



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:11 PM EST

PDB ID : 7JMI
EMDB ID : EMD-22395
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 29 - State 3 (S3)
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2020-07-31
Resolution : 4.50 Å(reported)
Based on initial model : 5TB4

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

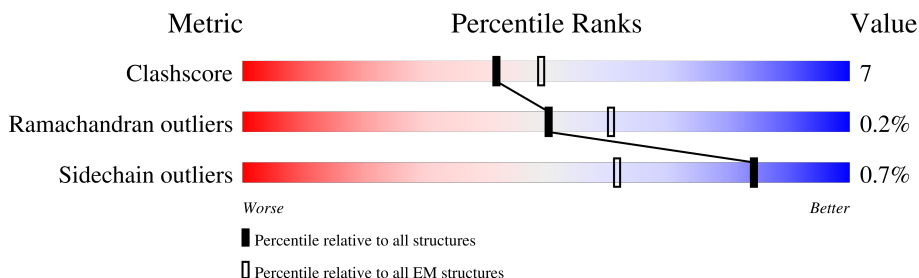
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	107	
1	F	107	
1	H	107	
1	J	107	
2	B	4687	
2	E	4687	
2	G	4687	
2	I	4687	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called ryanodine receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

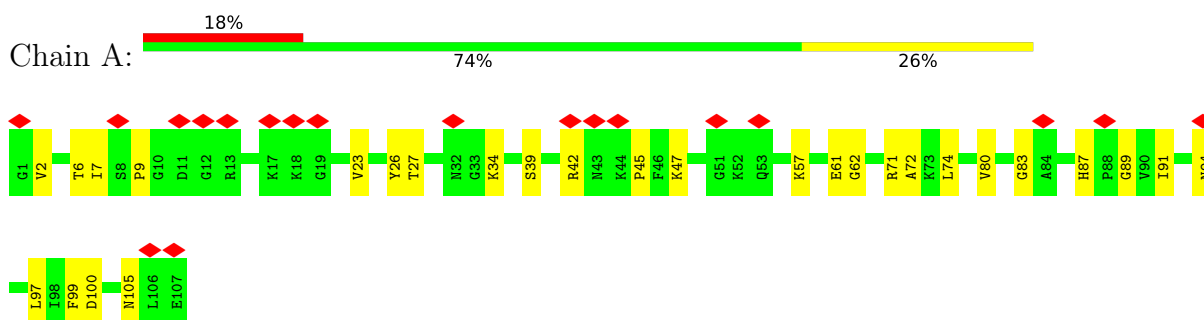
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0

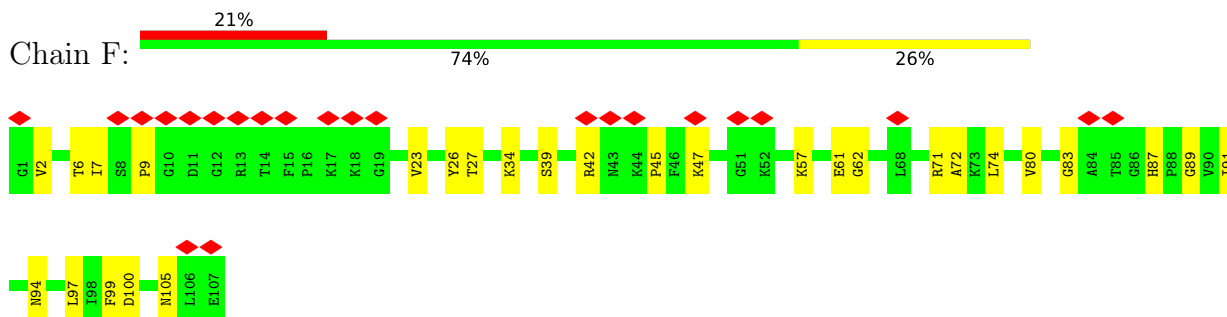
3 Residue-property plots [i](#)

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.

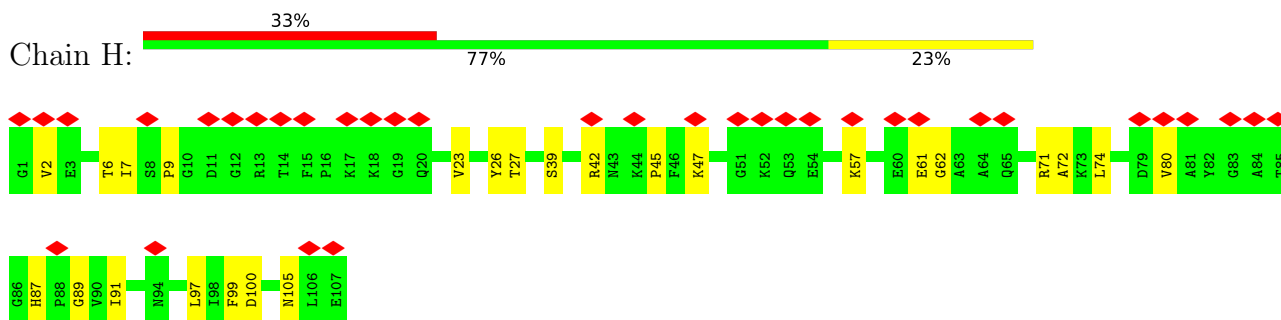
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



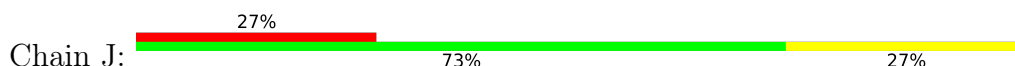
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

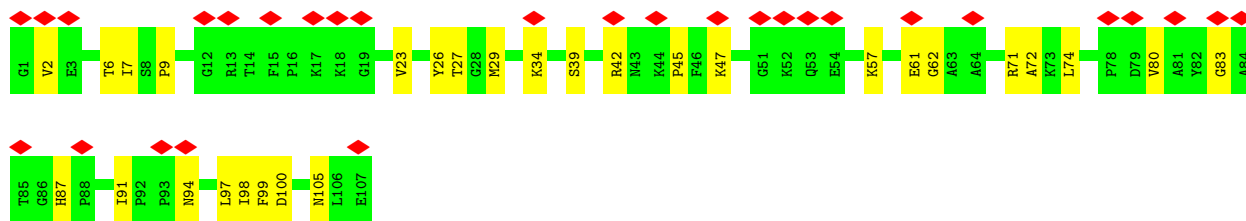


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

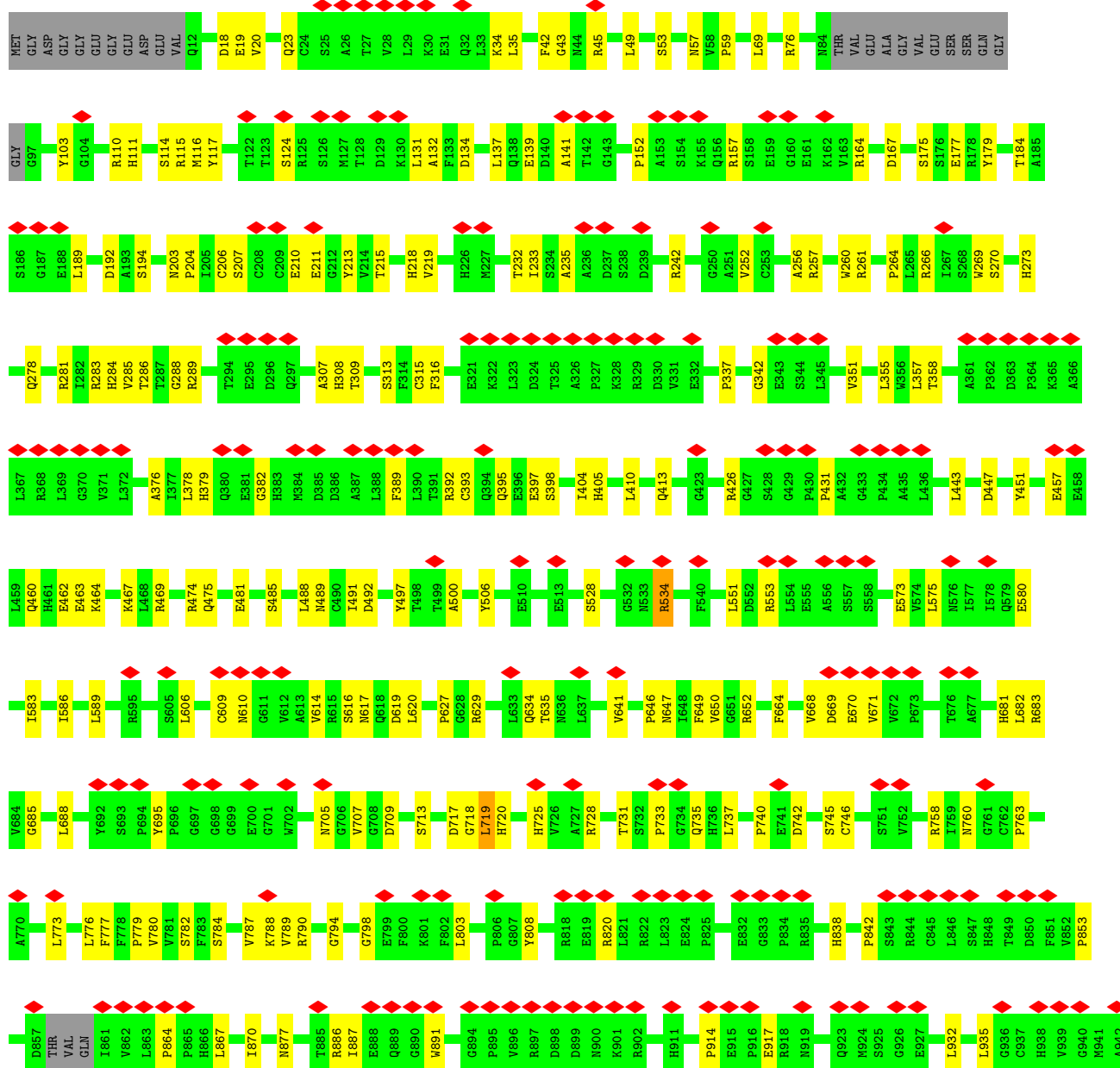
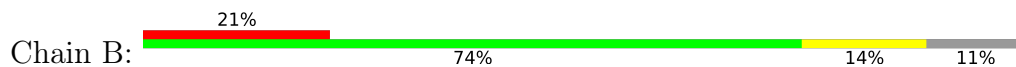


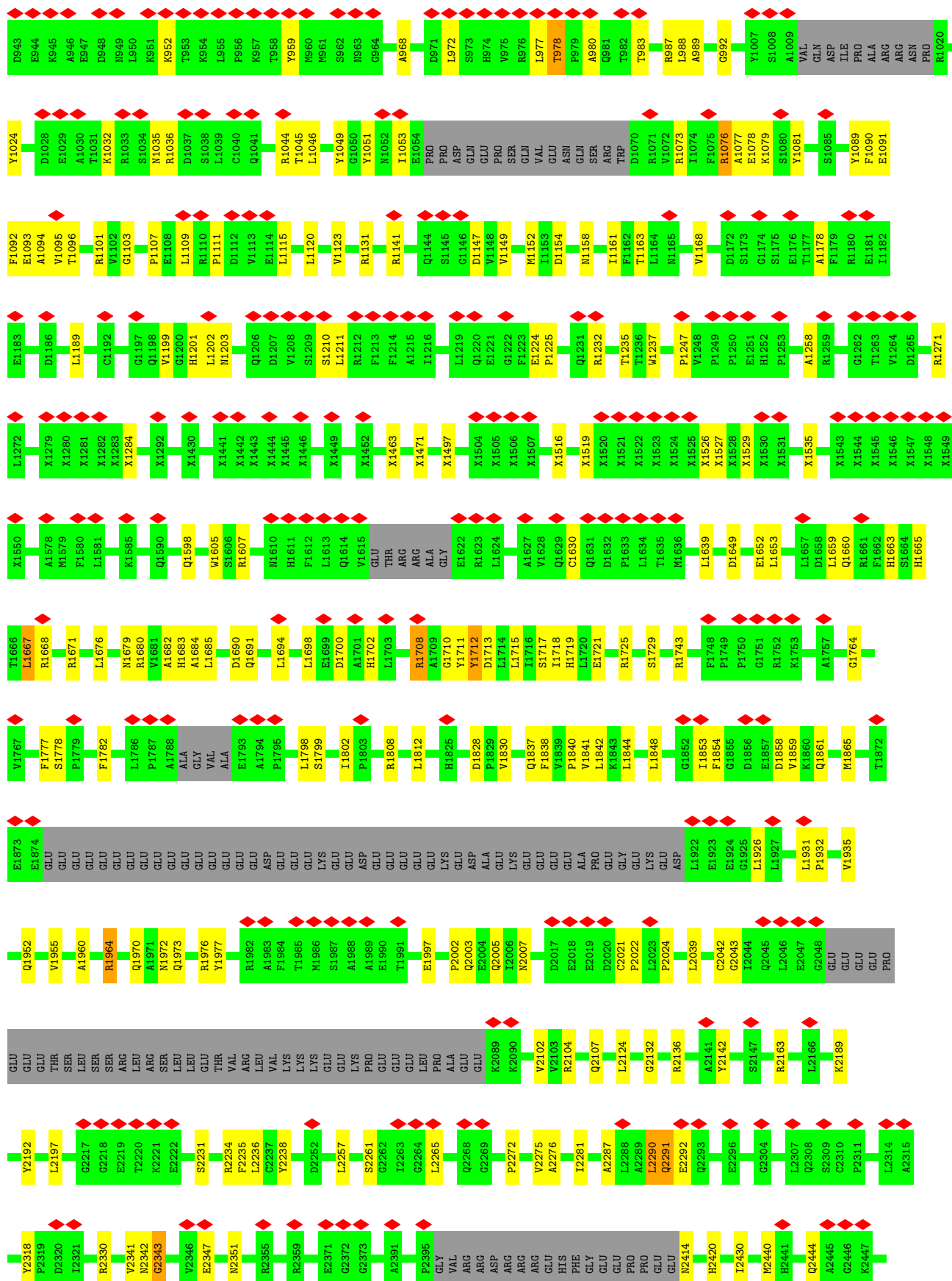
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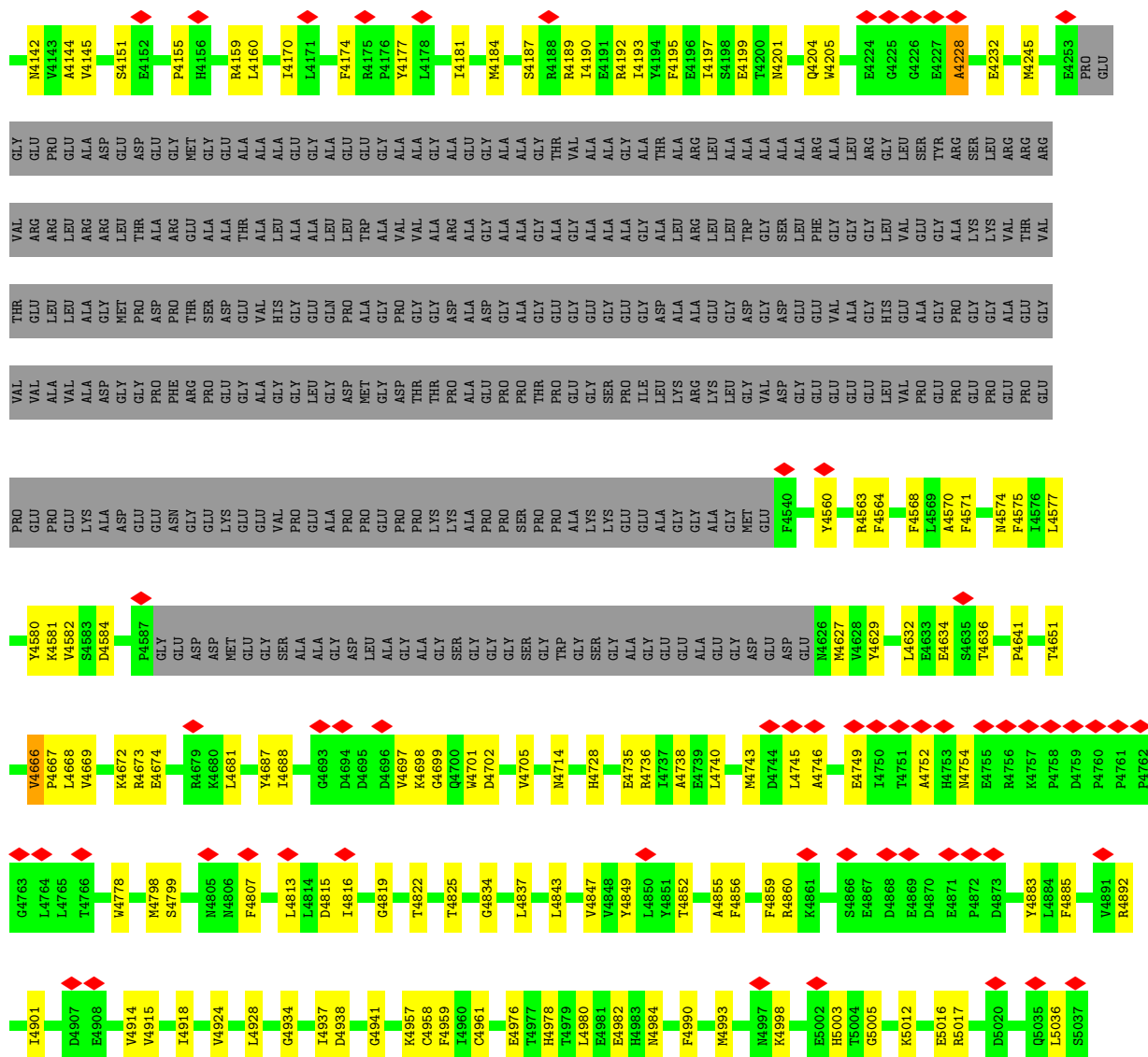


• Molecule 2: ryanodine receptor type 1

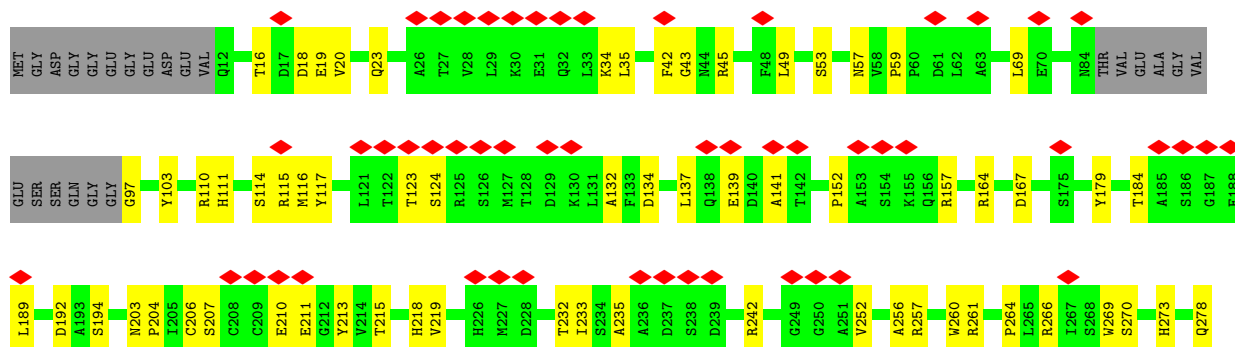
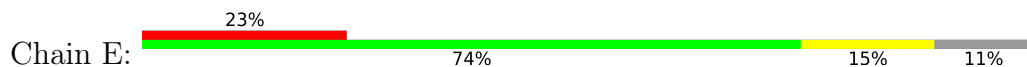




