



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:20 AM UTC

PDB ID : 4ATX / pdb_00004atx
EMDB ID : EMD-2098
Title : Rigor kinesin motor domain with an ordered neck-linker, docked on tubulin dimer, modelled into the 8A cryo-EM map of doublecortin- microtubules decorated with kinesin
Authors : Liu, J.S.; Schubert, C.R.; Fu, X.; Fourniol, F.J.; Jaiswal, J.K.; Houdusse, A.; Stultz, C.M.; Moores, C.A.; Walsh, C.A.
Deposited on : 2012-05-10
Resolution : 8.20 Å(reported)
Based on initial models : 1BG2, 2XRP

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:

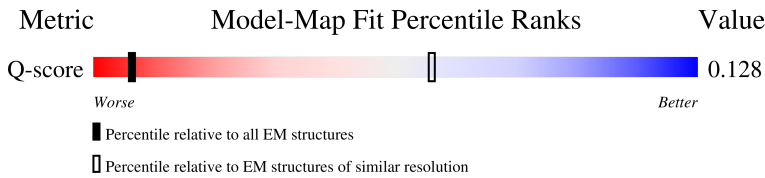
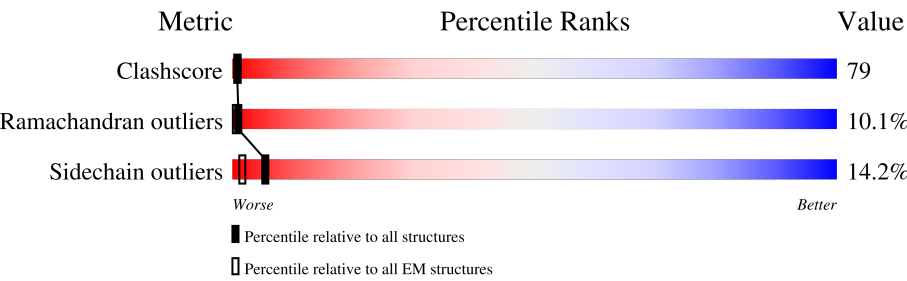
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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)

1 Overall quality at a glance i

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

The reported resolution of this entry is 8.20 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	A	445	10% 16% 56% 21% • •
2	B	452	10% 16% 56% 21% • 5%
3	C	340	17% 39% 44% 8% • 9%

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9183 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 TUBULIN BETA-2B CHAIN.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	THR	conflict	UNP Q6B856
A	172	VAL	MET	conflict	UNP Q6B856
A	298	ALA	SER	conflict	UNP Q6B856
A	318	VAL	ILE	conflict	UNP Q6B856

- Molecule 2 is a protein called TUBULIN ALPHA-1D CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3334	2114	569	630	21		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	ILE	VAL	conflict	UNP Q2HJ86
B	114	ILE	LEU	conflict	UNP Q2HJ86
B	136	SER	LEU	conflict	UNP Q2HJ86
B	137	VAL	ILE	conflict	UNP Q2HJ86
B	265	GLY	ILE	conflict	UNP Q2HJ86
B	358	GLU	GLN	conflict	UNP Q2HJ86
B	437	VAL	MET	conflict	UNP Q2HJ86
B	450	GLU	ASP	conflict	UNP Q2HJ86

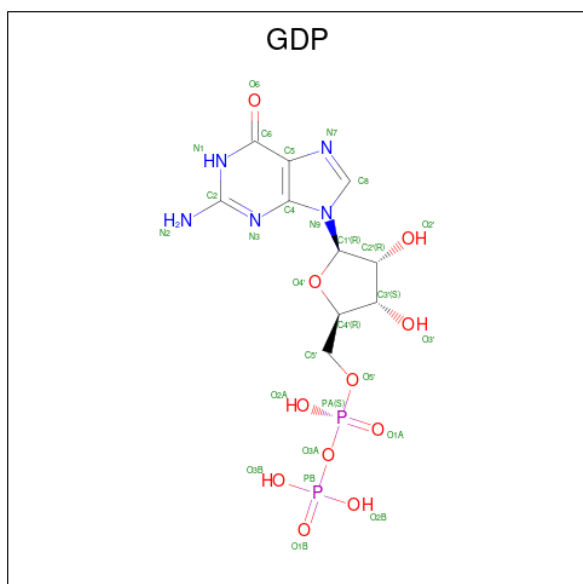
- Molecule 3 is a protein called KINESIN-1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	310	Total	C	N	O	S	0	1
			2438	1517	420	485	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	92	ASN	THR	engineered mutation	UNP Q2PQA9

