Full wwPDB EM Validation Report (i)

Apr 28, 2024 – 08:47 am BST

PDB ID	:	4CRM
EMDB ID	:	EMD-2598
Title	:	Cryo-EM of a pre-recycling complex with eRF1 and ABCE1
Authors	:	Preis, A.; Heuer, A.; Barrio-Garcia, C.; Hauser, A.; Eyler, D.; Berninghausen, O.; Green, R.; Becker, T.; Beckmann, R.
Deposited on	:	2014-02-28
Resolution	:	8.75 Å(reported)
Based on initial model	:	1DT9

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 (i) 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 (1)) were used in the production of this report:

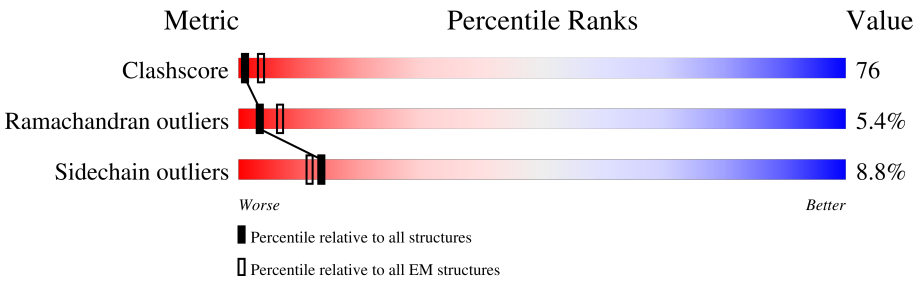
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.75 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 <=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	P	608	21% 31% 63% 5%
2	X	282	30% 44% 32% 16% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	P	1609	-	-	X	-
4	SF4	P	1610	-	-	X	-
4	SF4	P	1611	-	-	X	-
5	ADP	P	1612	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	P	1613	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7090 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.

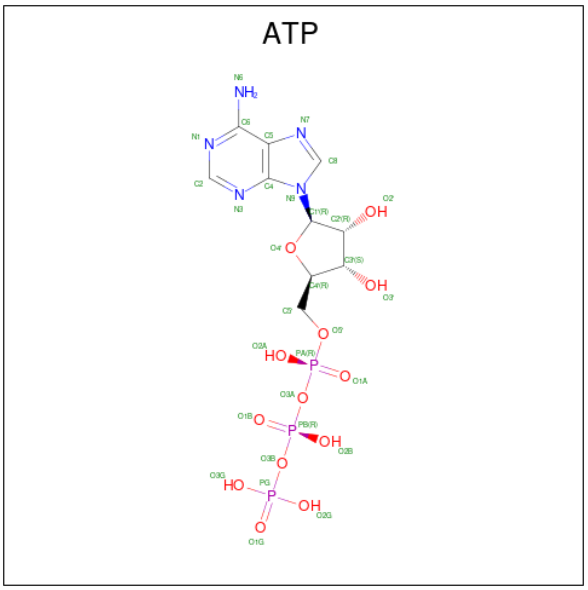
- Molecule 1 is a protein called TRANSLATION INITIATION FACTOR RLI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	P	608	4804	3065	831	884	24	0	0

- Molecule 2 is a protein called EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1.

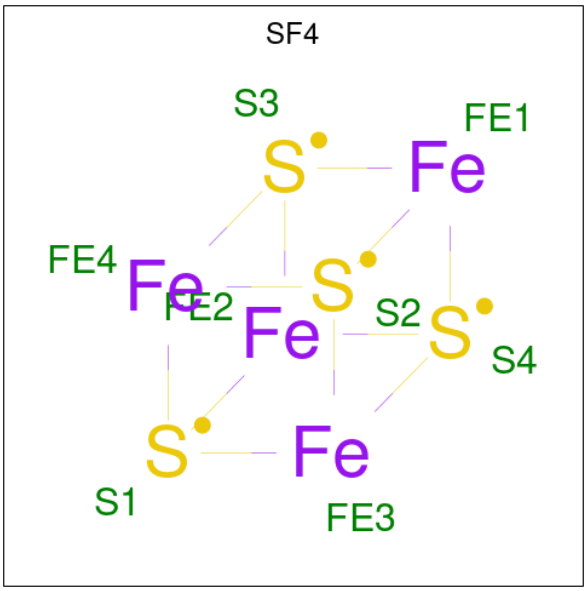
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	X	282	2210	1406	366	433	5	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



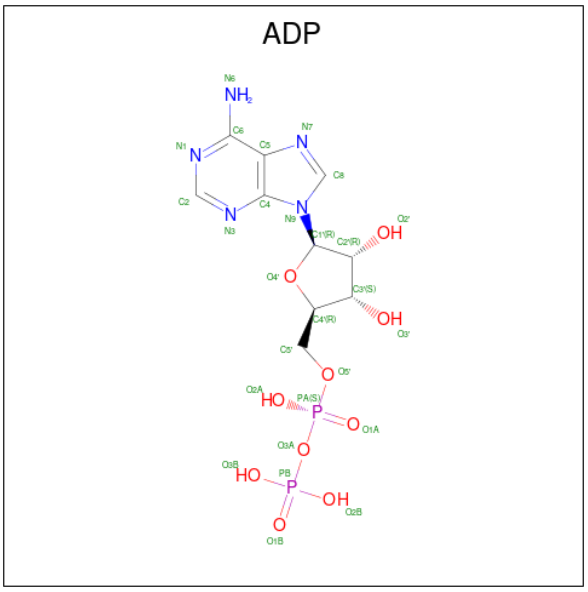
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	P	1	31	10	5	13	3	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
4	P	1	8	4	4	0
			Total	Fe	S	
4	P	1	8	4	4	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	P	1	27	10	5	10	2	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	P	1	1	1	0

- Molecule 7 is water.

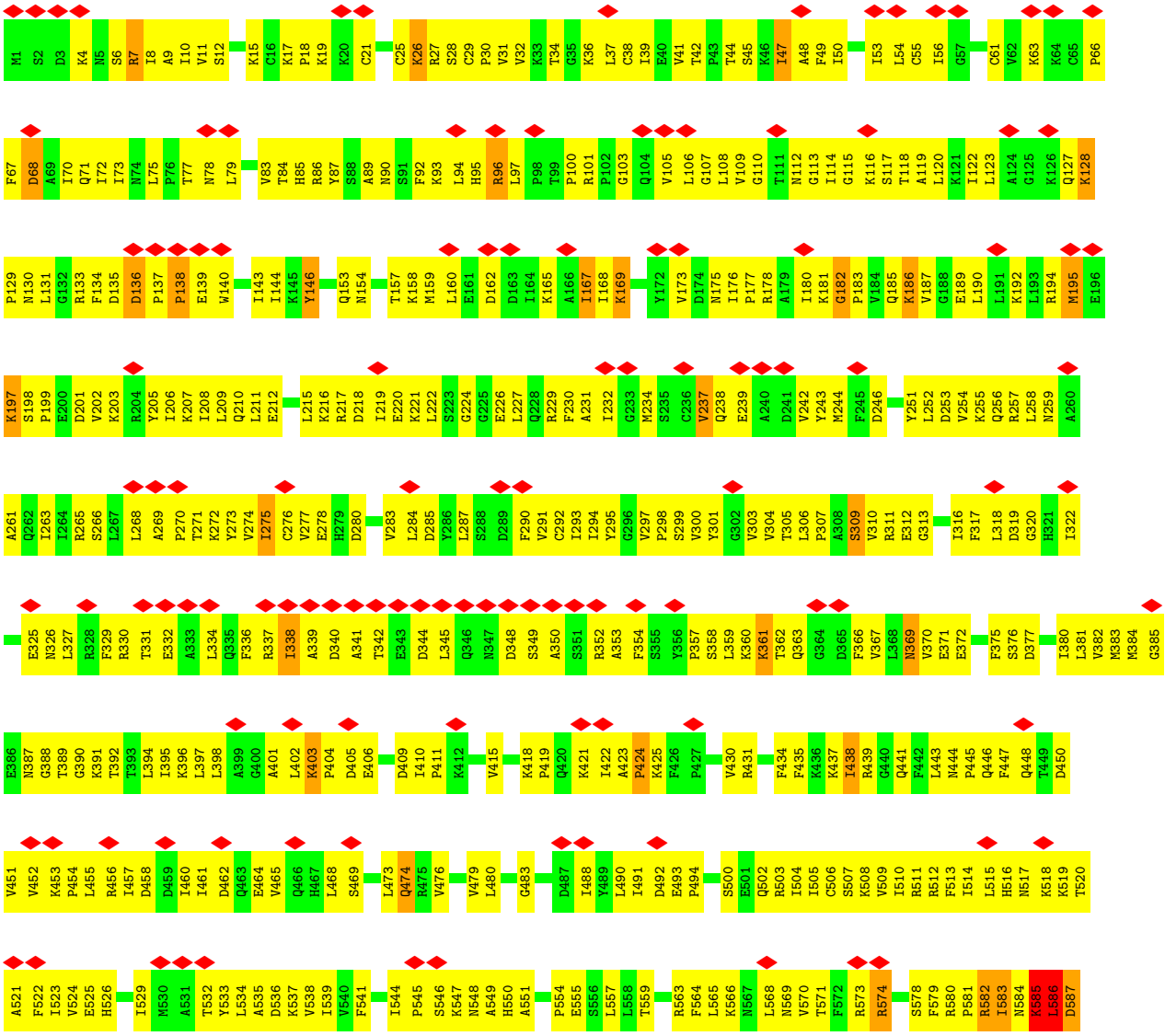
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
7	P	1	1	1	0

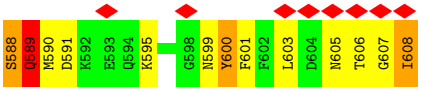
3 Residue-property plots (i)

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: TRANSLATION INITIATION FACTOR RLI1

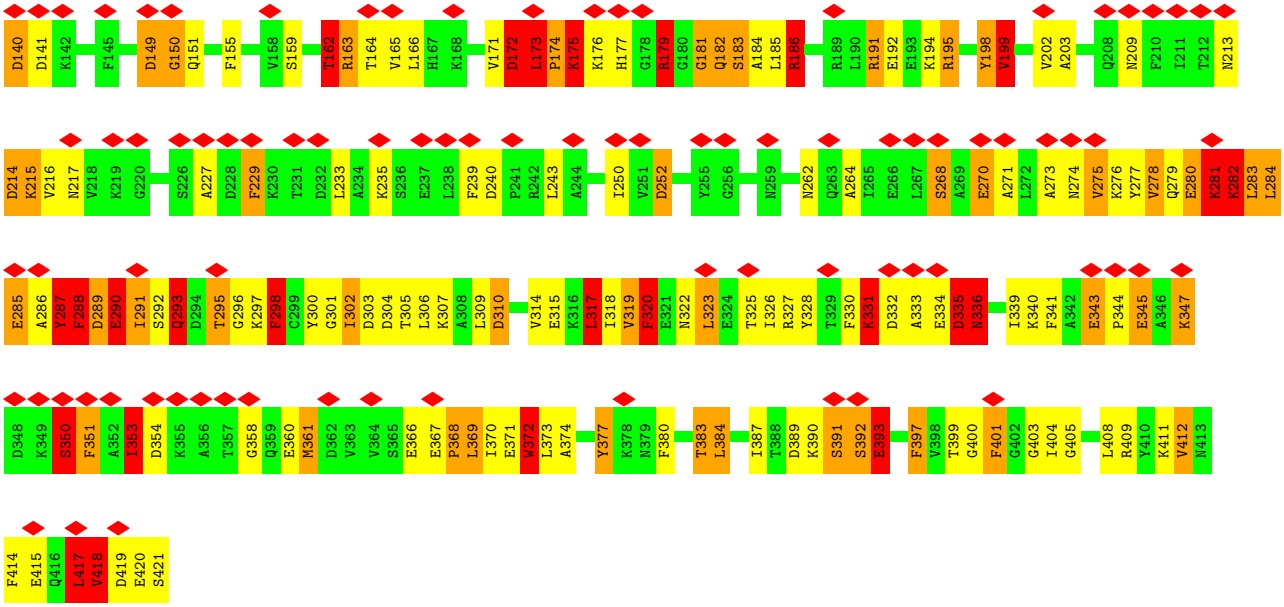
Chain P: 21% 31% 63% 5%





• Molecule 2: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39309	Depositor
Resolution determination method	Not provided	
CTF correction method	ON VOLUMES (SPIDER)	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	147136	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	1.329	Depositor
Minimum map value	-0.634	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.232	Depositor
Map size (Å)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ADP, ATP, MG

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	P	1.02	8/4893 (0.2%)	1.21	21/6603 (0.3%)
2	X	1.09	10/2246 (0.4%)	1.57	53/3021 (1.8%)
All	All	1.04	18/7139 (0.3%)	1.34	74/9624 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	2
2	X	1	17
All	All	1	19

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	150	GLY	C-N	18.11	1.75	1.34
1	P	608	ILE	C-O	-12.06	1.00	1.23
2	X	421	SER	C-OXT	-12.06	1.00	1.23
2	X	421	SER	C-O	-12.06	1.00	1.23
1	P	608	ILE	C-OXT	-12.03	1.00	1.23
2	X	186	ARG	CD-NE	10.40	1.64	1.46
1	P	309	SER	CA-CB	-10.32	1.37	1.52
1	P	589	GLN	CA-C	9.44	1.77	1.52
2	X	186	ARG	NE-CZ	9.01	1.44	1.33
1	P	589	GLN	CA-CB	8.04	1.71	1.53
2	X	150	GLY	N-CA	7.83	1.57	1.46
1	P	589	GLN	CB-CG	7.74	1.73	1.52
2	X	150	GLY	CA-C	7.16	1.63	1.51
2	X	181	GLY	CA-C	-6.54	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	302	ILE	C-N	6.39	1.48	1.34
1	P	589	GLN	N-CA	-5.71	1.34	1.46
2	X	186	ARG	CG-CD	5.36	1.65	1.51
1	P	589	GLN	CG-CD	5.03	1.62	1.51

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	149	ASP	O-C-N	-17.67	93.16	123.20
2	X	149	ASP	CA-C-N	14.81	145.82	116.20
2	X	298	PHE	CB-CG-CD1	-13.00	111.70	120.80
1	P	589	GLN	CA-CB-CG	12.85	141.68	113.40
1	P	588	SER	N-CA-CB	12.81	129.71	110.50
2	X	298	PHE	CB-CG-CD2	-11.46	112.78	120.80
1	P	589	GLN	CB-CG-CD	11.35	141.11	111.60
2	X	372	TRP	CB-CG-CD1	-11.34	112.26	127.00
1	P	589	GLN	N-CA-CB	-11.33	90.20	110.60
2	X	281	LYS	CA-CB-CG	11.31	138.29	113.40
2	X	186	ARG	NE-CZ-NH2	11.24	125.92	120.30
1	P	589	GLN	CB-CA-C	10.62	131.64	110.40
2	X	186	ARG	CA-CB-CG	10.55	136.62	113.40
1	P	589	GLN	CA-C-N	-9.65	95.98	117.20
2	X	298	PHE	CB-CA-C	-9.20	92.00	110.40
2	X	317	LEU	CB-CG-CD2	9.19	126.62	111.00
1	P	586	LEU	CB-CA-C	8.95	127.20	110.20
2	X	368	PRO	CA-N-CD	-8.62	99.43	111.50
2	X	293	GLN	N-CA-CB	8.57	126.02	110.60
1	P	585	LYS	CB-CA-C	8.21	126.81	110.40
2	X	183	SER	N-CA-CB	-8.11	98.34	110.50
1	P	573	ARG	NE-CZ-NH1	-7.97	116.31	120.30
2	X	195	ARG	NE-CZ-NH1	7.77	124.18	120.30
2	X	150	GLY	C-N-CA	-7.76	102.29	121.70
2	X	335	ASP	O-C-N	7.52	134.72	122.70
2	X	353	ILE	C-N-CA	7.40	140.20	121.70
2	X	179	ARG	NE-CZ-NH2	7.38	123.99	120.30
2	X	331	LYS	CA-CB-CG	7.30	129.46	113.40
2	X	361	MET	CG-SD-CE	-7.26	88.59	100.20
1	P	587	ASP	CA-CB-CG	7.19	129.21	113.40
1	P	586	LEU	CB-CG-CD2	7.06	123.01	111.00
2	X	372	TRP	CB-CA-C	-7.04	96.33	110.40
2	X	186	ARG	NH1-CZ-NH2	-6.99	111.71	119.40
2	X	186	ARG	CG-CD-NE	6.94	126.38	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	584	ASN	N-CA-C	-6.83	92.55	111.00
2	X	320	PHE	N-CA-CB	6.82	122.88	110.60
2	X	179	ARG	N-CA-CB	-6.61	98.71	110.60
2	X	412	VAL	CG1-CB-CG2	6.52	121.33	110.90
2	X	331	LYS	N-CA-C	6.51	128.57	111.00
2	X	369	LEU	CB-CA-C	-6.38	98.09	110.20
1	P	588	SER	N-CA-C	-6.25	94.14	111.00
2	X	175	LYS	N-CA-CB	6.17	121.71	110.60
2	X	295	THR	N-CA-CB	5.97	121.65	110.30
2	X	372	TRP	N-CA-CB	5.92	121.26	110.60
2	X	186	ARG	CD-NE-CZ	5.87	131.82	123.60
1	P	309	SER	N-CA-CB	-5.85	101.73	110.50
1	P	589	GLN	CA-C-O	5.83	132.35	120.10
2	X	335	ASP	CA-C-N	-5.74	104.58	117.20
2	X	320	PHE	N-CA-C	-5.66	95.72	111.00
2	X	307	LYS	N-CA-CB	5.64	120.75	110.60
1	P	600	TYR	CA-CB-CG	-5.60	102.76	113.40
2	X	140	ASP	CB-CG-OD1	-5.59	113.27	118.30
2	X	383	THR	N-CA-CB	5.59	120.92	110.30
2	X	179	ARG	N-CA-C	5.57	126.04	111.00
2	X	252	ASP	CB-CA-C	5.50	121.41	110.40
2	X	384	LEU	N-CA-C	5.50	125.84	111.00
2	X	214	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	P	41	VAL	CB-CA-C	-5.44	101.07	111.40
1	P	146	TYR	CA-CB-CG	-5.35	103.24	113.40
2	X	400	GLY	O-C-N	-5.32	114.19	122.70
2	X	421	SER	CA-C-O	-5.28	109.01	120.10
1	P	608	ILE	CA-C-O	-5.28	109.01	120.10
2	X	320	PHE	CB-CG-CD1	5.21	124.45	120.80
2	X	310	ASP	CB-CG-OD2	5.20	122.98	118.30
2	X	335	ASP	CB-CG-OD2	5.20	122.98	118.30
2	X	198	TYR	CB-CG-CD1	-5.19	117.89	121.00
2	X	397	PHE	O-C-N	-5.19	114.39	122.70
1	P	582	ARG	NE-CZ-NH1	5.17	122.88	120.30
2	X	229	PHE	CA-CB-CG	-5.12	101.61	113.90
2	X	336	ASN	N-CA-C	5.12	124.82	111.00
1	P	587	ASP	N-CA-CB	5.12	119.81	110.60
2	X	377	TYR	CB-CA-C	-5.08	100.23	110.40
2	X	281	LYS	CB-CA-C	-5.08	100.25	110.40
2	X	199	VAL	CA-CB-CG2	5.05	118.48	110.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	331	LYS	CA

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	574	ARG	Sidechain
1	P	589	GLN	Mainchain
2	X	140	ASP	Peptide
2	X	141	ASP	Sidechain,Peptide
2	X	149	ASP	Sidechain
2	X	174	PRO	Mainchain
2	X	179	ARG	Sidechain
2	X	191	ARG	Mainchain,Sidechain
2	X	192	GLU	Mainchain
2	X	198	TYR	Sidechain
2	X	214	ASP	Sidechain
2	X	217	ASN	Sidechain
2	X	240	ASP	Sidechain
2	X	262	ASN	Mainchain
2	X	298	PHE	Sidechain
2	X	392	SER	Peptide
2	X	401	PHE	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	P	4804	0	4945	829	0
2	X	2210	0	2182	251	0
3	P	31	0	12	29	0
4	P	16	0	0	16	0
5	P	27	0	12	20	0
6	P	1	0	0	2	0
7	P	1	0	0	0	0
All	All	7090	0	7151	1078	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 76.

