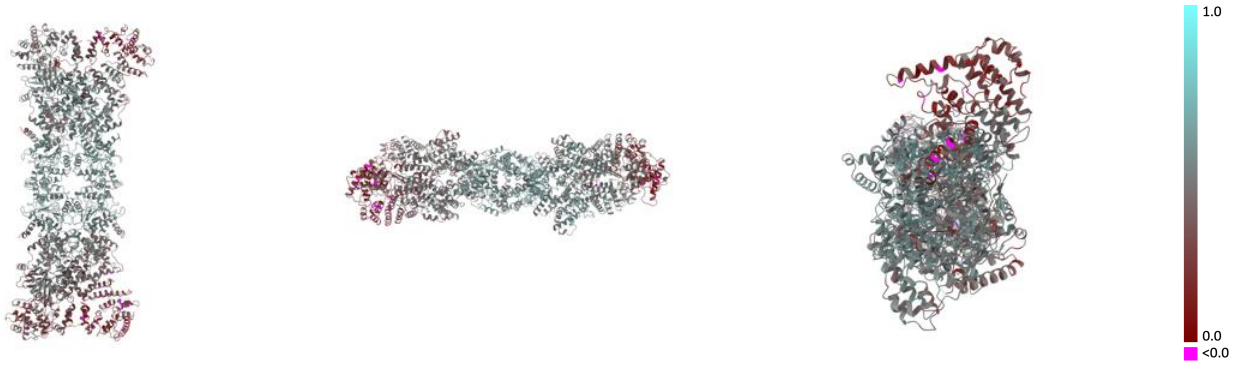
Y



Z

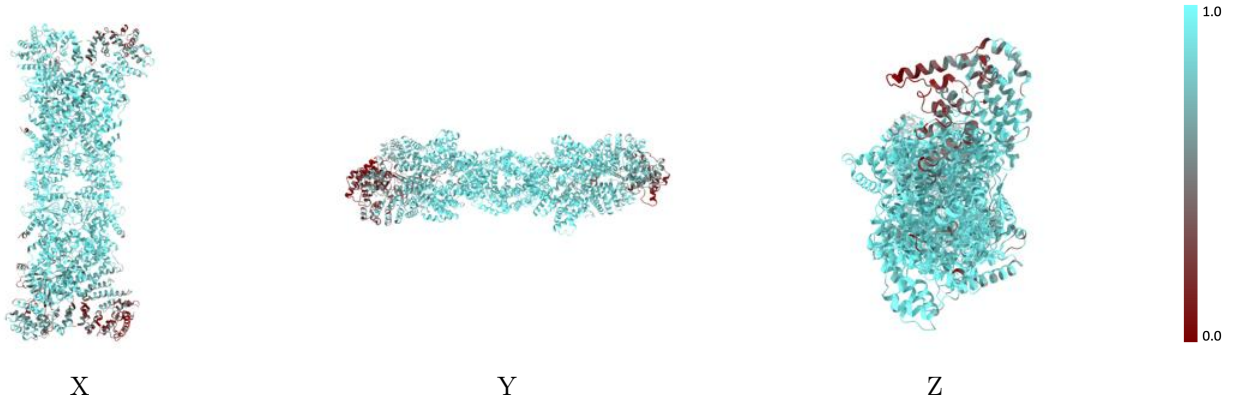
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



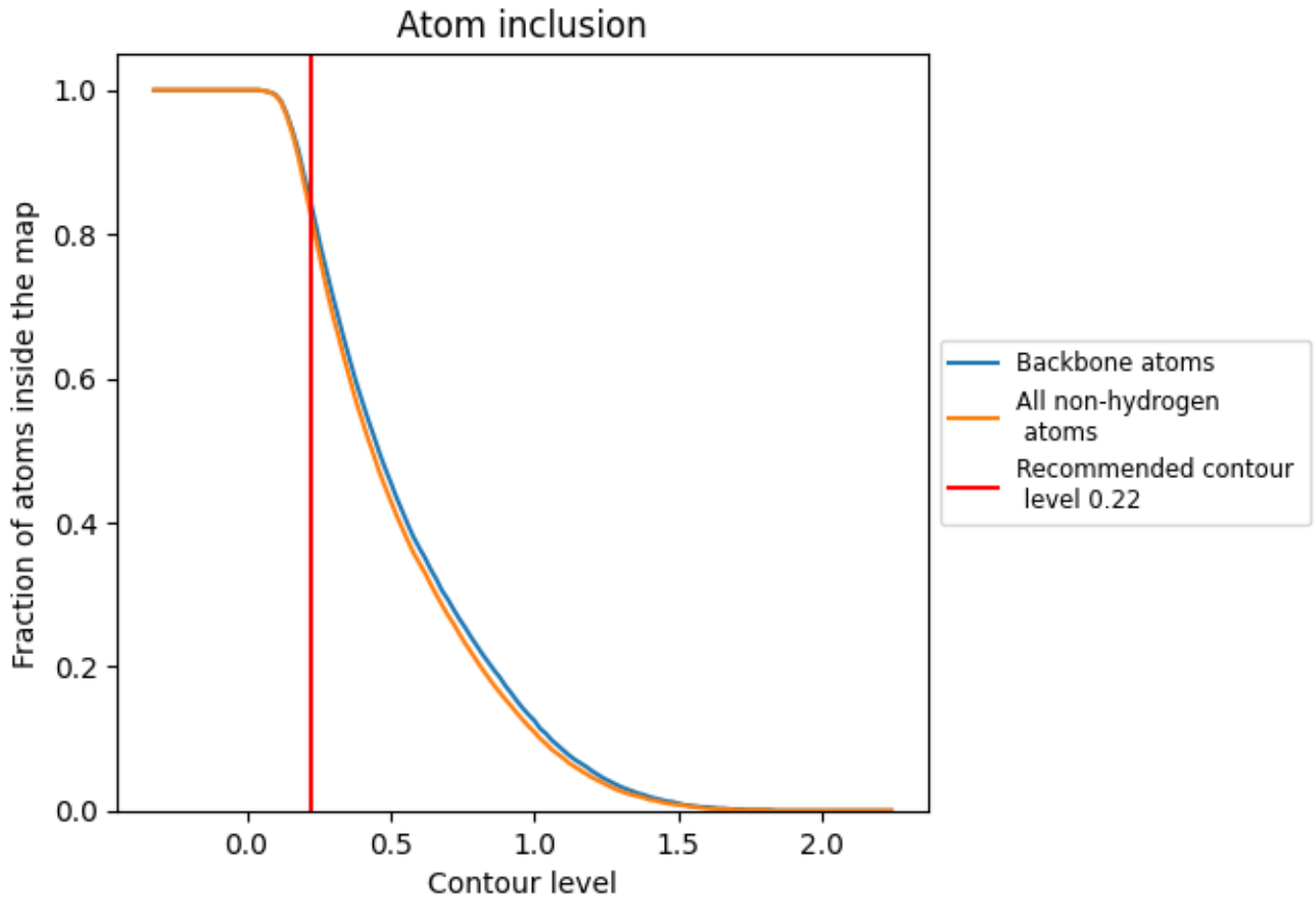
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



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 (0.22).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.4550
A	0.8370	0.4570
B	0.9400	0.5220
C	0.8180	0.4530
D	0.7600	0.4070
E	0.8580	0.4500
F	0.4520	0.3410