



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:28 AM UTC

PDB ID : 4CRM / pdb_00004crm
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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

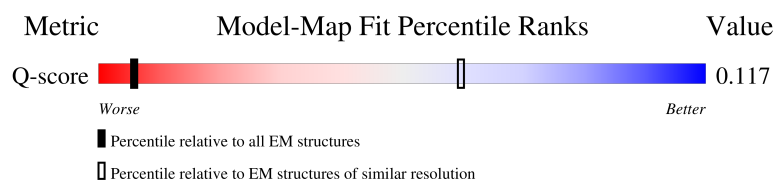
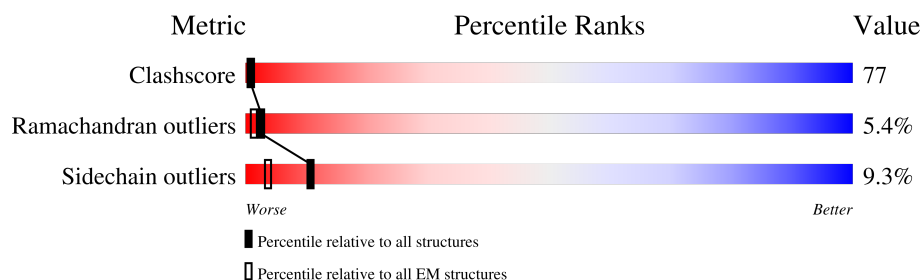
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	252 (8.25 - 9.25)

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

Mol	Chain	Length	Quality of chain
1	P	608	
2	X	282	

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	-
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.

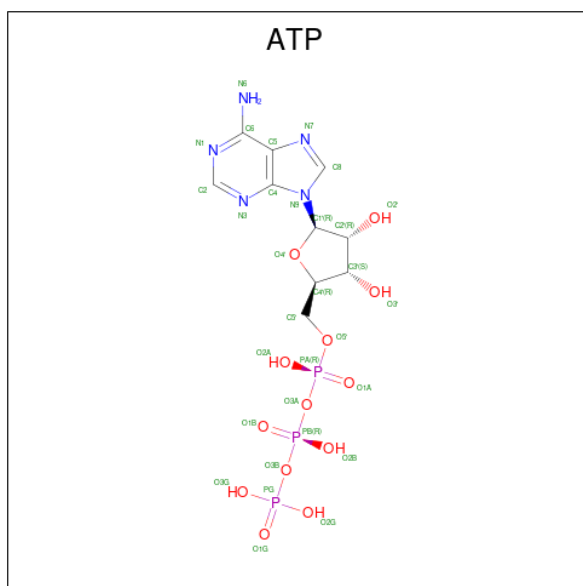
- Molecule 1 is a protein called TRANSLATION INITIATION FACTOR RLI1.

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 SUB-UNIT 1.

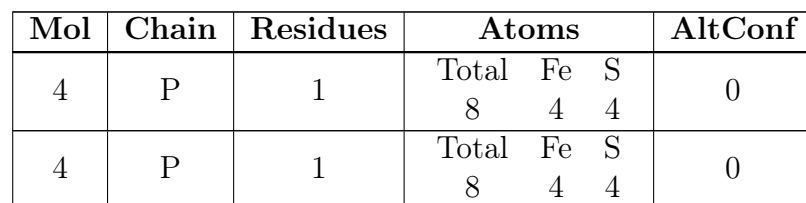
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	X	282	2210	1406	366	433	5	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: SF4) (formula: Fe_4S_4).



- # ADP

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

- 

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

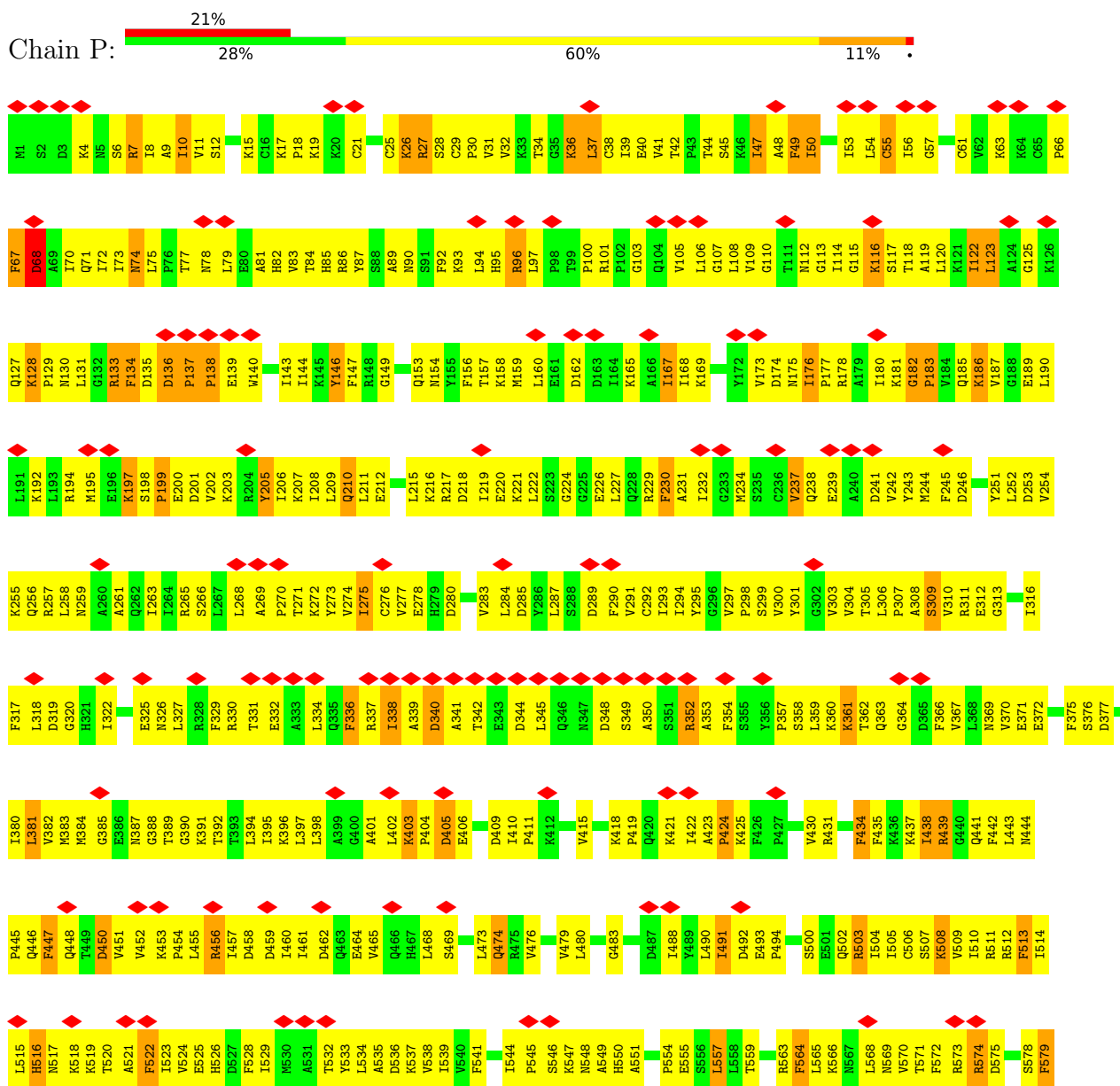
- Molecule 7 is water.

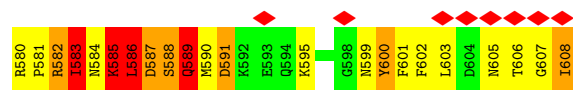
Mol	Chain	Residues	Atoms		AltConf
7	P	1	Total	O	0
			1	1	

3 Residue-property plots

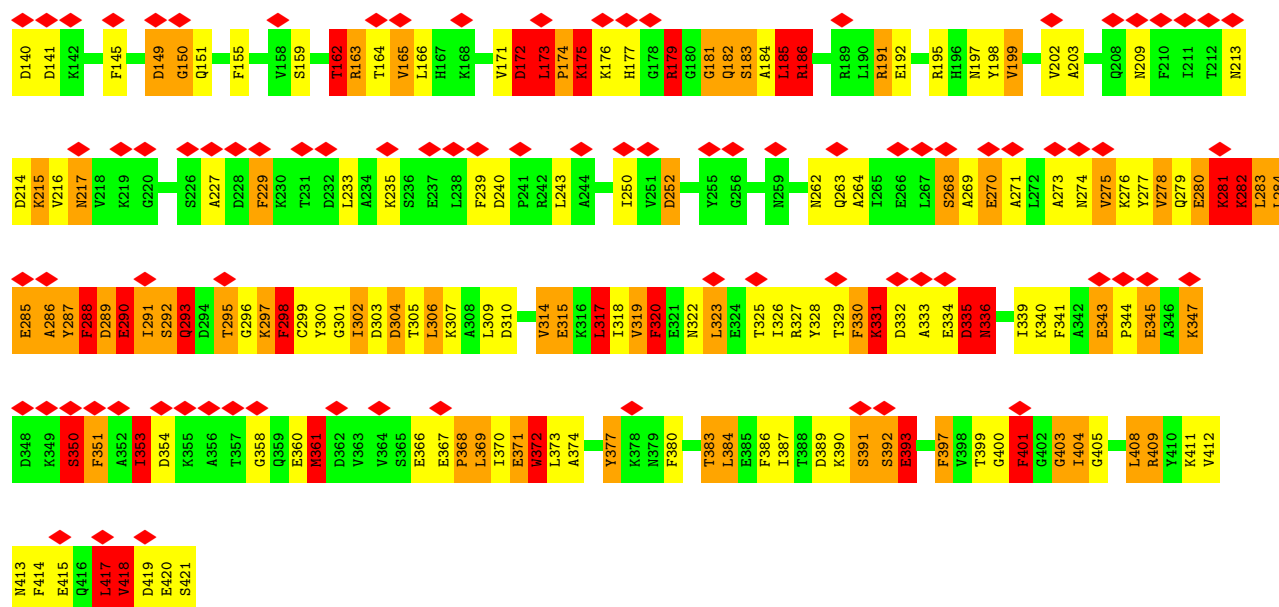
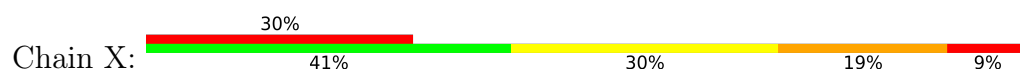
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 RL11