All (1078) 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:X:302:ILE:HD11	2:X:325:THR:CB	1.26	1.56
1:P:589:GLN:C	1:P:589:GLN:CA	1.77	1.50
2:X:328:TYR:CD1	2:X:366:GLU:HG2	1.45	1.49
2:X:150:GLY:C	2:X:151:GLN:N	1.75	1.37
2:X:323:LEU:CD1	2:X:370:ILE:CG1	1.94	1.37
2:X:323:LEU:HD12	2:X:370:ILE:CG1	1.50	1.36
2:X:302:ILE:C	2:X:340:LYS:NZ	1.75	1.36
2:X:287:TYR:OH	2:X:318:ILE:CD1	1.71	1.35
2:X:287:TYR:OH	2:X:318:ILE:HD11	1.19	1.29
2:X:302:ILE:CD1	2:X:325:THR:HB	1.60	1.29
2:X:310:ASP:OD1	2:X:380:PHE:HE1	1.15	1.25
2:X:287:TYR:HA	2:X:290:GLU:OE1	1.36	1.24
2:X:302:ILE:CD1	2:X:325:THR:CB	2.14	1.24
2:X:302:ILE:HD11	2:X:325:THR:CG2	1.69	1.22
1:P:37:LEU:HB2	1:P:54:LEU:HD12	1.22	1.20
1:P:396:LYS:HB3	1:P:402:LEU:HD13	1.19	1.18
2:X:328:TYR:CD1	2:X:366:GLU:CG	2.26	1.17
1:P:114:ILE:HD13	1:P:294:ILE:HD13	1.18	1.16
2:X:302:ILE:C	2:X:340:LYS:HZ2	1.35	1.15
1:P:195:MET:HA	1:P:237:VAL:HG22	1.26	1.15
1:P:21:CYS:SG	4:P:1611:SF4:S4	2.44	1.14
1:P:115:GLY:HA2	3:P:1609:ATP:O2A	1.45	1.14
2:X:310:ASP:OD1	2:X:380:PHE:CE1	1.98	1.14
2:X:173:LEU:C	2:X:173:LEU:HD13	1.69	1.13
1:P:120:LEU:HD21	1:P:168:ILE:HD13	1.31	1.12
2:X:347:LYS:O	2:X:350:SER:HB3	1.49	1.12
2:X:328:TYR:HE1	2:X:366:GLU:CD	1.53	1.11
1:P:18:PRO:HA	4:P:1611:SF4:S3	1.91	1.11
2:X:323:LEU:CD1	2:X:370:ILE:HG13	1.64	1.11
1:P:383:MET:HB2	1:P:524:VAL:HG12	1.34	1.10
2:X:290:GLU:OE2	2:X:291:ILE:HB	1.51	1.10
1:P:26:LYS:HD3	1:P:32:VAL:HG11	1.12	1.09
1:P:382:VAL:HG23	1:P:535:ALA:HB2	1.34	1.09
1:P:105:VAL:HG23	1:P:268:LEU:HD21	1.32	1.09
1:P:208:ILE:HG12	1:P:263:ILE:HD11	1.10	1.09
1:P:131:LEU:HD21	1:P:143:ILE:HD12	1.32	1.09
1:P:72:ILE:CG1	4:P:1610:SF4:S1	2.41	1.08
1:P:450:ASP:HA	1:P:505:ILE:HD11	1.27	1.08
2:X:328:TYR:CE1	2:X:366:GLU:CD	2.26	1.08
1:P:86:ARG:HG3	1:P:93:LYS:HG2	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:380:ILE:HD11	1:P:534:LEU:HB3	1.36	1.08
2:X:323:LEU:CD1	2:X:370:ILE:HG12	1.51	1.08
1:P:380:ILE:HG21	1:P:514:ILE:HD13	1.33	1.07
1:P:61:CYS:SG	4:P:1610:SF4:S1	2.53	1.07
1:P:338:ILE:HG23	1:P:340:ASP:H	1.18	1.06
2:X:302:ILE:HD11	2:X:325:THR:HB	1.13	1.06
1:P:72:ILE:CD1	4:P:1610:SF4:S1	0.96	1.05
1:P:84:THR:HG21	1:P:94:LEU:HD12	1.31	1.05
1:P:349:SER:HA	1:P:352:ARG:HG2	1.33	1.05
2:X:171:VAL:O	2:X:172:ASP:HB3	1.57	1.04
1:P:120:LEU:HD11	1:P:168:ILE:HD11	1.37	1.04
1:P:293:ILE:HD11	1:P:322:ILE:HD12	1.37	1.03
2:X:291:ILE:HG22	2:X:291:ILE:O	1.57	1.03
1:P:92:PHE:HB3	3:P:1609:ATP:H1'	1.38	1.02
1:P:120:LEU:HG	1:P:244:MET:HE2	1.41	1.02
1:P:568:LEU:HD12	1:P:570:VAL:HG22	1.38	1.01
2:X:334:GLU:O	2:X:335:ASP:CG	1.99	1.01
1:P:299:SER:HA	3:P:1609:ATP:O3'	1.59	1.01
1:P:72:ILE:HD11	4:P:1610:SF4:S1	0.67	1.00
1:P:31:VAL:HG12	1:P:36:LYS:HB2	1.44	1.00
1:P:114:ILE:HD11	1:P:116:LYS:HG3	1.01	1.00
1:P:280:ASP:HB3	1:P:283:VAL:HG22	1.44	1.00
1:P:183:PRO:HA	1:P:218:ASP:HB3	1.43	0.99
1:P:97:LEU:HG	1:P:122:ILE:HD11	1.43	0.99
1:P:403:LYS:HE3	1:P:403:LYS:HA	1.45	0.98
2:X:287:TYR:OH	2:X:318:ILE:HD13	1.63	0.98
2:X:328:TYR:HD1	2:X:366:GLU:CG	1.68	0.98
1:P:115:GLY:N	3:P:1609:ATP:O1B	1.96	0.97
2:X:281:LYS:HB3	2:X:391:SER:CB	1.93	0.97
1:P:130:ASN:HA	1:P:135:ASP:HB3	1.46	0.97
1:P:112:ASN:HB3	3:P:1609:ATP:O2G	1.65	0.97
2:X:323:LEU:HD12	2:X:370:ILE:HG13	1.20	0.97
2:X:328:TYR:CE1	2:X:366:GLU:CG	2.47	0.97
1:P:114:ILE:HD11	1:P:116:LYS:CG	1.95	0.96
2:X:377:TYR:CD1	2:X:384:LEU:HD13	1.99	0.96
2:X:173:LEU:C	2:X:173:LEU:CD1	2.32	0.96
2:X:303:ASP:N	2:X:340:LYS:HZ2	1.62	0.96
1:P:390:GLY:HA2	5:P:1612:ADP:O1A	1.63	0.96
1:P:337:ARG:HG3	1:P:608:ILE:HG22	1.48	0.96
1:P:56:ILE:HD12	2:X:399:THR:HB	1.46	0.95
1:P:493:GLU:H	1:P:524:VAL:HG23	1.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:368:PRO:HG2	2:X:371:GLU:HB2	1.47	0.95
1:P:537:LYS:HD3	1:P:554:PRO:HB2	1.48	0.95
1:P:434:PHE:CZ	1:P:476:VAL:HG13	2.02	0.94
1:P:388:GLY:HA2	5:P:1612:ADP:H5'2	1.49	0.94
1:P:334:LEU:HD22	1:P:504:ILE:HG21	1.48	0.94
1:P:494:PRO:HG2	1:P:523:ILE:HD11	1.50	0.94
1:P:468:LEU:HG	1:P:469:SER:H	1.33	0.93
2:X:287:TYR:HH	2:X:318:ILE:CD1	1.69	0.93
1:P:511:ARG:CG	1:P:608:ILE:HG12	1.99	0.93
2:X:282:LYS:HG2	2:X:283:LEU:N	1.83	0.93
1:P:133:ARG:HD3	1:P:134:PHE:CE2	2.04	0.93
1:P:403:LYS:HE2	1:P:404:PRO:HD2	1.49	0.92
2:X:287:TYR:CG	2:X:288:PHE:N	2.36	0.92
1:P:92:PHE:CB	3:P:1609:ATP:H1'	2.00	0.92
1:P:492:ASP:HA	1:P:524:VAL:HG22	1.48	0.92
1:P:173:VAL:HB	1:P:251:TYR:HE2	1.34	0.92
1:P:453:LYS:HB2	1:P:454:PRO:HD3	1.51	0.92
1:P:322:ILE:CG2	1:P:325:GLU:HB2	2.00	0.91
1:P:544:ILE:HG23	1:P:547:LYS:HB3	1.49	0.91
1:P:511:ARG:HG3	1:P:608:ILE:HG12	1.53	0.91
2:X:334:GLU:O	2:X:335:ASP:OD1	1.88	0.91
1:P:589:GLN:CA	1:P:590:MET:N	2.34	0.91
1:P:334:LEU:CD2	1:P:504:ILE:HG21	2.01	0.90
1:P:337:ARG:HG3	1:P:608:ILE:HA	1.51	0.90
2:X:287:TYR:HH	2:X:318:ILE:HD11	1.21	0.90
1:P:114:ILE:CD1	1:P:294:ILE:HD13	2.00	0.90
1:P:280:ASP:HB3	1:P:283:VAL:CG2	2.00	0.90
1:P:388:GLY:CA	5:P:1612:ADP:H5'2	2.02	0.90
1:P:380:ILE:CG2	1:P:514:ILE:HD13	2.03	0.89
1:P:544:ILE:HG13	1:P:545:PRO:HD2	1.54	0.89
1:P:338:ILE:HG23	1:P:340:ASP:N	1.86	0.89
2:X:288:PHE:HD1	2:X:288:PHE:C	1.76	0.89
1:P:194:ARG:HD3	1:P:234:MET:HB2	1.54	0.89
1:P:491:ILE:HG21	1:P:494:PRO:HG3	1.54	0.89
1:P:380:ILE:CD1	1:P:534:LEU:HB3	2.03	0.89
2:X:302:ILE:O	2:X:340:LYS:NZ	2.06	0.89
1:P:349:SER:CA	1:P:352:ARG:HG2	2.04	0.88
1:P:105:VAL:HG23	1:P:268:LEU:CD2	2.02	0.88
1:P:396:LYS:CB	1:P:402:LEU:HD13	2.01	0.88
1:P:26:LYS:CD	1:P:32:VAL:HG11	2.00	0.88
1:P:322:ILE:HG23	1:P:325:GLU:HB2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:297:VAL:HB	1:P:300:VAL:CG2	2.05	0.87
1:P:86:ARG:CZ	1:P:93:LYS:HD3	2.04	0.87
1:P:117:SER:HG	6:P:1613:MG:MG	0.80	0.87
1:P:389:THR:HG22	5:P:1612:ADP:O2B	1.73	0.87
2:X:173:LEU:HD23	2:X:191:ARG:HG3	1.55	0.87
2:X:302:ILE:HD11	2:X:325:THR:HG21	1.55	0.86
1:P:37:LEU:CB	1:P:54:LEU:HD12	2.05	0.86
2:X:172:ASP:O	2:X:173:LEU:HB3	1.74	0.86
2:X:281:LYS:HB3	2:X:391:SER:HB2	1.56	0.86
2:X:368:PRO:CG	2:X:371:GLU:OE1	2.23	0.86
1:P:447:PHE:CE1	1:P:479:VAL:HG23	2.10	0.86
2:X:326:ILE:HG23	2:X:367:GLU:O	1.75	0.86
1:P:86:ARG:CG	1:P:93:LYS:HG2	2.06	0.86
2:X:331:LYS:HB3	2:X:336:ASN:HA	1.55	0.86
2:X:305:THR:O	2:X:309:LEU:HG	1.74	0.86
1:P:297:VAL:HB	1:P:300:VAL:HG21	1.57	0.85
1:P:383:MET:CB	1:P:524:VAL:HG12	2.06	0.85
1:P:494:PRO:CG	1:P:523:ILE:HD11	2.06	0.85
1:P:194:ARG:CD	1:P:234:MET:HB2	2.07	0.85
1:P:114:ILE:CD1	1:P:294:ILE:HG21	2.06	0.85
1:P:31:VAL:O	1:P:34:THR:HG22	1.77	0.85
1:P:140:TRP:O	1:P:143:ILE:HG22	1.76	0.85
1:P:97:LEU:CG	1:P:122:ILE:HD11	2.05	0.85
2:X:273:ALA:O	2:X:277:TYR:CD2	2.30	0.84
1:P:117:SER:OG	6:P:1613:MG:MG	1.19	0.84
1:P:242:VAL:HG13	1:P:273:TYR:CE2	2.12	0.84
2:X:302:ILE:CD1	2:X:325:THR:CG2	2.52	0.84
1:P:131:LEU:HD21	1:P:143:ILE:CD1	2.08	0.84
1:P:94:LEU:HD13	1:P:95:HIS:N	1.93	0.84
1:P:306:LEU:HD12	1:P:307:PRO:HD2	1.59	0.84
1:P:339:ALA:HB2	1:P:606:THR:HG23	1.59	0.84
2:X:408:LEU:HD13	2:X:412:VAL:HG13	1.60	0.83
1:P:49:PHE:CE1	1:P:89:ALA:HB1	2.12	0.83
1:P:154:ASN:O	1:P:157:THR:HG22	1.78	0.83
2:X:368:PRO:HG2	2:X:371:GLU:OE1	1.77	0.83
1:P:382:VAL:HG23	1:P:535:ALA:CB	2.08	0.83
1:P:37:LEU:HB2	1:P:54:LEU:CD1	2.06	0.83
1:P:568:LEU:HD12	1:P:570:VAL:CG2	2.09	0.83
2:X:302:ILE:HD13	2:X:325:THR:HB	1.57	0.83
2:X:302:ILE:HD11	2:X:325:THR:OG1	1.77	0.82
1:P:502:GLN:O	1:P:505:ILE:HG22	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:173:LEU:HD13	2:X:174:PRO:N	1.93	0.82
1:P:388:GLY:C	5:P:1612:ADP:H5'2	1.99	0.82
1:P:252:LEU:HB3	1:P:256:GLN:HG3	1.58	0.82
1:P:105:VAL:CG2	1:P:268:LEU:HD11	2.10	0.82
1:P:533:TYR:O	1:P:607:GLY:HA2	1.80	0.82
2:X:288:PHE:CD1	2:X:289:ASP:N	2.48	0.82
1:P:114:ILE:CD1	1:P:116:LYS:HG3	1.97	0.82
1:P:114:ILE:HD13	1:P:294:ILE:CD1	2.05	0.81
1:P:167:ILE:HD13	1:P:168:ILE:N	1.94	0.81
1:P:208:ILE:CG1	1:P:263:ILE:HD11	2.03	0.81
1:P:258:LEU:HD12	1:P:568:LEU:HD21	1.60	0.81
1:P:96:ARG:O	1:P:97:LEU:HD22	1.78	0.81
1:P:275:ILE:HD13	1:P:276:CYS:N	1.95	0.81
1:P:380:ILE:HG13	1:P:535:ALA:HA	1.63	0.81
1:P:320:GLY:HA2	1:P:329:PHE:CZ	2.13	0.81
1:P:49:PHE:HE1	1:P:89:ALA:HB1	1.45	0.81
1:P:337:ARG:CG	1:P:608:ILE:HA	2.09	0.81
1:P:26:LYS:HD3	1:P:32:VAL:CG1	2.04	0.81
1:P:199:PRO:O	1:P:202:VAL:HG12	1.80	0.80
1:P:337:ARG:CG	1:P:608:ILE:HG22	2.10	0.80
2:X:309:LEU:O	2:X:380:PHE:HD1	1.64	0.80
1:P:491:ILE:HB	1:P:523:ILE:CD1	2.11	0.80
1:P:492:ASP:HA	1:P:524:VAL:CG2	2.12	0.80
2:X:290:GLU:O	2:X:291:ILE:HG12	1.81	0.80
2:X:264:ALA:O	2:X:268:SER:HB2	1.80	0.80
1:P:252:LEU:HA	1:P:256:GLN:HE21	1.46	0.80
1:P:363:GLN:HG2	5:P:1612:ADP:C5	2.17	0.80
1:P:383:MET:CE	1:P:539:ILE:HD12	2.11	0.80
1:P:506:CYS:O	1:P:509:VAL:HG12	1.81	0.80
1:P:21:CYS:SG	4:P:1611:SF4:FE2	1.74	0.80
1:P:514:ILE:HG23	1:P:519:LYS:O	1.82	0.80
1:P:135:ASP:OD1	1:P:139:GLU:HB2	1.81	0.79
1:P:159:MET:HE3	1:P:159:MET:HA	1.62	0.79
1:P:529:ILE:O	1:P:532:THR:HG22	1.82	0.79
2:X:291:ILE:O	2:X:291:ILE:CG2	2.30	0.79
1:P:86:ARG:HG3	1:P:93:LYS:CG	2.12	0.79
1:P:381:LEU:HD11	1:P:539:ILE:CD1	2.12	0.79
1:P:458:ASP:O	1:P:461:ILE:HG12	1.83	0.79
1:P:116:LYS:N	3:P:1609:ATP:O1B	2.14	0.79
1:P:380:ILE:HG21	1:P:514:ILE:CD1	2.12	0.79
2:X:150:GLY:C	2:X:151:GLN:CA	2.51	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:353:ALA:HB1	1:P:375:PHE:CE1	2.18	0.78
2:X:326:ILE:HG23	2:X:368:PRO:HA	1.65	0.78
2:X:323:LEU:HD12	2:X:370:ILE:CA	2.12	0.78
1:P:568:LEU:HD13	1:P:568:LEU:O	1.84	0.78
1:P:363:GLN:HG2	5:P:1612:ADP:C6	2.19	0.78
1:P:388:GLY:H	5:P:1612:ADP:PB	2.05	0.78
2:X:173:LEU:CD1	2:X:173:LEU:O	2.32	0.78
1:P:66:PRO:HD2	4:P:1611:SF4:S4	2.24	0.78
1:P:79:LEU:HD23	1:P:95:HIS:CE1	2.18	0.78
1:P:173:VAL:HB	1:P:251:TYR:CE2	2.19	0.78
1:P:72:ILE:HD13	4:P:1610:SF4:S1	1.37	0.78
2:X:172:ASP:O	2:X:173:LEU:CB	2.31	0.78
1:P:120:LEU:HD11	1:P:168:ILE:CD1	2.12	0.77
1:P:207:LYS:HA	1:P:212:GLU:OE2	1.83	0.77
1:P:444:ASN:HB2	1:P:445:PRO:HD2	1.64	0.77
1:P:108:LEU:HD23	1:P:109:VAL:N	1.99	0.77
1:P:187:VAL:HG13	1:P:230:PHE:CD1	2.20	0.77
1:P:244:MET:HA	1:P:275:ILE:HG22	1.66	0.77
1:P:92:PHE:CD2	3:P:1609:ATP:O4'	2.38	0.77
1:P:182:GLY:HA3	1:P:185:GLN:O	1.85	0.77
1:P:300:VAL:HG23	1:P:301:TYR:CD1	2.19	0.77
2:X:290:GLU:OE2	2:X:291:ILE:CB	2.30	0.76
2:X:301:GLY:O	2:X:305:THR:HG23	1.84	0.76
1:P:120:LEU:HD21	1:P:168:ILE:CD1	2.14	0.76
1:P:318:LEU:CD1	1:P:580:ARG:HB3	2.15	0.76
2:X:302:ILE:CD1	2:X:325:THR:HG21	2.15	0.76
1:P:273:TYR:OH	1:P:275:ILE:HB	1.85	0.76
1:P:31:VAL:CG1	1:P:36:LYS:HB2	2.15	0.76
1:P:360:LYS:HE2	1:P:369:ASN:CG	2.05	0.76
1:P:108:LEU:CD2	1:P:116:LYS:HG2	2.15	0.76
1:P:231:ALA:O	1:P:234:MET:HG2	1.84	0.76
1:P:491:ILE:HB	1:P:523:ILE:HD12	1.68	0.76
1:P:557:LEU:H	1:P:557:LEU:HD22	1.50	0.76
1:P:18:PRO:CA	4:P:1611:SF4:S3	2.72	0.76
1:P:338:ILE:HD13	1:P:338:ILE:O	1.86	0.76
1:P:491:ILE:CG2	1:P:494:PRO:HG3	2.15	0.76
1:P:106:LEU:HD23	1:P:290:PHE:HB2	1.68	0.75
1:P:517:ASN:OD1	1:P:519:LYS:HG2	1.87	0.75
1:P:388:GLY:N	5:P:1612:ADP:O3B	2.17	0.75
1:P:380:ILE:HD11	1:P:534:LEU:CB	2.14	0.75
2:X:288:PHE:C	2:X:288:PHE:CD1	2.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:97:LEU:CD1	1:P:122:ILE:HD11	2.17	0.75
1:P:337:ARG:HG3	1:P:608:ILE:CG2	2.16	0.75
1:P:589:GLN:C	1:P:589:GLN:HA	2.04	0.75
1:P:34:THR:CG2	1:P:36:LYS:HG3	2.17	0.74
1:P:380:ILE:HD11	1:P:534:LEU:C	2.07	0.74
1:P:105:VAL:CG2	1:P:268:LEU:HD21	2.14	0.74
2:X:171:VAL:O	2:X:172:ASP:CB	2.34	0.74
1:P:381:LEU:HD11	1:P:539:ILE:HG13	1.68	0.74
2:X:271:ALA:O	2:X:275:VAL:HG23	1.88	0.74
1:P:476:VAL:O	1:P:480:LEU:HG	1.87	0.74
2:X:323:LEU:HD12	2:X:370:ILE:CB	2.18	0.74
2:X:343:GLU:H	2:X:344:PRO:HD2	1.52	0.74
1:P:84:THR:HG22	1:P:94:LEU:O	1.86	0.74
2:X:302:ILE:CA	2:X:340:LYS:HZ3	1.90	0.74
1:P:92:PHE:HB2	3:P:1609:ATP:O2'	1.88	0.74
1:P:397:LEU:HD23	1:P:402:LEU:HB2	1.68	0.74
1:P:115:GLY:O	1:P:118:THR:HG22	1.87	0.74
1:P:242:VAL:HG13	1:P:273:TYR:CD2	2.21	0.74
1:P:112:ASN:CB	3:P:1609:ATP:O2G	2.36	0.73
1:P:114:ILE:HD13	1:P:294:ILE:HG21	1.69	0.73
1:P:128:LYS:HD2	1:P:128:LYS:O	1.87	0.73
1:P:185:GLN:HG3	1:P:189:GLU:OE1	1.88	0.73
