Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:16 AM UTC

PDB ID	:	7M7H / pdb_00007m7h
EMDB ID	:	EMD-23713
Title	:	6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 1'
Authors	:	Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.
Deposited on	:	2021-03-28
Resolution	:	4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

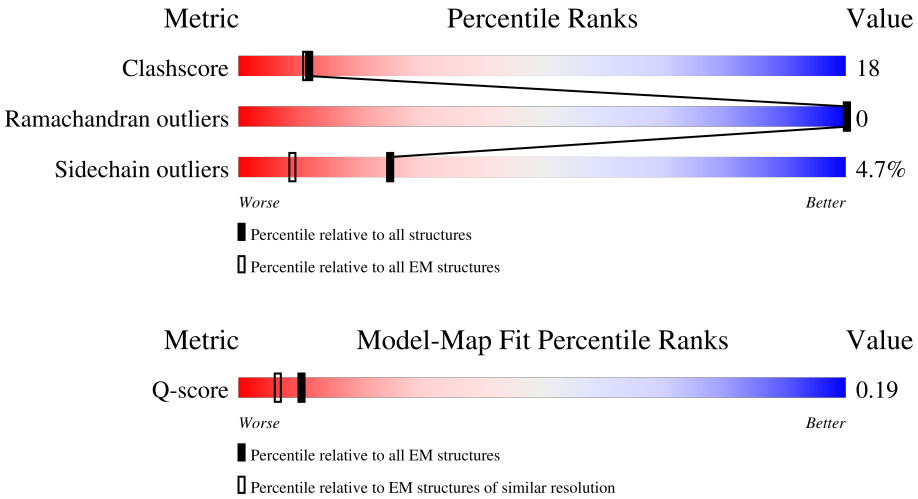
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 4.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1784	19% 48% 28% • 22%
1	B	1784	17% 50% 29% • 20%
2	C	249	53% 28% • 18%
2	E	249	53% 29% • 18%

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Mol	Chain	Length	Quality of chain
3	D	236	
3	F	236	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27046 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 EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1425	Total	C	N	O	S	0	0
			10513	6533	1929	2016	35		
1	A	1390	Total	C	N	O	S	0	0
			10319	6413	1899	1972	35		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ARG	-	expression tag	UNP Q5UNP6
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1486	THR	-	linker	UNP Q5UNP6
B	1487	SER	-	linker	UNP Q5UNP6
B	1488	GLU	-	linker	UNP Q5UNP6
B	1489	LEU	-	linker	UNP Q5UNP6
B	1490	GLY	-	linker	UNP Q5UNP6
B	1768	SER	-	expression tag	UNP Q03133
B	1769	SER	-	expression tag	UNP Q03133
B	1770	VAL	-	expression tag	UNP Q03133
B	1771	ASP	-	expression tag	UNP Q03133
B	1772	LYS	-	expression tag	UNP Q03133
B	1773	LEU	-	expression tag	UNP Q03133
B	1774	ALA	-	expression tag	UNP Q03133
B	1775	ALA	-	expression tag	UNP Q03133
B	1776	ALA	-	expression tag	UNP Q03133
B	1777	LEU	-	expression tag	UNP Q03133
B	1778	GLU	-	expression tag	UNP Q03133
B	1779	HIS	-	expression tag	UNP Q03133
B	1780	HIS	-	expression tag	UNP Q03133
B	1781	HIS	-	expression tag	UNP Q03133
B	1782	HIS	-	expression tag	UNP Q03133
B	1783	HIS	-	expression tag	UNP Q03133
B	1784	HIS	-	expression tag	UNP Q03133
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1486	THR	-	linker	UNP Q5UNP6
A	1487	SER	-	linker	UNP Q5UNP6
A	1488	GLU	-	linker	UNP Q5UNP6
A	1489	LEU	-	linker	UNP Q5UNP6
A	1490	GLY	-	linker	UNP Q5UNP6
A	1768	SER	-	expression tag	UNP Q03133
A	1769	SER	-	expression tag	UNP Q03133
A	1770	VAL	-	expression tag	UNP Q03133
A	1771	ASP	-	expression tag	UNP Q03133
A	1772	LYS	-	expression tag	UNP Q03133
A	1773	LEU	-	expression tag	UNP Q03133
A	1774	ALA	-	expression tag	UNP Q03133
A	1775	ALA	-	expression tag	UNP Q03133
A	1776	ALA	-	expression tag	UNP Q03133
A	1777	LEU	-	expression tag	UNP Q03133
A	1778	GLU	-	expression tag	UNP Q03133
A	1779	HIS	-	expression tag	UNP Q03133
A	1780	HIS	-	expression tag	UNP Q03133
A	1781	HIS	-	expression tag	UNP Q03133
A	1782	HIS	-	expression tag	UNP Q03133
A	1783	HIS	-	expression tag	UNP Q03133
A	1784	HIS	-	expression tag	UNP Q03133

- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

- Molecule 3 is a protein called 1B2 (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

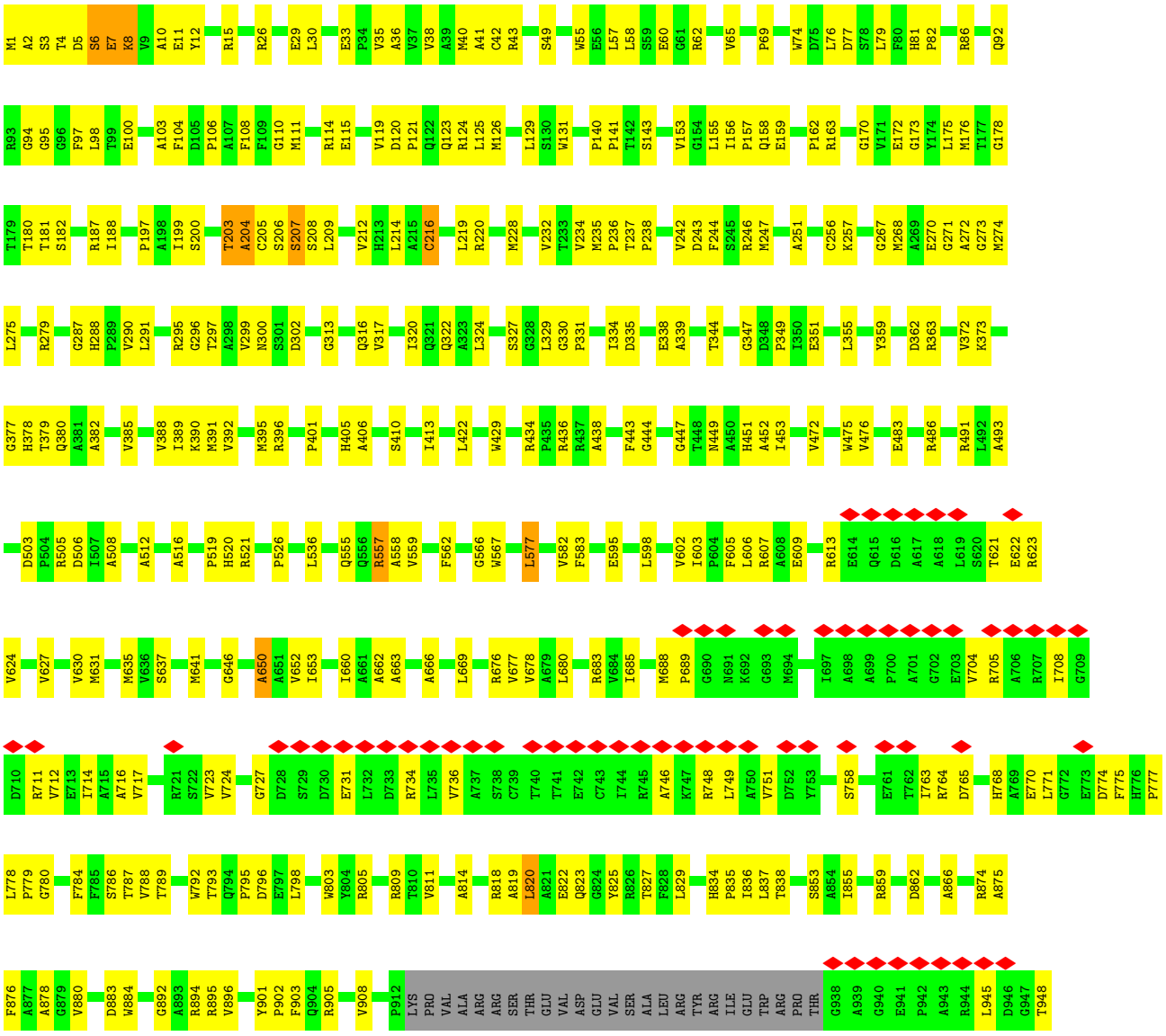
3 Residue-property plots (i)

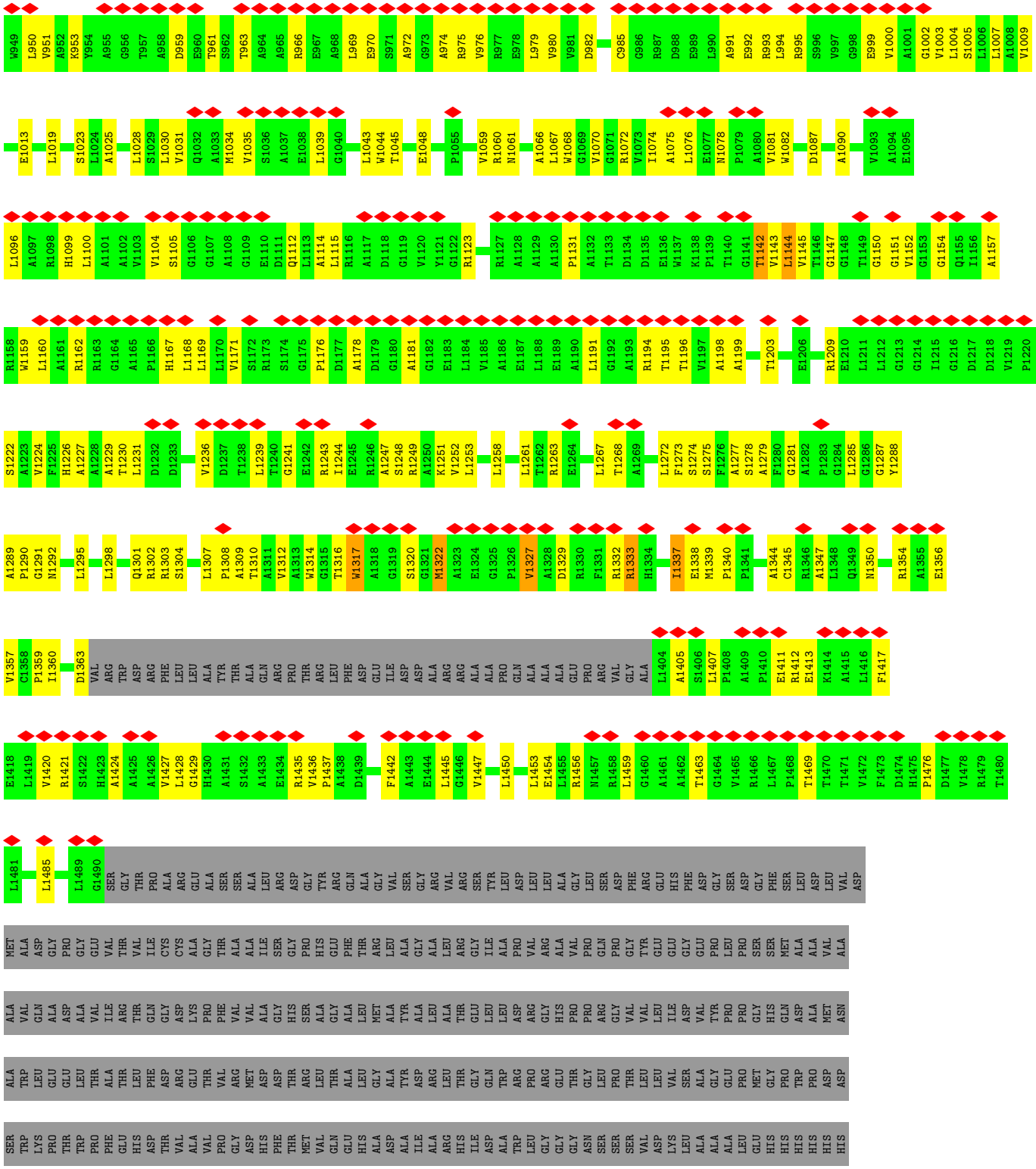
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

Chain B:



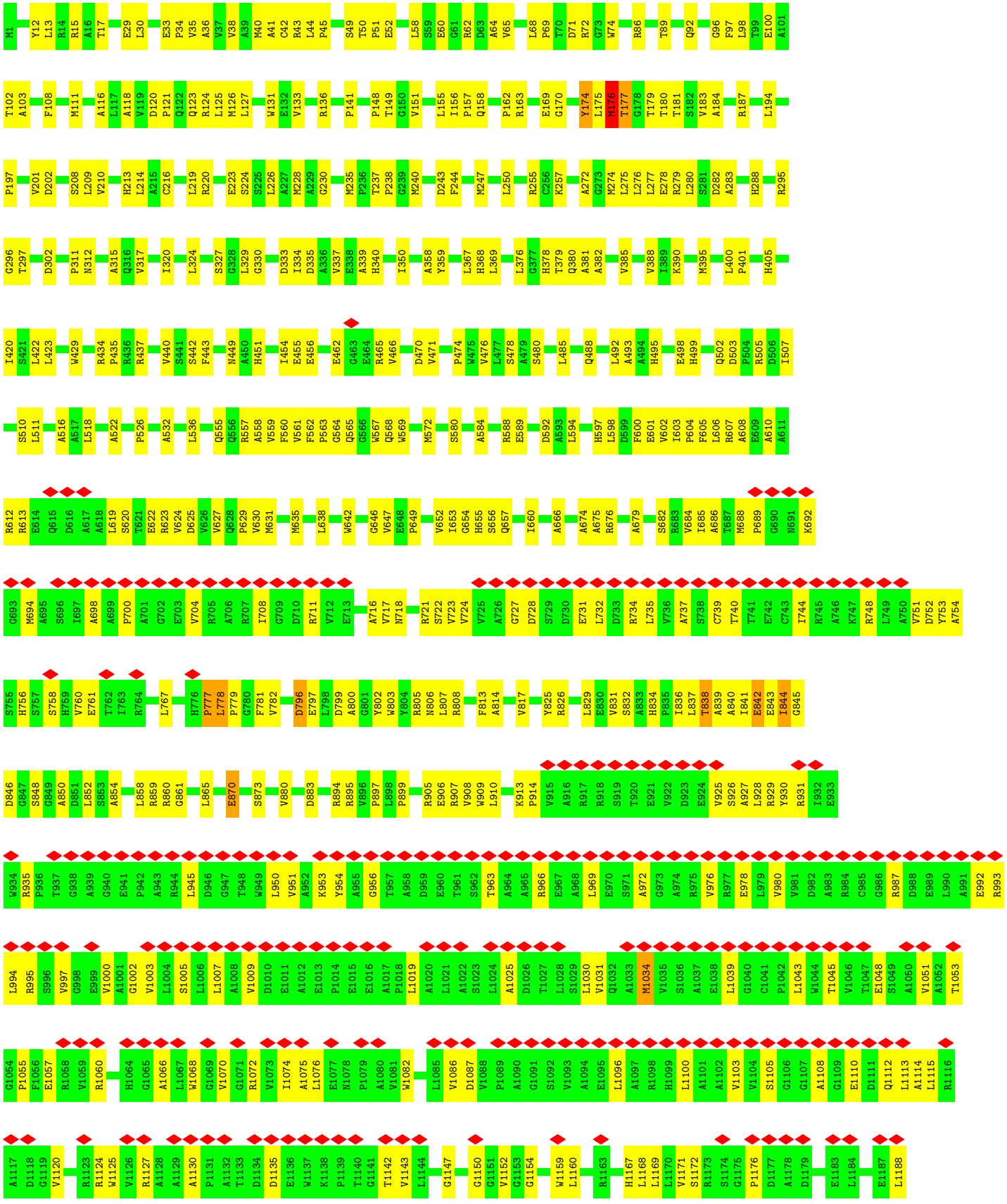


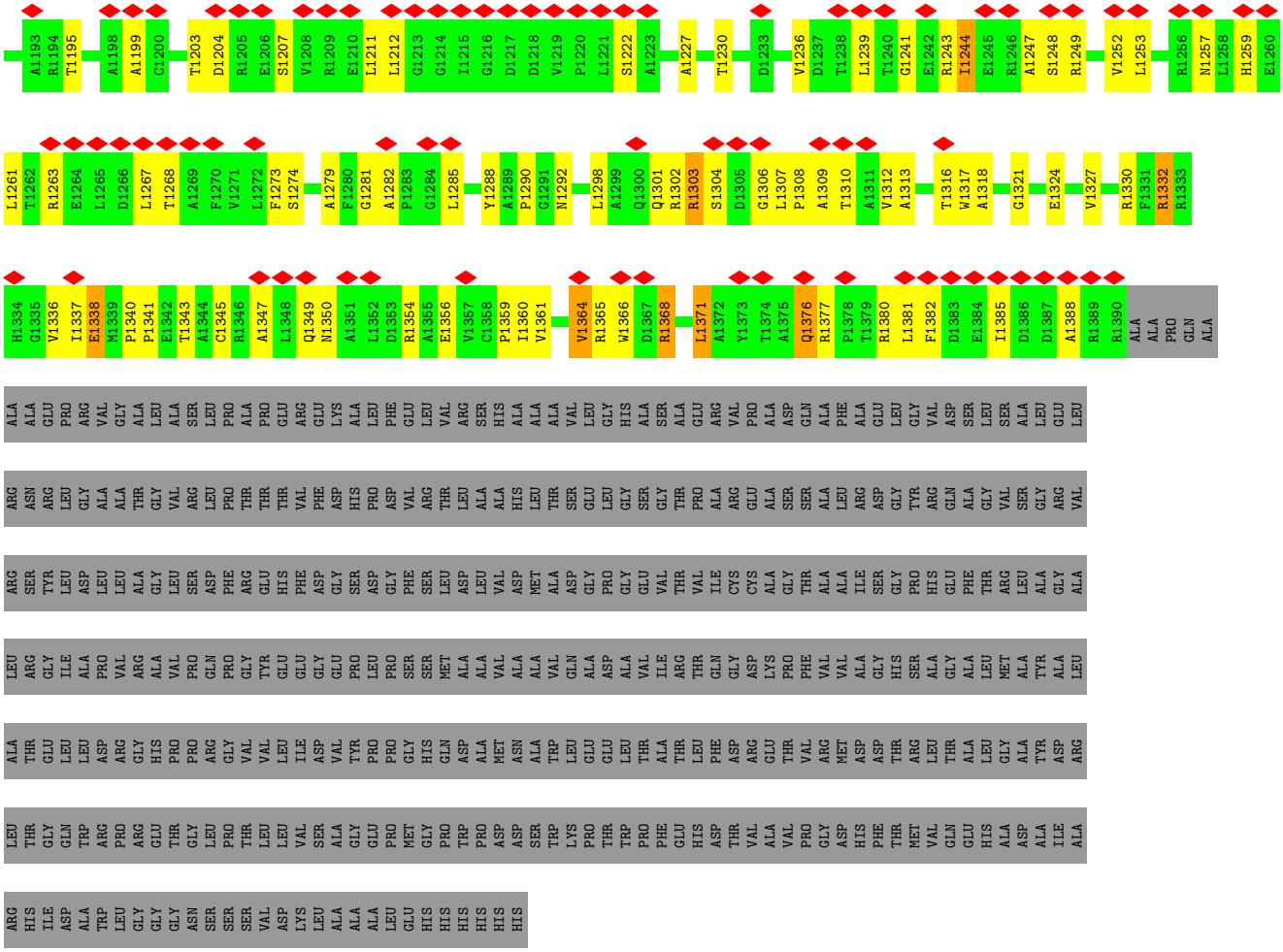


• Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

Chain A:



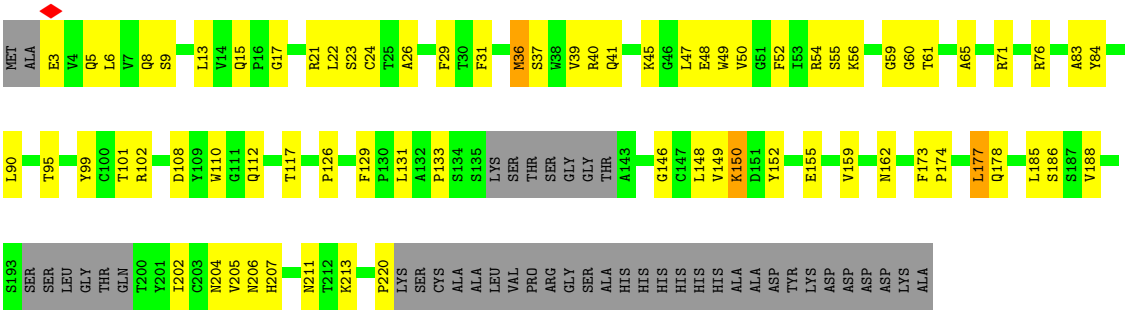




• Molecule 2: 1B2 (heavy chain)

Chain C:

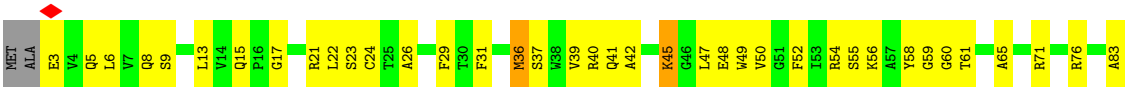


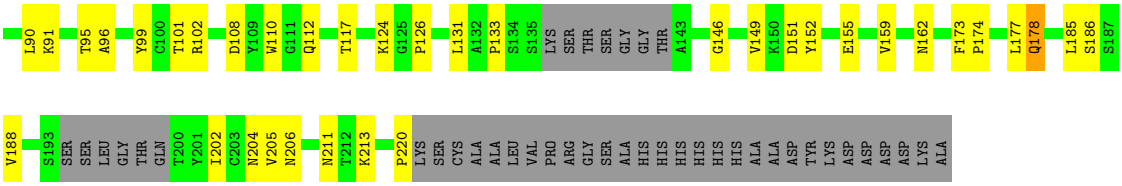


• Molecule 2: 1B2 (heavy chain)

Chain E:



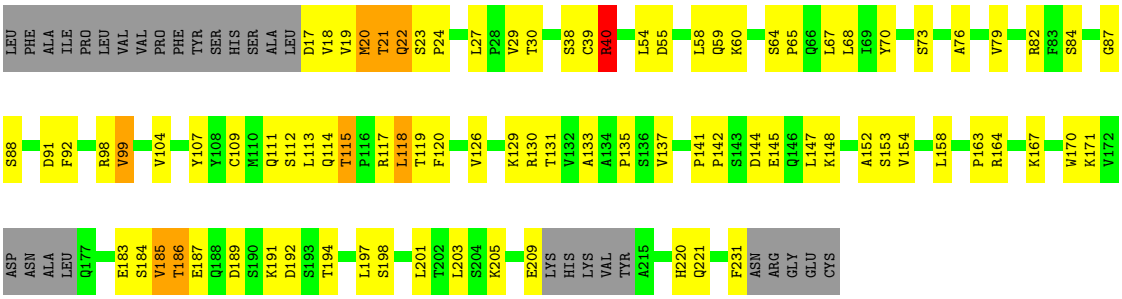




• Molecule 3: 1B2 (light chain)

Chain D:

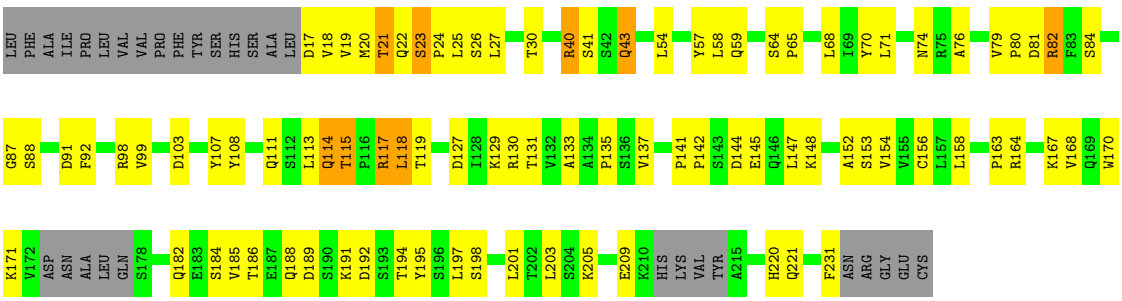




• Molecule 3: 1B2 (light chain)

Chain F:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.525	Depositor
Minimum map value	-0.358	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.28	0/10522	0.52	4/14323 (0.0%)
1	B	0.28	0/10715	0.55	6/14587 (0.0%)
2	C	0.26	0/1575	0.55	0/2141
2	E	0.23	0/1575	0.52	0/2141
3	D	0.50	0/1601	0.75	3/2175 (0.1%)
3	F	0.50	0/1601	0.71	0/2174
All	All	0.31	0/27589	0.56	13/37541 (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	C	0	1
2	E	0	1
3	D	0	1
3	F	0	1
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	197	PRO	CB-CA-C	-8.67	100.44	111.71
3	D	24	PRO	N-CA-C	-7.64	96.72	112.47
1	A	838	THR	N-CA-C	-7.33	104.31	113.18
1	B	650	ALA	N-CA-C	-6.61	104.85	113.12
1	A	176	MET	N-CA-C	-6.20	107.56	114.62
1	A	839	ALA	N-CA-C	-5.70	105.15	111.36
3	D	40	ARG	CB-CG-CD	5.69	124.39	111.30
1	A	842	GLU	N-CA-C	-5.68	105.00	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	CYS	N-CA-C	-5.66	105.11	111.28
1	B	204	ALA	CB-CA-C	-5.56	110.15	116.54
1	B	380	GLN	CB-CA-C	-5.52	109.72	117.23
1	B	10	ALA	N-CA-C	-5.21	105.61	111.28
3	D	120	PHE	N-CA-C	-5.05	107.17	113.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	155	GLU	Peptide
3	D	115	THR	Peptide
2	E	155	GLU	Peptide
3	F	115	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10319	0	10164	392	0
1	B	10513	0	10362	394	0
2	C	1539	0	1511	54	0
2	E	1539	0	1511	53	0
3	D	1568	0	1528	52	0
3	F	1568	0	1533	57	0
All	All	27046	0	26609	949	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 18.