• Molecule 2: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.44	17/4893 (0.3%)	1.77	102/6603 (1.5%)
2	X	1.48	20/2246 (0.9%)	1.98	84/3021 (2.8%)
All	All	1.45	37/7139 (0.5%)	1.84	186/9624 (1.9%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	150	GLY	C-N	30.02	1.75	1.33
1	P	589	GLN	CA-C	19.57	1.77	1.52
2	X	186	ARG	CD-NE	12.77	1.64	1.46
2	X	302	ILE	C-N	12.41	1.48	1.33
1	P	589	GLN	CA-CB	11.57	1.71	1.53
1	P	608	ILE	C-O	-11.56	1.00	1.23
2	X	421	SER	C-OXT	-11.55	1.00	1.23
2	X	421	SER	C-O	-11.55	1.00	1.23
1	P	608	ILE	C-OXT	-11.53	1.00	1.23
2	X	186	ARG	NE-CZ	10.65	1.44	1.33
1	P	309	SER	CA-CB	-9.80	1.37	1.53
2	X	150	GLY	N-CA	9.74	1.57	1.45
1	P	588	SER	CA-C	-9.64	1.40	1.53
2	X	181	GLY	CA-C	-9.55	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	589	GLN	N-CA	-9.53	1.34	1.46
2	X	150	GLY	CA-C	9.15	1.63	1.51
2	X	330	PHE	C-N	8.83	1.41	1.33
1	P	584	ASN	CA-C	-8.69	1.42	1.52
2	X	281	LYS	CA-C	-8.17	1.41	1.52
2	X	331	LYS	C-N	8.03	1.45	1.33
1	P	176	ILE	CA-CB	-7.09	1.50	1.54
2	X	314	VAL	CA-CB	-7.01	1.45	1.53
1	P	589	GLN	CB-CG	7.00	1.73	1.52
2	X	372	TRP	CA-C	-6.98	1.43	1.52
1	P	137	PRO	CA-C	-6.76	1.48	1.51
1	P	591	ASP	CA-C	-6.59	1.44	1.52
1	P	586	LEU	CA-C	-6.20	1.44	1.52
1	P	308	ALA	C-N	-6.13	1.25	1.33
2	X	369	LEU	CA-C	-6.02	1.45	1.52
2	X	335	ASP	C-N	5.94	1.41	1.33
1	P	309	SER	N-CA	-5.66	1.38	1.45
2	X	286	ALA	C-N	5.64	1.41	1.33
2	X	179	ARG	CD-NE	5.48	1.53	1.46
1	P	40	GLU	C-N	-5.30	1.25	1.33
2	X	297	LYS	C-N	5.29	1.40	1.33
2	X	179	ARG	NE-CZ	5.24	1.38	1.33
1	P	602	PHE	CA-C	-5.06	1.46	1.52