1:P:242:VAL:HG22	1:P:273:TYR:HD2	1.52	0.73
1:P:381:LEU:HD13	1:P:522:PHE:HE1	1.53	0.73
1:P:424:PRO:HB3	1:P:465:VAL:HG12	1.70	0.73
1:P:381:LEU:HD11	1:P:539:ILE:CG1	2.19	0.73
1:P:392:THR:O	1:P:395:ILE:HG22	1.88	0.73
1:P:176:ILE:HB	1:P:177:PRO:HD3	1.68	0.73
1:P:8:ILE:HG22	1:P:10:ILE:CD1	2.18	0.73
1:P:194:ARG:HB3	1:P:237:VAL:CG1	2.19	0.73
1:P:544:ILE:HG23	1:P:547:LYS:CB	2.18	0.73
2:X:173:LEU:O	2:X:173:LEU:HD12	1.89	0.73
1:P:136:ASP:HB3	1:P:137:PRO:HD2	1.70	0.73
1:P:383:MET:SD	1:P:539:ILE:HD12	2.29	0.73
1:P:120:LEU:CD1	1:P:246:ASP:HB2	2.19	0.72
2:X:317:LEU:HB3	2:X:384:LEU:HD11	1.71	0.72
1:P:160:LEU:O	1:P:160:LEU:HD23	1.89	0.72
1:P:532:THR:OG1	1:P:605:ASN:HB2	1.89	0.72
2:X:389:ASP:O	2:X:390:LYS:CG	2.38	0.72
1:P:25:CYS:SG	1:P:70:ILE:HD11	2.30	0.72
1:P:195:MET:HA	1:P:237:VAL:CG2	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:544:ILE:CG1	1:P:545:PRO:HD2	2.20	0.72
1:P:566:LYS:O	1:P:566:LYS:HD3	1.89	0.72
2:X:320:PHE:CG	2:X:403:GLY:HA2	2.25	0.72
1:P:47:ILE:HD13	1:P:48:ALA:H	1.55	0.71
2:X:278:VAL:O	2:X:282:LYS:HD2	1.89	0.71
1:P:144:ILE:HG23	1:P:153:GLN:HG3	1.72	0.71
1:P:431:ARG:NH1	1:P:431:ARG:HB3	2.05	0.71
1:P:120:LEU:HG	1:P:244:MET:CE	2.20	0.71
1:P:195:MET:CA	1:P:237:VAL:HG22	2.16	0.71
1:P:339:ALA:HB2	1:P:606:THR:CG2	2.19	0.71
2:X:368:PRO:HG3	2:X:371:GLU:OE1	1.90	0.71
1:P:435:PHE:HE1	1:P:439:ARG:HD3	1.54	0.71
2:X:326:ILE:HG23	2:X:368:PRO:CA	2.21	0.71
2:X:389:ASP:O	2:X:390:LYS:HG3	1.91	0.71
2:X:390:LYS:O	2:X:391:SER:CB	2.39	0.71
1:P:337:ARG:HG3	1:P:608:ILE:CA	2.20	0.71
1:P:511:ARG:HG2	1:P:608:ILE:HG12	1.72	0.71
2:X:173:LEU:HD23	2:X:191:ARG:CG	2.21	0.70
1:P:306:LEU:CD1	1:P:307:PRO:HD2	2.21	0.70
1:P:269:ALA:HB3	1:P:270:PRO:HD3	1.73	0.70
1:P:450:ASP:CA	1:P:505:ILE:HD11	2.13	0.70
2:X:273:ALA:HB1	2:X:277:TYR:CZ	2.27	0.70
1:P:387:ASN:CA	5:P:1612:ADP:O3B	2.39	0.70
1:P:409:ASP:C	1:P:411:PRO:HD3	2.12	0.70
1:P:438:ILE:HG13	1:P:483:GLY:O	1.91	0.70
1:P:268:LEU:HD12	1:P:268:LEU:H	1.57	0.70
1:P:354:PHE:HB3	1:P:375:PHE:CZ	2.26	0.70
2:X:273:ALA:HB1	2:X:277:TYR:OH	1.92	0.70
2:X:302:ILE:C	2:X:340:LYS:HZ3	1.65	0.70
1:P:265:ARG:O	1:P:268:LEU:HD13	1.89	0.70
2:X:271:ALA:O	2:X:275:VAL:CG2	2.40	0.70
1:P:266:SER:O	1:P:270:PRO:HD2	1.92	0.69
1:P:369:ASN:HD22	1:P:370:VAL:N	1.89	0.69
1:P:72:ILE:HD12	4:P:1610:SF4:S1	1.29	0.69
1:P:194:ARG:HB3	1:P:237:VAL:HG11	1.74	0.69
1:P:140:TRP:HB2	1:P:160:LEU:HD12	1.74	0.69
1:P:180:ILE:HD11	1:P:190:LEU:HD11	1.74	0.69
1:P:381:LEU:HD11	1:P:539:ILE:HD11	1.72	0.69
1:P:461:ILE:HG13	1:P:462:ASP:N	2.07	0.69
2:X:326:ILE:CG2	2:X:367:GLU:O	2.39	0.69
1:P:252:LEU:HB2	1:P:257:ARG:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:563:ARG:HE	1:P:563:ARG:HA	1.56	0.69
1:P:130:ASN:CA	1:P:135:ASP:HB3	2.20	0.69
1:P:173:VAL:CB	1:P:251:TYR:HE2	2.04	0.69
1:P:384:MET:HG3	1:P:385:GLY:H	1.58	0.69
1:P:392:THR:O	1:P:396:LYS:HD3	1.92	0.69
2:X:274:ASN:HA	2:X:277:TYR:HD2	1.56	0.69
1:P:47:ILE:HD13	1:P:48:ALA:N	2.08	0.69
1:P:180:ILE:CG2	1:P:219:ILE:HG12	2.23	0.69
1:P:265:ARG:HA	1:P:268:LEU:HD13	1.74	0.68
1:P:194:ARG:HD3	1:P:234:MET:CB	2.23	0.68
1:P:295:TYR:CZ	1:P:303:VAL:HG13	2.29	0.68
1:P:186:LYS:HB3	1:P:217:ARG:O	1.93	0.68
1:P:108:LEU:HA	1:P:292:CYS:SG	2.33	0.68
1:P:120:LEU:HA	1:P:244:MET:HE1	1.75	0.68
1:P:568:LEU:CD1	1:P:570:VAL:HG13	2.24	0.68
2:X:309:LEU:O	2:X:380:PHE:CD1	2.47	0.68
1:P:403:LYS:HA	1:P:403:LYS:CE	2.23	0.68
1:P:9:ALA:C	1:P:10:ILE:HD12	2.13	0.68
1:P:507:SER:O	1:P:534:LEU:HD21	1.94	0.68
2:X:281:LYS:HB3	2:X:391:SER:HB3	1.74	0.68
1:P:105:VAL:HG23	1:P:268:LEU:CG	2.24	0.68
1:P:185:GLN:HG3	1:P:189:GLU:CD	2.15	0.68
1:P:358:SER:N	1:P:372:GLU:HG3	2.09	0.68
1:P:434:PHE:CD2	1:P:480:LEU:HD21	2.29	0.68
1:P:493:GLU:N	1:P:524:VAL:HG23	2.04	0.68
1:P:162:ASP:OD1	1:P:165:LYS:HE3	1.93	0.68
2:X:347:LYS:O	2:X:350:SER:CB	2.35	0.68
1:P:384:MET:HG3	1:P:385:GLY:N	2.09	0.67
1:P:447:PHE:O	1:P:451:VAL:HG12	1.95	0.67
1:P:354:PHE:HB3	1:P:375:PHE:CE2	2.30	0.67
1:P:457:ILE:O	1:P:461:ILE:HG23	1.94	0.67
2:X:270:GLU:OE1	2:X:270:GLU:HA	1.95	0.67
1:P:544:ILE:CG2	1:P:547:LYS:HB3	2.24	0.67
2:X:273:ALA:C	2:X:277:TYR:CE2	2.69	0.67
1:P:8:ILE:HG22	1:P:10:ILE:HD11	1.76	0.67
2:X:332:ASP:N	2:X:335:ASP:O	2.27	0.67
1:P:78:ASN:CG	1:P:79:LEU:HD12	2.14	0.66
1:P:403:LYS:CE	1:P:404:PRO:HD2	2.24	0.66
1:P:511:ARG:CZ	1:P:607:GLY:HA3	2.25	0.66
2:X:328:TYR:HD1	2:X:366:GLU:HG2	0.77	0.66
1:P:349:SER:HA	1:P:352:ARG:CG	2.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:395:ILE:HD11	1:P:490:LEU:HB3	1.78	0.66
2:X:282:LYS:CG	2:X:283:LEU:N	2.50	0.66
1:P:382:VAL:CG2	1:P:535:ALA:HB2	2.20	0.66
1:P:511:ARG:HB2	1:P:534:LEU:HD23	1.77	0.66
2:X:368:PRO:HG2	2:X:371:GLU:CB	2.24	0.66
1:P:26:LYS:HD2	1:P:26:LYS:C	2.15	0.66
1:P:305:THR:HG22	1:P:306:LEU:H	1.59	0.66
1:P:352:ARG:HB3	1:P:376:SER:HB2	1.78	0.66
1:P:198:SER:HB3	1:P:199:PRO:HD2	1.78	0.65
1:P:557:LEU:HG	1:P:606:THR:HG22	1.78	0.65
1:P:198:SER:H	1:P:201:ASP:HB2	1.61	0.65
2:X:172:ASP:CG	2:X:173:LEU:N	2.50	0.65
1:P:322:ILE:HG21	1:P:325:GLU:HB2	1.76	0.65
2:X:330:PHE:O	2:X:331:LYS:HB2	1.95	0.65
1:P:336:PHE:CE1	1:P:529:ILE:HG23	2.32	0.65
1:P:392:THR:CG2	1:P:396:LYS:HE3	2.27	0.65
2:X:159:SER:H	2:X:162:THR:HG22	1.61	0.65
2:X:309:LEU:HD23	2:X:314:VAL:HB	1.79	0.65
1:P:175:ASN:O	1:P:178:ARG:HG2	1.96	0.65
1:P:159:MET:HA	1:P:159:MET:CE	2.27	0.65
1:P:305:THR:HG22	1:P:306:LEU:N	2.11	0.65
1:P:387:ASN:HA	5:P:1612:ADP:O3B	1.96	0.65
2:X:328:TYR:HE1	2:X:366:GLU:OE1	1.80	0.64
2:X:418:VAL:O	2:X:420:GLU:N	2.31	0.64
1:P:589:GLN:HG3	1:P:590:MET:SD	2.37	0.64
2:X:289:ASP:O	2:X:291:ILE:N	2.30	0.64
1:P:56:ILE:CD1	2:X:399:THR:HB	2.25	0.64
1:P:120:LEU:CD1	1:P:168:ILE:HD11	2.22	0.64
1:P:128:LYS:HG2	1:P:138:PRO:N	2.12	0.64
1:P:194:ARG:CB	1:P:237:VAL:HG11	2.27	0.64
2:X:290:GLU:OE2	2:X:291:ILE:N	2.30	0.64
1:P:105:VAL:HG23	1:P:268:LEU:HD11	1.78	0.64
1:P:336:PHE:CZ	1:P:529:ILE:HG23	2.33	0.64
1:P:353:ALA:HB2	1:P:377:ASP:OD1	1.97	0.64
1:P:510:ILE:HG22	1:P:514:ILE:HD12	1.80	0.64
2:X:326:ILE:HG12	2:X:368:PRO:HA	1.80	0.64
1:P:120:LEU:O	1:P:120:LEU:HD23	1.98	0.64
1:P:363:GLN:HG2	5:P:1612:ADP:C4	2.33	0.64
2:X:331:LYS:HB3	2:X:336:ASN:CA	2.28	0.64
1:P:26:LYS:HA	1:P:39:ILE:HG21	1.80	0.64
2:X:173:LEU:CD2	2:X:191:ARG:HG3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:38:CYS:SG	1:P:55:CYS:HA	2.39	0.63
1:P:234:MET:O	1:P:237:VAL:HG12	1.98	0.63
1:P:360:LYS:HE2	1:P:369:ASN:OD1	1.98	0.63
2:X:273:ALA:HB1	2:X:277:TYR:CE2	2.33	0.63
1:P:47:ILE:HD12	1:P:48:ALA:O	1.99	0.63
1:P:61:CYS:N	4:P:1610:SF4:S2	2.71	0.63
1:P:291:VAL:HG21	1:P:313:GLY:HA3	1.81	0.63
1:P:344:ASP:O	1:P:345:LEU:HD23	1.98	0.63
1:P:451:VAL:HG13	1:P:452:VAL:N	2.14	0.63
1:P:183:PRO:O	1:P:186:LYS:HD2	1.99	0.62
1:P:358:SER:HB3	1:P:372:GLU:OE2	2.00	0.62
1:P:329:PHE:CD1	1:P:330:ARG:HG3	2.35	0.62
1:P:410:ILE:O	1:P:410:ILE:HG13	1.97	0.62
1:P:515:LEU:CD1	1:P:608:ILE:HG13	2.29	0.62
2:X:326:ILE:HG23	2:X:367:GLU:C	2.19	0.62
1:P:4:LYS:HG2	1:P:77:THR:CG2	2.30	0.62
1:P:490:LEU:C	1:P:491:ILE:HD12	2.20	0.62
1:P:430:VAL:O	1:P:434:PHE:HD1	1.83	0.62
1:P:491:ILE:HD12	1:P:491:ILE:N	2.14	0.62
1:P:108:LEU:HD22	1:P:116:LYS:HG2	1.82	0.62
1:P:265:ARG:HA	1:P:268:LEU:CD1	2.30	0.62
1:P:258:LEU:HD12	1:P:568:LEU:CD2	2.29	0.62
1:P:353:ALA:HB3	1:P:375:PHE:O	2.00	0.62
2:X:347:LYS:C	2:X:350:SER:HB3	2.18	0.62
1:P:201:ASP:O	1:P:205:TYR:HD1	1.82	0.62
1:P:352:ARG:HD3	1:P:376:SER:HB3	1.82	0.62
1:P:383:MET:HB2	1:P:524:VAL:CG1	2.21	0.62
1:P:208:ILE:HG12	1:P:263:ILE:CD1	2.06	0.61
1:P:101:ARG:O	1:P:273:TYR:HD1	1.83	0.61
1:P:265:ARG:CA	1:P:268:LEU:HD13	2.29	0.61
1:P:268:LEU:HD12	1:P:268:LEU:N	2.14	0.61
1:P:555:GLU:OE1	1:P:559:THR:HG22	2.01	0.61
2:X:282:LYS:CG	2:X:283:LEU:H	2.12	0.61
2:X:343:GLU:O	2:X:345:GLU:HG3	2.00	0.61
1:P:66:PRO:CD	4:P:1611:SF4:S4	2.87	0.61
2:X:287:TYR:CA	2:X:290:GLU:OE1	2.30	0.61
2:X:301:GLY:O	2:X:305:THR:CG2	2.48	0.61
2:X:278:VAL:O	2:X:282:LYS:CD	2.48	0.61
1:P:87:TYR:CE2	3:P:1609:ATP:C5	2.89	0.61
1:P:185:GLN:HA	1:P:189:GLU:OE1	2.00	0.61
1:P:116:LYS:NZ	3:P:1609:ATP:O3G	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:120:LEU:HD12	1:P:246:ASP:HB2	1.82	0.61
1:P:177:PRO:HD3	1:P:227:LEU:HD21	1.82	0.61
1:P:275:ILE:HD13	1:P:276:CYS:H	1.65	0.61
1:P:357:PRO:C	1:P:372:GLU:HG3	2.21	0.61
1:P:84:THR:HG22	1:P:94:LEU:C	2.21	0.61
1:P:169:LYS:HE3	1:P:246:ASP:O	2.00	0.61
1:P:194:ARG:NE	1:P:234:MET:HB2	2.15	0.61
1:P:357:PRO:HA	1:P:372:GLU:HG3	1.81	0.61
1:P:415:VAL:HG22	1:P:488:ILE:HD11	1.83	0.61
2:X:408:LEU:HD13	2:X:412:VAL:CG1	2.30	0.61
1:P:100:PRO:HB3	1:P:273:TYR:CZ	2.36	0.60
1:P:114:ILE:HD12	1:P:116:LYS:N	2.16	0.60
1:P:437:LYS:O	1:P:438:ILE:HG12	2.01	0.60
1:P:352:ARG:CD	1:P:376:SER:HB3	2.31	0.60
1:P:202:VAL:O	1:P:206:ILE:HG23	2.02	0.60
2:X:374:ALA:HA	2:X:377:TYR:CZ	2.36	0.60
1:P:280:ASP:CB	1:P:283:VAL:HG22	2.26	0.60
1:P:352:ARG:HB2	1:P:376:SER:HA	1.81	0.60
1:P:300:VAL:HG23	1:P:301:TYR:N	2.14	0.60
2:X:333:ALA:O	2:X:334:GLU:HG3	2.01	0.60
1:P:25:CYS:HB3	1:P:39:ILE:HD13	1.84	0.60
1:P:84:THR:HG21	1:P:94:LEU:CD1	2.19	0.60
1:P:285:ASP:OD1	1:P:310:VAL:HG22	2.02	0.60
1:P:544:ILE:HG22	1:P:548:ASN:OD1	2.02	0.60
1:P:574:ARG:HD2	1:P:603:LEU:HD12	1.82	0.60
1:P:294:ILE:HG13	1:P:303:VAL:O	2.02	0.60
2:X:377:TYR:CZ	2:X:384:LEU:HD22	2.36	0.60
1:P:8:ILE:CG2	1:P:10:ILE:HD11	2.32	0.60
1:P:430:VAL:CG1	1:P:434:PHE:HE1	2.15	0.60
1:P:338:ILE:HG21	1:P:340:ASP:HB3	1.83	0.60
1:P:242:VAL:HG22	1:P:273:TYR:CD2	2.34	0.60
1:P:50:ILE:N	1:P:50:ILE:HD12	2.16	0.59
1:P:114:ILE:CG1	1:P:294:ILE:HG21	2.32	0.59
1:P:114:ILE:HG12	1:P:294:ILE:CG2	2.32	0.59
1:P:209:LEU:O	1:P:210:GLN:HG2	2.02	0.59
1:P:568:LEU:CD1	1:P:570:VAL:HG22	2.25	0.59
1:P:360:LYS:HE2	1:P:369:ASN:ND2	2.17	0.59
1:P:115:GLY:CA	3:P:1609:ATP:O2A	2.35	0.59
2:X:282:LYS:O	2:X:283:LEU:C	2.39	0.59
2:X:343:GLU:HB2	2:X:344:PRO:HD3	1.83	0.59
1:P:515:LEU:HD11	1:P:608:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:326:ILE:CG2	2:X:368:PRO:HA	2.32	0.59
2:X:377:TYR:CE1	2:X:384:LEU:HD13	2.37	0.59
1:P:44:THR:HG23	1:P:45:SER:N	2.17	0.59
1:P:53:ILE:HG23	1:P:54:LEU:N	2.16	0.59
1:P:222:LEU:HD22	1:P:226:GLU:OE1	2.03	0.59
2:X:277:TYR:O	2:X:281:LYS:HG3	2.01	0.59
1:P:278:GLU:OE1	1:P:283:VAL:HG21	2.03	0.59
1:P:369:ASN:HD22	1:P:370:VAL:H	1.50	0.59
1:P:509:VAL:O	1:P:513:PHE:HD1	1.84	0.59
2:X:390:LYS:O	2:X:391:SER:HB3	2.03	0.59
1:P:338:ILE:CG2	1:P:341:ALA:H	2.14	0.59
1:P:397:LEU:HD23	1:P:402:LEU:CB	2.33	0.59
1:P:10:ILE:HD12	1:P:10:ILE:N	2.16	0.59
1:P:73:ILE:HG23	1:P:75:LEU:CD2	2.33	0.59
1:P:136:ASP:HB3	1:P:137:PRO:CD	2.31	0.59
1:P:180:ILE:HG23	1:P:219:ILE:HG12	1.84	0.59
1:P:448:GLN:O	1:P:453:LYS:HG2	2.03	0.58
1:P:25:CYS:HB3	1:P:39:ILE:CD1	2.33	0.58
1:P:391:LYS:HG2	1:P:524:VAL:HG11	1.86	0.58
1:P:84:THR:HG23	1:P:85:HIS:N	2.18	0.58
1:P:271:THR:O	1:P:271:THR:HG22	2.03	0.58
1:P:116:LYS:HZ2	3:P:1609:ATP:PB	2.25	0.58
1:P:383:MET:HE2	1:P:539:ILE:HD12	1.86	0.58
2:X:323:LEU:HD12	2:X:370:ILE:HA	1.86	0.58
1:P:219:ILE:HD11	1:P:227:LEU:HD12	1.85	0.58
1:P:242:VAL:HG13	1:P:273:TYR:HE2	1.68	0.58
1:P:306:LEU:HD12	1:P:307:PRO:CD	2.32	0.58
1:P:418:LYS:HD3	1:P:419:PRO:O	2.04	0.58
2:X:273:ALA:O	2:X:277:TYR:CE2	2.57	0.58
2:X:203:ALA:HB1	2:X:243:LEU:HD21	1.84	0.58
2:X:314:VAL:HG22	2:X:408:LEU:HD23	1.86	0.58
1:P:206:ILE:HG13	1:P:207:LYS:N	2.19	0.57
1:P:381:LEU:C	1:P:381:LEU:HD23	2.24	0.57
2:X:374:ALA:HA	2:X:377:TYR:CE2	2.39	0.57
1:P:6:SER:OG	1:P:77:THR:HG22	2.04	0.57
1:P:159:MET:HE2	1:P:159:MET:O	2.04	0.57
1:P:211:LEU:O	1:P:215:LEU:HD12	2.04	0.57
1:P:253:ASP:O	1:P:257:ARG:HD3	2.04	0.57
1:P:293:ILE:O	1:P:293:ILE:HG13	2.04	0.57
1:P:352:ARG:HD3	1:P:376:SER:CB	2.33	0.57
1:P:254:VAL:HG23	1:P:255:LYS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:418:VAL:C	2:X:420:GLU:H	2.08	0.57
1:P:110:GLY:HA3	1:P:294:ILE:CG2	2.35	0.57
1:P:219:ILE:HG23	1:P:220:GLU:N	2.19	0.57
1:P:450:ASP:HA	1:P:505:ILE:CD1	2.19	0.57
1:P:78:ASN:ND2	1:P:79:LEU:HD12	2.20	0.57
