



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:29 PM UTC

PDB ID : 3J6P / pdb_00003j6p
EMDB ID : EMD-5931
Title : Pseudo-atomic model of dynein microtubule binding domain-tubulin complex based on a cryoEM map
Authors : Uchimura, S.; Fujii, T.; Takazaki, H.; Ayukawa, R.; Nishikawa, Y.; Minoura, I.; Hachikubo, Y.; Kurisu, G.; Sutoh, K.; Kon, T.; Namba, K.; Muto, E.
Deposited on : 2014-03-20
Resolution : 8.20 Å (reported)
Based on initial models : 1JFF, 3VKH

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

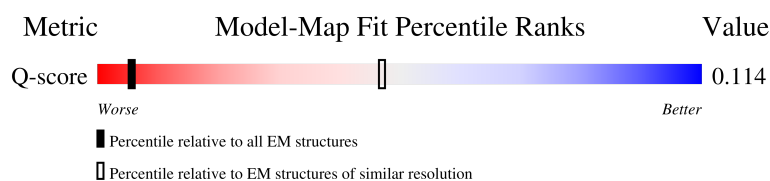
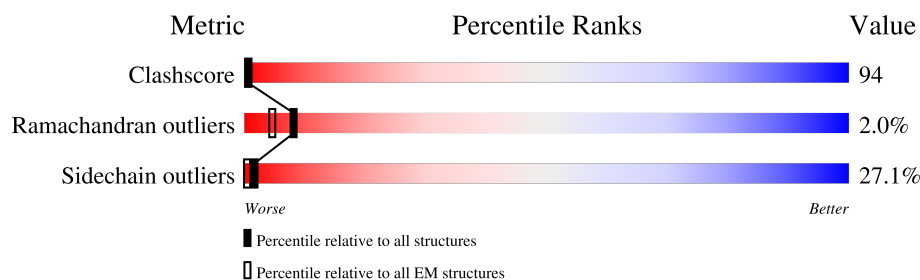
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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	337 (7.70 - 8.70)

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	D	108	43% 19% 56% 23% .
2	A	451	14% 18% 50% 22% . 9%
3	B	445	12% 14% 55% 23% . .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7563 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	108	Total	C	N	O	S	0	0
			862	557	141	157	7		

- Molecule 2 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

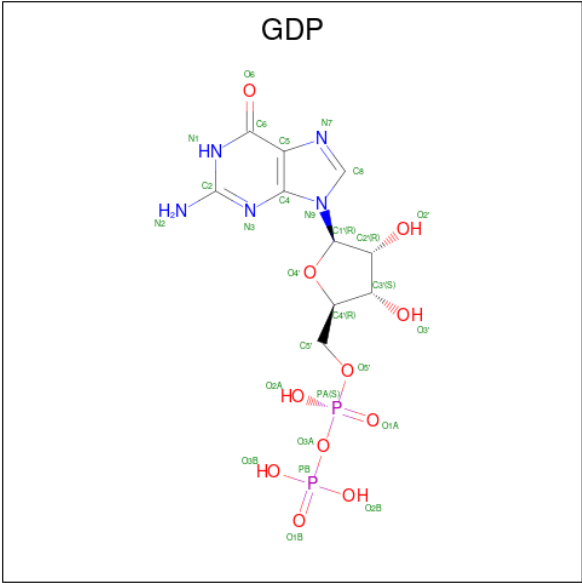
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



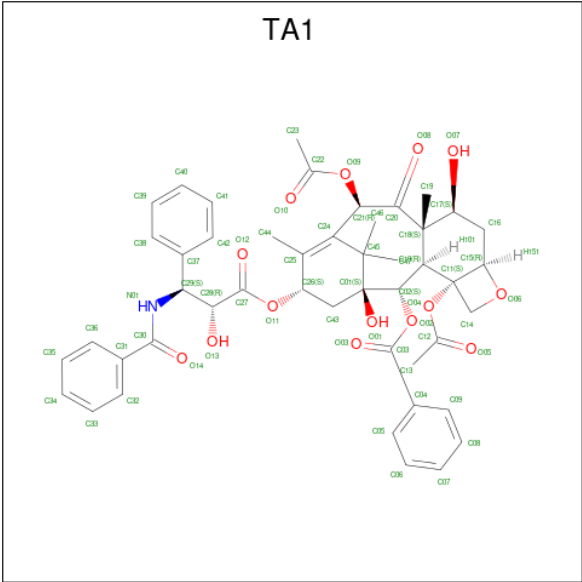
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).

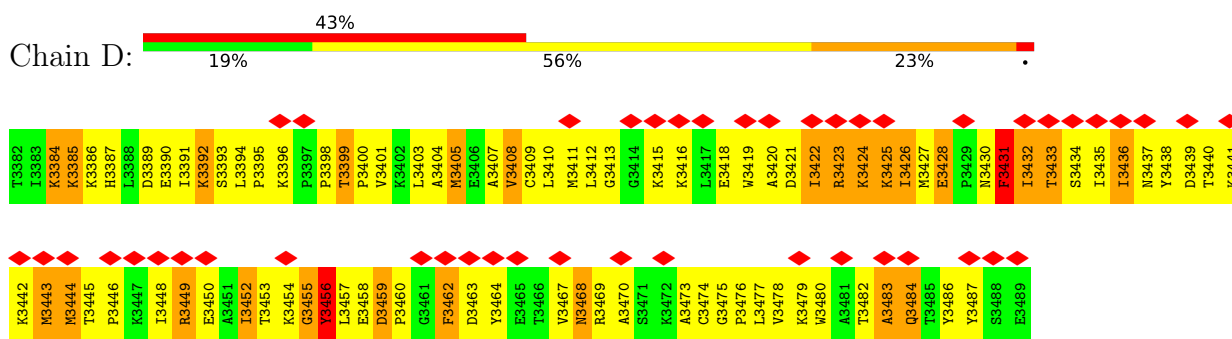


Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			62	47	1	14	

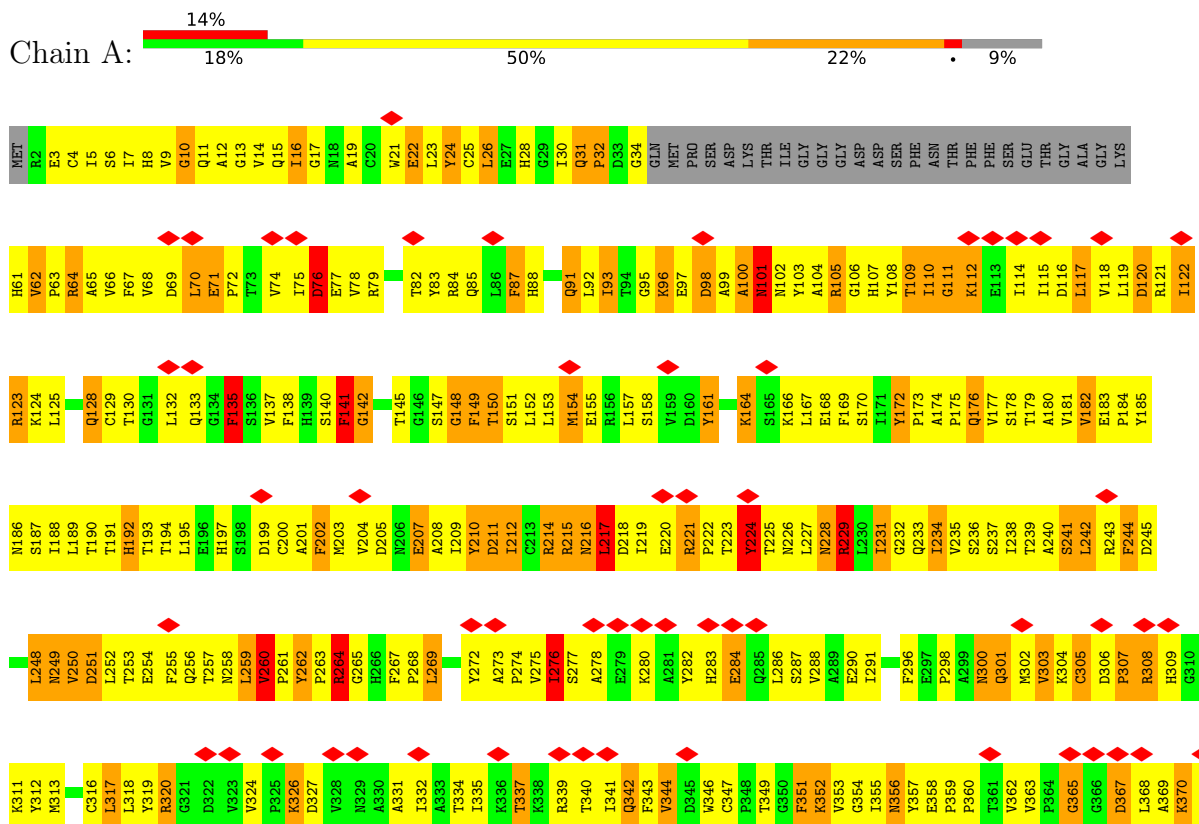
3 Residue-property plots

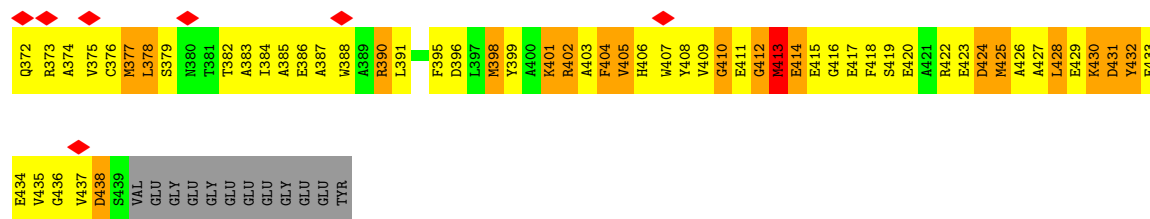
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

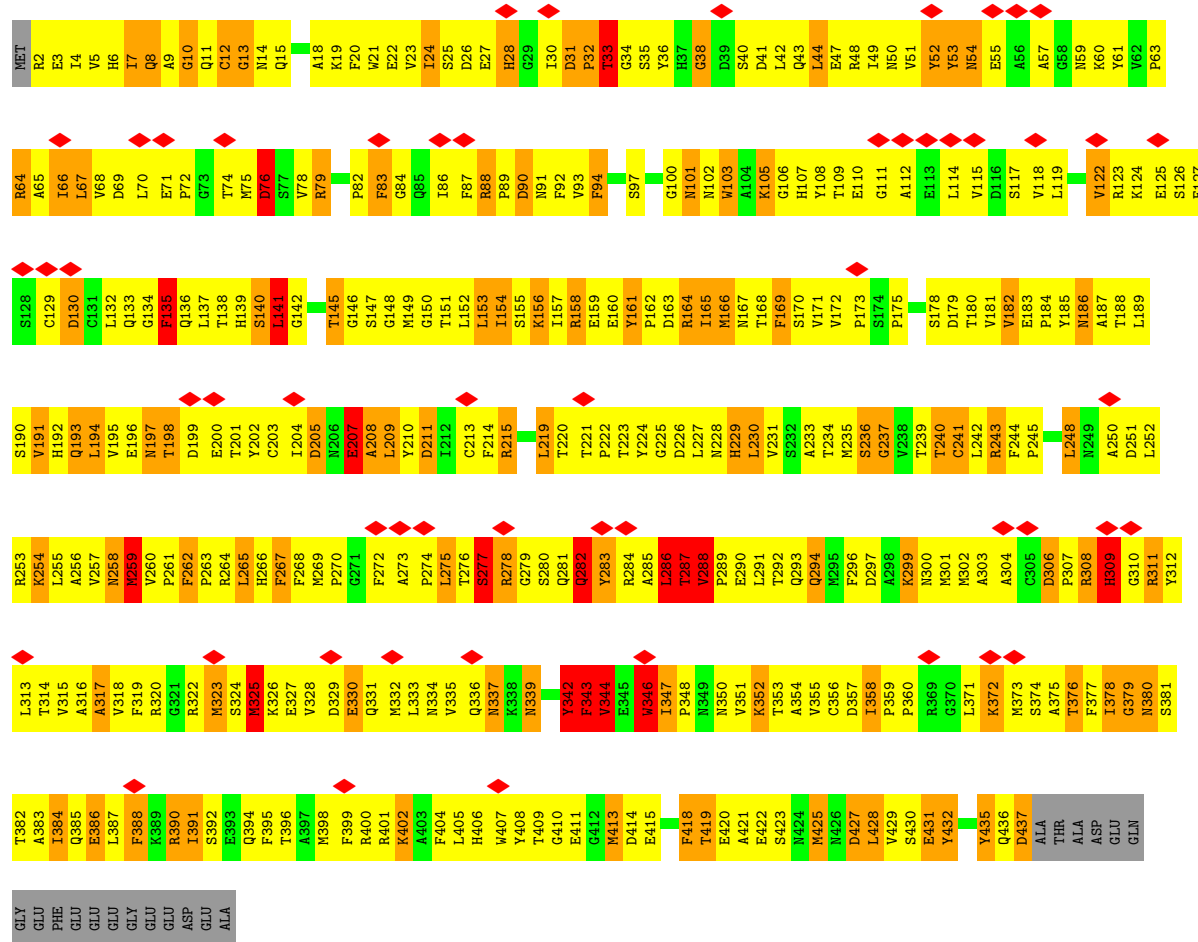
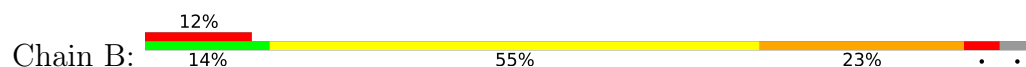


• Molecule 2: Tubulin alpha-1A chain





• Molecule 3: Tubulin beta chain



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	CTFFIND3 Each particle	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	109489	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	0.389	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	137.0, 137.0, 137.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, GTP, TA1

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	D	1.41	0/881	1.63	5/1186 (0.4%)
2	A	1.44	2/3300 (0.1%)	1.72	46/4482 (1.0%)
3	B	1.42	0/3426	1.72	59/4642 (1.3%)
All	All	1.43	2/7607 (0.0%)	1.71	110/10310 (1.1%)

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	D	0	1
2	A	0	12
3	B	0	10
All	All	0	23

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	30	ILE	C-N	9.37	1.52	1.33
2	A	410	GLY	CA-C	-6.91	1.44	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	PHE	CA-CB-CG	-13.25	100.55	113.80
2	A	404	PHE	CA-CB-CG	-10.12	103.67	113.80
2	A	62	VAL	CA-C-N	9.96	129.90	120.03
2	A	62	VAL	C-N-CA	9.96	129.90	120.03
3	B	83	PHE	CA-CB-CG	-9.58	104.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3431	PHE	CA-CB-CG	-9.14	104.66	113.80
3	B	28	HIS	CA-CB-CG	-8.81	104.99	113.80
3	B	296	PHE	CA-CB-CG	-8.64	105.16	113.80
2	A	367	ASP	CA-CB-CG	-8.59	104.02	112.60
3	B	388	PHE	CA-CB-CG	-8.56	105.24	113.80
1	D	3462	PHE	CA-CB-CG	-8.51	105.29	113.80
3	B	343	PHE	CA-CB-CG	-8.49	105.31	113.80
3	B	13	GLY	CA-C-N	8.40	132.21	120.29
3	B	13	GLY	C-N-CA	8.40	132.21	120.29
2	A	142	GLY	N-CA-C	-8.20	104.81	113.58
2	A	30	ILE	O-C-N	-8.13	112.07	122.32
2	A	296	PHE	CA-CB-CG	-8.12	105.67	113.80
2	A	216	ASN	CA-CB-CG	-7.58	105.02	112.60
3	B	248	LEU	CA-C-N	-7.56	112.57	123.00
3	B	248	LEU	C-N-CA	-7.56	112.57	123.00
1	D	3456	TYR	N-CA-C	-7.49	103.12	111.28
2	A	161	TYR	CA-CB-CG	-7.41	100.57	113.90
3	B	267	PHE	CA-CB-CG	-7.34	106.45	113.80
1	D	3468	ASN	CA-CB-CG	-7.25	105.35	112.60
3	B	283	TYR	CA-CB-CG	-7.01	101.28	113.90
3	B	346	TRP	CA-C-N	-6.97	117.86	122.60
3	B	346	TRP	C-N-CA	-6.97	117.86	122.60
2	A	217	LEU	N-CA-CB	6.93	121.70	110.40
3	B	103	TRP	N-CA-C	-6.76	103.91	111.28
3	B	306	ASP	CA-CB-CG	-6.76	105.84	112.60
3	B	197	ASN	CA-CB-CG	-6.66	105.94	112.60
3	B	358	ILE	CA-C-O	6.65	123.90	119.38
2	A	265	GLY	N-CA-C	-6.59	106.59	115.36
2	A	87	PHE	CA-CB-CG	-6.55	107.25	113.80
2	A	396	ASP	CA-CB-CG	-6.50	106.11	112.60
2	A	249	ASN	CA-CB-CG	-6.48	106.12	112.60
2	A	403	ALA	CA-C-N	6.29	131.23	120.72
2	A	403	ALA	C-N-CA	6.29	131.23	120.72
2	A	228	ASN	CA-CB-CG	-6.26	106.34	112.60
2	A	149	PHE	CA-CB-CG	-6.19	107.61	113.80
3	B	357	ASP	CA-CB-CG	-6.19	106.41	112.60
3	B	237	GLY	N-CA-C	-6.14	105.36	112.73
3	B	334	ASN	CA-CB-CG	-6.12	106.48	112.60
3	B	309	HIS	CA-CB-CG	-6.08	107.72	113.80
2	A	259	LEU	CA-C-N	-6.05	116.72	123.02
2	A	259	LEU	C-N-CA	-6.05	116.72	123.02
1	D	3421	ASP	CA-CB-CG	-6.04	106.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	340	THR	N-CA-C	-6.02	104.84	111.82
2	A	76	ASP	CA-CB-CG	-5.99	106.61	112.60
2	A	351	PHE	CA-CB-CG	-5.93	107.87	113.80
3	B	437	ASP	CA-CB-CG	-5.91	106.69	112.60
3	B	410	GLY	N-CA-C	-5.90	105.65	112.73
3	B	90	ASP	N-CA-C	-5.86	105.02	111.82
3	B	418	PHE	CA-CB-CG	-5.85	107.95	113.80
3	B	339	ASN	CA-CB-CG	-5.82	106.78	112.60
3	B	76	ASP	CA-CB-CG	-5.82	106.78	112.60
2	A	169	PHE	CA-CB-CG	-5.82	107.98	113.80
3	B	101	ASN	CA-CB-CG	-5.79	106.81	112.60
3	B	347	ILE	CA-C-O	5.79	122.36	119.12
3	B	52	TYR	CA-CB-CG	-5.76	103.53	113.90
3	B	215	ARG	CB-CA-C	-5.73	102.07	110.95
3	B	262	PHE	CA-CB-CG	-5.71	108.09	113.80
2	A	141	PHE	CA-CB-CG	-5.70	108.10	113.80
2	A	10	GLY	N-CA-C	-5.70	105.25	112.65
2	A	28	HIS	CA-CB-CG	-5.69	108.11	113.80
2	A	260	VAL	CA-C-O	5.68	123.35	119.20
2	A	202	PHE	CA-CB-CG	-5.65	108.15	113.80
3	B	342	TYR	N-CA-CB	5.65	119.04	110.28
3	B	254	LYS	N-CA-C	-5.63	105.04	111.07
3	B	402	LYS	CB-CA-C	-5.60	104.01	111.63
2	A	403	ALA	CB-CA-C	-5.60	108.50	116.34
3	B	357	ASP	CA-C-N	-5.58	117.30	123.43
3	B	357	ASP	C-N-CA	-5.58	117.30	123.43
3	B	207	GLU	N-CA-C	-5.57	105.29	111.36
3	B	309	HIS	CA-C-N	5.55	131.70	121.70
3	B	309	HIS	C-N-CA	5.55	131.70	121.70
3	B	259	MET	CA-C-N	-5.50	116.58	122.85
3	B	259	MET	C-N-CA	-5.50	116.58	122.85
2	A	365	GLY	CA-C-N	-5.49	110.64	121.41
2	A	365	GLY	C-N-CA	-5.49	110.64	121.41
2	A	258	ASN	CA-CB-CG	-5.49	107.11	112.60
3	B	435	TYR	CA-CB-CG	-5.48	104.04	113.90
2	A	71	GLU	CA-C-N	5.46	125.29	119.28
2	A	71	GLU	C-N-CA	5.46	125.29	119.28
3	B	169	PHE	CA-CB-CG	-5.45	108.35	113.80
2	A	357	TYR	CA-CB-CG	-5.43	104.13	113.90
3	B	258	ASN	CA-CB-CG	-5.42	107.18	112.60
2	A	211	ASP	CA-CB-CG	-5.38	107.22	112.60
3	B	205	ASP	CA-CB-CG	-5.34	107.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	70	LEU	CA-C-N	5.29	128.97	121.61
2	A	70	LEU	C-N-CA	5.29	128.97	121.61
3	B	317	ALA	CA-C-N	-5.29	116.39	122.95
3	B	317	ALA	C-N-CA	-5.29	116.39	122.95
2	A	343	PHE	CA-CB-CG	-5.29	108.51	113.80
2	A	438	ASP	CA-CB-CG	-5.26	107.34	112.60
3	B	208	ALA	N-CA-C	-5.25	105.56	111.28
2	A	224	TYR	N-CA-C	-5.24	105.65	111.36
2	A	101	ASN	CB-CA-C	-5.24	104.49	111.88
3	B	308	ARG	N-CA-C	-5.22	105.70	111.71
2	A	135	PHE	CA-CB-CG	-5.19	108.61	113.80
3	B	10	GLY	N-CA-C	-5.18	106.15	112.68
3	B	31	ASP	CA-CB-CG	-5.17	107.43	112.60
3	B	135	PHE	CA-CB-CG	-5.17	108.63	113.80
2	A	262	TYR	CA-CB-CG	-5.11	104.70	113.90
3	B	404	PHE	CA-C-N	5.10	127.12	120.28
3	B	404	PHE	C-N-CA	5.10	127.12	120.28
3	B	325	MET	N-CA-C	-5.07	105.83	111.36
3	B	358	ILE	CA-C-N	5.04	125.57	120.38
3	B	358	ILE	C-N-CA	5.04	125.57	120.38
2	A	356	ASN	CA-CB-CG	-5.04	107.56	112.60

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	110	ILE	Peptide
2	A	141	PHE	Peptide
2	A	176	GLN	Peptide
2	A	182	VAL	Peptide
2	A	221	ARG	Peptide
2	A	229	ARG	Sidechain
2	A	264	ARG	Peptide
2	A	283	HIS	Peptide
2	A	309	HIS	Peptide
2	A	365	GLY	Peptide
2	A	415	GLU	Peptide
2	A	64	ARG	Peptide
3	B	12	CYS	Peptide
3	B	141	LEU	Peptide
3	B	182	VAL	Peptide
3	B	277	SER	Peptide

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Mol	Chain	Res	Type	Group
3	B	286	LEU	Peptide
3	B	287	THR	Peptide
3	B	288	VAL	Peptide
3	B	33	THR	Peptide
3	B	379	GLY	Peptide
3	B	83	PHE	Peptide
1	D	3455	GLY	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	D	862	0	902	209	0
2	A	3227	0	3143	610	0
3	B	3351	0	3229	658	0
4	A	1	0	0	0	0
5	A	32	0	12	3	0
6	B	28	0	12	1	0
7	B	62	0	51	7	0
All	All	7563	0	7349	1401	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 94.