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V4049	S3931	K3715	K3716	X3424	X3248	X3016	G2899	ARG	E2779	X2673	R2458
F4050	D3932	L3716	D3717	X3425	X3249	X3017	G2900	LYS	N2780		S2459
S4051	Y3935	Q3829	Q3830	X3426	X3250	X3020	G2901	ILE	V2781		L2460
E4056	S3936	S3831	X3720	X3427	X3251	X3021	H2902	SER	D2782	X2692	L2463
L4059	Y3937	X3832	X3735	X3428	X3252	X3022	G2903	GLN	E2783	X2693	D2464
F4062	S3938	X3833	E3736	X3429	X3253	X3023	L2904	ALA	E2784	X2694	D2465
D4063	Q3939	X3834	E3737	X3430	X3254	X3027	L2905	GLN	L2785	X2695	L2466
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	Q3963	G3854	GLU	X3512	X3280	X3050	A2913		P2793	X2703	L2487
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	V3990	T3864	A3659	X3523	X3292	X3060	E2921		E2741	E2741	X2511
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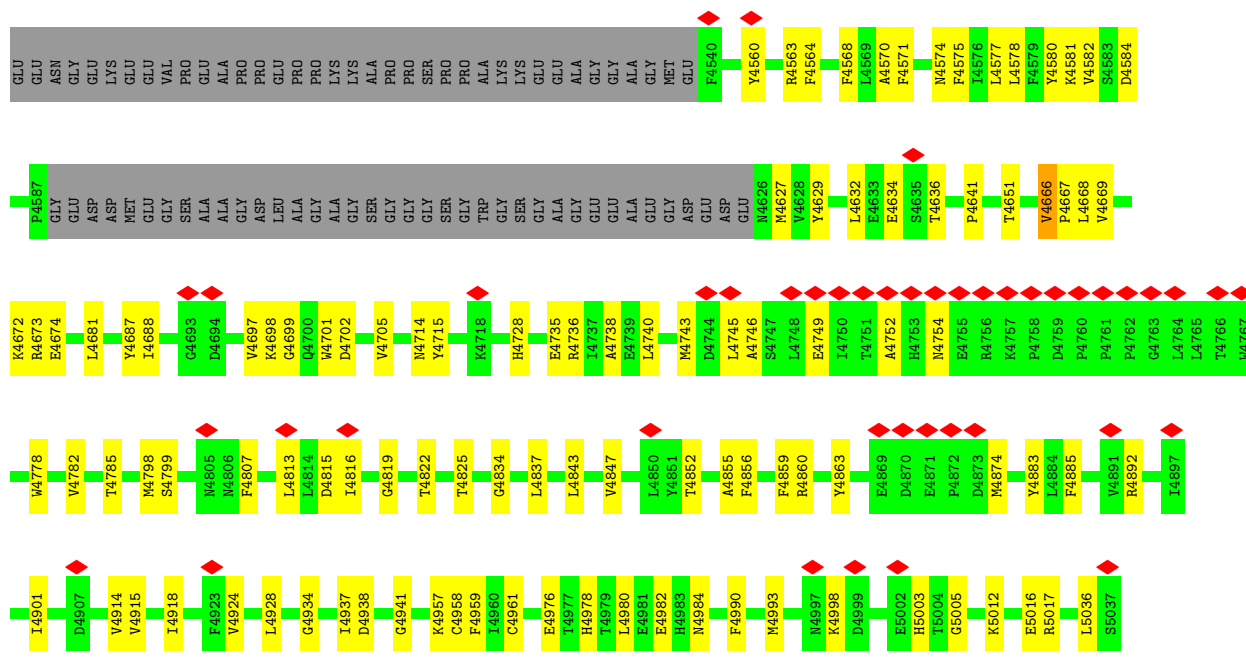
• Molecule 2: ryanodine receptor type 1



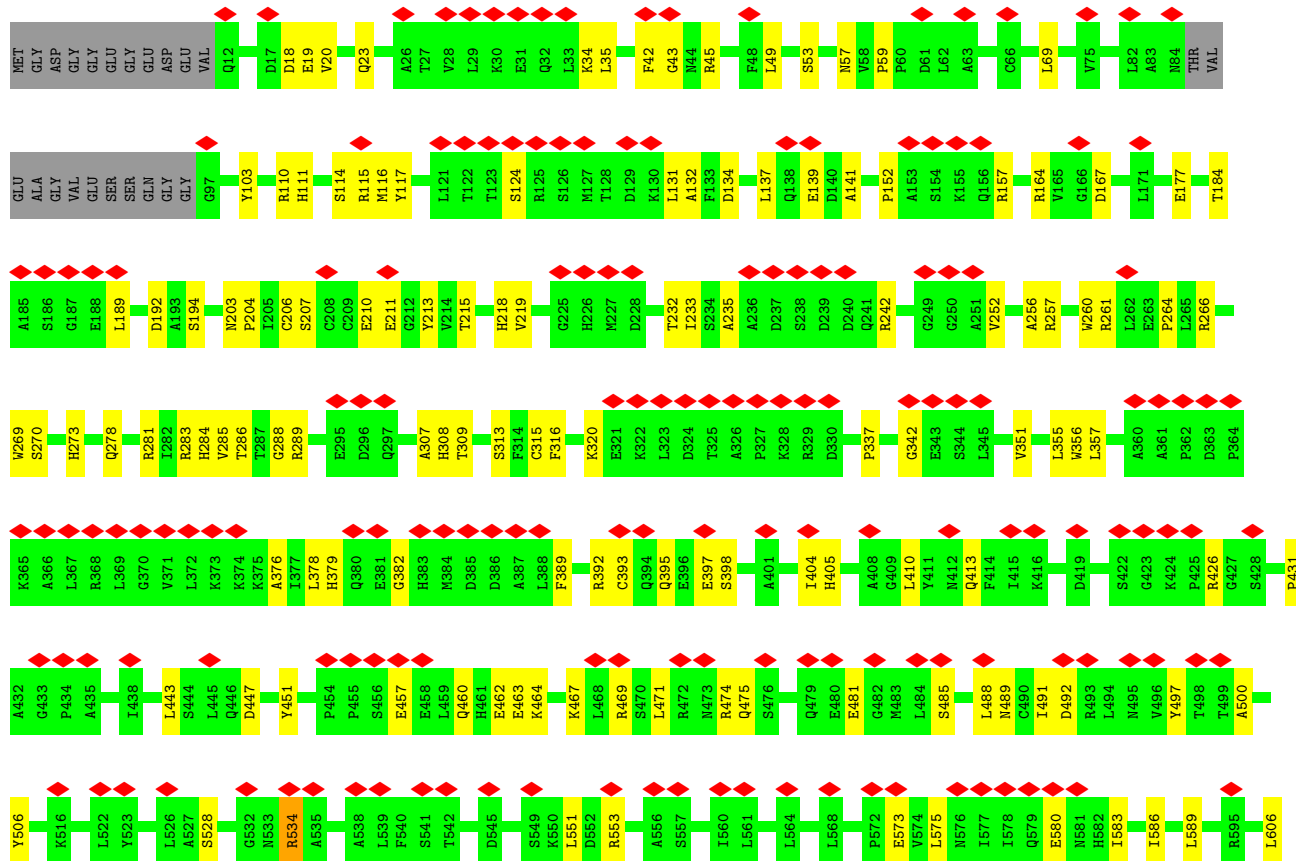
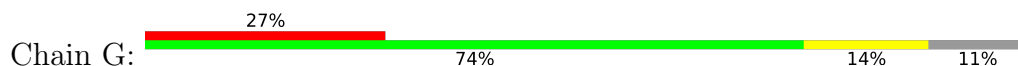








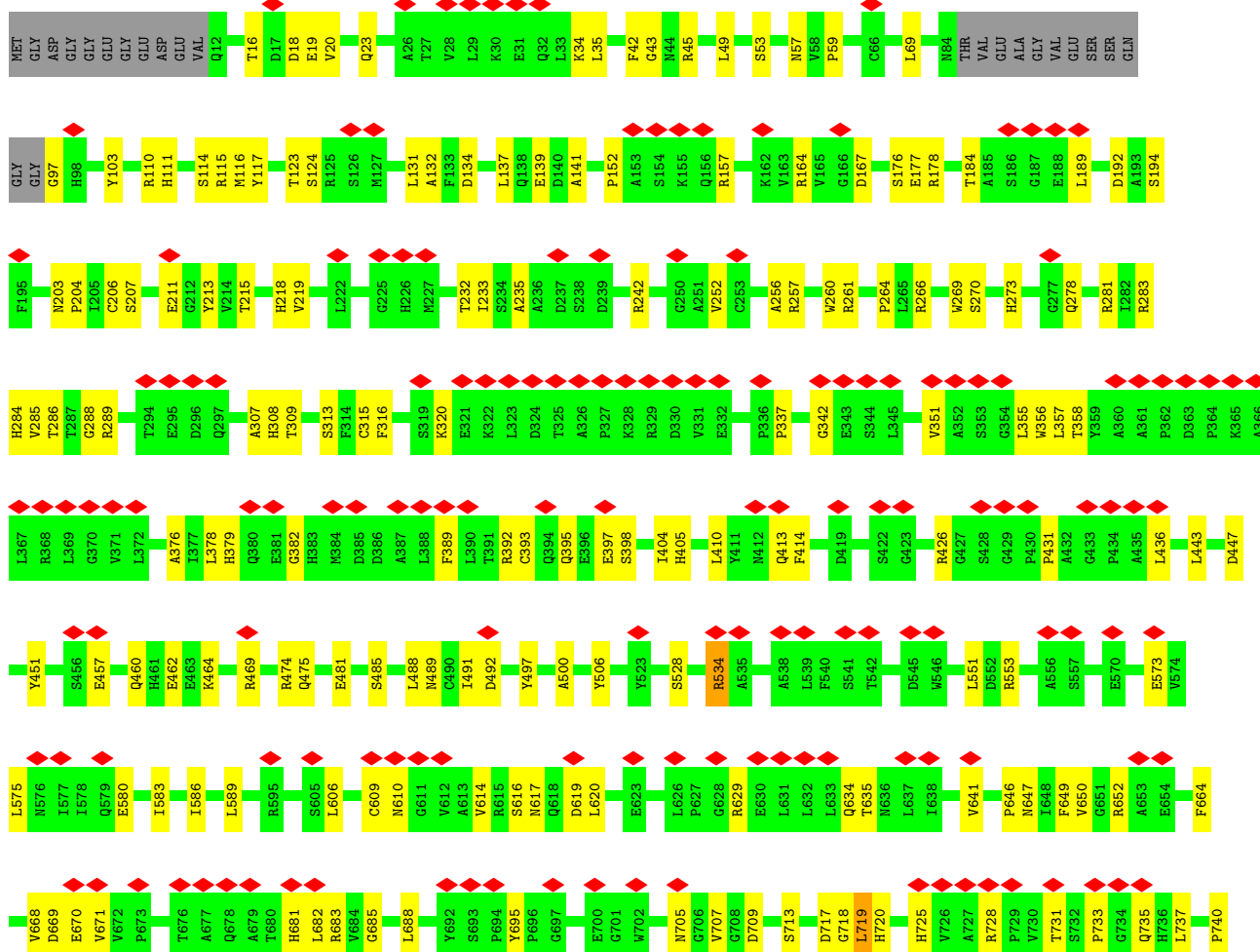
• Molecule 2: ryanodine receptor type 1







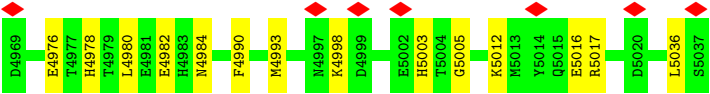
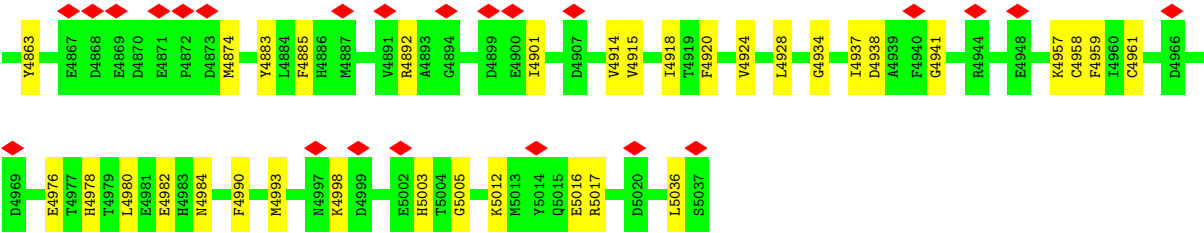








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V4582	S4583	D4584	P4587	GLY	GLU	ASP	ASP	GLY	GLY	GLY	SER	ALA	ALA	ALA	ALA	GLY	GLY	GLY	SER	GLY	TRP	GLY	GLY	GLY	ALA	GLY	GLY	GLY	GLY	M4626	M4627	V4628	Y4629	L4632	E4633	E4634	S4635	T4636	G4637	P4641	T4651	L4652	V4653					
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PRO	PHE	ARG	PRO	GLY	GLY	GLY	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	SER	ILE	LEU	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
ALA	ARG	GLY	ALA	THR	ALA	LEU	ALA	GLY	ALA	TRP	GLY	VAL	VAL	ALA	ALA	ALA	GLY	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	SER	LEU	PHE	GLY	GLY	GLY	VAL	THR	VAL	VAL	THR	GLY	LEU	ALA	ALA	GLY	PRO	
ASP	PRO	ASP	GLY	GLY	VAL	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
GLY	GLY	MET	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.549	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/834	0.56	0/1123
1	F	0.31	0/834	0.56	0/1123
1	H	0.31	0/834	0.56	0/1123
1	J	0.31	0/834	0.56	0/1123
2	B	0.30	0/25428	0.55	5/34534 (0.0%)
2	E	0.30	0/25428	0.55	5/34534 (0.0%)
2	G	0.30	0/25428	0.55	5/34534 (0.0%)
2	I	0.30	0/25428	0.55	5/34534 (0.0%)
All	All	0.30	0/105048	0.55	20/142628 (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
2	B	0	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	719	LEU	CA-CB-CG	6.09	129.30	115.30
2	G	719	LEU	CA-CB-CG	6.08	129.29	115.30
2	E	719	LEU	CA-CB-CG	6.08	129.28	115.30
2	I	719	LEU	CA-CB-CG	6.07	129.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1667	LEU	CA-CB-CG	5.71	128.43	115.30
2	B	1667	LEU	CA-CB-CG	5.70	128.42	115.30
2	E	1667	LEU	CA-CB-CG	5.69	128.40	115.30
2	I	1667	LEU	CA-CB-CG	5.69	128.39	115.30
2	B	977	LEU	CA-CB-CG	5.51	127.98	115.30
2	I	977	LEU	CA-CB-CG	5.51	127.97	115.30
2	E	977	LEU	CA-CB-CG	5.49	127.93	115.30
2	G	977	LEU	CA-CB-CG	5.47	127.88	115.30
2	I	2290	LEU	CA-CB-CG	5.17	127.20	115.30
2	G	2290	LEU	CA-CB-CG	5.15	127.15	115.30
2	B	2290	LEU	CA-CB-CG	5.14	127.11	115.30
2	E	2290	LEU	CA-CB-CG	5.13	127.10	115.30
2	E	2291	GLN	C-N-CA	5.04	134.29	121.70
2	I	2291	GLN	C-N-CA	5.03	134.29	121.70
2	B	2291	GLN	C-N-CA	5.03	134.28	121.70
2	G	2291	GLN	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2292	GLU	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4228	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	137	LEU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	E	2291	GLN	Peptide
2	E	2292	GLU	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4228	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
2	G	137	LEU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2292	GLU	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4228	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
2	I	137	LEU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2292	GLU	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4228	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	I	808	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	18	0
1	F	818	0	824	17	0
1	H	818	0	824	17	0
1	J	818	0	824	18	0
2	B	29369	0	24711	395	0
2	E	29369	0	24713	406	0
2	G	29369	0	24713	395	0
2	I	29369	0	24712	397	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102145	1629	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 7.