1:P:114:ILE:HG12	1:P:294:ILE:HG21	1.87	0.57
1:P:116:LYS:HD2	1:P:277:VAL:CG1	2.35	0.57
1:P:244:MET:HA	1:P:275:ILE:CG2	2.35	0.57
1:P:117:SER:HB2	3:P:1609:ATP:O1A	2.05	0.57
1:P:192:LYS:O	1:P:195:MET:HG3	2.05	0.57
1:P:503:ARG:O	1:P:506:CYS:HB3	2.05	0.57
1:P:529:ILE:HD12	1:P:529:ILE:N	2.19	0.57
2:X:163:ARG:HD2	2:X:163:ARG:O	2.04	0.57
2:X:368:PRO:HD2	2:X:368:PRO:O	2.05	0.57
1:P:114:ILE:HD12	1:P:115:GLY:N	2.20	0.57
1:P:243:TYR:CE2	1:P:272:LYS:HD3	2.39	0.57
2:X:287:TYR:CZ	2:X:318:ILE:HD11	2.31	0.57
1:P:173:VAL:CG2	1:P:251:TYR:HE2	2.18	0.56
1:P:295:TYR:HE1	1:P:305:THR:HG1	1.53	0.56
2:X:343:GLU:HB2	2:X:344:PRO:CD	2.35	0.56
1:P:42:THR:OG1	1:P:47:ILE:HG22	2.04	0.56
1:P:78:ASN:OD1	1:P:79:LEU:HD12	2.05	0.56
1:P:265:ARG:C	1:P:268:LEU:HD13	2.25	0.56
1:P:295:TYR:OH	1:P:325:GLU:HG2	2.05	0.56
1:P:316:ILE:HA	1:P:319:ASP:OD1	2.06	0.56
1:P:468:LEU:HG	1:P:469:SER:N	2.11	0.56
2:X:389:ASP:C	2:X:390:LYS:HG3	2.24	0.56
1:P:105:VAL:HG23	1:P:268:LEU:CD1	2.36	0.56
1:P:190:LEU:HB3	1:P:230:PHE:HZ	1.70	0.56
1:P:106:LEU:HD13	1:P:107:GLY:O	2.05	0.56
1:P:120:LEU:CD2	1:P:168:ILE:HD13	2.21	0.56
1:P:565:LEU:CD1	1:P:600:TYR:HB3	2.35	0.56
1:P:451:VAL:HG13	1:P:452:VAL:HG23	1.87	0.56
1:P:96:ARG:C	1:P:97:LEU:HD22	2.26	0.56
1:P:114:ILE:HD12	1:P:114:ILE:C	2.26	0.56
1:P:180:ILE:HG21	1:P:219:ILE:HG12	1.88	0.56
1:P:568:LEU:HD12	1:P:570:VAL:HG13	1.87	0.56
1:P:37:LEU:HD12	1:P:37:LEU:N	2.21	0.56
1:P:39:ILE:HG13	1:P:49:PHE:O	2.06	0.56
1:P:187:VAL:HG13	1:P:230:PHE:HD1	1.67	0.56
1:P:476:VAL:O	1:P:479:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:492:ASP:OD1	1:P:524:VAL:HG21	2.06	0.56
1:P:571:THR:HG23	1:P:595:LYS:NZ	2.21	0.56
2:X:319:VAL:HG12	2:X:320:PHE:H	1.70	0.56
1:P:167:ILE:HG21	1:P:243:TYR:CD1	2.41	0.55
1:P:538:VAL:HG12	1:P:539:ILE:N	2.21	0.55
2:X:318:ILE:O	2:X:405:GLY:N	2.40	0.55
1:P:92:PHE:CB	3:P:1609:ATP:C1'	2.80	0.55
1:P:383:MET:SD	1:P:539:ILE:HB	2.47	0.55
1:P:337:ARG:CD	1:P:608:ILE:HA	2.37	0.55
2:X:287:TYR:CD2	2:X:288:PHE:N	2.75	0.55
1:P:86:ARG:NE	1:P:93:LYS:HD3	2.20	0.55
1:P:108:LEU:HD21	1:P:116:LYS:HG2	1.89	0.55
1:P:112:ASN:HA	3:P:1609:ATP:O3G	2.06	0.55
1:P:520:THR:HG22	1:P:521:ALA:N	2.21	0.55
1:P:569:ASN:OD1	1:P:595:LYS:HE2	2.07	0.55
1:P:202:VAL:HG13	1:P:203:LYS:N	2.21	0.55
1:P:381:LEU:HD12	1:P:554:PRO:HB3	1.86	0.55
1:P:144:ILE:CG2	1:P:153:GLN:HG3	2.37	0.55
1:P:186:LYS:HG2	1:P:216:LYS:O	2.06	0.55
1:P:380:ILE:CG1	1:P:535:ALA:HA	2.35	0.55
2:X:418:VAL:C	2:X:420:GLU:N	2.60	0.55
1:P:342:THR:HA	1:P:608:ILE:OXT	2.07	0.55
2:X:292:SER:O	2:X:298:PHE:CZ	2.59	0.55
2:X:343:GLU:N	2:X:344:PRO:HD2	2.20	0.55
1:P:252:LEU:CB	1:P:257:ARG:HG3	2.36	0.55
2:X:274:ASN:HA	2:X:277:TYR:CD2	2.39	0.55
2:X:322:ASN:O	2:X:323:LEU:C	2.45	0.55
2:X:339:ILE:HG22	2:X:340:LYS:N	2.22	0.55
1:P:387:ASN:CB	5:P:1612:ADP:O3B	2.55	0.55
1:P:75:LEU:HB3	1:P:78:ASN:OD1	2.07	0.54
1:P:252:LEU:HB2	1:P:257:ARG:CG	2.36	0.54
1:P:31:VAL:CG2	1:P:56:ILE:HG12	2.38	0.54
1:P:133:ARG:HG3	1:P:135:ASP:H	1.73	0.54
1:P:4:LYS:HG2	1:P:77:THR:HG21	1.88	0.54
1:P:26:LYS:HA	1:P:39:ILE:CG2	2.37	0.54
1:P:34:THR:HG21	1:P:36:LYS:HE2	1.88	0.54
1:P:106:LEU:HD13	1:P:106:LEU:C	2.28	0.54
1:P:203:LYS:O	1:P:206:ILE:HG12	2.07	0.54
1:P:268:LEU:H	1:P:268:LEU:CD1	2.18	0.54
1:P:493:GLU:H	1:P:524:VAL:CG2	2.10	0.54
1:P:67:PHE:HE2	4:P:1611:SF4:S1	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:337:ARG:CZ	1:P:341:ALA:HB1	2.38	0.54
1:P:218:ASP:OD1	1:P:221:LYS:HB2	2.07	0.54
1:P:589:GLN:CA	1:P:590:MET:H	2.20	0.54
1:P:318:LEU:HD12	1:P:580:ARG:HB3	1.88	0.54
1:P:529:ILE:HD12	1:P:529:ILE:H	1.73	0.54
1:P:61:CYS:SG	1:P:72:ILE:HD11	2.48	0.53
1:P:84:THR:CG2	1:P:94:LEU:HB3	2.37	0.53
1:P:224:GLY:HA3	1:P:251:TYR:CD1	2.43	0.53
1:P:243:TYR:HE2	1:P:272:LYS:HD3	1.72	0.53
1:P:339:ALA:HA	1:P:606:THR:OG1	2.08	0.53
2:X:353:ILE:CG1	2:X:354:ASP:H	2.21	0.53
1:P:87:TYR:CD2	3:P:1609:ATP:C6	2.95	0.53
1:P:295:TYR:CZ	1:P:325:GLU:HG2	2.43	0.53
1:P:585:LYS:HG2	1:P:588:SER:HA	1.89	0.53
2:X:328:TYR:CD1	2:X:366:GLU:CD	2.69	0.53
1:P:394:LEU:O	1:P:398:LEU:HD23	2.09	0.53
1:P:464:GLU:OE1	1:P:464:GLU:HA	2.08	0.53
1:P:87:TYR:CD2	3:P:1609:ATP:C5	2.97	0.53
1:P:106:LEU:HD23	1:P:290:PHE:CB	2.36	0.53
1:P:422:ILE:HG23	1:P:422:ILE:O	2.08	0.53
1:P:357:PRO:CA	1:P:372:GLU:HG3	2.39	0.53
1:P:390:GLY:CA	5:P:1612:ADP:O1A	2.47	0.53
1:P:392:THR:HG23	1:P:396:LYS:HE3	1.91	0.53
1:P:493:GLU:N	1:P:494:PRO:HD3	2.23	0.53
2:X:278:VAL:O	2:X:282:LYS:HB3	2.07	0.53
1:P:7:ARG:HB3	1:P:7:ARG:CZ	2.39	0.53
1:P:25:CYS:CB	1:P:39:ILE:HD13	2.39	0.53
1:P:67:PHE:CE2	4:P:1611:SF4:S1	3.02	0.53
1:P:293:ILE:HD11	1:P:322:ILE:CD1	2.24	0.53
1:P:388:GLY:HA2	5:P:1612:ADP:C5'	2.33	0.53
1:P:331:THR:HG23	1:P:332:GLU:N	2.24	0.53
1:P:563:ARG:HE	1:P:563:ARG:CA	2.21	0.53
1:P:254:VAL:HG12	1:P:526:HIS:O	2.09	0.53
2:X:155:PHE:O	2:X:165:VAL:CG1	2.57	0.53
1:P:26:LYS:HD2	1:P:26:LYS:O	2.09	0.52
1:P:509:VAL:HG13	1:P:510:ILE:N	2.24	0.52
1:P:11:VAL:HG22	1:P:90:ASN:HB3	1.90	0.52
1:P:67:PHE:O	1:P:68:ASP:HB2	2.09	0.52
1:P:94:LEU:HD13	1:P:95:HIS:H	1.73	0.52
1:P:280:ASP:HB3	1:P:283:VAL:HG21	1.88	0.52
1:P:371:GLU:HG2	1:P:550:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:395:ILE:HG23	1:P:396:LYS:N	2.24	0.52
1:P:532:THR:HG23	1:P:533:TYR:N	2.24	0.52
1:P:182:GLY:O	1:P:186:LYS:HA	2.09	0.52
1:P:360:LYS:HG3	1:P:406:GLU:OE1	2.09	0.52
1:P:140:TRP:HB2	1:P:160:LEU:CD1	2.39	0.52
1:P:515:LEU:HD12	1:P:608:ILE:HD11	1.90	0.52
1:P:108:LEU:HD13	1:P:277:VAL:HG22	1.91	0.52
1:P:297:VAL:HB	1:P:300:VAL:HG22	1.87	0.52
1:P:110:GLY:HA3	1:P:294:ILE:HG22	1.91	0.52
1:P:425:LYS:O	1:P:425:LYS:HG3	2.09	0.52
1:P:395:ILE:HG23	1:P:396:LYS:HD2	1.92	0.52
1:P:500:SER:O	1:P:504:ILE:HG12	2.10	0.52
2:X:165:VAL:HG12	2:X:166:LEU:H	1.74	0.52
1:P:130:ASN:O	1:P:133:ARG:HG2	2.10	0.52
1:P:565:LEU:HD13	1:P:600:TYR:HB3	1.92	0.52
2:X:290:GLU:O	2:X:291:ILE:CG1	2.55	0.52
1:P:569:ASN:ND2	1:P:586:LEU:HG	2.25	0.51
1:P:190:LEU:CB	1:P:230:PHE:CZ	2.93	0.51
1:P:409:ASP:O	1:P:411:PRO:HD3	2.09	0.51
1:P:112:ASN:OD1	3:P:1609:ATP:O3G	2.28	0.51
1:P:252:LEU:CA	1:P:256:GLN:HE21	2.19	0.51
1:P:511:ARG:HE	1:P:608:ILE:N	2.07	0.51
1:P:190:LEU:CD1	1:P:230:PHE:CZ	2.94	0.51
1:P:295:TYR:CE2	1:P:303:VAL:CG1	2.93	0.51
1:P:349:SER:O	1:P:350:ALA:HB3	2.11	0.51
1:P:387:ASN:HB3	5:P:1612:ADP:O3B	2.10	0.51
1:P:12:SER:OG	1:P:15:LYS:HD2	2.11	0.51
1:P:31:VAL:HG12	1:P:36:LYS:CB	2.28	0.51
1:P:31:VAL:HG22	1:P:56:ILE:HG12	1.93	0.51
1:P:87:TYR:HB3	3:P:1609:ATP:C2	2.44	0.51
1:P:253:ASP:OD1	1:P:256:GLN:HG2	2.11	0.51
1:P:317:PHE:O	1:P:329:PHE:HZ	1.94	0.51
1:P:565:LEU:HD12	1:P:600:TYR:HB2	1.91	0.51
1:P:388:GLY:N	5:P:1612:ADP:PB	2.81	0.51
1:P:238:GLN:HG3	1:P:239:GLU:N	2.25	0.51
1:P:334:LEU:HD22	1:P:504:ILE:CG2	2.31	0.51
2:X:305:THR:O	2:X:309:LEU:CG	2.55	0.51
2:X:326:ILE:HG22	2:X:327:ARG:N	2.25	0.51
1:P:336:PHE:CZ	1:P:529:ILE:CG2	2.94	0.51
1:P:384:MET:HG2	1:P:564:PHE:CE1	2.46	0.51
2:X:314:VAL:HG22	2:X:408:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:328:TYR:CE1	2:X:366:GLU:OE2	2.64	0.51
1:P:381:LEU:HD13	1:P:522:PHE:CE1	2.40	0.50
2:X:173:LEU:HD13	2:X:174:PRO:C	2.32	0.50
1:P:176:ILE:HB	1:P:227:LEU:HD21	1.91	0.50
2:X:339:ILE:CG2	2:X:340:LYS:N	2.74	0.50
1:P:87:TYR:CB	3:P:1609:ATP:C2	2.93	0.50
1:P:183:PRO:HA	1:P:218:ASP:CB	2.29	0.50
1:P:230:PHE:CE2	1:P:234:MET:CE	2.94	0.50
1:P:322:ILE:HG12	1:P:325:GLU:OE1	2.11	0.50
2:X:287:TYR:O	2:X:288:PHE:C	2.49	0.50
2:X:331:LYS:CB	2:X:336:ASN:HA	2.34	0.50
1:P:106:LEU:CD2	1:P:290:PHE:HB2	2.39	0.50
1:P:338:ILE:HD13	1:P:338:ILE:C	2.31	0.50
1:P:362:THR:HG22	1:P:405:ASP:OD2	2.12	0.50
1:P:570:VAL:HG23	1:P:570:VAL:O	2.11	0.50
2:X:318:ILE:O	2:X:404:ILE:C	2.49	0.50
1:P:229:ARG:HA	1:P:232:ILE:HD12	1.93	0.50
1:P:352:ARG:CB	1:P:376:SER:HA	2.41	0.50
1:P:310:VAL:HG13	1:P:311:ARG:N	2.27	0.50
2:X:285:GLU:HB2	2:X:393:GLU:HB2	1.93	0.50
2:X:309:LEU:HD11	2:X:317:LEU:HG	1.93	0.50
1:P:105:VAL:HG22	1:P:274:VAL:HB	1.94	0.50
1:P:122:ILE:HG21	1:P:129:PRO:HG3	1.93	0.50
1:P:215:LEU:HD12	1:P:215:LEU:H	1.77	0.50
1:P:336:PHE:CE1	1:P:529:ILE:CG2	2.94	0.50
1:P:516:HIS:O	1:P:518:LYS:HD2	2.12	0.50
1:P:359:LEU:HD11	1:P:409:ASP:OD2	2.11	0.50
1:P:382:VAL:HG12	1:P:383:MET:N	2.27	0.50
1:P:523:ILE:HG23	1:P:523:ILE:O	2.12	0.50
1:P:17:LYS:O	4:P:1611:SF4:S1	2.69	0.49
1:P:455:LEU:N	1:P:455:LEU:HD12	2.27	0.49
1:P:589:GLN:N	1:P:590:MET:N	2.60	0.49
2:X:367:GLU:HB3	2:X:372:TRP:CD1	2.47	0.49
1:P:244:MET:HG2	1:P:275:ILE:HG21	1.94	0.49
1:P:353:ALA:CB	1:P:375:PHE:CD1	2.95	0.49
1:P:366:PHE:HZ	1:P:549:ALA:HB2	1.77	0.49
1:P:384:MET:CG	1:P:564:PHE:CE1	2.95	0.49
1:P:585:LYS:HE3	1:P:588:SER:CB	2.42	0.49
1:P:122:ILE:CG2	1:P:129:PRO:HG3	2.41	0.49
1:P:293:ILE:CD1	1:P:322:ILE:HD12	2.25	0.49
1:P:295:TYR:HE1	1:P:305:THR:OG1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:430:VAL:CG1	1:P:434:PHE:CE1	2.96	0.49
1:P:504:ILE:O	1:P:504:ILE:HG22	2.13	0.49
2:X:350:SER:O	2:X:351:PHE:O	2.30	0.49
1:P:334:LEU:HD21	1:P:504:ILE:HG21	1.91	0.49
1:P:367:VAL:O	1:P:367:VAL:HG13	2.12	0.49
1:P:533:TYR:CZ	1:P:608:ILE:CG2	2.95	0.49
1:P:31:VAL:HG11	1:P:38:CYS:HB2	1.94	0.49
1:P:565:LEU:HD12	1:P:600:TYR:CB	2.42	0.49
2:X:326:ILE:CG2	2:X:367:GLU:C	2.80	0.49
2:X:408:LEU:CD1	2:X:412:VAL:HG22	2.43	0.49
1:P:75:LEU:HG	1:P:79:LEU:HD13	1.94	0.49
1:P:116:LYS:HD2	1:P:277:VAL:HG11	1.94	0.49
1:P:269:ALA:CB	1:P:270:PRO:HD3	2.42	0.49
1:P:431:ARG:HB3	1:P:431:ARG:HH11	1.75	0.49
1:P:568:LEU:HD12	1:P:570:VAL:CG1	2.43	0.49
1:P:27:ARG:O	1:P:28:SER:HB2	2.11	0.49
1:P:269:ALA:HB3	1:P:270:PRO:CD	2.40	0.49
1:P:354:PHE:CB	1:P:375:PHE:CZ	2.94	0.49
2:X:289:ASP:O	2:X:290:GLU:C	2.51	0.49
1:P:362:THR:HG23	1:P:362:THR:O	2.12	0.49
1:P:488:ILE:HG13	1:P:488:ILE:O	2.12	0.49
1:P:580:ARG:HH22	1:P:582:ARG:HH11	1.61	0.49
1:P:381:LEU:HD22	1:P:522:PHE:HD1	1.76	0.49
1:P:589:GLN:C	1:P:589:GLN:N	2.54	0.49
2:X:322:ASN:O	2:X:323:LEU:O	2.30	0.49
1:P:338:ILE:HG23	1:P:341:ALA:H	1.78	0.48
2:X:181:GLY:C	2:X:183:SER:H	2.16	0.48
1:P:7:ARG:HB3	1:P:7:ARG:NH1	2.29	0.48
1:P:181:LYS:HA	1:P:219:ILE:CG2	2.42	0.48
1:P:546:SER:HA	5:P:1612:ADP:O3'	2.13	0.48
1:P:557:LEU:HD22	1:P:557:LEU:N	2.24	0.48
1:P:568:LEU:HD13	1:P:568:LEU:C	2.33	0.48
1:P:585:LYS:HD3	1:P:585:LYS:H	1.78	0.48
2:X:339:ILE:HB	2:X:341:PHE:CE2	2.47	0.48
1:P:295:TYR:CZ	1:P:303:VAL:CG1	2.95	0.48
1:P:453:LYS:CB	1:P:454:PRO:HD3	2.33	0.48
2:X:215:LYS:HG2	2:X:216:VAL:H	1.78	0.48
1:P:73:ILE:CG2	1:P:75:LEU:HD21	2.44	0.48
1:P:138:PRO:HB2	1:P:140:TRP:NE1	2.28	0.48
1:P:169:LYS:C	1:P:169:LYS:HD2	2.34	0.48
1:P:97:LEU:HD11	1:P:122:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:198:SER:O	1:P:201:ASP:HB3	2.14	0.48
1:P:510:ILE:HB	1:P:534:LEU:CD2	2.44	0.48
1:P:303:VAL:HG22	1:P:304:VAL:N	2.28	0.48
1:P:380:ILE:HD11	1:P:534:LEU:O	2.13	0.48
1:P:8:ILE:HG22	1:P:10:ILE:HD12	1.94	0.47
1:P:291:VAL:CG2	1:P:313:GLY:HA3	2.44	0.47
1:P:295:TYR:CD1	1:P:295:TYR:N	2.81	0.47
1:P:457:ILE:O	1:P:457:ILE:HG22	2.14	0.47
2:X:289:ASP:OD1	2:X:290:GLU:N	2.46	0.47
2:X:334:GLU:O	2:X:335:ASP:CB	2.62	0.47
1:P:34:THR:HG21	1:P:36:LYS:HG3	1.96	0.47
1:P:75:LEU:N	1:P:75:LEU:HD22	2.29	0.47
1:P:511:ARG:NE	1:P:607:GLY:HA3	2.29	0.47
2:X:389:ASP:O	2:X:390:LYS:HG2	2.13	0.47
1:P:114:ILE:HD12	1:P:116:LYS:H	1.79	0.47
1:P:337:ARG:HE	1:P:337:ARG:HA	1.79	0.47
1:P:510:ILE:HG22	1:P:514:ILE:CD1	2.44	0.47
2:X:150:GLY:C	2:X:151:GLN:C	2.72	0.47
1:P:34:THR:HG23	1:P:36:LYS:HG3	1.93	0.47
2:X:183:SER:HB2	2:X:186:ARG:HB3	1.96	0.47
2:X:331:LYS:HG3	2:X:332:ASP:HB2	1.97	0.47
1:P:32:VAL:HG21	1:P:39:ILE:HG22	1.96	0.47
1:P:190:LEU:CB	1:P:230:PHE:HZ	2.28	0.47
1:P:529:ILE:H	1:P:529:ILE:CD1	2.27	0.47
2:X:173:LEU:HD13	2:X:173:LEU:O	2.01	0.47
2:X:289:ASP:CG	2:X:290:GLU:N	2.68	0.47
2:X:302:ILE:CD1	2:X:340:LYS:HD3	2.45	0.47
2:X:159:SER:N	2:X:162:THR:HG22	2.26	0.47
2:X:183:SER:HB2	2:X:186:ARG:CB	2.45	0.47
2:X:347:LYS:H	2:X:347:LYS:HD2	1.79	0.47
1:P:392:THR:HG22	1:P:396:LYS:CE	2.45	0.47
1:P:541:PHE:CE2	1:P:551:ALA:HB2	2.49	0.47
2:X:274:ASN:OD1	2:X:274:ASN:C	2.53	0.47