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	149	ASP	O-C-N	-25.71	93.16	122.72
1	P	589	GLN	CB-CG-CD	16.77	141.11	112.60
1	P	587	ASP	CA-CB-CG	16.61	129.21	112.60
2	X	331	LYS	N-CA-C	14.86	128.57	108.07
1	P	589	GLN	CA-CB-CG	13.79	141.68	114.10
1	P	589	GLN	N-CA-CB	-13.70	90.20	110.07
1	P	588	SER	N-CA-CB	13.48	129.71	110.44
1	P	589	GLN	CB-CA-C	13.13	131.64	110.90
1	P	588	SER	N-CA-C	-12.71	94.14	110.53
1	P	137	PRO	O-C-N	12.66	127.13	121.31
2	X	229	PHE	CA-CB-CG	-12.20	101.61	113.80
2	X	281	LYS	CA-CB-CG	12.10	138.29	114.10
1	P	589	GLN	CA-C-O	11.31	132.35	120.70
2	X	186	ARG	CA-CB-CG	11.26	136.62	114.10
1	P	336	PHE	CA-CB-CG	-10.97	102.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	336	ASN	N-CA-C	10.64	124.82	108.96
1	P	584	ASN	N-CA-C	-10.58	92.55	109.59
1	P	586	LEU	CB-CA-C	10.26	127.20	109.65
2	X	384	LEU	N-CA-C	10.09	125.84	109.40
2	X	150	GLY	CA-C-N	-10.08	102.29	121.54
2	X	150	GLY	C-N-CA	-10.08	102.29	121.54
2	X	353	ILE	CA-C-N	9.77	140.20	121.54
2	X	353	ILE	C-N-CA	9.77	140.20	121.54
2	X	372	TRP	CB-CG-CD1	-9.76	112.26	126.90
1	P	447	PHE	CA-CB-CG	-9.69	104.11	113.80
1	P	589	GLN	CA-C-N	9.52	133.99	120.28
1	P	589	GLN	C-N-CA	9.52	133.99	120.28
1	P	585	LYS	CB-CA-C	9.43	126.81	109.46
1	P	230	PHE	CA-CB-CG	-9.21	104.59	113.80
2	X	293	GLN	N-CA-CB	9.19	126.02	110.49
2	X	335	ASP	O-C-N	9.12	134.72	122.59
2	X	368	PRO	CA-N-CD	-8.98	99.43	112.00
1	P	147	PHE	CA-CB-CG	-8.73	105.07	113.80
2	X	298	PHE	CB-CA-C	-8.58	92.00	110.45
2	X	372	TRP	CB-CA-C	-8.54	96.33	110.85
2	X	183	SER	N-CA-CB	-8.37	98.34	111.39
2	X	252	ASP	CA-CB-CG	8.31	120.91	112.60
2	X	369	LEU	CB-CA-C	-8.11	98.09	110.90
1	P	137	PRO	N-CA-C	-7.91	102.88	110.47
2	X	361	MET	N-CA-C	7.91	120.15	108.60
2	X	306	LEU	N-CA-C	7.84	119.61	111.14
1	P	309	SER	N-CA-C	7.81	120.60	110.53
2	X	331	LYS	CA-CB-CG	7.68	129.46	114.10
1	P	67	PHE	CA-CB-CG	-7.65	106.15	113.80
2	X	297	LYS	N-CA-C	-7.60	100.43	111.30
1	P	289	ASP	CA-CB-CG	-7.59	105.00	112.60
1	P	585	LYS	CA-C-N	7.56	131.60	120.87
1	P	585	LYS	C-N-CA	7.56	131.60	120.87
1	P	183	PRO	N-CA-C	-7.51	103.34	113.40
2	X	372	TRP	N-CA-CB	7.50	121.26	110.16
2	X	186	ARG	NE-CZ-NH2	7.46	125.92	119.20
2	X	307	LYS	N-CA-CB	7.41	120.75	110.01
2	X	320	PHE	N-CA-CB	7.33	122.88	110.49
2	X	397	PHE	O-C-N	-7.29	114.39	122.12
1	P	41	VAL	CB-CA-C	-7.19	101.07	110.84
2	X	179	ARG	N-CA-C	7.16	126.04	110.80
2	X	320	PHE	N-CA-C	-7.08	95.72	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	27	ARG	N-CA-C	-7.07	100.59	110.35
1	P	584	ASN	CA-CB-CG	-7.07	105.53	112.60
1	P	583	ILE	N-CA-C	-7.04	100.50	109.30
1	P	49	PHE	CA-CB-CG	-7.03	106.77	113.80
2	X	179	ARG	N-CA-CB	-6.97	98.71	110.49
2	X	252	ASP	CB-CA-C	6.96	121.41	109.51
1	P	588	SER	CA-C-N	-6.81	111.18	120.44
1	P	588	SER	C-N-CA	-6.81	111.18	120.44
1	P	602	PHE	CA-CB-CG	-6.71	107.09	113.80
1	P	459	ASP	CA-C-N	6.70	131.28	120.30
1	P	459	ASP	C-N-CA	6.70	131.28	120.30
1	P	245	PHE	CA-CB-CG	-6.69	107.11	113.80
2	X	175	LYS	N-CA-CB	6.64	121.71	110.49
1	P	442	PHE	CA-CB-CG	-6.62	107.17	113.80
2	X	295	THR	N-CA-CB	6.60	121.65	110.49
1	P	137	PRO	CB-CA-C	6.60	117.59	111.39
2	X	369	LEU	N-CA-CB	6.59	119.63	110.07
2	X	400	GLY	O-C-N	-6.54	114.19	122.70
2	X	186	ARG	CG-CD-NE	6.53	126.38	112.00
1	P	513	PHE	CA-CB-CG	-6.44	107.36	113.80
2	X	336	ASN	CA-C-N	6.41	132.87	122.81
2	X	336	ASN	C-N-CA	6.41	132.87	122.81
1	P	528	PHE	CA-CB-CG	-6.34	107.45	113.80
1	P	585	LYS	O-C-N	-6.32	115.82	122.96
2	X	302	ILE	O-C-N	6.30	128.45	121.90
1	P	156	PHE	CA-CB-CG	-6.29	107.51	113.80
1	P	81	ALA	CA-C-N	6.25	133.77	121.58
1	P	81	ALA	C-N-CA	6.25	133.77	121.58
1	P	456	ARG	CA-C-N	6.21	130.49	120.30
1	P	456	ARG	C-N-CA	6.21	130.49	120.30
1	P	600	TYR	CA-CB-CG	-6.19	102.76	113.90
1	P	364	GLY	N-CA-C	-6.11	106.09	114.64
1	P	309	SER	N-CA-CB	-6.09	101.73	110.44
2	X	383	THR	N-CA-CB	6.09	120.92	110.68
1	P	122	ILE	N-CA-CB	6.09	118.82	110.54
2	X	145	PHE	CA-CB-CG	6.04	119.84	113.80
1	P	199	PRO	N-CA-C	-5.99	105.57	113.65
1	P	36	LYS	CA-C-N	5.95	133.85	121.94
1	P	36	LYS	C-N-CA	5.95	133.85	121.94
1	P	74	ASN	CA-CB-CG	-5.95	106.65	112.60
1	P	146	TYR	CA-CB-CG	-5.92	103.24	113.90
1	P	434	PHE	CB-CA-C	-5.92	100.79	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	186	ARG	NH1-CZ-NH2	-5.84	111.71	119.30
1	P	564	PHE	CA-CB-CG	-5.83	107.97	113.80
1	P	37	LEU	N-CA-C	5.81	120.23	113.20
2	X	386	PHE	N-CA-C	-5.75	100.81	109.95
1	P	582	ARG	N-CA-C	-5.74	99.82	109.07
2	X	292	SER	CA-C-O	-5.73	114.31	121.02
2	X	331	LYS	CB-CA-C	-5.73	101.22	114.41
2	X	372	TRP	N-CA-C	-5.72	105.12	111.36
1	P	57	GLY	N-CA-C	-5.71	107.37	115.43
2	X	384	LEU	CD1-CG-CD2	5.71	123.37	110.80
1	P	174	ASP	CA-CB-CG	-5.70	106.90	112.60
2	X	299	CYS	CA-C-N	5.70	131.44	122.21
2	X	299	CYS	C-N-CA	5.70	131.44	122.21
2	X	217	ASN	CA-CB-CG	5.69	118.29	112.60
2	X	150	GLY	O-C-N	5.65	128.84	122.34
1	P	55	CYS	CA-C-N	5.63	129.56	120.55
1	P	55	CYS	C-N-CA	5.63	129.56	120.55
2	X	409	ARG	CB-CA-C	-5.62	101.30	110.85
1	P	149	GLY	N-CA-C	-5.62	107.57	115.32
2	X	361	MET	CG-SD-CE	-5.60	88.59	100.90
1	P	133	ARG	CA-C-N	5.58	128.79	120.31
1	P	133	ARG	C-N-CA	5.58	128.79	120.31
2	X	315	GLU	CB-CA-C	-5.57	102.14	110.88
1	P	522	PHE	CA-CB-CG	-5.55	108.25	113.80
1	P	68	ASP	CA-C-N	5.52	128.70	120.31
1	P	68	ASP	C-N-CA	5.52	128.70	120.31
2	X	286	ALA	CA-C-O	-5.50	112.64	120.51
2	X	401	PHE	CA-CB-CG	-5.47	108.33	113.80
1	P	589	GLN	CG-CD-NE2	5.47	124.60	116.40
1	P	210	GLN	CA-C-N	5.45	132.21	121.58
1	P	210	GLN	C-N-CA	5.45	132.21	121.58
1	P	585	LYS	N-CA-CB	-5.44	102.03	110.29
1	P	503	ARG	CA-C-N	5.43	129.06	120.47
1	P	503	ARG	C-N-CA	5.43	129.06	120.47
1	P	352	ARG	N-CA-C	-5.43	105.05	110.97
2	X	330	PHE	CA-C-O	-5.42	114.70	120.40
1	P	583	ILE	CA-CB-CG1	5.41	119.60	110.40
1	P	41	VAL	N-CA-CB	5.39	117.46	110.99
1	P	572	PHE	CA-CB-CG	-5.37	108.43	113.80
1	P	137	PRO	N-CA-CB	5.36	106.19	103.19
1	P	340	ASP	CA-C-N	5.35	128.45	120.31
1	P	340	ASP	C-N-CA	5.35	128.45	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	588	SER	CA-CB-OG	5.35	121.79	111.10
1	P	134	PHE	CA-CB-CG	-5.34	108.46	113.80
2	X	179	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	X	413	ASN	N-CA-C	-5.31	100.52	109.07
1	P	82	HIS	N-CA-C	5.31	119.61	113.18
2	X	317	LEU	CB-CG-CD2	5.31	126.62	110.70
2	X	186	ARG	CD-NE-CZ	5.30	131.82	124.40
2	X	298	PHE	CB-CG-CD1	-5.29	111.70	120.70
2	X	185	LEU	CB-CA-C	5.29	115.98	109.16
2	X	403	GLY	N-CA-C	-5.28	106.42	115.08
1	P	176	ILE	CB-CA-C	-5.25	107.12	114.00
2	X	304	ASP	N-CA-CB	5.25	117.59	109.98
2	X	377	TYR	CB-CA-C	-5.23	100.23	110.11
2	X	306	LEU	CB-CA-C	-5.22	102.65	110.90
1	P	205	TYR	CA-CB-CG	-5.20	104.53	113.90
1	P	439	ARG	CA-C-N	5.20	125.72	120.00
1	P	439	ARG	C-N-CA	5.20	125.72	120.00
1	P	125	GLY	N-CA-C	-5.19	108.16	115.32
1	P	573	ARG	NE-CZ-NH1	-5.18	116.31	121.50
2	X	293	GLN	CA-C-N	5.18	131.44	121.54
2	X	293	GLN	C-N-CA	5.18	131.44	121.54
2	X	263	GLN	OE1-CD-NE2	-5.18	117.42	122.60
2	X	397	PHE	CA-C-O	5.15	126.01	120.55
2	X	408	LEU	CA-C-N	5.15	127.60	120.29
2	X	408	LEU	C-N-CA	5.15	127.60	120.29
1	P	516	HIS	CA-C-N	5.15	128.13	120.31
1	P	516	HIS	C-N-CA	5.15	128.13	120.31
1	P	450	ASP	N-CA-C	5.14	117.67	111.40
2	X	329	THR	CA-C-N	-5.12	115.59	123.07
2	X	329	THR	C-N-CA	-5.12	115.59	123.07
1	P	579	PHE	CA-CB-CG	-5.12	108.68	113.80
2	X	197	ASN	CA-CB-CG	5.12	117.72	112.60
2	X	281	LYS	CB-CA-C	-5.11	100.25	110.42
2	X	371	GLU	CA-C-N	5.11	127.55	120.29
2	X	371	GLU	C-N-CA	5.11	127.55	120.29
1	P	123	LEU	CA-C-N	5.10	128.07	120.31
1	P	123	LEU	C-N-CA	5.10	128.07	120.31
2	X	408	LEU	N-CA-C	5.10	118.43	110.32
1	P	405	ASP	N-CA-C	-5.10	105.80	111.36
1	P	459	ASP	CA-CB-CG	-5.06	107.54	112.60
1	P	241	ASP	CA-CB-CG	-5.04	107.56	112.60
1	P	200	GLU	N-CA-C	-5.02	106.00	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	329	THR	O-C-N	-5.02	117.45	123.27
1	P	575	ASP	N-CA-C	-5.01	103.46	109.72
2	X	179	ARG	CA-C-O	-5.01	113.35	120.51

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	Peptide,Sidechain
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

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	843	0
2	X	2210	0	2182	259	0
3	P	31	0	12	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1100	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 77.