All (1629) 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)
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.88	0.72
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.88	0.71
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.88	0.71
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.56	0.71
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.56	0.70
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.89	0.70
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.74	0.69
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.74	0.69
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.75	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.75	0.68
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.56	0.68
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.74	0.68
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.75	0.68
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.59	0.68
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.59	0.68
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.75	0.68
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.59	0.68
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.59	0.67
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.74	0.67
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.77	0.66
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.77	0.66
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.78	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.43	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.43	0.66
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.78	0.65
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.78	0.65
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.29	0.65
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.78	0.65
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.78	0.65
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.29	0.65
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.78	0.65
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.79	0.65
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.29	0.65
2:G:379:HIS:HD2	2:G:382:GLY:H	1.43	0.65
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.79	0.65
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.29	0.65
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.78	0.64
2:B:4961:CYS:SG	2:B:4978:HIS:NE2	2.71	0.64
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.78	0.64
2:B:1232:ARG:HD2	2:B:1702:HIS:HB3	1.80	0.64
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.78	0.64
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.31	0.64
2:I:4961:CYS:SG	2:I:4978:HIS:NE2	2.71	0.64
2:B:379:HIS:HD2	2:B:382:GLY:H	1.43	0.64
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.31	0.64
2:G:4961:CYS:SG	2:G:4978:HIS:NE2	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.31	0.64
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.78	0.63
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.80	0.63
2:E:1232:ARG:HD2	2:E:1702:HIS:HB3	1.80	0.63
2:E:4961:CYS:SG	2:E:4978:HIS:NE2	2.71	0.63
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.31	0.63
2:I:606:LEU:O	2:I:617:ASN:ND2	2.32	0.63
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.81	0.63
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.81	0.63
2:B:606:LEU:O	2:B:617:ASN:ND2	2.32	0.63
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.81	0.63
2:E:606:LEU:O	2:E:617:ASN:ND2	2.32	0.63
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.63
2:G:606:LEU:O	2:G:617:ASN:ND2	2.32	0.62
2:I:1232:ARG:HD2	2:I:1702:HIS:HB3	1.80	0.62
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.32	0.62
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.32	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.62
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.32	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:E:4918:ILE:HG23	2:G:4892:ARG:HD3	1.81	0.62
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.81	0.62
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.62
2:B:4934:GLY:HA3	2:E:4937:ILE:HD12	1.81	0.62
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.32	0.62
1:A:34:LYS:NZ	2:B:635:THR:O	2.33	0.62
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.81	0.62
2:G:1232:ARG:HD2	2:G:1702:HIS:HB3	1.80	0.62
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.33	0.62
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.33	0.62
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.66	0.61
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.81	0.61
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.61
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.66	0.61
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.61
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.33	0.61
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.33	0.61
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.66	0.61
2:E:4144:ALA:HB2	2:E:4170:ILE:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.84	0.60
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.81	0.60
2:G:111:HIS:HD2	2:G:114:SER:H	1.49	0.60
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.84	0.60
2:I:111:HIS:HD2	2:I:114:SER:H	1.49	0.60
2:G:4144:ALA:HB2	2:G:4170:ILE:HG22	1.84	0.60
2:B:4144:ALA:HB2	2:B:4170:ILE:HG22	1.84	0.60
2:I:4144:ALA:HB2	2:I:4170:ILE:HG22	1.84	0.60
2:B:111:HIS:HD2	2:B:114:SER:H	1.49	0.60
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.84	0.60
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.67	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.49	0.59
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.66	0.59
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.67	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.59
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.36	0.59
2:B:4847:VAL:HG11	2:B:4924:VAL:HG11	1.85	0.59
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.84	0.59
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	1.85	0.59
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.85	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.59
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.84	0.59
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	1.85	0.59
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.67	0.59
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.59
2:I:132:ALA:HA	2:I:194:SER:HB2	1.84	0.59
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.85	0.59
2:B:315:CYS:SG	2:B:316:PHE:N	2.75	0.59
2:I:315:CYS:SG	2:I:316:PHE:N	2.75	0.59
2:E:315:CYS:SG	2:E:316:PHE:N	2.75	0.59
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.67	0.59
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.36	0.59
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.85	0.59
2:B:132:ALA:HA	2:B:194:SER:HB2	1.84	0.58
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.36	0.58
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	1.85	0.58
2:I:4847:VAL:HG11	2:I:4924:VAL:HG11	1.85	0.58
2:B:1973:GLN:O	2:B:1977:TYR:N	2.35	0.58
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	1.85	0.58
2:E:3761:GLN:HB3	2:E:4754:ASN:HA	1.85	0.58
2:G:132:ALA:HA	2:G:194:SER:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.37	0.58
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.36	0.58
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.85	0.58
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.58
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.69	0.58
1:H:6:THR:HA	1:H:72:ALA:HA	1.85	0.58
2:I:3761:GLN:HB3	2:I:4754:ASN:HA	1.86	0.58
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.69	0.58
2:E:3767:GLN:HB3	2:E:3772:THR:HG22	1.86	0.58
2:G:3761:GLN:HB3	2:G:4754:ASN:HA	1.86	0.58
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.85	0.58
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.36	0.58
2:B:3761:GLN:HB3	2:B:4754:ASN:HA	1.86	0.58
2:E:132:ALA:HA	2:E:194:SER:HB2	1.84	0.58
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.85	0.58
2:E:4847:VAL:HG11	2:E:4924:VAL:HG11	1.85	0.58
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.85	0.58
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.69	0.58
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.85	0.58
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.58
2:G:315:CYS:SG	2:G:316:PHE:N	2.75	0.58
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.69	0.58
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.69	0.58
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.58
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.58
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.85	0.58
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.85	0.57
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.69	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.57
2:G:4847:VAL:HG11	2:G:4924:VAL:HG11	1.85	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.36	0.57
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.57
2:E:842:PRO:HD3	2:E:1073:ARG:HG3	1.87	0.57
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	1.86	0.57
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.37	0.57
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.86	0.57
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.86	0.57
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.86	0.57
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.86	0.57
1:J:6:THR:HA	1:J:72:ALA:HA	1.85	0.57
1:A:6:THR:HA	1:A:72:ALA:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:842:PRO:HD3	2:I:1073:ARG:HG3	1.87	0.57
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.85	0.57
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.86	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
1:F:6:THR:HA	1:F:72:ALA:HA	1.85	0.57
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.86	0.57
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.69	0.57
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.37	0.57
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.37	0.57
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.57
2:E:4581:LYS:HB2	2:E:4632:LEU:HB2	1.86	0.57
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.86	0.57
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.85	0.57
2:B:842:PRO:HD3	2:B:1073:ARG:HG3	1.87	0.57
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.87	0.57
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.37	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.57
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.57
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.87	0.57
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.86	0.57
2:G:3767:GLN:HB3	2:G:3772:THR:HG22	1.86	0.57
2:G:4059:LEU:O	2:G:4063:ASP:N	2.36	0.57
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.85	0.57
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.87	0.57
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.57
2:I:3767:GLN:HB3	2:I:3772:THR:HG22	1.86	0.57
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.38	0.56
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.37	0.56
2:I:4581:LYS:HB2	2:I:4632:LEU:HB2	1.86	0.56
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.87	0.56
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.87	0.56
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.56
2:G:4581:LYS:HB2	2:G:4632:LEU:HB2	1.86	0.56
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.56
2:I:4059:LEU:O	2:I:4063:ASP:N	2.36	0.56
2:B:4581:LYS:HB2	2:B:4632:LEU:HB2	1.86	0.56
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.88	0.56
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.87	0.56
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.71	0.56
2:G:1237:TRP:HH2	2:G:1652:GLU:HA	1.71	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.36	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.56
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.88	0.56
2:E:1237:TRP:HH2	2:E:1652:GLU:HA	1.71	0.56
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.69	0.56
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.37	0.56
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.70	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.56
2:I:1237:TRP:HH2	2:I:1652:GLU:HA	1.71	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.56
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.70	0.56
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.56
2:B:3767:GLN:HB3	2:B:3772:THR:HG22	1.86	0.56
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.79	0.56
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.88	0.56
2:G:728:ARG:NH2	2:G:1527:UNK:O	2.38	0.56
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.71	0.56
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.88	0.56
2:B:1237:TRP:HH2	2:B:1652:GLU:HA	1.71	0.56
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.71	0.56
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.79	0.56
2:E:4059:LEU:O	2:E:4063:ASP:N	2.36	0.56
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.87	0.56
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.56
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.88	0.56
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.88	0.56
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.86	0.56
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.87	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.39	0.55
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.88	0.55
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.88	0.55
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.70	0.55
2:I:1973:GLN:O	2:I:1977:TYR:N	2.35	0.55
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.71	0.55
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.70	0.55
2:B:4980:LEU:O	2:B:4984:ASN:ND2	2.40	0.55
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.71	0.55
2:I:4056:GLU:HA	2:I:4059:LEU:HB2	1.89	0.55
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.88	0.55
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.88	0.55
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.89	0.55
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.40	0.55
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.40	0.55
2:B:4056:GLU:HA	2:B:4059:LEU:HB2	1.89	0.55
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.79	0.55
2:G:4134:GLU:HG3	2:G:4135:PRO:HD3	1.89	0.55
2:I:4134:GLU:HG3	2:I:4135:PRO:HD3	1.89	0.55
2:B:4134:GLU:HG3	2:B:4135:PRO:HD3	1.89	0.55
2:E:4201:ASN:O	2:E:4205:TRP:N	2.40	0.55
2:E:4980:LEU:O	2:E:4984:ASN:ND2	2.40	0.55
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.40	0.55
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.88	0.55
2:I:4980:LEU:O	2:I:4984:ASN:ND2	2.40	0.55
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.88	0.55
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.88	0.55
2:E:4056:GLU:HA	2:E:4059:LEU:HB2	1.89	0.55
2:E:4134:GLU:HG3	2:E:4135:PRO:HD3	1.89	0.55
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.79	0.55
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.40	0.55
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.40	0.55
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.55
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.40	0.55
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.88	0.55
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.40	0.55
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.55
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.40	0.55
2:G:1973:GLN:O	2:G:1977:TYR:N	2.35	0.55
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.40	0.55
2:G:4201:ASN:O	2:G:4205:TRP:N	2.40	0.55
2:I:451:TYR:O	2:I:474:ARG:NH1	2.40	0.55
2:I:1667:LEU:O	2:I:1671:ARG:NH1	2.40	0.55
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.88	0.55
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.88	0.54
2:B:488:LEU:O	2:B:492:ASP:N	2.40	0.54
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.89	0.54
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.54
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.40	0.54
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.90	0.54
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.72	0.54
2:I:4201:ASN:O	2:I:4205:TRP:N	2.40	0.54
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.40	0.54
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.54
2:B:1667:LEU:O	2:B:1671:ARG:NH1	2.40	0.54
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.89	0.54
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.72	0.54
2:B:4187:SER:HB2	2:B:4189:ARG:HH21	1.73	0.54
2:B:4201:ASN:O	2:B:4205:TRP:N	2.40	0.54
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.88	0.54
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.88	0.54
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.88	0.54
2:E:4187:SER:HB2	2:E:4189:ARG:HH21	1.73	0.54
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.88	0.54
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.54
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.72	0.54
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.88	0.54
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.88	0.54
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.88	0.54
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.72	0.54
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.54
2:G:264:PRO:HG2	2:G:270:SER:HB2	1.90	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.54
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.89	0.54
2:B:4059:LEU:O	2:B:4063:ASP:N	2.36	0.54
2:E:1973:GLN:O	2:E:1977:TYR:N	2.35	0.54
2:G:4980:LEU:O	2:G:4984:ASN:ND2	2.40	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.40	0.54
2:E:451:TYR:O	2:E:474:ARG:NH1	2.40	0.54
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.90	0.54
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.41	0.54
2:I:23:GLN:HE21	2:I:34:LYS:HB3	1.73	0.54
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.41	0.54
2:E:264:PRO:HG2	2:E:270:SER:HB2	1.90	0.54
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.90	0.54
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1667:LEU:O	2:G:1671:ARG:NH1	2.40	0.54
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.90	0.54
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.90	0.54
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.41	0.54
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.40	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:E:3843:ASP:H	2:E:3874:VAL:HG13	1.73	0.54
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.41	0.54
2:G:451:TYR:O	2:G:474:ARG:NH1	2.40	0.54
2:G:1777:PHE:HA	2:G:1799:SER:HB2	1.90	0.54
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.90	0.54
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.54
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.41	0.54
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.41	0.53
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.41	0.53
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.41	0.53
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.53
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.40	0.53
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.53
2:I:4187:SER:HB2	2:I:4189:ARG:HH21	1.73	0.53
2:E:1667:LEU:O	2:E:1671:ARG:NH1	2.40	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.40	0.53
2:I:4563:ARG:NH1	2:I:4815:ASP:OD2	2.41	0.53
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.90	0.53
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.72	0.53
2:E:488:LEU:O	2:E:492:ASP:N	2.40	0.53
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.72	0.53
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.40	0.53
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.91	0.53
2:G:4056:GLU:HA	2:G:4059:LEU:HB2	1.89	0.53
2:I:157:ARG:NH2	2:I:167:ASP:OD1	2.38	0.53
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.90	0.53
2:I:1777:PHE:HA	2:I:1799:SER:HB2	1.90	0.53
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.53
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.40	0.53
2:I:4914:VAL:HG13	2:I:4915:VAL:HG23	1.90	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.53
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.91	0.53
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.91	0.53
2:G:731:THR:OG1	2:G:1519:UNK:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.90	0.53
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.90	0.53
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.90	0.53
2:E:4563:ARG:NH1	2:E:4815:ASP:OD2	2.41	0.53
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.74	0.53
2:G:488:LEU:O	2:G:492:ASP:N	2.40	0.53
2:G:685:GLY:N	2:G:780:VAL:O	2.38	0.53
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.41	0.53
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.41	0.53
2:B:4702:ASP:HA	2:B:4778:TRP:HE1	1.74	0.53
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.74	0.53
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.53
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.53
2:E:647:ASN:ND2	2:E:820:ARG:O	2.40	0.53
2:G:4187:SER:HB2	2:G:4189:ARG:HH21	1.73	0.53
2:G:4815:ASP:O	2:G:4819:GLY:N	2.42	0.53
2:I:111:HIS:N	2:I:116:MET:O	2.40	0.53