1:P:208:ILE:HG23	1:P:209:LEU:N	2.29	0.47
1:P:460:ILE:HG22	1:P:460:ILE:O	2.15	0.47
1:P:585:LYS:HE3	1:P:588:SER:HB2	1.97	0.47
2:X:328:TYR:CE1	2:X:366:GLU:CB	2.98	0.47
1:P:37:LEU:CA	1:P:54:LEU:HD12	2.45	0.46
1:P:381:LEU:HB3	1:P:522:PHE:CD1	2.51	0.46
1:P:455:LEU:O	1:P:456:ARG:HB2	2.16	0.46
1:P:557:LEU:H	1:P:557:LEU:CD2	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:300:TYR:CE1	2:X:401:PHE:CD1	3.03	0.46
1:P:252:LEU:HD22	1:P:256:GLN:NE2	2.30	0.46
1:P:415:VAL:CG2	1:P:488:ILE:HD11	2.45	0.46
2:X:301:GLY:O	2:X:305:THR:OG1	2.19	0.46
1:P:173:VAL:CG2	1:P:251:TYR:CE2	2.98	0.46
1:P:318:LEU:HA	1:P:330:ARG:HH22	1.81	0.46
1:P:511:ARG:HG2	1:P:608:ILE:H	1.80	0.46
2:X:327:ARG:HE	2:X:369:LEU:HD21	1.79	0.46
1:P:84:THR:O	1:P:131:LEU:HA	2.15	0.46
1:P:329:PHE:CE1	1:P:330:ARG:HG3	2.50	0.46
2:X:317:LEU:CB	2:X:384:LEU:HD11	2.42	0.46
1:P:352:ARG:HB3	1:P:376:SER:CB	2.45	0.46
2:X:199:VAL:HG11	2:X:233:LEU:HD13	1.97	0.46
2:X:377:TYR:OH	2:X:384:LEU:HD22	2.16	0.46
1:P:130:ASN:O	1:P:131:LEU:HB2	2.16	0.46
1:P:300:VAL:CG2	1:P:301:TYR:CD1	2.95	0.46
1:P:491:ILE:HB	1:P:523:ILE:HD13	1.93	0.46
1:P:162:ASP:CG	1:P:165:LYS:HE3	2.36	0.46
1:P:295:TYR:CE2	1:P:325:GLU:HG2	2.51	0.46
1:P:423:ALA:HB1	1:P:424:PRO:HD2	1.98	0.46
2:X:271:ALA:O	2:X:275:VAL:HG22	2.16	0.46
1:P:94:LEU:HD23	1:P:115:GLY:HA3	1.98	0.45
1:P:474:GLN:CA	1:P:474:GLN:HE21	2.27	0.45
1:P:444:ASN:CB	1:P:445:PRO:HD2	2.37	0.45
1:P:32:VAL:HG12	1:P:32:VAL:O	2.16	0.45
1:P:544:ILE:HG23	1:P:544:ILE:O	2.16	0.45
2:X:155:PHE:O	2:X:165:VAL:HG12	2.16	0.45
2:X:326:ILE:CG2	2:X:327:ARG:N	2.79	0.45
1:P:167:ILE:HG23	1:P:167:ILE:O	2.16	0.45
1:P:197:LYS:HG3	1:P:201:ASP:OD2	2.16	0.45
1:P:297:VAL:HG12	1:P:298:PRO:N	2.31	0.45
1:P:568:LEU:CD1	1:P:570:VAL:CG1	2.94	0.45
2:X:390:LYS:O	2:X:391:SER:OG	2.34	0.45
1:P:122:ILE:HG13	1:P:123:LEU:N	2.30	0.45
1:P:133:ARG:HD3	1:P:134:PHE:CD2	2.51	0.45
1:P:381:LEU:HD23	1:P:382:VAL:O	2.17	0.45
2:X:309:LEU:HD23	2:X:314:VAL:CB	2.44	0.45
1:P:17:LYS:NZ	1:P:19:LYS:HB2	2.31	0.45
1:P:510:ILE:CG2	1:P:514:ILE:CD1	2.95	0.45
1:P:443:LEU:N	1:P:443:LEU:HD22	2.32	0.45
1:P:510:ILE:HG23	1:P:514:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:585:LYS:O	1:P:591:ASP:HB2	2.16	0.45
1:P:600:TYR:CD1	1:P:600:TYR:N	2.83	0.45
1:P:338:ILE:CG2	1:P:340:ASP:HB3	2.46	0.45
1:P:167:ILE:HD13	1:P:167:ILE:C	2.36	0.45
1:P:186:LYS:H	1:P:186:LYS:HD3	1.81	0.45
1:P:285:ASP:OD2	1:P:583:ILE:HG22	2.16	0.45
1:P:571:THR:HG23	1:P:595:LYS:HZ2	1.79	0.45
2:X:155:PHE:O	2:X:165:VAL:HG13	2.17	0.45
2:X:373:LEU:O	2:X:377:TYR:CD1	2.69	0.45
1:P:300:VAL:HG23	1:P:301:TYR:H	1.80	0.44
1:P:353:ALA:CB	1:P:375:PHE:CE1	2.94	0.44
2:X:368:PRO:CG	2:X:371:GLU:HB2	2.33	0.44
1:P:100:PRO:HA	1:P:273:TYR:CE1	2.53	0.44
1:P:256:GLN:HA	1:P:259:ASN:HD22	1.82	0.44
1:P:444:ASN:OD1	1:P:447:PHE:HB2	2.17	0.44
1:P:274:VAL:HG12	1:P:275:ILE:N	2.32	0.44
1:P:421:LYS:N	1:P:421:LYS:HD3	2.31	0.44
2:X:233:LEU:HD11	2:X:239:PHE:CD1	2.51	0.44
2:X:293:GLN:HB3	2:X:297:LYS:HB2	1.98	0.44
2:X:328:TYR:CE1	2:X:366:GLU:HB3	2.52	0.44
1:P:219:ILE:HD11	1:P:227:LEU:CD1	2.47	0.44
1:P:401:ALA:C	1:P:402:LEU:HD12	2.38	0.44
1:P:402:LEU:HD12	1:P:402:LEU:N	2.32	0.44
1:P:515:LEU:CD1	1:P:608:ILE:CG1	2.95	0.44
1:P:533:TYR:OH	1:P:608:ILE:HG21	2.17	0.44
2:X:273:ALA:C	2:X:277:TYR:CD2	2.85	0.44
1:P:92:PHE:CD2	3:P:1609:ATP:C4'	3.01	0.44
1:P:138:PRO:HB2	1:P:140:TRP:CD1	2.52	0.44
1:P:143:ILE:HG23	1:P:144:ILE:N	2.32	0.44
2:X:290:GLU:HG2	2:X:291:ILE:HG12	1.99	0.44
2:X:318:ILE:N	2:X:405:GLY:O	2.39	0.44
1:P:103:GLY:HA2	1:P:271:THR:HA	1.99	0.44
1:P:128:LYS:HD3	1:P:136:ASP:O	2.18	0.44
1:P:453:LYS:HB2	1:P:454:PRO:CD	2.36	0.44
2:X:417:LEU:HB3	2:X:418:VAL:H	1.49	0.44
1:P:114:ILE:CG1	1:P:294:ILE:CG2	2.95	0.44
1:P:133:ARG:HG3	1:P:134:PHE:N	2.32	0.44
1:P:305:THR:CG2	1:P:306:LEU:N	2.80	0.44
1:P:491:ILE:HG22	1:P:492:ASP:N	2.31	0.44
1:P:11:VAL:HG22	1:P:90:ASN:CB	2.47	0.44
1:P:283:VAL:O	1:P:287:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:338:ILE:HD12	1:P:340:ASP:HB2	2.00	0.44
1:P:415:VAL:HG22	1:P:488:ILE:CG1	2.48	0.44
1:P:176:ILE:CB	1:P:177:PRO:HD3	2.42	0.43
1:P:182:GLY:N	1:P:183:PRO:HD3	2.33	0.43
1:P:320:GLY:CA	1:P:329:PHE:CZ	2.95	0.43
1:P:578:SER:OG	1:P:580:ARG:HG2	2.17	0.43
1:P:536:ASP:CA	1:P:557:LEU:HD11	2.48	0.43
2:X:163:ARG:HH11	2:X:163:ARG:HD3	1.67	0.43
2:X:285:GLU:CB	2:X:393:GLU:HB2	2.48	0.43
2:X:297:LYS:O	2:X:298:PHE:CZ	2.70	0.43
1:P:70:ILE:HG22	1:P:71:GLN:N	2.32	0.43
1:P:283:VAL:HG23	1:P:284:LEU:N	2.33	0.43
1:P:445:PRO:HG2	1:P:446:GLN:OE1	2.18	0.43
1:P:304:VAL:HG12	1:P:305:THR:O	2.18	0.43
1:P:357:PRO:HA	1:P:372:GLU:CG	2.46	0.43
1:P:468:LEU:HD23	1:P:473:LEU:HB2	2.00	0.43
1:P:510:ILE:CG2	1:P:514:ILE:HD11	2.48	0.43
1:P:306:LEU:HG	1:P:307:PRO:N	2.34	0.43
1:P:352:ARG:CD	1:P:376:SER:CB	2.95	0.43
1:P:353:ALA:HB3	1:P:375:PHE:CD1	2.54	0.43
1:P:430:VAL:HG13	1:P:434:PHE:HE1	1.83	0.43
2:X:290:GLU:C	2:X:291:ILE:HG12	2.37	0.43
1:P:108:LEU:CD1	1:P:116:LYS:HG2	2.48	0.43
1:P:348:ASP:O	1:P:352:ARG:HG2	2.18	0.43
1:P:588:SER:H	1:P:591:ASP:HB2	1.83	0.43
1:P:49:PHE:C	1:P:50:ILE:HD12	2.38	0.43
1:P:96:ARG:HD2	1:P:304:VAL:O	2.18	0.43
1:P:120:LEU:HD23	1:P:120:LEU:C	2.39	0.43
1:P:183:PRO:O	1:P:186:LYS:HG3	2.19	0.43
1:P:194:ARG:HB2	1:P:237:VAL:HG11	2.00	0.43
1:P:180:ILE:HG23	1:P:180:ILE:O	2.17	0.43
1:P:202:VAL:CG1	1:P:203:LYS:N	2.82	0.43
1:P:468:LEU:CG	1:P:469:SER:H	2.16	0.43
2:X:195:ARG:O	2:X:199:VAL:HG23	2.19	0.43
2:X:368:PRO:O	2:X:372:TRP:CD1	2.72	0.43
1:P:97:LEU:HD11	1:P:122:ILE:HD11	1.94	0.43
1:P:157:THR:HG23	1:P:158:LYS:N	2.33	0.43
1:P:198:SER:HB3	1:P:199:PRO:CD	2.45	0.43
1:P:261:ALA:HB1	1:P:287:LEU:CD1	2.49	0.43
1:P:588:SER:H	1:P:591:ASP:CB	2.31	0.43
2:X:330:PHE:CE1	2:X:341:PHE:CE2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:73:ILE:CG2	1:P:75:LEU:CD2	2.97	0.42
1:P:451:VAL:HG13	1:P:452:VAL:H	1.84	0.42
1:P:532:THR:CG2	1:P:533:TYR:N	2.82	0.42
2:X:323:LEU:HD12	2:X:370:ILE:N	2.34	0.42
2:X:155:PHE:CE1	2:X:202:VAL:HG13	2.54	0.42
2:X:417:LEU:O	2:X:418:VAL:HG23	2.19	0.42
1:P:322:ILE:HG23	1:P:322:ILE:O	2.18	0.42
1:P:491:ILE:N	1:P:491:ILE:CD1	2.82	0.42
1:P:114:ILE:CD1	1:P:116:LYS:N	2.82	0.42
1:P:529:ILE:N	1:P:529:ILE:CD1	2.83	0.42
2:X:383:THR:C	2:X:384:LEU:HD12	2.40	0.42
1:P:87:TYR:CD2	3:P:1609:ATP:C4	3.07	0.42
1:P:116:LYS:HZ2	1:P:116:LYS:HB2	1.84	0.42
1:P:160:LEU:HD23	1:P:160:LEU:C	2.39	0.42
1:P:237:VAL:CG1	1:P:238:GLN:N	2.82	0.42
1:P:363:GLN:HB3	5:P:1612:ADP:C2	2.54	0.42
2:X:199:VAL:CG1	2:X:233:LEU:HD13	2.49	0.42
2:X:268:SER:O	2:X:271:ALA:N	2.53	0.42
1:P:112:ASN:HA	3:P:1609:ATP:PG	2.58	0.42
1:P:190:LEU:HB2	1:P:230:PHE:CE1	2.54	0.42
1:P:268:LEU:CD1	1:P:268:LEU:N	2.81	0.42
1:P:384:MET:HG3	1:P:564:PHE:CE1	2.54	0.42
2:X:317:LEU:HB3	2:X:384:LEU:HD21	2.00	0.42
1:P:120:LEU:CG	1:P:244:MET:HE2	2.30	0.42
1:P:127:GLN:OE1	1:P:127:GLN:HA	2.20	0.42
1:P:143:ILE:CG2	1:P:144:ILE:N	2.82	0.42
1:P:231:ALA:HA	1:P:234:MET:CE	2.50	0.42
1:P:520:THR:CG2	1:P:521:ALA:N	2.83	0.42
2:X:306:LEU:HD11	2:X:369:LEU:HD21	2.02	0.42
1:P:39:ILE:HD11	1:P:48:ALA:HB1	2.01	0.42
1:P:50:ILE:N	1:P:50:ILE:CD1	2.83	0.42
1:P:219:ILE:HD12	1:P:222:LEU:HD12	2.02	0.42
1:P:430:VAL:HG12	1:P:434:PHE:CE1	2.55	0.42
1:P:607:GLY:C	1:P:608:ILE:O	2.57	0.42
1:P:114:ILE:HG12	1:P:294:ILE:HG23	2.01	0.42
1:P:331:THR:CG2	1:P:332:GLU:N	2.83	0.42
1:P:395:ILE:CG2	1:P:396:LYS:N	2.83	0.42
1:P:444:ASN:ND2	1:P:447:PHE:CD2	2.86	0.42
1:P:505:ILE:CG2	1:P:506:CYS:N	2.82	0.42
1:P:509:VAL:CG1	1:P:510:ILE:N	2.82	0.42
2:X:326:ILE:HA	2:X:369:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:39:ILE:O	1:P:39:ILE:HG23	2.19	0.42
1:P:73:ILE:HG21	1:P:75:LEU:HD21	2.02	0.42
1:P:129:PRO:HB2	1:P:143:ILE:HD13	2.01	0.42
1:P:363:GLN:HG2	5:P:1612:ADP:C2	2.55	0.42
1:P:455:LEU:HD12	1:P:455:LEU:H	1.85	0.42
1:P:538:VAL:CG1	1:P:539:ILE:N	2.83	0.42
2:X:310:ASP:HA	2:X:380:PHE:CD1	2.55	0.41
1:P:47:ILE:CD1	1:P:48:ALA:N	2.82	0.41
1:P:157:THR:CG2	1:P:158:LYS:N	2.82	0.41
1:P:168:ILE:HG23	1:P:168:ILE:O	2.19	0.41
1:P:169:LYS:HD2	1:P:169:LYS:O	2.20	0.41
1:P:261:ALA:CB	1:P:287:LEU:HD11	2.50	0.41
1:P:389:THR:O	1:P:549:ALA:CB	2.67	0.41
2:X:195:ARG:NH1	2:X:229:PHE:CD2	2.88	0.41
2:X:288:PHE:CG	2:X:289:ASP:N	2.83	0.41
1:P:53:ILE:CG2	1:P:54:LEU:N	2.82	0.41
1:P:87:TYR:CE1	1:P:92:PHE:HD2	2.38	0.41
1:P:97:LEU:CD1	1:P:122:ILE:CD1	2.93	0.41
1:P:118:THR:HG23	1:P:119:ALA:N	2.34	0.41
1:P:273:TYR:HH	1:P:275:ILE:HB	1.80	0.41
1:P:392:THR:CG2	1:P:396:LYS:CE	2.96	0.41
1:P:441:GLN:O	1:P:447:PHE:HD2	2.03	0.41
1:P:565:LEU:CD1	1:P:600:TYR:CB	2.98	0.41
1:P:574:ARG:HD3	1:P:580:ARG:O	2.20	0.41
1:P:578:SER:O	1:P:579:PHE:HB2	2.19	0.41
2:X:368:PRO:O	2:X:368:PRO:CD	2.68	0.41
2:X:408:LEU:HD11	2:X:412:VAL:HG22	2.02	0.41
1:P:305:THR:CG2	1:P:306:LEU:H	2.30	0.41
1:P:382:VAL:CG1	1:P:383:MET:N	2.82	0.41
1:P:444:ASN:OD1	1:P:447:PHE:CD2	2.73	0.41
1:P:505:ILE:HG23	1:P:506:CYS:N	2.35	0.41
1:P:517:ASN:O	1:P:518:LYS:HB2	2.21	0.41
2:X:317:LEU:HD22	2:X:319:VAL:HG23	2.02	0.41
1:P:100:PRO:CB	1:P:273:TYR:CE1	3.03	0.41
1:P:291:VAL:HG22	1:P:309:SER:O	2.20	0.41
1:P:309:SER:OG	1:P:312:GLU:HB2	2.19	0.41
1:P:371:GLU:CG	1:P:550:HIS:CE1	3.03	0.41
1:P:581:PRO:HB3	1:P:601:PHE:CE1	2.56	0.41
1:P:84:THR:CG2	1:P:85:HIS:N	2.83	0.41
1:P:599:ASN:HD22	1:P:599:ASN:N	2.19	0.41
2:X:377:TYR:CE1	2:X:384:LEU:HD22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:97:LEU:HG	1:P:122:ILE:CD1	2.32	0.41
1:P:113:GLY:H	3:P:1609:ATP:PG	2.42	0.41
1:P:524:VAL:O	1:P:525:GLU:HG2	2.20	0.41
1:P:92:PHE:CG	3:P:1609:ATP:C1'	3.03	0.41
1:P:198:SER:CB	1:P:199:PRO:HD2	2.42	0.41
1:P:316:ILE:O	1:P:316:ILE:HG22	2.20	0.41
2:X:278:VAL:HG12	2:X:279:GLN:N	2.36	0.41
1:P:44:THR:CG2	1:P:45:SER:N	2.82	0.41
1:P:83:VAL:O	1:P:146:TYR:CZ	2.74	0.41
1:P:100:PRO:CB	1:P:273:TYR:CZ	3.02	0.41
1:P:112:ASN:CA	3:P:1609:ATP:O2G	2.68	0.41
1:P:194:ARG:HB3	1:P:237:VAL:HG13	1.99	0.41
1:P:326:ASN:O	1:P:327:LEU:HD23	2.21	0.41
2:X:280:GLU:HB3	2:X:281:LYS:H	1.61	0.41
2:X:326:ILE:CG1	2:X:368:PRO:HA	2.50	0.41
2:X:397:PHE:O	2:X:401:PHE:N	2.54	0.41
1:P:84:THR:HG23	1:P:94:LEU:HB3	2.02	0.41
1:P:244:MET:HG2	1:P:275:ILE:CG2	2.51	0.41
1:P:511:ARG:O	1:P:515:LEU:HG	2.20	0.41
2:X:290:GLU:OE2	2:X:291:ILE:CA	2.69	0.41
1:P:128:LYS:HE3	1:P:137:PRO:HA	2.03	0.40
1:P:159:MET:CE	1:P:159:MET:CA	2.95	0.40
1:P:457:ILE:HA	1:P:460:ILE:HB	2.03	0.40
1:P:511:ARG:HG2	1:P:608:ILE:HG23	2.02	0.40
2:X:173:LEU:HD13	2:X:175:LYS:N	2.36	0.40
2:X:173:LEU:CD1	2:X:175:LYS:N	2.84	0.40
2:X:289:ASP:C	2:X:291:ILE:N	2.73	0.40
2:X:309:LEU:C	2:X:380:PHE:HD1	2.24	0.40
1:P:29:CYS:HA	1:P:30:PRO:HD2	1.87	0.40
1:P:114:ILE:HD13	1:P:294:ILE:CG2	2.45	0.40
1:P:115:GLY:C	1:P:118:THR:HG22	2.42	0.40
1:P:167:ILE:HG22	1:P:243:TYR:HA	2.03	0.40
1:P:182:GLY:H	1:P:183:PRO:HD3	1.86	0.40
1:P:441:GLN:OE1	1:P:447:PHE:CD2	2.75	0.40
2:X:293:GLN:CB	2:X:297:LYS:HB2	2.51	0.40
2:X:319:VAL:HG13	2:X:323:LEU:HD11	2.04	0.40
2:X:325:THR:O	2:X:369:LEU:HB2	2.20	0.40
1:P:94:LEU:HD23	1:P:118:THR:HG21	2.04	0.40
1:P:219:ILE:CG2	1:P:220:GLU:N	2.83	0.40
1:P:254:VAL:CG2	1:P:255:LYS:N	2.84	0.40
1:P:291:VAL:O	1:P:291:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:415:VAL:HG22	1:P:488:ILE:CD1	2.48	0.40
1:P:424:PRO:HB3	1:P:465:VAL:CG1	2.48	0.40
2:X:315:GLU:HG3	2:X:409:ARG:HG2	2.04	0.40
1:P:117:SER:N	3:P:1609:ATP:O2B	2.48	0.40
1:P:435:PHE:CD2	1:P:435:PHE:C	2.95	0.40
1:P:508:LYS:CG	1:P:512:ARG:HD2	2.51	0.40
2:X:165:VAL:HG12	2:X:166:LEU:N	2.35	0.40
1:P:38:CYS:SG	1:P:55:CYS:CA	3.08	0.40
1:P:130:ASN:C	1:P:135:ASP:HB3	2.40	0.40
1:P:146:TYR:CD2	1:P:146:TYR:O	2.75	0.40
1:P:190:LEU:HB2	1:P:230:PHE:CZ	2.57	0.40
1:P:361:LYS:HD3	1:P:362:THR:N	2.36	0.40
1:P:515:LEU:HD12	1:P:608:ILE:CD1	2.51	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	P	606/608 (100%)	563 (93%)	35 (6%)	8 (1%)	12 48
2	X	280/282 (99%)	197 (70%)	43 (15%)	40 (14%)	0 4
All	All	886/890 (100%)	760 (86%)	78 (9%)	48 (5%)	3 19