All (1100) 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	1.55
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	1.42
2:X:302:ILE:C	2:X:340:LYS:NZ	1.75	1.40
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: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
2:X:302:ILE:C	2:X:340:LYS:HZ2	1.35	1.20
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:173:LEU:C	2:X:173:LEU:HD13	1.69	1.17
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:328:TYR:HE1	2:X:366:GLU:CD	1.53	1.16
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:328:TYR:CE1	2:X:366:GLU:CD	2.26	1.12
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
1:P:18:PRO:HA	4:P:1611:SF4:S3	1.91	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:86:ARG:HG3	1:P:93:LYS:HG2	1.31	1.08
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
2:X:334:GLU:O	2:X:335:ASP:CG	1.99	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
1:P:120:LEU:HG	1:P:244:MET:HE2	1.39	1.04
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:159:MET:HE3	1:P:159:MET:HA	1.39	1.01
1:P:568:LEU:HD12	1:P:570:VAL:HG22	1.38	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:173:LEU:C	2:X:173:LEU:CD1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:X:288:PHE:HD1	2:X:288:PHE:C	1.76	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:231:ALA:HA	1:P:234:MET:HE3	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:388:GLY:C	5:P:1612:ADP:H5'2	1.99	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:288:PHE:C	2:X:288:PHE:CD1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:150:GLY:C	2:X:151:GLN:CA	2.51	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
2:X:173:LEU:HD13	2:X:174:PRO:N	1.93	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:360:LYS:HE2	1:P:369:ASN:CG	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:380:ILE:HD11	1:P:534:LEU:C	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:P:589:GLN:C	1:P:589:GLN:HA	2.04	0.75
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:34:THR:CG2	1:P:36:LYS:HG3	2.17	0.74
1:P:409:ASP:C	1:P:411:PRO:HD3	2.12	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
2:X:302:ILE:C	2:X:340:LYS:HZ3	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:ALA:C	1:P:10:ILE:HD12	2.13	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:185:GLN:HG3	1:P:189:GLU:CD	2.15	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
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:78:ASN:CG	1:P:79:LEU:HD12	2.14	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:273:ALA:C	2:X:277:TYR:CE2	2.69	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:26:LYS:HD2	1:P:26:LYS:C	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:438:ILE:HG13	1:P:483:GLY:O	1.91	0.70
2:X:172:ASP:CG	2:X:173:LEU:N	2.50	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
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
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:383:MET:HE1	1:P:539:ILE:HD12	1.74	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: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:120:LEU:HA	1:P:244:MET:HE1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:120:LEU:HG	1:P:244:MET:CE	2.20	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
2:X:326:ILE:HG23	2:X:367:GLU:C	2.19	0.67
1:P:490:LEU:C	1:P:491:ILE:HD12	2.20	0.67
1:P:544:ILE:CG2	1:P:547:LYS:HB3	2.24	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: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:347:LYS:C	2:X:350:SER:HB3	2.18	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
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:305:THR:HG22	1:P:306:LEU:H	1.59	0.66
1:P:159:MET:HE3	1:P:159:MET:CA	2.21	0.66
1:P:357:PRO:C	1:P:372:GLU:HG3	2.21	0.66
1:P:84:THR:HG22	1:P:94:LEU:C	2.21	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
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: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:418:VAL:O	2:X:420:GLU:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:282:LYS:O	2:X:283:LEU:C	2.39	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
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:589:GLN:C	1:P:589:GLN:N	2.54	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
1:P:4:LYS:HG2	1:P:77:THR:CG2	2.30	0.62
1:P:381:LEU:C	1:P:381:LEU:HD23	2.24	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
2:X:418:VAL:C	2:X:420:GLU:H	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:353:ALA:HB3	1:P:375:PHE:O	2.00	0.62
1:P:201:ASP:O	1:P:205:TYR:HD1	1.82	0.62
1:P:265:ARG:C	1:P:268:LEU:HD13	2.25	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
2:X:328:TYR:HE1	2:X:366:GLU:OE1	1.80	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
2:X:389:ASP:C	2:X:390:LYS:HG3	2.24	0.61
1:P:116:LYS:NZ	3:P:1609:ATP:O3G	2.25	0.61
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: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:96:ARG:C	1:P:97:LEU:HD22	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:114:ILE:HD12	1:P:114:ILE:C	2.26	0.60
1:P:430:VAL:CG1	1:P:434:PHE:HE1	2.15	0.60
1:P:192:LYS:O	1:P:195:MET:HE3	2.02	0.60
1:P:300:VAL:HG23	1:P:301:TYR:N	2.14	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
2:X:322:ASN:O	2:X:323:LEU:C	2.45	0.59
1:P:115:GLY:CA	3:P:1609:ATP:O2A	2.35	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
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:106:LEU:HD13	1:P:106:LEU:C	2.28	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
2:X:301:GLY:O	2:X:305:THR:OG1	2.19	0.59
1:P:448:GLN:O	1:P:453:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:323:LEU:HD12	2:X:370:ILE:HA	1.86	0.58
2:X:328:TYR:CD1	2:X:366:GLU:CD	2.69	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
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: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
2:X:150:GLY:C	2:X:151:GLN:C	2.72	0.57
2:X:418:VAL:C	2:X:420:GLU:N	2.60	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:383:MET:HE1	1:P:539:ILE:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:ILE:HG13	1:P:207:LYS:N	2.19	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
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:159:MET:HA	1:P:159:MET:CE	2.27	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:180:ILE:HG21	1:P:219:ILE:HG12	1.88	0.56
1:P:338:ILE:HD13	1:P:338:ILE:C	2.31	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
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
2:X:173:LEU:HD13	2:X:174:PRO:C	2.32	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
2:X:287:TYR:O	2:X:288:PHE:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:380:ILE:CG1	1:P:535:ALA:HA	2.35	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:318:ILE:O	2:X:404:ILE:C	2.49	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: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
2:X:326:ILE:CG2	2:X:367:GLU:C	2.80	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: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
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
2:X:302:ILE:C	2:X:340:LYS:HZ1	2.06	0.54
1:P:202:VAL:HG13	1:P:203:LYS:N	2.21	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
2:X:289:ASP:O	2:X:290:GLU:C	2.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:181:GLY:C	2:X:183:SER:H	2.16	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
1:P:568:LEU:HD13	1:P:568:LEU:C	2.33	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:169:LYS:C	1:P:169:LYS:HD2	2.34	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
1:P:331:THR:HG23	1:P:332:GLU:N	2.24	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
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: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:425:LYS:O	1:P:425:LYS:HG3	2.09	0.52
1:P:565:LEU:HD13	1:P:600:TYR:HB3	1.92	0.52
2:X:289:ASP:CG	2:X:290:GLU:N	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:X:274:ASN:OD1	2:X:274:ASN:C	2.53	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:395:ILE:HG23	1:P:396:LYS:N	2.24	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
1:P:162:ASP:CG	1:P:165:LYS:HE3	2.36	0.50
1:P:381:LEU:HD13	1:P:522:PHE:CE1	2.40	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: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: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
1:P:229:ARG:HA	1:P:232:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:ILE:HD13	1:P:167:ILE:C	2.36	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:354:PHE:CB	1:P:375:PHE:CZ	2.94	0.49
2:X:273:ALA:C	2:X:277:TYR:CD2	2.85	0.49
1:P:362:THR:HG23	1:P:362:THR:O	2.12	0.49
1:P:401:ALA:C	1:P:402:LEU:HD12	2.38	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
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
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: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:230:PHE:CE2	1:P:234:MET:HE2	2.48	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
2:X:290:GLU:C	2:X:291:ILE:HG12	2.37	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:97:LEU:HD11	1:P:122:ILE:CD1	2.43	0.48
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:120:LEU:HD23	1:P:120:LEU:C	2.39	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:49:PHE:C	1:P:50:ILE:HD12	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:510:ILE:HG22	1:P:514:ILE:CD1	2.44	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:160:LEU:HD23	1:P:160:LEU:C	2.39	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: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
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
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
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
2:X:383:THR:C	2:X:384:LEU:HD12	2.40	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:295:TYR:CE2	1:P:325:GLU:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:P:32:VAL:HG12	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
2:X:328:TYR:CE1	2:X:366:GLU:OE2	2.64	0.45
2:X:309:LEU:C	2:X:380:PHE:HD1	2.24	0.45
1:P:115:GLY:C	1:P:118:THR:HG22	2.42	0.45
1:P:167:ILE:O	1:P:167:ILE:HG23	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:435:PHE:CD2	1:P:435:PHE:C	2.95	0.45
1:P:510:ILE:CG2	1:P:514:ILE:CD1	2.95	0.45
1:P:130:ASN:C	1:P:135:ASP:HB3	2.40	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
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
2:X:289:ASP:C	2:X:291:ILE:N	2.73	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
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:309:LEU:C	2:X:380:PHE:CD1	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:P:92:PHE:CD2	3:P:1609:ATP:C4'	3.01	0.44
1:P:120:LEU:CG	1:P:244:MET:HE2	2.27	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:74:ASN:C	1:P:75:LEU:HD22	2.42	0.44
1:P:114:ILE:CG1	1:P:294:ILE:CG2	2.95	0.44
1:P:305:THR:CG2	1:P:306:LEU:N	2.80	0.44
1:P:320:GLY:C	1:P:329:PHE:CE2	2.96	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
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
2:X:172:ASP:CG	2:X:173:LEU:H	2.24	0.44
2:X:291:ILE:O	2:X:292:SER:C	2.61	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
2:X:268:SER:O	2:X:269:ALA:C	2.60	0.43
1:P:133:ARG:HG3	1:P:134:PHE:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:492:ASP:CG	1:P:524:VAL:HG21	2.42	0.43
1:P:571:THR:HG23	1:P:595:LYS:HZ2	1.81	0.43
2:X:183:SER:C	2:X:185:LEU:H	2.27	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
2:X:331:LYS:CE	2:X:361:MET:HE1	2.49	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:280:GLU:O	2:X:281:LYS:C	2.61	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:96:ARG:HD2	1:P:304:VAL:O	2.18	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:588:SER:C	1:P:589:GLN:C	2.87	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:108:LEU:HD23	1:P:108:LEU:C	2.43	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
1:P:73:ILE:CG2	1:P:75:LEU:CD2	2.97	0.42
1:P:253:ASP:CG	1:P:256:GLN:HG2	2.44	0.42
1:P:381:LEU:HD23	1:P:382:VAL:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:P:607:GLY:C	1:P:608:ILE:O	2.57	0.42
2:X:181:GLY:C	2:X:183:SER:N	2.78	0.42
2:X:317:LEU:HB3	2:X:384:LEU:HD21	2.00	0.42
1:P:127:GLN:OE1	1:P:127:GLN:HA	2.20	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: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:509:VAL:CG1	1:P:510:ILE:N	2.82	0.42
1:P:564:PHE:CD2	1:P:564:PHE:C	2.96	0.42
2:X:326:ILE:HA	2:X:369:LEU:H	1.84	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:338:ILE:C	1:P:338:ILE:CD1	2.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:108:LEU:CD2	1:P:108:LEU:C	2.94	0.41
1:P:112:ASN:CA	3:P:1609:ATP:O2G	2.68	0.41
1:P:134:PHE:CD1	1:P:134:PHE:C	2.98	0.41
1:P:167:ILE:C	1:P:167:ILE:CD1	2.94	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
1:P:505:ILE:CG2	1:P:506:CYS:N	2.82	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:120:LEU:CD2	1:P:120:LEU:C	2.94	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:160:LEU:C	1:P:160:LEU:CD2	2.94	0.40
1:P:237:VAL:CG1	1:P:238:GLN:N	2.82	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
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: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:143:ILE:CG2	1:P:144:ILE:N	2.82	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:38:CYS:SG	1:P:55:CYS:CA	3.08	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%)	9	42
2	X	280/282 (99%)	197 (70%)	43 (15%)	40 (14%)	0	3
All	All	886/890 (100%)	760 (86%)	78 (9%)	48 (5%)	2	15