All (1401) 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)
3:B:191:VAL:HA	3:B:194:LEU:HD12	1.21	1.17
3:B:250:ALA:HA	3:B:254:LYS:HE2	1.21	1.16
2:A:11:GLN:HG3	2:A:74:VAL:HG11	1.26	1.13
2:A:259:LEU:HD11	2:A:378:LEU:HD13	1.27	1.12
2:A:151:SER:HB3	2:A:193:THR:HG21	1.32	1.11
3:B:234:THR:HG21	3:B:270:PRO:HB3	1.21	1.10
2:A:71:GLU:HG3	3:B:2:ARG:HH21	1.15	1.08
2:A:316:CYS:HB2	2:A:378:LEU:HD11	1.27	1.08
1:D:3416:LYS:HG3	1:D:3418:GLU:H	1.14	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:VAL:HG13	2:A:305:CYS:H	1.18	1.08
3:B:57:ALA:HB2	3:B:60:LYS:HD2	1.30	1.08
1:D:3424:LYS:HB2	3:B:159:GLU:HB2	1.34	1.07
2:A:311:LYS:HG2	2:A:344:VAL:HG13	1.23	1.07
3:B:324:SER:HB3	3:B:327:GLU:HG2	1.08	1.06
2:A:119:LEU:HA	2:A:122:ILE:HD11	1.37	1.04
2:A:7:ILE:HG12	2:A:137:VAL:HG22	1.35	1.02
3:B:102:ASN:HB3	3:B:105:LYS:H	1.22	1.02
3:B:133:GLN:HE21	3:B:252:LEU:HB2	1.20	1.02
1:D:3387:HIS:HD2	1:D:3473:ALA:HB2	1.24	1.02
2:A:66:VAL:HG12	2:A:91:GLN:HG3	1.41	1.02
2:A:115:ILE:HD11	2:A:153:LEU:HD13	1.40	1.02
2:A:269:LEU:HD22	2:A:384:ILE:HD11	1.42	1.01
3:B:269:MET:HE3	3:B:301:MET:HE2	1.38	1.01
3:B:251:ASP:H	3:B:254:LYS:HG3	1.27	1.00
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.40	0.99
3:B:210:TYR:CE1	3:B:227:LEU:HD11	1.97	0.99
3:B:21:TRP:HA	3:B:24:ILE:HG22	1.42	0.98
1:D:3424:LYS:HZ2	3:B:159:GLU:HB3	1.26	0.98
2:A:286:LEU:HG	2:A:290:GLU:HB2	1.45	0.98
3:B:133:GLN:HG2	3:B:252:LEU:HD12	1.46	0.98
3:B:275:LEU:HD23	3:B:300:ASN:HD21	1.29	0.97
2:A:362:VAL:HG13	2:A:368:LEU:HB2	1.45	0.97
1:D:3390:GLU:HG3	2:A:402:ARG:HH22	1.29	0.97
2:A:102:ASN:HB2	2:A:408:TYR:CE1	2.00	0.96
2:A:219:ILE:HB	2:A:222:PRO:HG3	1.46	0.96
1:D:3464:TYR:CE1	1:D:3478:VAL:HG11	2.00	0.96
1:D:3416:LYS:HE2	1:D:3418:GLU:HB2	1.45	0.95
3:B:147:SER:HB3	3:B:190:SER:HB3	1.48	0.94
1:D:3455:GLY:HA2	1:D:3458:GLU:H	1.32	0.94
3:B:241:CYS:HB2	3:B:320:ARG:HE	1.31	0.94
2:A:69:ASP:HB2	2:A:75:ILE:HD11	1.50	0.94
3:B:319:PHE:CD2	3:B:375:ALA:HB2	2.03	0.94
1:D:3423:ARG:HH12	3:B:158:ARG:HD2	1.30	0.93
2:A:26:LEU:HD21	2:A:363:VAL:HG13	1.49	0.93
3:B:264:ARG:HB2	3:B:266:HIS:CD2	2.03	0.93
3:B:269:MET:SD	3:B:303:ALA:HB3	2.09	0.93
3:B:48:ARG:HG2	3:B:243:ARG:HB3	1.48	0.92
2:A:210:TYR:HE1	2:A:227:LEU:HD21	1.32	0.92
3:B:57:ALA:HB3	3:B:60:LYS:H	1.32	0.92
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:VAL:CG2	3:B:258:ASN:HB3	2.00	0.91
3:B:133:GLN:CG	3:B:252:LEU:HD12	1.99	0.91
3:B:269:MET:HE3	3:B:301:MET:CE	1.99	0.91
2:A:316:CYS:HB2	2:A:378:LEU:CD1	2.00	0.91
3:B:140:SER:HB2	3:B:142:GLY:CA	2.00	0.91
3:B:27:GLU:OE1	7:B:502:TA1:H411	1.68	0.91
3:B:6:HIS:HB3	3:B:65:ALA:HB2	1.53	0.90
1:D:3387:HIS:CD2	1:D:3473:ALA:HB2	2.07	0.90
2:A:167:LEU:HD23	2:A:202:PHE:CE2	2.07	0.90
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.51	0.90
2:A:104:ALA:HB1	2:A:411:GLU:HB2	1.54	0.90
2:A:276:ILE:HG23	2:A:369:ALA:CB	2.01	0.90
1:D:3424:LYS:HE2	3:B:156:LYS:HD2	1.52	0.90
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.51	0.90
3:B:140:SER:HB2	3:B:142:GLY:HA3	1.53	0.90
1:D:3431:PHE:CE1	1:D:3435:ILE:HD11	2.06	0.89
2:A:179:THR:HG21	3:B:248:LEU:CD2	2.02	0.89
2:A:311:LYS:CG	2:A:344:VAL:HG13	2.03	0.89
1:D:3384:LYS:HD3	1:D:3386:LYS:HB2	1.54	0.89
1:D:3416:LYS:HG3	1:D:3418:GLU:N	1.88	0.89
3:B:132:LEU:HB3	3:B:164:ARG:HD3	1.54	0.89
3:B:241:CYS:HB2	3:B:320:ARG:NE	1.88	0.88
2:A:154:MET:HA	2:A:157:LEU:HD12	1.53	0.88
3:B:264:ARG:HB2	3:B:266:HIS:HD2	1.36	0.88
1:D:3445:THR:HB	1:D:3446:PRO:HD3	1.54	0.88
1:D:3457:LEU:HA	1:D:3462:PHE:HD2	1.39	0.88
1:D:3464:TYR:HB2	1:D:3478:VAL:HG21	1.54	0.88
2:A:110:ILE:HG23	2:A:111:GLY:H	1.39	0.87
2:A:422:ARG:HH12	2:A:426:ALA:HB2	1.39	0.87
3:B:75:MET:HE1	3:B:94:PHE:HB3	1.54	0.87
1:D:3424:LYS:HZ1	3:B:156:LYS:HA	1.40	0.87
3:B:269:MET:HB2	3:B:301:MET:HE3	1.55	0.86
2:A:132:LEU:CD2	2:A:164:LYS:HE3	2.04	0.86
2:A:181:VAL:HG23	3:B:258:ASN:HB3	1.56	0.86
2:A:155:GLU:HG2	2:A:197:HIS:CE1	2.10	0.86
2:A:174:ALA:HB3	2:A:177:VAL:HB	1.55	0.86
2:A:362:VAL:CG1	2:A:368:LEU:HB2	2.06	0.86
1:D:3394:LEU:HB3	2:A:410:GLY:HA2	1.58	0.85
3:B:315:VAL:HG13	3:B:377:PHE:CE1	2.11	0.85
2:A:66:VAL:CG1	2:A:91:GLN:HG3	2.05	0.85
3:B:301:MET:HE1	3:B:377:PHE:HE2	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3394:LEU:CB	2:A:410:GLY:HA2	2.07	0.85
2:A:119:LEU:O	2:A:122:ILE:HG12	1.76	0.85
2:A:229:ARG:HG2	2:A:229:ARG:HH11	1.40	0.85
2:A:115:ILE:HD13	2:A:152:LEU:HD11	1.58	0.85
3:B:285:ALA:HB1	3:B:290:GLU:HG2	1.59	0.84
1:D:3464:TYR:CB	1:D:3478:VAL:HG21	2.07	0.84
1:D:3475:GLY:O	1:D:3478:VAL:HG12	1.76	0.84
3:B:105:LYS:HG3	3:B:110:GLU:HG2	1.58	0.84
2:A:317:LEU:HG	2:A:377:MET:HB2	1.58	0.84
3:B:256:ALA:O	3:B:260:VAL:HG22	1.76	0.84
3:B:319:PHE:HA	3:B:375:ALA:HA	1.57	0.84
3:B:189:LEU:HD23	3:B:421:ALA:CB	2.08	0.84
2:A:274:PRO:HG2	2:A:374:ALA:CB	2.06	0.83
3:B:6:HIS:HB3	3:B:65:ALA:CB	2.08	0.83
3:B:8:GLN:OE1	3:B:67:LEU:HD22	1.78	0.83
2:A:112:LYS:O	2:A:115:ILE:HG22	1.78	0.83
2:A:174:ALA:HB1	2:A:207:GLU:HG2	1.60	0.83
3:B:105:LYS:CG	3:B:110:GLU:HG2	2.08	0.83
3:B:168:THR:HB	3:B:201:THR:HG23	1.60	0.83
2:A:311:LYS:HG2	2:A:344:VAL:CG1	2.08	0.83
2:A:71:GLU:HG3	3:B:2:ARG:NH2	1.93	0.83
2:A:151:SER:HB3	2:A:193:THR:CG2	2.08	0.83
2:A:276:ILE:O	2:A:369:ALA:HB2	1.79	0.83
3:B:243:ARG:HH22	3:B:252:LEU:HG	1.43	0.83
1:D:3424:LYS:NZ	3:B:156:LYS:HA	1.93	0.83
2:A:68:VAL:HG13	2:A:93:ILE:CG2	2.09	0.83
3:B:30:ILE:HD12	3:B:53:TYR:CE2	2.14	0.83
2:A:223:THR:HG22	2:A:224:TYR:H	1.44	0.82
3:B:75:MET:CE	3:B:94:PHE:HB3	2.09	0.82
3:B:133:GLN:NE2	3:B:252:LEU:HB2	1.94	0.82
2:A:305:CYS:SG	2:A:384:ILE:HD13	2.18	0.82
2:A:115:ILE:CD1	2:A:153:LEU:HD13	2.08	0.82
2:A:242:LEU:HG	2:A:250:VAL:O	1.78	0.82
3:B:275:LEU:HD23	3:B:300:ASN:ND2	1.93	0.82
1:D:3464:TYR:CG	1:D:3478:VAL:HG21	2.15	0.81
3:B:172:VAL:HG11	3:B:387:LEU:CD2	2.09	0.81
3:B:274:PRO:O	3:B:275:LEU:HD13	1.80	0.81
1:D:3482:THR:HG23	1:D:3486:TYR:CD2	2.16	0.81
2:A:225:THR:O	2:A:229:ARG:HG3	1.80	0.81
2:A:276:ILE:HG23	2:A:369:ALA:HB2	1.61	0.81
2:A:301:GLN:HE22	2:A:307:PRO:HD3	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:189:LEU:HD23	3:B:421:ALA:HB3	1.62	0.81
2:A:22:GLU:HG2	2:A:83:TYR:CE1	2.15	0.81
3:B:103:TRP:HD1	3:B:147:SER:HB2	1.43	0.81
3:B:155:SER:HA	3:B:197:ASN:HD21	1.46	0.81
2:A:107:HIS:HB2	2:A:148:GLY:HA2	1.62	0.80
2:A:362:VAL:HG21	2:A:370:LYS:N	1.97	0.80
3:B:70:LEU:H	3:B:145:THR:HG21	1.46	0.80
1:D:3464:TYR:CD1	1:D:3478:VAL:HG11	2.15	0.80
2:A:103:TYR:HD2	2:A:413:MET:HE2	1.47	0.80
2:A:119:LEU:HA	2:A:122:ILE:CD1	2.11	0.80
3:B:323:MET:HE3	3:B:373:MET:SD	2.21	0.80
1:D:3432:ILE:HD13	1:D:3433:THR:H	1.46	0.80
2:A:66:VAL:HA	2:A:91:GLN:HG2	1.62	0.80
3:B:234:THR:CG2	3:B:270:PRO:HB3	2.10	0.80
3:B:149:MET:O	3:B:153:LEU:HD22	1.83	0.79
2:A:223:THR:HB	2:A:225:THR:HG22	1.63	0.79
2:A:286:LEU:HG	2:A:290:GLU:CB	2.12	0.79
1:D:3433:THR:O	1:D:3436:ILE:HG12	1.83	0.79
1:D:3455:GLY:HA2	1:D:3457:LEU:HG	1.64	0.79
2:A:132:LEU:HD21	2:A:164:LYS:HE3	1.63	0.79
3:B:4:ILE:HD11	3:B:252:LEU:CD1	2.11	0.79
1:D:3464:TYR:CD1	1:D:3478:VAL:HG21	2.18	0.79
2:A:301:GLN:HB2	2:A:303:VAL:H	1.48	0.79
1:D:3394:LEU:HD22	2:A:410:GLY:CA	2.13	0.78
2:A:431:ASP:O	2:A:435:VAL:HG23	1.82	0.78
1:D:3428:GLU:HG2	1:D:3431:PHE:H	1.47	0.78
3:B:31:ASP:O	3:B:34:GLY:HA3	1.83	0.78
3:B:148:GLY:O	3:B:151:THR:HG22	1.83	0.78
1:D:3457:LEU:HA	1:D:3462:PHE:CD2	2.17	0.78
2:A:188:ILE:HG23	2:A:425:MET:SD	2.23	0.78
2:A:211:ASP:O	2:A:215:ARG:HG2	1.84	0.78
3:B:210:TYR:HE1	3:B:227:LEU:HD11	1.45	0.77
2:A:151:SER:CB	2:A:193:THR:HG21	2.11	0.77
3:B:150:GLY:HA2	3:B:153:LEU:CD2	2.15	0.77
3:B:250:ALA:HB1	3:B:254:LYS:HB2	1.67	0.77
3:B:324:SER:HB3	3:B:327:GLU:CG	2.03	0.77
3:B:189:LEU:O	3:B:192:HIS:HB3	1.85	0.77
3:B:286:LEU:HD22	3:B:291:LEU:HD11	1.65	0.77
3:B:115:VAL:HG13	3:B:153:LEU:CD1	2.15	0.77
3:B:184:PRO:HG3	3:B:394:GLN:CB	2.14	0.77
2:A:303:VAL:HG13	2:A:305:CYS:N	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:250:ALA:CA	3:B:254:LYS:HE2	2.11	0.76
2:A:72:PRO:HG3	2:A:96:LYS:HA	1.67	0.76
2:A:104:ALA:CB	2:A:411:GLU:HB2	2.15	0.76
3:B:30:ILE:HG22	3:B:31:ASP:O	1.86	0.76
2:A:205:ASP:HB3	2:A:208:ALA:CB	2.15	0.76
2:A:199:ASP:HB3	2:A:256:GLN:NE2	2.01	0.76
3:B:242:LEU:HD22	3:B:250:ALA:O	1.86	0.75
2:A:74:VAL:O	2:A:77:GLU:HB2	1.86	0.75
3:B:323:MET:HG3	3:B:328:VAL:CG2	2.17	0.75
2:A:183:GLU:HB3	2:A:184:PRO:HD3	1.68	0.75
2:A:362:VAL:HG21	2:A:370:LYS:H	1.52	0.75
3:B:204:ILE:HG21	3:B:209:LEU:HD21	1.69	0.75
3:B:108:TYR:CE1	3:B:413:MET:HE1	2.21	0.75
2:A:199:ASP:HB3	2:A:256:GLN:HE21	1.51	0.75
3:B:21:TRP:HA	3:B:24:ILE:CG2	2.17	0.75
2:A:422:ARG:NH1	2:A:426:ALA:HB2	2.01	0.75
3:B:243:ARG:NH2	3:B:252:LEU:HG	2.00	0.75
3:B:149:MET:C	3:B:153:LEU:HD22	2.12	0.75
3:B:151:THR:O	3:B:154:ILE:HG13	1.86	0.75
3:B:286:LEU:HD13	3:B:373:MET:O	1.87	0.75
3:B:323:MET:HG3	3:B:328:VAL:HG21	1.68	0.75
2:A:69:ASP:HB3	2:A:75:ILE:CG1	2.17	0.75
3:B:325:MET:HE3	3:B:355:VAL:HG21	1.68	0.75
1:D:3455:GLY:CA	1:D:3458:GLU:H	2.00	0.74
3:B:19:LYS:O	3:B:22:GLU:HB2	1.86	0.74
3:B:57:ALA:HB2	3:B:60:LYS:CD	2.14	0.74
3:B:237:GLY:O	3:B:241:CYS:HB3	1.87	0.74
3:B:324:SER:O	3:B:328:VAL:HG23	1.86	0.74
3:B:371:LEU:HG	3:B:372:LYS:N	2.00	0.74
3:B:172:VAL:HG11	3:B:387:LEU:HD23	1.67	0.74
3:B:201:THR:OG1	3:B:265:LEU:HD11	1.87	0.74
1:D:3459:ASP:HB2	1:D:3462:PHE:HB3	1.67	0.74
2:A:7:ILE:CG1	2:A:137:VAL:HG22	2.15	0.74
3:B:10:GLY:O	3:B:13:GLY:HA3	1.87	0.74
3:B:103:TRP:CD1	3:B:147:SER:HB2	2.22	0.74
3:B:119:LEU:HA	3:B:122:VAL:CG1	2.16	0.74
2:A:9:VAL:HG11	2:A:150:THR:OG1	1.87	0.74
2:A:177:VAL:HG21	2:A:207:GLU:HB3	1.69	0.74
2:A:210:TYR:CE1	2:A:227:LEU:HD21	2.20	0.74
3:B:332:MET:HE2	3:B:353:THR:OG1	1.87	0.74
1:D:3404:ALA:O	1:D:3408:VAL:HG22	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3405:MET:HA	1:D:3408:VAL:CG2	2.17	0.74
2:A:7:ILE:CG1	2:A:137:VAL:HG13	2.18	0.74
3:B:318:VAL:HA	3:B:354:ALA:HB3	1.68	0.74
3:B:230:LEU:HD21	3:B:302:MET:CE	2.17	0.74
3:B:234:THR:HG23	3:B:376:THR:CG2	2.18	0.74
3:B:310:GLY:O	3:B:342:TYR:HB3	1.88	0.74
1:D:3444:MET:HG2	1:D:3446:PRO:HD2	1.69	0.74
2:A:31:GLN:HB3	2:A:32:PRO:CD	2.18	0.74
2:A:274:PRO:O	2:A:276:ILE:HG22	1.87	0.74
3:B:54:ASN:HD21	3:B:64:ARG:HB2	1.53	0.73
3:B:192:HIS:O	3:B:195:VAL:HG12	1.88	0.73
2:A:155:GLU:HA	2:A:197:HIS:ND1	2.02	0.73
2:A:252:LEU:O	2:A:255:PHE:HB2	1.88	0.73
1:D:3424:LYS:HE2	3:B:156:LYS:CD	2.17	0.73
3:B:209:LEU:HD11	3:B:302:MET:HE2	1.70	0.73
3:B:234:THR:HG23	3:B:376:THR:HG22	1.68	0.73
3:B:275:LEU:HB2	3:B:294:GLN:OE1	1.88	0.73
3:B:259:MET:O	3:B:261:PRO:HD3	1.89	0.73
2:A:241:SER:O	2:A:244:PHE:HB3	1.88	0.73
2:A:402:ARG:HE	2:A:405:VAL:HG12	1.52	0.73
3:B:270:PRO:O	3:B:302:MET:HG3	1.88	0.73
2:A:7:ILE:HG13	2:A:137:VAL:HG13	1.71	0.73
3:B:184:PRO:HG3	3:B:394:GLN:HB3	1.69	0.73
3:B:315:VAL:HG13	3:B:377:PHE:HE1	1.52	0.73
3:B:8:GLN:CD	3:B:67:LEU:HD22	2.13	0.73
3:B:154:ILE:HG22	3:B:166:MET:SD	2.28	0.73
3:B:219:LEU:HD21	3:B:226:ASP:OD2	1.89	0.73
3:B:21:TRP:CZ3	3:B:63:PRO:HB3	2.23	0.73
3:B:141:LEU:HB3	3:B:187:ALA:HA	1.71	0.73
1:D:3408:VAL:HA	1:D:3411:MET:HE2	1.70	0.72
2:A:133:GLN:HB2	2:A:243:ARG:HH12	1.52	0.72
3:B:188:THR:HG23	3:B:425:MET:HE2	1.70	0.72
3:B:100:GLY:HA3	3:B:105:LYS:HE2	1.70	0.72
3:B:169:PHE:CZ	3:B:235:MET:HB3	2.24	0.72
2:A:255:PHE:O	2:A:259:LEU:HB2	1.88	0.72
3:B:35:SER:HB3	3:B:59:ASN:OD1	1.88	0.72
2:A:362:VAL:HG21	2:A:370:LYS:CA	2.20	0.72
3:B:67:LEU:HD12	3:B:92:PHE:CD1	2.24	0.72
2:A:105:ARG:HG2	2:A:411:GLU:HG3	1.70	0.72
3:B:273:ALA:CB	3:B:375:ALA:H	2.02	0.72
3:B:199:ASP:O	3:B:265:LEU:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:286:LEU:HD11	3:B:371:LEU:HD21	1.72	0.72
3:B:396:THR:HG23	3:B:422:GLU:OE2	1.90	0.72
3:B:413:MET:HG2	3:B:418:PHE:HE1	1.55	0.72
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.70	0.72
3:B:304:ALA:HB3	3:B:387:LEU:CD1	2.20	0.72
3:B:57:ALA:CB	3:B:60:LYS:HD2	2.16	0.72
2:A:69:ASP:HB3	2:A:75:ILE:HG12	1.72	0.71
2:A:214:ARG:O	2:A:218:ASP:HA	1.89	0.71
2:A:242:LEU:HD21	2:A:250:VAL:HB	1.71	0.71
3:B:175:PRO:HD2	3:B:207:GLU:OE2	1.90	0.71
3:B:191:VAL:HA	3:B:194:LEU:CD1	2.12	0.71
3:B:286:LEU:O	3:B:291:LEU:HD13	1.90	0.71
1:D:3444:MET:O	1:D:3448:ILE:HB	1.90	0.71
2:A:175:PRO:HD2	2:A:207:GLU:HG2	1.73	0.71
2:A:179:THR:HG21	3:B:248:LEU:HD22	1.71	0.71
3:B:7:ILE:HB	3:B:137:LEU:CD1	2.20	0.71
1:D:3433:THR:HA	1:D:3436:ILE:HD13	1.73	0.71
3:B:102:ASN:ND2	3:B:408:TYR:HA	2.06	0.71
2:A:174:ALA:CB	2:A:177:VAL:HB	2.20	0.71
2:A:385:ALA:HB2	2:A:432:TYR:HB3	1.72	0.71
1:D:3449:ARG:O	1:D:3453:THR:HG23	1.90	0.70
2:A:166:LYS:HE3	2:A:197:HIS:O	1.91	0.70
2:A:274:PRO:HG2	2:A:374:ALA:HB1	1.73	0.70
2:A:133:GLN:CB	2:A:243:ARG:HH12	2.04	0.70
3:B:48:ARG:CG	3:B:243:ARG:HB3	2.21	0.70
3:B:250:ALA:HA	3:B:254:LYS:CE	2.12	0.70
3:B:274:PRO:CG	3:B:374:SER:HB3	2.22	0.70
2:A:19:ALA:HB2	2:A:228:ASN:HB3	1.73	0.70
3:B:119:LEU:HD11	3:B:156:LYS:CG	2.21	0.70
2:A:7:ILE:HG12	2:A:137:VAL:CG2	2.16	0.70
3:B:268:PHE:HB3	3:B:379:GLY:H	1.57	0.70
2:A:14:VAL:HG21	2:A:75:ILE:CD1	2.22	0.70
2:A:119:LEU:HD23	2:A:122:ILE:HD11	1.72	0.70
2:A:303:VAL:CG1	2:A:305:CYS:HB2	2.20	0.70
3:B:140:SER:C	3:B:142:GLY:HA3	2.17	0.70
3:B:6:HIS:HD1	3:B:21:TRP:HE1	1.39	0.70
3:B:23:VAL:HG13	7:B:502:TA1:H321	1.73	0.70
1:D:3439:ASP:HB3	1:D:3442:LYS:HG2	1.74	0.69
2:A:405:VAL:O	2:A:409:VAL:HG23	1.92	0.69
3:B:119:LEU:HA	3:B:122:VAL:HG13	1.74	0.69
1:D:3468:ASN:OD1	1:D:3475:GLY:HA2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:115:VAL:HG13	3:B:153:LEU:HD12	1.74	0.69
1:D:3424:LYS:CE	3:B:156:LYS:HD2	2.20	0.69
1:D:3459:ASP:HB2	1:D:3462:PHE:CB	2.22	0.69
2:A:207:GLU:O	2:A:210:TYR:HB2	1.91	0.69
3:B:89:PRO:HA	3:B:92:PHE:CE2	2.26	0.69
3:B:385:GLN:HG2	3:B:386:GLU:N	2.05	0.69
3:B:251:ASP:N	3:B:254:LYS:HG3	2.05	0.69
3:B:346:TRP:O	3:B:348:PRO:HD3	1.93	0.69
2:A:184:PRO:O	2:A:188:ILE:HG12	1.92	0.69
3:B:10:GLY:HA2	3:B:145:THR:HB	1.74	0.69
3:B:150:GLY:HA2	3:B:153:LEU:HD22	1.73	0.69
2:A:84:ARG:HG2	2:A:84:ARG:HH11	1.57	0.68
2:A:205:ASP:HB3	2:A:208:ALA:HB3	1.74	0.68
3:B:140:SER:HB2	3:B:142:GLY:HA2	1.74	0.68
2:A:5:ILE:O	2:A:135:PHE:HA	1.93	0.68
3:B:230:LEU:HD23	3:B:231:VAL:N	2.08	0.68
2:A:201:ALA:O	2:A:268:PRO:HD2	1.94	0.68
1:D:3392:LYS:HE3	1:D:3423:ARG:NH2	2.09	0.68
3:B:207:GLU:HG2	3:B:208:ALA:N	2.08	0.68
2:A:79:ARG:O	2:A:84:ARG:HG3	1.94	0.68
3:B:69:ASP:OD1	3:B:71:GLU:HB3	1.94	0.68
1:D:3390:GLU:CG	2:A:402:ARG:HH22	2.04	0.68
2:A:167:LEU:HD23	2:A:202:PHE:HE2	1.57	0.68
3:B:6:HIS:HB3	3:B:21:TRP:HZ2	1.59	0.68
2:A:103:TYR:CD2	2:A:413:MET:HE2	2.29	0.68
2:A:188:ILE:HG13	2:A:395:PHE:CD2	2.29	0.68
3:B:4:ILE:HD11	3:B:252:LEU:HD11	1.74	0.68
3:B:24:ILE:HD11	3:B:52:TYR:CE2	2.28	0.68
2:A:371:VAL:HG12	2:A:373:ARG:H	1.59	0.67
2:A:242:LEU:HD23	2:A:255:PHE:HE1	1.58	0.67
2:A:66:VAL:HG12	2:A:91:GLN:CG	2.21	0.67
3:B:173:PRO:HB3	3:B:183:GLU:CG	2.24	0.67
1:D:3464:TYR:HB2	1:D:3478:VAL:CG2	2.23	0.67
2:A:188:ILE:HD12	2:A:425:MET:SD	2.34	0.67
2:A:301:GLN:NE2	2:A:307:PRO:HD3	2.08	0.67
2:A:250:VAL:HG21	2:A:318:LEU:HD21	1.76	0.67
2:A:105:ARG:HB2	2:A:110:ILE:HG22	1.77	0.67
3:B:289:PRO:HG3	3:B:331:GLN:OE1	1.95	0.67
1:D:3473:ALA:O	1:D:3476:PRO:HD2	1.94	0.67
3:B:371:LEU:HG	3:B:372:LYS:H	1.59	0.67
1:D:3424:LYS:HE2	3:B:156:LYS:CE	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:242:LEU:HD23	2:A:255:PHE:CE1	2.30	0.67
2:A:251:ASP:H	2:A:254:GLU:HG3	1.60	0.67
3:B:155:SER:HA	3:B:197:ASN:ND2	2.10	0.66
3:B:413:MET:HG3	3:B:414:ASP:N	2.08	0.66
3:B:36:TYR:OH	3:B:43:GLN:HB2	1.96	0.66
2:A:69:ASP:CB	2:A:75:ILE:HD11	2.23	0.66
2:A:103:TYR:H	2:A:408:TYR:HE1	1.43	0.66
1:D:3457:LEU:HD12	1:D:3458:GLU:N	2.11	0.66
2:A:172:TYR:HE2	2:A:388:TRP:CZ3	2.12	0.66
3:B:11:GLN:HG3	3:B:74:THR:CG2	2.25	0.66
3:B:204:ILE:CG2	3:B:209:LEU:HD21	2.25	0.66
2:A:11:GLN:O	2:A:14:VAL:HB	1.96	0.66
2:A:227:LEU:O	2:A:231:ILE:HG12	1.95	0.66
2:A:242:LEU:HD11	2:A:250:VAL:HG23	1.76	0.66
3:B:70:LEU:O	3:B:72:PRO:HD3	1.96	0.66
3:B:21:TRP:CA	3:B:24:ILE:HG22	2.20	0.66
3:B:100:GLY:CA	3:B:105:LYS:HE2	2.26	0.66
3:B:332:MET:HE1	3:B:351:VAL:HG11	1.77	0.66
2:A:256:GLN:O	2:A:260:VAL:HG13	1.94	0.66
2:A:360:PRO:HG3	2:A:374:ALA:HB3	1.78	0.66
3:B:390:ARG:O	3:B:394:GLN:HG3	1.95	0.66
2:A:62:VAL:HG13	2:A:63:PRO:HD2	1.78	0.65
3:B:264:ARG:O	3:B:265:LEU:HD23	1.96	0.65
2:A:68:VAL:HA	2:A:93:ILE:HG22	1.78	0.65
2:A:98:ASP:O	2:A:110:ILE:HD13	1.97	0.65
3:B:71:GLU:HG2	3:B:74:THR:H	1.62	0.65
2:A:217:LEU:H	2:A:217:LEU:HD23	1.60	0.65
3:B:31:ASP:HB2	3:B:34:GLY:HA2	1.78	0.65
3:B:336:GLN:HE22	3:B:350:ASN:H	1.43	0.65
2:A:101:ASN:ND2	3:B:254:LYS:HD2	2.10	0.65
3:B:132:LEU:O	3:B:164:ARG:HG2	1.96	0.65
3:B:173:PRO:HD2	3:B:391:ILE:HD11	1.78	0.65
3:B:339:ASN:HB3	3:B:342:TYR:CE1	2.31	0.65
1:D:3399:THR:OG1	1:D:3400:PRO:HD3	1.95	0.65
1:D:3430:ASN:O	1:D:3434:SER:HB2	1.97	0.65
3:B:209:LEU:CD1	3:B:230:LEU:HD21	2.25	0.65
3:B:259:MET:HA	3:B:314:THR:HG21	1.79	0.65
2:A:242:LEU:HD21	2:A:318:LEU:HD21	1.79	0.65
3:B:119:LEU:HD11	3:B:156:LYS:HG2	1.77	0.65
3:B:272:PHE:CE2	3:B:274:PRO:HD2	2.32	0.65
2:A:132:LEU:O	2:A:132:LEU:HG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:384:ILE:HG22	2:A:388:TRP:CD1	2.31	0.65
3:B:202:TYR:HE2	3:B:378:ILE:HG21	1.61	0.65
2:A:405:VAL:HG13	2:A:409:VAL:CG2	2.27	0.65
3:B:282:GLN:O	3:B:282:GLN:HG2	1.96	0.65
1:D:3392:LYS:HE2	1:D:3393:SER:HA	1.79	0.65
3:B:172:VAL:HG11	3:B:387:LEU:HD21	1.77	0.65
3:B:188:THR:HG23	3:B:425:MET:CE	2.26	0.65
1:D:3424:LYS:HZ2	3:B:159:GLU:CB	2.05	0.64
2:A:82:THR:HG22	2:A:83:TYR:CD1	2.32	0.64
2:A:242:LEU:CD1	2:A:318:LEU:HD22	2.27	0.64
3:B:151:THR:HA	3:B:154:ILE:HD11	1.79	0.64
2:A:176:GLN:OE1	3:B:333:LEU:HD11	1.96	0.64
3:B:6:HIS:CE1	3:B:8:GLN:HG2	2.32	0.64
3:B:241:CYS:O	3:B:244:PHE:HB2	1.96	0.64
3:B:325:MET:CE	3:B:355:VAL:HG21	2.27	0.64
1:D:3398:PRO:HB2	1:D:3401:VAL:HG23	1.78	0.64
1:D:3455:GLY:HA3	1:D:3458:GLU:CG	2.27	0.64
2:A:104:ALA:CB	2:A:413:MET:HG2	2.28	0.64
3:B:110:GLU:HA	3:B:110:GLU:OE1	1.98	0.64
3:B:319:PHE:CG	3:B:375:ALA:HB2	2.31	0.64
1:D:3394:LEU:HD13	2:A:409:VAL:C	2.21	0.64
1:D:3419:TRP:CE3	1:D:3422:ILE:HG12	2.33	0.64
2:A:185:TYR:OH	2:A:399:TYR:HA	1.98	0.64
2:A:203:MET:HG3	2:A:267:PHE:HB3	1.77	0.64
2:A:416:GLY:O	2:A:420:GLU:HG2	1.96	0.64
3:B:264:ARG:HG3	3:B:264:ARG:HH11	1.62	0.64
3:B:320:ARG:HA	3:B:356:CYS:HB3	1.80	0.64
1:D:3423:ARG:NH2	3:B:162:PRO:HB3	2.12	0.64
2:A:248:LEU:HB2	2:A:355:ILE:H	1.61	0.64
2:A:386:GLU:OE1	2:A:386:GLU:HA	1.96	0.64
3:B:261:PRO:HB2	3:B:262:PHE:CD2	2.33	0.64
1:D:3384:LYS:HZ1	1:D:3386:LYS:HE3	1.62	0.64
3:B:102:ASN:HD21	3:B:408:TYR:HA	1.62	0.64
3:B:173:PRO:HG2	3:B:391:ILE:HD13	1.78	0.64
2:A:66:VAL:HG12	2:A:91:GLN:HA	1.79	0.64
2:A:109:THR:HG22	2:A:110:ILE:N	2.12	0.64
2:A:311:LYS:H	2:A:382:THR:HB	1.63	0.64
3:B:106:GLY:O	3:B:111:GLY:HA3	1.97	0.64
2:A:105:ARG:C	2:A:110:ILE:HG22	2.23	0.64
2:A:362:VAL:HG21	2:A:370:LYS:HA	1.78	0.64
3:B:31:ASP:HB3	3:B:32:PRO:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:76:ASP:HA	3:B:79:ARG:HG3	1.80	0.64
2:A:167:LEU:HA	2:A:200:CYS:O	1.98	0.63
2:A:324:VAL:HG12	2:A:326:LYS:H	1.62	0.63
2:A:298:PRO:HA	2:A:301:GLN:OE1	1.99	0.63
3:B:7:ILE:HB	3:B:137:LEU:HD13	1.80	0.63
3:B:66:ILE:C	3:B:67:LEU:HD23	2.23	0.63
3:B:288:VAL:HG12	3:B:289:PRO:CD	2.28	0.63
1:D:3394:LEU:CG	2:A:410:GLY:HA2	2.29	0.63
1:D:3419:TRP:O	1:D:3422:ILE:HG13	1.98	0.63
2:A:106:GLY:O	2:A:111:GLY:HA2	1.99	0.63
2:A:238:ILE:HD12	2:A:255:PHE:CE2	2.32	0.63
2:A:278:ALA:HB2	2:A:367:ASP:O	1.99	0.63
1:D:3455:GLY:CA	1:D:3458:GLU:HG3	2.29	0.63
1:D:3455:GLY:HA3	1:D:3458:GLU:HG3	1.79	0.63
3:B:94:PHE:HD1	3:B:94:PHE:H	1.46	0.63
2:A:23:LEU:HD22	2:A:232:GLY:C	2.23	0.63
2:A:132:LEU:CG	2:A:164:LYS:HE3	2.28	0.63
3:B:328:VAL:O	3:B:332:MET:HG2	1.99	0.63
1:D:3390:GLU:CD	2:A:402:ARG:HH12	2.06	0.63
1:D:3416:LYS:CG	1:D:3418:GLU:H	2.03	0.63
3:B:229:HIS:HD1	3:B:229:HIS:C	2.05	0.63
3:B:286:LEU:HD22	3:B:291:LEU:CD1	2.28	0.63
3:B:330:GLU:HG3	3:B:331:GLN:N	2.13	0.63
1:D:3469:ARG:HG3	1:D:3469:ARG:HH11	1.64	0.63
2:A:84:ARG:HG2	2:A:84:ARG:NH1	2.12	0.63
3:B:89:PRO:HA	3:B:92:PHE:HE2	1.63	0.63
1:D:3436:ILE:HG13	1:D:3437:ASN:HD22	1.64	0.63
2:A:117:LEU:HD11	2:A:121:ARG:HH22	1.64	0.63
2:A:225:THR:HG23	2:A:226:ASN:HD22	1.64	0.63
3:B:198:THR:O	3:B:265:LEU:HD13	1.98	0.63
2:A:317:LEU:HB3	2:A:319:TYR:HE1	1.64	0.62
2:A:401:LYS:HE3	3:B:346:TRP:HB3	1.80	0.62
3:B:182:VAL:HB	3:B:186:ASN:HD21	1.64	0.62
3:B:184:PRO:HG3	3:B:394:GLN:HB2	1.81	0.62
7:B:502:TA1:H463	7:B:502:TA1:H261	1.80	0.62
3:B:220:THR:O	3:B:222:PRO:HD3	1.99	0.62
2:A:178:SER:HB2	2:A:183:GLU:OE2	1.98	0.62
3:B:67:LEU:HD23	3:B:67:LEU:N	2.12	0.62
1:D:3483:ALA:HB1	1:D:3484:GLN:NE2	2.15	0.62
2:A:68:VAL:HG13	2:A:93:ILE:HG22	1.81	0.62
2:A:179:THR:HG22	3:B:352:LYS:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:GLN:HB2	2:A:303:VAL:N	2.15	0.62
2:A:412:GLY:HA2	2:A:413:MET:O	2.00	0.62
3:B:119:LEU:C	3:B:122:VAL:HG13	2.25	0.62
2:A:179:THR:HG23	3:B:353:THR:HB	1.81	0.62