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	68	ASP
1	P	138	PRO
1	P	197	LYS
2	X	162	THR
2	X	172	ASP

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Mol	Chain	Res	Type
2	X	173	LEU
2	X	175	LYS
2	X	213	ASN
2	X	280	GLU
2	X	282	LYS
2	X	284	LEU
2	X	286	ALA
2	X	288	PHE
2	X	290	GLU
2	X	293	GLN
2	X	351	PHE
2	X	360	GLU
2	X	391	SER
2	X	392	SER
2	X	393	GLU
2	X	411	LYS
2	X	179	ARG
2	X	184	ALA
2	X	227	ALA
2	X	281	LYS
2	X	291	ILE
2	X	295	THR
2	X	323	LEU
2	X	335	ASP
2	X	417	LEU
2	X	418	VAL
2	X	419	ASP
1	P	136	ASP
2	X	320	PHE
2	X	350	SER
1	P	96	ARG
2	X	177	HIS
2	X	182	GLN
2	X	283	LEU
2	X	343	GLU
2	X	353	ILE
2	X	287	TYR
1	P	182	GLY
1	P	438	ILE
2	X	319	VAL
1	P	424	PRO
2	X	296	GLY

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Mol	Chain	Res	Type
2	X	358	GLY

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	P	537/537 (100%)	516 (96%)	21 (4%)	32 56
2	X	234/234 (100%)	187 (80%)	47 (20%)	1 7
All	All	771/771 (100%)	703 (91%)	68 (9%)	13 31

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

Mol	Chain	Res	Type
1	P	7	ARG
1	P	26	LYS
1	P	47	ILE
1	P	63	LYS
1	P	128	LYS
1	P	167	ILE
1	P	169	LYS
1	P	186	LYS
1	P	195	MET
1	P	237	VAL
1	P	275	ILE
1	P	338	ILE
1	P	361	LYS
1	P	369	ASN
1	P	403	LYS
1	P	474	GLN
1	P	583	ILE
1	P	585	LYS
1	P	586	LEU
1	P	587	ASP
1	P	589	GLN
2	X	162	THR

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Mol	Chain	Res	Type
2	X	163	ARG
2	X	164	THR
2	X	172	ASP
2	X	173	LEU
2	X	176	LYS
2	X	179	ARG
2	X	182	GLN
2	X	185	LEU
2	X	186	ARG
2	X	194	LYS
2	X	199	VAL
2	X	209	ASN
2	X	215	LYS
2	X	235	LYS
2	X	250	ILE
2	X	252	ASP
2	X	268	SER
2	X	270	GLU
2	X	275	VAL
2	X	276	LYS
2	X	278	VAL
2	X	281	LYS
2	X	282	LYS
2	X	284	LEU
2	X	285	GLU
2	X	287	TYR
2	X	288	PHE
2	X	289	ASP
2	X	290	GLU
2	X	304	ASP
2	X	317	LEU
2	X	320	PHE
2	X	331	LYS
2	X	336	ASN
2	X	345	GLU
2	X	347	LYS
2	X	350	SER
2	X	353	ILE
2	X	361	MET
2	X	372	TRP
2	X	387	ILE
2	X	393	GLU