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
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

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Mol	Chain	Res	Type
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
2	X	358	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	537/537 (100%)	512 (95%)	25 (5%)	23	45
2	X	234/234 (100%)	187 (80%)	47 (20%)	1	7
All	All	771/771 (100%)	699 (91%)	72 (9%)	11	26

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	7	ARG
1	P	10	ILE
1	P	26	LYS
1	P	47	ILE
1	P	50	ILE
1	P	63	LYS
1	P	116	LYS
1	P	128	LYS
1	P	167	ILE
1	P	186	LYS
1	P	237	VAL
1	P	275	ILE
1	P	338	ILE
1	P	361	LYS
1	P	381	LEU
1	P	403	LYS
1	P	474	GLN
1	P	491	ILE
1	P	508	LYS
1	P	557	LEU
1	P	583	ILE
1	P	585	LYS
1	P	586	LEU
1	P	587	ASP
1	P	589	GLN
2	X	162	THR
2	X	163	ARG
2	X	164	THR
2	X	165	VAL
2	X	172	ASP
2	X	173	LEU
2	X	176	LYS
2	X	179	ARG
2	X	182	GLN

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Mol	Chain	Res	Type
2	X	185	LEU
2	X	186	ARG
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	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
2	X	404	ILE
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	71	GLN
1	P	85	HIS
1	P	95	HIS
1	P	210	GLN
1	P	238	GLN
1	P	256	GLN
1	P	259	ASN
1	P	262	GLN
1	P	347	ASN
1	P	369	ASN
1	P	432	GLN
1	P	448	GLN
1	P	463	GLN
1	P	467	HIS
1	P	474	GLN
1	P	526	HIS
1	P	562	ASN
1	P	594	GLN
1	P	605	ASN
2	X	196	HIS
2	X	197	ASN

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](#)

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
3	ATP	P	1609	6	32,33,33	2.39	7 (21%)	48,52,52	3.06	13 (27%)
4	SF4	P	1611	1	0,12,12	-	-	-	-	-
5	ADP	P	1612	-	28,29,29	1.03	3 (10%)	43,45,45	0.98	2 (4%)
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
3	ATP	P	1609	6	-	2/22/38/38	0/3/3/3
4	SF4	P	1611	1	-	-	0/6/5/5
5	ADP	P	1612	-	-	4/16/32/32	0/3/3/3
4	SF4	P	1610	1	-	-	0/6/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1609	ATP	PB-O3A	8.91	1.69	1.59
3	P	1609	ATP	C4-N3	5.11	1.44	1.34
3	P	1609	ATP	O5'-C5'	-4.61	1.27	1.44
3	P	1609	ATP	PA-O5'	-3.09	1.47	1.59
5	P	1612	ADP	PB-O3B	2.73	1.64	1.54
5	P	1612	ADP	C4-N3	2.53	1.39	1.34
3	P	1609	ATP	C3'-C4'	-2.21	1.47	1.53
3	P	1609	ATP	PB-O1B	-2.15	1.43	1.50
5	P	1612	ADP	PB-O2B	-2.03	1.47	1.54
3	P	1609	ATP	O4'-C1'	2.00	1.46	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1609	ATP	O5'-C5'-C4'	12.42	151.28	108.99
3	P	1609	ATP	O3A-PB-O1B	-8.02	86.57	110.70
3	P	1609	ATP	O5'-PA-O1A	-6.37	83.69	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1609	ATP	PA-O5'-C5'	5.86	154.90	121.35
3	P	1609	ATP	C5'-C4'-C3'	-5.45	95.58	115.21
3	P	1609	ATP	O2A-PA-O3A	4.79	120.21	107.27
3	P	1609	ATP	O4'-C4'-C3'	4.68	114.45	105.15
3	P	1609	ATP	O2B-PB-O3B	4.40	119.17	107.27
5	P	1612	ADP	O2B-PB-O3A	2.81	114.06	104.64
3	P	1609	ATP	C3'-C2'-C1'	2.56	106.31	101.46
3	P	1609	ATP	O2A-PA-O1A	2.28	123.07	112.44
3	P	1609	ATP	O2A-PA-O5'	-2.15	97.82	107.57
5	P	1612	ADP	O4'-C1'-C2'	-2.11	102.11	106.62
3	P	1609	ATP	O2B-PB-O1B	2.11	122.25	112.44
3	P	1609	ATP	O3B-PB-O1B	2.04	116.83	110.70