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

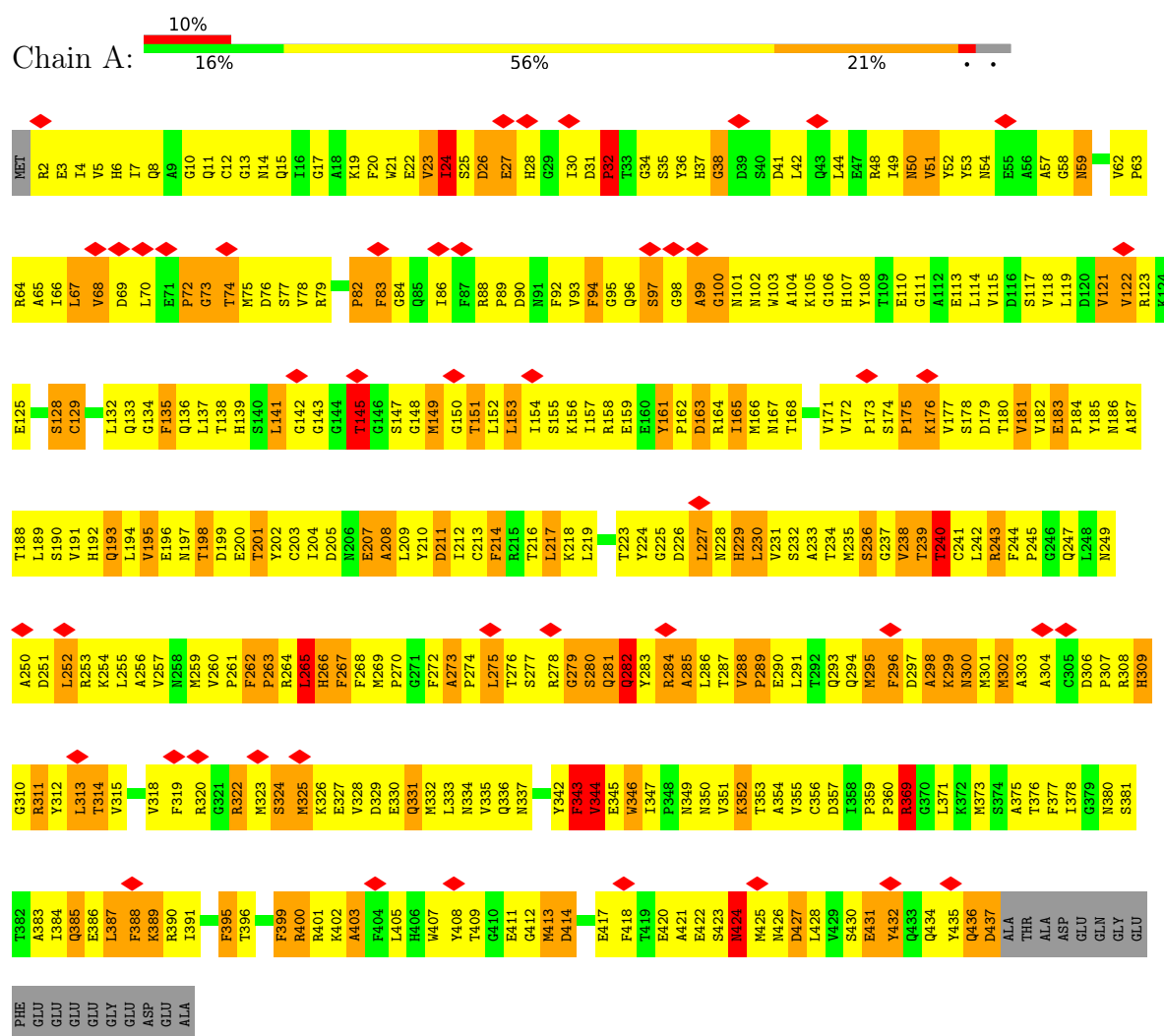


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	32	10	5	14	3	0