All (949) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1333:ARG:HD3	1:A:927:ALA:HB1	1.63	0.81
1:B:1144:LEU:HD13	1:B:1169:LEU:HD23	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:184:SER:HB3	3:D:198:SER:HB3	1.64	0.79
1:A:158:GLN:NE2	1:A:235:MET:SD	2.60	0.74
1:A:1019:LEU:HD13	1:A:1244:ILE:HG22	1.67	0.74
2:C:41:GLN:HB2	2:C:47:LEU:HD23	1.70	0.71
3:F:164:ARG:HE	3:F:185:VAL:HG11	1.55	0.71
1:B:123:GLN:NE2	1:B:180:THR:O	2.25	0.70
1:B:157:PRO:HB3	1:A:157:PRO:HB3	1.73	0.70
2:E:41:GLN:NE2	2:E:42:ALA:O	2.23	0.70
1:A:148:PRO:HB2	1:A:224:SER:HA	1.74	0.70
1:B:162:PRO:HA	1:A:163:ARG:HH22	1.55	0.70
1:B:559:VAL:HG11	1:B:820:LEU:HD11	1.74	0.70
1:B:1244:ILE:HD13	1:B:1290:PRO:HG2	1.74	0.69
1:A:208:SER:HB2	1:A:385:VAL:HB	1.72	0.69
1:A:1252:VAL:HG23	1:A:1253:LEU:HD12	1.74	0.69
1:A:235:MET:HE2	1:A:240:MET:H	1.56	0.69
1:A:685:ILE:HG12	1:A:753:TYR:HD2	1.57	0.69
3:F:18:VAL:HA	3:F:114:GLN:HE22	1.56	0.69
3:F:19:VAL:HG22	3:F:43:GLN:HB2	1.73	0.69
1:A:213:HIS:HD2	1:A:214:LEU:HD22	1.57	0.69
2:C:24:CYS:HB3	2:C:83:ALA:HB3	1.75	0.69
1:B:2:ALA:HB1	1:B:8:LYS:H	1.56	0.69
1:B:120:ASP:HB3	1:B:123:GLN:HG3	1.73	0.69
1:B:275:LEU:HD11	1:B:388:VAL:HG11	1.74	0.69
1:B:491:ARG:HD3	1:B:902:PRO:HG3	1.74	0.69
1:B:646:GLY:HA3	1:B:883:ASP:HB2	1.75	0.69
2:E:174:PRO:HD3	3:F:186:THR:HG22	1.75	0.68
1:B:176:MET:HE3	1:A:243:ASP:HB3	1.75	0.68
1:A:704:VAL:HG21	1:A:723:VAL:HG21	1.75	0.68
1:A:777:PRO:HB3	1:A:796:ASP:HA	1.76	0.68
2:E:24:CYS:HB3	2:E:83:ALA:HB3	1.75	0.68
1:A:228:MET:HE3	1:A:274:MET:HG3	1.76	0.67
1:A:629:PRO:HG3	1:A:679:ALA:HA	1.76	0.67
1:B:124:ARG:NH1	1:B:908:VAL:O	2.24	0.67
1:A:844:ILE:HG22	1:A:852:LEU:HD21	1.76	0.67
1:A:120:ASP:HB2	1:A:179:THR:HA	1.76	0.67
1:B:58:LEU:HB3	1:B:401:PRO:HB3	1.77	0.67
1:B:235:MET:HE3	1:B:236:PRO:HD2	1.77	0.67
1:A:120:ASP:HB3	1:A:123:GLN:HG3	1.77	0.67
1:B:660:ILE:HG21	1:B:678:VAL:HB	1.77	0.67
3:D:40:ARG:HA	3:D:40:ARG:NE	2.10	0.66
1:B:1428:LEU:HD21	1:B:1447:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:MET:HE2	1:B:237:THR:O	1.95	0.66
1:B:1194:ARG:NH1	1:B:1196:THR:OG1	2.29	0.66
1:B:111:MET:SD	1:B:187:ARG:NH1	2.69	0.66
1:B:1143:VAL:HG11	1:B:1160:LEU:HD13	1.77	0.66
1:B:344:THR:HG23	1:B:347:GLY:H	1.60	0.66
2:C:146:GLY:HA3	2:C:188:VAL:HG22	1.78	0.66
3:D:158:LEU:HB2	3:D:197:LEU:HB3	1.77	0.66
1:B:205:CYS:HB3	1:B:378:HIS:HE2	1.60	0.66
1:B:688:MET:HE2	1:B:763:ILE:HD12	1.77	0.66
3:D:21:THR:HA	3:D:40:ARG:O	1.95	0.66
1:B:1066:ALA:HB1	1:B:1290:PRO:HB3	1.78	0.65
1:A:565:GLN:OE1	1:A:657:GLN:NE2	2.29	0.65
1:B:558:ALA:HB2	1:B:880:VAL:HG13	1.78	0.65
1:B:603:ILE:HG22	1:B:607:ARG:HH21	1.62	0.65
1:B:980:VAL:O	1:B:993:ARG:NH1	2.30	0.65
1:B:1252:VAL:HG23	1:B:1253:LEU:HD12	1.79	0.65
1:A:466:VAL:HG23	1:A:505:ARG:HH22	1.61	0.64
1:A:1337:ILE:HG12	1:A:1338:GLU:HG2	1.79	0.64
1:B:680:LEU:HA	1:B:683:ARG:HE	1.60	0.64
1:B:1275:SER:HA	1:B:1314:TRP:H	1.62	0.64
1:A:478:SER:H	1:A:488:GLN:HE22	1.45	0.64
2:E:146:GLY:HA3	2:E:188:VAL:HG22	1.78	0.64
3:F:158:LEU:HB2	3:F:197:LEU:HB3	1.77	0.64
1:B:1034:MET:HE2	1:B:1081:VAL:HG13	1.79	0.64
1:B:1000:VAL:HG12	1:B:1002:GLY:H	1.62	0.64
1:A:219:LEU:O	1:A:279:ARG:NH1	2.28	0.64
1:B:503:ASP:OD2	1:B:505:ARG:NH1	2.30	0.64
1:B:1450:LEU:HD13	1:A:247:MET:HA	1.78	0.64
1:A:485:LEU:HD21	1:A:522:ALA:HB2	1.80	0.64
1:A:1000:VAL:HG12	1:A:1002:GLY:H	1.63	0.64
1:A:980:VAL:O	1:A:993:ARG:NH1	2.31	0.64
1:B:1005:SER:HB2	1:B:1045:THR:HA	1.80	0.63
1:B:663:ALA:HB1	1:B:669:LEU:HB2	1.80	0.63
1:A:610:ALA:HB2	1:A:613:ARG:HH21	1.63	0.63
1:B:15:ARG:HH21	3:F:76:ALA:HB1	1.63	0.63
2:C:3:GLU:HG3	2:C:5:GLN:HE22	1.63	0.63
1:B:1034:MET:HE1	1:B:1043:LEU:HB2	1.79	0.63
1:A:565:GLN:HE21	1:A:751:VAL:HG11	1.63	0.63
1:B:1302:ARG:HH11	1:B:1309:ALA:HB2	1.64	0.63
1:A:1087:ASP:HB3	1:A:1114:ALA:HA	1.80	0.63
1:A:330:GLY:N	3:F:98:ARG:HH12	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:144:ASP:HA	3:D:147:LEU:HD12	1.81	0.63
2:E:3:GLU:HG3	2:E:5:GLN:HE22	1.63	0.62
1:B:748:ARG:NH1	1:B:749:LEU:O	2.32	0.62
1:B:969:LEU:HD11	1:B:1004:LEU:HD12	1.81	0.62
1:B:959:ASP:HB3	1:B:961:THR:HG22	1.82	0.62
3:D:145:GLU:HA	3:D:148:LYS:HG2	1.81	0.62
3:F:144:ASP:HA	3:F:147:LEU:HD12	1.81	0.62
1:A:29:GLU:HA	1:A:33:GLU:HB2	1.82	0.62
1:B:244:PHE:HD2	1:B:268:MET:HE1	1.65	0.62
1:A:1176:PRO:HD2	1:A:1199:ALA:HB2	1.81	0.61
1:A:40:MET:HG3	1:A:275:LEU:HD22	1.81	0.61
1:B:330:GLY:N	3:D:98:ARG:HH12	1.98	0.61
1:A:17:THR:HG23	3:F:74:ASN:HD21	1.64	0.61
1:A:1076:LEU:HD13	1:A:1281:GLY:HA3	1.83	0.61
3:F:145:GLU:HA	3:F:148:LYS:HG2	1.81	0.61
1:B:121:PRO:HB2	1:B:234:VAL:HG11	1.83	0.61
1:A:613:ARG:NH2	1:A:620:SER:OG	2.33	0.61
3:D:163:PRO:HD2	3:D:221:GLN:HE21	1.64	0.61
1:B:555:GLN:NE2	1:B:878:ALA:O	2.34	0.61
1:A:388:VAL:HG12	1:A:454:ILE:HD11	1.82	0.61
1:A:717:VAL:O	1:A:814:ALA:N	2.34	0.61
1:B:156:ILE:HD11	1:B:204:ALA:HA	1.83	0.61
1:A:35:VAL:HG12	1:A:277:LEU:HD12	1.82	0.61
3:F:163:PRO:HD2	3:F:221:GLN:HE21	1.64	0.60
1:A:734:ARG:HA	1:A:737:ALA:HB3	1.83	0.60
3:F:130:ARG:HH12	3:F:133:ALA:HB2	1.66	0.60
1:A:1072:ARG:HG2	1:A:1112:GLN:HE21	1.66	0.60
3:D:147:LEU:O	3:D:205:LYS:NZ	2.28	0.60
3:F:99:VAL:HG13	3:F:103:ASP:HB2	1.82	0.60
1:B:40:MET:HE1	1:B:392:VAL:HB	1.84	0.60
1:A:642:TRP:HB3	1:A:647:VAL:HB	1.82	0.60
2:E:162:ASN:N	2:E:202:ILE:O	2.32	0.60
1:B:121:PRO:HA	1:B:124:ARG:HG2	1.82	0.60
1:A:684:VAL:HB	1:A:767:LEU:HD21	1.83	0.60
1:B:705:ARG:HH11	1:B:708:ILE:HD11	1.66	0.60
1:A:36:ALA:N	1:A:278:GLU:O	2.35	0.60
1:B:1087:ASP:HB3	1:B:1114:ALA:HA	1.84	0.59
1:A:1354:ARG:HB2	1:A:1356:GLU:HG2	1.84	0.59
1:B:1048:GLU:HG3	1:B:1090:ALA:HA	1.84	0.59
1:A:567:TRP:HB3	1:A:836:ILE:HG12	1.84	0.59
1:B:602:VAL:HG12	1:B:630:VAL:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:PRO:HB3	1:B:798:LEU:H	1.68	0.59
1:B:835:PRO:O	1:B:838:THR:OG1	2.21	0.59
2:C:162:ASN:N	2:C:202:ILE:O	2.32	0.59
1:B:1072:ARG:HG2	1:B:1112:GLN:HE21	1.67	0.59
1:B:1000:VAL:HB	1:B:1039:LEU:HD21	1.84	0.59
1:A:505:ARG:HH21	1:A:894:ARG:HH22	1.51	0.59
2:C:149:VAL:HG11	2:C:205:VAL:HG11	1.83	0.59
1:B:1301:GLN:O	1:B:1304:SER:OG	2.21	0.59
1:B:60:GLU:HG3	1:B:62:ARG:HG3	1.85	0.58
1:B:97:PHE:HA	1:B:270:GLU:HG2	1.85	0.58
1:A:121:PRO:HA	1:A:124:ARG:HG2	1.83	0.58
1:A:1239:LEU:HD23	1:A:1243:ARG:HD3	1.85	0.58
1:A:1302:ARG:HH11	1:A:1309:ALA:HB2	1.67	0.58
1:B:334:ILE:O	1:B:363:ARG:NH1	2.32	0.58
1:B:1151:GLY:HA3	1:B:1320:SER:HB2	1.84	0.58
1:B:1176:PRO:HD2	1:B:1199:ALA:HB2	1.84	0.58
1:A:379:THR:HB	1:A:382:ALA:HB3	1.86	0.58
1:A:945:LEU:HD21	1:A:1105:SER:HB3	1.84	0.58
1:A:395:MET:SD	1:A:456:GLU:HA	2.43	0.58
3:D:130:ARG:HH12	3:D:133:ALA:HB2	1.66	0.58
1:B:1236:VAL:HA	1:B:1239:LEU:HB2	1.84	0.58
2:E:54:ARG:HD2	2:E:60:GLY:HA3	1.86	0.58
1:B:1150:GLY:O	1:B:1154:GLY:N	2.35	0.58
1:A:727:GLY:H	1:A:732:LEU:HD22	1.69	0.58
2:C:40:ARG:NH1	2:C:48:GLU:OE1	2.36	0.58
3:D:54:LEU:HD13	3:D:92:PHE:CD2	2.38	0.58
2:E:40:ARG:NH1	2:E:48:GLU:OE1	2.36	0.58
1:A:1168:LEU:HD13	1:A:1195:THR:HG22	1.86	0.58
1:A:1259:HIS:O	1:A:1263:ARG:HD3	2.04	0.58
1:A:493:ALA:HB2	1:A:536:LEU:HB3	1.85	0.57
1:A:1337:ILE:HG12	1:A:1338:GLU:H	1.68	0.57
1:B:1076:LEU:HD13	1:B:1281:GLY:HA3	1.85	0.57
1:A:45:PRO:HD2	1:A:376:LEU:HD23	1.86	0.57
1:A:560:PHE:HB2	1:A:652:VAL:HG12	1.85	0.57
1:A:602:VAL:HG13	1:A:630:VAL:HG22	1.85	0.57
2:E:133:PRO:HG2	2:E:220:PRO:HB3	1.87	0.57
1:B:12:TYR:HE1	3:F:70:TYR:HB2	1.68	0.57
1:B:583:PHE:HD1	1:B:641:MET:HE3	1.69	0.57
1:B:1068:TRP:HZ2	1:B:1087:ASP:HB2	1.69	0.57
1:A:69:PRO:HG2	1:A:72:ARG:HH21	1.69	0.57
1:B:1437:PRO:HG2	1:B:1445:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:MET:O	1:A:748:ARG:NH2	2.37	0.57
1:A:685:ILE:HD11	1:A:754:ALA:HB3	1.86	0.57
1:B:1332:ARG:HA	1:A:1365:ARG:CZ	2.35	0.57
1:A:213:HIS:CD2	1:A:214:LEU:HD22	2.39	0.57
1:A:1171:VAL:HG21	1:A:1211:LEU:HD21	1.86	0.57
2:C:49:TRP:HB3	3:D:118:LEU:HA	1.85	0.57
3:D:54:LEU:HD13	3:D:92:PHE:HD2	1.68	0.57
1:B:1167:HIS:CD2	1:B:1194:ARG:HG2	2.39	0.57
1:A:158:GLN:HE22	1:A:240:MET:HG2	1.68	0.57
1:A:118:ALA:HB3	1:A:174:TYR:HB2	1.86	0.57
1:A:395:MET:HE1	1:A:454:ILE:HG22	1.86	0.57
1:A:1005:SER:HB2	1:A:1045:THR:HA	1.85	0.57
1:A:1222:SER:HB3	1:A:1268:THR:H	1.69	0.57
2:C:54:ARG:HD2	2:C:60:GLY:HA3	1.86	0.57
2:E:36:MET:H	2:E:76:ARG:HH12	1.52	0.57
1:A:567:TRP:CD2	1:A:832:SER:HB2	2.39	0.57
2:C:133:PRO:HG2	2:C:220:PRO:HB3	1.87	0.57
1:B:624:VAL:HA	1:B:627:VAL:HG12	1.87	0.56
1:B:1251:LYS:HE3	1:B:1291:GLY:HA3	1.86	0.56
1:B:1347:ALA:HA	1:B:1350:ASN:HD21	1.69	0.56
1:B:1337:ILE:HG22	1:B:1363:ASP:HB2	1.86	0.56
1:A:718:ASN:HA	1:A:813:PHE:HB3	1.88	0.56
2:C:173:PHE:CD2	3:D:198:SER:HB2	2.40	0.56
1:B:621:THR:HB	1:B:627:VAL:HG23	1.88	0.56
1:B:1159:TRP:CD1	1:B:1345:CYS:HB2	2.40	0.56
1:A:700:PRO:HA	1:A:721:ARG:HA	1.87	0.56
3:F:130:ARG:HH21	3:F:194:THR:HG22	1.69	0.56
1:A:1068:TRP:HZ2	1:A:1087:ASP:HB2	1.70	0.56
1:B:296:GLY:HA3	1:B:327:SER:HB3	1.87	0.56
1:B:566:GLY:HA3	1:B:836:ILE:HG12	1.88	0.56
1:B:1339:MET:HE2	1:B:1344:ALA:HA	1.86	0.56
1:A:608:ALA:HB1	1:A:612:ARG:HG3	1.86	0.56
3:F:30:THR:HB	3:F:129:LYS:HB3	1.88	0.56
1:B:287:GLY:O	1:B:895:ARG:NH1	2.38	0.56
1:A:127:LEU:HD21	1:A:187:ARG:HB3	1.88	0.56
1:A:1212:LEU:HD13	1:A:1261:LEU:HG	1.88	0.56
3:D:130:ARG:HH21	3:D:194:THR:HG22	1.69	0.56
2:E:49:TRP:HB3	3:F:118:LEU:HA	1.87	0.56
1:B:5:ASP:HA	1:B:8:LYS:HB2	1.88	0.56
1:B:637:SER:O	1:B:641:MET:HG2	2.05	0.56
2:C:36:MET:H	2:C:76:ARG:HH12	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ALA:HB3	1:A:376:LEU:HA	1.88	0.56
1:A:330:GLY:CA	3:F:98:ARG:HH12	2.19	0.56
1:B:999:GLU:HB2	1:B:1405:ALA:HA	1.88	0.56
1:A:1000:VAL:HB	1:A:1039:LEU:HD21	1.88	0.56
1:A:1236:VAL:HA	1:A:1239:LEU:HB2	1.87	0.56
1:A:1263:ARG:HA	1:A:1307:LEU:HD11	1.88	0.56
3:D:17:ASP:OD1	3:D:18:VAL:N	2.35	0.56
3:D:30:THR:HB	3:D:129:LYS:HB3	1.88	0.55
1:B:1356:GLU:HB3	1:B:1359:PRO:HG3	1.87	0.55
1:A:162:PRO:HD2	1:A:910:LEU:HG	1.88	0.55
1:A:320:ILE:O	1:A:324:LEU:HB2	2.06	0.55
1:A:928:LEU:HB3	1:A:1361:VAL:HG13	1.88	0.55
1:A:474:PRO:HB3	1:A:873:SER:HB2	1.88	0.55
1:A:558:ALA:HB2	1:A:880:VAL:HG13	1.89	0.55
1:A:562:PHE:HB2	1:A:654:GLY:HA2	1.89	0.55
1:B:244:PHE:CD2	1:B:268:MET:HE1	2.41	0.55
1:B:1310:THR:HG22	1:B:1312:VAL:HG13	1.89	0.55
1:B:1420:VAL:HG22	1:B:1459:LEU:HD11	1.89	0.55
1:B:1272:LEU:HD21	1:B:1298:LEU:HD23	1.88	0.55
1:B:950:LEU:HB2	1:B:1003:VAL:HG22	1.88	0.55
1:A:1142:THR:HA	1:A:1167:HIS:HB2	1.88	0.55
1:A:930:TYR:O	1:A:1360:ILE:N	2.39	0.55
2:C:110:TRP:HB3	3:D:64:SER:HB2	1.89	0.55
1:B:338:GLU:HB2	1:B:391:MET:HE3	1.89	0.55
1:A:42:CYS:HB2	1:A:44:LEU:HD23	1.89	0.55
1:A:646:GLY:HA3	1:A:883:ASP:HB3	1.89	0.55
1:A:1301:GLN:O	1:A:1304:SER:OG	2.25	0.55
1:B:712:VAL:HG22	1:B:727:GLY:HA3	1.89	0.55
1:A:43:ARG:HG2	1:A:125:LEU:HD22	1.88	0.55
1:A:124:ARG:NH1	1:A:908:VAL:O	2.40	0.55
1:A:698:ALA:HA	1:A:722:SER:HA	1.89	0.55
1:B:1230:THR:OG1	1:B:1247:ALA:O	2.22	0.55
2:E:55:SER:O	2:E:59:GLY:N	2.37	0.55
2:E:21:ARG:HE	2:E:22:LEU:H	1.54	0.54
1:B:205:CYS:HB2	1:B:444:GLY:HA2	1.90	0.54
1:B:1360:ILE:HG13	1:B:1360:ILE:O	2.07	0.54
1:B:788:VAL:HG13	1:B:789:THR:HG23	1.88	0.54
1:A:12:TYR:HE1	3:D:70:TYR:HB2	1.71	0.54
1:A:1150:GLY:O	1:A:1154:GLY:N	2.40	0.54
1:A:50:THR:HG1	1:A:136:ARG:HH12	1.48	0.54
1:A:526:PRO:HG3	1:A:532:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:GLY:HA2	1:A:1324:GLU:HB3	1.90	0.54
2:C:49:TRP:CZ2	2:C:52:PHE:HD1	2.25	0.54
2:E:49:TRP:CZ2	2:E:52:PHE:HD1	2.25	0.54
1:A:1031:VAL:HG21	1:A:1074:ILE:HD13	1.90	0.54
1:B:82:PRO:HB3	1:A:1306:GLY:HA2	1.89	0.54
2:E:41:GLN:HB2	2:E:47:LEU:HD23	1.90	0.54
1:B:41:ALA:O	1:B:274:MET:N	2.39	0.54
1:B:155:LEU:HB2	1:B:181:THR:HG23	1.90	0.54
1:B:158:GLN:OE1	1:B:235:MET:HE1	2.08	0.54
1:B:291:LEU:HA	1:B:396:ARG:HH22	1.71	0.54
1:A:756:HIS:ND1	1:A:806:ASN:O	2.41	0.54
2:C:21:ARG:HE	2:C:22:LEU:H	1.55	0.54
3:F:184:SER:HB3	3:F:198:SER:HB3	1.90	0.54
1:B:786:SER:OG	1:B:793:THR:OG1	2.25	0.54
1:A:797:GLU:HB2	1:A:805:ARG:HH22	1.72	0.54
2:C:55:SER:O	2:C:59:GLY:N	2.38	0.54
1:B:379:THR:HB	1:B:382:ALA:HB3	1.90	0.54
1:A:642:TRP:HZ3	1:A:831:VAL:HG13	1.73	0.54
1:A:1188:LEU:HB3	1:A:1195:THR:HG21	1.90	0.54
1:A:1055:PRO:HB3	1:A:1303:ARG:HH22	1.72	0.53
1:A:368:HIS:HB3	1:A:423:LEU:HD21	1.89	0.53
1:A:859:ARG:HH12	1:A:870:GLU:CD	2.16	0.53
1:A:1336:VAL:HG12	1:A:1364:VAL:HA	1.90	0.53
1:B:680:LEU:HD23	1:B:771:LEU:HA	1.89	0.53
1:A:1125:TRP:CH2	1:A:1279:ALA:HB1	2.44	0.53
1:B:945:LEU:N	1:B:972:ALA:O	2.41	0.53
1:B:1456:ARG:NH1	1:B:1469:THR:O	2.41	0.53
1:B:2:ALA:HB1	1:B:7:GLU:HB2	1.91	0.53
1:B:1144:LEU:HB3	1:B:1224:VAL:HA	1.91	0.53
1:B:948:THR:HG22	1:B:975:ARG:HE	1.74	0.53
1:A:98:LEU:HD13	1:A:100:GLU:HB2	1.91	0.53
1:A:385:VAL:HA	1:A:388:VAL:HG22	1.91	0.53
1:A:950:LEU:HB2	1:A:1003:VAL:HG22	1.91	0.53
1:A:43:ARG:NH1	1:A:49:SER:OG	2.42	0.53
1:B:3:SER:HB3	1:B:6:SER:HB2	1.91	0.53
1:A:945:LEU:N	1:A:972:ALA:O	2.42	0.53
1:A:1230:THR:OG1	1:A:1247:ALA:O	2.23	0.53
2:C:31:PHE:O	2:C:76:ARG:NH2	2.41	0.53
2:E:31:PHE:O	2:E:76:ARG:NH2	2.41	0.53
1:B:1226:HIS:HD2	1:B:1258:LEU:HD12	1.74	0.52
1:B:1004:LEU:HD23	1:B:1044:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HB3	1:A:420:ILE:HG12	1.92	0.52
1:A:1108:ALA:O	1:A:1380:ARG:NH1	2.42	0.52
1:B:717:VAL:O	1:B:814:ALA:N	2.39	0.52
1:B:1463:THR:HG21	1:B:1485:LEU:HD21	1.90	0.52
1:A:43:ARG:O	1:A:272:ALA:N	2.39	0.52
1:B:76:LEU:H	1:B:79:LEU:HD13	1.74	0.52
1:B:961:THR:HG21	1:B:1009:VAL:HG21	1.92	0.52
1:A:180:THR:O	1:A:183:VAL:HG22	2.09	0.52
1:A:279:ARG:NE	1:A:282:ASP:OD2	2.41	0.52
1:B:351:GLU:HG3	1:B:443:PHE:HE2	1.72	0.52
1:B:390:LYS:HE2	1:B:401:PRO:HB2	1.91	0.52
1:A:625:ASP:HB3	1:A:686:ALA:HB2	1.92	0.52
1:A:826:ARG:HH22	1:A:850:ALA:HB1	1.75	0.52
1:B:49:SER:OG	1:B:100:GLU:OE2	2.25	0.52
1:B:320:ILE:HG22	1:B:451:HIS:CG	2.44	0.52
1:B:1068:TRP:CZ2	1:B:1087:ASP:HB2	2.45	0.52
2:C:54:ARG:HH11	2:C:61:THR:H	1.56	0.52
1:A:330:GLY:HA3	3:F:98:ARG:HH12	1.74	0.52
1:A:778:LEU:HG	1:A:779:PRO:HD2	1.91	0.52
1:B:295:ARG:HD3	1:B:329:LEU:HD11	1.90	0.52
1:B:798:LEU:HD11	1:B:803:TRP:CH2	2.44	0.52
1:B:1278:SER:OG	1:B:1289:ALA:O	2.28	0.52
1:B:1248:SER:O	1:B:1252:VAL:HG22	2.10	0.52
1:A:65:VAL:HG12	1:A:96:GLY:N	2.25	0.52
1:A:156:ILE:HG13	1:A:381:ALA:HB2	1.92	0.52
1:A:228:MET:CE	1:A:274:MET:HG3	2.38	0.52
1:A:302:ASP:OD1	1:A:449:ASN:ND2	2.40	0.52
1:B:114:ARG:HB2	1:B:1429:GLY:HA3	1.93	0.52
1:A:817:VAL:HG11	1:A:844:ILE:HG21	1.92	0.52
2:C:126:PRO:HB3	2:C:152:TYR:HB3	1.91	0.52
2:E:126:PRO:HB3	2:E:152:TYR:HB3	1.91	0.52