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

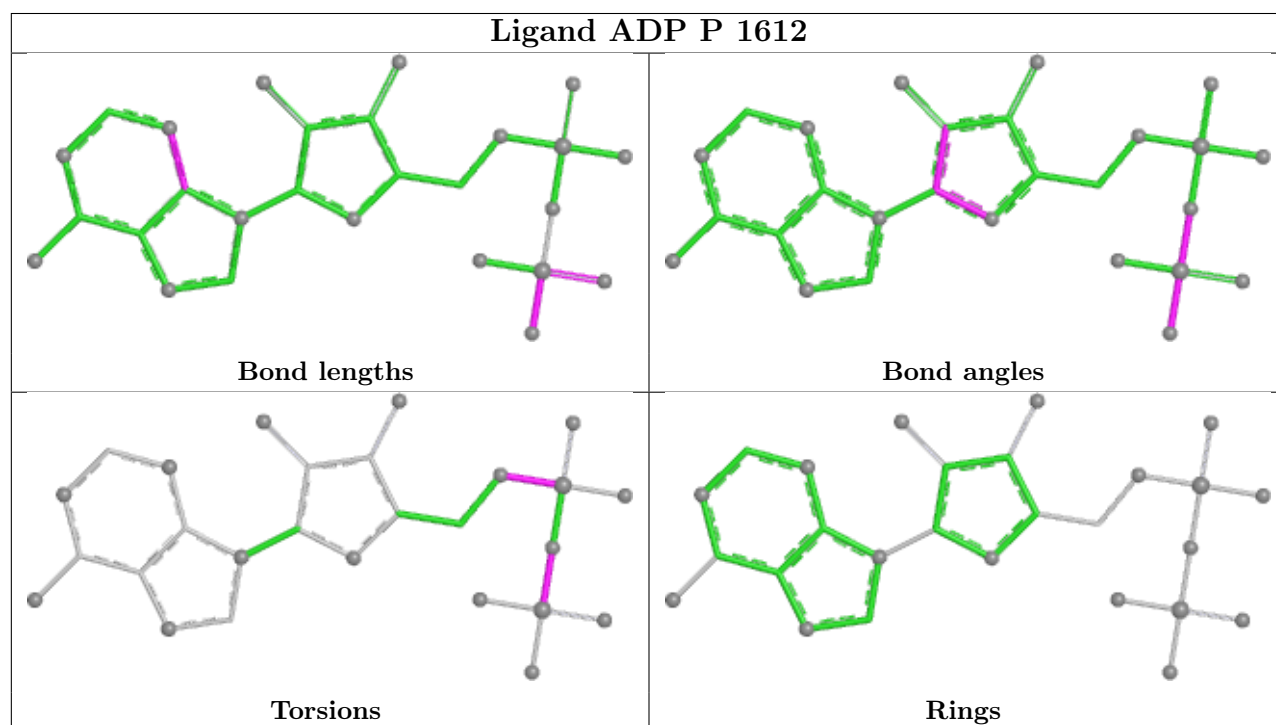
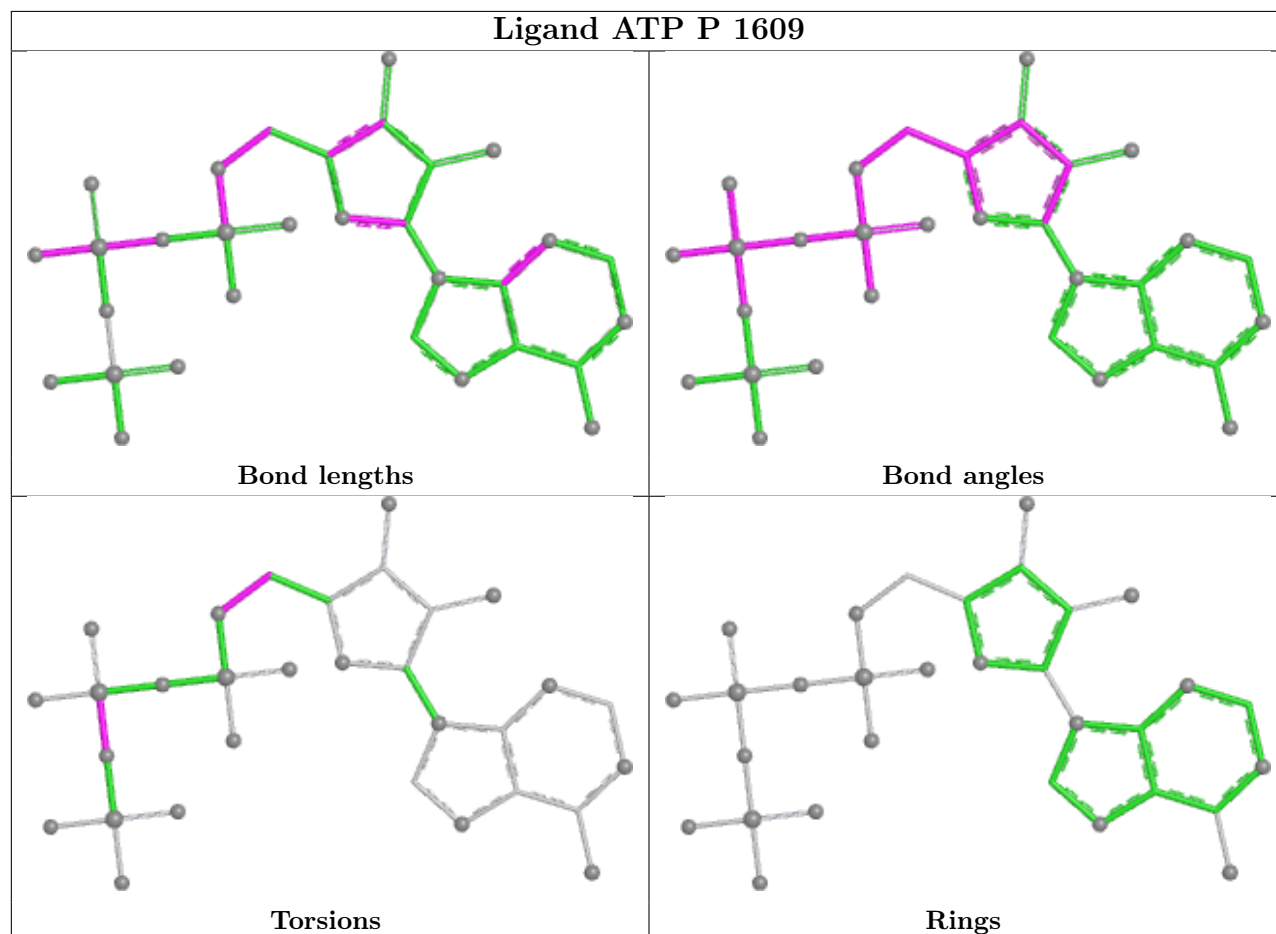
There are no ring outliers.

4 monomers are involved in 65 short contacts:

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



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

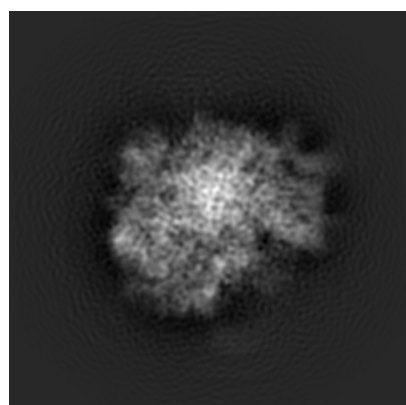
6 Map visualisation [i](#)

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.

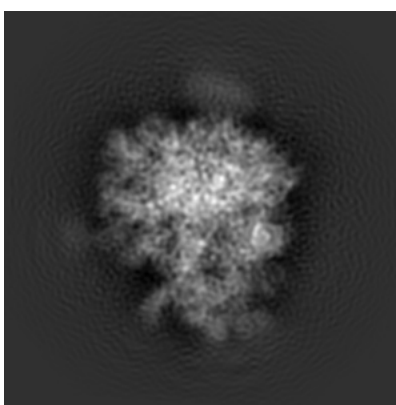
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

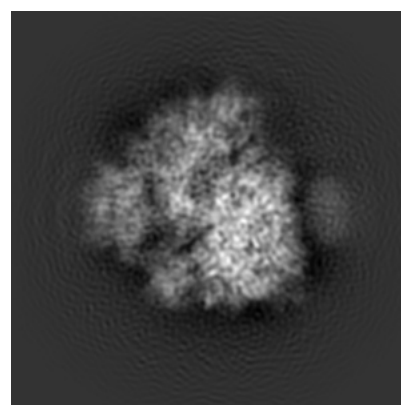
6.1.1 Primary map



X



Y

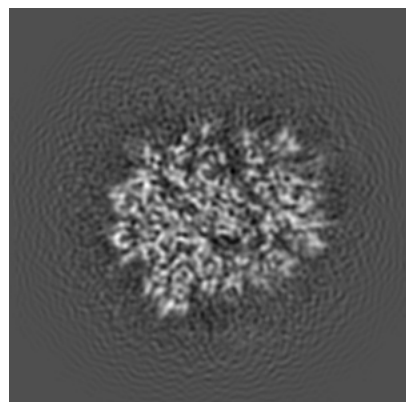


Z

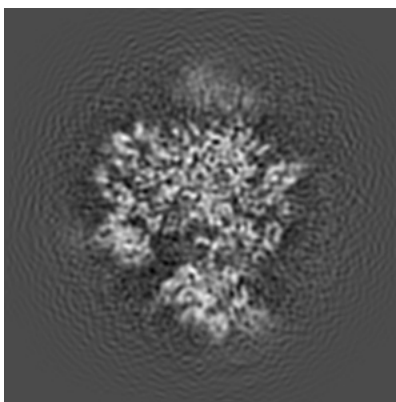
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

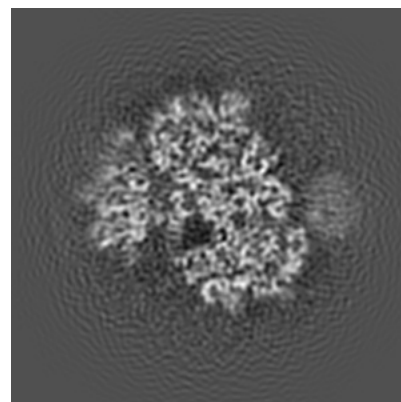
6.2.1 Primary map



X Index: 184



Y Index: 184

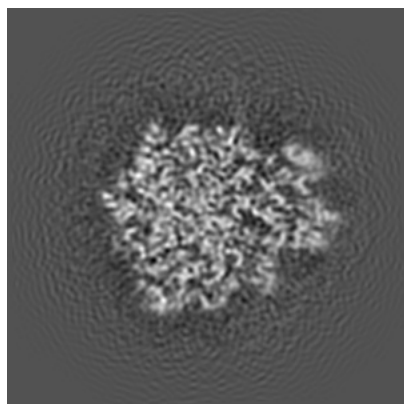


Z Index: 184

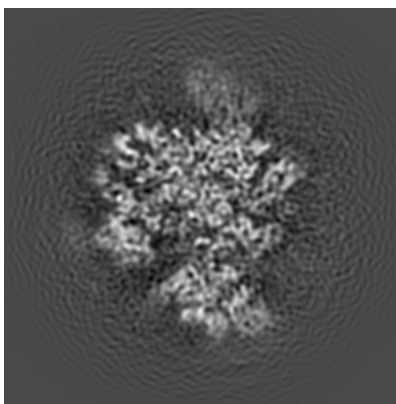
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

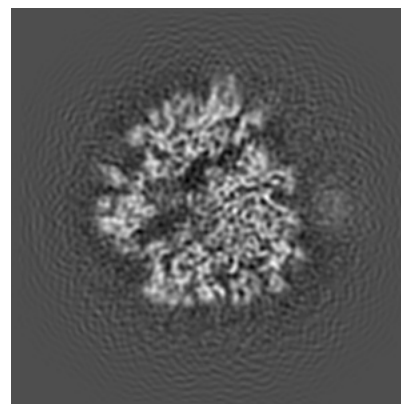
6.3.1 Primary map



X Index: 197



Y Index: 186

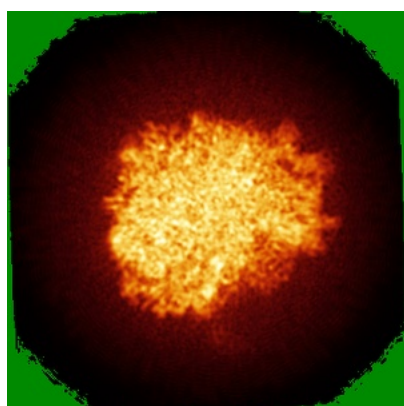


Z Index: 168

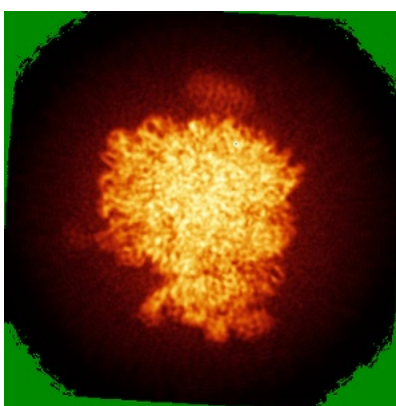
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

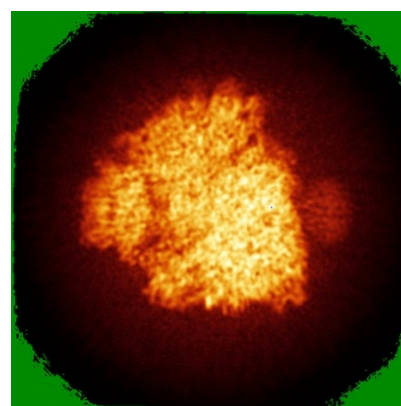
6.4.1 Primary map



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



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.