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.91	0.53
2:B:131:LEU:HB3	2:E:2459:SER:HB2	1.91	0.53
2:B:451:TYR:O	2:B:474:ARG:NH1	2.40	0.53
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.91	0.53
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.90	0.53
2:B:3843:ASP:H	2:B:3874:VAL:HG13	1.73	0.53
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.41	0.53
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.73	0.53
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.91	0.53
2:E:4702:ASP:HA	2:E:4778:TRP:HE1	1.74	0.53
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.41	0.53
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.91	0.53
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.41	0.53
2:B:264:PRO:HG2	2:B:270:SER:HB2	1.90	0.53
2:E:731:THR:OG1	2:E:1519:UNK:O	2.26	0.53
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.72	0.53
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.90	0.53
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.91	0.53
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.91	0.53
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.73	0.53
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.90	0.53
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.91	0.53
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.41	0.53
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.40	0.53
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.74	0.53
2:I:488:LEU:O	2:I:492:ASP:N	2.40	0.53
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.90	0.53
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.91	0.52
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.91	0.52
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.90	0.52
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.40	0.52
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.89	0.52
2:I:4702:ASP:HA	2:I:4778:TRP:HE1	1.74	0.52
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.41	0.52
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.90	0.52
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.90	0.52
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.43	0.52
2:G:4563:ARG:NH1	2:G:4815:ASP:OD2	2.41	0.52
2:I:264:PRO:HG2	2:I:270:SER:HB2	1.90	0.52
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.91	0.52
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.91	0.52
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.92	0.52
2:B:4914:VAL:HG13	2:B:4915:VAL:HG23	1.90	0.52
2:G:647:ASN:ND2	2:G:820:ARG:O	2.40	0.52
2:G:3843:ASP:H	2:G:3874:VAL:HG13	1.73	0.52
1:J:7:ILE:HG22	1:J:9:PRO:HD2	1.91	0.52
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.74	0.52
2:B:1777:PHE:HA	2:B:1799:SER:HB2	1.90	0.52
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.91	0.52
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.43	0.52
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.92	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.52
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.91	0.52
2:G:3840:SER:OG	2:G:3875:MET:O	2.25	0.52
2:I:1729:SER:O	2:I:2163:ARG:NH1	2.43	0.52
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.43	0.52
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.92	0.52
2:E:1777:PHE:HA	2:E:1799:SER:HB2	1.90	0.52
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.92	0.52
1:F:7:ILE:HG22	1:F:9:PRO:HD2	1.91	0.52
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.73	0.52
2:G:111:HIS:N	2:G:116:MET:O	2.40	0.52
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.91	0.52
2:G:4702:ASP:HA	2:G:4778:TRP:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1729:SER:O	2:B:2163:ARG:NH1	2.43	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.52
2:B:4151:SER:HA	2:B:4160:LEU:HD21	1.92	0.52
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.92	0.52
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.91	0.52
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.91	0.52
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.91	0.52
2:G:4914:VAL:HG13	2:G:4915:VAL:HG23	1.90	0.52
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.91	0.52
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.91	0.52
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.92	0.52
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.92	0.52
2:G:4834:GLY:HA2	2:G:4837:LEU:HD12	1.92	0.52
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.92	0.52
2:B:157:ARG:NH2	2:B:167:ASP:OD1	2.38	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.52
2:E:111:HIS:N	2:E:116:MET:O	2.40	0.52
2:E:4834:GLY:HA2	2:E:4837:LEU:HD12	1.92	0.52
2:G:1729:SER:O	2:G:2163:ARG:NH1	2.43	0.52
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.92	0.52
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.91	0.52
2:B:728:ARG:NH2	2:B:1527:UNK:O	2.43	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.41	0.52
2:B:4024:VAL:HG23	2:B:4027:LEU:HD12	1.92	0.52
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.91	0.52
2:E:4815:ASP:O	2:E:4819:GLY:N	2.42	0.52
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.91	0.52
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.92	0.52
2:I:3843:ASP:H	2:I:3874:VAL:HG13	1.73	0.52
2:B:111:HIS:N	2:B:116:MET:O	2.40	0.52
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.90	0.52
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.92	0.52
2:E:4914:VAL:HG13	2:E:4915:VAL:HG23	1.90	0.52
2:B:4815:ASP:O	2:B:4819:GLY:N	2.41	0.51
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.41	0.51
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.92	0.51
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.92	0.51
2:E:278:GLN:N	2:E:315:CYS:SG	2.83	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.51
2:I:4151:SER:HA	2:I:4160:LEU:HD21	1.92	0.51
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.91	0.51
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.93	0.51
2:I:4834:GLY:HA2	2:I:4837:LEU:HD12	1.92	0.51
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.75	0.51
2:B:1258:ALA:HB3	2:B:1271:ARG:HB3	1.93	0.51
2:E:1729:SER:O	2:E:2163:ARG:NH1	2.43	0.51
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.92	0.51
2:G:1258:ALA:HB3	2:G:1271:ARG:HB3	1.93	0.51
2:I:1258:ALA:HB3	2:I:1271:ARG:HB3	1.93	0.51
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.92	0.51
2:E:395:GLN:HG3	2:E:397:GLU:H	1.76	0.51
2:E:1258:ALA:HB3	2:E:1271:ARG:HB3	1.93	0.51
2:G:157:ARG:NH2	2:G:167:ASP:OD1	2.38	0.51
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.29	0.51
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.91	0.51
2:I:647:ASN:ND2	2:I:820:ARG:O	2.40	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.91	0.51
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.92	0.51
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.92	0.51
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.93	0.51
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.92	0.51
2:I:3817:LEU:HD22	2:I:3899:PHE:HB2	1.93	0.51
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.43	0.51
2:B:278:GLN:N	2:B:315:CYS:SG	2.83	0.51
2:E:4024:VAL:HG23	2:E:4027:LEU:HD12	1.92	0.51
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.44	0.51
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.92	0.51
2:I:395:GLN:HG3	2:I:397:GLU:H	1.76	0.51
2:I:635:THR:O	1:J:34:LYS:NZ	2.44	0.51
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.92	0.51
2:I:4815:ASP:O	2:I:4819:GLY:N	2.42	0.51
2:B:794:GLY:H	2:B:798:GLY:HA3	1.76	0.51
2:B:4834:GLY:HA2	2:B:4837:LEU:HD12	1.92	0.51
2:E:261:ARG:N	2:E:283:ARG:O	2.40	0.51
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.44	0.51
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.51
1:H:7:ILE:HG22	1:H:9:PRO:HD2	1.91	0.51
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.93	0.51
1:A:7:ILE:HG22	1:A:9:PRO:HD2	1.91	0.51
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.92	0.51
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.76	0.51
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.93	0.51
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.92	0.51
2:E:4151:SER:HA	2:E:4160:LEU:HD21	1.92	0.51
2:B:647:ASN:ND2	2:B:820:ARG:O	2.40	0.51
2:B:4892:ARG:HD3	2:I:4918:ILE:HG23	1.91	0.51
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.93	0.51
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.76	0.51
2:I:4024:VAL:HG23	2:I:4027:LEU:HD12	1.92	0.51
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.94	0.50
2:B:709:ASP:O	2:B:725:HIS:ND1	2.44	0.50
2:B:3817:LEU:HD22	2:B:3899:PHE:HB2	1.93	0.50
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.50
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.77	0.50
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.76	0.50
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.77	0.50
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.93	0.50
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.92	0.50
2:G:4151:SER:HA	2:G:4160:LEU:HD21	1.92	0.50
2:G:4860:ARG:NH2	2:I:4629:TYR:OH	2.43	0.50
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.92	0.50
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.92	0.50
2:B:3767:GLN:HA	2:B:3770:LEU:HB2	1.93	0.50
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.92	0.50
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.92	0.50
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.93	0.50
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.29	0.50
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.44	0.50
2:I:728:ARG:NH2	2:I:1527:UNK:O	2.44	0.50
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.92	0.50
2:E:794:GLY:H	2:E:798:GLY:HA3	1.76	0.50
2:E:3817:LEU:HD22	2:E:3899:PHE:HB2	1.93	0.50
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.45	0.50
2:G:278:GLN:N	2:G:315:CYS:SG	2.83	0.50
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.92	0.50
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.93	0.50
2:I:3767:GLN:HA	2:I:3770:LEU:HB2	1.93	0.50
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.94	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.50
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.94	0.50
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4571:PHE:O	2:I:4575:PHE:N	2.44	0.50
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.29	0.50
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.45	0.50
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.94	0.50
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.45	0.50
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.77	0.50
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.93	0.50
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.92	0.50
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.77	0.50
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.94	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.93	0.50
2:E:3767:GLN:HA	2:E:3770:LEU:HB2	1.93	0.50
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.30	0.50
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.93	0.50
2:I:3963:ASN:O	2:I:3966:THR:OG1	2.28	0.50
1:A:27:THR:HB	1:A:100:ASP:HB3	1.94	0.50
2:G:395:GLN:HG3	2:G:397:GLU:H	1.76	0.50
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.45	0.50
2:I:794:GLY:H	2:I:798:GLY:HA3	1.76	0.50
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.94	0.50
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.94	0.50
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.93	0.50
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.94	0.50
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.94	0.50
2:E:4934:GLY:O	2:E:4938:ASP:N	2.42	0.50
2:G:709:ASP:O	2:G:725:HIS:ND1	2.44	0.50
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.94	0.50
2:B:43:GLY:N	2:B:447:ASP:OD2	2.44	0.49
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.30	0.49
2:B:3840:SER:OG	2:B:3875:MET:O	2.25	0.49
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.77	0.49
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.94	0.49
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.94	0.49
2:G:4024:VAL:HG23	2:G:4027:LEU:HD12	1.92	0.49
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.94	0.49
2:I:709:ASP:O	2:I:725:HIS:ND1	2.44	0.49
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.94	0.49
2:B:313:SER:HB3	2:B:351:VAL:HB	1.95	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.76	0.49
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.92	0.49
2:B:4197:ILE:HG21	2:B:4990:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.94	0.49
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.94	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.92	0.49
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.45	0.49
1:J:27:THR:HB	1:J:100:ASP:HB3	1.94	0.49
2:B:34:LYS:H	2:B:53:SER:HG	1.60	0.49
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.29	0.49
2:E:3840:SER:OG	2:E:3875:MET:O	2.25	0.49
1:F:27:THR:HB	1:F:100:ASP:HB3	1.94	0.49
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.94	0.49
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.94	0.49
2:G:3817:LEU:HD22	2:G:3899:PHE:HB2	1.93	0.49
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.94	0.49
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.94	0.49
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.94	0.49
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.45	0.49
2:I:4177:TYR:HE1	2:I:4199:GLU:HB2	1.78	0.49
2:G:1972:ASN:HD21	2:G:2024:PRO:HB3	1.78	0.49
2:G:4177:TYR:HE1	2:G:4199:GLU:HB2	1.78	0.49
2:B:76:ARG:HB3	2:E:3935:TRP:HB3	1.95	0.49
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.48	0.49
2:B:485:SER:O	2:B:489:ASN:N	2.46	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.49
2:B:4570:ALA:O	2:B:4574:ASN:ND2	2.45	0.49
2:E:313:SER:HB3	2:E:351:VAL:HB	1.95	0.49
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.94	0.49
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.94	0.49
1:H:87:HIS:N	1:H:91:ILE:O	2.45	0.49
2:I:313:SER:HB3	2:I:351:VAL:HB	1.95	0.49
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.94	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.49
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.30	0.49
2:E:709:ASP:O	2:E:725:HIS:ND1	2.44	0.49
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.45	0.49
2:E:4197:ILE:HG21	2:E:4990:PHE:HB3	1.94	0.49
2:G:313:SER:HB3	2:G:351:VAL:HB	1.95	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.76	0.49
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.93	0.49
2:I:278:GLN:N	2:I:315:CYS:SG	2.83	0.49
2:I:1972:ASN:HD21	2:I:2024:PRO:HB3	1.78	0.49
2:I:4570:ALA:O	2:I:4574:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:87:HIS:N	1:J:91:ILE:O	2.45	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:B:4822:THR:O	2:B:4825:THR:OG1	2.30	0.49
2:E:34:LYS:N	2:E:53:SER:OG	2.42	0.49
1:F:87:HIS:N	1:F:91:ILE:O	2.45	0.49
2:G:261:ARG:N	2:G:283:ARG:O	2.40	0.49
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.94	0.49
1:H:27:THR:HB	1:H:100:ASP:HB3	1.94	0.49
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.94	0.49
2:E:4822:THR:O	2:E:4825:THR:OG1	2.30	0.49
2:G:3767:GLN:HA	2:G:3770:LEU:HB2	1.93	0.49
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.94	0.49
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.49
2:B:4563:ARG:NH1	2:B:4815:ASP:OD2	2.41	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.49
2:E:2440:MET:O	2:E:2444:GLN:N	2.40	0.49
2:E:3766:GLN:HE21	2:E:3767:GLN:HE22	1.61	0.49
2:G:3766:GLN:HE21	2:G:3767:GLN:HE22	1.61	0.49
2:I:43:GLY:N	2:I:447:ASP:OD2	2.44	0.49
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.94	0.49
2:B:3766:GLN:HE21	2:B:3767:GLN:HE22	1.61	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:4560:TYR:O	2:I:4564:PHE:N	2.45	0.49
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.94	0.48
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.45	0.48
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.95	0.48
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.45	0.48
2:G:4192:ARG:HH12	2:G:4982:GLU:HG2	1.78	0.48
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.46	0.48
1:A:87:HIS:N	1:A:91:ILE:O	2.45	0.48
2:B:685:GLY:N	2:B:780:VAL:O	2.38	0.48
2:B:731:THR:OG1	2:B:1519:UNK:O	2.31	0.48
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.94	0.48
2:B:4177:TYR:HE1	2:B:4199:GLU:HB2	1.78	0.48
2:E:43:GLY:N	2:E:447:ASP:OD2	2.44	0.48
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.48	0.48
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.47	0.48
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.78	0.48
2:E:4697:VAL:O	2:E:4701:TRP:N	2.46	0.48
2:G:4197:ILE:HG21	2:G:4990:PHE:HB3	1.94	0.48
2:G:4697:VAL:O	2:G:4701:TRP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.95	0.48
2:I:3766:GLN:HE21	2:I:3767:GLN:HE22	1.61	0.48
2:I:4192:ARG:HH12	2:I:4982:GLU:HG2	1.78	0.48
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.95	0.48
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.95	0.48
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.78	0.48
2:E:4177:TYR:HE1	2:E:4199:GLU:HB2	1.78	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.47	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.46	0.48
2:I:4197:ILE:HG21	2:I:4990:PHE:HB3	1.94	0.48
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.96	0.48
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.46	0.48
2:B:4192:ARG:HH12	2:B:4982:GLU:HG2	1.78	0.48
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	1.96	0.48
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.46	0.48
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.48
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	1.96	0.48
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.45	0.48
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.47	0.48
2:G:1713:ASP:O	2:G:1717:SER:N	2.45	0.48
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.96	0.48
2:I:4697:VAL:O	2:I:4701:TRP:N	2.46	0.48
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.47	0.48
2:B:2868:SER:O	2:B:2872:GLN:N	2.47	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.48
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.94	0.48
2:G:4184:MET:HB2	2:G:4190:ILE:HD13	1.95	0.48
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.95	0.48
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.48	0.48
2:I:460:GLN:HG2	2:I:462:GLU:H	1.79	0.48
2:I:2440:MET:O	2:I:2444:GLN:N	2.40	0.48
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.94	0.48
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.96	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.47	0.48
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.96	0.48
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.95	0.48
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.48
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.94	0.48
2:I:2347:GLU:O	2:I:2351:ASN:N	2.45	0.48
2:B:1659:LEU:O	2:B:1663:HIS:N	2.44	0.48
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.48	0.48
2:E:1713:ASP:O	2:E:1717:SER:N	2.45	0.48
2:E:4192:ARG:HH12	2:E:4982:GLU:HG2	1.78	0.48
2:G:34:LYS:N	2:G:53:SER:OG	2.42	0.48
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.95	0.48
2:G:4822:THR:O	2:G:4825:THR:OG1	2.30	0.48
2:I:34:LYS:N	2:I:53:SER:OG	2.42	0.48
2:I:685:GLY:N	2:I:780:VAL:O	2.38	0.48
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.94	0.48
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.94	0.48
1:J:91:ILE:HD12	1:J:97:LEU:HD11	1.96	0.48
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.48
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.79	0.48
2:E:4184:MET:HB2	2:E:4190:ILE:HD13	1.95	0.48
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.46	0.48
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.95	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.47	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.46	0.48
2:I:731:THR:OG1	2:I:1519:UNK:O	2.32	0.48
2:B:460:GLN:HG2	2:B:462:GLU:H	1.79	0.47
2:E:3963:ASN:O	2:E:3966:THR:OG1	2.29	0.47
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.46	0.47
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.96	0.47
2:B:2440:MET:O	2:B:2444:GLN:N	2.40	0.47
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.95	0.47
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.46	0.47
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.96	0.47
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.96	0.47
2:I:1659:LEU:O	2:I:1663:HIS:N	2.44	0.47
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.95	0.47
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.96	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.46	0.47
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.96	0.47
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.96	0.47
2:G:59:PRO:HG3	2:G:307:ALA:HB3	1.96	0.47
1:H:91:ILE:HD12	1:H:97:LEU:HD11	1.96	0.47
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.79	0.47
2:I:4184:MET:HB2	2:I:4190:ILE:HD13	1.96	0.47
2:B:983:THR:O	2:B:987:ARG:N	2.45	0.47
2:B:4937:ILE:HD12	2:I:4934:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.47	0.47
2:E:3832:ILE:O	2:E:3836:MET:N	2.45	0.47
1:F:91:ILE:HD12	1:F:97:LEU:HD11	1.96	0.47
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.49	0.47
1:H:62:GLY:HA3	1:H:74:LEU:HD21	1.97	0.47