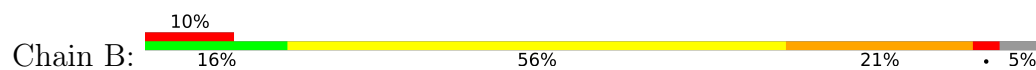
3 Residue-property plots

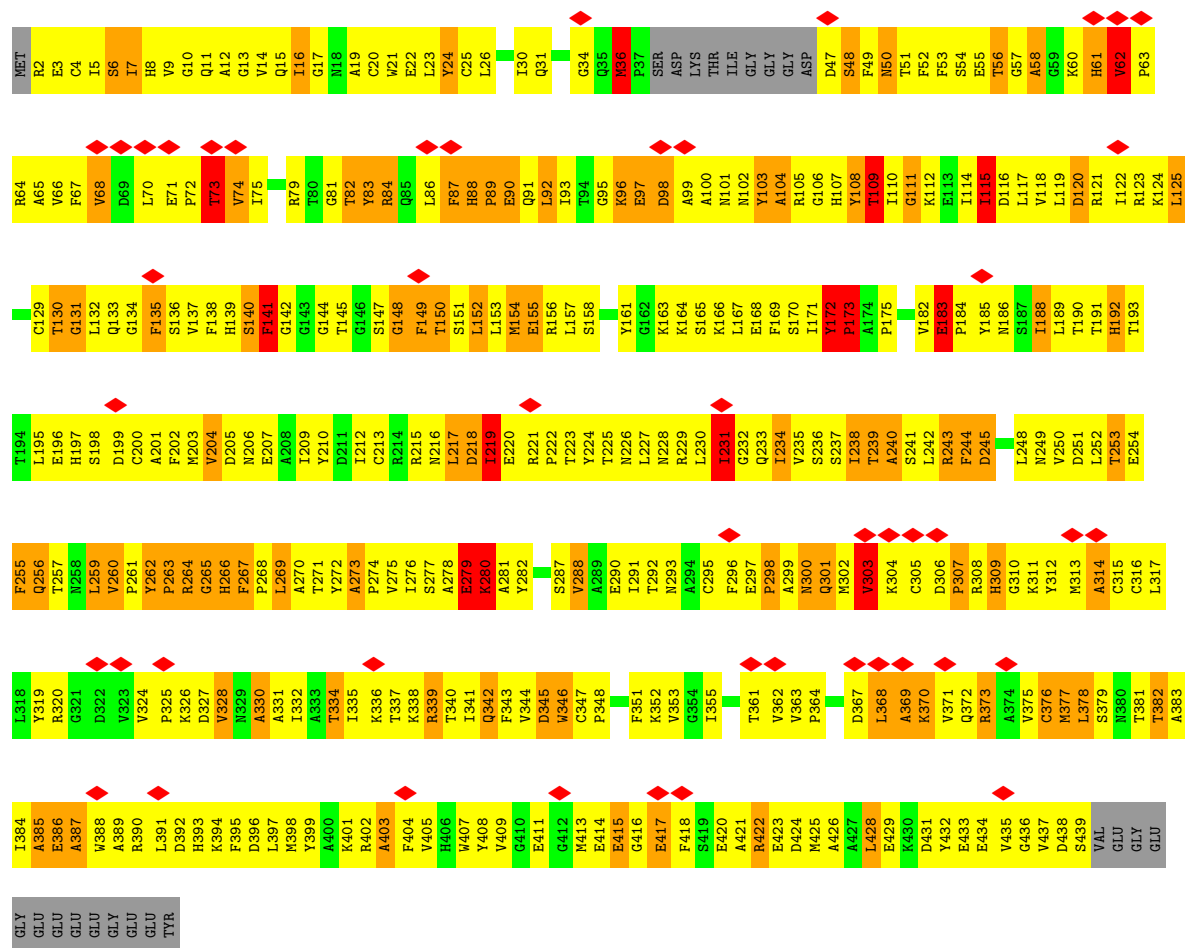
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: TUBULIN BETA-2B CHAIN