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Mol	Chain	Res	Type
2	X	414	PHE
2	X	415	GLU
2	X	417	LEU
2	X	418	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	85	HIS
1	P	95	HIS
1	P	112	ASN
1	P	210	GLN
1	P	238	GLN
1	P	256	GLN
1	P	259	ASN
1	P	347	ASN
1	P	369	ASN
1	P	432	GLN
1	P	448	GLN
1	P	463	GLN
1	P	474	GLN
1	P	562	ASN
1	P	599	ASN
1	P	605	ASN
2	X	151	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	P	1612	-	24,29,29	1.16	4 (16%)	29,45,45	1.27	4 (13%)
3	ATP	P	1609	6	26,33,33	2.19	8 (30%)	31,52,52	3.26	10 (32%)
4	SF4	P	1611	1	0,12,12	-	-	-		
4	SF4	P	1610	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	P	1610	1	-	-	0/6/5/5
3	ATP	P	1609	6	-	2/18/38/38	0/3/3/3
4	SF4	P	1611	1	-	-	0/6/5/5
5	ADP	P	1612	-	-	4/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1609	ATP	C4-N3	6.03	1.44	1.35
3	P	1609	ATP	O5'-C5'	-4.58	1.27	1.44
3	P	1609	ATP	O4'-C1'	3.97	1.46	1.41
3	P	1609	ATP	PA-O5'	-2.97	1.47	1.59
5	P	1612	ADP	PB-O3B	2.62	1.64	1.54
5	P	1612	ADP	C4-N3	2.54	1.39	1.35
3	P	1609	ATP	C3'-C4'	-2.20	1.47	1.53
3	P	1609	ATP	C8-N7	-2.19	1.30	1.34
3	P	1609	ATP	C2-N3	2.17	1.35	1.32
3	P	1609	ATP	PB-O1B	-2.13	1.43	1.50
5	P	1612	ADP	C8-N7	-2.10	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	1612	ADP	C2-N3	2.06	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	1609	ATP	O5'-C5'-C4'	12.29	151.28	108.99
3	P	1609	ATP	O5'-PA-O1A	-6.50	83.69	109.07
3	P	1609	ATP	PA-O5'-C5'	5.67	154.90	121.68
3	P	1609	ATP	C5'-C4'-C3'	-5.23	95.58	115.18
3	P	1609	ATP	O4'-C4'-C3'	4.72	114.45	105.11
3	P	1609	ATP	C3'-C2'-C1'	3.54	106.31	100.98
5	P	1612	ADP	O4'-C1'-C2'	-3.30	102.11	106.93
5	P	1612	ADP	O2B-PB-O3A	2.81	114.06	104.64
3	P	1609	ATP	C4-C5-N7	2.72	112.23	109.40
5	P	1612	ADP	C3'-C2'-C1'	2.55	104.81	100.98
5	P	1612	ADP	C4-C5-N7	2.43	111.93	109.40
3	P	1609	ATP	O2A-PA-O1A	2.19	123.07	112.24
3	P	1609	ATP	O2A-PA-O5'	-2.14	97.82	107.75
3	P	1609	ATP	O2B-PB-O1B	2.02	122.25	112.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	1609	ATP	C4'-C5'-O5'-PA
5	P	1612	ADP	C5'-O5'-PA-O1A
5	P	1612	ADP	C5'-O5'-PA-O3A
3	P	1609	ATP	PG-O3B-PB-O2B
5	P	1612	ADP	PA-O3A-PB-O2B
5	P	1612	ADP	PA-O3A-PB-O3B

There are no ring outliers.

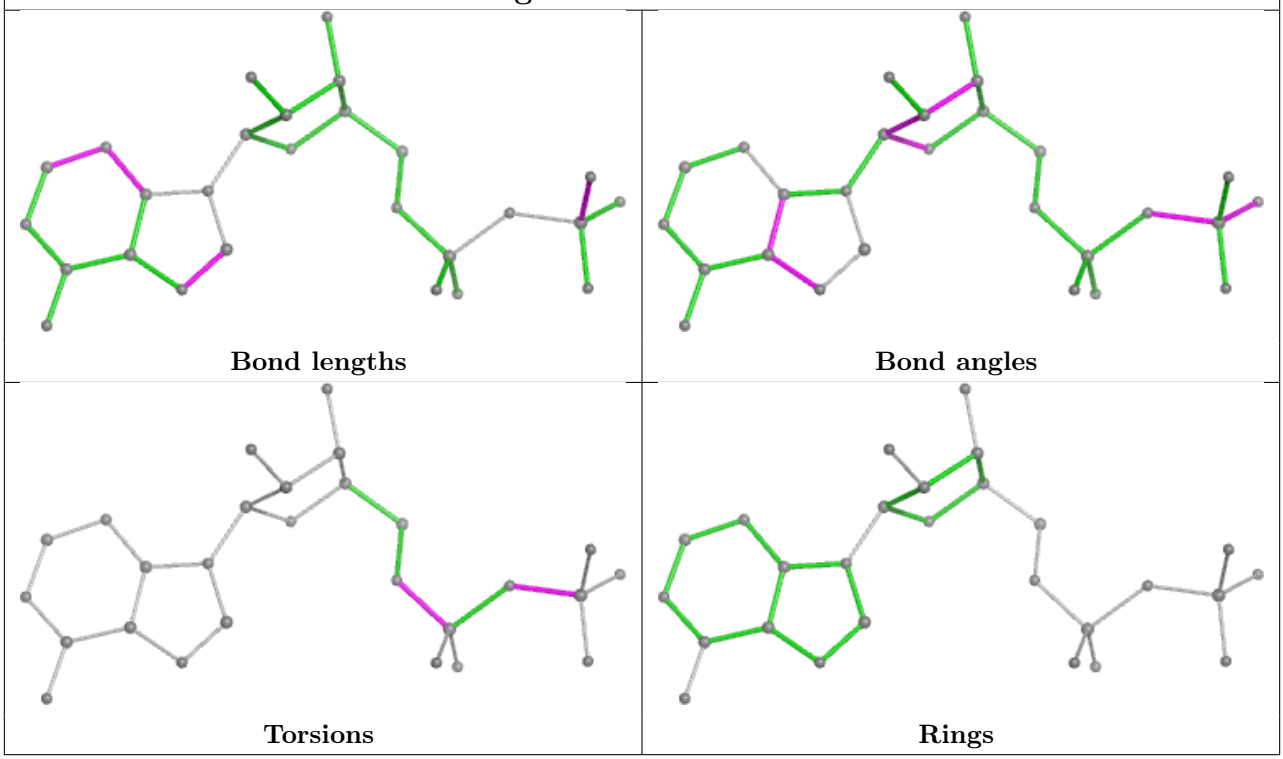
4 monomers are involved in 65 short contacts:

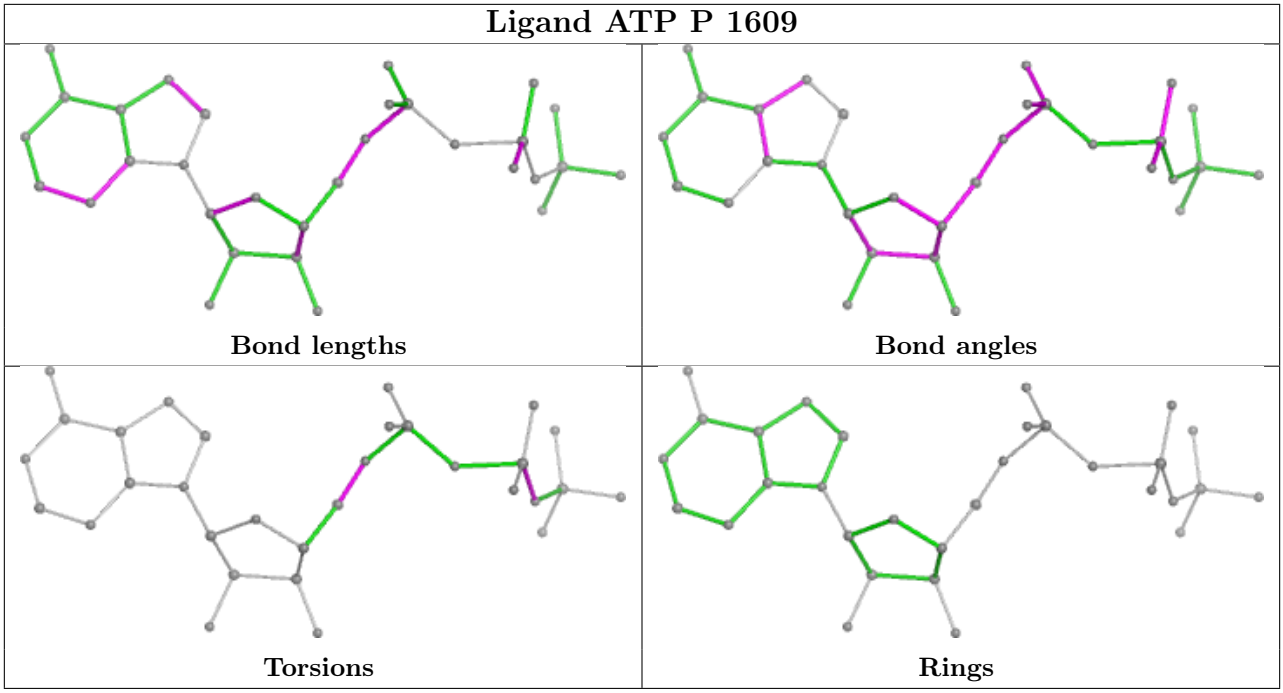
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	1612	ADP	20	0
3	P	1609	ATP	29	0
4	P	1611	SF4	9	0
4	P	1610	SF4	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

Ligand ADP P 1612





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	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	150:GLY	C	151:GLN	N	1.75

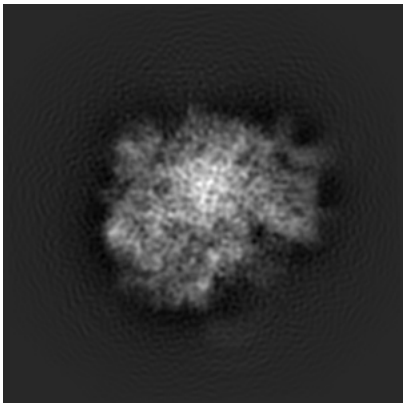
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2598. These allow visual inspection of the internal detail of the map and identification of artifacts.

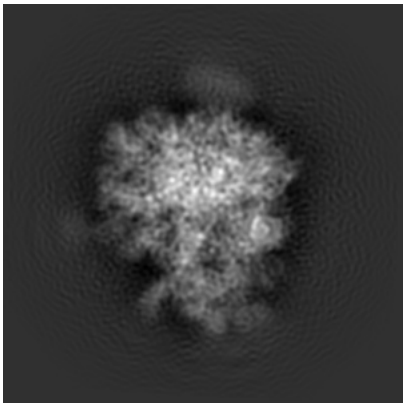
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

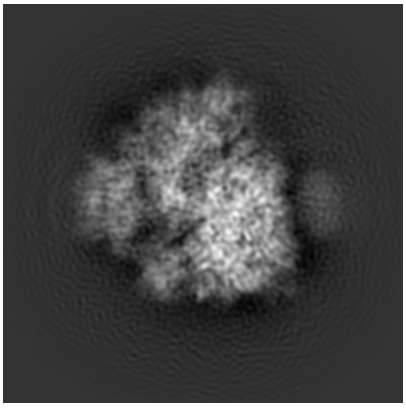
6.1.1 Primary map



X



Y

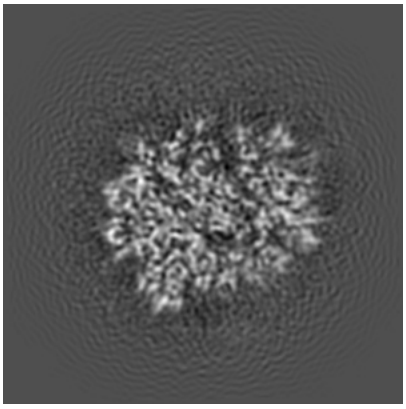


Z

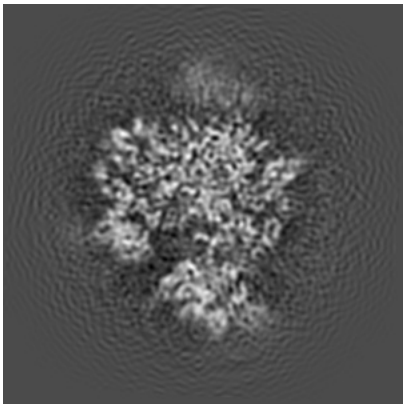
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

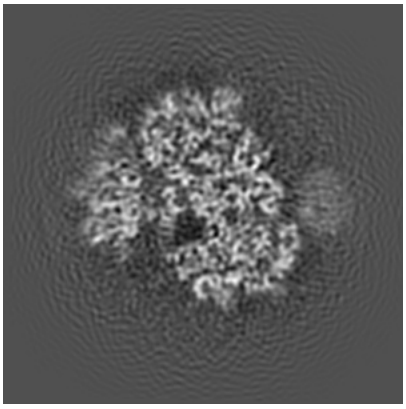
6.2.1 Primary map



X Index: 184



Y Index: 184

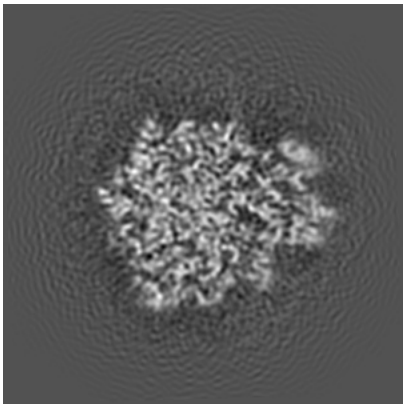


Z Index: 184

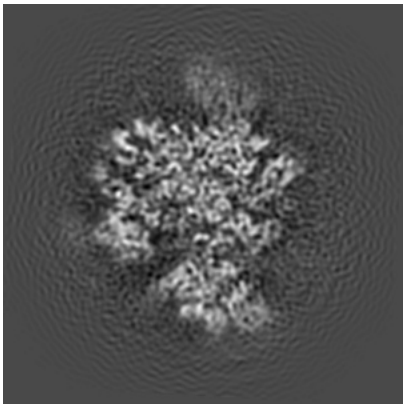
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

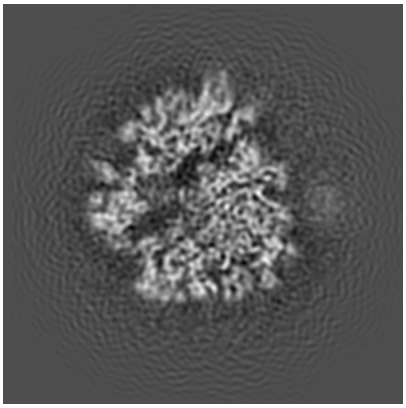
6.3.1 Primary map



X Index: 197



Y Index: 186

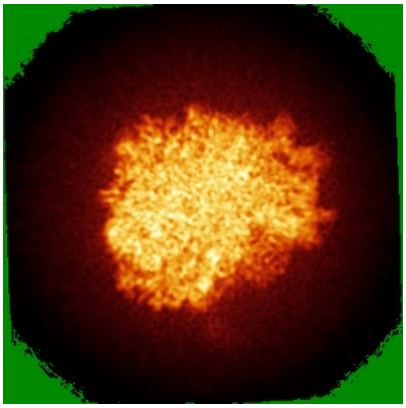


Z Index: 168

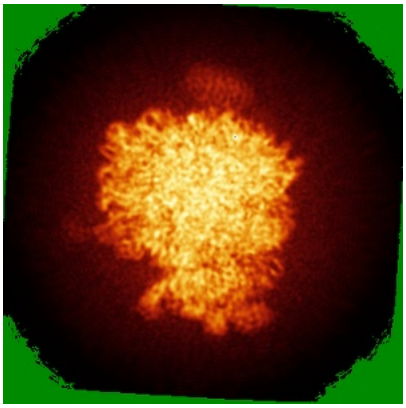
The images above show the largest variance slices of the map in three orthogonal directions.