2:A:221:ARG:HG2	2:A:221:ARG:O	1.99	0.62
2:A:303:VAL:HG11	2:A:305:CYS:HB2	1.81	0.62
2:A:320:ARG:HB2	2:A:358:GLU:O	1.99	0.62
2:A:363:VAL:H	2:A:368:LEU:HD12	1.65	0.62
2:A:9:VAL:HG21	2:A:149:PHE:HD1	1.65	0.62
3:B:20:PHE:CZ	3:B:24:ILE:HD13	2.34	0.62
2:A:193:THR:HG23	2:A:194:THR:N	2.15	0.62
2:A:275:VAL:HG11	2:A:300:ASN:HD21	1.64	0.62
1:D:3416:LYS:HE2	1:D:3418:GLU:CB	2.23	0.62
2:A:362:VAL:CG2	2:A:370:LYS:HA	2.28	0.62
3:B:55:GLU:HG2	3:B:61:TYR:CE1	2.35	0.62
2:A:118:VAL:O	2:A:122:ILE:HD13	2.00	0.61
2:A:132:LEU:HG	2:A:164:LYS:HE3	1.81	0.61
2:A:175:PRO:HG2	2:A:304:LYS:CD	2.29	0.61
3:B:157:ILE:HG21	3:B:166:MET:SD	2.39	0.61
3:B:283:TYR:O	3:B:284:ARG:HB2	2.00	0.61
1:D:3408:VAL:HG12	1:D:3411:MET:HE2	1.81	0.61
3:B:150:GLY:HA2	3:B:153:LEU:HD23	1.82	0.61
3:B:288:VAL:HG12	3:B:289:PRO:N	2.15	0.61
1:D:3450:GLU:HA	1:D:3453:THR:OG1	2.01	0.61
2:A:107:HIS:HD2	2:A:108:TYR:CD1	2.17	0.61
2:A:250:VAL:CG2	2:A:318:LEU:HD21	2.31	0.61
2:A:408:TYR:CG	2:A:418:PHE:HZ	2.18	0.61
3:B:182:VAL:HG12	3:B:185:TYR:HB2	1.82	0.61
3:B:326:LYS:HE3	3:B:330:GLU:HB3	1.82	0.61
3:B:119:LEU:CA	3:B:122:VAL:HG13	2.31	0.61
3:B:278:ARG:HB3	3:B:279:GLY:CA	2.31	0.61
3:B:312:TYR:HE2	3:B:377:PHE:HZ	1.49	0.61
3:B:408:TYR:CD2	3:B:418:PHE:HZ	2.18	0.61
2:A:110:ILE:HG23	2:A:111:GLY:N	2.14	0.61
2:A:261:PRO:HB2	2:A:262:TYR:CD2	2.36	0.61
3:B:314:THR:H	3:B:380:ASN:HB3	1.66	0.61
3:B:388:PHE:HB2	3:B:429:VAL:HG22	1.83	0.61
1:D:3384:LYS:HD3	1:D:3386:LYS:CB	2.28	0.61
3:B:172:VAL:HG23	3:B:203:CYS:HB3	1.81	0.61
3:B:372:LYS:HG3	3:B:373:MET:HB2	1.83	0.61
1:D:3422:ILE:HG13	1:D:3423:ARG:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:68:VAL:HG13	2:A:93:ILE:HG21	1.83	0.61
1:D:3384:LYS:CD	1:D:3386:LYS:HB2	2.29	0.61
3:B:188:THR:HG21	3:B:422:GLU:HA	1.82	0.60
3:B:209:LEU:HD11	3:B:302:MET:CE	2.31	0.60
2:A:115:ILE:CD1	2:A:152:LEU:HD11	2.28	0.60
2:A:223:THR:HG22	2:A:224:TYR:N	2.14	0.60
2:A:244:PHE:HD1	2:A:245:ASP:N	1.99	0.60
2:A:269:LEU:CD2	2:A:384:ILE:HD11	2.26	0.60
2:A:419:SER:O	2:A:422:ARG:HB3	2.01	0.60
3:B:172:VAL:CG1	3:B:173:PRO:HD2	2.31	0.60
3:B:297:ASP:OD2	3:B:299:LYS:HE2	2.01	0.60
3:B:269:MET:CE	3:B:301:MET:HE2	2.22	0.60
3:B:327:GLU:HA	3:B:330:GLU:HG2	1.83	0.60
2:A:205:ASP:HB3	2:A:208:ALA:HB2	1.81	0.60
2:A:275:VAL:HG21	2:A:300:ASN:OD1	2.01	0.60
2:A:316:CYS:CB	2:A:378:LEU:HD11	2.18	0.60
3:B:315:VAL:CG1	3:B:351:VAL:HG13	2.31	0.60
3:B:408:TYR:O	3:B:411:GLU:HB2	2.02	0.60
1:D:3418:GLU:O	1:D:3422:ILE:HG23	2.01	0.60
2:A:274:PRO:CG	2:A:374:ALA:HA	2.32	0.60
3:B:102:ASN:HB3	3:B:105:LYS:N	2.06	0.60
3:B:258:ASN:HD22	3:B:352:LYS:HG3	1.66	0.60
1:D:3436:ILE:HG13	1:D:3437:ASN:ND2	2.17	0.60
1:D:3456:TYR:HA	1:D:3459:ASP:OD1	2.01	0.60
2:A:317:LEU:HB3	2:A:319:TYR:CE1	2.35	0.60
3:B:168:THR:CB	3:B:201:THR:HG23	2.30	0.60
2:A:424:ASP:O	2:A:427:ALA:HB3	2.01	0.60
3:B:19:LYS:HG3	3:B:228:ASN:HB3	1.84	0.60
3:B:332:MET:CE	3:B:351:VAL:HG11	2.31	0.60
2:A:152:LEU:HD12	2:A:152:LEU:C	2.26	0.59
2:A:175:PRO:HG2	2:A:304:LYS:CE	2.32	0.59
3:B:119:LEU:HD11	3:B:156:LYS:CB	2.32	0.59
2:A:119:LEU:O	2:A:123:ARG:HG2	2.03	0.59
2:A:303:VAL:HG13	2:A:305:CYS:HB2	1.84	0.59
3:B:107:HIS:CE1	3:B:152:LEU:HD13	2.37	0.59
3:B:133:GLN:HG3	3:B:252:LEU:HD12	1.81	0.59
1:D:3456:TYR:O	1:D:3459:ASP:HB2	2.02	0.59
2:A:228:ASN:HA	2:A:231:ILE:HG13	1.83	0.59
3:B:49:ILE:HG13	3:B:50:ASN:N	2.16	0.59
1:D:3395:PRO:HD2	2:A:410:GLY:HA3	1.84	0.59
1:D:3423:ARG:CZ	3:B:162:PRO:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:248:LEU:HD23	3:B:353:THR:O	2.02	0.59
2:A:239:THR:O	2:A:243:ARG:HG2	2.01	0.59
3:B:11:GLN:HG3	3:B:74:THR:HG21	1.84	0.59
3:B:150:GLY:CA	3:B:153:LEU:HD22	2.33	0.59
3:B:167:ASN:HB3	3:B:202:TYR:HE1	1.67	0.59
3:B:255:LEU:O	3:B:259:MET:HG3	2.01	0.59
3:B:107:HIS:HB3	3:B:108:TYR:CD1	2.36	0.59
3:B:173:PRO:HG2	3:B:391:ILE:CD1	2.32	0.59
3:B:273:ALA:CB	3:B:274:PRO:HD3	2.28	0.59
1:D:3405:MET:SD	1:D:3408:VAL:HG23	2.42	0.59
3:B:172:VAL:HB	3:B:205:ASP:OD1	2.02	0.59
3:B:198:THR:O	3:B:265:LEU:HD22	2.03	0.59
3:B:209:LEU:HD11	3:B:230:LEU:HD21	1.85	0.59
1:D:3424:LYS:CE	3:B:156:LYS:HA	2.32	0.59
1:D:3424:LYS:CB	3:B:159:GLU:HB2	2.22	0.59
2:A:11:GLN:HG3	2:A:74:VAL:CG1	2.17	0.59
2:A:173:PRO:HG2	2:A:391:LEU:HD11	1.85	0.59
3:B:139:HIS:HB2	3:B:146:GLY:O	2.03	0.59
3:B:48:ARG:O	3:B:51:VAL:HG23	2.03	0.59
3:B:156:LYS:HD2	3:B:156:LYS:N	2.18	0.59
1:D:3419:TRP:CZ3	1:D:3422:ILE:HG12	2.37	0.59
2:A:407:TRP:HE1	3:B:260:VAL:CG2	2.15	0.59
3:B:165:ILE:HG22	3:B:199:ASP:OD2	2.03	0.59
2:A:231:ILE:HA	2:A:234:ILE:CG2	2.32	0.58
3:B:54:ASN:ND2	3:B:64:ARG:HB2	2.17	0.58
2:A:120:ASP:O	2:A:124:LYS:HB2	2.03	0.58
2:A:273:ALA:CB	2:A:274:PRO:HD3	2.24	0.58
3:B:273:ALA:HB1	3:B:291:LEU:HG	1.84	0.58
2:A:179:THR:HG21	3:B:248:LEU:HD21	1.81	0.58
2:A:176:GLN:HB3	3:B:333:LEU:HD13	1.85	0.58
2:A:256:GLN:HG3	2:A:257:THR:N	2.18	0.58
3:B:185:TYR:OH	3:B:399:PHE:HA	2.04	0.58
3:B:266:HIS:HB3	3:B:432:TYR:OH	2.02	0.58
2:A:203:MET:HE2	2:A:267:PHE:HB2	1.86	0.58
2:A:423:GLU:O	2:A:426:ALA:HB3	2.03	0.58
3:B:125:GLU:HA	3:B:125:GLU:OE1	2.04	0.58
2:A:9:VAL:HG22	2:A:10:GLY:N	2.19	0.58
2:A:66:VAL:HA	2:A:91:GLN:CG	2.34	0.58
2:A:70:LEU:HD12	2:A:145:THR:OG1	2.03	0.58
2:A:209:ILE:HG12	2:A:302:MET:HG2	1.83	0.58
3:B:5:VAL:CG2	3:B:135:PHE:HD2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3412:LEU:HD21	1:D:3435:ILE:CD1	2.33	0.58
2:A:166:LYS:HE2	2:A:199:ASP:OD1	2.03	0.58
2:A:167:LEU:HD23	2:A:202:PHE:CZ	2.38	0.58
3:B:185:TYR:HD1	3:B:395:PHE:CE1	2.22	0.58
3:B:314:THR:HG22	3:B:315:VAL:N	2.18	0.58
1:D:3455:GLY:HA3	1:D:3458:GLU:HB2	1.84	0.58
2:A:317:LEU:HD23	2:A:375:VAL:HG11	1.86	0.58
2:A:413:MET:O	2:A:414:GLU:HG3	2.04	0.58
1:D:3469:ARG:HG3	1:D:3469:ARG:NH1	2.18	0.58
2:A:24:TYR:CE1	2:A:240:ALA:HB2	2.39	0.58
2:A:274:PRO:HG2	2:A:374:ALA:CA	2.34	0.58
3:B:171:VAL:HA	3:B:204:ILE:O	2.04	0.58
1:D:3405:MET:O	1:D:3408:VAL:HG23	2.03	0.57
1:D:3464:TYR:HE1	1:D:3468:ASN:OD1	1.87	0.57
2:A:259:LEU:HD11	2:A:378:LEU:CD1	2.17	0.57
3:B:119:LEU:O	3:B:122:VAL:HG13	2.04	0.57
3:B:199:ASP:C	3:B:265:LEU:HB2	2.29	0.57
1:D:3445:THR:O	1:D:3449:ARG:HB3	2.04	0.57
2:A:231:ILE:O	2:A:234:ILE:HG23	2.04	0.57
1:D:3392:LYS:HE3	3:B:158:ARG:HH12	1.69	0.57
1:D:3477:LEU:N	1:D:3477:LEU:HD12	2.19	0.57
2:A:105:ARG:CB	2:A:110:ILE:HG22	2.34	0.57
2:A:401:LYS:HD3	3:B:346:TRP:CD2	2.39	0.57
3:B:135:PHE:HZ	3:B:161:TYR:CE1	2.22	0.57
1:D:3424:LYS:HE2	3:B:156:LYS:HE2	1.87	0.57
3:B:273:ALA:HB2	3:B:375:ALA:H	1.68	0.57
2:A:217:LEU:HG	2:A:219:ILE:CD1	2.34	0.57
2:A:168:GLU:HG3	2:A:201:ALA:CB	2.34	0.57
2:A:405:VAL:HG13	2:A:409:VAL:HG23	1.86	0.57
3:B:55:GLU:HG2	3:B:61:TYR:HE1	1.70	0.57
3:B:359:PRO:HB2	3:B:371:LEU:O	2.05	0.57
2:A:220:GLU:HA	2:A:220:GLU:OE1	2.05	0.57
3:B:107:HIS:HE1	3:B:152:LEU:HD13	1.68	0.57
3:B:211:ASP:OD2	3:B:215:ARG:HD2	2.05	0.57
2:A:141:PHE:N	2:A:142:GLY:HA3	2.19	0.57
2:A:185:TYR:HD1	2:A:395:PHE:CE2	2.22	0.57
3:B:67:LEU:HD12	3:B:92:PHE:CE1	2.39	0.57
2:A:248:LEU:CB	2:A:355:ILE:H	2.18	0.57
3:B:4:ILE:HD11	3:B:252:LEU:HD12	1.86	0.57
3:B:229:HIS:C	3:B:229:HIS:ND1	2.62	0.57
3:B:307:PRO:O	3:B:310:GLY:HA3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3452:ILE:HG22	1:D:3453:THR:N	2.19	0.57
3:B:272:PHE:HD2	3:B:274:PRO:O	1.87	0.57
2:A:331:ALA:O	2:A:335:ILE:HG12	2.04	0.56
3:B:21:TRP:CE3	3:B:24:ILE:HG21	2.40	0.56
1:D:3392:LYS:HE3	3:B:158:ARG:NH1	2.21	0.56
2:A:229:ARG:HH11	2:A:229:ARG:CG	2.16	0.56
2:A:274:PRO:HG2	2:A:374:ALA:HA	1.87	0.56
3:B:180:THR:HG22	3:B:182:VAL:H	1.69	0.56
3:B:299:LYS:HD3	3:B:299:LYS:N	2.20	0.56
2:A:168:GLU:HG3	2:A:201:ALA:HB1	1.88	0.56
2:A:209:ILE:O	2:A:212:ILE:HB	2.04	0.56
2:A:241:SER:HB2	2:A:356:ASN:ND2	2.20	0.56
2:A:371:VAL:HG12	2:A:372:GLN:N	2.20	0.56
3:B:86:ILE:HG23	3:B:87:PHE:N	2.18	0.56
3:B:175:PRO:HD2	3:B:207:GLU:CD	2.30	0.56
3:B:230:LEU:HD21	3:B:302:MET:HE3	1.87	0.56
3:B:268:PHE:HB3	3:B:379:GLY:N	2.20	0.56
3:B:272:PHE:CD2	3:B:274:PRO:HD2	2.39	0.56
1:D:3416:LYS:CE	1:D:3418:GLU:HB2	2.28	0.56
1:D:3428:GLU:HG2	1:D:3431:PHE:HB2	1.88	0.56
2:A:67:PHE:CE2	2:A:87:PHE:CE2	2.94	0.56
3:B:352:LYS:HD3	3:B:352:LYS:C	2.30	0.56
2:A:208:ALA:HB1	2:A:303:VAL:C	2.31	0.56
2:A:250:VAL:HG13	2:A:254:GLU:OE1	2.06	0.56
3:B:413:MET:CG	3:B:418:PHE:HE1	2.18	0.56
2:A:76:ASP:HA	2:A:79:ARG:HG3	1.87	0.56
3:B:64:ARG:HD2	3:B:125:GLU:HB3	1.88	0.56
3:B:275:LEU:CD2	3:B:300:ASN:HD21	2.11	0.56
1:D:3407:ALA:O	1:D:3410:LEU:HB3	2.04	0.56
2:A:362:VAL:HG13	2:A:368:LEU:CB	2.28	0.56
3:B:273:ALA:HB3	3:B:375:ALA:H	1.69	0.56
3:B:428:LEU:HD12	3:B:428:LEU:O	2.05	0.56
1:D:3422:ILE:O	1:D:3425:LYS:HB2	2.05	0.56
2:A:16:ILE:HG22	2:A:17:GLY:N	2.20	0.56
2:A:92:LEU:HD12	2:A:92:LEU:N	2.21	0.56
2:A:152:LEU:HD12	2:A:153:LEU:HA	1.86	0.56
2:A:237:SER:HB3	2:A:376:CYS:SG	2.46	0.56
3:B:180:THR:HB	3:B:183:GLU:OE1	2.06	0.56
3:B:388:PHE:CB	3:B:429:VAL:HG22	2.36	0.56
2:A:219:ILE:HG22	2:A:222:PRO:HD3	1.87	0.56
3:B:36:TYR:CE2	3:B:44:LEU:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:132:LEU:HD23	3:B:164:ARG:HD2	1.88	0.56
3:B:288:VAL:CB	3:B:289:PRO:HD3	2.35	0.56
1:D:3394:LEU:HD13	2:A:409:VAL:O	2.06	0.55
2:A:229:ARG:HG2	2:A:229:ARG:NH1	2.10	0.55
2:A:225:THR:HG23	2:A:226:ASN:N	2.21	0.55
3:B:103:TRP:NE1	3:B:148:GLY:H	2.05	0.55
3:B:260:VAL:HG23	3:B:260:VAL:O	2.04	0.55
2:A:189:LEU:O	2:A:193:THR:HG22	2.07	0.55
3:B:315:VAL:CG1	3:B:377:PHE:HE1	2.18	0.55
1:D:3432:ILE:HD13	1:D:3433:THR:N	2.18	0.55
2:A:66:VAL:HG12	2:A:91:GLN:CA	2.36	0.55
2:A:103:TYR:N	2:A:408:TYR:HE1	2.04	0.55
2:A:152:LEU:HD12	2:A:153:LEU:N	2.21	0.55
3:B:122:VAL:HG22	3:B:123:ARG:N	2.21	0.55
2:A:242:LEU:HD13	2:A:318:LEU:HD22	1.87	0.55
3:B:297:ASP:CG	3:B:299:LYS:HE2	2.31	0.55
1:D:3392:LYS:NZ	3:B:158:ARG:HH12	2.04	0.55
1:D:3431:PHE:CZ	1:D:3435:ILE:HD11	2.42	0.55
2:A:175:PRO:HG2	2:A:304:LYS:HE2	1.87	0.55
3:B:132:LEU:HD23	3:B:164:ARG:CD	2.36	0.55
3:B:231:VAL:HA	3:B:302:MET:HE1	1.88	0.55
1:D:3392:LYS:HE2	1:D:3392:LYS:C	2.32	0.55
2:A:21:TRP:O	2:A:24:TYR:HB2	2.06	0.55
2:A:23:LEU:CD2	2:A:233:GLN:HA	2.37	0.55
2:A:359:PRO:HB3	2:A:372:GLN:O	2.06	0.55
3:B:7:ILE:HB	3:B:137:LEU:HD12	1.87	0.55
3:B:172:VAL:CG2	3:B:203:CYS:HB3	2.36	0.55
3:B:223:THR:HG22	3:B:224:TYR:N	2.21	0.55
2:A:185:TYR:CD1	2:A:395:PHE:CE2	2.95	0.55
3:B:173:PRO:HB3	3:B:183:GLU:HG2	1.89	0.55
3:B:188:THR:CG2	3:B:422:GLU:HA	2.37	0.55
2:A:154:MET:HE1	2:A:166:LYS:CB	2.37	0.54
3:B:202:TYR:HE2	3:B:378:ILE:CG2	2.19	0.54
2:A:9:VAL:HG21	2:A:149:PHE:CD1	2.41	0.54
2:A:114:ILE:HG22	2:A:118:VAL:CG2	2.37	0.54
3:B:283:TYR:HB3	3:B:285:ALA:H	1.72	0.54
1:D:3478:VAL:HG13	1:D:3479:LYS:N	2.22	0.54
3:B:264:ARG:HA	3:B:264:ARG:NE	2.23	0.54
2:A:104:ALA:HB1	2:A:413:MET:HG2	1.90	0.54
2:A:331:ALA:O	2:A:334:THR:HG22	2.06	0.54
2:A:204:VAL:CG2	2:A:302:MET:HE3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:299:LYS:HD3	3:B:299:LYS:H	1.71	0.54
1:D:3409:CYS:O	1:D:3412:LEU:HB2	2.08	0.54
1:D:3484:GLN:NE2	1:D:3484:GLN:H	2.05	0.54
2:A:412:GLY:N	2:A:413:MET:HB2	2.23	0.54
3:B:132:LEU:CB	3:B:164:ARG:HD3	2.35	0.54
3:B:102:ASN:HB2	3:B:105:LYS:HB2	1.89	0.54
1:D:3392:LYS:CE	3:B:158:ARG:HH12	2.21	0.54
1:D:3438:TYR:CZ	1:D:3443:MET:HB2	2.43	0.54
1:D:3455:GLY:HA3	1:D:3458:GLU:CB	2.38	0.54
2:A:301:GLN:O	2:A:302:MET:HB2	2.08	0.54
3:B:135:PHE:CE1	3:B:157:ILE:HG23	2.43	0.54
3:B:189:LEU:HA	3:B:421:ALA:HB1	1.89	0.54
3:B:195:VAL:HG13	3:B:196:GLU:N	2.21	0.54
3:B:198:THR:HG22	3:B:265:LEU:HD13	1.89	0.54
2:A:63:PRO:HG2	2:A:87:PHE:HA	1.89	0.54
2:A:177:VAL:HG21	2:A:207:GLU:CB	2.38	0.54
2:A:210:TYR:OH	3:B:325:MET:HB3	2.07	0.54
2:A:301:GLN:CB	2:A:303:VAL:HG12	2.38	0.54
2:A:401:LYS:HZ2	3:B:346:TRP:CD1	2.25	0.54
3:B:179:ASP:HB2	6:B:501:GDP:H3'	1.90	0.54
3:B:234:THR:HG21	3:B:270:PRO:CB	2.15	0.54
3:B:299:LYS:H	3:B:299:LYS:CD	2.20	0.54
2:A:26:LEU:CD2	2:A:363:VAL:HG13	2.30	0.54
2:A:237:SER:HA	2:A:241:SER:OG	2.08	0.54
2:A:66:VAL:HB	2:A:91:GLN:O	2.08	0.53
2:A:172:TYR:OH	2:A:387:ALA:HB1	2.07	0.53
2:A:172:TYR:CE2	2:A:388:TRP:CZ3	2.95	0.53
3:B:264:ARG:HG3	3:B:264:ARG:NH1	2.23	0.53
3:B:18:ALA:O	3:B:22:GLU:HG3	2.09	0.53
3:B:288:VAL:HG12	3:B:289:PRO:HD3	1.91	0.53
3:B:318:VAL:HG23	3:B:378:ILE:HD11	1.90	0.53
3:B:6:HIS:O	3:B:65:ALA:HB1	2.07	0.53
3:B:42:LEU:HD21	3:B:245:PRO:HD2	1.89	0.53
2:A:118:VAL:HG11	2:A:153:LEU:HD22	1.90	0.53
2:A:298:PRO:O	2:A:301:GLN:HG2	2.09	0.53
2:A:402:ARG:O	2:A:402:ARG:HG3	2.08	0.53
2:A:11:GLN:CG	2:A:74:VAL:HG11	2.19	0.53
2:A:274:PRO:HB3	2:A:371:VAL:HG21	1.91	0.53
3:B:5:VAL:HG21	3:B:135:PHE:HD2	1.73	0.53
3:B:337:ASN:N	3:B:337:ASN:HD22	2.05	0.53
3:B:415:GLU:OE2	3:B:415:GLU:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3394:LEU:HD13	2:A:410:GLY:HA2	1.90	0.53
2:A:261:PRO:HG2	2:A:313:MET:SD	2.49	0.53
2:A:269:LEU:N	2:A:269:LEU:HD23	2.24	0.53
2:A:115:ILE:HG23	2:A:116:ASP:N	2.24	0.53
2:A:212:ILE:HD11	2:A:302:MET:H	1.73	0.53
2:A:337:THR:O	2:A:339:ARG:HB2	2.08	0.53
3:B:119:LEU:HA	3:B:122:VAL:HG11	1.91	0.53
3:B:182:VAL:HG12	3:B:182:VAL:O	2.09	0.53
1:D:3403:LEU:HD23	1:D:3403:LEU:N	2.24	0.53
2:A:68:VAL:HG22	2:A:93:ILE:CG2	2.39	0.53
2:A:101:ASN:O	2:A:182:VAL:HG21	2.08	0.53
2:A:192:HIS:HB2	2:A:424:ASP:OD2	2.09	0.53
3:B:31:ASP:C	3:B:34:GLY:HA3	2.34	0.53
3:B:168:THR:CG2	3:B:201:THR:HG23	2.38	0.53
3:B:181:VAL:O	3:B:398:MET:HE1	2.08	0.53
3:B:204:ILE:HG22	3:B:205:ASP:N	2.24	0.53
3:B:285:ALA:CB	3:B:290:GLU:HG2	2.36	0.53
3:B:360:PRO:HB2	7:B:502:TA1:H281	1.91	0.53
1:D:3428:GLU:HG3	1:D:3430:ASN:OD1	2.09	0.53
2:A:78:VAL:HG11	2:A:92:LEU:HD21	1.91	0.53
2:A:6:SER:O	2:A:65:ALA:HB1	2.09	0.52
2:A:155:GLU:HA	2:A:197:HIS:CE1	2.43	0.52
2:A:204:VAL:CG2	2:A:302:MET:HB3	2.39	0.52
2:A:217:LEU:HG	2:A:219:ILE:HD11	1.89	0.52
3:B:4:ILE:CD1	3:B:252:LEU:HD11	2.40	0.52
3:B:135:PHE:CZ	3:B:161:TYR:CE1	2.97	0.52
3:B:167:ASN:HA	3:B:200:GLU:O	2.08	0.52
3:B:201:THR:HG22	3:B:202:TYR:N	2.24	0.52
3:B:172:VAL:CG1	3:B:387:LEU:HD21	2.39	0.52
2:A:304:LYS:O	2:A:304:LYS:HG3	2.10	0.52
2:A:402:ARG:O	2:A:405:VAL:HB	2.08	0.52
3:B:3:GLU:OE2	3:B:130:ASP:HB3	2.08	0.52
3:B:52:TYR:OH	3:B:239:THR:HG21	2.09	0.52
2:A:332:ILE:HD13	2:A:351:PHE:CD1	2.45	0.52
3:B:9:ALA:O	3:B:13:GLY:HA2	2.09	0.52
3:B:52:TYR:HB2	3:B:53:TYR:CE1	2.45	0.52
3:B:57:ALA:HB3	3:B:60:LYS:N	2.12	0.52
3:B:275:LEU:HD23	3:B:300:ASN:CG	2.34	0.52
3:B:309:HIS:N	3:B:310:GLY:HA3	2.25	0.52
1:D:3455:GLY:HA2	1:D:3458:GLU:N	2.13	0.52
2:A:76:ASP:HA	2:A:79:ARG:CG	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:250:VAL:HG21	2:A:318:LEU:CD2	2.39	0.52
3:B:10:GLY:HA3	3:B:146:GLY:HA2	1.91	0.52
2:A:88:HIS:O	2:A:92:LEU:HD12	2.10	0.52
2:A:251:ASP:O	2:A:255:PHE:HD1	1.93	0.52
2:A:288:VAL:HG23	2:A:373:ARG:HH11	1.74	0.52
1:D:3394:LEU:HD22	2:A:410:GLY:N	2.24	0.52
2:A:388:TRP:CZ3	2:A:391:LEU:HD22	2.45	0.52
1:D:3426:ILE:HG22	1:D:3427:MET:N	2.25	0.52
2:A:34:GLY:C	2:A:61:HIS:N	2.68	0.52
2:A:185:TYR:O	2:A:189:LEU:HG	2.10	0.52
2:A:251:ASP:N	2:A:254:GLU:HG3	2.24	0.52
2:A:377:MET:O	2:A:377:MET:HG3	2.08	0.52
2:A:105:ARG:NH2	2:A:110:ILE:HD12	2.24	0.52
2:A:185:TYR:HD2	2:A:408:TYR:HE2	1.59	0.52
2:A:217:LEU:HA	2:A:277:SER:HB3	1.92	0.52
3:B:4:ILE:N	3:B:51:VAL:HG12	2.25	0.52
3:B:184:PRO:HD2	3:B:398:MET:HE1	1.92	0.51
3:B:253:ARG:O	3:B:257:VAL:HG23	2.10	0.51
1:D:3395:PRO:HG2	2:A:411:GLU:OE2	2.10	0.51
1:D:3422:ILE:C	1:D:3422:ILE:HD12	2.35	0.51
2:A:352:LYS:HE2	2:A:353:VAL:O	2.10	0.51
3:B:44:LEU:O	3:B:44:LEU:HD12	2.09	0.51
2:A:372:GLN:HE21	2:A:372:GLN:CA	2.23	0.51
3:B:64:ARG:HG3	3:B:125:GLU:OE2	2.11	0.51
3:B:313:LEU:HD23	3:B:313:LEU:N	2.25	0.51
1:D:3392:LYS:HD2	1:D:3423:ARG:NE	2.26	0.51
1:D:3412:LEU:HD21	1:D:3435:ILE:HD11	1.91	0.51
3:B:127:GLU:HA	3:B:127:GLU:OE1	2.10	0.51
1:D:3444:MET:CE	1:D:3448:ILE:HG12	2.40	0.51
2:A:63:PRO:HB2	2:A:91:GLN:OE1	2.09	0.51
2:A:248:LEU:O	2:A:248:LEU:HD12	2.11	0.51
2:A:282:TYR:CD1	2:A:284:GLU:CG	2.94	0.51
3:B:182:VAL:HG11	3:B:408:TYR:OH	2.10	0.51
2:A:147:SER:HB2	2:A:190:THR:OG1	2.10	0.51
2:A:221:ARG:N	2:A:222:PRO:HD3	2.25	0.51
2:A:363:VAL:HG23	2:A:368:LEU:HD11	1.93	0.51
2:A:402:ARG:HE	2:A:405:VAL:CG1	2.22	0.51
1:D:3390:GLU:O	1:D:3394:LEU:HG	2.11	0.51
2:A:408:TYR:CB	2:A:418:PHE:HZ	2.24	0.51
3:B:111:GLY:O	3:B:115:VAL:HG23	2.11	0.51
3:B:134:GLY:HA3	3:B:165:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:205:ASP:O	3:B:209:LEU:HD22	2.11	0.51
2:A:429:GLU:HG3	2:A:430:LYS:N	2.26	0.51
1:D:3392:LYS:HE2	1:D:3393:SER:CA	2.41	0.51
3:B:4:ILE:H	3:B:51:VAL:HG12	1.76	0.50
3:B:287:THR:HG22	3:B:288:VAL:H	1.76	0.50
2:A:154:MET:HE1	2:A:166:LYS:HB3	1.93	0.50
2:A:407:TRP:HE1	3:B:260:VAL:HG23	1.75	0.50
2:A:407:TRP:NE1	3:B:257:VAL:HA	2.27	0.50
3:B:42:LEU:HD21	3:B:245:PRO:CD	2.41	0.50
2:A:102:ASN:ND2	2:A:105:ARG:H	2.09	0.50
2:A:114:ILE:HG22	2:A:118:VAL:HG23	1.93	0.50
2:A:118:VAL:O	2:A:121:ARG:HB2	2.12	0.50
2:A:311:LYS:HD3	2:A:342:GLN:O	2.12	0.50
3:B:230:LEU:O	3:B:233:ALA:HB3	2.11	0.50
1:D:3408:VAL:HG12	1:D:3411:MET:CE	2.41	0.50
1:D:3412:LEU:CD2	1:D:3431:PHE:CE1	2.95	0.50
2:A:152:LEU:HD12	2:A:153:LEU:CA	2.42	0.50
3:B:28:HIS:ND1	3:B:49:ILE:HG22	2.27	0.50
3:B:173:PRO:HD2	3:B:391:ILE:CD1	2.40	0.50
2:A:103:TYR:CD2	2:A:189:LEU:CD1	2.94	0.50
2:A:123:ARG:HA	2:A:161:TYR:OH	2.11	0.50
2:A:241:SER:HB2	2:A:356:ASN:HD22	1.76	0.50
2:A:287:SER:HA	2:A:373:ARG:CZ	2.42	0.50
3:B:8:GLN:HG3	3:B:66:ILE:O	2.12	0.50
3:B:123:ARG:O	3:B:127:GLU:HG2	2.12	0.50
1:D:3394:LEU:HA	2:A:410:GLY:HA3	1.93	0.50
1:D:3449:ARG:HH21	1:D:3449:ARG:CG	2.24	0.50
2:A:201:ALA:O	2:A:267:PHE:HA	2.12	0.50
2:A:224:TYR:CE1	3:B:325:MET:HG2	2.47	0.50
1:D:3428:GLU:HG2	1:D:3428:GLU:O	2.11	0.50
1:D:3455:GLY:CA	1:D:3458:GLU:HB2	2.41	0.50
2:A:22:GLU:HG2	2:A:83:TYR:HE1	1.72	0.50
2:A:92:LEU:HD12	2:A:92:LEU:H	1.76	0.50
2:A:107:HIS:HA	2:A:148:GLY:C	2.37	0.50
2:A:238:ILE:HD12	2:A:255:PHE:CZ	2.46	0.50
2:A:372:GLN:HE21	2:A:372:GLN:HA	1.75	0.50
3:B:135:PHE:HZ	3:B:161:TYR:CD1	2.30	0.50
3:B:172:VAL:HG12	3:B:173:PRO:HD2	1.94	0.50
3:B:287:THR:HG22	3:B:288:VAL:N	2.26	0.50
1:D:3394:LEU:HD22	2:A:410:GLY:HA3	1.91	0.50
1:D:3438:TYR:CE2	1:D:3443:MET:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:LEU:HD21	2:A:233:GLN:HA	1.93	0.50
2:A:103:TYR:CD2	2:A:189:LEU:HD12	2.47	0.50
3:B:5:VAL:CG2	3:B:135:PHE:CD2	2.95	0.50
3:B:307:PRO:HB3	3:B:312:TYR:CE1	2.47	0.50
2:A:407:TRP:CZ2	3:B:256:ALA:HB1	2.47	0.49
3:B:52:TYR:CB	3:B:53:TYR:CE1	2.95	0.49
2:A:105:ARG:HB2	2:A:110:ILE:CG2	2.40	0.49
2:A:276:ILE:HG12	2:A:277:SER:N	2.27	0.49
2:A:107:HIS:CD2	2:A:108:TYR:CE1	3.00	0.49
2:A:288:VAL:HA	2:A:291:ILE:HD11	1.94	0.49
2:A:313:MET:HE2	2:A:435:VAL:HG11	1.93	0.49
3:B:250:ALA:HB1	3:B:254:LYS:CB	2.41	0.49
2:A:262:TYR:HB3	2:A:263:PRO:HD2	1.93	0.49
2:A:401:LYS:CD	3:B:346:TRP:CD2	2.94	0.49
2:A:67:PHE:HE2	2:A:87:PHE:CE2	2.29	0.49
2:A:107:HIS:HD2	2:A:108:TYR:CE1	2.31	0.49
2:A:107:HIS:CD2	2:A:108:TYR:CD1	2.99	0.49
2:A:118:VAL:HG11	2:A:153:LEU:CD2	2.42	0.49
2:A:412:GLY:H	2:A:413:MET:HB2	1.77	0.49
3:B:10:GLY:C	3:B:13:GLY:HA3	2.36	0.49
3:B:52:TYR:HB2	3:B:53:TYR:CD1	2.48	0.49
3:B:89:PRO:O	3:B:92:PHE:HD2	1.94	0.49
1:D:3412:LEU:CD2	1:D:3431:PHE:CZ	2.95	0.49
1:D:3449:ARG:HH21	1:D:3449:ARG:HG2	1.77	0.49
3:B:135:PHE:CE1	3:B:157:ILE:CG2	2.95	0.49
2:A:219:ILE:C	2:A:222:PRO:HD3	2.38	0.49
2:A:161:TYR:HB3	2:A:164:LYS:HB2	1.93	0.49
2:A:312:TYR:CE2	2:A:377:MET:HE1	2.48	0.49
3:B:52:TYR:CB	3:B:53:TYR:CD1	2.95	0.49
3:B:313:LEU:HB2	3:B:380:ASN:HB3	1.95	0.49
2:A:3:GLU:C	2:A:243:ARG:HH11	2.21	0.49
2:A:97:GLU:HB2	2:A:110:ILE:HD11	1.95	0.49
2:A:168:GLU:CG	2:A:201:ALA:HB2	2.43	0.49
3:B:7:ILE:HD13	3:B:66:ILE:HD11	1.94	0.49
3:B:12:CYS:HB3	3:B:140:SER:OG	2.13	0.49
3:B:332:MET:HE1	3:B:351:VAL:CG1	2.41	0.49
3:B:346:TRP:CE3	3:B:347:ILE:HG12	2.46	0.49
2:A:108:TYR:CE1	2:A:413:MET:SD	3.06	0.49
2:A:268:PRO:HA	2:A:379:SER:O	2.13	0.48
2:A:324:VAL:HG12	2:A:326:LYS:N	2.26	0.48
2:A:426:ALA:O	2:A:429:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:24:ILE:CD1	3:B:52:TYR:CE2	2.95	0.48
3:B:94:PHE:CD1	3:B:94:PHE:N	2.81	0.48
2:A:65:ALA:O	2:A:91:GLN:HG2	2.13	0.48
2:A:166:LYS:H	2:A:199:ASP:CG	2.20	0.48
2:A:229:ARG:NH2	2:A:363:VAL:HG11	2.28	0.48
2:A:248:LEU:HB3	2:A:354:GLY:HA2	1.94	0.48
3:B:274:PRO:HG2	3:B:374:SER:HB3	1.93	0.48
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.49	0.48
2:A:275:VAL:CG1	2:A:300:ASN:HD21	2.26	0.48
2:A:405:VAL:HG12	2:A:406:HIS:N	2.26	0.48
3:B:89:PRO:HA	3:B:92:PHE:CD2	2.48	0.48
3:B:286:LEU:CD1	3:B:371:LEU:HD21	2.41	0.48
2:A:103:TYR:CD2	2:A:413:MET:CE	2.94	0.48
2:A:244:PHE:CD1	2:A:245:ASP:N	2.80	0.48
2:A:267:PHE:CD1	2:A:267:PHE:N	2.81	0.48
2:A:317:LEU:HD23	2:A:375:VAL:CG1	2.42	0.48
3:B:67:LEU:HD21	3:B:87:PHE:CE2	2.48	0.48
2:A:210:TYR:CE1	2:A:227:LEU:CD2	2.94	0.48
2:A:274:PRO:HG3	2:A:374:ALA:HA	1.96	0.48
2:A:308:ARG:HH11	2:A:390:ARG:HH12	1.60	0.48
3:B:70:LEU:HG	3:B:145:THR:HG23	1.95	0.48
3:B:75:MET:HE2	3:B:94:PHE:HB3	1.95	0.48
3:B:318:VAL:HG13	3:B:354:ALA:HB3	1.96	0.48