1:B:156:ILE:HG21	1:B:158:GLN:HE21	1.75	0.51
1:A:50:THR:OG1	1:A:136:ARG:NH1	2.28	0.51
1:A:133:VAL:HG11	1:A:228:MET:CE	2.40	0.51
1:A:502:GLN:HB3	1:A:507:ILE:HD11	1.92	0.51
1:A:638:LEU:HB3	1:A:642:TRP:CZ3	2.46	0.51
1:A:752:ASP:OD1	1:A:752:ASP:N	2.42	0.51
1:B:892:GLY:O	1:B:894:ARG:NH1	2.44	0.51
1:B:1168:LEU:HD12	1:B:1195:THR:HG22	1.91	0.51
1:A:492:LEU:HD23	1:A:536:LEU:HD21	1.92	0.51
1:A:1159:TRP:CG	1:A:1345:CYS:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ARG:HH11	2:E:61:THR:H	1.56	0.51
1:B:1354:ARG:HB2	1:B:1356:GLU:HG2	1.91	0.51
1:B:1421:ARG:NH2	1:B:1436:VAL:H	2.08	0.51
1:B:77:ASP:OD2	1:A:931:ARG:NE	2.31	0.51
1:B:622:GLU:OE1	1:B:623:ARG:NH1	2.44	0.51
1:B:829:LEU:HD11	1:B:880:VAL:HG21	1.92	0.51
1:A:209:LEU:HD11	1:A:440:VAL:HG12	1.93	0.51
1:A:758:SER:HA	1:A:761:GLU:HB2	1.92	0.51
1:A:1068:TRP:CZ2	1:A:1087:ASP:HB2	2.46	0.51
3:D:58:LEU:HB2	3:D:68:LEU:HD11	1.93	0.51
1:B:43:ARG:O	1:B:272:ALA:N	2.42	0.51
1:B:291:LEU:O	1:B:396:ARG:NH2	2.44	0.51
3:F:147:LEU:O	3:F:205:LYS:NZ	2.28	0.51
1:B:36:ALA:HB1	1:B:290:VAL:HG13	1.92	0.51
1:A:71:ASP:O	1:A:907:ARG:NH2	2.44	0.51
1:A:711:ARG:NH2	1:A:758:SER:H	2.08	0.51
1:B:395:MET:O	1:B:436:ARG:NH2	2.43	0.51
3:F:70:TYR:N	3:F:74:ASN:O	2.42	0.51
1:B:30:LEU:HD13	1:A:30:LEU:HD22	1.92	0.51
1:B:1450:LEU:O	1:B:1454:GLU:HG2	2.10	0.51
1:B:1459:LEU:O	1:B:1463:THR:OG1	2.24	0.51
1:A:1066:ALA:HB1	1:A:1290:PRO:HB3	1.92	0.51
1:B:685:ILE:HA	1:B:688:MET:HE3	1.91	0.50
1:B:1239:LEU:HD23	1:B:1243:ARG:HD3	1.93	0.50
1:A:244:PHE:HB3	1:A:250:LEU:CD2	2.41	0.50
2:E:31:PHE:CE2	2:E:76:ARG:HB2	2.46	0.50
1:A:711:ARG:HH22	1:A:758:SER:H	1.59	0.50
1:B:338:GLU:OE2	1:B:372:VAL:N	2.39	0.50
1:B:1142:THR:HA	1:B:1167:HIS:HB2	1.94	0.50
1:B:1203:THR:HG21	1:B:1249:ARG:HE	1.75	0.50
1:A:966:ARG:HB2	1:A:976:VAL:HG21	1.93	0.50
2:E:8:GLN:H	2:E:112:GLN:HE22	1.59	0.50
3:F:58:LEU:HB2	3:F:68:LEU:HD11	1.93	0.50
1:B:716:ALA:HB3	1:B:724:VAL:HB	1.93	0.50
1:B:216:CYS:HB3	1:B:220:ARG:HE	1.76	0.50
1:A:480:SER:HB2	1:A:518:LEU:HD22	1.93	0.50
1:A:826:ARG:HG3	1:A:852:LEU:HA	1.93	0.50
1:B:7:GLU:HG3	2:E:58:TYR:CE2	2.47	0.50
1:B:704:VAL:HG23	1:B:714:ILE:HD11	1.92	0.50
1:B:1347:ALA:HA	1:B:1350:ASN:ND2	2.27	0.50
2:E:21:ARG:HE	2:E:22:LEU:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:982:ASP:HB3	1:B:985:CYS:HB3	1.93	0.50
1:B:1025:ALA:HB2	1:B:1241:GLY:HA3	1.94	0.50
2:C:31:PHE:CE2	2:C:76:ARG:HB2	2.47	0.50
3:F:127:ASP:HB3	3:F:188:GLN:NE2	2.27	0.50
1:B:76:LEU:HD23	1:B:79:LEU:HD22	1.94	0.50
1:B:410:SER:HB3	1:B:413:ILE:HD12	1.94	0.50
1:B:1453:LEU:O	1:B:1456:ARG:HG2	2.11	0.50
1:A:682:SER:HA	1:A:685:ILE:HG22	1.92	0.50
2:C:8:GLN:H	2:C:112:GLN:HE22	1.59	0.50
3:D:22:GLN:HG2	3:D:40:ARG:HB2	1.93	0.50
1:A:716:ALA:HB3	1:A:724:VAL:HB	1.94	0.49
1:A:800:ALA:HA	1:A:803:TRP:CD1	2.47	0.49
3:D:142:PRO:HD3	3:D:154:VAL:HB	1.94	0.49
1:B:519:PRO:O	1:B:520:HIS:ND1	2.45	0.49
1:B:567:TRP:HB3	1:B:834:HIS:HB3	1.94	0.49
1:B:602:VAL:O	1:B:606:LEU:N	2.40	0.49
1:B:652:VAL:HB	1:B:784:PHE:HD1	1.76	0.49
1:A:1248:SER:O	1:A:1252:VAL:HG22	2.11	0.49
1:B:963:THR:HA	1:B:966:ARG:HG2	1.94	0.49
1:A:466:VAL:HG23	1:A:505:ARG:NH2	2.26	0.49
1:A:692:LYS:HB2	1:A:728:ASP:HA	1.93	0.49
1:A:1143:VAL:HG11	1:A:1160:LEU:HD13	1.93	0.49
1:A:1340:PRO:HB2	1:A:1343:THR:HG22	1.94	0.49
2:C:21:ARG:HE	2:C:22:LEU:N	2.10	0.49
1:B:339:ALA:HB2	1:B:355:LEU:HD11	1.93	0.49
1:B:512:ALA:HB1	1:B:884:TRP:HB3	1.95	0.49
1:B:627:VAL:O	1:B:631:MET:HG2	2.12	0.49
1:B:1031:VAL:HG21	1:B:1074:ILE:HD13	1.95	0.49
1:B:1152:VAL:HG21	1:B:1322:MET:HB3	1.94	0.49
1:B:74:TRP:CD1	1:B:238:PRO:HD3	2.48	0.49
1:A:966:ARG:HA	1:A:969:LEU:HB2	1.94	0.49
1:B:300:ASN:O	1:B:449:ASN:N	2.41	0.49
1:B:1332:ARG:HG3	1:A:1365:ARG:NH2	2.28	0.49
1:B:1411:GLU:C	1:B:1413:GLU:N	2.70	0.49
3:F:88:SER:N	3:F:91:ASP:O	2.43	0.49
1:A:339:ALA:HB2	1:A:369:LEU:HD11	1.95	0.49
2:C:49:TRP:HZ2	2:C:52:PHE:HD1	1.61	0.49
3:F:142:PRO:HD3	3:F:154:VAL:HB	1.94	0.49
1:B:247:MET:HE1	1:A:176:MET:HE1	1.95	0.49
1:B:945:LEU:HD21	1:B:1105:SER:HB3	1.93	0.49
1:B:1209:ARG:HA	1:B:1261:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1249:ARG:HB2	1:B:1253:LEU:HD13	1.93	0.49
1:B:1316:THR:O	1:B:1338:GLU:HA	2.12	0.49
1:B:1337:ILE:HA	1:A:1365:ARG:NH2	2.28	0.49
1:A:601:GLU:HG3	1:A:603:ILE:H	1.78	0.49
3:F:114:GLN:H	3:F:117:ARG:HH22	1.60	0.49
1:A:15:ARG:HH21	3:D:76:ALA:HB1	1.78	0.49
1:A:390:LYS:HE3	1:A:401:PRO:HG2	1.95	0.49
1:A:624:VAL:HA	1:A:627:VAL:HG22	1.94	0.49
1:A:369:LEU:HB3	1:A:422:LEU:HD23	1.95	0.49
1:A:1310:THR:HG22	1:A:1312:VAL:HG13	1.95	0.49
2:C:207:HIS:N	2:C:213:LYS:HZ3	2.11	0.49
1:B:562:PHE:CE1	1:B:652:VAL:HG13	2.48	0.48
1:A:1025:ALA:HB2	1:A:1241:GLY:HA3	1.95	0.48
1:A:1159:TRP:CZ2	1:A:1349:GLN:HB2	2.48	0.48
1:A:1368:ARG:HE	1:A:1368:ARG:HB2	1.45	0.48
3:D:29:VAL:HG23	3:D:99:VAL:HG11	1.95	0.48
1:B:43:ARG:CG	1:B:129:LEU:HD21	2.43	0.48
1:A:330:GLY:HA3	3:F:98:ARG:NH1	2.28	0.48
1:A:627:VAL:O	1:A:631:MET:N	2.40	0.48
1:A:660:ILE:HG22	1:A:674:ALA:HB1	1.94	0.48
1:B:251:ALA:H	1:B:267:GLY:H	1.60	0.48
1:B:557:ARG:HG3	1:B:650:ALA:HB2	1.95	0.48
1:B:1251:LYS:HD2	1:B:1295:LEU:HD11	1.94	0.48
1:B:1274:SER:HB2	1:B:1292:ASN:HB3	1.94	0.48
1:A:240:MET:HE3	1:A:244:PHE:CE2	2.49	0.48
1:A:329:LEU:C	3:F:98:ARG:HH12	2.21	0.48
1:A:1316:THR:O	1:A:1338:GLU:HA	2.13	0.48
3:F:185:VAL:HG22	3:F:197:LEU:HA	1.96	0.48
1:B:331:PRO:HB3	1:B:359:TYR:HA	1.95	0.48
1:B:792:TRP:HZ3	1:B:819:ALA:HB1	1.79	0.48
1:B:1171:VAL:HG12	1:B:1198:ALA:HB3	1.94	0.48
1:B:1004:LEU:HD21	1:B:1104:VAL:HG11	1.94	0.48
1:A:235:MET:SD	1:A:240:MET:HG2	2.53	0.48
1:A:717:VAL:HG23	1:A:723:VAL:HG12	1.96	0.48
3:F:127:ASP:HB3	3:F:188:GLN:HE22	1.78	0.48
1:B:953:LYS:HA	1:B:1007:LEU:HB3	1.94	0.48
1:B:1074:ILE:HG22	1:B:1082:TRP:HB2	1.94	0.48
1:B:1442:PHE:N	1:B:1476:PRO:O	2.44	0.48
1:A:17:THR:HG23	3:F:74:ASN:ND2	2.29	0.48
1:A:761:GLU:HG3	1:A:808:ARG:HD2	1.94	0.48
3:F:130:ARG:NH1	3:F:131:THR:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLN:O	1:B:320:ILE:HG12	2.13	0.48
1:A:111:MET:HE1	1:A:116:ALA:HA	1.94	0.48
1:B:114:ARG:NE	1:B:170:GLY:O	2.47	0.48
1:B:558:ALA:HA	1:B:827:THR:HG23	1.95	0.48
1:B:1152:VAL:HA	1:B:1317:TRP:HZ2	1.78	0.48
3:D:189:ASP:OD1	3:D:189:ASP:N	2.42	0.48
1:B:855:ILE:HG12	1:B:875:ALA:HA	1.96	0.48
1:B:1285:LEU:HG	1:B:1327:VAL:HG11	1.96	0.48
1:A:244:PHE:HB3	1:A:250:LEU:HD21	1.95	0.48
1:B:558:ALA:HB1	1:B:829:LEU:HD13	1.96	0.48
1:A:963:THR:HA	1:A:966:ARG:HG2	1.96	0.47
2:C:31:PHE:HE2	2:C:76:ARG:HB2	1.79	0.47
3:D:29:VAL:HG21	3:D:99:VAL:HG21	1.96	0.47
3:D:130:ARG:NH1	3:D:131:THR:O	2.47	0.47
1:A:1074:ILE:HG22	1:A:1082:TRP:HB2	1.95	0.47
3:D:163:PRO:O	3:D:220:HIS:NE2	2.47	0.47
2:E:31:PHE:HE2	2:E:76:ARG:HB2	1.79	0.47
1:B:69:PRO:HD3	1:B:97:PHE:CG	2.50	0.47
1:B:677:VAL:HG11	1:B:803:TRP:CE2	2.49	0.47
1:A:568:GLN:O	1:A:860:ARG:NH1	2.47	0.47
1:A:600:PHE:HE2	1:A:605:PHE:HB2	1.79	0.47
2:C:9:SER:OG	2:C:23:SER:OG	2.32	0.47
3:F:59:GLN:HA	3:F:65:PRO:HA	1.96	0.47
1:B:104:PHE:HB2	1:B:124:ARG:HD3	1.96	0.47
1:B:1123:ARG:HH22	1:B:1279:ALA:HA	1.78	0.47
1:A:149:THR:HB	1:A:194:LEU:HD22	1.95	0.47
1:A:471:VAL:HG11	1:A:865:LEU:HD23	1.96	0.47
1:A:1222:SER:HB3	1:A:1268:THR:HG22	1.96	0.47
3:D:54:LEU:HD11	3:D:109:CYS:SG	2.54	0.47
3:D:118:LEU:H	3:D:118:LEU:HG	1.44	0.47
1:B:583:PHE:CD1	1:B:641:MET:HE3	2.48	0.47
1:B:736:VAL:HG22	1:B:746:ALA:HB3	1.97	0.47
1:B:1007:LEU:HD23	1:B:1007:LEU:H	1.80	0.47
1:B:1048:GLU:O	1:B:1060:ARG:NE	2.44	0.47
1:B:1417:PHE:CZ	1:B:1421:ARG:HD2	2.49	0.47
1:A:1356:GLU:HB3	1:A:1359:PRO:HG3	1.95	0.47
2:E:49:TRP:HZ2	2:E:52:PHE:HD1	1.61	0.47
3:F:130:ARG:HD2	3:F:131:THR:N	2.29	0.47
1:B:521:ARG:HD3	1:B:876:PHE:O	2.14	0.47
1:A:69:PRO:HG3	1:A:97:PHE:HB3	1.96	0.47
3:F:40:ARG:HD2	3:F:40:ARG:HA	1.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:LEU:HD12	1:B:779:PRO:HD2	1.96	0.47
1:B:1068:TRP:O	1:B:1072:ARG:HG3	2.13	0.47
1:A:35:VAL:HG23	1:A:220:ARG:HE	1.79	0.47
1:A:174:TYR:HA	1:A:177:THR:HG22	1.96	0.47
1:A:295:ARG:HG3	1:A:329:LEU:HD11	1.97	0.47
1:A:605:PHE:CZ	1:A:627:VAL:HG12	2.50	0.47
2:E:173:PHE:CD2	3:F:198:SER:HB2	2.50	0.47
3:F:163:PRO:O	3:F:220:HIS:NE2	2.47	0.47
1:B:966:ARG:HB2	1:B:976:VAL:HG21	1.95	0.47
1:A:51:PRO:HD2	1:A:136:ARG:CZ	2.44	0.47
1:A:739:CYS:HB3	1:A:744:ILE:HG22	1.97	0.47
1:A:954:TYR:HD2	1:A:956:GLY:H	1.63	0.47
1:A:1068:TRP:O	1:A:1072:ARG:HG3	2.15	0.47
3:D:59:GLN:HA	3:D:65:PRO:HA	1.96	0.47
1:B:777:PRO:HB2	1:B:796:ASP:OD1	2.15	0.47
1:B:1427:VAL:HG23	1:B:1454:GLU:HG3	1.96	0.47
1:A:50:THR:HG23	1:A:52:GLU:HG3	1.97	0.47
1:A:842:GLU:HG3	1:A:854:ALA:HB3	1.97	0.47
1:B:140:PRO:HB2	1:B:143:SER:HB3	1.95	0.47
1:B:859:ARG:HB3	1:B:862:ASP:HB2	1.96	0.47
2:C:71:ARG:HH21	2:C:90:LEU:HA	1.80	0.47
2:C:112:GLN:OE1	2:C:112:GLN:N	2.43	0.47
2:C:150:LYS:HB3	2:C:150:LYS:HE2	1.50	0.47
1:B:1048:GLU:HB3	1:B:1060:ARG:HE	1.80	0.46
1:B:1226:HIS:HE1	1:B:1251:LYS:HA	1.80	0.46
3:F:17:ASP:OD1	3:F:18:VAL:N	2.47	0.46
1:B:624:VAL:HG11	1:B:685:ILE:HG22	1.96	0.46
1:B:1009:VAL:HA	1:B:1048:GLU:HB2	1.97	0.46
1:B:1178:ALA:HB3	1:B:1181:ALA:HB2	1.97	0.46
1:A:257:LYS:HE3	1:A:257:LYS:HB3	1.77	0.46
1:A:929:ARG:HG3	1:A:1359:PRO:HB3	1.97	0.46
2:C:50:VAL:O	2:C:65:ALA:N	2.46	0.46
3:D:130:ARG:HD2	3:D:131:THR:N	2.29	0.46
2:E:112:GLN:OE1	2:E:112:GLN:N	2.43	0.46
1:B:331:PRO:O	1:B:363:ARG:NH1	2.47	0.46
1:B:577:LEU:HA	1:B:583:PHE:HB3	1.97	0.46
1:A:201:VAL:HG21	1:A:210:VAL:HG12	1.97	0.46
1:A:838:THR:HA	1:A:841:ILE:HB	1.98	0.46
1:A:1312:VAL:HG12	1:A:1359:PRO:HB2	1.97	0.46
3:D:38:SER:OG	3:D:39:CYS:N	2.47	0.46
3:D:88:SER:N	3:D:91:ASP:O	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:50:VAL:O	2:E:65:ALA:N	2.46	0.46
1:B:373:LYS:O	1:B:377:GLY:N	2.46	0.46
1:B:1028:LEU:HD11	1:B:1244:ILE:HD12	1.96	0.46
2:C:39:VAL:O	2:C:99:TYR:N	2.38	0.46
1:B:623:ARG:O	1:B:627:VAL:N	2.37	0.46
1:A:13:LEU:HD21	3:F:71:LEU:HD11	1.96	0.46
1:A:584:ALA:O	1:A:588:ARG:HG2	2.15	0.46
1:A:619:LEU:H	1:A:623:ARG:HG3	1.79	0.46
2:E:9:SER:OG	2:E:23:SER:OG	2.32	0.46
1:B:951:VAL:HG13	1:B:951:VAL:O	2.16	0.46
1:B:1222:SER:HB3	1:B:1268:THR:H	1.81	0.46
1:B:1291:GLY:O	1:B:1295:LEU:HG	2.16	0.46
1:B:660:ILE:HD13	1:B:803:TRP:CZ3	2.51	0.46
1:B:1453:LEU:HA	1:B:1456:ARG:NE	2.31	0.46
1:A:470:ASP:CG	1:A:471:VAL:H	2.24	0.46
2:C:95:THR:HG23	2:C:117:THR:HG23	1.98	0.46
1:B:631:MET:O	1:B:635:MET:HB2	2.16	0.46
1:A:43:ARG:HB3	1:A:272:ALA:HB3	1.97	0.46
1:A:841:ILE:HG22	1:A:854:ALA:HB2	1.98	0.46
1:A:845:GLY:HA2	1:A:848:SER:HB2	1.98	0.46
1:A:1147:GLY:N	1:A:1171:VAL:O	2.42	0.46
2:C:102:ARG:HB3	2:C:108:ASP:OD1	2.16	0.46
1:B:652:VAL:HG21	1:B:666:ALA:HB2	1.97	0.46
1:B:1435:ARG:NH1	1:B:1437:PRO:HA	2.31	0.46
1:A:1318:ALA:HB3	1:A:1341:PRO:HD3	1.97	0.46
2:E:71:ARG:HH21	2:E:90:LEU:HA	1.80	0.46
2:E:110:TRP:HB3	3:F:64:SER:HB2	1.97	0.46
3:F:57:TYR:HB2	3:F:108:TYR:HB2	1.98	0.46
1:A:40:MET:HB2	1:A:51:PRO:HG2	1.98	0.46
1:A:141:PRO:HG2	1:A:516:ALA:HB2	1.98	0.46
1:A:567:TRP:CZ2	1:A:635:MET:HE2	2.50	0.46
1:A:721:ARG:NH2	1:A:846:ASP:H	2.14	0.46
3:F:58:LEU:HD13	3:F:107:TYR:CE1	2.51	0.46
1:B:43:ARG:HG3	1:B:129:LEU:HD21	1.98	0.45
1:B:1244:ILE:HG12	1:B:1287:GLY:HA2	1.97	0.45
1:A:340:HIS:HD2	1:A:442:SER:HA	1.81	0.45
1:A:594:LEU:HG	1:A:675:ALA:HB1	1.98	0.45
1:A:1285:LEU:HD22	1:A:1288:TYR:CD2	2.52	0.45
1:B:141:PRO:HD2	1:B:516:ALA:HB2	1.97	0.45
1:B:562:PHE:HD2	1:B:635:MET:HE3	1.81	0.45
1:A:1203:THR:OG1	1:A:1249:ARG:NH1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:HG13	1:B:288:HIS:HB3	1.99	0.45
1:B:329:LEU:HD12	1:B:453:ILE:HG21	1.98	0.45
1:B:676:ARG:HH21	1:B:775:PHE:HB3	1.81	0.45
1:B:712:VAL:HG21	1:B:731:GLU:HB2	1.98	0.45
1:A:208:SER:HB3	1:A:381:ALA:O	2.17	0.45
1:B:103:ALA:HB1	1:B:905:ARG:HB3	1.99	0.45
1:B:688:MET:N	1:B:689:PRO:HD3	2.31	0.45
1:A:92:GLN:HE21	1:A:250:LEU:HD12	1.81	0.45
1:A:760:VAL:HG21	1:A:807:LEU:HD22	1.98	0.45
1:B:493:ALA:HB2	1:B:536:LEU:HB3	1.98	0.45
1:B:582:VAL:C	1:B:641:MET:HE1	2.41	0.45
1:B:1303:ARG:HG2	1:B:1357:VAL:HG22	1.99	0.45
1:B:1424:ALA:HA	1:B:1427:VAL:HG12	1.98	0.45
1:A:126:MET:HE3	1:A:126:MET:HA	1.98	0.45
1:A:149:THR:HA	1:A:226:LEU:O	2.16	0.45
2:E:95:THR:HG23	2:E:117:THR:HG23	1.98	0.45
1:B:731:GLU:HA	1:B:734:ARG:HG2	1.99	0.45
1:B:805:ARG:HG2	1:B:809:ARG:HH12	1.80	0.45
1:A:235:MET:HG3	1:A:237:THR:O	2.16	0.45
1:A:756:HIS:H	1:A:807:LEU:HA	1.82	0.45
1:A:951:VAL:HG13	1:A:951:VAL:O	2.16	0.45
3:F:188:GLN:HG3	3:F:195:TYR:CZ	2.51	0.45
1:B:330:GLY:CA	3:D:98:ARG:HH12	2.30	0.45
1:B:555:GLN:HE21	1:B:827:THR:HB	1.81	0.45
1:B:749:LEU:HG	1:B:751:VAL:HG23	1.99	0.45
1:B:1019:LEU:HG	1:B:1252:VAL:HG21	1.98	0.45
1:B:1226:HIS:CE1	1:B:1251:LYS:HA	2.52	0.45
1:A:12:TYR:CE1	3:D:70:TYR:HB2	2.51	0.45
1:A:108:PHE:HZ	1:A:131:TRP:CE2	2.34	0.45
2:E:41:GLN:NE2	2:E:45:LYS:O	2.41	0.45
2:E:124:LYS:NZ	2:E:151:ASP:HB3	2.32	0.45
2:E:185:LEU:HD23	2:E:186:SER:N	2.32	0.45
3:F:135:PRO:HB2	3:F:158:LEU:HD12	1.99	0.45
1:B:1157:ALA:HA	1:B:1160:LEU:HD12	1.99	0.44
1:B:1277:ALA:HB2	1:B:1285:LEU:HD13	1.99	0.44
1:A:560:PHE:CE1	1:A:829:LEU:HD23	2.51	0.44
1:A:1110:GLU:HB2	1:A:1113:LEU:HD21	2.00	0.44
3:D:135:PRO:HB2	3:D:158:LEU:HD12	1.99	0.44
3:F:80:PRO:HB2	3:F:82:ARG:HG3	1.98	0.44
1:A:33:GLU:O	1:A:220:ARG:NE	2.50	0.44
1:A:334:ILE:HD13	1:A:359:TYR:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:87:GLY:HA3	3:D:92:PHE:HD1	1.82	0.44
1:B:42:CYS:HB3	1:B:389:ILE:HD13	2.00	0.44
1:B:966:ARG:HA	1:B:969:LEU:HB2	1.99	0.44
1:B:114:ARG:HH12	1:B:173:GLY:H	1.66	0.44
1:A:688:MET:N	1:A:689:PRO:HD2	2.32	0.44
1:A:987:ARG:NH1	1:A:1239:LEU:O	2.51	0.44
2:C:185:LEU:HD23	2:C:186:SER:N	2.32	0.44
1:B:81:HIS:CD2	1:B:82:PRO:HD2	2.52	0.44
1:B:243:ASP:HB3	1:A:176:MET:SD	2.57	0.44
1:B:1075:ALA:HB2	1:B:1082:TRP:HD1	1.82	0.44
1:A:1159:TRP:CD1	1:A:1345:CYS:HB2	2.52	0.44
2:E:102:ARG:HB3	2:E:108:ASP:OD1	2.16	0.44
3:F:87:GLY:HA3	3:F:92:PHE:HD1	1.82	0.44
1:B:555:GLN:NE2	1:B:827:THR:HB	2.33	0.44
1:B:780:GLY:H	1:B:795:PRO:HB2	1.82	0.44
1:B:1263:ARG:HA	1:B:1307:LEU:HD11	1.99	0.44
1:B:1298:LEU:O	1:B:1302:ARG:HG3	2.17	0.44
1:B:1337:ILE:HG13	1:A:1365:ARG:CZ	2.47	0.44
1:A:103:ALA:HB1	1:A:905:ARG:HB3	1.99	0.44
1:A:992:GLU:HA	1:A:995:ARG:HE	1.83	0.44
2:E:13:LEU:HD13	2:E:117:THR:HB	1.99	0.44
1:B:92:GLN:NE2	1:B:94:GLY:O	2.51	0.44
1:B:324:LEU:HB3	1:B:329:LEU:O	2.17	0.44
1:B:362:ASP:OD1	1:B:362:ASP:N	2.50	0.44
1:A:216:CYS:O	1:A:220:ARG:HG2	2.18	0.44
1:A:296:GLY:HA3	1:A:327:SER:HB3	2.00	0.44