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

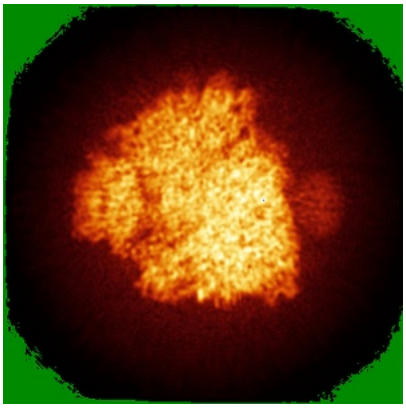
6.4.1 Primary map



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

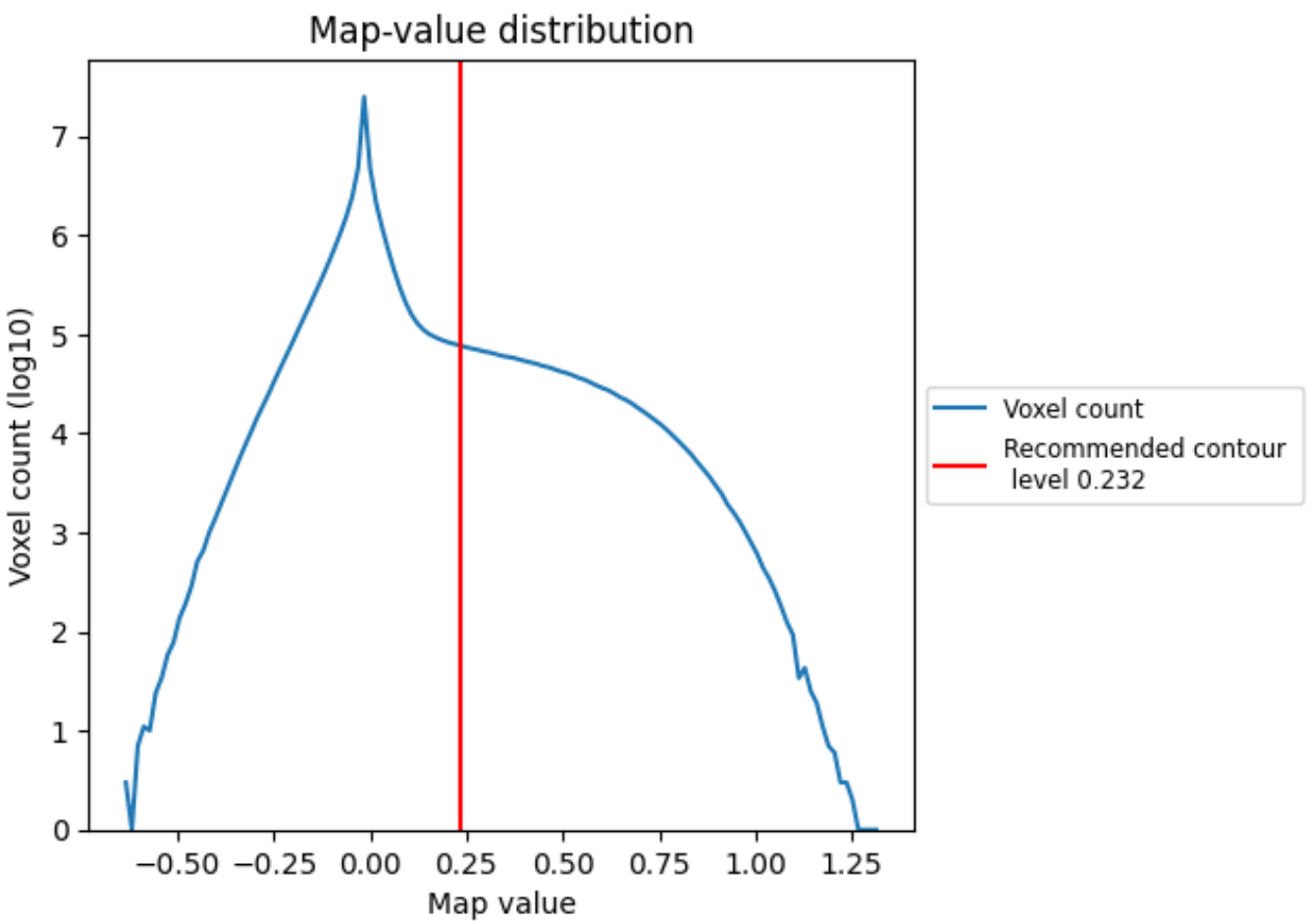
6.6 Mask visualisation (i)

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

7 Map analysis (i)

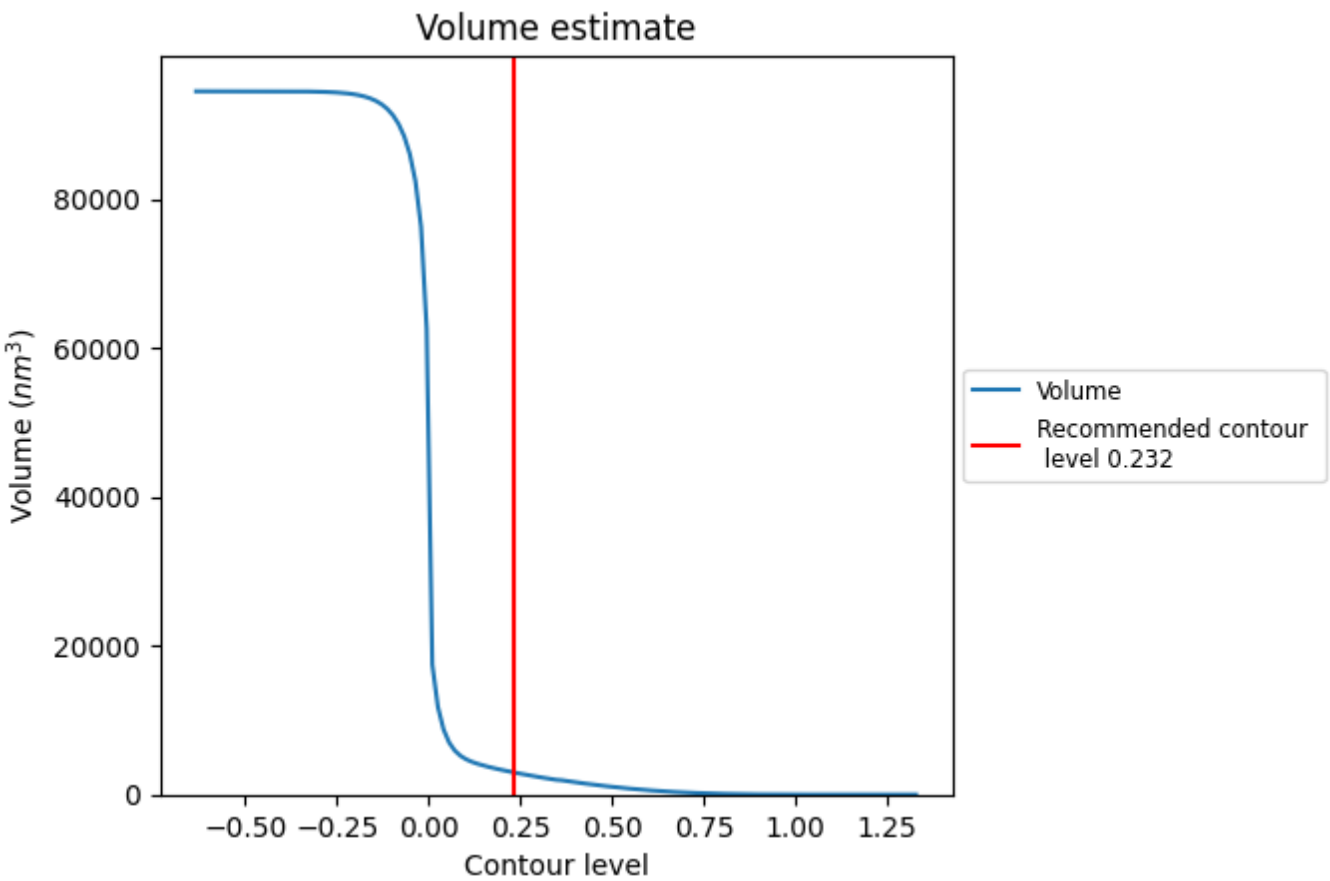
This section contains the results of statistical analysis of the map.

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.

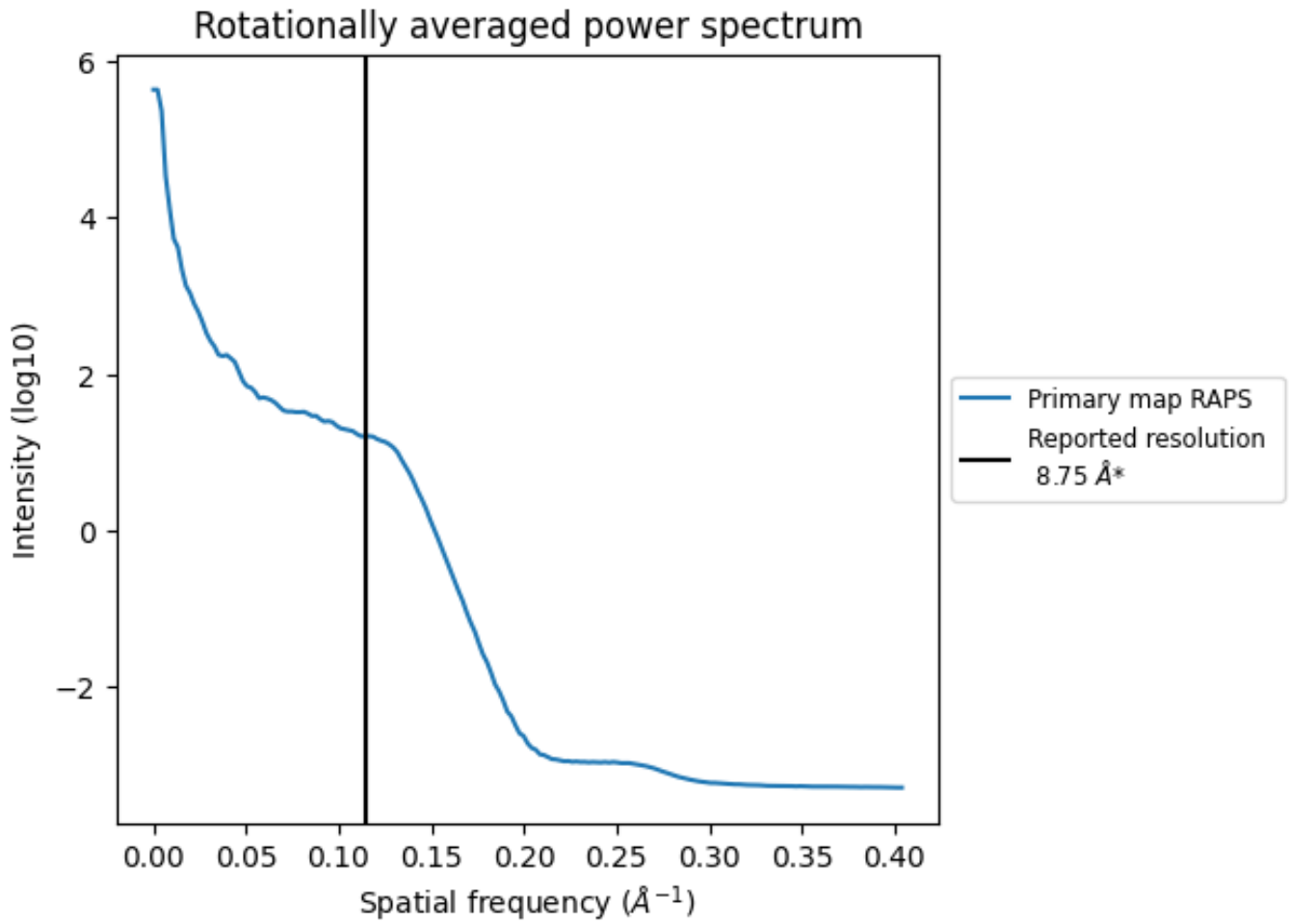
7.2 Volume estimate (i)



The volume at the recommended contour level is 2976 nm^3; this corresponds to an approximate mass of 2688 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 0.114 Å^{-1}

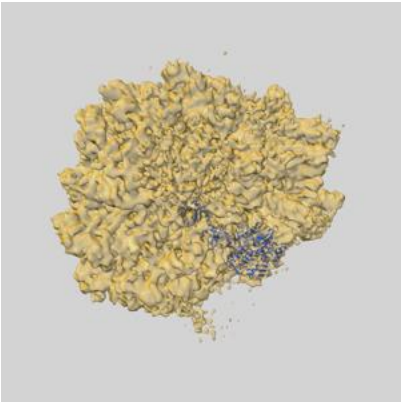
8 Fourier-Shell correlation (i)

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

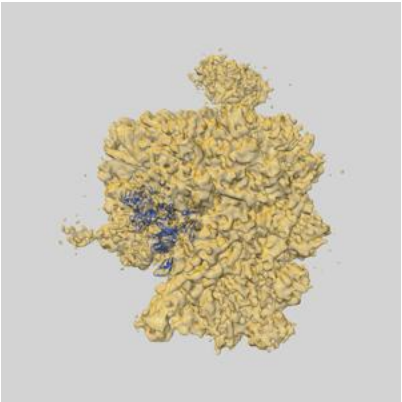
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2598 and PDB model 4CRM. Per-residue inclusion information can be found in section 3 on page 7.

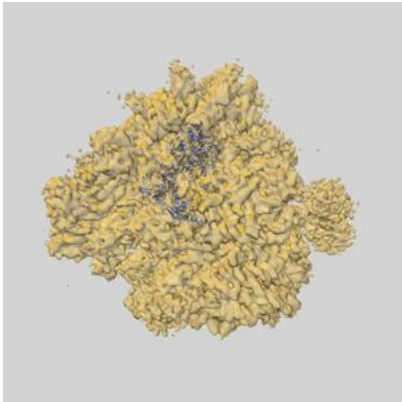
9.1 Map-model overlay (i)



X



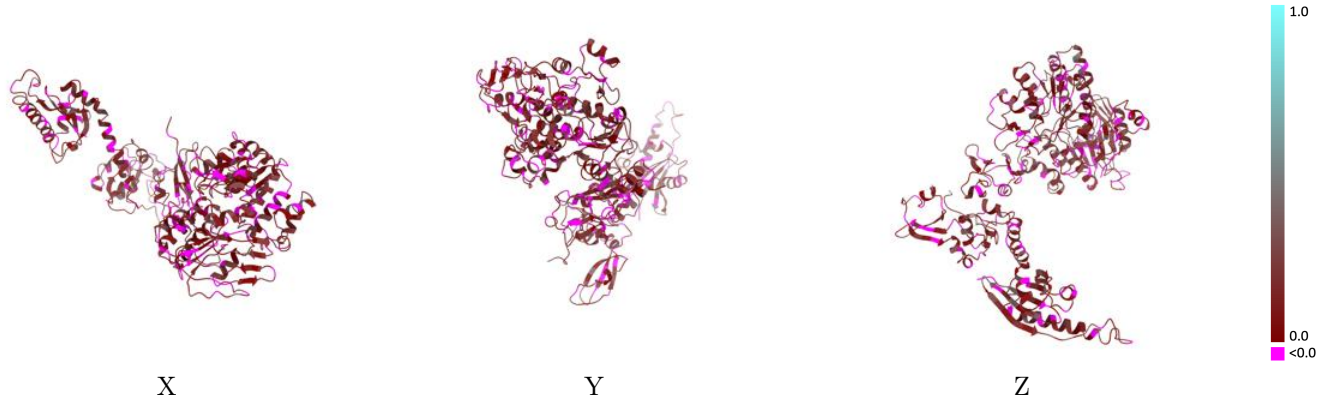
Y



Z

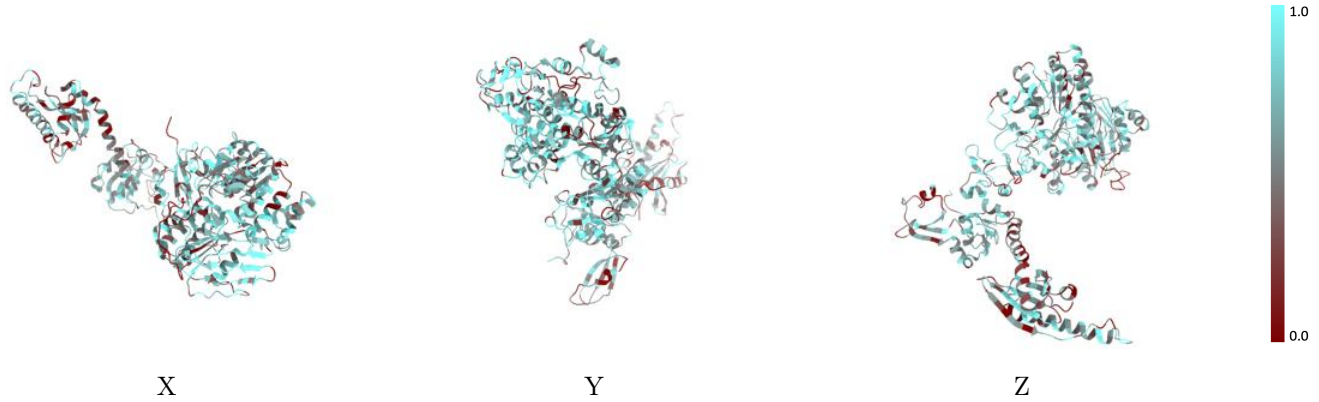
The images above show the 3D surface view of the map at the recommended contour level 0.232 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



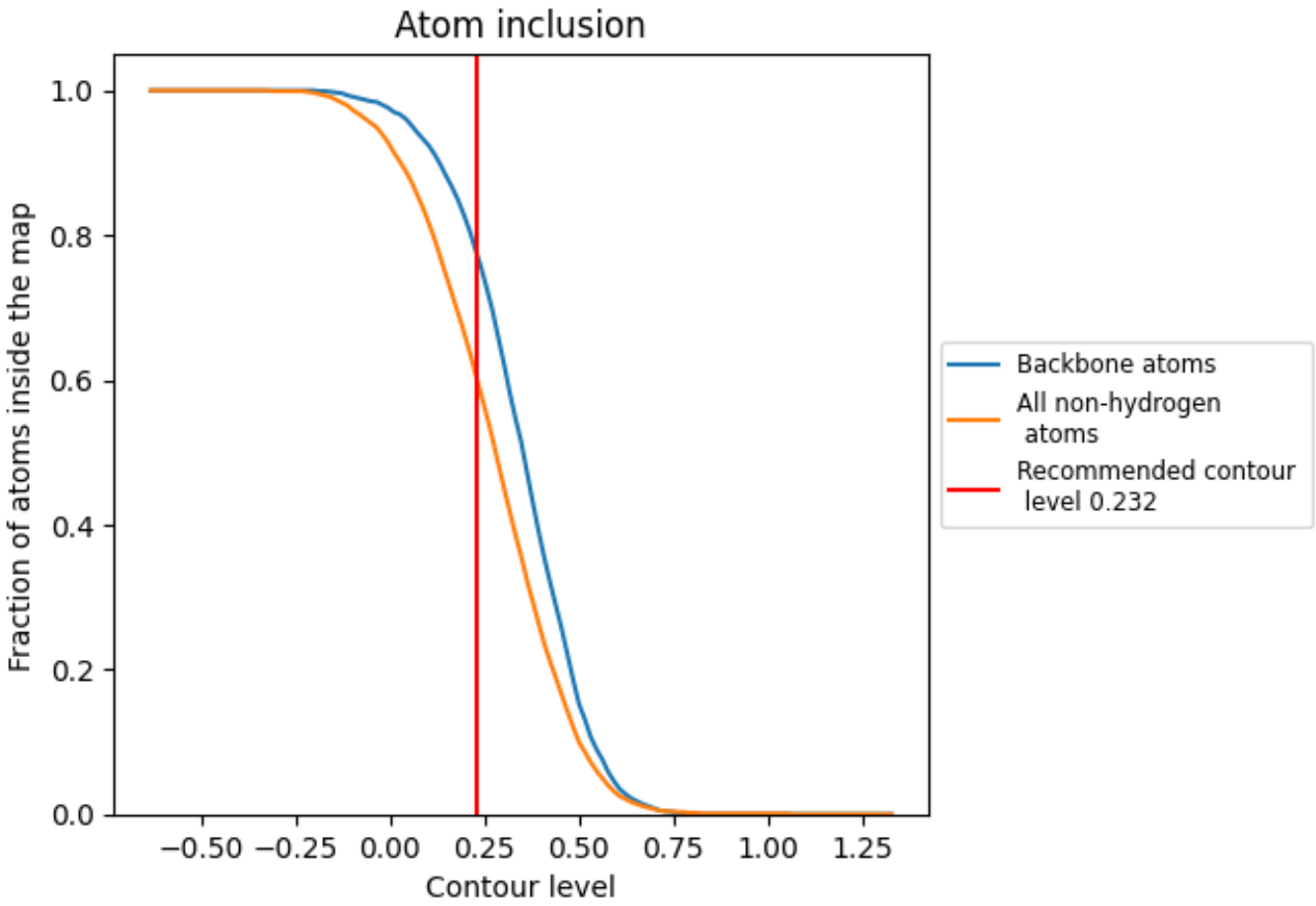
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.232).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.232) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.1170
P	0.6380	0.1130
X	0.5160	0.1260