3:B:408:TYR:CD2	3:B:418:PHE:CZ	2.99	0.48
2:A:132:LEU:HD21	2:A:164:LYS:CE	2.40	0.48
3:B:36:TYR:CZ	3:B:38:GLY:HA3	2.49	0.48
3:B:103:TRP:CD1	3:B:147:SER:CB	2.94	0.48
3:B:107:HIS:CE1	3:B:152:LEU:HB2	2.48	0.48
2:A:62:VAL:CG1	2:A:63:PRO:HD2	2.42	0.48
2:A:125:LEU:HD23	2:A:128:GLN:HE22	1.79	0.48
2:A:228:ASN:HA	2:A:231:ILE:CG1	2.44	0.48
3:B:241:CYS:SG	3:B:318:VAL:HG11	2.54	0.48
2:A:115:ILE:HD11	2:A:153:LEU:CD1	2.28	0.48
3:B:3:GLU:HA	3:B:51:VAL:HG13	1.96	0.48
3:B:42:LEU:HD12	3:B:47:GLU:OE1	2.14	0.48
1:D:3392:LYS:HD2	1:D:3423:ARG:CZ	2.44	0.48
2:A:9:VAL:HG22	2:A:10:GLY:H	1.78	0.48
2:A:107:HIS:CE1	2:A:152:LEU:HB3	2.48	0.48
2:A:341:ILE:HG23	2:A:342:GLN:N	2.29	0.48
1:D:3398:PRO:HG2	1:D:3401:VAL:HG21	1.96	0.48
2:A:11:GLN:HE21	2:A:74:VAL:CG1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:22:GLU:CG	2:A:83:TYR:CE1	2.94	0.48
2:A:172:TYR:CZ	2:A:391:LEU:HD13	2.48	0.48
2:A:301:GLN:HB2	2:A:303:VAL:HG12	1.96	0.48
3:B:94:PHE:O	3:B:114:LEU:HD11	2.14	0.48
1:D:3456:TYR:HA	1:D:3456:TYR:HD1	1.57	0.47
2:A:135:PHE:CD1	2:A:135:PHE:N	2.81	0.47
2:A:220:GLU:C	2:A:222:PRO:HD3	2.39	0.47
3:B:19:LYS:HG3	3:B:228:ASN:CB	2.44	0.47
2:A:102:ASN:HD21	2:A:105:ARG:H	1.62	0.47
2:A:346:TRP:HZ2	2:A:435:VAL:CG1	2.27	0.47
2:A:405:VAL:HA	2:A:408:TYR:HD2	1.78	0.47
3:B:255:LEU:O	3:B:259:MET:HB2	2.14	0.47
3:B:265:LEU:HG	3:B:266:HIS:N	2.15	0.47
1:D:3390:GLU:HG3	2:A:402:ARG:NH2	2.13	0.47
1:D:3392:LYS:HE2	1:D:3393:SER:N	2.29	0.47
1:D:3408:VAL:O	1:D:3412:LEU:HD13	2.14	0.47
2:A:17:GLY:HA3	2:A:67:PHE:HE1	1.80	0.47
2:A:108:TYR:CD1	2:A:108:TYR:N	2.82	0.47
2:A:210:TYR:HE1	2:A:227:LEU:CD2	2.16	0.47
3:B:31:ASP:HB3	3:B:32:PRO:CD	2.43	0.47
3:B:343:PHE:O	3:B:344:VAL:HB	2.14	0.47
3:B:428:LEU:HD12	3:B:428:LEU:C	2.40	0.47
3:B:428:LEU:HG	3:B:429:VAL:N	2.29	0.47
2:A:101:ASN:HD21	3:B:254:LYS:NZ	2.13	0.47
2:A:248:LEU:HB2	2:A:355:ILE:N	2.28	0.47
2:A:399:TYR:O	2:A:402:ARG:HA	2.13	0.47
3:B:33:THR:HG22	3:B:34:GLY:N	2.29	0.47
3:B:53:TYR:CD1	3:B:53:TYR:N	2.83	0.47
3:B:427:ASP:O	3:B:430:SER:HB3	2.14	0.47
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.79	0.47
2:A:168:GLU:O	2:A:201:ALA:HA	2.15	0.47
3:B:259:MET:CE	3:B:268:PHE:CZ	2.97	0.47
3:B:269:MET:CG	3:B:303:ALA:HB3	2.44	0.47
3:B:315:VAL:HB	3:B:351:VAL:HG13	1.96	0.47
2:A:164:LYS:HD3	2:A:164:LYS:HA	1.40	0.47
2:A:187:SER:O	2:A:191:THR:HG22	2.15	0.47
2:A:372:GLN:HA	2:A:372:GLN:NE2	2.30	0.47
2:A:398:MET:HB2	2:A:398:MET:HE3	1.42	0.47
3:B:272:PHE:CE1	7:B:502:TA1:H391	2.50	0.47
3:B:301:MET:HE1	3:B:377:PHE:CE2	2.32	0.47
3:B:312:TYR:HA	3:B:381:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3428:GLU:HG2	1:D:3431:PHE:N	2.22	0.47
3:B:3:GLU:HA	3:B:51:VAL:HA	1.96	0.47
3:B:105:LYS:HG2	3:B:110:GLU:HG2	1.92	0.47
3:B:316:ALA:O	3:B:378:ILE:HD12	2.15	0.47
1:D:3480:TRP:O	1:D:3483:ALA:HB3	2.15	0.47
2:A:9:VAL:O	2:A:13:GLY:HA3	2.15	0.47
2:A:175:PRO:HD2	2:A:207:GLU:CG	2.43	0.47
2:A:288:VAL:O	2:A:291:ILE:HG12	2.15	0.47
2:A:67:PHE:N	2:A:67:PHE:CD2	2.82	0.47
2:A:82:THR:HG22	2:A:83:TYR:N	2.29	0.47
2:A:224:TYR:CD1	3:B:325:MET:HG2	2.50	0.47
3:B:132:LEU:HB3	3:B:164:ARG:HH11	1.79	0.47
1:D:3449:ARG:HG2	1:D:3449:ARG:NH2	2.29	0.47
2:A:87:PHE:N	2:A:87:PHE:CD1	2.83	0.47
2:A:388:TRP:HZ3	2:A:391:LEU:HD22	1.79	0.47
3:B:70:LEU:H	3:B:145:THR:CG2	2.22	0.47
3:B:135:PHE:HD1	3:B:166:MET:HG2	1.79	0.47
3:B:262:PHE:HB3	3:B:263:PRO:HD2	1.97	0.47
3:B:267:PHE:CD1	3:B:267:PHE:N	2.82	0.47
3:B:318:VAL:HG13	3:B:354:ALA:CB	2.45	0.47
2:A:175:PRO:CG	2:A:304:LYS:HG2	2.46	0.46
2:A:191:THR:HG23	2:A:192:HIS:N	2.31	0.46
2:A:204:VAL:HG22	2:A:302:MET:HB3	1.97	0.46
2:A:224:TYR:CZ	3:B:325:MET:HG2	2.50	0.46
3:B:326:LYS:HE3	3:B:330:GLU:CB	2.44	0.46
3:B:352:LYS:HD3	3:B:353:THR:N	2.30	0.46
2:A:14:VAL:HG21	2:A:75:ILE:HD11	1.96	0.46
2:A:216:ASN:HD22	2:A:216:ASN:HA	1.54	0.46
2:A:242:LEU:HD11	2:A:318:LEU:CD2	2.45	0.46
3:B:324:SER:OG	3:B:326:LYS:HB3	2.16	0.46
1:D:3384:LYS:HD3	1:D:3386:LYS:CG	2.45	0.46
2:A:100:ALA:HB3	2:A:105:ARG:HG3	1.98	0.46
2:A:153:LEU:O	2:A:157:LEU:HG	2.14	0.46
2:A:177:VAL:HG13	3:B:329:ASP:HB3	1.96	0.46
3:B:48:ARG:HG2	3:B:243:ARG:CB	2.34	0.46
3:B:107:HIS:CD2	3:B:151:THR:CG2	2.98	0.46
3:B:332:MET:O	3:B:335:VAL:HB	2.16	0.46
2:A:11:GLN:HE21	2:A:74:VAL:CG2	2.29	0.46
2:A:244:PHE:HE2	2:A:358:GLU:OE1	1.98	0.46
2:A:259:LEU:O	2:A:261:PRO:HD3	2.14	0.46
3:B:135:PHE:CD1	3:B:135:PHE:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:315:VAL:HG12	3:B:351:VAL:HG13	1.97	0.46
1:D:3442:LYS:HA	1:D:3442:LYS:HD3	1.79	0.46
2:A:8:HIS:CD2	2:A:17:GLY:HA2	2.50	0.46
2:A:11:GLN:O	2:A:15:GLN:HG3	2.15	0.46
2:A:24:TYR:OH	2:A:239:THR:HB	2.15	0.46
3:B:319:PHE:HA	3:B:375:ALA:CA	2.36	0.46
1:D:3462:PHE:O	1:D:3467:VAL:HG23	2.15	0.46
2:A:22:GLU:HG2	2:A:83:TYR:CZ	2.49	0.46
2:A:436:GLY:C	2:A:438:ASP:H	2.23	0.46
3:B:108:TYR:CD1	3:B:108:TYR:N	2.82	0.46
3:B:169:PHE:CE2	3:B:235:MET:HB3	2.49	0.46
3:B:312:TYR:CD2	3:B:315:VAL:HG22	2.50	0.46
1:D:3410:LEU:C	1:D:3410:LEU:HD23	2.41	0.46
1:D:3438:TYR:CD1	1:D:3439:ASP:N	2.84	0.46
2:A:10:GLY:O	2:A:14:VAL:HG23	2.15	0.46
3:B:210:TYR:O	3:B:214:PHE:HB3	2.15	0.46
3:B:425:MET:HA	3:B:428:LEU:HD23	1.97	0.46
2:A:105:ARG:O	2:A:110:ILE:HG22	2.16	0.46
3:B:4:ILE:HD12	3:B:136:GLN:HE21	1.81	0.46
3:B:24:ILE:HD11	3:B:52:TYR:HE2	1.76	0.46
1:D:3394:LEU:CD1	2:A:410:GLY:HA2	2.46	0.46
1:D:3398:PRO:HB2	1:D:3401:VAL:CG2	2.44	0.46
1:D:3482:THR:HG23	1:D:3486:TYR:HD2	1.77	0.46
2:A:219:ILE:HG22	2:A:221:ARG:N	2.31	0.46
2:A:238:ILE:HD12	2:A:255:PHE:HE2	1.77	0.46
3:B:54:ASN:HD21	3:B:64:ARG:CB	2.22	0.46
3:B:278:ARG:HB3	3:B:279:GLY:HA3	1.97	0.46
3:B:323:MET:HE3	3:B:323:MET:HB3	1.81	0.46
2:A:26:LEU:HD23	2:A:363:VAL:HA	1.98	0.46
2:A:234:ILE:HD13	2:A:235:VAL:N	2.31	0.46
2:A:388:TRP:CE3	2:A:388:TRP:HA	2.51	0.46
2:A:412:GLY:CA	2:A:413:MET:HB2	2.46	0.46
3:B:70:LEU:HG	3:B:145:THR:CG2	2.46	0.46
3:B:161:TYR:CD1	3:B:161:TYR:N	2.82	0.46
3:B:172:VAL:HG13	3:B:173:PRO:HD2	1.98	0.46
3:B:236:SER:O	3:B:240:THR:HG23	2.15	0.45
3:B:325:MET:HE1	3:B:355:VAL:HB	1.96	0.45
2:A:72:PRO:HG3	2:A:95:GLY:O	2.17	0.45
2:A:251:ASP:CB	2:A:254:GLU:HG3	2.46	0.45
3:B:103:TRP:CD1	3:B:148:GLY:H	2.34	0.45
3:B:200:GLU:HA	3:B:265:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:230:LEU:HD23	3:B:231:VAL:HG23	1.99	0.45
1:D:3400:PRO:HA	1:D:3403:LEU:HG	1.98	0.45
1:D:3418:GLU:HG3	1:D:3420:ALA:H	1.82	0.45
1:D:3455:GLY:CA	1:D:3458:GLU:CB	2.95	0.45
2:A:99:ALA:HB1	5:A:502:GTP:O2G	2.16	0.45
2:A:172:TYR:CD1	2:A:172:TYR:C	2.94	0.45
2:A:181:VAL:HG21	3:B:258:ASN:HB3	1.93	0.45
3:B:187:ALA:O	3:B:191:VAL:HG12	2.16	0.45
3:B:425:MET:CG	3:B:428:LEU:HD23	2.47	0.45
2:A:5:ILE:HD13	2:A:125:LEU:HB3	1.98	0.45
2:A:204:VAL:HG21	2:A:302:MET:HE3	1.98	0.45
3:B:358:ILE:HA	3:B:359:PRO:HD3	1.50	0.45
2:A:119:LEU:CD2	2:A:153:LEU:CD1	2.95	0.45
2:A:119:LEU:CA	2:A:122:ILE:HD11	2.27	0.45
3:B:264:ARG:O	3:B:265:LEU:HB3	2.16	0.45
1:D:3399:THR:O	1:D:3403:LEU:HG	2.17	0.45
2:A:100:ALA:HB1	2:A:102:ASN:OD1	2.17	0.45
2:A:176:GLN:HB3	3:B:333:LEU:CD1	2.46	0.45
2:A:217:LEU:H	2:A:217:LEU:CD2	2.28	0.45
2:A:276:ILE:HG23	2:A:369:ALA:HB1	1.95	0.45
3:B:259:MET:HB3	3:B:259:MET:HE3	1.61	0.45
3:B:273:ALA:O	3:B:294:GLN:HG2	2.16	0.45
3:B:352:LYS:HZ2	3:B:352:LYS:HG2	1.40	0.45
3:B:413:MET:HG2	3:B:418:PHE:CE1	2.43	0.45
1:D:3464:TYR:CE1	1:D:3468:ASN:CG	2.95	0.45
2:A:217:LEU:CD2	2:A:217:LEU:N	2.80	0.45
3:B:64:ARG:HG3	3:B:125:GLU:CD	2.41	0.45
3:B:140:SER:CB	3:B:142:GLY:HA3	2.37	0.45
3:B:242:LEU:HD22	3:B:250:ALA:N	2.32	0.45
1:D:3431:PHE:HD1	1:D:3431:PHE:HA	1.43	0.45
1:D:3459:ASP:HB2	1:D:3462:PHE:HB2	1.97	0.45
7:B:502:TA1:H463	7:B:502:TA1:C26	2.46	0.45
1:D:3464:TYR:CD1	1:D:3478:VAL:CG1	2.94	0.45
2:A:21:TRP:HE3	2:A:21:TRP:N	2.14	0.45
2:A:182:VAL:HG11	3:B:257:VAL:CG1	2.46	0.45
3:B:6:HIS:CE1	3:B:8:GLN:HE21	2.35	0.45
3:B:11:GLN:O	3:B:15:GLN:N	2.41	0.45
3:B:43:GLN:O	3:B:49:ILE:HG23	2.17	0.45
3:B:288:VAL:HG12	3:B:289:PRO:CA	2.47	0.45
3:B:332:MET:CE	3:B:351:VAL:CG1	2.94	0.45
2:A:75:ILE:O	2:A:78:VAL:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:93:ILE:HD12	2:A:93:ILE:HA	1.76	0.45
2:A:6:SER:OG	2:A:65:ALA:HB2	2.17	0.44
2:A:203:MET:SD	2:A:388:TRP:CZ2	3.10	0.44
2:A:360:PRO:HG3	2:A:374:ALA:CB	2.46	0.44
3:B:169:PHE:HD2	3:B:204:ILE:HD11	1.82	0.44
2:A:12:ALA:HB2	5:A:502:GTP:C8	2.52	0.44
2:A:98:ASP:HB3	3:B:2:ARG:HH12	1.82	0.44
2:A:334:THR:HG23	2:A:335:ILE:N	2.32	0.44
2:A:432:TYR:HD1	2:A:432:TYR:HA	1.36	0.44
3:B:94:PHE:CD1	3:B:94:PHE:C	2.93	0.44
3:B:115:VAL:O	3:B:118:VAL:HB	2.17	0.44
3:B:230:LEU:HD21	3:B:302:MET:HE1	1.98	0.44
3:B:277:SER:N	3:B:281:GLN:HB3	2.32	0.44
3:B:346:TRP:CZ2	3:B:435:TYR:CD1	3.06	0.44
3:B:431:GLU:OE1	3:B:432:TYR:HA	2.17	0.44
1:D:3384:LYS:HG2	1:D:3387:HIS:ND1	2.32	0.44
1:D:3395:PRO:HB3	3:B:163:ASP:OD1	2.17	0.44
1:D:3410:LEU:C	1:D:3413:GLY:H	2.25	0.44
1:D:3418:GLU:HG3	1:D:3419:TRP:N	2.32	0.44
2:A:195:LEU:HD23	2:A:264:ARG:CZ	2.47	0.44
2:A:242:LEU:CD2	2:A:318:LEU:CD2	2.95	0.44
3:B:141:LEU:O	3:B:186:ASN:HB2	2.17	0.44
3:B:262:PHE:CE2	3:B:435:TYR:CE1	3.06	0.44
1:D:3394:LEU:CD2	2:A:410:GLY:CA	2.93	0.44
2:A:23:LEU:CD1	2:A:363:VAL:HG22	2.46	0.44
3:B:30:ILE:CD1	3:B:53:TYR:CE2	2.95	0.44
3:B:102:ASN:HD21	3:B:407:TRP:C	2.26	0.44
3:B:109:THR:HG22	3:B:110:GLU:OE2	2.17	0.44
2:A:5:ILE:HG23	2:A:64:ARG:O	2.17	0.44
2:A:22:GLU:CG	2:A:83:TYR:HE1	2.31	0.44
2:A:23:LEU:HD12	2:A:363:VAL:HG22	1.99	0.44
2:A:119:LEU:HD23	2:A:153:LEU:HD11	2.00	0.44
2:A:250:VAL:CG2	2:A:318:LEU:CD2	2.95	0.44
2:A:412:GLY:HA2	2:A:413:MET:C	2.42	0.44
3:B:30:ILE:HA	3:B:35:SER:O	2.18	0.44
3:B:209:LEU:HG	3:B:230:LEU:HD22	2.00	0.44
1:D:3427:MET:HE3	3:B:196:GLU:CD	2.43	0.44
1:D:3438:TYR:HD1	1:D:3439:ASP:N	2.15	0.44
2:A:23:LEU:HD23	2:A:236:SER:HB2	1.98	0.44
2:A:103:TYR:CG	2:A:189:LEU:HD12	2.53	0.44
2:A:140:SER:C	2:A:142:GLY:HA3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:154:MET:CE	2:A:166:LYS:HD2	2.48	0.44
2:A:272:TYR:HE1	2:A:376:CYS:HG	1.58	0.44
3:B:185:TYR:HD1	3:B:185:TYR:HA	1.69	0.44
2:A:82:THR:CG2	2:A:83:TYR:CD1	3.00	0.44
2:A:177:VAL:CG2	2:A:207:GLU:HB3	2.44	0.44
2:A:195:LEU:HD21	2:A:428:LEU:CD2	2.48	0.44
2:A:231:ILE:HG12	2:A:231:ILE:H	1.35	0.44
3:B:378:ILE:HG22	3:B:379:GLY:N	2.33	0.44
2:A:209:ILE:HG12	2:A:302:MET:CG	2.47	0.44
2:A:269:LEU:O	2:A:378:LEU:HA	2.17	0.44
2:A:413:MET:C	2:A:414:GLU:HG3	2.43	0.44
3:B:264:ARG:HG2	3:B:431:GLU:OE2	2.18	0.44
3:B:392:SER:O	3:B:395:PHE:HB3	2.17	0.44
2:A:282:TYR:HD1	2:A:282:TYR:HA	1.48	0.44
2:A:133:GLN:HB3	2:A:243:ARG:HH12	1.80	0.43
3:B:408:TYR:N	3:B:408:TYR:CD1	2.86	0.43
2:A:234:ILE:HD13	2:A:234:ILE:C	2.43	0.43
2:A:255:PHE:HE2	2:A:378:LEU:HD21	1.83	0.43
3:B:78:VAL:O	3:B:84:GLY:HA2	2.18	0.43
3:B:184:PRO:CB	3:B:395:PHE:HA	2.48	0.43
3:B:320:ARG:HB2	3:B:358:ILE:O	2.18	0.43
1:D:3405:MET:HA	1:D:3408:VAL:HG22	1.97	0.43
2:A:242:LEU:CD1	2:A:318:LEU:CD2	2.94	0.43
3:B:292:THR:HG21	3:B:331:GLN:HG2	1.98	0.43
3:B:314:THR:N	3:B:380:ASN:HB3	2.33	0.43
3:B:382:THR:HB	3:B:436:GLN:CD	2.43	0.43
3:B:425:MET:HE2	3:B:425:MET:HB3	1.42	0.43
2:A:286:LEU:O	2:A:291:ILE:HG23	2.18	0.43
3:B:36:TYR:CD2	3:B:44:LEU:HD22	2.53	0.43
3:B:168:THR:HG22	3:B:169:PHE:N	2.33	0.43
3:B:191:VAL:CA	3:B:194:LEU:HD12	2.15	0.43
3:B:382:THR:HG21	3:B:436:GLN:HA	2.00	0.43
3:B:388:PHE:HD1	3:B:388:PHE:HA	1.59	0.43
1:D:3391:ILE:HD13	1:D:3391:ILE:N	2.34	0.43
1:D:3459:ASP:HA	1:D:3460:PRO:HD3	1.46	0.43
2:A:168:GLU:CG	2:A:201:ALA:CB	2.96	0.43
2:A:244:PHE:CD1	2:A:244:PHE:C	2.95	0.43
2:A:248:LEU:HD13	2:A:248:LEU:HA	1.56	0.43
2:A:264:ARG:H	2:A:264:ARG:HG2	1.62	0.43
2:A:362:VAL:HB	2:A:370:LYS:HD3	2.00	0.43
3:B:204:ILE:CG2	3:B:209:LEU:CD2	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:420:GLU:CG	3:B:421:ALA:N	2.82	0.43
1:D:3432:ILE:CG1	1:D:3433:THR:N	2.81	0.43
1:D:3440:THR:CG2	1:D:3441:LYS:N	2.82	0.43
3:B:108:TYR:O	3:B:112:ALA:HB2	2.19	0.43
3:B:175:PRO:HD2	3:B:207:GLU:OE1	2.19	0.43
3:B:276:THR:HB	3:B:281:GLN:HG3	2.00	0.43
2:A:360:PRO:HG2	2:A:374:ALA:HB2	2.01	0.43
3:B:282:GLN:HE21	3:B:282:GLN:HB3	1.47	0.43
3:B:346:TRP:CE3	3:B:347:ILE:CG1	3.02	0.43
3:B:359:PRO:CB	3:B:360:PRO:HD2	2.47	0.43
1:D:3405:MET:SD	1:D:3408:VAL:CG2	3.07	0.43
1:D:3419:TRP:CE3	1:D:3419:TRP:HA	2.53	0.43
2:A:102:ASN:HD21	2:A:105:ARG:HG2	1.84	0.43
3:B:44:LEU:O	3:B:49:ILE:HG23	2.19	0.43
3:B:103:TRP:CE3	3:B:189:LEU:HD13	2.54	0.43
3:B:137:LEU:HD12	3:B:137:LEU:HA	1.88	0.43
3:B:230:LEU:CD2	3:B:302:MET:CE	2.93	0.43
1:D:3487:TYR:CD1	1:D:3487:TYR:C	2.94	0.43
2:A:142:GLY:HA2	2:A:183:GLU:OE1	2.18	0.43
2:A:262:TYR:HA	2:A:263:PRO:HD3	1.81	0.43
2:A:7:ILE:HG13	2:A:7:ILE:O	2.18	0.42
2:A:185:TYR:HD2	2:A:408:TYR:CE2	2.37	0.42
3:B:198:THR:O	3:B:198:THR:HG22	2.19	0.42
3:B:425:MET:CA	3:B:428:LEU:HD23	2.49	0.42
1:D:3455:GLY:HA2	1:D:3458:GLU:HG3	2.01	0.42
2:A:117:LEU:HD13	2:A:117:LEU:HA	1.76	0.42
2:A:225:THR:CG2	2:A:226:ASN:N	2.82	0.42
2:A:341:ILE:CG2	2:A:342:GLN:N	2.82	0.42
3:B:7:ILE:CG2	3:B:137:LEU:CD1	2.97	0.42
3:B:158:ARG:HA	3:B:158:ARG:HD3	1.75	0.42
3:B:276:THR:HB	3:B:281:GLN:CG	2.49	0.42
1:D:3392:LYS:CE	1:D:3393:SER:HA	2.48	0.42
1:D:3457:LEU:HD12	1:D:3457:LEU:C	2.44	0.42
2:A:242:LEU:HD21	2:A:318:LEU:CD2	2.46	0.42
2:A:339:ARG:O	2:A:339:ARG:HG3	2.20	0.42
2:A:352:LYS:HD3	2:A:352:LYS:C	2.44	0.42
3:B:151:THR:CG2	3:B:152:LEU:N	2.82	0.42
3:B:275:LEU:HD23	3:B:300:ASN:OD1	2.19	0.42
3:B:288:VAL:CG1	3:B:289:PRO:HD3	2.48	0.42
1:D:3436:ILE:CG1	1:D:3437:ASN:N	2.82	0.42
2:A:288:VAL:HA	2:A:291:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:24:ILE:CG2	3:B:25:SER:N	2.82	0.42
3:B:102:ASN:HD21	3:B:408:TYR:CA	2.29	0.42
3:B:269:MET:HE3	3:B:301:MET:HE3	1.93	0.42
3:B:269:MET:HG2	3:B:303:ALA:CB	2.50	0.42
1:D:3385:LYS:NZ	3:B:196:GLU:HG2	2.34	0.42
1:D:3464:TYR:CD1	1:D:3478:VAL:CG2	2.96	0.42
2:A:68:VAL:HG11	2:A:149:PHE:CZ	2.55	0.42
2:A:147:SER:HB3	2:A:186:ASN:HB3	2.01	0.42
2:A:175:PRO:HD3	2:A:205:ASP:OD2	2.19	0.42
2:A:237:SER:CB	2:A:376:CYS:SG	3.07	0.42
2:A:371:VAL:CG1	2:A:372:GLN:N	2.82	0.42
2:A:407:TRP:NE1	3:B:260:VAL:CG2	2.82	0.42
2:A:419:SER:O	2:A:423:GLU:HG3	2.19	0.42
3:B:4:ILE:N	3:B:51:VAL:CG1	2.82	0.42
3:B:86:ILE:CG2	3:B:87:PHE:N	2.83	0.42
3:B:168:THR:CG2	3:B:169:PHE:N	2.83	0.42
3:B:195:VAL:CG1	3:B:196:GLU:N	2.81	0.42
3:B:270:PRO:HB2	3:B:302:MET:SD	2.59	0.42
3:B:311:ARG:HH11	3:B:311:ARG:CG	2.32	0.42
3:B:319:PHE:N	3:B:319:PHE:CD1	2.87	0.42
3:B:399:PHE:HE2	3:B:419:THR:HG23	1.85	0.42
2:A:208:ALA:CB	2:A:303:VAL:C	2.93	0.42
2:A:234:ILE:HG21	2:A:302:MET:HE1	2.02	0.42
3:B:6:HIS:CB	3:B:21:TRP:HZ2	2.28	0.42
3:B:40:SER:OG	3:B:43:GLN:HG3	2.19	0.42
3:B:133:GLN:HA	3:B:133:GLN:OE1	2.19	0.42
3:B:185:TYR:HA	3:B:395:PHE:CE1	2.54	0.42
3:B:270:PRO:C	3:B:302:MET:HG3	2.45	0.42
3:B:310:GLY:HA2	3:B:383:ALA:HB2	2.00	0.42
1:D:3464:TYR:HE1	1:D:3468:ASN:CG	2.28	0.42
3:B:241:CYS:SG	3:B:318:VAL:CG1	3.08	0.42
3:B:289:PRO:HA	3:B:292:THR:HG23	2.01	0.42
3:B:390:ARG:HD2	3:B:390:ARG:HA	1.57	0.42
1:D:3474:CYS:O	1:D:3477:LEU:HB2	2.20	0.42
1:D:3478:VAL:CG1	1:D:3479:LYS:N	2.82	0.42
2:A:15:GLN:NE2	5:A:502:GTP:N7	2.67	0.42
2:A:215:ARG:HG2	2:A:215:ARG:H	1.65	0.42
2:A:324:VAL:HB	2:A:327:ASP:CG	2.45	0.42
3:B:185:TYR:CD1	3:B:395:PHE:CE1	3.06	0.42
1:D:3384:LYS:HB2	1:D:3384:LYS:NZ	2.35	0.42
1:D:3436:ILE:CG1	1:D:3437:ASN:HD22	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3467:VAL:O	1:D:3470:ALA:HB3	2.19	0.42
2:A:7:ILE:CD1	2:A:137:VAL:HG22	2.49	0.42
2:A:152:LEU:O	2:A:155:GLU:HB3	2.20	0.42
2:A:193:THR:CG2	2:A:194:THR:N	2.83	0.42
2:A:291:ILE:CD1	2:A:373:ARG:HG3	2.49	0.42
2:A:305:CYS:SG	2:A:383:ALA:CB	3.08	0.42
2:A:414:GLU:HB2	2:A:416:GLY:HA3	2.02	0.42
3:B:68:VAL:CG1	3:B:149:MET:SD	3.07	0.42
3:B:230:LEU:CD2	3:B:302:MET:HE1	2.50	0.42
3:B:317:ALA:CB	3:B:319:PHE:CE1	3.03	0.42
2:A:158:SER:HB2	2:A:197:HIS:ND1	2.35	0.42
2:A:301:GLN:NE2	2:A:306:ASP:H	2.17	0.42
3:B:140:SER:O	3:B:142:GLY:HA3	2.19	0.42
3:B:311:ARG:HA	3:B:342:TYR:O	2.19	0.42
2:A:9:VAL:HG12	2:A:138:PHE:O	2.19	0.41
2:A:117:LEU:HD12	2:A:121:ARG:NH1	2.35	0.41
2:A:133:GLN:HG2	2:A:252:LEU:HB2	2.01	0.41
2:A:175:PRO:HG2	2:A:304:LYS:CG	2.50	0.41
2:A:175:PRO:HG3	2:A:304:LYS:HG2	2.02	0.41
3:B:24:ILE:HG23	3:B:25:SER:N	2.34	0.41
3:B:28:HIS:O	3:B:36:TYR:CE1	2.73	0.41
3:B:88:ARG:HA	3:B:89:PRO:HD3	1.87	0.41
3:B:141:LEU:N	3:B:141:LEU:CD1	2.83	0.41
3:B:141:LEU:HD13	3:B:170:SER:HB2	2.01	0.41
2:A:103:TYR:CD2	2:A:189:LEU:HD13	2.55	0.41
3:B:44:LEU:O	3:B:49:ILE:HG12	2.20	0.41
3:B:52:TYR:HB3	3:B:53:TYR:CE1	2.55	0.41
3:B:115:VAL:HG21	3:B:152:LEU:HD23	2.02	0.41
3:B:156:LYS:HZ2	3:B:156:LYS:HG3	1.69	0.41
3:B:320:ARG:CB	3:B:356:CYS:HB3	2.49	0.41
1:D:3384:LYS:NZ	1:D:3386:LYS:HE3	2.34	0.41
2:A:119:LEU:C	2:A:123:ARG:HD3	2.45	0.41
2:A:269:LEU:HD22	2:A:384:ILE:CD1	2.32	0.41
2:A:430:LYS:O	2:A:434:GLU:HG3	2.20	0.41
3:B:86:ILE:HG23	3:B:87:PHE:CD1	2.54	0.41
3:B:107:HIS:NE2	3:B:151:THR:HG23	2.35	0.41
3:B:223:THR:CG2	3:B:224:TYR:N	2.82	0.41
3:B:390:ARG:HH11	3:B:390:ARG:HD3	1.75	0.41
1:D:3457:LEU:O	1:D:3463:ASP:HB3	2.20	0.41
2:A:110:ILE:CG2	2:A:111:GLY:N	2.82	0.41
2:A:141:PHE:HB2	2:A:173:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:190:THR:O	2:A:193:THR:HG22	2.20	0.41
2:A:229:ARG:HH22	2:A:363:VAL:HG11	1.84	0.41
2:A:301:GLN:HE21	2:A:303:VAL:HG12	1.84	0.41
3:B:28:HIS:O	3:B:36:TYR:HE1	2.03	0.41
3:B:67:LEU:HD21	3:B:87:PHE:CD2	2.55	0.41
3:B:151:THR:OG1	3:B:193:GLN:HB2	2.20	0.41
3:B:346:TRP:CD1	3:B:346:TRP:H	2.37	0.41
1:D:3427:MET:HG3	3:B:196:GLU:OE1	2.20	0.41
1:D:3432:ILE:CD1	1:D:3433:THR:N	2.82	0.41
2:A:31:GLN:CB	2:A:32:PRO:CD	2.91	0.41
2:A:149:PHE:O	2:A:152:LEU:HG	2.20	0.41
3:B:325:MET:HE1	3:B:355:VAL:CB	2.51	0.41
2:A:104:ALA:CB	2:A:413:MET:CG	2.97	0.41
2:A:210:TYR:HD1	2:A:210:TYR:HA	1.56	0.41
2:A:217:LEU:HD23	2:A:217:LEU:N	2.32	0.41
2:A:238:ILE:HD13	2:A:238:ILE:HA	1.89	0.41
3:B:242:LEU:HB3	3:B:250:ALA:O	2.20	0.41
3:B:267:PHE:HB2	3:B:384:ILE:CD1	2.51	0.41
1:D:3385:LYS:HZ1	3:B:196:GLU:HG2	1.86	0.41
1:D:3438:TYR:CD1	1:D:3438:TYR:C	2.94	0.41
1:D:3444:MET:HB3	1:D:3444:MET:HE2	1.58	0.41
1:D:3456:TYR:O	1:D:3462:PHE:HB3	2.20	0.41
1:D:3457:LEU:CD1	1:D:3458:GLU:N	2.83	0.41
2:A:19:ALA:CB	2:A:228:ASN:HB3	2.46	0.41
3:B:281:GLN:OE1	3:B:281:GLN:HA	2.20	0.41
1:D:3422:ILE:C	1:D:3422:ILE:CD1	2.94	0.41
1:D:3433:THR:HA	1:D:3436:ILE:CD1	2.46	0.41
2:A:204:VAL:HG23	2:A:302:MET:HE3	2.01	0.41
2:A:407:TRP:HE1	3:B:260:VAL:HG22	1.86	0.41
2:A:422:ARG:HH12	2:A:426:ALA:CB	2.22	0.41
3:B:408:TYR:CG	3:B:418:PHE:HZ	2.39	0.41
1:D:3384:LYS:HG3	1:D:3386:LYS:HB2	2.03	0.41
1:D:3423:ARG:NH1	3:B:158:ARG:HD2	2.14	0.41
1:D:3424:LYS:HE3	3:B:155:SER:O	2.20	0.41
1:D:3457:LEU:HD12	1:D:3458:GLU:CA	2.51	0.41
2:A:63:PRO:CG	2:A:87:PHE:HA	2.51	0.41
2:A:69:ASP:CB	2:A:75:ILE:CD1	2.94	0.41
2:A:119:LEU:HA	2:A:122:ILE:CG1	2.51	0.41
2:A:185:TYR:HD1	2:A:185:TYR:HA	1.57	0.41
2:A:244:PHE:HD1	2:A:245:ASP:H	1.65	0.41
3:B:76:ASP:HA	3:B:79:ARG:CG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:88:ARG:O	3:B:91:ASN:HB2	2.21	0.41
3:B:133:GLN:HG2	3:B:252:LEU:CD1	2.34	0.41
3:B:314:THR:CG2	3:B:315:VAL:N	2.83	0.41
2:A:359:PRO:HA	2:A:360:PRO:HD3	1.92	0.41
2:A:371:VAL:HG12	2:A:373:ARG:N	2.30	0.41
2:A:407:TRP:NE1	3:B:260:VAL:HG23	2.36	0.41
3:B:64:ARG:HG2	3:B:125:GLU:HB3	2.02	0.41
3:B:133:GLN:HE22	3:B:253:ARG:HG3	1.86	0.41
3:B:223:THR:HG22	3:B:225:GLY:H	1.86	0.41
1:D:3412:LEU:HD22	1:D:3431:PHE:HZ	1.85	0.40
1:D:3477:LEU:HD12	1:D:3477:LEU:H	1.85	0.40
2:A:404:PHE:CE2	3:B:258:ASN:O	2.74	0.40
3:B:4:ILE:CG2	3:B:136:GLN:HG2	2.51	0.40
3:B:7:ILE:CD1	3:B:66:ILE:HD11	2.51	0.40
3:B:7:ILE:CB	3:B:137:LEU:CD1	2.95	0.40
3:B:184:PRO:HB3	3:B:394:GLN:HB2	2.03	0.40
3:B:259:MET:CE	3:B:268:PHE:CE1	3.04	0.40
3:B:261:PRO:HB2	3:B:262:PHE:HD2	1.80	0.40
3:B:325:MET:CE	3:B:355:VAL:CG2	2.98	0.40
2:A:72:PRO:HG3	2:A:96:LYS:CA	2.44	0.40
2:A:276:ILE:HD13	2:A:277:SER:O	2.22	0.40
3:B:165:ILE:HG22	3:B:199:ASP:CG	2.46	0.40
3:B:167:ASN:HB3	3:B:202:TYR:CE1	2.50	0.40
3:B:288:VAL:HB	3:B:289:PRO:HD3	2.03	0.40
3:B:396:THR:HA	3:B:399:PHE:HB3	2.02	0.40
3:B:406:HIS:CE1	3:B:407:TRP:CE2	3.09	0.40
1:D:3418:GLU:CG	1:D:3419:TRP:N	2.85	0.40
1:D:3462:PHE:O	1:D:3462:PHE:CD1	2.74	0.40
2:A:233:GLN:HG3	2:A:272:TYR:CZ	2.56	0.40
2:A:117:LEU:CD1	2:A:121:ARG:HH22	2.31	0.40
3:B:276:THR:O	7:B:502:TA1:H192	2.21	0.40
3:B:278:ARG:C	3:B:278:ARG:CD	2.94	0.40
1:D:3477:LEU:N	1:D:3477:LEU:CD1	2.84	0.40
2:A:26:LEU:HD12	2:A:26:LEU:HA	1.90	0.40
2:A:180:ALA:HB3	2:A:183:GLU:HB2	2.04	0.40
2:A:219:ILE:O	2:A:222:PRO:HD3	2.22	0.40
2:A:402:ARG:NE	2:A:405:VAL:HG12	2.28	0.40
3:B:199:ASP:HA	3:B:265:LEU:HB2	2.04	0.40
3:B:425:MET:HA	3:B:428:LEU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	D	106/108 (98%)	100 (94%)	5 (5%)	1 (1%)	14	51
2	A	408/451 (90%)	374 (92%)	23 (6%)	11 (3%)	4	25
3	B	424/445 (95%)	386 (91%)	31 (7%)	7 (2%)	7	36
All	All	938/1004 (93%)	860 (92%)	59 (6%)	19 (2%)	8	31