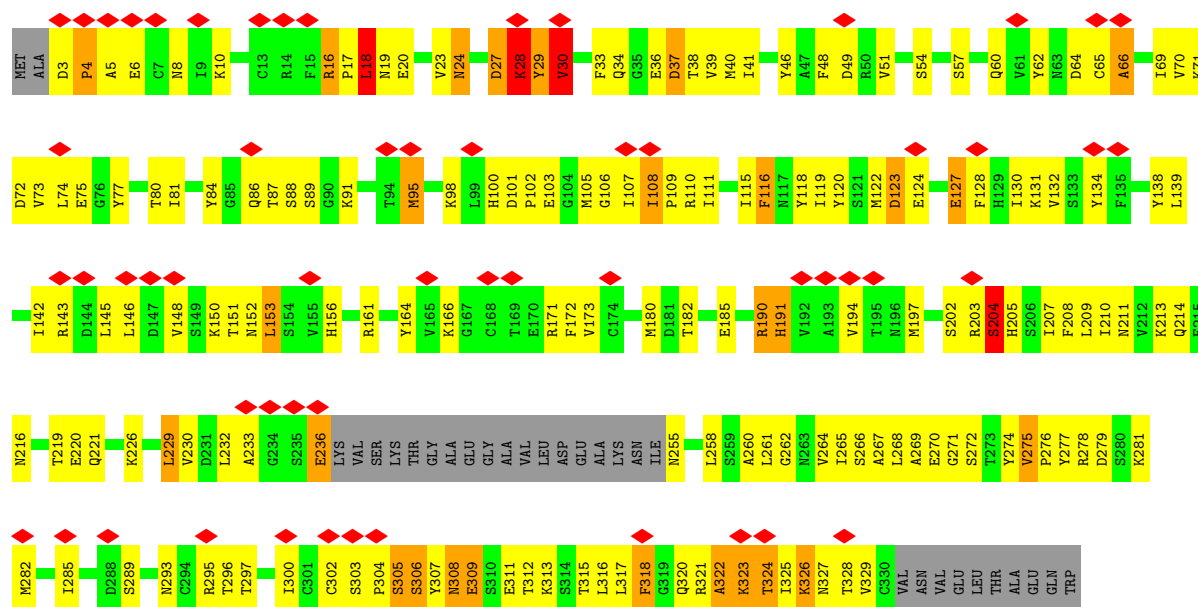


• Molecule 2: TUBULIN ALPHA-1D CHAIN





• Molecule 3: KINESIN-1 HEAVY CHAIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	168000	Depositor
Resolution determination method	Not provided	
CTF correction method	DONE WITH FREALIGN	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	760	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	11.104	Depositor
Minimum map value	-8.071	Depositor
Average map value	0.544	Depositor
Map value standard deviation	1.797	Depositor
Recommended contour level	1.55	Depositor
Map size (Å)	238.0, 140.0, 282.8	wwPDB
Map dimensions	85, 50, 101	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.8, 2.8, 2.8	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/3426	1.11	22/4642 (0.5%)
2	B	1.33	4/3410 (0.1%)	1.12	22/4629 (0.5%)
3	C	1.35	4/2477 (0.2%)	1.63	43/3339 (1.3%)
All	All	1.13	8/9313 (0.1%)	1.27	87/12610 (0.7%)

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
3	C	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	92	LEU	C-N	52.06	1.98	1.33
2	B	298	PRO	C-N	35.33	1.73	1.33
2	B	68	VAL	C-N	24.43	1.67	1.33
2	B	36	MET	SD-CE	7.60	1.98	1.79
3	C	108	ILE	CA-CB	-6.66	1.50	1.54
3	C	18	LEU	CA-C	-5.87	1.45	1.52
3	C	329	VAL	C-N	-5.25	1.26	1.33
3	C	327	ASN	CA-C	-5.06	1.46	1.53