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.95	0.47
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.97	0.47
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.97	0.47
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.96	0.47
2:B:1713:ASP:O	2:B:1717:SER:N	2.45	0.47
2:B:4184:MET:HB2	2:B:4190:ILE:HD13	1.95	0.47
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.79	0.47
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.97	0.47
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.97	0.47
2:E:983:THR:O	2:E:987:ARG:N	2.45	0.47
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.95	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.97	0.47
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.49	0.47
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	1.97	0.47
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.79	0.47
2:E:59:PRO:HG3	2:E:307:ALA:HB3	1.96	0.47
1:F:62:GLY:HA3	1:F:74:LEU:HD21	1.97	0.47
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.47
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.96	0.47
1:A:91:ILE:HD12	1:A:97:LEU:HD11	1.96	0.47
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.47
2:B:4860:ARG:NH2	2:E:4629:TYR:OH	2.47	0.47
2:E:460:GLN:HG2	2:E:462:GLU:H	1.79	0.47
2:E:4571:PHE:O	2:E:4575:PHE:N	2.44	0.47
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	1.97	0.47
2:G:1090:PHE:HD2	2:G:1202:LEU:HD11	1.80	0.47
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	1.97	0.47
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.97	0.47
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.97	0.47
2:E:157:ARG:NH2	2:E:167:ASP:OD1	2.38	0.47
2:G:215:THR:HG22	2:G:273:HIS:HA	1.97	0.47
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.79	0.47
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.49	0.47
2:I:983:THR:O	2:I:987:ARG:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.96	0.47
2:B:1203:ASN:ND2	2:B:1210:SER:O	2.48	0.47
2:E:1668:ARG:HA	2:E:1671:ARG:HH11	1.80	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.46	0.47
2:I:3840:SER:OG	2:I:3875:MET:O	2.25	0.47
2:I:4204:GLN:NE2	2:I:4245:MET:SD	2.88	0.47
2:B:1668:ARG:HA	2:B:1671:ARG:HH11	1.80	0.47
2:B:4885:PHE:HE2	2:B:4901:ILE:HD11	1.80	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.97	0.47
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.97	0.47
2:E:1203:ASN:ND2	2:E:1210:SER:O	2.48	0.47
2:E:4885:PHE:HE2	2:E:4901:ILE:HD11	1.80	0.47
2:G:2347:GLU:O	2:G:2351:ASN:N	2.45	0.47
2:G:4745:LEU:O	2:G:4749:GLU:N	2.47	0.47
2:I:59:PRO:HG3	2:I:307:ALA:HB3	1.96	0.47
2:E:215:THR:HG22	2:E:273:HIS:HA	1.97	0.46
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	1.97	0.46
2:E:4204:GLN:NE2	2:E:4245:MET:SD	2.88	0.46
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.98	0.46
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.79	0.46
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.97	0.46
2:I:988:LEU:O	2:I:992:GLY:N	2.49	0.46
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.97	0.46
2:I:4201:ASN:ND2	2:I:4993:MET:SD	2.89	0.46
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.97	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.97	0.46
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.97	0.46
2:B:1090:PHE:HD2	2:B:1202:LEU:HD11	1.80	0.46
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.97	0.46
2:E:164:ARG:N	2:E:167:ASP:OD2	2.48	0.46
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.46
2:E:4174:PHE:HA	2:E:4177:TYR:HD2	1.81	0.46
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.97	0.46
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.79	0.46
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.97	0.46
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.49	0.46
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.97	0.46
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.79	0.46
2:B:3963:ASN:O	2:B:3966:THR:OG1	2.28	0.46
2:B:4204:GLN:NE2	2:B:4245:MET:SD	2.88	0.46
2:B:4571:PHE:O	2:B:4575:PHE:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:232:THR:HB	2:E:252:VAL:HG11	1.97	0.46
2:E:4852:THR:HG21	2:E:4883:TYR:HB2	1.98	0.46
2:G:983:THR:O	2:G:987:ARG:N	2.45	0.46
2:G:988:LEU:O	2:G:992:GLY:N	2.48	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.48	0.46
2:I:215:THR:HG22	2:I:273:HIS:HA	1.97	0.46
2:B:1091:GLU:HB3	2:B:1203:ASN:HB3	1.98	0.46
2:B:4201:ASN:ND2	2:B:4993:MET:SD	2.89	0.46
2:E:988:LEU:O	2:E:992:GLY:N	2.48	0.46
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.25	0.46
2:I:4083:ASP:HA	2:I:4085:ARG:HH11	1.81	0.46
2:B:59:PRO:HB3	2:B:281:ARG:HD3	1.98	0.46
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.80	0.46
2:B:4697:VAL:O	2:B:4701:TRP:N	2.46	0.46
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.81	0.46
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.49	0.46
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.98	0.46
2:G:43:GLY:N	2:G:447:ASP:OD2	2.44	0.46
2:G:460:GLN:HG2	2:G:462:GLU:H	1.79	0.46
2:G:876:GLU:O	2:G:880:GLU:N	2.47	0.46
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.97	0.46
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.80	0.46
2:I:1091:GLU:HB3	2:I:1203:ASN:HB3	1.98	0.46
2:I:1970:GLN:HB2	2:I:3642:TYR:HA	1.98	0.46
2:B:59:PRO:HG3	2:B:307:ALA:HB3	1.96	0.46
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.97	0.46
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.80	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.96	0.46
2:G:1668:ARG:HA	2:G:1671:ARG:HH11	1.80	0.46
2:B:232:THR:HB	2:B:252:VAL:HG11	1.97	0.46
2:B:261:ARG:N	2:B:283:ARG:O	2.40	0.46
2:B:583:ILE:HA	2:B:586:ILE:HD12	1.98	0.46
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.98	0.46
2:B:4174:PHE:HA	2:B:4177:TYR:HD2	1.80	0.46
2:E:876:GLU:O	2:E:880:GLU:N	2.47	0.46
2:E:3759:GLU:HA	2:E:3762:ARG:HH11	1.81	0.46
2:G:184:THR:HB	2:G:189:LEU:HG	1.98	0.46
2:G:1091:GLU:HB3	2:G:1203:ASN:HB3	1.98	0.46
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	1.98	0.46
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.98	0.46
2:I:2235:PHE:HA	2:I:2238:TYR:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4040:ILE:O	2:I:4044:MET:N	2.47	0.46
2:B:164:ARG:N	2:B:167:ASP:OD2	2.48	0.46
2:B:1830:VAL:HB	2:B:1837:GLN:HA	1.98	0.46
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.97	0.46
2:E:3696:ASP:OD2	2:E:3771:HIS:NE2	2.49	0.46
2:G:1684:ALA:HA	2:G:1782:PHE:HZ	1.81	0.46
2:I:1203:ASN:ND2	2:I:1210:SER:O	2.48	0.46
2:I:1668:ARG:HA	2:I:1671:ARG:HH11	1.80	0.46
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.97	0.46
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.98	0.46
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.80	0.46
2:B:1970:GLN:HB2	2:B:3642:TYR:HA	1.98	0.46
2:B:4852:THR:HG21	2:B:4883:TYR:HB2	1.98	0.46
2:E:184:THR:HB	2:E:189:LEU:HG	1.98	0.46
2:E:260:TRP:CE2	2:E:284:HIS:HD2	2.34	0.46
2:E:1091:GLU:HB3	2:E:1203:ASN:HB3	1.98	0.46
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.98	0.46
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.97	0.46
2:G:260:TRP:CE2	2:G:284:HIS:HD2	2.34	0.46
2:G:583:ILE:HA	2:G:586:ILE:HD12	1.98	0.46
2:I:583:ILE:HA	2:I:586:ILE:HD12	1.98	0.46
2:I:1841:VAL:HA	2:I:1844:LEU:HB3	1.98	0.46
2:I:4937:ILE:O	2:I:4941:GLY:N	2.49	0.46
2:B:215:THR:HG22	2:B:273:HIS:HA	1.97	0.46
2:B:742:ASP:OD1	2:B:760:ASN:ND2	2.49	0.46
2:E:59:PRO:HB3	2:E:281:ARG:HD3	1.98	0.46
2:E:1286:UNK:HA	2:E:1461:UNK:HA	1.97	0.46
2:E:4745:LEU:O	2:E:4749:GLU:N	2.47	0.46
2:G:177:GLU:HG3	2:I:2452:ARG:HH12	1.81	0.46
2:G:1970:GLN:HB2	2:G:3642:TYR:HA	1.98	0.46
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.46
2:G:3927:GLN:O	2:G:3931:SER:N	2.46	0.46
2:G:4174:PHE:HA	2:G:4177:TYR:HD2	1.80	0.46
2:G:4204:GLN:NE2	2:G:4245:MET:SD	2.88	0.46
2:I:59:PRO:HB3	2:I:281:ARG:HD3	1.98	0.46
2:I:260:TRP:CE2	2:I:284:HIS:HD2	2.34	0.46
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.97	0.46
2:I:1092:PHE:N	2:I:1149:VAL:O	2.38	0.46
2:I:3832:ILE:O	2:I:3836:MET:N	2.45	0.46
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.97	0.46
2:B:184:THR:HB	2:B:189:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:260:TRP:CE2	2:B:284:HIS:HD2	2.34	0.45
2:B:870:ILE:HA	2:B:870:ILE:HD12	1.85	0.45
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.81	0.45
2:B:4083:ASP:HA	2:B:4085:ARG:HH11	1.81	0.45
2:E:742:ASP:OD1	2:E:760:ASN:ND2	2.49	0.45
2:E:1032:LYS:O	2:E:1036:ARG:N	2.45	0.45
2:E:1516:UNK:N	2:E:1529:UNK:O	2.49	0.45
2:E:1970:GLN:HB2	2:E:3642:TYR:HA	1.98	0.45
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.98	0.45
2:E:3927:GLN:O	2:E:3931:SER:N	2.46	0.45
2:G:629:ARG:NH2	1:H:89:GLY:O	2.49	0.45
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.97	0.45
2:G:3759:GLU:HA	2:G:3762:ARG:HH11	1.81	0.45
2:G:4083:ASP:HA	2:G:4085:ARG:HH11	1.81	0.45
2:I:3696:ASP:OD2	2:I:3771:HIS:NE2	2.49	0.45
2:I:4852:THR:HG21	2:I:4883:TYR:HB2	1.98	0.45
2:E:485:SER:O	2:E:489:ASN:N	2.46	0.45
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.98	0.45
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.99	0.45
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	1.98	0.45
2:E:4201:ASN:ND2	2:E:4993:MET:SD	2.89	0.45
2:G:164:ARG:N	2:G:167:ASP:OD2	2.48	0.45
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.98	0.45
2:G:670:GLU:H	2:G:740:PRO:HB3	1.81	0.45
2:G:1203:ASN:ND2	2:G:1210:SER:O	2.49	0.45
2:G:4201:ASN:ND2	2:G:4993:MET:SD	2.89	0.45
2:G:4852:THR:HG21	2:G:4883:TYR:HB2	1.98	0.45
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.81	0.45
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.97	0.45
2:I:1684:ALA:HA	2:I:1782:PHE:HZ	1.81	0.45
1:J:39:SER:HB2	1:J:45:PRO:HA	1.99	0.45
2:B:978:THR:HB	2:B:980:ALA:H	1.81	0.45
2:E:583:ILE:HA	2:E:586:ILE:HD12	1.98	0.45
2:E:4934:GLY:HA3	2:G:4937:ILE:HD12	1.98	0.45
2:G:232:THR:HB	2:G:252:VAL:HG11	1.97	0.45
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.81	0.45
2:I:1639:LEU:HD12	2:I:1653:LEU:HD21	1.99	0.45
2:I:1713:ASP:O	2:I:1717:SER:N	2.45	0.45
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.81	0.45
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.81	0.45
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3759:GLU:HA	2:B:3762:ARG:HH11	1.81	0.45
2:B:4934:GLY:O	2:B:4938:ASP:N	2.42	0.45
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.81	0.45
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.99	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.97	0.45
2:I:742:ASP:OD1	2:I:760:ASN:ND2	2.49	0.45
2:I:1090:PHE:HD2	2:I:1202:LEU:HD11	1.80	0.45
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.99	0.45
2:B:134:ASP:HA	2:B:192:ASP:HA	1.99	0.45
2:B:670:GLU:H	2:B:740:PRO:HB3	1.82	0.45
2:B:1841:VAL:HA	2:B:1844:LEU:HB3	1.98	0.45
2:B:2235:PHE:HA	2:B:2238:TYR:HD2	1.81	0.45
2:E:1090:PHE:HD2	2:E:1202:LEU:HD11	1.80	0.45
2:G:1830:VAL:HB	2:G:1837:GLN:HA	1.98	0.45
2:G:3696:ASP:OD2	2:G:3771:HIS:NE2	2.49	0.45
2:I:184:THR:HB	2:I:189:LEU:HG	1.98	0.45
2:I:261:ARG:HB3	2:I:283:ARG:HB3	1.99	0.45
2:I:1830:VAL:HB	2:I:1837:GLN:HA	1.98	0.45
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.97	0.45
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.99	0.45
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.80	0.45
2:E:635:THR:O	1:F:34:LYS:NZ	2.49	0.45
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.97	0.45
2:G:2235:PHE:HA	2:G:2238:TYR:HD2	1.81	0.45
2:G:4885:PHE:HE2	2:G:4901:ILE:HD11	1.80	0.45
2:I:232:THR:HB	2:I:252:VAL:HG11	1.97	0.45
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.97	0.45
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.81	0.45
2:I:4174:PHE:HA	2:I:4177:TYR:HD2	1.81	0.45
2:I:4934:GLY:O	2:I:4938:ASP:N	2.42	0.45
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.98	0.45
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.99	0.45
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.32	0.45
2:G:2257:LEU:O	2:G:2261:SER:N	2.50	0.45
2:G:3832:ILE:O	2:G:3836:MET:N	2.45	0.45
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.98	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.90	0.45
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.32	0.45
2:E:670:GLU:H	2:E:740:PRO:HB3	1.81	0.45
2:E:1659:LEU:O	2:E:1663:HIS:N	2.44	0.45
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.97	0.45
2:G:4937:ILE:O	2:G:4941:GLY:N	2.49	0.45
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.97	0.45
2:I:670:GLU:H	2:I:740:PRO:HB3	1.81	0.45
2:I:3759:GLU:HA	2:I:3762:ARG:HH11	1.81	0.45
1:A:89:GLY:O	2:B:629:ARG:NH2	2.50	0.45
2:B:988:LEU:O	2:B:992:GLY:N	2.49	0.45
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.97	0.45
2:B:3696:ASP:OD2	2:B:3771:HIS:NE2	2.49	0.45
2:E:1235:THR:OG1	2:E:1607:ARG:NE	2.50	0.45
2:E:1830:VAL:HB	2:E:1837:GLN:HA	1.98	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.90	0.45
2:G:261:ARG:HB3	2:G:283:ARG:HB3	1.99	0.45
2:G:3963:ASN:O	2:G:3966:THR:OG1	2.28	0.45
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	1.98	0.45
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.99	0.45
1:A:39:SER:HB2	1:A:45:PRO:HA	1.99	0.45
2:B:1092:PHE:N	2:B:1149:VAL:O	2.38	0.45
2:B:1639:LEU:HD12	2:B:1653:LEU:HD21	1.99	0.45
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.99	0.45
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.98	0.45
2:E:134:ASP:HA	2:E:192:ASP:HA	1.99	0.45
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.52	0.45
2:E:2257:LEU:O	2:E:2261:SER:N	2.50	0.45
2:G:59:PRO:HB3	2:G:281:ARG:HD3	1.98	0.45
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.52	0.45
2:G:978:THR:HB	2:G:980:ALA:H	1.81	0.45
2:G:1639:LEU:HD12	2:G:1653:LEU:HD21	1.99	0.45
2:G:1841:VAL:HA	2:G:1844:LEU:HB3	1.98	0.45
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.97	0.45
2:I:1235:THR:OG1	2:I:1607:ARG:NE	2.50	0.45
2:I:4012:LEU:O	2:I:4016:LEU:N	2.50	0.45
2:I:4885:PHE:HE2	2:I:4901:ILE:HD11	1.80	0.45
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.32	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.52	0.44
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.98	0.44
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.97	0.44
2:E:978:THR:HB	2:E:980:ALA:H	1.81	0.44
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.81	0.44
2:B:2257:LEU:O	2:B:2261:SER:N	2.50	0.44
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1841:VAL:HA	2:E:1844:LEU:HB3	1.98	0.44
2:E:2235:PHE:HA	2:E:2238:TYR:HD2	1.81	0.44
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.98	0.44
2:G:124:SER:HA	2:G:132:ALA:HB3	2.00	0.44
2:I:124:SER:HA	2:I:132:ALA:HB3	1.99	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.90	0.44
2:E:4560:TYR:O	2:E:4564:PHE:N	2.45	0.44
2:E:4998:LYS:HB3	2:E:5003:HIS:HE1	1.83	0.44
2:G:742:ASP:OD1	2:G:760:ASN:ND2	2.49	0.44
2:G:1659:LEU:O	2:G:1663:HIS:N	2.44	0.44
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.97	0.44
1:H:39:SER:HB2	1:H:45:PRO:HA	1.99	0.44
2:B:475:GLN:NE2	2:B:528:SER:O	2.51	0.44
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.36	0.44
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.52	0.44
2:G:627:PRO:HG3	1:H:89:GLY:H	1.82	0.44
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.44
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.30	0.44
2:I:4822:THR:O	2:I:4825:THR:OG1	2.30	0.44
2:E:2347:GLU:O	2:E:2351:ASN:N	2.45	0.44
1:F:39:SER:HB2	1:F:45:PRO:HA	1.99	0.44
2:G:1235:THR:OG1	2:G:1607:ARG:NE	2.50	0.44
2:G:4571:PHE:O	2:G:4575:PHE:N	2.44	0.44
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.00	0.44
2:I:2257:LEU:O	2:I:2261:SER:N	2.50	0.44
2:B:1235:THR:OG1	2:B:1607:ARG:NE	2.50	0.44
2:E:179:TYR:OH	2:G:2359:ARG:NH1	2.51	0.44
2:E:475:GLN:NE2	2:E:528:SER:O	2.51	0.44
2:E:627:PRO:HG3	1:F:89:GLY:H	1.83	0.44
2:E:685:GLY:N	2:E:780:VAL:O	2.38	0.44
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.99	0.44
2:E:1684:ALA:HA	2:E:1782:PHE:HZ	1.81	0.44
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.83	0.44
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.52	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.99	0.44
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.44
2:G:5012:LYS:O	2:G:5016:GLU:N	2.49	0.44
2:I:4736:ARG:O	2:I:4740:LEU:N	2.51	0.44
2:I:4998:LYS:HB3	2:I:5003:HIS:HE1	1.83	0.44
2:B:261:ARG:HB3	2:B:283:ARG:HB3	1.99	0.44
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	1.98	0.44
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.99	0.44
2:E:4083:ASP:HA	2:E:4085:ARG:HH11	1.81	0.44
2:G:475:GLN:NE2	2:G:528:SER:O	2.51	0.44
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.00	0.44
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.98	0.44
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.53	0.44
2:I:838:HIS:CE1	2:I:1201:HIS:HD2	2.36	0.44
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.44
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.99	0.44
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.52	0.44
2:B:838:HIS:CE1	2:B:1201:HIS:HD2	2.36	0.44
2:B:1685:LEU:HD22	2:B:1718:ILE:HD13	1.99	0.44
2:B:1976:ARG:NH1	2:B:1997:GLU:OE2	2.36	0.44
2:B:3927:GLN:O	2:B:3931:SER:N	2.46	0.44
2:B:4228:ALA:O	2:B:4232:GLU:N	2.51	0.44
2:E:1092:PHE:N	2:E:1149:VAL:O	2.38	0.44
2:E:1639:LEU:HD12	2:E:1653:LEU:HD21	1.99	0.44
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.53	0.44
2:I:206:CYS:SG	2:I:207:SER:N	2.90	0.44
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.32	0.44
2:I:3552:UNK:O	2:I:3556:UNK:N	2.50	0.44
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.99	0.44
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.52	0.44
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.51	0.44
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.00	0.44
2:G:134:ASP:HA	2:G:192:ASP:HA	1.99	0.44
2:G:355:LEU:HB3	2:G:378:LEU:HB3	2.00	0.44
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.83	0.44
2:G:3713:LYS:HG2	2:G:3715:LYS:H	1.83	0.44
2:G:4041:ALA:HA	2:G:4044:MET:HB2	2.00	0.44
2:I:134:ASP:HA	2:I:192:ASP:HA	1.99	0.44
2:I:978:THR:HB	2:I:980:ALA:H	1.81	0.44
2:B:124:SER:HA	2:B:132:ALA:HB3	1.99	0.43
2:B:175:SER:O	2:E:2452:ARG:NE	2.52	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.43
2:B:4041:ALA:HA	2:B:4044:MET:HB2	2.00	0.43
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.83	0.43
2:B:4998:LYS:HB3	2:B:5003:HIS:HE1	1.83	0.43
2:E:261:ARG:HB3	2:E:283:ARG:HB3	1.99	0.43
2:E:728:ARG:NH2	2:E:1527:UNK:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4937:ILE:O	2:E:4941:GLY:N	2.49	0.43
2:G:131:LEU:HB3	2:I:2459:SER:HB2	2.00	0.43
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.99	0.43
2:I:139:GLU:O	2:I:141:ALA:N	2.51	0.43
2:I:233:ILE:HD11	2:I:242:ARG:HH21	1.83	0.43
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.52	0.43
2:I:4978:HIS:ND1	2:I:4982:GLU:OE1	2.51	0.43
2:B:1663:HIS:O	2:B:1667:LEU:N	2.49	0.43
2:B:1684:ALA:HA	2:B:1782:PHE:HZ	1.81	0.43
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.83	0.43
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.51	0.43
2:E:4012:LEU:O	2:E:4016:LEU:N	2.50	0.43
2:G:139:GLU:O	2:G:141:ALA:N	2.51	0.43
2:G:342:GLY:HA2	2:G:389:PHE:HD2	1.83	0.43
2:I:1685:LEU:HD22	2:I:1718:ILE:HD13	1.99	0.43
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	2.00	0.43
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.83	0.43
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.54	0.43
2:B:4745:LEU:O	2:B:4749:GLU:N	2.47	0.43
2:B:4918:ILE:HG23	2:E:4892:ARG:HD3	1.99	0.43
2:E:355:LEU:HB3	2:E:378:LEU:HB3	2.00	0.43
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.01	0.43
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.53	0.43
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.43
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.51	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.43
2:G:4918:ILE:HG23	2:I:4892:ARG:HD3	2.00	0.43
2:I:4228:ALA:O	2:I:4232:GLU:N	2.51	0.43
2:I:4976:GLU:O	2:I:4980:LEU:N	2.44	0.43
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.52	0.43
2:B:3832:ILE:O	2:B:3836:MET:N	2.45	0.43
2:B:4705:VAL:HB	2:B:4778:TRP:CD1	2.54	0.43
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.52	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:4228:ALA:O	2:E:4232:GLU:N	2.51	0.43
2:E:4705:VAL:HB	2:E:4778:TRP:CD1	2.54	0.43
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.51	0.43
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.01	0.43
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.53	0.43
2:B:1694:LEU:HD23	2:B:1715:LEU:HD13	2.01	0.43
2:B:2039:LEU:HA	2:B:2042:CYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2517:UNK:O	2:B:2521:UNK:N	2.52	0.43
2:B:4560:TYR:O	2:B:4564:PHE:N	2.45	0.43
2:E:124:SER:HA	2:E:132:ALA:HB3	2.00	0.43
2:E:457:GLU:OE1	2:E:464:LYS:NZ	2.51	0.43
2:E:1685:LEU:HD22	2:E:1718:ILE:HD13	1.99	0.43
2:E:1778:SER:N	2:E:1799:SER:O	2.52	0.43
2:E:2517:UNK:O	2:E:2521:UNK:N	2.51	0.43
2:E:3713:LYS:HG2	2:E:3715:LYS:H	1.83	0.43
2:G:838:HIS:CE1	2:G:1201:HIS:HD2	2.36	0.43
2:G:1685:LEU:HD22	2:G:1718:ILE:HD13	1.99	0.43
2:I:355:LEU:HB3	2:I:378:LEU:HB3	2.00	0.43
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.51	0.43
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.52	0.43
2:I:1679:ASN:O	2:I:1683:HIS:ND1	2.37	0.43
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.53	0.43
2:B:139:GLU:O	2:B:141:ALA:N	2.51	0.43
2:B:233:ILE:HD11	2:B:242:ARG:HH21	1.83	0.43
2:B:3993:LEU:HA	2:B:3996:PHE:HB2	2.00	0.43
2:E:139:GLU:O	2:E:141:ALA:N	2.51	0.43
2:E:4181:ILE:HG23	2:E:4195:PHE:HE1	1.83	0.43
2:G:4040:ILE:O	2:G:4044:MET:N	2.47	0.43