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	276	ILE
2	A	437	VAL
3	B	38	GLY
3	B	130	ASP
3	B	282	GLN
3	B	287	THR
3	B	344	VAL
2	A	100	ALA
2	A	111	GLY
2	A	249	ASN
1	D	3483	ALA
2	A	342	GLN
2	A	413	MET
2	A	148	GLY
2	A	31	GLN
2	A	307	PRO
3	B	82	PRO
2	A	412	GLY
3	B	32	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	95/95 (100%)	68 (72%)	27 (28%)	0	2
2	A	347/377 (92%)	261 (75%)	86 (25%)	1	4
3	B	367/381 (96%)	261 (71%)	106 (29%)	0	2
All	All	809/853 (95%)	590 (73%)	219 (27%)	2	3

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3384	LYS
1	D	3385	LYS
1	D	3389	ASP
1	D	3392	LYS
1	D	3396	LYS
1	D	3399	THR
1	D	3405	MET
1	D	3408	VAL
1	D	3415	LYS
1	D	3422	ILE
1	D	3423	ARG
1	D	3424	LYS
1	D	3425	LYS
1	D	3426	ILE
1	D	3428	GLU
1	D	3431	PHE
1	D	3432	ILE
1	D	3433	THR
1	D	3436	ILE
1	D	3443	MET
1	D	3444	MET
1	D	3449	ARG
1	D	3452	ILE
1	D	3454	LYS
1	D	3456	TYR
1	D	3459	ASP