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	307	TYR	CA-CB-CG	-12.24	91.87	113.90
2	B	68	VAL	O-C-N	-10.89	111.34	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	TYR	CA-C-N	10.70	133.22	119.84
2	B	172	TYR	C-N-CA	10.70	133.22	119.84
1	A	262	PHE	CA-C-N	10.01	132.36	119.84
1	A	262	PHE	C-N-CA	10.01	132.36	119.84
3	C	28	LYS	CA-C-N	-9.59	109.48	123.00
3	C	28	LYS	C-N-CA	-9.59	109.48	123.00
3	C	327	ASN	CA-CB-CG	-8.51	104.09	112.60
2	B	298	PRO	O-C-N	-7.92	111.94	122.64
1	A	77	SER	N-CA-C	-7.91	104.23	114.04
1	A	159	GLU	N-CA-C	-7.82	104.23	114.31
1	A	313	LEU	N-CA-C	-7.68	103.87	113.55
2	B	428	LEU	N-CA-C	-7.55	104.31	113.97
1	A	208	ALA	N-CA-C	-7.47	102.81	112.23
3	C	66	ALA	N-CA-C	7.44	120.84	111.69
1	A	293	GLN	N-CA-C	-7.38	102.92	110.97
3	C	103	GLU	CA-C-N	7.30	129.49	120.22
3	C	103	GLU	C-N-CA	7.30	129.49	120.22
3	C	116	PHE	CA-CB-CG	-7.15	106.65	113.80
1	A	385	GLN	N-CA-C	-7.08	103.49	111.14
1	A	388	PHE	N-CA-C	-6.99	104.01	112.54
1	A	22	GLU	N-CA-C	-6.98	103.37	110.97
2	B	301	GLN	N-CA-C	6.98	121.48	112.41
1	A	399	PHE	N-CA-C	-6.94	103.64	111.07
3	C	204	SER	CB-CA-C	-6.87	97.83	109.72
3	C	27	ASP	CA-CB-CG	-6.84	105.76	112.60
1	A	389	LYS	N-CA-C	-6.83	103.52	110.97
2	B	422	ARG	N-CA-C	-6.83	103.06	111.40
3	C	29	TYR	CA-CB-CG	-6.81	101.65	113.90
3	C	36	GLU	CB-CA-C	-6.76	99.35	110.85
3	C	309	GLU	N-CA-C	-6.72	104.03	111.36
2	B	385	ALA	N-CA-C	-6.69	103.24	111.33
2	B	188	ILE	N-CA-C	-6.68	103.20	113.16
3	C	190	ARG	CA-C-N	6.66	129.75	120.29
3	C	190	ARG	C-N-CA	6.66	129.75	120.29
2	B	92	LEU	O-C-N	6.57	129.61	122.64
2	B	123	ARG	N-CA-C	-6.49	105.94	114.31
3	C	30	VAL	CA-C-N	-6.47	114.08	123.00
3	C	30	VAL	C-N-CA	-6.47	114.08	123.00
1	A	217	LEU	N-CA-C	-6.44	96.47	107.23
1	A	27	GLU	N-CA-C	-6.23	106.04	113.21
3	C	304	PRO	O-C-N	6.14	130.78	122.37
3	C	191	HIS	CB-CA-C	-6.13	100.43	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	30	VAL	N-CA-C	6.11	116.16	110.42
1	A	181	VAL	N-CA-C	6.07	116.82	111.90
1	A	243	ARG	N-CA-C	-6.01	106.60	112.97
1	A	88	ARG	N-CA-C	-6.00	102.21	109.83
3	C	322	ALA	CA-C-N	-5.97	114.48	122.72
3	C	322	ALA	C-N-CA	-5.97	114.48	122.72
3	C	324	THR	CA-C-N	-5.92	114.44	122.91
3	C	324	THR	C-N-CA	-5.92	114.44	122.91
2	B	231	ILE	N-CA-C	-5.86	103.94	110.62
2	B	264	ARG	N-CA-C	-5.85	101.64	110.24
3	C	100	HIS	CA-CB-CG	-5.80	108.00	113.80
1	A	296	PHE	N-CA-C	5.73	119.90	113.02
1	A	247	GLN	N-CA-C	-5.72	105.04	111.28
3	C	128	PHE	CA-CB-CG	-5.64	108.16	113.80
2	B	415	GLU	N-CA-C	-5.59	105.56	112.38
2	B	262	TYR	CA-C-N	5.57	126.81	119.84
2	B	262	TYR	C-N-CA	5.57	126.81	119.84
3	C	36	GLU	CB-CG-CD	-5.57	103.14	112.60
3	C	24	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	59	ASN	N-CA-C	-5.48	105.60	114.09
2	B	259	LEU	N-CA-C	5.48	120.98	113.97
2	B	280	LYS	N-CA-C	-5.43	106.16	112.89
3	C	33	PHE	CA-CB-CG	-5.42	108.38	113.80
3	C	308	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	436	GLN	N-CA-C	-5.35	106.44	112.87
2	B	429	GLU	N-CA-C	-5.34	105.90	112.90
3	C	64	ASP	CA-CB-CG	-5.28	107.33	112.60
3	C	19	ASN	CA-CB-CG	-5.26	107.33	112.60
3	C	271	GLY	N-CA-C	-5.26	107.53	115.32
3	C	65	CYS	N-CA-C	5.21	117.97	111.24
3	C	323	LYS	CA-C-O	5.18	126.08	120.43
1	A	289	PRO	N-CA-C	-5.17	107.12	113.84
3	C	37	ASP	N-CA-C	5.17	119.64	113.23
3	C	18	LEU	CB-CA-C	-5.12	100.03	109.46
2	B	421	ALA	N-CA-C	-5.11	107.07	113.72
2	B	89	PRO	N-CA-C	-5.10	106.42	113.81
3	C	318	PHE	CA-CB-CG	-5.08	108.72	113.80
2	B	140	SER	N-CA-C	5.06	116.30	109.11
3	C	18	LEU	N-CA-CB	5.03	117.94	110.29
3	C	275	VAL	CA-C-N	5.03	126.13	119.84
3	C	275	VAL	C-N-CA	5.03	126.13	119.84
3	C	123	ASP	CA-CB-CG	-5.02	107.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	108	ILE	CB-CA-C	-5.02	107.43	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	16	ARG	Sidechain
3	C	27	ASP	Peptide
3	C	28	LYS	Peptide
3	C	30	VAL	Peptide
3	C	305	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3351	0	3229	587	0
2	B	3334	0	3223	667	0
3	C	2438	0	2397	192	0
4	A	28	0	12	1	0
5	B	32	0	12	5	0
All	All	9183	0	8873	1422	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 79.