1:A:688:MET:HE1	1:A:760:VAL:HA	1.99	0.44
1:A:1076:LEU:HG	1:A:1376:GLN:HE22	1.83	0.44
3:D:189:ASP:OD2	3:D:192:ASP:HB3	2.17	0.44
1:B:108:PHE:HZ	1:B:131:TRP:CE2	2.35	0.44
1:B:110:GLY:O	1:B:111:MET:HE2	2.18	0.44
1:B:115:GLU:O	1:B:119:VAL:HG23	2.18	0.44
1:B:299:VAL:HG12	1:A:197:PRO:HA	2.00	0.44
1:B:322:GLN:HE22	1:A:223:GLU:HG3	1.83	0.44
1:B:731:GLU:HG2	1:B:734:ARG:HH11	1.83	0.44
1:A:41:ALA:HB2	1:A:133:VAL:HB	1.98	0.44
1:A:103:ALA:HB1	1:A:905:ARG:HD3	2.00	0.44
1:A:1222:SER:HA	1:A:1267:LEU:HA	1.98	0.44
1:A:1302:ARG:NH2	1:A:1307:LEU:HB3	2.33	0.44
2:E:3:GLU:HG3	2:E:5:GLN:NE2	2.33	0.44
1:B:35:VAL:HA	1:B:279:ARG:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:HIS:HD2	1:B:836:ILE:HG13	1.83	0.44
1:A:58:LEU:HD13	1:A:390:LYS:HG3	2.00	0.44
1:A:103:ALA:HA	1:A:906:GLU:O	2.18	0.44
1:A:748:ARG:NH2	1:A:752:ASP:HB3	2.32	0.44
1:A:802:TYR:HA	1:A:805:ARG:HE	1.82	0.44
1:A:834:HIS:HA	1:A:858:LEU:O	2.18	0.44
1:A:841:ILE:HA	1:A:844:ILE:HB	1.99	0.44
1:A:906:GLU:HG2	1:A:907:ARG:H	1.83	0.44
2:C:110:TRP:CE2	3:D:65:PRO:HB2	2.53	0.44
3:F:189:ASP:OD2	3:F:192:ASP:HB3	2.17	0.44
1:B:175:LEU:HB2	1:A:243:ASP:OD2	2.17	0.43
1:B:475:TRP:CE2	1:B:526:PRO:HG3	2.53	0.43
1:B:787:THR:HB	1:B:811:VAL:HG13	2.00	0.43
1:B:1333:ARG:HG2	1:A:1127:ARG:HH12	1.82	0.43
1:A:337:VAL:HG23	1:A:367:LEU:HD11	2.00	0.43
1:A:1005:SER:OG	1:A:1043:LEU:HD11	2.18	0.43
3:D:20:MET:HB3	3:D:22:GLN:HE22	1.83	0.43
1:B:120:ASP:HB2	1:B:178:GLY:O	2.17	0.43
1:B:627:VAL:HG22	1:B:631:MET:HG2	2.00	0.43
1:A:60:GLU:OE2	1:A:62:ARG:NH2	2.51	0.43
1:A:317:VAL:HG13	1:A:358:ALA:HB2	1.99	0.43
1:A:559:VAL:HG21	1:A:825:TYR:HB3	2.00	0.43
1:A:1086:VAL:HA	1:A:1113:LEU:HB2	1.99	0.43
1:A:1096:LEU:HD22	1:A:1100:LEU:HD11	1.99	0.43
1:A:1147:GLY:HA2	1:A:1172:SER:HB3	2.00	0.43
1:B:2:ALA:HB3	1:B:8:LYS:HE2	2.00	0.43
1:B:55:TRP:CZ3	1:B:401:PRO:HG3	2.53	0.43
1:B:157:PRO:HG3	1:A:181:THR:H	1.83	0.43
1:B:182:SER:HB2	1:A:202:ASP:OD1	2.18	0.43
1:B:434:ARG:HE	1:B:434:ARG:HB3	1.61	0.43
1:B:705:ARG:CZ	1:B:714:ILE:HD12	2.48	0.43
1:B:834:HIS:O	1:B:836:ILE:HD12	2.17	0.43
1:B:1272:LEU:HD23	1:B:1295:LEU:HD22	2.00	0.43
1:A:42:CYS:HB2	1:A:44:LEU:CD2	2.48	0.43
2:C:149:VAL:CG1	2:C:205:VAL:HG11	2.48	0.43
1:B:1229:ALA:HB1	1:B:1288:TYR:HE1	1.83	0.43
1:A:569:TRP:CZ3	1:A:861:GLY:HA2	2.54	0.43
1:A:1302:ARG:NH1	1:A:1308:PRO:O	2.39	0.43
2:E:8:GLN:HB2	2:E:112:GLN:HE22	1.84	0.43
1:B:7:GLU:O	1:B:11:GLU:N	2.47	0.43
1:A:589:GLU:HA	1:A:592:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1350:ASN:C	1:A:1350:ASN:HD22	2.26	0.43
1:B:12:TYR:CE1	3:F:70:TYR:HB2	2.52	0.43
1:B:206:SER:O	1:B:207:SER:C	2.61	0.43
1:B:663:ALA:HB2	1:B:798:LEU:HD21	2.00	0.43
1:A:283:ALA:HB1	1:A:288:HIS:HB2	1.99	0.43
1:A:320:ILE:HA	1:A:451:HIS:CD2	2.54	0.43
1:A:462:GLU:O	1:A:465:ARG:HG2	2.19	0.43
1:A:652:VAL:HG21	1:A:666:ALA:HB2	2.00	0.43
1:A:1227:ALA:HB2	1:A:1273:PHE:HD2	1.83	0.43
3:D:152:ALA:HB3	3:D:203:LEU:HB3	2.01	0.43
1:A:133:VAL:HG11	1:A:228:MET:HE1	2.00	0.43
1:A:155:LEU:HD11	1:A:184:ALA:HB3	2.00	0.43
1:A:563:PRO:HB2	1:A:567:TRP:CD1	2.54	0.43
1:A:619:LEU:HD23	1:A:622:GLU:HB2	2.00	0.43
1:A:781:PHE:CD2	1:A:782:VAL:HG12	2.53	0.43
1:B:98:LEU:HD11	1:B:271:GLY:HA2	2.00	0.43
1:B:472:VAL:HG21	1:B:866:ALA:HA	2.01	0.43
1:B:652:VAL:HG11	1:B:662:ALA:HA	1.99	0.43
1:B:1227:ALA:HB2	1:B:1273:PHE:HD2	1.84	0.43
1:A:470:ASP:OD2	1:A:471:VAL:HG12	2.18	0.43
1:A:498:GLU:HG3	1:A:499:HIS:CE1	2.54	0.43
1:A:560:PHE:CG	1:A:649:PRO:HB3	2.54	0.43
1:A:1274:SER:HB2	1:A:1292:ASN:HB3	2.00	0.43
1:B:205:CYS:HB3	1:B:378:HIS:NE2	2.29	0.43
1:B:390:LYS:HG2	1:B:391:MET:HE2	2.00	0.43
1:A:34:PRO:HB2	1:A:280:LEU:HB2	2.01	0.43
1:B:1031:VAL:O	1:B:1035:VAL:HG23	2.19	0.43
1:B:1147:GLY:N	1:B:1171:VAL:O	2.51	0.43
1:B:1152:VAL:HA	1:B:1317:TRP:CZ2	2.53	0.43
1:A:169:GLU:HG2	1:A:170:GLY:N	2.34	0.43
2:C:3:GLU:HG3	2:C:5:GLN:NE2	2.33	0.43
2:C:8:GLN:HB2	2:C:112:GLN:HE22	1.83	0.43
2:C:13:LEU:HD13	2:C:117:THR:HB	2.00	0.43
2:E:36:MET:HE3	2:E:36:MET:HA	2.01	0.43
3:F:152:ALA:HB3	3:F:203:LEU:HB3	2.01	0.43
1:B:2:ALA:CA	1:B:7:GLU:HB2	2.49	0.42
1:B:42:CYS:HA	1:B:273:GLY:HA2	2.00	0.42
1:B:57:LEU:HD12	1:B:62:ARG:HB2	2.00	0.42
1:B:188:ILE:HD12	1:B:188:ILE:H	1.84	0.42
1:B:429:TRP:HH2	1:B:438:ALA:HB2	1.83	0.42
1:B:1302:ARG:NH1	1:B:1308:PRO:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:THR:O	1:A:1257:ASN:ND2	2.52	0.42
1:A:1327:VAL:HA	1:A:1330:ARG:HD2	2.01	0.42
2:C:108:ASP:HA	3:D:67:LEU:HB2	2.01	0.42
1:B:950:LEU:HD13	1:B:979:LEU:HD22	2.01	0.42
1:B:1030:LEU:HD23	1:B:1034:MET:SD	2.59	0.42
1:A:255:ARG:HG2	1:A:405:HIS:NE2	2.34	0.42
1:A:1125:TRP:N	1:A:1381:LEU:O	2.47	0.42
2:C:211:ASN:HA	2:C:213:LYS:HE3	2.01	0.42
2:E:211:ASN:HA	2:E:213:LYS:HE3	2.01	0.42
1:B:104:PHE:O	1:B:106:PRO:HD3	2.20	0.42
1:B:209:LEU:HD12	1:B:209:LEU:HA	1.84	0.42
1:B:1028:LEU:HD21	1:B:1070:VAL:HG21	2.00	0.42
1:A:68:LEU:HD22	1:A:74:TRP:HZ3	1.84	0.42
1:A:333:ASP:O	1:A:434:ARG:NH1	2.52	0.42
1:A:564:GLY:N	1:A:655:HIS:HB3	2.35	0.42
1:B:29:GLU:HA	1:B:33:GLU:HB2	2.02	0.42
1:B:257:LYS:HG3	1:B:405:HIS:HB3	2.02	0.42
1:B:483:GLU:OE1	1:B:486:ARG:NH2	2.50	0.42
1:B:711:ARG:NH1	1:B:758:SER:OG	2.52	0.42
1:B:765:ASP:OD1	1:B:765:ASP:N	2.52	0.42
1:A:613:ARG:NH2	1:A:620:SER:HG	2.16	0.42
1:A:1075:ALA:HB1	1:A:1377:ARG:HD3	2.01	0.42
1:A:1096:LEU:HA	1:A:1100:LEU:HG	2.01	0.42
1:A:1282:ALA:HB1	1:A:1285:LEU:HD12	2.01	0.42
2:E:6:LEU:HD23	2:E:6:LEU:HA	1.95	0.42
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.93	0.42
1:B:764:ARG:HE	1:B:768:HIS:CD2	2.37	0.42
1:A:226:LEU:HD21	1:A:276:LEU:HD11	2.00	0.42
1:A:608:ALA:HA	1:A:612:ARG:HE	1.85	0.42
1:A:1108:ALA:C	1:A:1380:ARG:HH12	2.26	0.42
1:B:126:MET:HG3	1:B:153:VAL:HG11	2.00	0.42
1:B:1131:PRO:N	1:B:1354:ARG:HH22	2.18	0.42
1:B:1239:LEU:HD22	1:B:1244:ILE:HG13	2.01	0.42
1:A:335:ASP:OD2	1:A:434:ARG:NH2	2.52	0.42
3:D:107:TYR:CD1	3:D:126:VAL:HG21	2.55	0.42
1:B:331:PRO:HA	1:B:359:TYR:HD1	1.84	0.42
1:B:970:GLU:HA	1:B:974:ALA:O	2.20	0.42
1:B:1078:ASN:CG	1:B:1081:VAL:HB	2.44	0.42
1:A:257:LYS:HD2	1:A:405:HIS:HB3	2.01	0.42
1:A:476:VAL:O	1:A:511:LEU:HG	2.19	0.42
1:A:568:GLN:HA	1:A:572:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:VAL:O	1:A:708:ILE:HG23	2.18	0.42
1:A:721:ARG:HH22	1:A:846:ASP:H	1.68	0.42
1:A:1298:LEU:O	1:A:1302:ARG:HG3	2.19	0.42
2:C:36:MET:HE3	2:C:36:MET:HA	2.01	0.42
2:C:174:PRO:HD3	3:D:186:THR:HG23	2.01	0.42
2:E:204:ASN:N	2:E:204:ASN:OD1	2.53	0.42
1:B:297:THR:HG23	1:B:452:ALA:HB2	2.01	0.42
1:B:562:PHE:CD2	1:B:635:MET:HE3	2.55	0.42
1:B:705:ARG:HA	1:B:705:ARG:HD3	1.83	0.42
1:A:69:PRO:HG2	1:A:72:ARG:NH2	2.33	0.42
1:A:151:VAL:HA	1:A:228:MET:HB3	2.02	0.42
1:A:580:SER:HB3	1:A:865:LEU:HD22	2.00	0.42
1:A:913:LYS:N	1:A:914:PRO:HD3	2.34	0.42
1:A:1103:VAL:HG13	1:A:1113:LEU:HG	2.02	0.42
2:C:129:PHE:O	2:C:148:LEU:N	2.52	0.42
3:F:171:LYS:HA	3:F:171:LYS:HD3	1.92	0.42
1:B:232:VAL:HG23	1:B:272:ALA:HB2	2.02	0.42
1:B:1143:VAL:HG11	1:B:1160:LEU:CD1	2.48	0.42
1:A:86:ARG:HB3	1:A:89:THR:OG1	2.20	0.42
1:A:555:GLN:O	1:A:557:ARG:HG2	2.19	0.42
1:A:605:PHE:CD2	1:A:630:VAL:HG11	2.55	0.42
1:A:978:GLU:OE1	1:A:978:GLU:N	2.52	0.42
3:F:137:VAL:HG22	3:F:158:LEU:HD11	2.01	0.42
1:B:329:LEU:C	3:D:98:ARG:HH12	2.28	0.42
1:B:1096:LEU:HD22	1:B:1100:LEU:HD11	2.02	0.42
1:A:302:ASP:O	1:A:312:ASN:ND2	2.53	0.42
1:A:378:HIS:CD2	1:A:380:GLN:H	2.38	0.42
1:A:619:LEU:HB3	1:A:623:ARG:HG2	2.00	0.42
1:A:1009:VAL:HA	1:A:1048:GLU:OE1	2.19	0.42
1:A:1034:MET:HE2	1:A:1034:MET:HB2	1.60	0.42
1:B:834:HIS:CD2	1:B:836:ILE:HG13	2.55	0.41
1:B:1162:ARG:HG2	1:B:1191:LEU:HD22	2.02	0.41
1:A:935:ARG:HB2	1:A:1124:ARG:HG3	2.02	0.41
1:A:1366:TRP:HE1	1:A:1382:PHE:HD1	1.66	0.41
1:B:131:TRP:HE1	1:B:901:TYR:HB2	1.85	0.41
1:B:385:VAL:HA	1:B:388:VAL:HG12	2.01	0.41
1:B:512:ALA:HB1	1:B:884:TRP:CG	2.55	0.41
1:B:1222:SER:HB3	1:B:1268:THR:HG22	2.01	0.41
1:A:38:VAL:HB	1:A:276:LEU:HD23	2.01	0.41
1:A:435:PRO:HA	1:A:456:GLU:OE2	2.20	0.41
1:A:731:GLU:O	1:A:735:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:VAL:HG13	1:A:1347:ALA:HA	2.02	0.41
2:C:17:GLY:N	2:C:90:LEU:O	2.53	0.41
2:E:41:GLN:O	2:E:96:ALA:HB1	2.21	0.41
1:B:114:ARG:CZ	1:B:172:GLU:H	2.33	0.41
1:B:156:ILE:HG22	1:B:158:GLN:HG2	2.02	0.41
1:B:475:TRP:CD1	1:B:508:ALA:HB2	2.54	0.41
1:B:853:SER:HB3	1:B:878:ALA:HB1	2.02	0.41
1:B:1096:LEU:HA	1:B:1100:LEU:HG	2.00	0.41
1:A:43:ARG:HD2	1:A:100:GLU:HG3	2.02	0.41
1:A:311:PRO:HG2	1:A:350:ILE:HD12	2.01	0.41
1:A:572:MET:O	1:A:606:LEU:HB2	2.21	0.41
1:A:953:LYS:HA	1:A:1007:LEU:HB3	2.02	0.41
3:D:164:ARG:HE	3:D:185:VAL:HG11	1.85	0.41
2:E:39:VAL:O	2:E:99:TYR:N	2.37	0.41
1:B:82:PRO:HG2	1:A:1308:PRO:HG3	2.02	0.41
1:B:131:TRP:HB3	1:B:903:PHE:HZ	1.86	0.41
1:B:242:VAL:O	1:B:246:ARG:NH1	2.54	0.41
1:A:74:TRP:CD1	1:A:238:PRO:HD3	2.56	0.41
1:A:503:ASP:O	1:A:507:ILE:HG12	2.20	0.41
1:A:604:PRO:HB3	1:A:607:ARG:HH21	1.85	0.41
2:C:159:VAL:HG13	2:C:205:VAL:HG22	2.02	0.41
3:F:23:SER:HA	3:F:24:PRO:HD2	1.93	0.41
1:B:125:LEU:O	1:B:129:LEU:HD23	2.20	0.41
1:B:506:ASP:HB3	1:B:896:VAL:HG21	2.02	0.41
1:B:605:PHE:CD2	1:B:630:VAL:HG11	2.55	0.41
1:B:763:ILE:O	1:B:763:ILE:HG22	2.20	0.41
1:B:992:GLU:HA	1:B:995:ARG:HE	1.85	0.41
1:B:1013:GLU:HB2	1:B:1061:ASN:HD21	1.86	0.41
1:B:1059:VAL:O	1:B:1301:GLN:NE2	2.54	0.41
1:A:176:MET:SD	1:A:176:MET:N	2.94	0.41
1:A:340:HIS:CD2	1:A:443:PHE:H	2.39	0.41
1:A:597:HIS:CE1	1:A:676:ARG:HB2	2.56	0.41
1:A:610:ALA:HA	1:A:613:ARG:HE	1.84	0.41
1:A:737:ALA:HA	1:A:740:THR:HG22	2.02	0.41
2:E:17:GLY:N	2:E:90:LEU:O	2.53	0.41
1:B:43:ARG:HH21	1:B:905:ARG:NH2	2.18	0.41
1:B:219:LEU:O	1:B:279:ARG:NH1	2.53	0.41
1:B:228:MET:HE3	1:B:274:MET:HE2	2.03	0.41
1:B:302:ASP:N	1:B:447:GLY:O	2.49	0.41
1:B:603:ILE:HD13	1:B:606:LEU:HD12	2.03	0.41
1:B:609:GLU:O	1:B:613:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:LEU:HD13	1:B:1288:TYR:HB2	2.03	0.41
1:A:102:THR:HG22	1:A:909:TRP:CD2	2.56	0.41
1:A:994:LEU:HA	1:A:997:VAL:HG12	2.01	0.41
3:D:137:VAL:HG22	3:D:158:LEU:HD11	2.02	0.41
2:E:159:VAL:HG13	2:E:205:VAL:HG22	2.02	0.41
3:F:141:PRO:HB3	3:F:231:PHE:HB2	2.02	0.41
1:B:335:ASP:HB2	1:B:429:TRP:CZ2	2.56	0.41
1:B:406:ALA:HB1	1:B:422:LEU:HD21	2.02	0.41
1:B:683:ARG:HD2	1:B:770:GLU:HG2	2.03	0.41
1:B:704:VAL:HG21	1:B:723:VAL:HG11	2.03	0.41
1:A:30:LEU:O	1:A:220:ARG:HB3	2.21	0.41
1:A:312:ASN:HD22	1:A:315:ALA:HB2	1.85	0.41
1:A:400:LEU:HG	1:A:429:TRP:HB2	2.02	0.41
1:A:564:GLY:HA3	1:A:656:SER:OG	2.20	0.41
1:A:602:VAL:HG12	1:A:606:LEU:HD23	2.03	0.41
1:A:1125:TRP:HH2	1:A:1279:ALA:HB1	1.85	0.41
1:A:1313:ALA:HB3	1:A:1360:ILE:HG23	2.03	0.41
2:C:177:LEU:HD13	2:C:177:LEU:HA	1.93	0.41
3:F:156:CYS:HB3	3:F:168:VAL:HG11	2.02	0.41
1:B:313:GLY:O	1:B:317:VAL:HG23	2.21	0.41
1:B:476:VAL:HG11	1:B:884:TRP:CZ2	2.55	0.41
1:B:836:ILE:HG22	1:B:837:LEU:CD2	2.51	0.41
1:A:156:ILE:HD12	1:A:380:GLN:OE1	2.20	0.41
1:A:495:HIS:NE2	1:A:897:PRO:O	2.53	0.41
1:A:561:VAL:HA	1:A:653:ILE:HG23	2.02	0.41
2:C:26:ALA:HB1	2:C:29:PHE:CE1	2.56	0.41
3:F:21:THR:HG21	3:F:111:GLN:HB3	2.03	0.41
1:B:2:ALA:CB	1:B:7:GLU:HB2	2.51	0.41
1:B:256:CYS:SG	1:B:378:HIS:N	2.94	0.41
1:B:349:PRO:HA	1:B:413:ILE:HG12	2.03	0.41
1:B:605:PHE:HD2	1:B:630:VAL:HG11	1.86	0.41
1:B:1222:SER:HA	1:B:1267:LEU:HA	2.03	0.41
1:B:1340:PRO:HG2	1:A:1332:ARG:HH21	1.86	0.41
1:A:213:HIS:HB2	1:A:297:THR:HB	2.03	0.41
1:A:437:ARG:HG2	1:A:455:GLU:HG3	2.03	0.41
1:A:1048:GLU:O	1:A:1060:ARG:NE	2.54	0.41
2:C:21:ARG:HH22	2:C:84:TYR:HB3	1.86	0.41
3:D:141:PRO:HB3	3:D:231:PHE:HB2	2.02	0.41
2:E:37:SER:HB2	2:E:101:THR:OG1	2.20	0.41
1:B:330:GLY:HA3	3:D:98:ARG:HH12	1.86	0.41
1:A:929:ARG:HH22	1:A:1354:ARG:NH1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:LEU:O	1:A:1171:VAL:HG23	2.20	0.41
1:A:1204:ASP:HB3	1:A:1207:SER:HB3	2.02	0.41
1:A:1385:ILE:HB	1:A:1388:ALA:HB2	2.02	0.41
2:C:206:ASN:C	2:C:213:LYS:HZ3	2.29	0.41
3:D:170:TRP:CE3	3:D:201:LEU:HD22	2.56	0.41
1:B:121:PRO:HB2	1:B:234:VAL:CG1	2.50	0.40
1:A:568:GLN:HA	1:A:572:MET:CE	2.49	0.40
1:A:926:SER:HB3	1:A:1130:ALA:HB3	2.04	0.40
1:A:1337:ILE:HG23	1:A:1338:GLU:N	2.36	0.40
2:E:26:ALA:HB1	2:E:29:PHE:CE1	2.56	0.40
2:E:149:VAL:HG13	2:E:205:VAL:HG11	2.02	0.40
2:E:206:ASN:C	2:E:213:LYS:HZ3	2.29	0.40
1:B:26:ARG:HA	1:B:29:GLU:HG2	2.03	0.40
1:B:86:ARG:NH1	1:A:1135:ASP:OD2	2.47	0.40
1:B:595:GLU:HA	1:B:598:LEU:O	2.21	0.40
1:A:230:GLY:HA3	1:A:274:MET:HA	2.02	0.40
1:A:510:SER:HB3	1:A:895:ARG:HA	2.03	0.40
1:A:594:LEU:O	1:A:598:LEU:N	2.54	0.40
1:A:1110:GLU:OE2	1:A:1380:ARG:HD2	2.20	0.40
1:A:1115:LEU:HD22	1:A:1120:VAL:HG12	2.04	0.40
2:C:6:LEU:HD23	2:C:6:LEU:HA	1.95	0.40
2:C:37:SER:HB2	2:C:101:THR:OG1	2.21	0.40
2:C:204:ASN:OD1	2:C:204:ASN:N	2.53	0.40
2:E:36:MET:H	2:E:76:ARG:NH1	2.17	0.40
2:E:178:GLN:HE21	2:E:178:GLN:HB2	1.70	0.40
3:F:170:TRP:CE3	3:F:201:LEU:HD22	2.56	0.40
1:B:65:VAL:HG13	1:B:95:GLY:H	1.86	0.40
1:B:203:THR:OG1	1:B:207:SER:HA	2.21	0.40
1:B:1099:HIS:HB2	1:B:1115:LEU:HD13	2.03	0.40
1:A:312:ASN:HB3	1:A:315:ALA:HB3	2.02	0.40
1:A:495:HIS:CG	1:A:899:PRO:HD3	2.57	0.40
1:A:837:LEU:HD12	1:A:840:ALA:HB3	2.04	0.40
2:C:36:MET:H	2:C:76:ARG:NH1	2.18	0.40
1:B:157:PRO:HD2	1:A:180:THR:HG23	2.04	0.40
1:B:324:LEU:HD13	1:B:331:PRO:HD3	2.04	0.40
1:B:991:ALA:HA	1:B:994:LEU:HD12	2.04	0.40
1:B:1023:SER:HB2	1:B:1067:LEU:HD21	2.03	0.40
1:B:1227:ALA:HB2	1:B:1273:PHE:CD2	2.56	0.40
1:A:1019:LEU:HD23	1:A:1019:LEU:HA	1.93	0.40
1:A:1152:VAL:HG22	1:A:1317:TRP:CD1	2.57	0.40
3:D:171:LYS:HA	3:D:171:LYS:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:TYR:O	1:B:363:ARG:HG2	2.20	0.40
1:B:823:GLN:C	1:B:825:TYR:H	2.30	0.40
1:B:855:ILE:HG23	1:B:874:ARG:HG3	2.02	0.40
1:A:1371:LEU:HD12	1:A:1371:LEU:HA	1.83	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	1388/1784 (78%)	1303 (94%)	85 (6%)	0	100	100
1	B	1419/1784 (80%)	1353 (95%)	66 (5%)	0	100	100
2	C	199/249 (80%)	186 (94%)	13 (6%)	0	100	100
2	E	199/249 (80%)	187 (94%)	12 (6%)	0	100	100
3	D	200/236 (85%)	182 (91%)	18 (9%)	0	100	100
3	F	200/236 (85%)	183 (92%)	17 (8%)	0	100	100
All	All	3605/4538 (79%)	3394 (94%)	211 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1028/1325 (78%)	1003 (98%)	25 (2%)	43 63
1	B	1047/1325 (79%)	1015 (97%)	32 (3%)	35 56
2	C	170/203 (84%)	162 (95%)	8 (5%)	23 47
2	E	170/203 (84%)	162 (95%)	8 (5%)	23 47
3	D	182/208 (88%)	151 (83%)	31 (17%)	2 12
3	F	182/208 (88%)	156 (86%)	26 (14%)	3 16
All	All	2779/3472 (80%)	2649 (95%)	130 (5%)	25 47