2:I:733:PRO:HD2	2:I:763:PRO:HD2	2.00	0.43
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	2.01	0.43
2:I:3805:LEU:H	2:I:3805:LEU:HG	1.72	0.43
2:I:3993:LEU:HA	2:I:3996:PHE:HB2	2.00	0.43
2:B:1679:ASN:O	2:B:1683:HIS:ND1	2.37	0.43
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	2.01	0.43
2:B:2347:GLU:O	2:B:2351:ASN:N	2.45	0.43
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	2.01	0.43
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.43
2:E:4041:ALA:HA	2:E:4044:MET:HB2	2.01	0.43
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.83	0.43
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.52	0.43
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	2.01	0.43
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.83	0.43
2:I:1694:LEU:HD23	2:I:1715:LEU:HD13	2.01	0.43
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.53	0.43
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.00	0.43
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.99	0.43
2:B:1778:SER:N	2:B:1799:SER:O	2.52	0.43
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:233:ILE:HD11	2:G:242:ARG:HH21	1.83	0.43
2:G:3805:LEU:H	2:G:3805:LEU:HG	1.72	0.43
2:G:4055:VAL:O	2:G:4059:LEU:N	2.49	0.43
2:G:4228:ALA:O	2:G:4232:GLU:N	2.51	0.43
2:G:4934:GLY:O	2:G:4938:ASP:N	2.42	0.43
2:I:1931:LEU:HD22	2:I:1935:VAL:HG11	2.01	0.43
2:I:2039:LEU:HA	2:I:2042:CYS:HB3	2.01	0.43
2:I:3927:GLN:O	2:I:3931:SER:N	2.46	0.43
2:B:932:LEU:HD23	2:B:935:LEU:HD12	2.01	0.43
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	2.00	0.43
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.01	0.43
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.99	0.43
2:B:4138:ASP:O	2:B:4142:ASN:ND2	2.52	0.43
2:B:5012:LYS:O	2:B:5016:GLU:N	2.49	0.43
2:E:2132:GLY:O	2:E:2136:ARG:N	2.52	0.43
1:F:7:ILE:HB	1:F:71:ARG:HB3	2.01	0.43
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.52	0.43
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	2.01	0.43
2:G:2440:MET:O	2:G:2444:GLN:N	2.41	0.43
2:G:4998:LYS:HB3	2:G:5003:HIS:HE1	1.83	0.43
2:I:475:GLN:NE2	2:I:528:SER:O	2.51	0.43
2:I:932:LEU:HD23	2:I:935:LEU:HD12	2.01	0.43
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.43
2:I:4041:ALA:HA	2:I:4044:MET:HB2	2.00	0.43
2:B:2459:SER:HB2	2:I:131:LEU:HB3	2.00	0.43
2:E:233:ILE:HD11	2:E:242:ARG:HH21	1.83	0.43
2:E:733:PRO:HD2	2:E:763:PRO:HD2	2.00	0.43
2:E:1694:LEU:HD23	2:E:1715:LEU:HD13	2.01	0.43
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.34	0.43
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.53	0.43
2:E:4976:GLU:O	2:E:4980:LEU:N	2.44	0.43
2:G:733:PRO:HD2	2:G:763:PRO:HD2	2.00	0.43
2:G:914:PRO:O	2:G:918:ARG:N	2.50	0.43
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.99	0.43
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	2.01	0.43
2:G:1952:GLN:HA	2:G:1955:VAL:HG12	2.01	0.43
2:G:3993:LEU:HA	2:G:3996:PHE:HB2	2.00	0.43
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.53	0.43
2:I:342:GLY:HA2	2:I:389:PHE:HD2	1.84	0.43
2:I:876:GLU:O	2:I:880:GLU:N	2.47	0.43
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4705:VAL:HB	2:I:4778:TRP:CD1	2.54	0.43
2:B:733:PRO:HD2	2:B:763:PRO:HD2	2.00	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.53	0.42
2:B:4105:GLY:HA2	2:B:4108:ILE:HD12	2.01	0.42
2:E:16:THR:OG1	2:E:97:GLY:O	2.36	0.42
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.00	0.42
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.01	0.42
2:E:4125:PHE:HA	2:E:4128:PHE:HB3	2.01	0.42
2:G:1663:HIS:O	2:G:1667:LEU:N	2.49	0.42
2:G:1694:LEU:HD23	2:G:1715:LEU:HD13	2.01	0.42
2:G:1778:SER:N	2:G:1799:SER:O	2.52	0.42
2:G:2517:UNK:O	2:G:2521:UNK:N	2.52	0.42
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.53	0.42
2:I:110:ARG:HA	2:I:117:TYR:HA	2.01	0.42
2:I:4181:ILE:HG23	2:I:4195:PHE:HE1	1.83	0.42
2:I:4745:LEU:O	2:I:4749:GLU:N	2.47	0.42
2:I:5012:LYS:O	2:I:5016:GLU:N	2.49	0.42
2:E:110:ARG:HA	2:E:117:TYR:HA	2.02	0.42
2:E:1497:UNK:HA	2:E:1535:UNK:HA	2.00	0.42
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.53	0.42
2:G:3992:PHE:O	2:G:3996:PHE:N	2.48	0.42
2:I:652:ARG:HB3	2:I:773:LEU:HD13	2.02	0.42
2:I:4105:GLY:HA2	2:I:4108:ILE:HD12	2.01	0.42
2:E:342:GLY:HA2	2:E:389:PHE:HD2	1.84	0.42
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	2.01	0.42
2:E:1952:GLN:HA	2:E:1955:VAL:HG12	2.01	0.42
2:G:758:ARG:NH2	2:G:803:LEU:O	2.53	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.42
2:G:4181:ILE:HG23	2:G:4195:PHE:HE1	1.83	0.42
2:G:4705:VAL:HB	2:G:4778:TRP:CD1	2.54	0.42
2:G:4976:GLU:O	2:G:4980:LEU:N	2.44	0.42
2:I:1094:ALA:HB3	2:I:1147:ASP:HB3	2.02	0.42
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.01	0.42
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.83	0.42
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	2.01	0.42
2:B:266:ARG:NH2	2:B:269:TRP:O	2.52	0.42
2:B:355:LEU:HB3	2:B:378:LEU:HB3	2.00	0.42
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.01	0.42
2:B:758:ARG:NH2	2:B:803:LEU:O	2.53	0.42
2:B:1865:MET:SD	2:B:1865:MET:N	2.93	0.42
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4736:ARG:O	2:B:4740:LEU:N	2.51	0.42
2:B:4849:TYR:HE1	2:E:4578:LEU:HD21	1.84	0.42
2:B:4937:ILE:O	2:B:4941:GLY:N	2.49	0.42
2:E:488:LEU:HD23	2:E:491:ILE:HD12	2.01	0.42
2:E:652:ARG:HB3	2:E:773:LEU:HD13	2.02	0.42
2:E:4105:GLY:HA2	2:E:4108:ILE:HD12	2.01	0.42
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.52	0.42
2:G:266:ARG:NH2	2:G:269:TRP:O	2.52	0.42
2:G:652:ARG:HB3	2:G:773:LEU:HD13	2.02	0.42
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.42
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.52	0.42
2:B:614:VAL:HG22	2:B:616:SER:H	1.85	0.42
2:B:1094:ALA:HB3	2:B:1147:ASP:HB3	2.02	0.42
2:E:870:ILE:HD12	2:E:870:ILE:HA	1.85	0.42
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.30	0.42
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.01	0.42
2:G:4012:LEU:O	2:G:4016:LEU:N	2.50	0.42
2:G:4105:GLY:HA2	2:G:4108:ILE:HD12	2.02	0.42
1:H:7:ILE:HB	1:H:71:ARG:HB3	2.01	0.42
2:I:266:ARG:NH2	2:I:269:TRP:O	2.52	0.42
2:I:758:ARG:NH2	2:I:803:LEU:O	2.53	0.42
2:I:1778:SER:N	2:I:1799:SER:O	2.52	0.42
2:I:1865:MET:SD	2:I:1865:MET:N	2.93	0.42
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.01	0.42
2:B:2132:GLY:O	2:B:2136:ARG:N	2.52	0.42
2:B:4012:LEU:O	2:B:4016:LEU:N	2.50	0.42
2:E:932:LEU:HD23	2:E:935:LEU:HD12	2.01	0.42
2:G:110:ARG:HA	2:G:117:TYR:HA	2.01	0.42
2:G:1094:ALA:HB3	2:G:1147:ASP:HB3	2.02	0.42
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.01	0.42
2:G:3733:CYS:O	2:G:3737:GLU:N	2.49	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.01	0.42
2:B:342:GLY:HA2	2:B:389:PHE:HD2	1.84	0.42
2:B:3713:LYS:HG2	2:B:3715:LYS:H	1.83	0.42
2:E:614:VAL:HG22	2:E:616:SER:H	1.85	0.42
2:E:1211:LEU:HD11	2:E:1225:PRO:HB3	2.02	0.42
2:G:457:GLU:OE1	2:G:464:LYS:NZ	2.51	0.42
2:G:488:LEU:HD23	2:G:491:ILE:HD12	2.01	0.42
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	2.01	0.42
2:G:2021:CYS:HA	2:G:2022:PRO:HD3	1.90	0.42
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	2.01	0.42
2:I:3713:LYS:HG2	2:I:3715:LYS:H	1.83	0.42
2:I:4863:TYR:HB2	2:I:4874:MET:HE2	2.01	0.42
1:A:89:GLY:H	2:B:627:PRO:HG3	1.85	0.42
2:B:110:ARG:HA	2:B:117:TYR:HA	2.01	0.42
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.42
2:B:4181:ILE:HG23	2:B:4195:PHE:HE1	1.83	0.42
2:B:4629:TYR:OH	2:I:4860:ARG:NH2	2.51	0.42
2:E:266:ARG:NH2	2:E:269:TRP:O	2.52	0.42
2:E:3993:LEU:HA	2:E:3996:PHE:HB2	2.00	0.42
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.00	0.42
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.93	0.42
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.85	0.42
2:I:2517:UNK:O	2:I:2521:UNK:N	2.53	0.42
2:B:2142:TYR:CG	2:B:2197:LEU:HD13	2.55	0.42
2:G:2039:LEU:HA	2:G:2042:CYS:HB3	2.01	0.42
2:G:4934:GLY:HA3	2:I:4937:ILE:HD12	2.01	0.42
2:I:392:ARG:HH12	2:I:398:SER:HB2	1.85	0.42
2:I:1516:UNK:N	2:I:1529:UNK:O	2.53	0.42
1:J:7:ILE:HB	1:J:71:ARG:HB3	2.01	0.42
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.93	0.42
2:B:652:ARG:HB3	2:B:773:LEU:HD13	2.02	0.42
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.42
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.02	0.42
2:E:758:ARG:NH2	2:E:803:LEU:O	2.53	0.42
2:E:1094:ALA:HB3	2:E:1147:ASP:HB3	2.02	0.42
2:E:1865:MET:SD	2:E:1865:MET:N	2.93	0.42
2:E:2142:TYR:CG	2:E:2197:LEU:HD13	2.55	0.42
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.01	0.42
2:E:4813:LEU:HA	2:E:4816:ILE:HG12	2.01	0.42
2:G:210:GLU:HG3	2:G:337:PRO:HG3	2.02	0.42
2:G:392:ARG:HH12	2:G:398:SER:HB2	1.85	0.42
2:G:1032:LYS:O	2:G:1036:ARG:N	2.45	0.42
2:I:261:ARG:N	2:I:283:ARG:O	2.40	0.42
2:I:1952:GLN:HA	2:I:1955:VAL:HG12	2.01	0.42
2:I:2142:TYR:CG	2:I:2197:LEU:HD13	2.55	0.42
1:J:83:GLY:HA2	1:J:94:ASN:H	1.85	0.42
1:A:7:ILE:HB	1:A:71:ARG:HB3	2.01	0.41
2:B:914:PRO:HD2	2:B:917:GLU:HB2	2.02	0.41
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.53	0.41
2:B:4568:PHE:HA	2:B:4571:PHE:HD2	1.85	0.41
2:E:392:ARG:HH12	2:E:398:SER:HB2	1.85	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.93	0.41
2:E:2039:LEU:HA	2:E:2042:CYS:HB3	2.01	0.41
2:E:2810:LYS:O	2:E:2814:LYS:N	2.49	0.41
2:E:4055:VAL:O	2:E:4059:LEU:N	2.49	0.41
2:E:4668:LEU:HG	2:E:4672:LYS:HE3	2.02	0.41
2:G:870:ILE:HA	2:G:870:ILE:HD12	1.85	0.41
2:G:1679:ASN:O	2:G:1683:HIS:ND1	2.37	0.41
2:G:2142:TYR:CG	2:G:2197:LEU:HD13	2.55	0.41
2:G:4125:PHE:HA	2:G:4128:PHE:HB3	2.01	0.41
2:I:242:ARG:O	2:I:289:ARG:NH1	2.53	0.41
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.41
2:I:4568:PHE:HA	2:I:4571:PHE:HD2	1.85	0.41
2:B:242:ARG:O	2:B:289:ARG:NH1	2.53	0.41
2:B:392:ARG:HH12	2:B:398:SER:HB2	1.85	0.41
2:B:457:GLU:OE1	2:B:464:LYS:NZ	2.51	0.41
2:B:1032:LYS:O	2:B:1036:ARG:N	2.45	0.41
2:B:1211:LEU:HD11	2:B:1225:PRO:HB3	2.02	0.41
2:B:2021:CYS:HA	2:B:2022:PRO:HD3	1.91	0.41
2:E:426:ARG:HG2	2:E:431:PRO:HA	2.02	0.41
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	2.01	0.41
2:E:1936:LYS:O	2:E:1940:CYS:N	2.47	0.41
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.03	0.41
2:E:4568:PHE:HA	2:E:4571:PHE:HD2	1.85	0.41
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:G:242:ARG:O	2:G:289:ARG:NH1	2.53	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.93	0.41
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	2.01	0.41
2:I:426:ARG:HG2	2:I:431:PRO:HA	2.03	0.41
2:I:457:GLU:OE1	2:I:464:LYS:NZ	2.51	0.41
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.01	0.41
2:I:1211:LEU:HD11	2:I:1225:PRO:HB3	2.02	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.01	0.41
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.03	0.41
2:E:2021:CYS:HA	2:E:2022:PRO:HD3	1.91	0.41
2:G:426:ARG:HG2	2:G:431:PRO:HA	2.02	0.41
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.03	0.41
2:G:1865:MET:SD	2:G:1865:MET:N	2.93	0.41
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4813:LEU:HA	2:I:4816:ILE:HG12	2.01	0.41
2:B:357:LEU:HD21	2:B:376:ALA:HB1	2.03	0.41
2:B:1952:GLN:HA	2:B:1955:VAL:HG12	2.01	0.41
2:B:3694:LYS:HA	2:B:3695:PRO:HD3	1.95	0.41
2:B:4125:PHE:HA	2:B:4128:PHE:HB3	2.01	0.41
2:B:4193:ILE:HD13	2:B:4193:ILE:HA	1.90	0.41
2:B:4668:LEU:HG	2:B:4672:LYS:HE3	2.02	0.41
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.94	0.41
2:E:242:ARG:O	2:E:289:ARG:NH1	2.53	0.41
2:E:3733:CYS:O	2:E:3737:GLU:N	2.49	0.41
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	2.02	0.41
2:G:2437:ALA:HA	2:G:2438:PRO:HD3	1.94	0.41
2:I:614:VAL:HG22	2:I:616:SER:H	1.85	0.41
2:I:914:PRO:O	2:I:918:ARG:N	2.50	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.56	0.41
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.02	0.41
2:I:2437:ALA:HA	2:I:2438:PRO:HD3	1.94	0.41
2:I:4958:CYS:SG	2:I:4959:PHE:N	2.94	0.41
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.02	0.41
2:B:1089:TYR:N	2:B:1224:GLU:O	2.54	0.41
2:B:2880:GLU:O	2:B:2884:ASN:N	2.49	0.41
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	2.01	0.41
2:B:4852:THR:O	2:B:4856:PHE:N	2.53	0.41
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.41
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.53	0.41
2:E:4193:ILE:HD13	2:E:4193:ILE:HA	1.90	0.41
2:G:932:LEU:HD23	2:G:935:LEU:HD12	2.01	0.41
2:G:2132:GLY:O	2:G:2136:ARG:N	2.52	0.41
2:G:4813:LEU:HA	2:G:4816:ILE:HG12	2.01	0.41
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.02	0.41
2:I:668:VAL:HG22	2:I:789:VAL:HG23	2.03	0.41
2:I:2132:GLY:O	2:I:2136:ARG:N	2.52	0.41
2:I:3930:ILE:HG23	2:I:3951:PHE:HE1	1.86	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:4813:LEU:HA	2:B:4816:ILE:HG12	2.01	0.41
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	2.02	0.41
2:E:4040:ILE:O	2:E:4044:MET:N	2.47	0.41
1:F:23:VAL:HB	1:F:105:ASN:HA	2.02	0.41
2:G:3930:ILE:HG23	2:G:3951:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4668:LEU:HG	2:G:4672:LYS:HE3	2.02	0.41
2:G:4852:THR:O	2:G:4856:PHE:N	2.53	0.41
2:I:488:LEU:HD23	2:I:491:ILE:HD12	2.01	0.41
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.53	0.41
2:I:4125:PHE:HA	2:I:4128:PHE:HB3	2.01	0.41
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.85	0.41
2:B:426:ARG:HG2	2:B:431:PRO:HA	2.03	0.41
2:B:488:LEU:HD23	2:B:491:ILE:HD12	2.01	0.41
2:E:210:GLU:HG3	2:E:337:PRO:HG3	2.02	0.41
2:E:357:LEU:HD21	2:E:376:ALA:HB1	2.03	0.41
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.33	0.41
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	2.01	0.41
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.03	0.41
2:E:4852:THR:O	2:E:4856:PHE:N	2.53	0.41
2:G:357:LEU:HD21	2:G:376:ALA:HB1	2.03	0.41
2:G:1211:LEU:HD11	2:G:1225:PRO:HB3	2.02	0.41
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.03	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.54	0.41
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.53	0.41
2:G:4560:TYR:O	2:G:4564:PHE:N	2.45	0.41
2:G:4958:CYS:SG	2:G:4959:PHE:N	2.94	0.41
1:H:7:ILE:N	1:H:71:ARG:O	2.45	0.41
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.02	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.49	0.41
2:B:1046:LEU:HD12	2:B:1053:ILE:HD11	2.03	0.41
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.03	0.41
2:E:1046:LEU:HD12	2:E:1053:ILE:HD11	2.03	0.41
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.94	0.41
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.02	0.41
2:G:4863:TYR:HB2	2:G:4874:MET:HE2	2.03	0.41
2:I:16:THR:OG1	2:I:97:GLY:O	2.36	0.41
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.53	0.41
2:I:4668:LEU:HG	2:I:4672:LYS:HE3	2.02	0.41
1:A:83:GLY:HA2	1:A:94:ASN:H	1.85	0.41
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.39	0.41
2:B:3930:ILE:HG23	2:B:3951:PHE:HE1	1.86	0.41
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.03	0.41
2:B:4976:GLU:O	2:B:4980:LEU:N	2.44	0.41
2:E:379:HIS:CD2	2:E:381:GLU:H	2.39	0.41
2:E:385:ASP:N	2:E:385:ASP:OD1	2.54	0.41
2:E:414:PHE:HE1	2:E:436:LEU:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:467:LYS:O	2:E:471:LEU:N	2.54	0.41
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	2.01	0.41
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.03	0.41
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.03	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.03	0.41
2:G:776:LEU:HG	2:G:848:HIS:HA	2.03	0.41
2:G:914:PRO:HD2	2:G:917:GLU:HB2	2.02	0.41
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.02	0.41
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.03	0.41
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.03	0.41
2:G:4736:ARG:O	2:G:4740:LEU:N	2.51	0.41
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.39	0.41
2:I:668:VAL:O	2:I:741:GLU:N	2.53	0.41
2:I:1089:TYR:N	2:I:1224:GLU:O	2.54	0.41
2:I:1497:UNK:HA	2:I:1535:UNK:HA	2.02	0.41
2:I:4204:GLN:HE22	2:I:4245:MET:HA	1.86	0.41
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.03	0.41
2:I:4852:THR:O	2:I:4856:PHE:N	2.53	0.41
1:A:23:VAL:HB	1:A:105:ASN:HA	2.03	0.41
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.03	0.41
2:E:3698:LEU:HD23	2:E:3771:HIS:CE1	2.56	0.41
2:E:4863:TYR:HB2	2:E:4874:MET:HE2	2.02	0.41
1:F:83:GLY:HA2	1:F:94:ASN:H	1.85	0.41
2:G:1046:LEU:HD12	2:G:1053:ILE:HD11	2.03	0.41
2:G:4059:LEU:HD13	2:G:4166:LEU:HB3	2.03	0.41
1:J:23:VAL:HB	1:J:105:ASN:HA	2.03	0.41
1:J:29:MET:HB3	1:J:98:ILE:HB	2.03	0.41
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.87	0.40
2:B:3698:LEU:HD23	2:B:3771:HIS:CE1	2.56	0.40
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.03	0.40
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.04	0.40
2:E:914:PRO:O	2:E:918:ARG:N	2.50	0.40
2:E:1089:TYR:N	2:E:1224:GLU:O	2.54	0.40
2:E:1154:ASP:O	2:E:1158:ASN:N	2.55	0.40
2:E:3930:ILE:HG23	2:E:3951:PHE:HE1	1.86	0.40
2:E:3999:MET:HA	2:E:4002:LYS:HB3	2.03	0.40
2:E:4736:ARG:O	2:E:4740:LEU:N	2.51	0.40
2:G:1089:TYR:N	2:G:1224:GLU:O	2.54	0.40
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.03	0.40
2:G:4782:VAL:O	2:G:4785:THR:OG1	2.30	0.40
2:I:357:LEU:HD21	2:I:376:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:776:LEU:HG	2:I:848:HIS:HA	2.03	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.03	0.40
2:I:4848:VAL:HG12	2:I:4920:PHE:HZ	1.86	0.40
2:B:1497:UNK:HA	2:B:1535:UNK:HA	2.03	0.40
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.85	0.40
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.39	0.40
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.03	0.40
2:E:914:PRO:HD2	2:E:917:GLU:HB2	2.02	0.40
2:G:320:LYS:HG2	2:G:356:TRP:CD1	2.56	0.40
2:G:614:VAL:HG22	2:G:616:SER:H	1.85	0.40
2:G:668:VAL:HG22	2:G:789:VAL:HG23	2.03	0.40
2:G:1936:LYS:O	2:G:1940:CYS:N	2.47	0.40
2:I:320:LYS:HG2	2:I:356:TRP:CD1	2.56	0.40
2:I:1046:LEU:HD12	2:I:1053:ILE:HD11	2.03	0.40
2:I:3362:UNK:O	2:I:3366:UNK:N	2.54	0.40
2:I:3698:LEU:HD23	2:I:3771:HIS:CE1	2.56	0.40
2:I:4055:VAL:O	2:I:4059:LEU:N	2.49	0.40
2:B:668:VAL:HG22	2:B:789:VAL:HG23	2.03	0.40
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.03	0.40
2:B:4204:GLN:HE22	2:B:4245:MET:HA	1.87	0.40
2:E:663:TYR:HB2	2:E:808:TYR:HB3	2.04	0.40
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.03	0.40
2:E:5012:LYS:O	2:E:5016:GLU:N	2.49	0.40
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.55	0.40
2:G:1269:CYS:HA	2:G:1473:UNK:HA	2.04	0.40
2:G:1720:LEU:HB2	2:G:1847:THR:HG23	2.03	0.40
1:H:23:VAL:HB	1:H:105:ASN:HA	2.03	0.40
2:I:914:PRO:HD2	2:I:917:GLU:HB2	2.02	0.40
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.02	0.40
2:B:210:GLU:HG3	2:B:337:PRO:HG3	2.02	0.40
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.03	0.40
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.53	0.40
2:B:1154:ASP:O	2:B:1158:ASN:N	2.55	0.40
2:B:1284:UNK:HA	2:B:1463:UNK:HA	2.03	0.40
2:B:4651:THR:HA	2:B:4799:SER:HB3	2.02	0.40
2:E:320:LYS:HG2	2:E:356:TRP:CD1	2.56	0.40
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.86	0.40
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.02	0.40
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	2.03	0.40
2:E:2950:UNK:O	2:E:2954:UNK:N	2.55	0.40
2:E:3362:UNK:O	2:E:3366:UNK:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4651:THR:HA	2:E:4799:SER:HB3	2.03	0.40
2:G:467:LYS:O	2:G:471:LEU:N	2.54	0.40
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.87	0.40
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.53	0.40
2:G:1497:UNK:HA	2:G:1535:UNK:HA	2.03	0.40
2:I:176:SER:HB2	2:I:178:ARG:HD3	2.04	0.40
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.86	0.40
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	2.02	0.40
2:I:4059:LEU:HD13	2:I:4166:LEU:HB3	2.04	0.40
2:I:4651:THR:HA	2:I:4799:SER:HB3	2.02	0.40
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.03	0.40
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.04	0.40
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.55	0.40
2:B:1516:UNK:N	2:B:1529:UNK:O	2.54	0.40
2:B:2950:UNK:O	2:B:2954:UNK:N	2.55	0.40
2:G:1092:PHE:N	2:G:1149:VAL:O	2.38	0.40
2:G:1863:LEU:HB3	2:G:1870:VAL:HG11	2.03	0.40
2:G:3999:MET:HA	2:G:4002:LYS:HB3	2.03	0.40
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.86	0.40
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.04	0.40
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.03	0.40
2:I:1720:LEU:HB2	2:I:1847:THR:HG23	2.03	0.40
2:I:1863:LEU:HB3	2:I:1870:VAL:HG11	2.03	0.40
1:J:7:ILE:N	1:J:71:ARG:O	2.45	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	105/107 (98%)	92 (88%)	13 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	H	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	J	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4687 (69%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	E	3235/4687 (69%)	2887 (89%)	342 (11%)	6 (0%)	47	81
2	G	3235/4687 (69%)	2892 (89%)	337 (10%)	6 (0%)	47	81
2	I	3235/4687 (69%)	2889 (89%)	340 (10%)	6 (0%)	47	81
All	All	13360/19176 (70%)	11926 (89%)	1410 (11%)	24 (0%)	50	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	B	1932	PRO
2	E	1932	PRO
2	G	1932	PRO
2	I	1932	PRO
2	B	1840	PRO
2	B	4667	PRO
2	E	1840	PRO
2	E	4667	PRO
2	G	1840	PRO
2	G	4667	PRO
2	I	1840	PRO
2	I	4667	PRO
2	B	2343	GLY
2	E	2343	GLY
2	G	2343	GLY
2	I	2343	GLY
2	B	4641	PRO
2	E	4641	PRO
2	G	4641	PRO
2	I	4641	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	88/88 (100%)	88 (100%)	0	100	100
1	F	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	J	88/88 (100%)	88 (100%)	0	100	100
2	B	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
All	All	10324/13188 (78%)	10256 (99%)	68 (1%)	84	90