All (1422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:PHE:CE1	2:B:341:ILE:HD11	1.32	1.63
2:B:298:PRO:C	2:B:299:ALA:N	1.73	1.44
2:B:5:ILE:HG12	2:B:64:ARG:NH1	1.27	1.42
2:B:57:GLY:HA3	2:B:58:ALA:CB	1.45	1.42
2:B:3:GLU:CG	2:B:51:THR:HA	1.57	1.34
2:B:296:PHE:CE1	2:B:341:ILE:CD1	2.11	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:PRO:HG2	2:B:91:GLN:OE1	1.29	1.31
2:B:3:GLU:HG2	2:B:51:THR:CA	1.60	1.29
2:B:57:GLY:CA	2:B:58:ALA:HB2	1.63	1.28
1:A:264:ARG:HD3	3:C:278:ARG:NH2	1.45	1.27
2:B:62:VAL:CG1	2:B:63:PRO:HD2	1.67	1.23
1:A:264:ARG:NH1	3:C:278:ARG:NE	1.89	1.21
2:B:92:LEU:C	2:B:93:ILE:N	1.98	1.21
2:B:5:ILE:CG1	2:B:64:ARG:NH1	2.05	1.20
2:B:217:LEU:HD12	2:B:277:SER:CB	1.72	1.16
2:B:62:VAL:HG12	2:B:63:PRO:CD	1.76	1.15
2:B:5:ILE:CD1	2:B:64:ARG:HH12	1.57	1.15
2:B:70:LEU:HD13	2:B:145:THR:OG1	1.49	1.13
2:B:296:PHE:CE2	2:B:335:ILE:HG21	1.84	1.13
1:A:234:THR:HG21	1:A:270:PRO:HB2	1.23	1.12
2:B:243:ARG:NH2	2:B:252:LEU:H	1.45	1.12
2:B:30:ILE:HG12	2:B:36:MET:HB3	1.19	1.10
2:B:67:PHE:HE2	2:B:87:PHE:CE2	1.68	1.10
2:B:274:PRO:C	2:B:275:VAL:N	2.09	1.10
1:A:93:VAL:HG11	1:A:118:VAL:HG22	1.30	1.08
2:B:298:PRO:HB3	2:B:307:PRO:HD2	1.36	1.06
2:B:11:GLN:HG3	2:B:74:VAL:HG11	1.34	1.05
1:A:172:VAL:HG11	1:A:387:LEU:HD21	1.37	1.05
2:B:109:THR:HG22	2:B:110:ILE:N	1.71	1.05
2:B:296:PHE:CD1	2:B:341:ILE:CD1	2.40	1.04
2:B:217:LEU:CD1	2:B:277:SER:HB3	1.87	1.04
2:B:67:PHE:CE2	2:B:87:PHE:CE2	2.45	1.04
2:B:63:PRO:HG2	2:B:91:GLN:CD	1.85	1.02
1:A:299:LYS:H	1:A:299:LYS:HD3	1.24	1.02
1:A:264:ARG:HD3	3:C:278:ARG:CZ	1.88	1.02
3:C:219:THR:HG22	3:C:221:GLN:HG2	1.36	1.02
2:B:56:THR:O	2:B:58:ALA:HB3	1.59	1.02
1:A:236:SER:O	1:A:240:THR:HG23	1.61	1.01
2:B:243:ARG:HH21	2:B:252:LEU:N	1.57	1.01
2:B:5:ILE:HG12	2:B:64:ARG:CZ	1.90	1.00
2:B:5:ILE:CG1	2:B:64:ARG:HH12	1.67	1.00
2:B:88:HIS:HB2	2:B:91:GLN:HE21	1.22	1.00
2:B:52:PHE:HZ	2:B:239:THR:HG21	1.27	0.99
2:B:276:ILE:HG23	2:B:369:ALA:HB2	1.43	0.99
2:B:30:ILE:HD11	2:B:61:HIS:CE1	1.97	0.99
2:B:296:PHE:HE1	2:B:341:ILE:HD11	1.21	0.99
3:C:98:LYS:HD3	3:C:101:ASP:HB2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:HE3	1:A:351:VAL:HG11	1.45	0.98
3:C:134:TYR:CD1	3:C:145:LEU:HD12	1.98	0.97
3:C:17:PRO:HA	3:C:54:SER:HB3	1.48	0.95