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Mol	Chain	Res	Type
1	D	3484	GLN
2	A	4	CYS
2	A	16	ILE
2	A	22	GLU
2	A	24	TYR
2	A	25	CYS
2	A	26	LEU
2	A	32	PRO
2	A	76	ASP
2	A	85	GLN
2	A	91	GLN
2	A	93	ILE
2	A	96	LYS
2	A	98	ASP
2	A	101	ASN
2	A	105	ARG
2	A	109	THR
2	A	112	LYS
2	A	117	LEU
2	A	120	ASP
2	A	122	ILE
2	A	123	ARG
2	A	128	GLN
2	A	129	CYS
2	A	130	THR
2	A	135	PHE
2	A	141	PHE
2	A	150	THR
2	A	154	MET
2	A	164	LYS
2	A	170	SER
2	A	172	TYR
2	A	192	HIS
2	A	207	GLU
2	A	210	TYR
2	A	212	ILE
2	A	214	ARG
2	A	215	ARG
2	A	217	LEU
2	A	224	TYR
2	A	229	ARG
2	A	231	ILE

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Mol	Chain	Res	Type
2	A	234	ILE
2	A	241	SER
2	A	242	LEU
2	A	244	PHE
2	A	248	LEU
2	A	250	VAL
2	A	251	ASP
2	A	253	THR
2	A	260	VAL
2	A	264	ARG
2	A	269	LEU
2	A	276	ILE
2	A	280	LYS
2	A	284	GLU
2	A	300	ASN
2	A	301	GLN
2	A	303	VAL
2	A	305	CYS
2	A	308	ARG
2	A	317	LEU
2	A	320	ARG
2	A	326	LYS
2	A	337	THR
2	A	344	VAL
2	A	347	CYS
2	A	349	THR
2	A	352	LYS
2	A	370	LYS
2	A	377	MET
2	A	378	LEU
2	A	390	ARG
2	A	398	MET
2	A	401	LYS
2	A	402	ARG
2	A	405	VAL
2	A	413	MET
2	A	414	GLU
2	A	417	GLU
2	A	424	ASP
2	A	425	MET
2	A	428	LEU
2	A	430	LYS