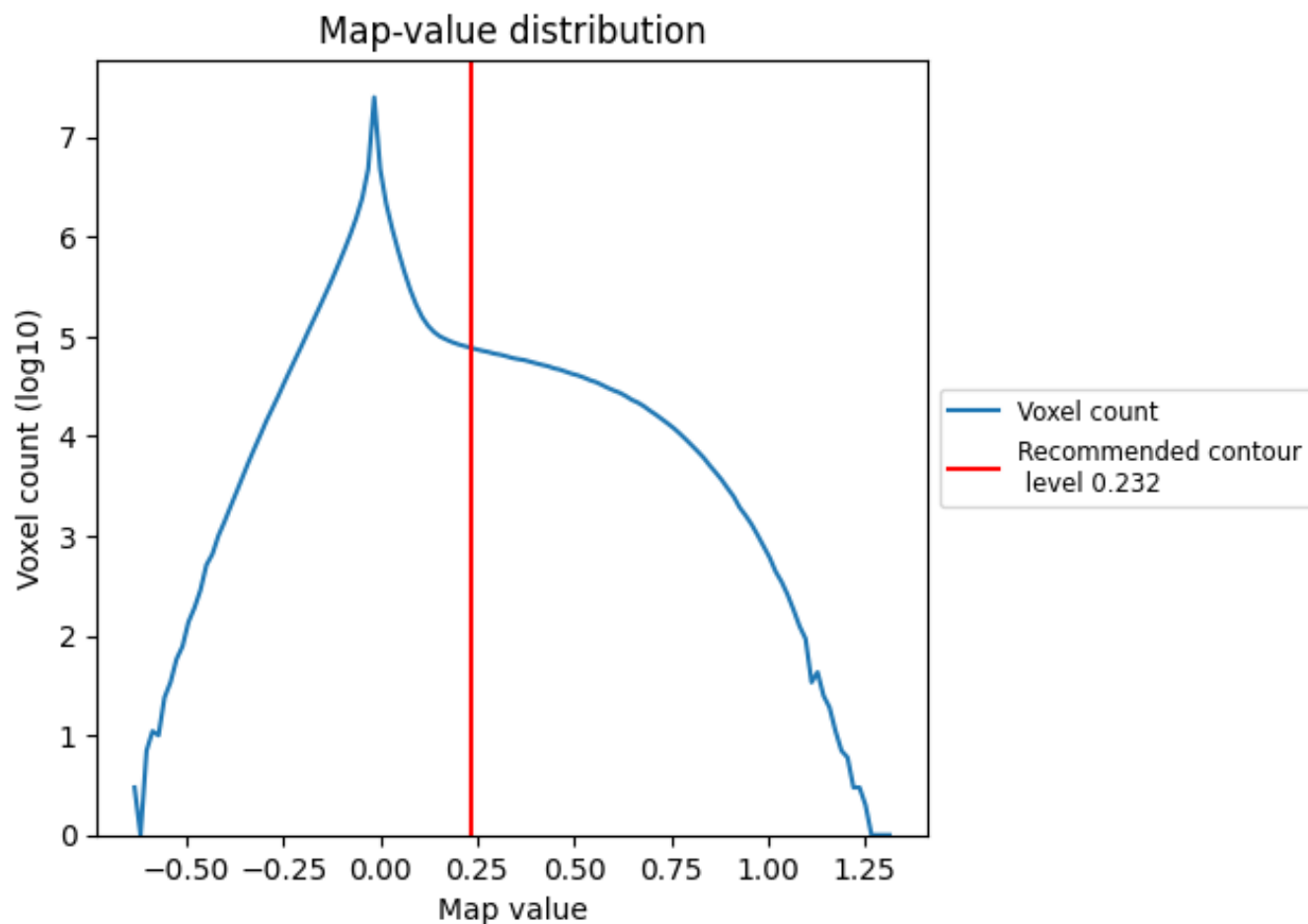
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

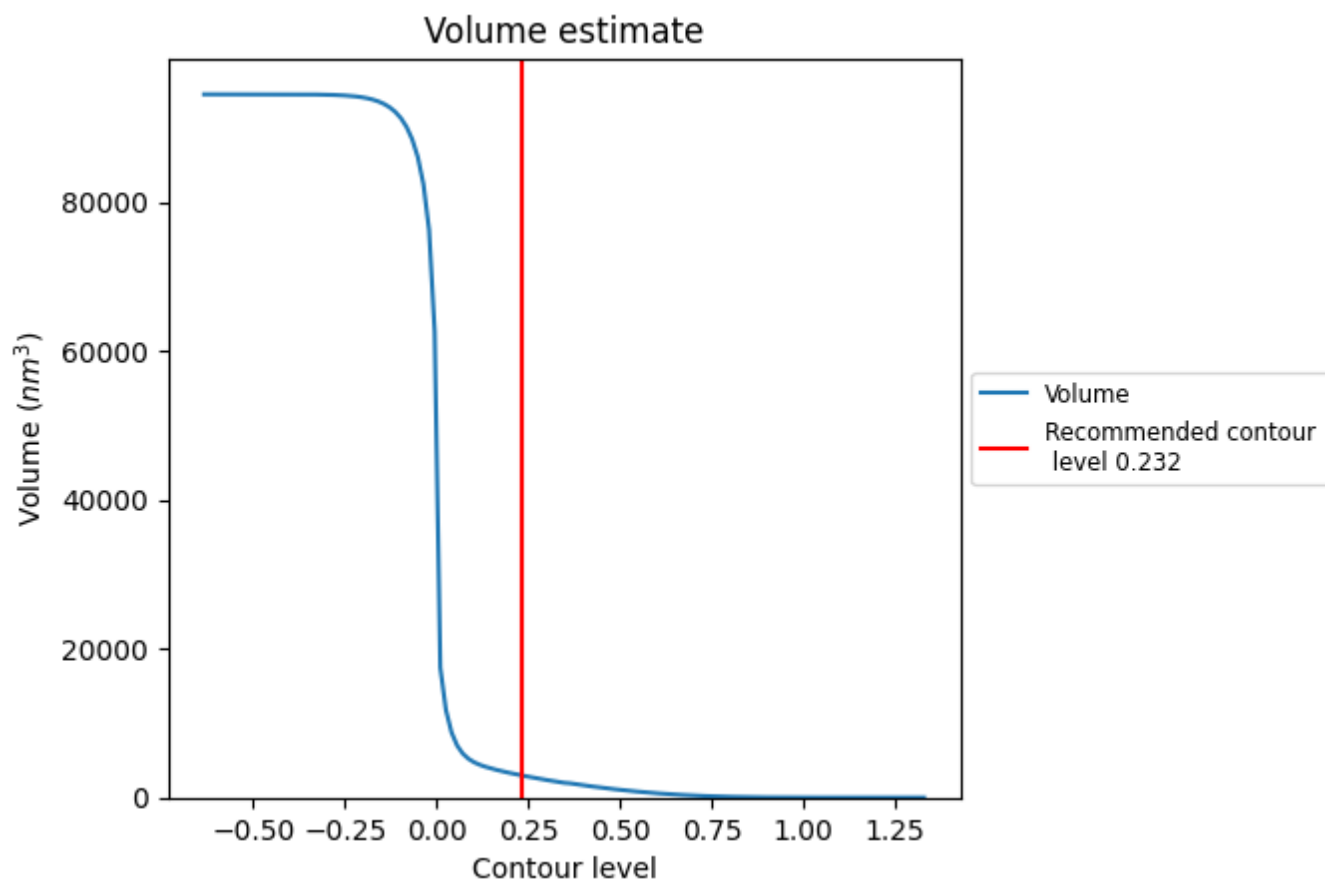
This section contains the results of statistical analysis of the map.

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.