2:B:57:GLY:CA	2:B:58:ALA:CB	2.30	0.95
2:B:62:VAL:HG12	2:B:63:PRO:HD2	0.97	0.95
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.48	0.95
1:A:281:GLN:O	1:A:283:TYR:N	2.00	0.95
2:B:278:ALA:O	2:B:279:GLU:HB3	1.66	0.95
2:B:316:CYS:HB3	2:B:378:LEU:HD11	1.49	0.95
1:A:264:ARG:NH1	3:C:278:ARG:CZ	2.30	0.94
2:B:251:ASP:N	2:B:254:GLU:HG3	1.82	0.94
2:B:259:LEU:HD11	2:B:378:LEU:HD13	1.47	0.94
2:B:98:ASP:HB2	2:B:105:ARG:HH21	1.31	0.94
2:B:217:LEU:HD12	2:B:277:SER:HB3	0.95	0.93
2:B:251:ASP:H	2:B:254:GLU:HG3	1.33	0.93
2:B:237:SER:HB2	2:B:376:CYS:SG	2.08	0.93
1:A:132:LEU:HD23	1:A:164:ARG:HG3	1.50	0.93
1:A:70:LEU:H	1:A:145:THR:HG21	1.33	0.92
2:B:70:LEU:CD1	2:B:145:THR:OG1	2.18	0.91
2:B:151:SER:HB3	2:B:193:THR:HG21	1.51	0.91
1:A:147:SER:O	1:A:151:THR:HB	1.71	0.91
3:C:219:THR:CG2	3:C:221:GLN:HG2	2.00	0.90
2:B:55:GLU:O	2:B:57:GLY:N	2.04	0.90
2:B:30:ILE:CD1	2:B:61:HIS:ND1	2.34	0.90
1:A:264:ARG:O	1:A:265:LEU:HB3	1.69	0.90
2:B:52:PHE:CE1	2:B:239:THR:HB	2.07	0.90
2:B:30:ILE:CG1	2:B:36:MET:HB3	2.02	0.90
2:B:63:PRO:CG	2:B:91:GLN:OE1	2.20	0.90
2:B:343:PHE:CZ	2:B:351:PHE:CE2	2.61	0.89
1:A:102:ASN:HD21	1:A:408:TYR:HA	1.38	0.89
2:B:110:ILE:HG23	2:B:111:GLY:H	1.38	0.89
3:C:208:PHE:HE2	3:C:210:ILE:HD11	1.38	0.89
2:B:296:PHE:CD1	2:B:341:ILE:HD11	2.03	0.88
2:B:147:SER:HB2	2:B:190:THR:OG1	1.73	0.88
1:A:8:GLN:OE1	1:A:67:LEU:HD22	1.73	0.88
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.08	0.88
2:B:109:THR:HG22	2:B:110:ILE:H	1.33	0.88
2:B:63:PRO:CD	2:B:87:PHE:HA	2.03	0.88
1:A:93:VAL:HG11	1:A:118:VAL:CG2	2.03	0.88
2:B:119:LEU:HD23	2:B:122:ILE:HD11	1.53	0.87
2:B:122:ILE:HD12	2:B:157:LEU:HD21	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:HD3	1:A:342:TYR:HA	1.56	0.87
2:B:30:ILE:CD1	2:B:61:HIS:CE1	2.57	0.87
1:A:323:MET:HE2	1:A:328:VAL:HG22	1.54	0.87
1:A:195:VAL:HG13	1:A:196:GLU:HG2	1.57	0.87
1:A:153:LEU:O	1:A:157:ILE:HG12	1.76	0.86
1:A:276:THR:HB	1:A:281:GLN:HG3	1.56	0.86
1:A:6:HIS:CE1	1:A:8:GLN:HG2	2.10	0.86
1:A:101:ASN:HD21	1:A:143:GLY:HA2	1.38	0.86
2:B:296:PHE:CD1	2:B:341:ILE:HD12	2.08	0.86
1:A:19:LYS:HG3	1:A:228:ASN:HB3	1.57	0.86
2:B:63:PRO:HD3	2:B:87:PHE:HA	1.56	0.86
2:B:52:PHE:CZ	2:B:239:THR:HG21	2.11	0.86