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	4	THR
1	B	6	SER
1	B	7	GLU
1	B	8	LYS
1	B	159	GLU
1	B	163	ARG
1	B	199	ILE
1	B	200	SER
1	B	203	THR
1	B	207	SER
1	B	208	SER
1	B	212	VAL
1	B	214	LEU
1	B	557	ARG
1	B	577	LEU
1	B	653	ILE
1	B	774	ASP
1	B	818	ARG
1	B	820	LEU
1	B	822	GLU
1	B	1142	THR
1	B	1144	LEU
1	B	1145	VAL
1	B	1317	TRP
1	B	1322	MET
1	B	1327	VAL
1	B	1329	ASP
1	B	1333	ARG
1	B	1337	ILE

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Mol	Chain	Res	Type
1	B	1407	LEU
1	B	1412	ARG
1	A	174	TYR
1	A	175	LEU
1	A	176	MET
1	A	177	THR
1	A	777	PRO
1	A	778	LEU
1	A	796	ASP
1	A	799	ASP
1	A	843	GLU
1	A	844	ILE
1	A	870	GLU
1	A	1030	LEU
1	A	1034	MET
1	A	1051	VAL
1	A	1053	THR
1	A	1057	GLU
1	A	1070	VAL
1	A	1244	ILE
1	A	1303	ARG
1	A	1332	ARG
1	A	1338	GLU
1	A	1364	VAL
1	A	1368	ARG
1	A	1371	LEU
1	A	1376	GLN
2	C	15	GLN
2	C	36	MET
2	C	45	LYS
2	C	56	LYS
2	C	131	LEU
2	C	150	LYS
2	C	177	LEU
2	C	178	GLN
3	D	19	VAL
3	D	20	MET
3	D	21	THR
3	D	22	GLN
3	D	23	SER
3	D	27	LEU
3	D	40	ARG