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	534	ARG
2	B	553	ARG
2	B	688	LEU
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4137	ARG
2	B	4798	MET
2	B	4957	LYS
2	E	534	ARG
2	E	553	ARG

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Mol	Chain	Res	Type
2	E	688	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1964	ARG
2	E	3663	LEU
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4137	ARG
2	E	4798	MET
2	E	4957	LYS
2	G	534	ARG
2	G	553	ARG
2	G	688	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4137	ARG
2	G	4798	MET
2	G	4957	LYS
2	I	534	ARG
2	I	553	ARG
2	I	688	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3805	LEU

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Mol	Chain	Res	Type
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4137	ARG
2	I	4798	MET
2	I	4957	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	203	ASN
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN
2	B	479	GLN
2	B	838	HIS
2	B	1035	ASN
2	B	1158	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1972	ASN
2	B	2127	GLN
2	B	2931	GLN
2	B	3766	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN

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Mol	Chain	Res	Type
2	B	4054	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4201	ASN
2	B	4728	HIS
2	B	5031	GLN
2	E	23	GLN
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	203	ASN
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	413	GLN
2	E	479	GLN
2	E	838	HIS
2	E	1035	ASN
2	E	1158	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1972	ASN
2	E	2127	GLN
2	E	3766	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4142	ASN
2	E	4201	ASN
2	E	4728	HIS
2	E	5031	GLN

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Mol	Chain	Res	Type
2	G	23	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	203	ASN
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	479	GLN
2	G	838	HIS
2	G	1035	ASN
2	G	1158	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1972	ASN
2	G	2127	GLN
2	G	3766	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4142	ASN
2	G	4201	ASN
2	G	4728	HIS
2	G	5031	GLN
1	H	25	HIS
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	203	ASN

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Mol	Chain	Res	Type
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	838	HIS
2	I	1035	ASN
2	I	1158	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1972	ASN
2	I	2127	GLN
2	I	2931	GLN
2	I	3766	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4201	ASN
2	I	4728	HIS
2	I	5031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	12
2	B	12
2	I	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	3613:UNK	C	3639:THR	N	44.80
1	B	3613:UNK	C	3639:THR	N	44.74
1	I	3613:UNK	C	3639:THR	N	44.65
1	E	3613:UNK	C	3639:THR	N	44.57
1	B	3163:UNK	C	3170:UNK	N	16.54
1	E	3163:UNK	C	3170:UNK	N	16.53
1	G	3163:UNK	C	3170:UNK	N	16.53
1	I	3163:UNK	C	3170:UNK	N	16.50
1	E	3468:UNK	C	3511:UNK	N	14.95

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3468:UNK	C	3511:UNK	N	14.94
1	G	3468:UNK	C	3511:UNK	N	14.91
1	I	3468:UNK	C	3511:UNK	N	14.90
1	E	3063:UNK	C	3134:UNK	N	14.65
1	B	3063:UNK	C	3134:UNK	N	14.64
1	I	3063:UNK	C	3134:UNK	N	14.62
1	G	3063:UNK	C	3134:UNK	N	14.60
1	G	2703:UNK	C	2734:ASN	N	14.51
1	I	2703:UNK	C	2734:ASN	N	14.47
1	E	2703:UNK	C	2734:ASN	N	14.44
1	B	2703:UNK	C	2734:ASN	N	14.32
1	E	3236:UNK	C	3241:UNK	N	13.44
1	B	3236:UNK	C	3241:UNK	N	13.43
1	I	3236:UNK	C	3241:UNK	N	13.42
1	G	3236:UNK	C	3241:UNK	N	13.41
1	G	1564:UNK	C	1573:MET	N	12.96
1	B	1564:UNK	C	1573:MET	N	12.89
1	I	1564:UNK	C	1573:MET	N	12.89
1	E	1564:UNK	C	1573:MET	N	12.80
1	E	2976:UNK	C	2995:UNK	N	12.34
1	I	2976:UNK	C	2995:UNK	N	12.34
1	B	2976:UNK	C	2995:UNK	N	12.33
1	G	2976:UNK	C	2995:UNK	N	12.32
1	G	3254:UNK	C	3261:UNK	N	8.64
1	I	3254:UNK	C	3261:UNK	N	8.64
1	B	3254:UNK	C	3261:UNK	N	8.62
1	E	3254:UNK	C	3261:UNK	N	8.61
1	B	1297:UNK	C	1430:UNK	N	5.93
1	I	1297:UNK	C	1430:UNK	N	5.91
1	E	1297:UNK	C	1430:UNK	N	5.78
1	G	1297:UNK	C	1430:UNK	N	5.58
1	B	2479:LEU	C	2487:UNK	N	3.79
1	G	2479:LEU	C	2487:UNK	N	3.71
1	I	2479:LEU	C	2487:UNK	N	3.68
1	E	2479:LEU	C	2487:UNK	N	3.62
1	B	2939:ARG	C	2942:UNK	N	3.60
1	E	2939:ARG	C	2942:UNK	N	3.56
1	I	2939:ARG	C	2942:UNK	N	3.52
1	G	2939:ARG	C	2942:UNK	N	3.42

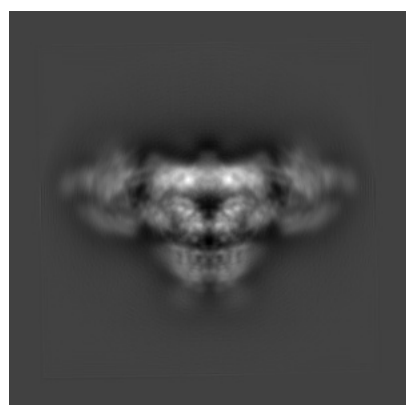
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22395. These allow visual inspection of the internal detail of the map and identification of artifacts.

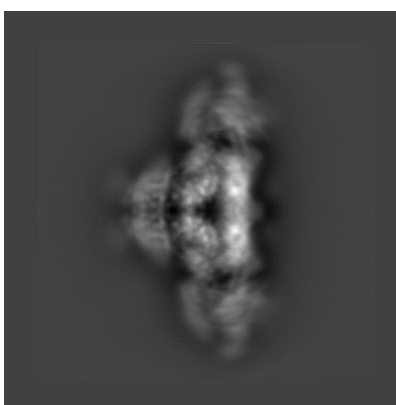
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

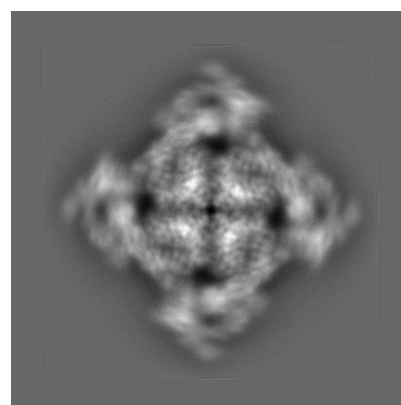
6.1.1 Primary map



X



Y

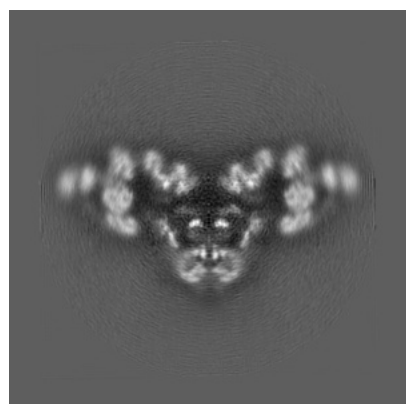


Z

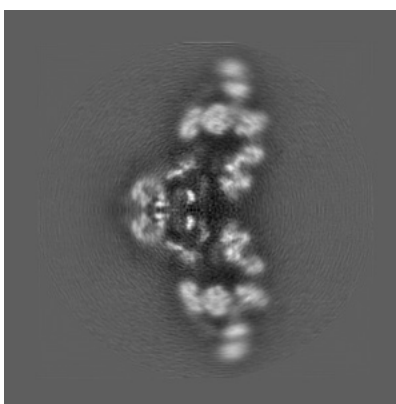
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

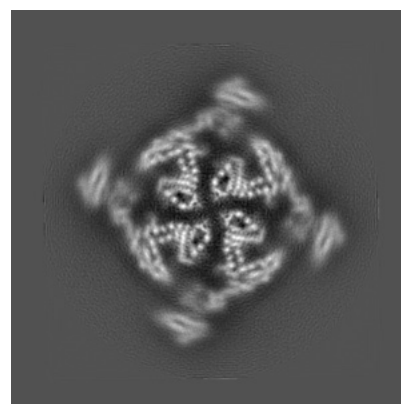
6.2.1 Primary map



X Index: 200



Y Index: 200

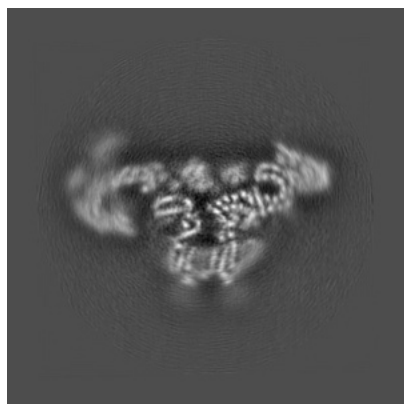


Z Index: 200

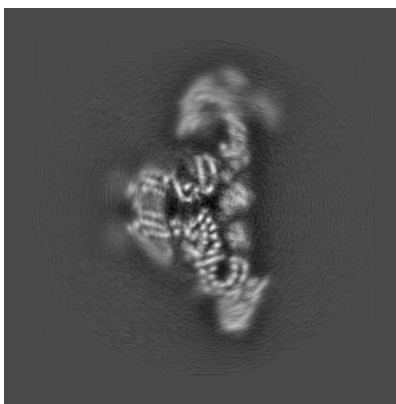
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

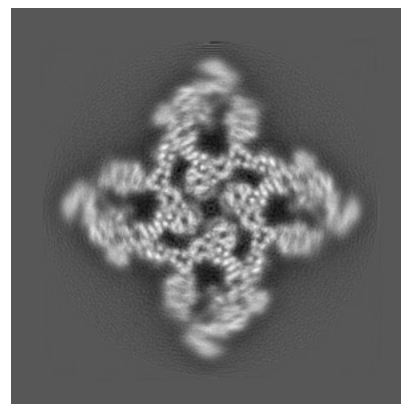
6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 230

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

6.4 Orthogonal surface views [i](#)

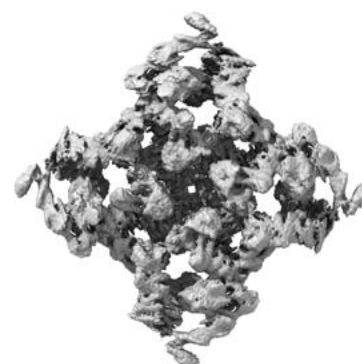
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