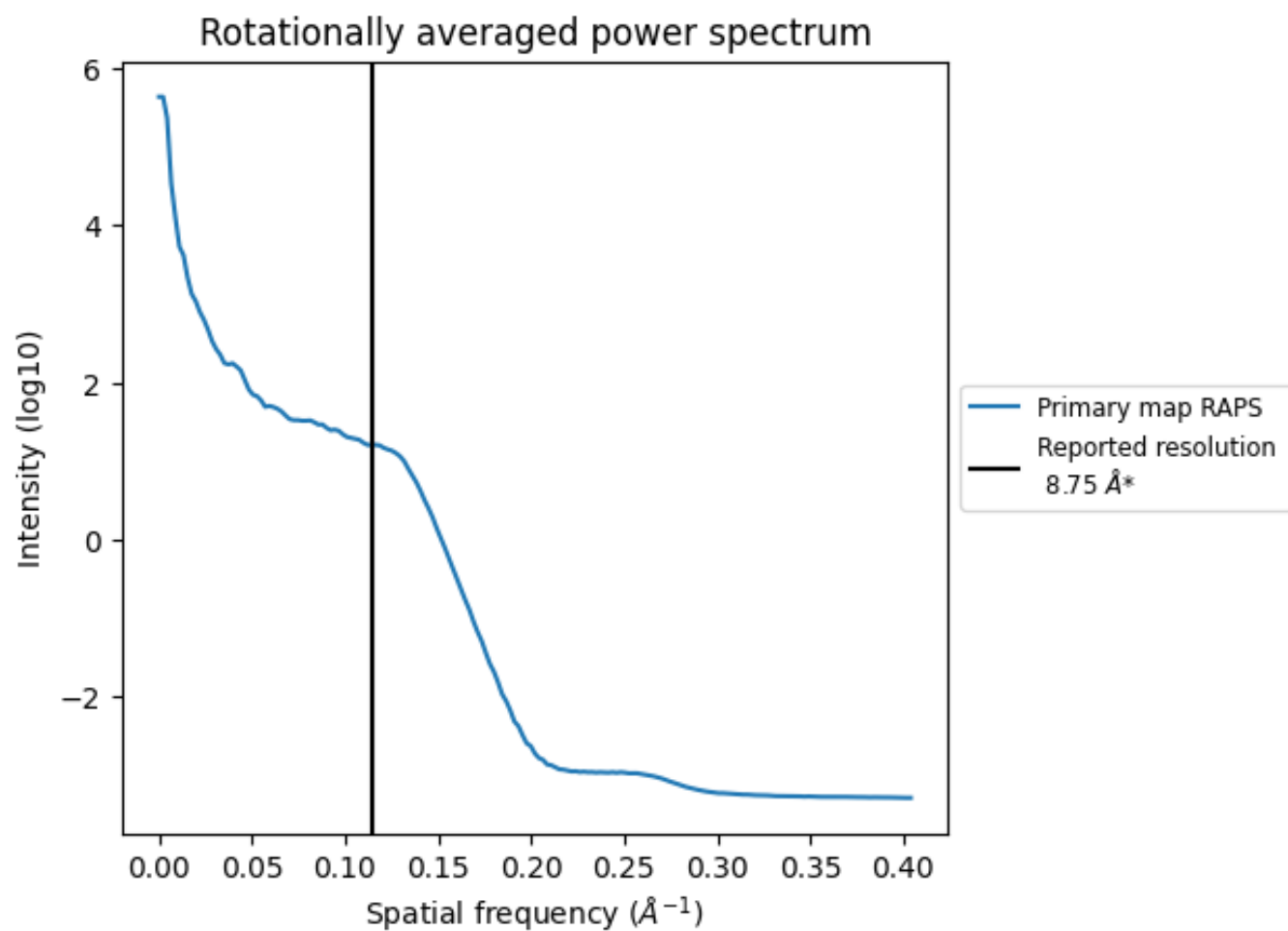
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2976 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

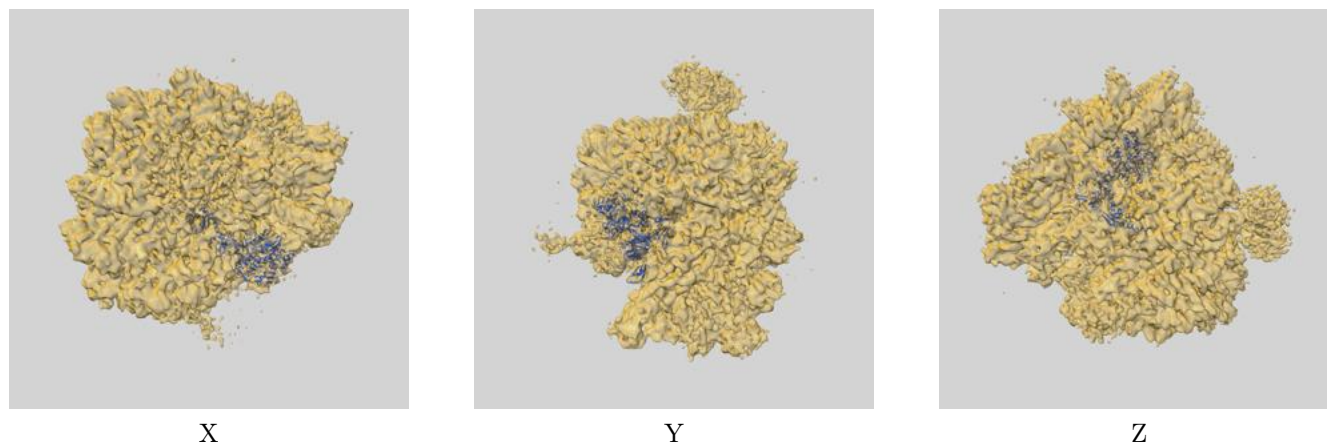
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

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

9.1 Map-model overlay [i](#)



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](#)

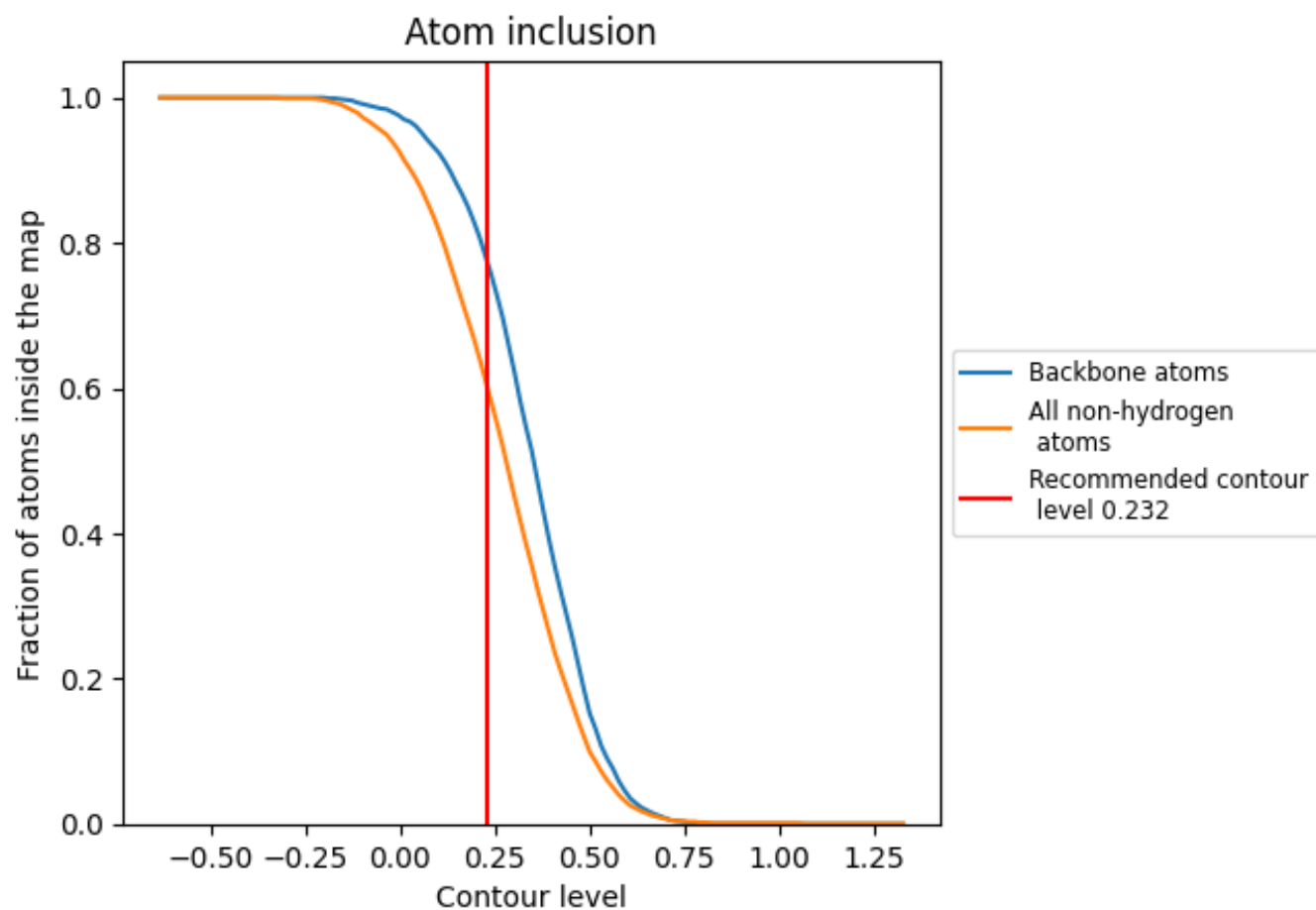


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

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 ⓘ

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