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Mol	Chain	Res	Type
3	D	55	ASP
3	D	60	LYS
3	D	73	SER
3	D	79	VAL
3	D	82	ARG
3	D	84	SER
3	D	99	VAL
3	D	104	VAL
3	D	111	GLN
3	D	112	SER
3	D	113	LEU
3	D	114	GLN
3	D	115	THR
3	D	117	ARG
3	D	118	LEU
3	D	119	THR
3	D	153	SER
3	D	167	LYS
3	D	183	GLU
3	D	185	VAL
3	D	186	THR
3	D	187	GLU
3	D	191	LYS
3	D	209	GLU
2	E	15	GLN
2	E	36	MET
2	E	45	LYS
2	E	56	LYS
2	E	91	LYS
2	E	131	LEU
2	E	177	LEU
2	E	178	GLN
3	F	20	MET
3	F	21	THR
3	F	22	GLN
3	F	23	SER
3	F	25	LEU
3	F	26	SER
3	F	27	LEU
3	F	40	ARG
3	F	41	SER
3	F	43	GLN

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Mol	Chain	Res	Type
3	F	54	LEU
3	F	79	VAL
3	F	81	ASP
3	F	82	ARG
3	F	84	SER
3	F	113	LEU
3	F	114	GLN
3	F	115	THR
3	F	117	ARG
3	F	118	LEU
3	F	119	THR
3	F	153	SER
3	F	167	LYS
3	F	182	GLN
3	F	191	LYS
3	F	209	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	300	ASN
1	B	375	ASN
1	B	405	HIS
1	B	555	GLN
1	B	1112	GLN
1	B	1226	HIS
1	B	1350	ASN
1	A	122	GLN
1	A	158	GLN
1	A	312	ASN
1	A	340	HIS
1	A	378	HIS
1	A	502	GLN
1	A	565	GLN
1	A	597	HIS
1	A	657	GLN
1	A	806	ASN
1	A	856	HIS
1	A	1112	GLN
1	A	1349	GLN
2	C	5	GLN
2	C	41	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	5	GLN
3	F	43	GLN
3	F	47	HIS
3	F	74	ASN
3	F	182	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

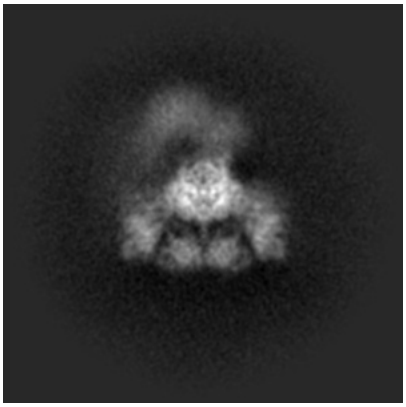
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23713. These allow visual inspection of the internal detail of the map and identification of artifacts.

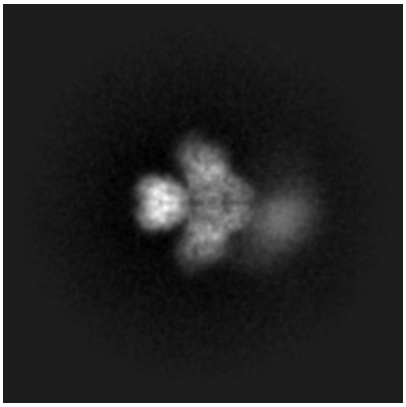
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

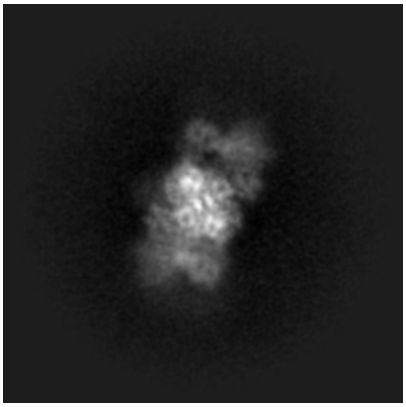
6.1.1 Primary map



X



Y

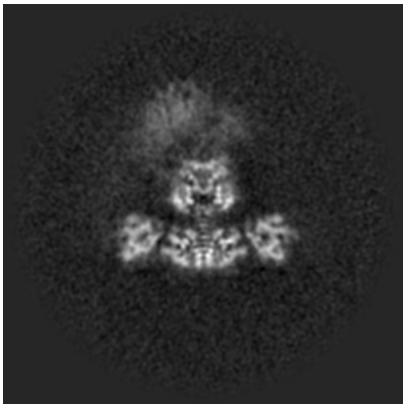


Z

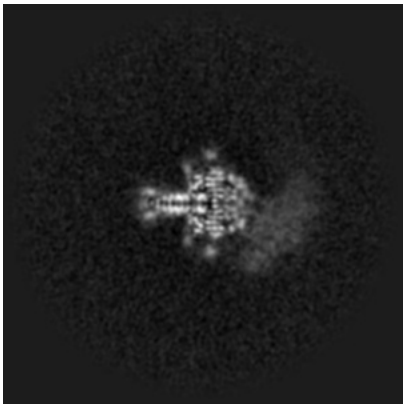
The images above show the map projected in three orthogonal directions.

6.2 Central slices

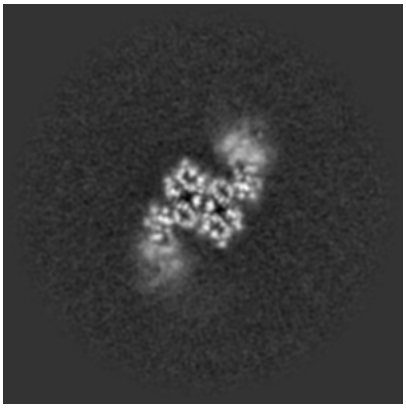
6.2.1 Primary map



X Index: 168



Y Index: 168

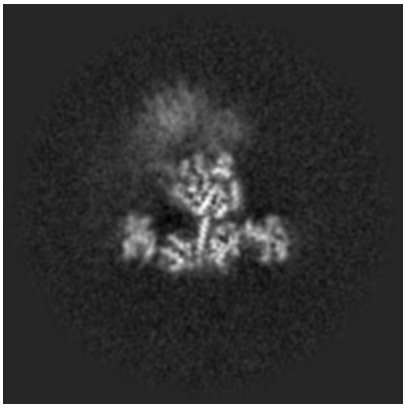


Z Index: 168

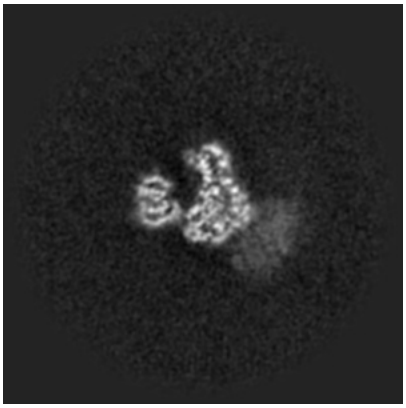
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

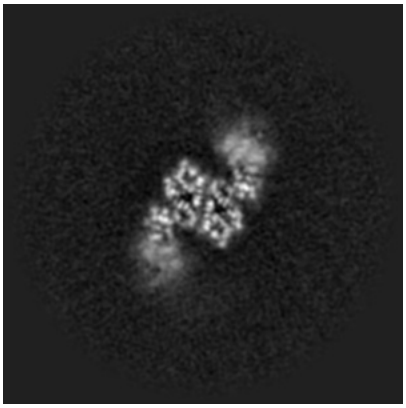
6.3.1 Primary map



X Index: 162



Y Index: 183

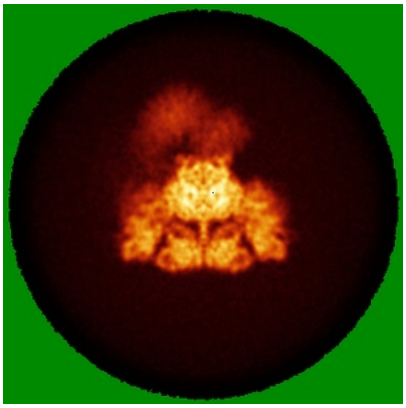


Z Index: 167

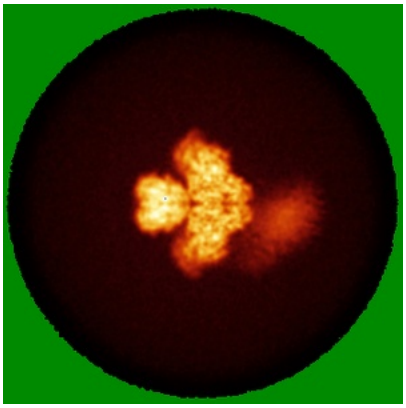
The images above show the largest variance slices of the map in three orthogonal directions.

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

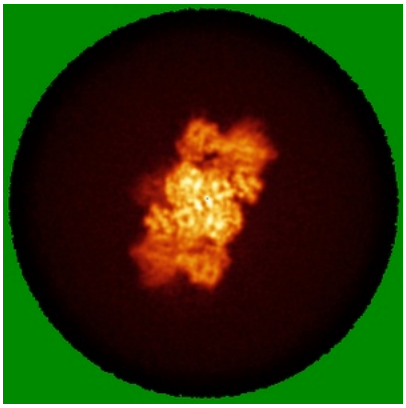
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

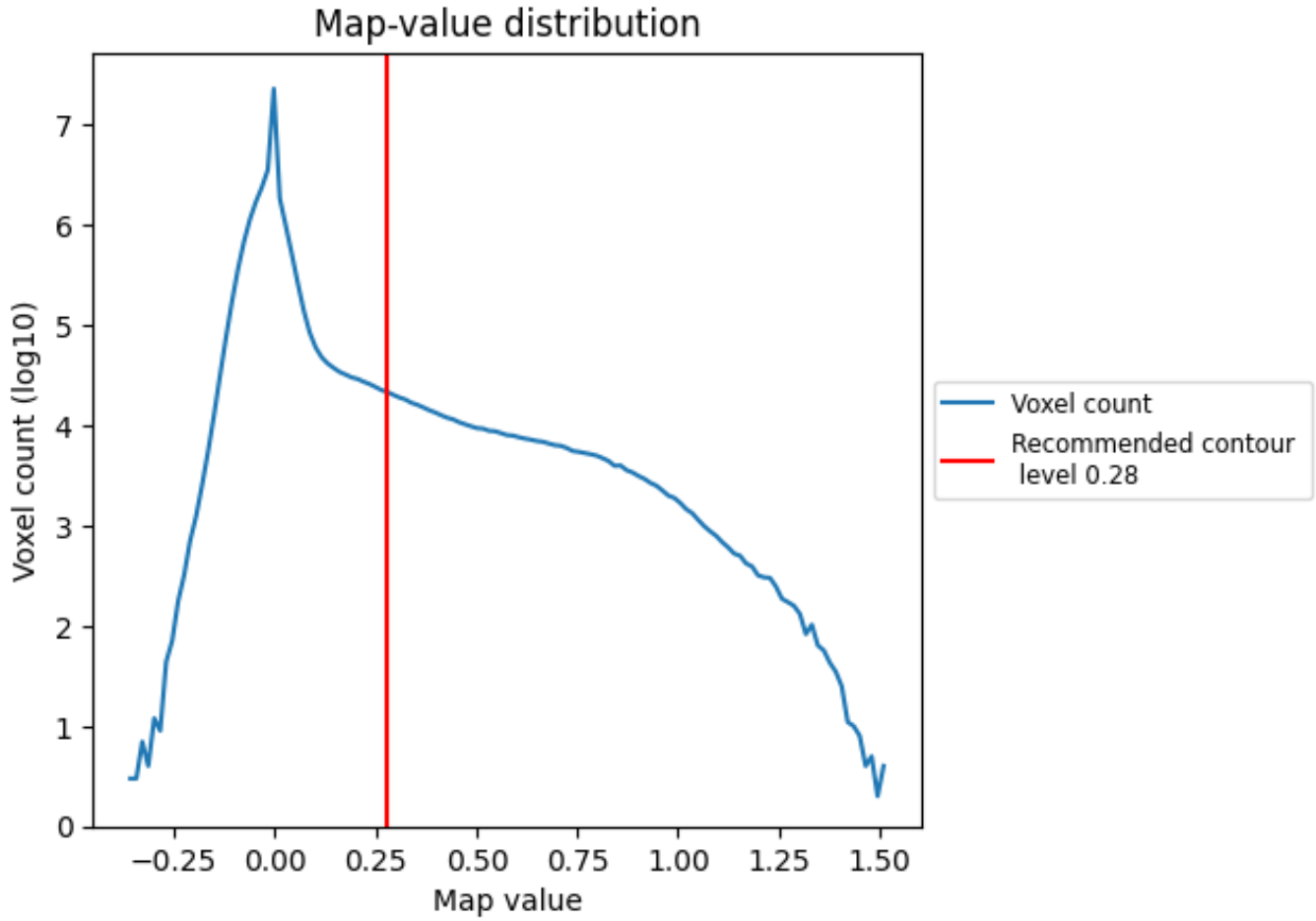
6.6 Mask visualisation (i)