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Mol	Chain	Res	Type
2	A	431	ASP
2	A	432	TYR
2	A	433	GLU
3	B	7	ILE
3	B	8	GLN
3	B	14	ASN
3	B	24	ILE
3	B	26	ASP
3	B	33	THR
3	B	41	ASP
3	B	44	LEU
3	B	53	TYR
3	B	54	ASN
3	B	64	ARG
3	B	66	ILE
3	B	67	LEU
3	B	76	ASP
3	B	79	ARG
3	B	88	ARG
3	B	90	ASP
3	B	94	PHE
3	B	97	SER
3	B	101	ASN
3	B	105	LYS
3	B	117	SER
3	B	122	VAL
3	B	124	LYS
3	B	126	SER
3	B	129	CYS
3	B	135	PHE
3	B	138	THR
3	B	140	SER
3	B	141	LEU
3	B	145	THR
3	B	153	LEU
3	B	154	ILE
3	B	156	LYS
3	B	158	ARG
3	B	160	GLU
3	B	161	TYR
3	B	164	ARG
3	B	165	ILE

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Mol	Chain	Res	Type
3	B	166	MET
3	B	178	SER
3	B	186	ASN
3	B	191	VAL
3	B	193	GLN
3	B	194	LEU
3	B	198	THR
3	B	207	GLU
3	B	209	LEU
3	B	211	ASP
3	B	213	CYS
3	B	219	LEU
3	B	221	THR
3	B	229	HIS
3	B	230	LEU
3	B	236	SER
3	B	240	THR
3	B	241	CYS
3	B	243	ARG
3	B	259	MET
3	B	265	LEU
3	B	275	LEU
3	B	277	SER
3	B	278	ARG
3	B	280	SER
3	B	282	GLN
3	B	286	LEU
3	B	288	VAL
3	B	293	GLN
3	B	294	GLN
3	B	299	LYS
3	B	306	ASP
3	B	308	ARG
3	B	309	HIS
3	B	311	ARG
3	B	322	ARG
3	B	323	MET
3	B	325	MET
3	B	330	GLU
3	B	337	ASN
3	B	342	TYR
3	B	343	PHE

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Mol	Chain	Res	Type
3	B	344	VAL
3	B	346	TRP
3	B	352	LYS
3	B	372	LYS
3	B	376	THR
3	B	378	ILE
3	B	380	ASN
3	B	384	ILE
3	B	386	GLU
3	B	390	ARG
3	B	391	ILE
3	B	400	ARG
3	B	401	ARG
3	B	402	LYS
3	B	405	LEU
3	B	409	THR
3	B	413	MET
3	B	419	THR
3	B	423	SER
3	B	425	MET
3	B	427	ASP
3	B	428	LEU
3	B	431	GLU
3	B	432	TYR
3	B	437	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3437	ASN
1	D	3484	GLN
2	A	11	GLN
2	A	15	GLN
2	A	101	ASN
2	A	102	ASN
2	A	107	HIS
2	A	128	GLN
2	A	139	HIS
2	A	186	ASN
2	A	226	ASN
2	A	256	GLN
2	A	266	HIS

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Mol	Chain	Res	Type
2	A	301	GLN
2	A	372	GLN
2	A	380	ASN
2	A	393	HIS
3	B	8	GLN
3	B	14	ASN
3	B	43	GLN
3	B	54	ASN
3	B	91	ASN
3	B	96	GLN
3	B	101	ASN
3	B	102	ASN
3	B	107	HIS
3	B	133	GLN
3	B	136	GLN
3	B	139	HIS
3	B	167	ASN
3	B	186	ASN
3	B	258	ASN
3	B	282	GLN
3	B	334	ASN
3	B	336	GLN
3	B	337	ASN
3	B	349	ASN
3	B	380	ASN
3	B	394	GLN
3	B	406	HIS
3	B	424	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	GTP	A	502	4	33,34,34	1.90	3 (9%)	50,54,54	0.91	3 (6%)
6	GDP	B	501	-	29,30,30	2.86	11 (37%)	45,47,47	3.47	16 (35%)
7	TA1	B	502	-	68,68,68	2.20	25 (36%)	105,105,105	1.49	13 (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
5	GTP	A	502	4	-	4/22/38/38	0/3/3/3
6	GDP	B	501	-	-	4/16/32/32	0/3/3/3
7	TA1	B	502	-	-	9/41/127/127	0/7/7/7

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	GDP	PA-O3A	7.65	1.67	1.59
7	B	502	TA1	C06-C05	6.47	1.50	1.38
5	A	502	GTP	PA-O3A	-5.96	1.53	1.59
6	B	501	GDP	O6-C6	5.92	1.34	1.23
6	B	501	GDP	C8-N9	5.84	1.50	1.37
5	A	502	GTP	PB-O3A	-5.73	1.53	1.59
7	B	502	TA1	C08-C07	-5.63	1.25	1.38
5	A	502	GTP	PB-O3B	5.55	1.65	1.59
7	B	502	TA1	C18-C10	5.33	1.68	1.57
7	B	502	TA1	C05-C04	4.85	1.46	1.39
6	B	501	GDP	C2-N1	4.74	1.49	1.37
7	B	502	TA1	C45-C24	4.25	1.61	1.54
6	B	501	GDP	PB-O2B	-3.91	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	TA1	C36-C31	3.74	1.45	1.39
7	B	502	TA1	O02-C03	3.57	1.42	1.34
7	B	502	TA1	C25-C24	3.43	1.39	1.34
6	B	501	GDP	O4'-C1'	3.39	1.49	1.42
7	B	502	TA1	C46-C45	3.17	1.59	1.53
7	B	502	TA1	C43-C01	3.14	1.60	1.54
7	B	502	TA1	C11-C10	3.13	1.61	1.54
6	B	501	GDP	C8-N7	3.04	1.41	1.32
7	B	502	TA1	C43-C26	2.88	1.58	1.52
6	B	501	GDP	C5-N7	-2.84	1.33	1.39
6	B	501	GDP	C5-C4	2.60	1.45	1.38
7	B	502	TA1	C26-C25	2.59	1.56	1.51
7	B	502	TA1	C18-C20	2.58	1.62	1.55
7	B	502	TA1	C01-C45	2.55	1.66	1.56
7	B	502	TA1	C04-C03	-2.52	1.44	1.50
6	B	501	GDP	C2-N3	-2.43	1.27	1.33
6	B	501	GDP	PB-O3B	2.41	1.63	1.54
7	B	502	TA1	C41-C42	2.33	1.42	1.38
7	B	502	TA1	C16-C15	2.31	1.56	1.52
7	B	502	TA1	O09-C21	2.16	1.49	1.44
7	B	502	TA1	C37-C29	2.15	1.54	1.52
7	B	502	TA1	C08-C09	2.13	1.42	1.38
7	B	502	TA1	C10-C02	2.13	1.62	1.57
7	B	502	TA1	C33-C32	2.07	1.42	1.38
7	B	502	TA1	C34-C33	2.05	1.42	1.38
7	B	502	TA1	C39-C38	2.03	1.42	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	N9-C8-N7	-10.74	93.48	113.40
6	B	501	GDP	C8-N7-C5	9.20	120.65	104.26
6	B	501	GDP	C6-C5-N7	8.57	145.89	130.29
6	B	501	GDP	N2-C2-N3	6.28	131.93	119.67
6	B	501	GDP	C6-C5-C4	-6.17	109.55	118.83
7	B	502	TA1	C06-C05-C04	-5.85	114.61	120.36
6	B	501	GDP	C8-N9-C4	5.83	116.96	106.03
7	B	502	TA1	C07-C08-C09	5.73	127.31	120.24
6	B	501	GDP	C5-C6-N1	4.48	124.67	113.25
6	B	501	GDP	N2-C2-N1	-4.23	107.83	116.76
6	B	501	GDP	C2-N3-C4	4.10	119.36	112.30
7	B	502	TA1	C05-C04-C03	-4.02	111.54	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	O6-C6-C5	-3.95	116.11	126.53
6	B	501	GDP	C4-C5-N7	-3.86	104.56	110.67
6	B	501	GDP	C2-N1-C6	-3.79	118.24	125.11
7	B	502	TA1	C09-C04-C03	3.64	128.41	120.40
6	B	501	GDP	C2'-C3'-C4'	3.40	109.17	102.61
7	B	502	TA1	C17-C18-C20	3.19	109.75	102.58
7	B	502	TA1	O04-C11-C14	-3.01	101.75	108.13
7	B	502	TA1	C45-C01-C02	2.95	115.17	111.93
6	B	501	GDP	C1'-N9-C8	-2.65	119.19	126.73
5	A	502	GTP	O2G-PG-O3B	2.65	113.52	104.64
7	B	502	TA1	O01-C01-C43	2.49	113.40	107.04
7	B	502	TA1	C14-C11-C15	-2.32	82.98	85.38
6	B	501	GDP	O2'-C2'-C3'	2.28	119.14	111.82
7	B	502	TA1	C08-C09-C04	-2.28	118.13	120.36
7	B	502	TA1	C10-C18-C17	-2.23	102.31	106.55
7	B	502	TA1	O06-C15-C11	2.18	92.96	90.58
5	A	502	GTP	O5'-C5'-C4'	2.10	116.14	108.99
6	B	501	GDP	C4'-O4'-C1'	2.05	114.00	109.47
5	A	502	GTP	O3G-PG-O3B	2.03	111.44	104.64
7	B	502	TA1	C21-O09-C22	2.01	120.10	115.95

There are no chirality outliers.

All (17) torsion outliers are listed below:

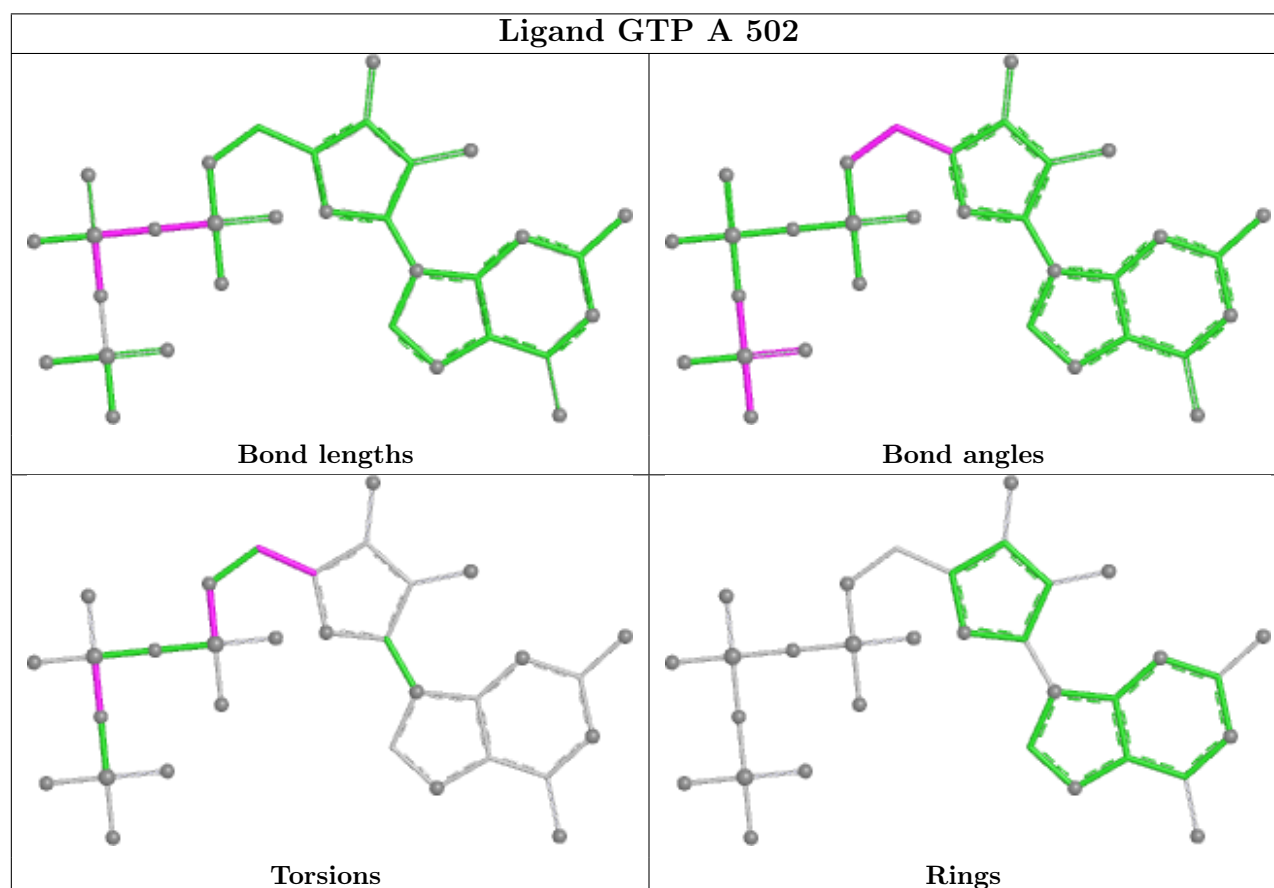
Mol	Chain	Res	Type	Atoms
6	B	501	GDP	PA-O3A-PB-O2B
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
7	B	502	TA1	O02-C03-C04-C05
7	B	502	TA1	O02-C03-C04-C09
7	B	502	TA1	O03-C03-C04-C09
7	B	502	TA1	O03-C03-C04-C05
7	B	502	TA1	N01-C30-C31-C36
7	B	502	TA1	O14-C30-C31-C36
7	B	502	TA1	N01-C30-C31-C32
7	B	502	TA1	O14-C30-C31-C32
5	A	502	GTP	C3'-C4'-C5'-O5'
5	A	502	GTP	C5'-O5'-PA-O1A
5	A	502	GTP	O4'-C4'-C5'-O5'
6	B	501	GDP	PA-O3A-PB-O3B
7	B	502	TA1	C15-C11-O04-C12
5	A	502	GTP	PG-O3B-PB-O2B

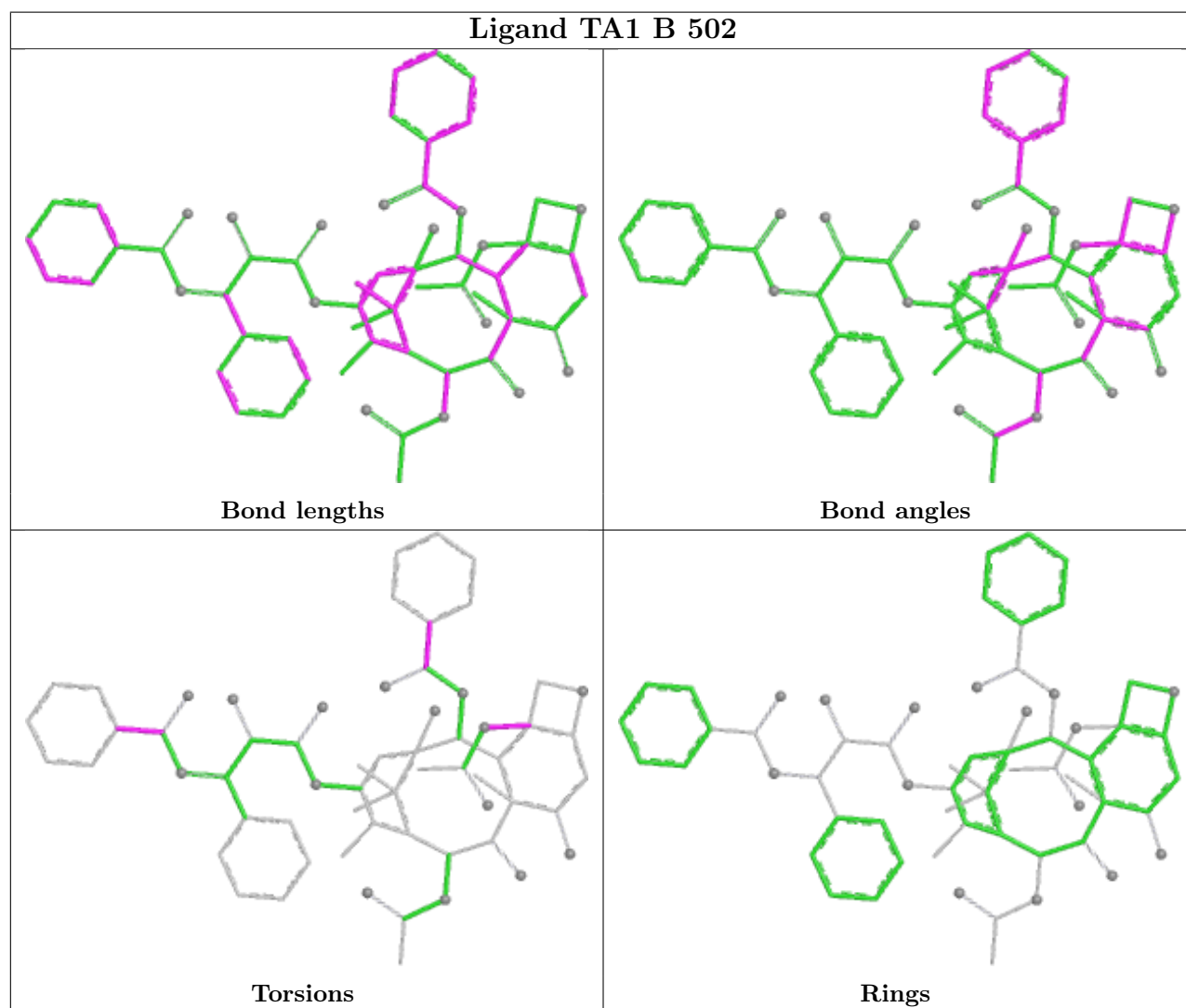
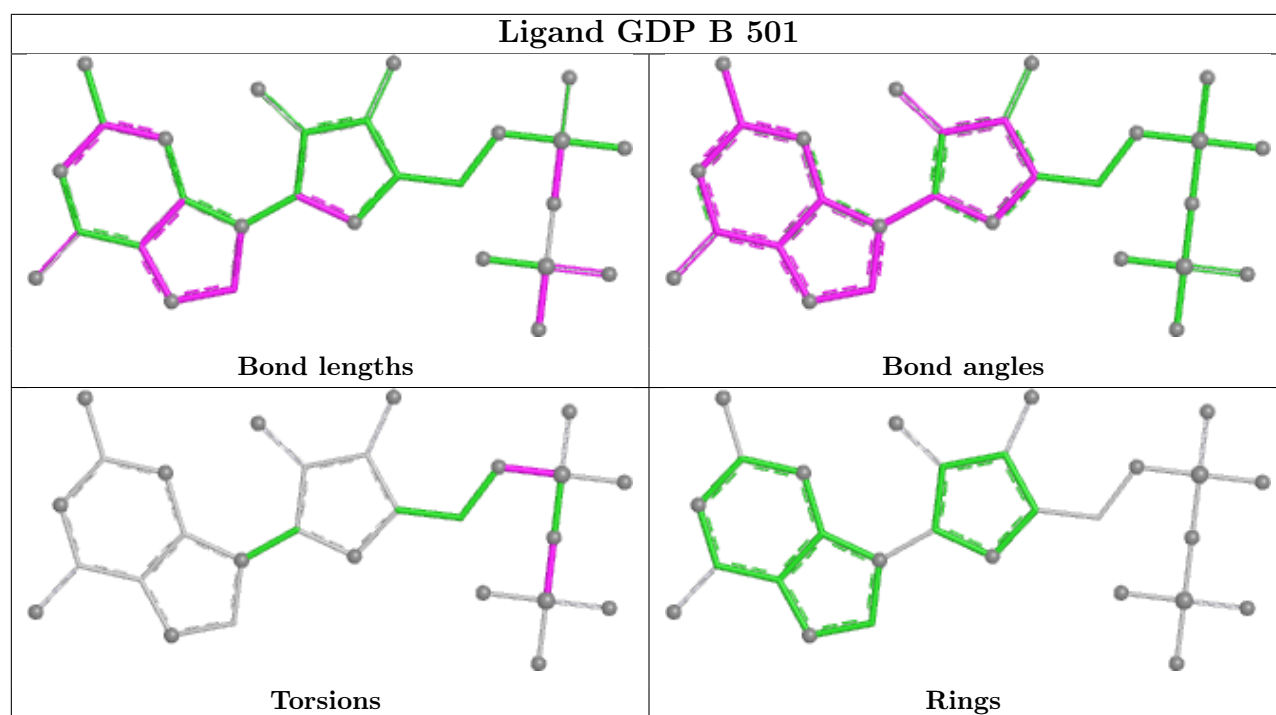
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	GTP	3	0
6	B	501	GDP	1	0
7	B	502	TA1	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](#)

There are no chain breaks in this entry.

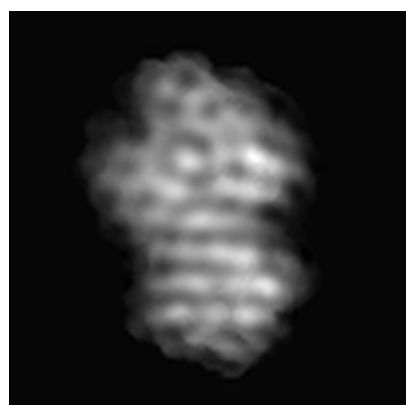
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5931. These allow visual inspection of the internal detail of the map and identification of artifacts.