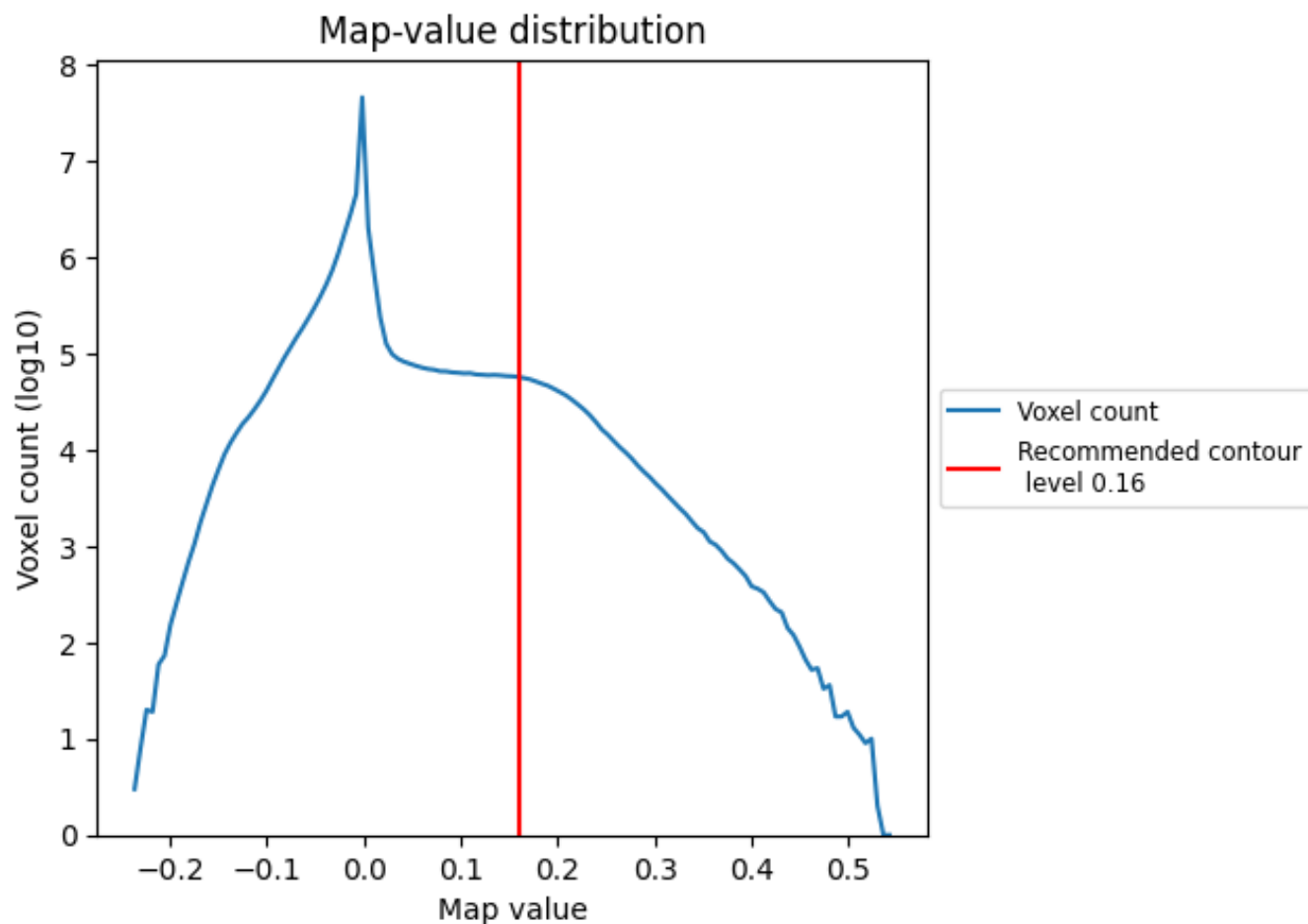
6.5 Mask visualisation

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

7 Map analysis [i](#)

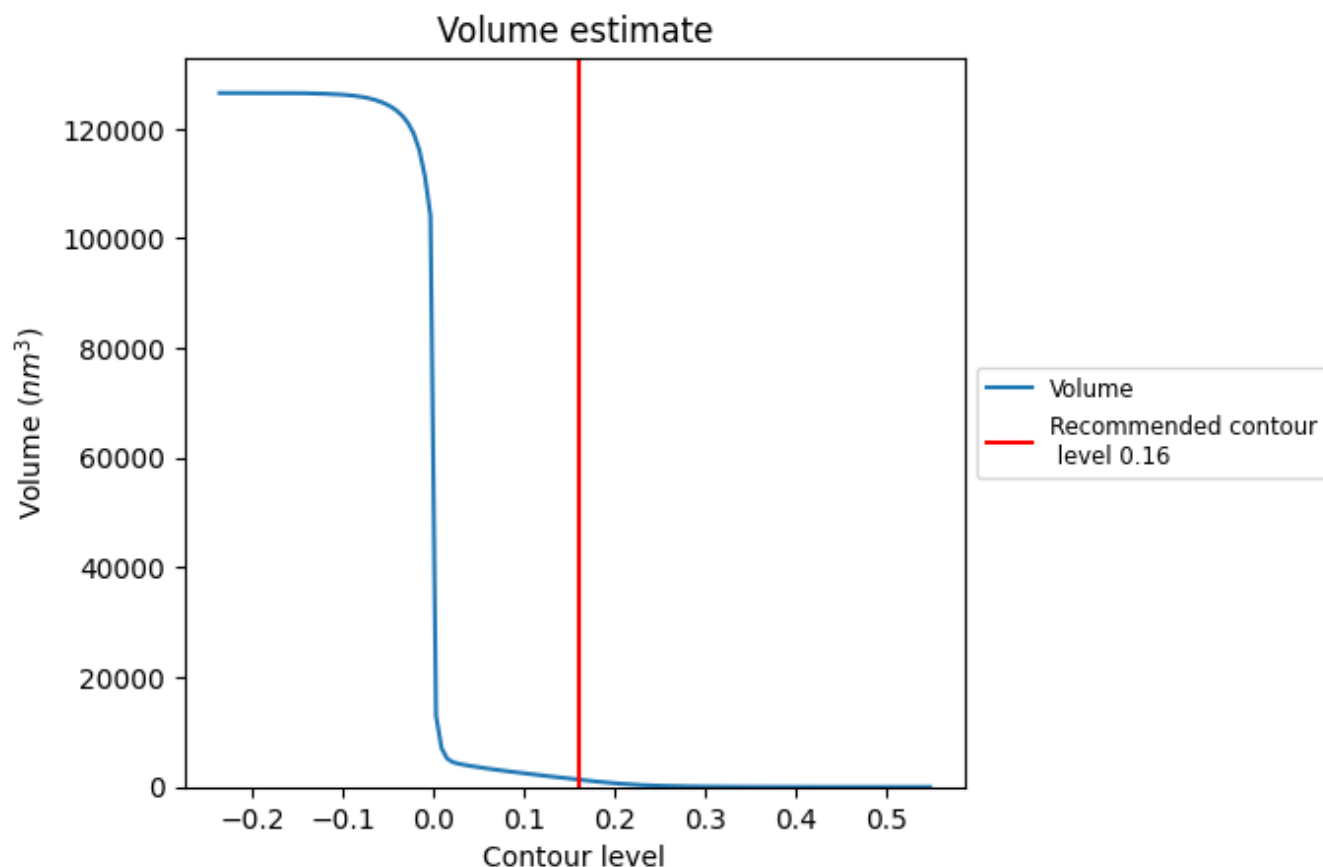
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

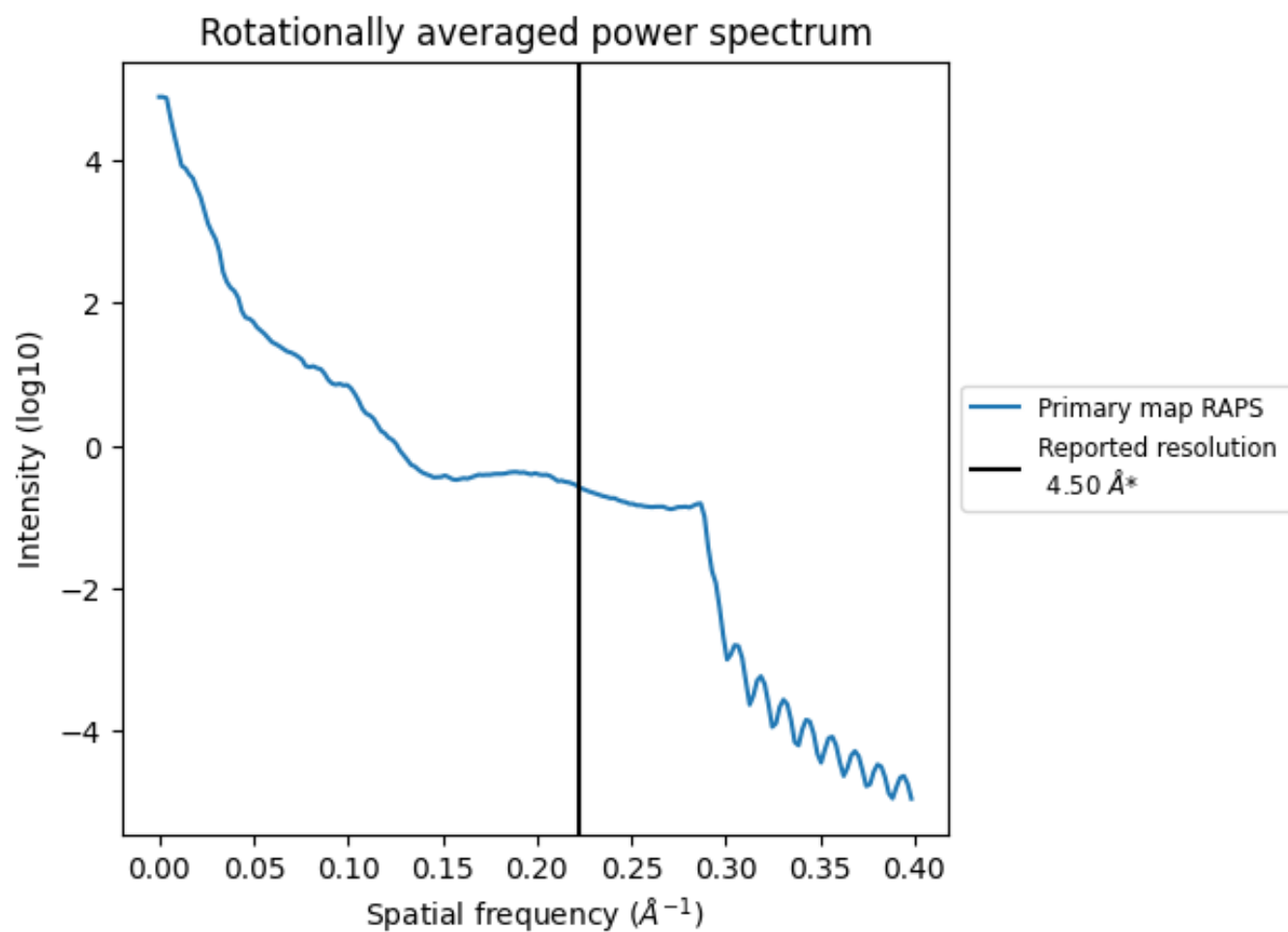
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1337 nm³; this corresponds to an approximate mass of 1208 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

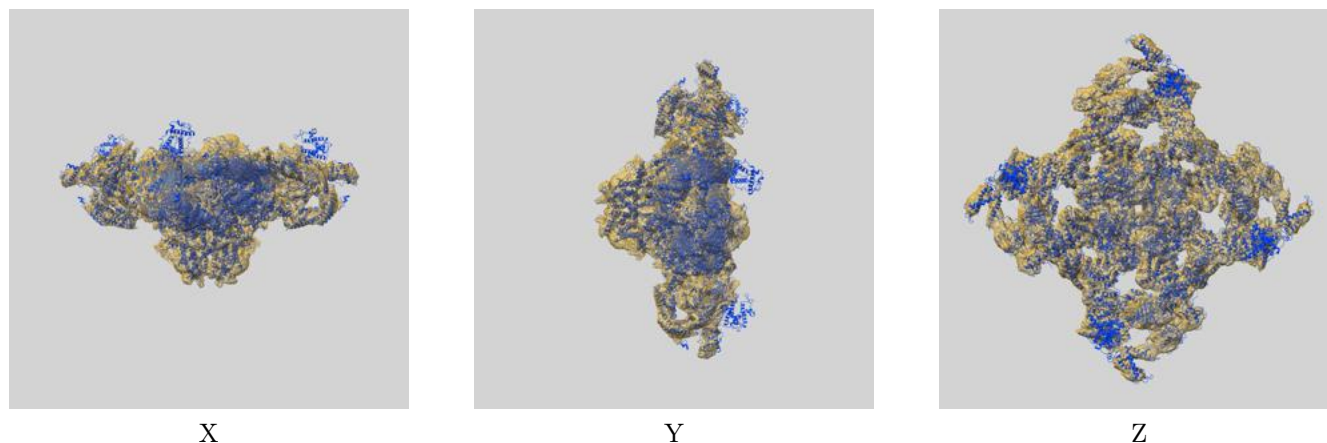
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

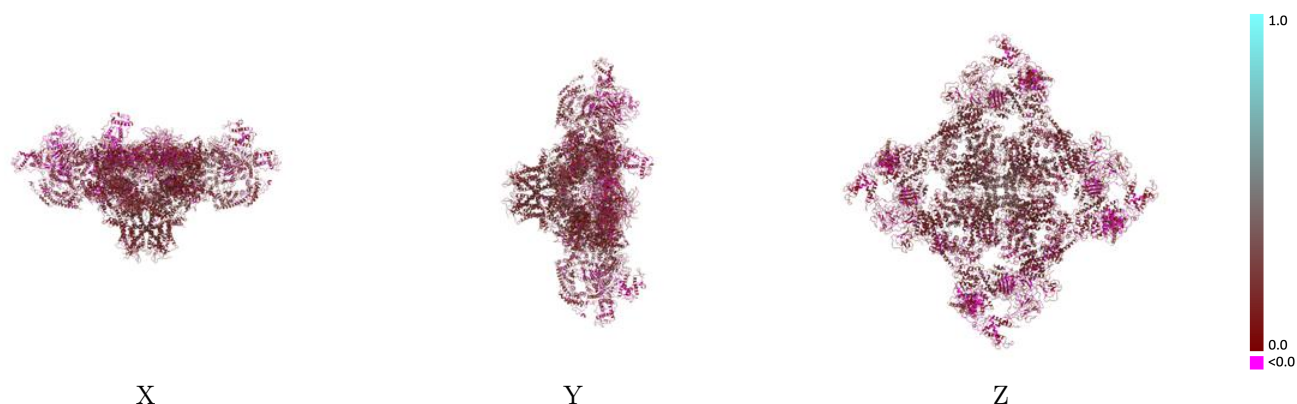
This section contains information regarding the fit between EMDB map EMD-22395 and PDB model 7JMI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



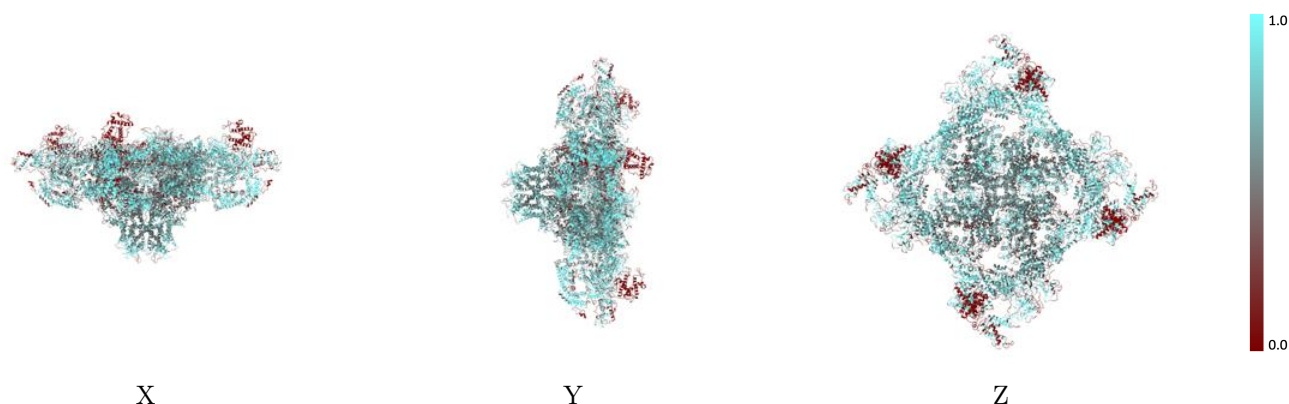
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



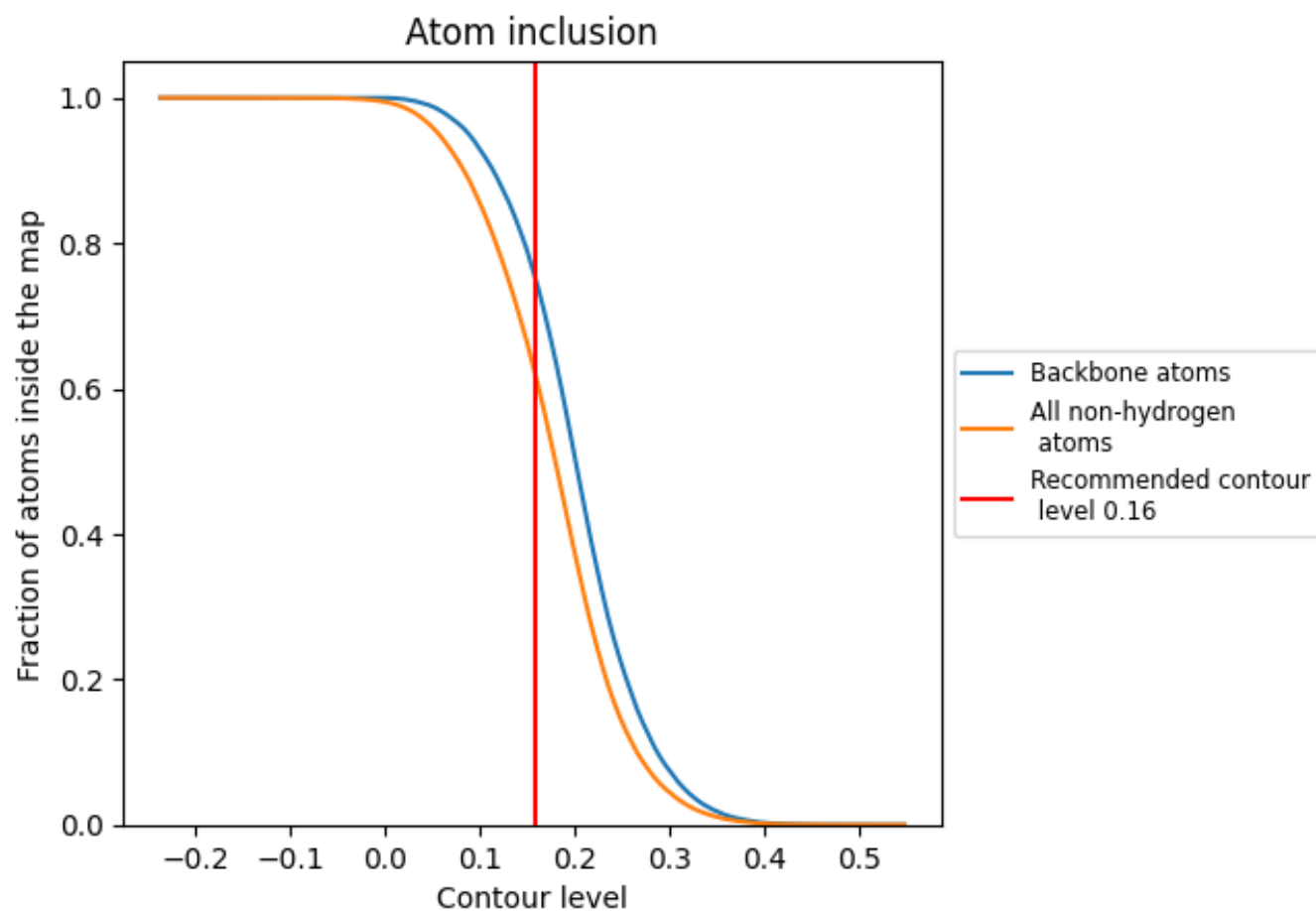
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6142	<div></div> 0.1530
A	<div></div> 0.7022	<div></div> 0.1430
B	<div></div> 0.6326	<div></div> 0.1730
E	<div></div> 0.6194	<div></div> 0.1580
F	<div></div> 0.6700	<div></div> 0.1150
G	<div></div> 0.5956	<div></div> 0.1340
H	<div></div> 0.6216	<div></div> 0.1130
I	<div></div> 0.6041	<div></div> 0.1490
J	<div></div> 0.6439	<div></div> 0.1220

1.0

0.0

<0.0