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

7 Map analysis

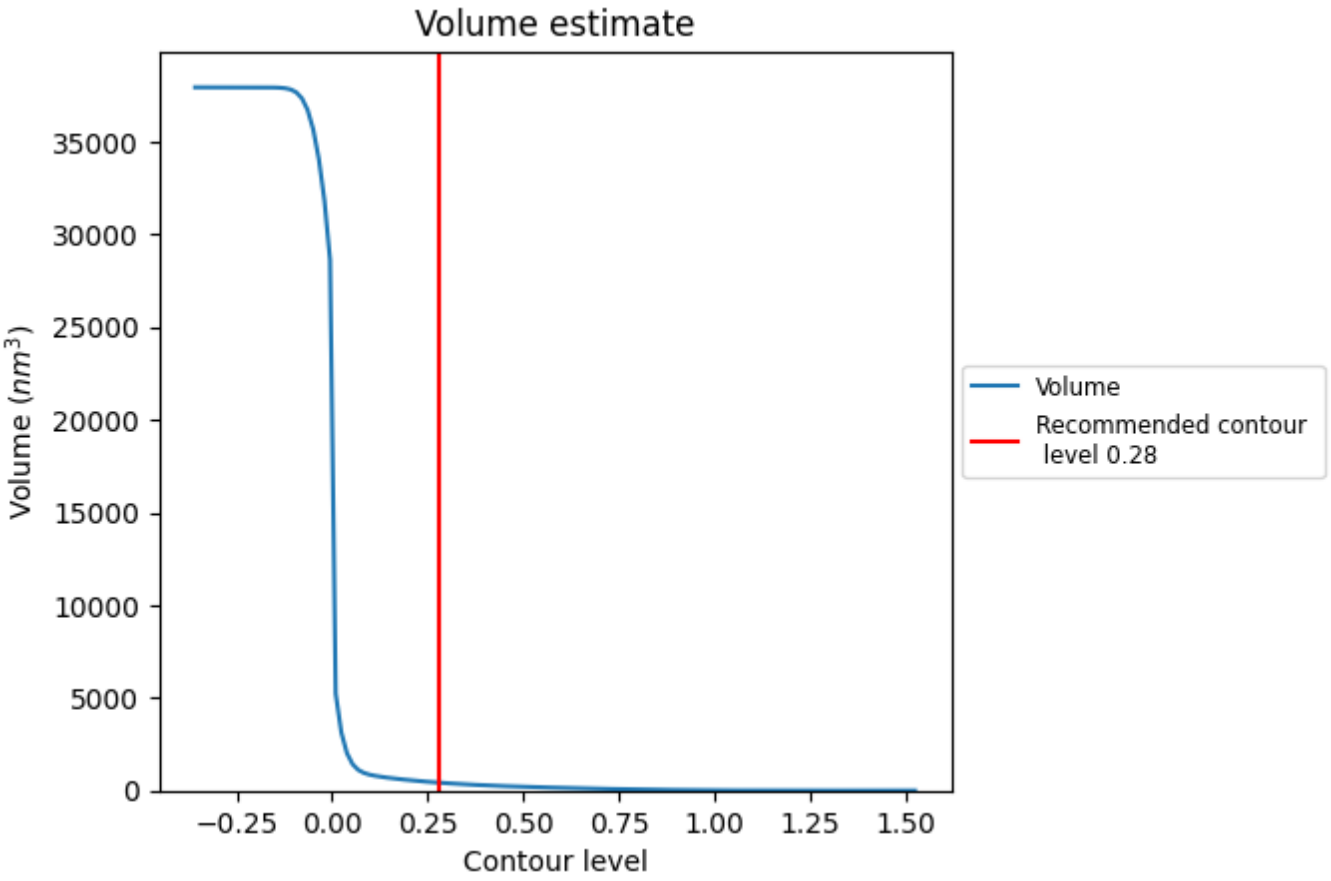
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

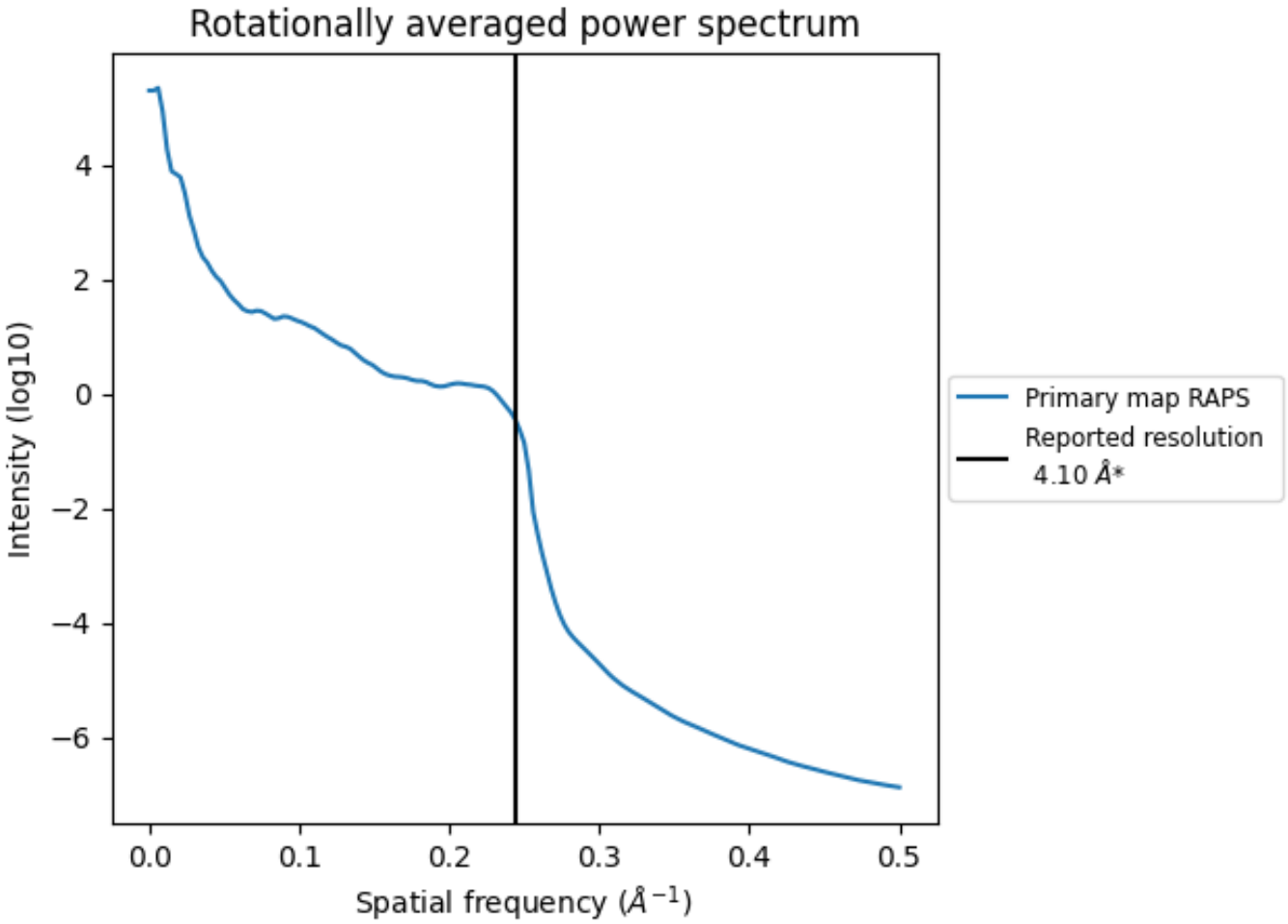
7.2 Volume estimate



The volume at the recommended contour level is 425 nm^3; this corresponds to an approximate mass of 384 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

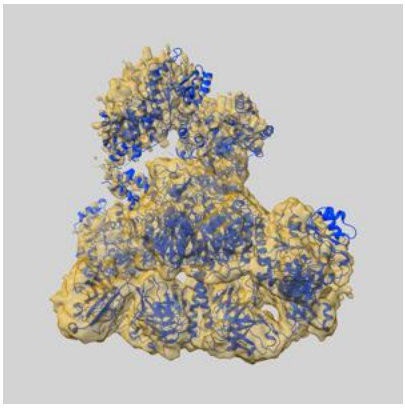
8 Fourier-Shell correlation (i)

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

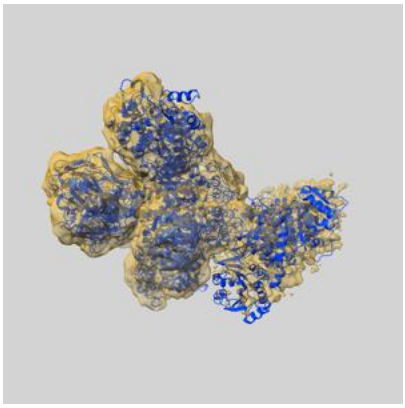
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23713 and PDB model 7M7H. Per-residue inclusion information can be found in section 3 on page 8.

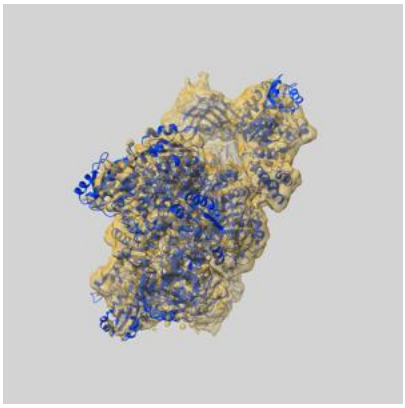
9.1 Map-model overlay



X



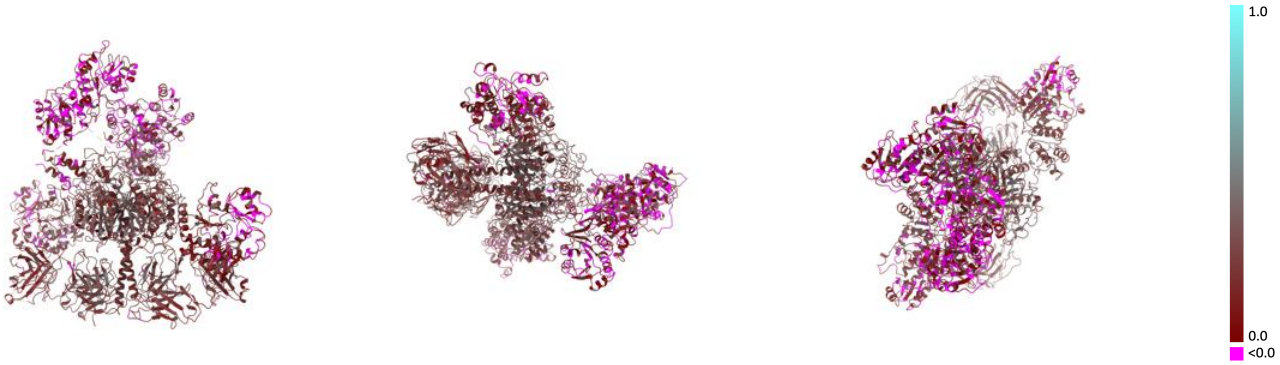
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28 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.

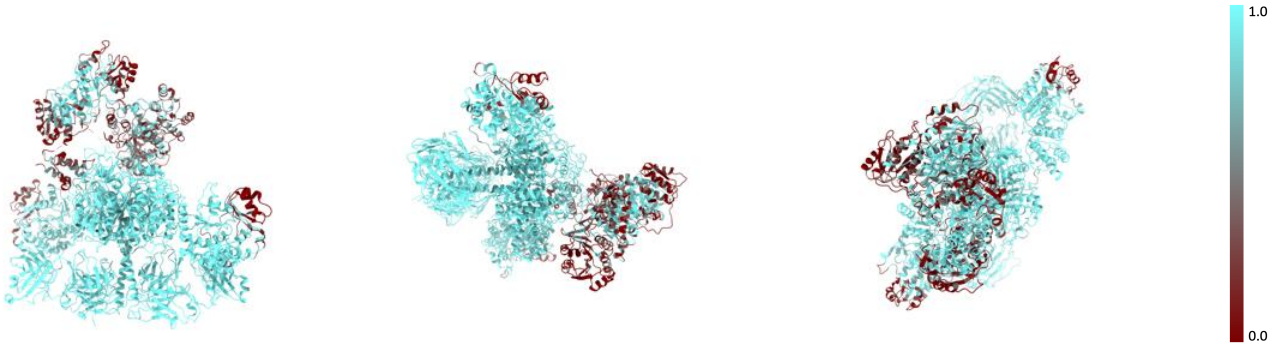
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

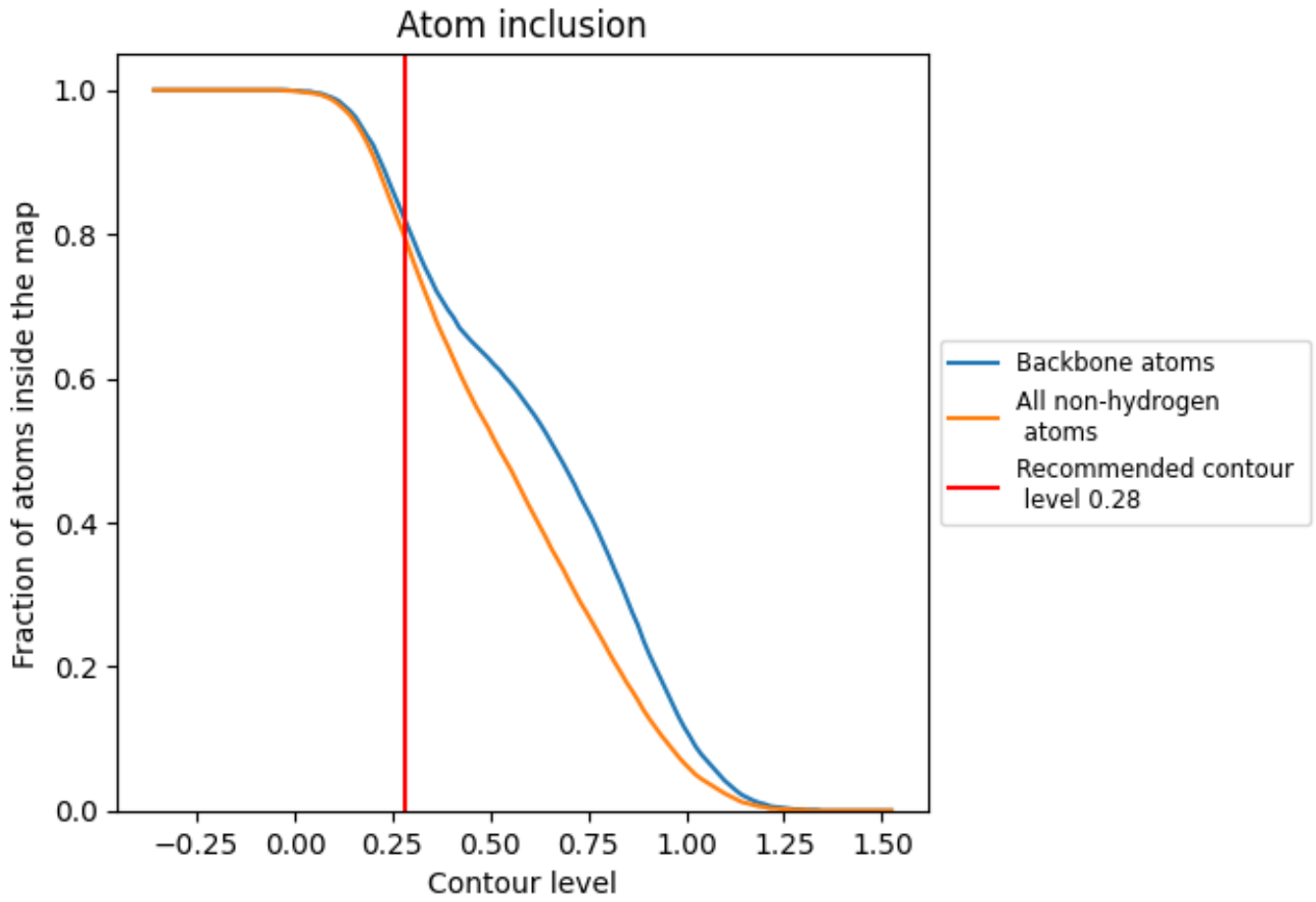
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.1900
A	0.7310	0.1780
B	0.7570	0.1670
C	0.9720	0.2360
D	0.9750	0.2620
E	0.9820	0.2410
F	0.9720	0.2610