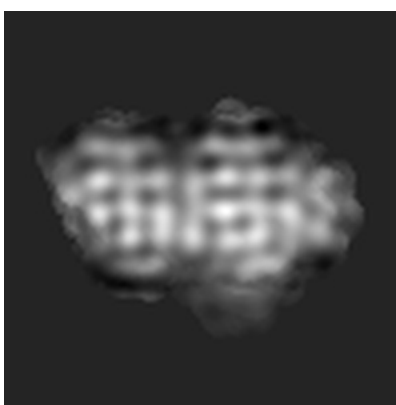
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

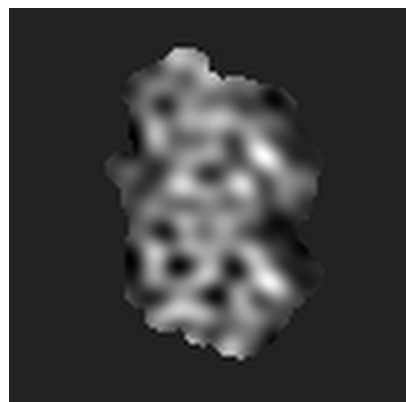


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 50



Y Index: 50

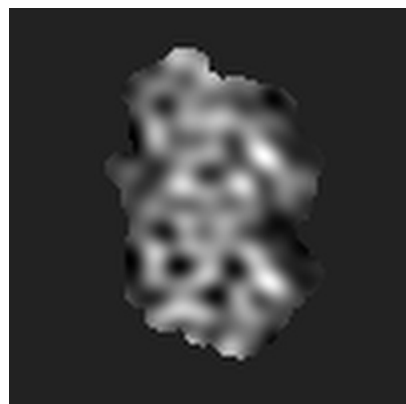


Z Index: 50

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

6.3 Largest variance slices [i](#)

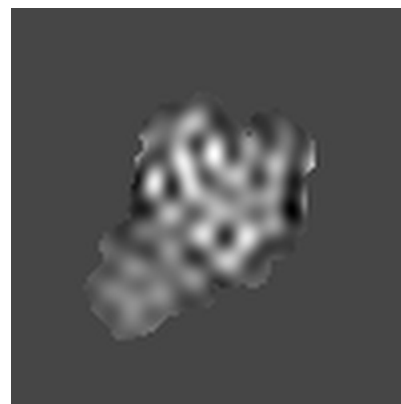
6.3.1 Primary map



X Index: 50



Y Index: 54



Z Index: 63

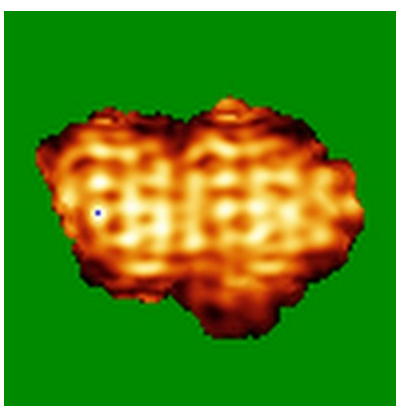
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y



Z

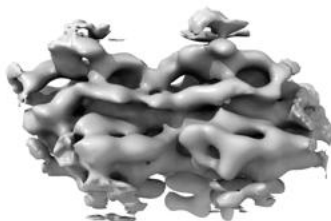
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

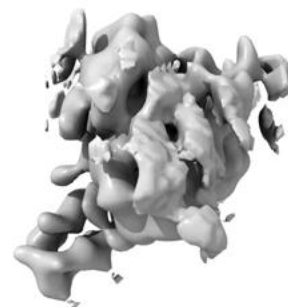
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

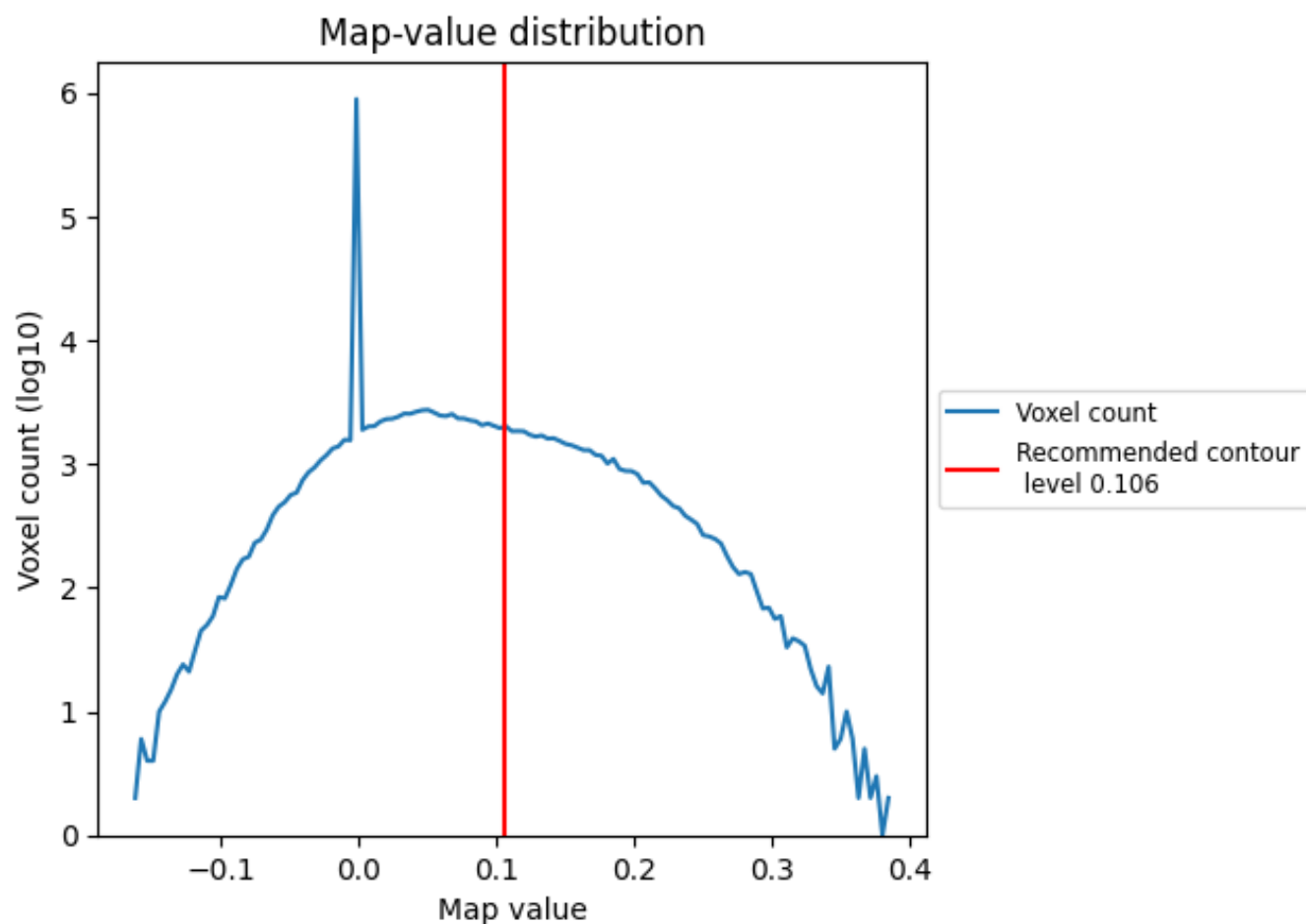
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

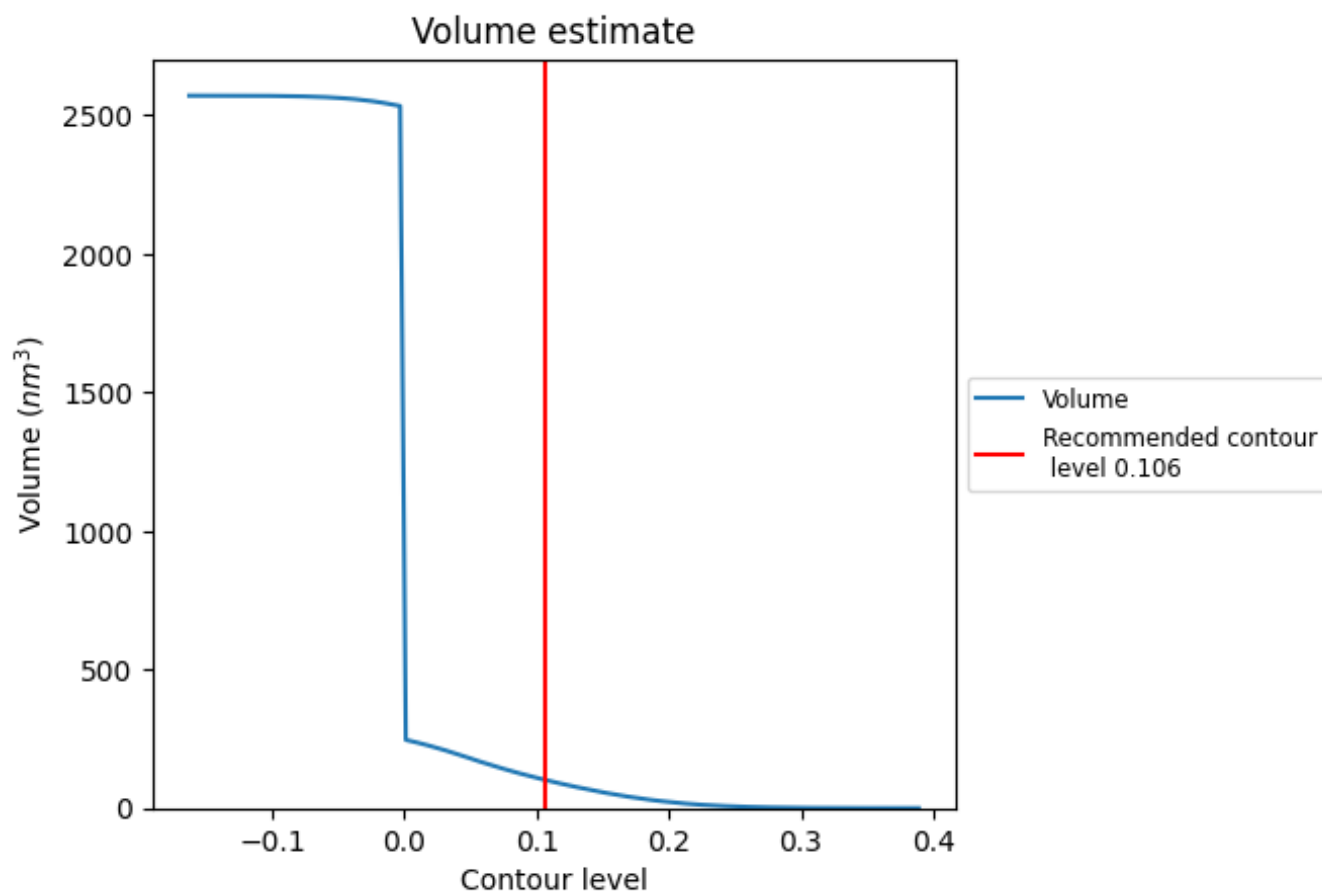
This section contains the results of statistical analysis of the map.

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.

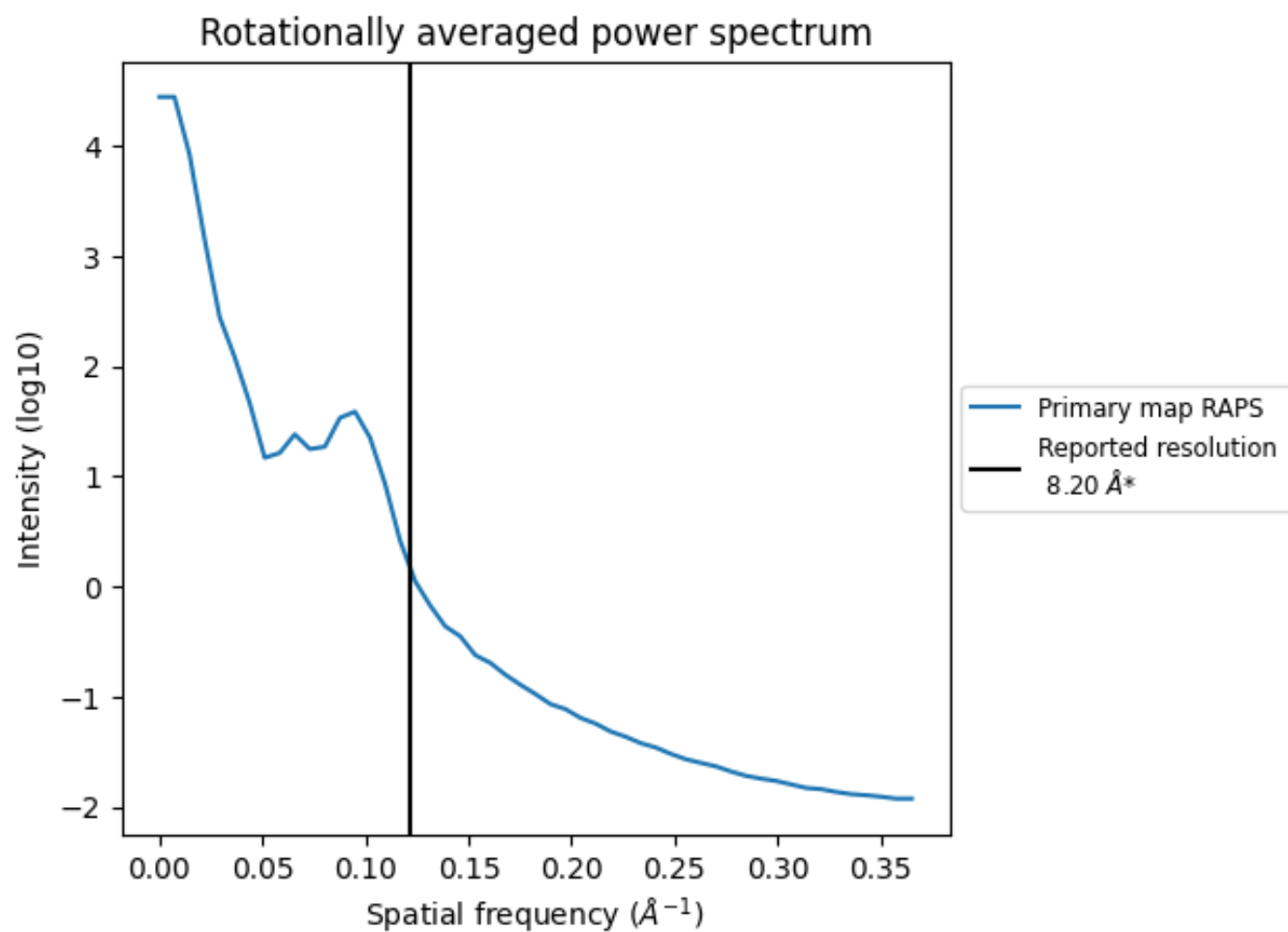
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm^3 ; this corresponds to an approximate mass of 93 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 0.122 Å⁻¹

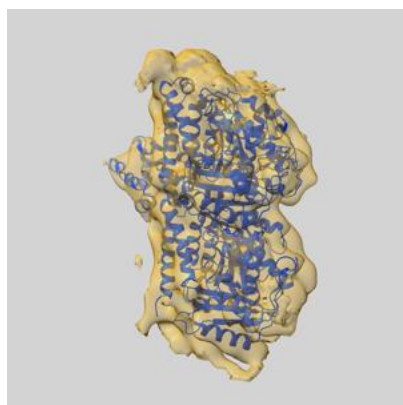
8 Fourier-Shell correlation

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

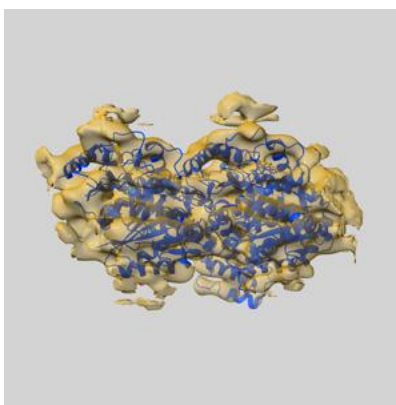
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5931 and PDB model 3J6P. Per-residue inclusion information can be found in section [3](#) on page [6](#).

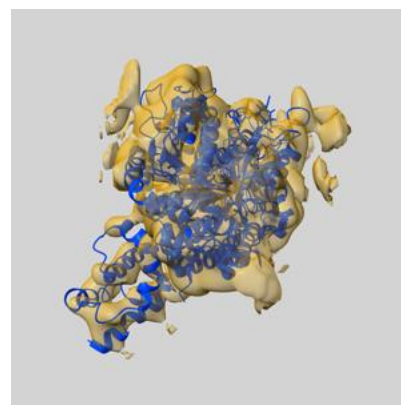
9.1 Map-model overlay [i](#)



X



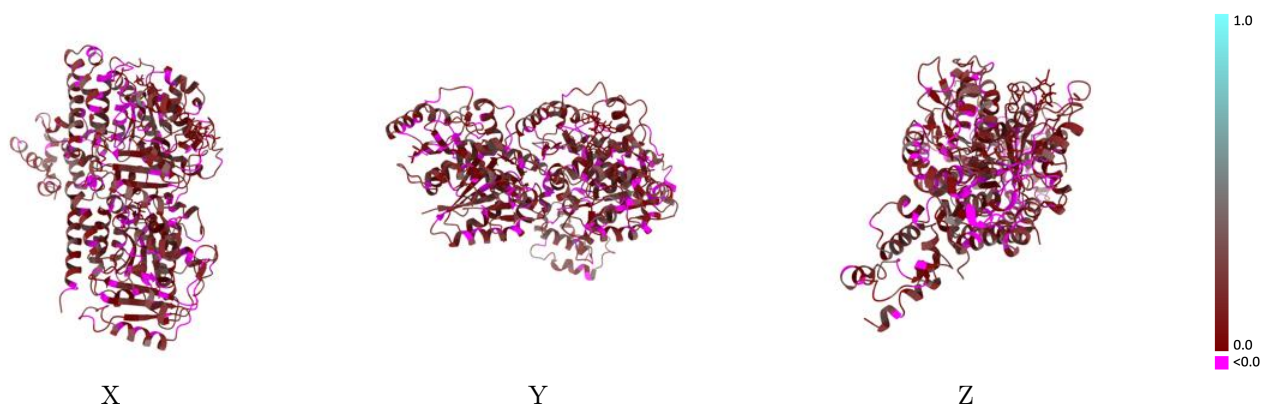
Y



Z

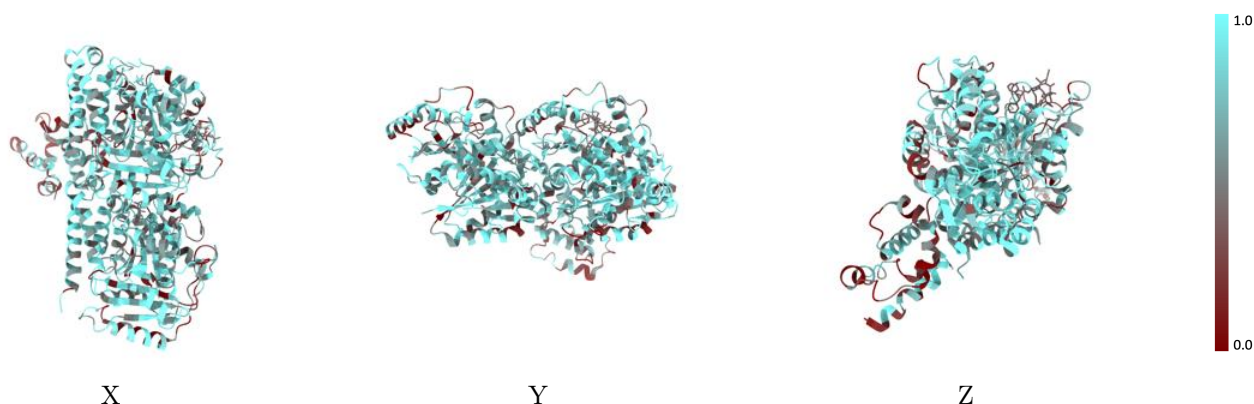
The images above show the 3D surface view of the map at the recommended contour level 0.106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



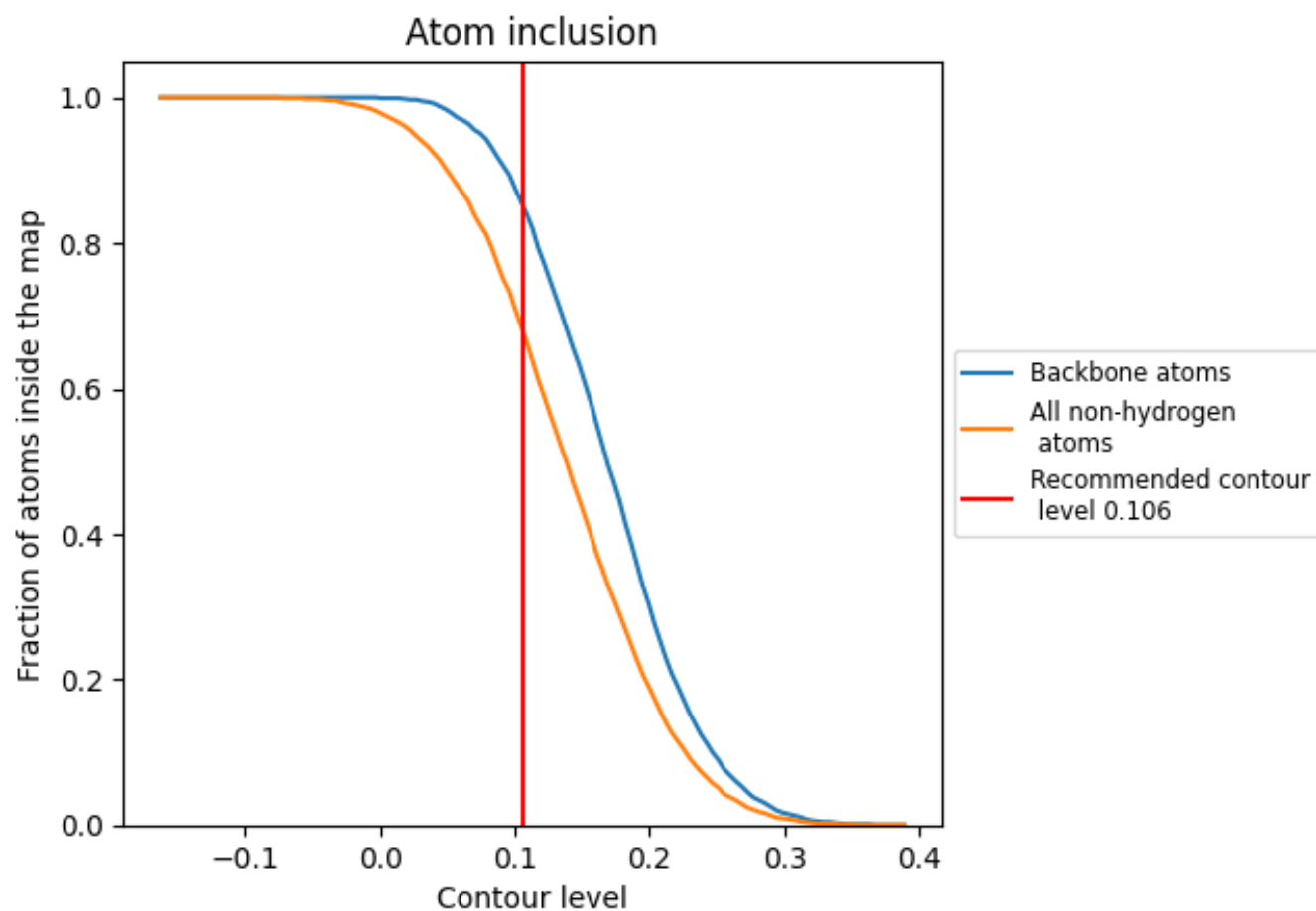
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.106).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 68% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6790	0.1140
A	0.6960	0.1060
B	0.7160	0.1140
D	0.4650	0.1430