2:B:220:GLU:C	2:B:222:PRO:HD3	2.02	0.85
1:A:10:GLY:HA2	1:A:145:THR:HB	1.55	0.85
2:B:264:ARG:O	2:B:266:HIS:N	2.09	0.85
1:A:242:LEU:HD22	1:A:250:ALA:H	1.41	0.85
1:A:360:PRO:HG2	1:A:371:LEU:HB3	1.56	0.85
1:A:4:ILE:HD13	1:A:136:GLN:HE21	1.42	0.84
2:B:234:ILE:HG13	2:B:270:ALA:HB1	1.59	0.84
3:C:48:PHE:CZ	3:C:316:LEU:HD22	2.13	0.84
1:A:234:THR:HG21	1:A:270:PRO:CB	2.06	0.84
1:A:20:PHE:CD1	1:A:235:MET:SD	2.71	0.84
1:A:209:LEU:HB3	1:A:227:LEU:HD22	1.59	0.84
2:B:264:ARG:HB2	2:B:266:HIS:CD2	2.13	0.84
1:A:191:VAL:HG11	1:A:425:MET:HG3	1.60	0.83
2:B:204:VAL:HG11	2:B:231:ILE:HD12	1.59	0.83
1:A:3:GLU:O	1:A:133:GLN:HB3	1.78	0.83
1:A:264:ARG:CD	3:C:278:ARG:CZ	2.55	0.83
1:A:287:THR:O	1:A:288:VAL:HG23	1.79	0.83
2:B:172:TYR:HD1	2:B:172:TYR:C	1.87	0.83
1:A:148:GLY:O	1:A:151:THR:HG22	1.79	0.83
1:A:324:SER:HB3	1:A:327:GLU:HG2	1.60	0.83
2:B:23:LEU:HD23	2:B:236:SER:HB2	1.60	0.83
2:B:217:LEU:CD1	2:B:277:SER:CA	2.56	0.83
2:B:316:CYS:HB3	2:B:378:LEU:CD1	2.08	0.83
1:A:150:GLY:HA2	1:A:153:LEU:HD22	1.60	0.83
2:B:106:GLY:O	2:B:111:GLY:HA3	1.78	0.83
1:A:156:LYS:HE2	1:A:156:LYS:HA	1.61	0.82
1:A:110:GLU:O	1:A:113:GLU:HG2	1.79	0.82
1:A:101:ASN:ND2	1:A:143:GLY:HA2	1.94	0.82
1:A:147:SER:HB2	1:A:190:SER:HB3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:PHE:CZ	2:B:239:THR:HB	2.14	0.82
2:B:151:SER:CB	2:B:193:THR:HG21	2.09	0.82
3:C:180:MET:HA	3:C:180:MET:HE2	1.61	0.82
3:C:108:ILE:HB	3:C:109:PRO:HD3	1.62	0.82
2:B:276:ILE:HG23	2:B:369:ALA:CB	2.10	0.81
2:B:248:LEU:HD23	2:B:353:VAL:O	1.80	0.81
1:A:20:PHE:CZ	1:A:24:ILE:HD12	2.15	0.81
2:B:67:PHE:CE2	2:B:87:PHE:HE2	1.96	0.81
2:B:6:SER:HB3	2:B:136:SER:OG	1.81	0.81
2:B:109:THR:CG2	2:B:110:ILE:N	2.44	0.81
3:C:138:TYR:CD2	3:C:139:LEU:HD23	2.15	0.80
2:B:70:LEU:CD1	2:B:145:THR:HG23	2.12	0.80
2:B:184:PRO:HG2	2:B:398:MET:HE1	1.64	0.80
2:B:217:LEU:CD1	2:B:277:SER:CB	2.55	0.80
1:A:236:SER:O	1:A:240:THR:CG2	2.29	0.80
2:B:234:ILE:HD13	2:B:234:ILE:O	1.81	0.80
2:B:132:LEU:H	2:B:132:LEU:HD23	1.46	0.80
2:B:241:SER:O	2:B:244:PHE:HB3	1.82	0.80
1:A:68:VAL:HG12	1:A:149:MET:SD	2.22	0.80
2:B:7:ILE:HG22	2:B:66:VAL:HG22	1.63	0.79
2:B:52:PHE:HZ	2:B:239:THR:CG2	1.94	0.79
1:A:264:ARG:HB2	1:A:266:HIS:HD2	1.45	0.79
1:A:413:MET:HG3	1:A:414:ASP:H	1.47	0.79
3:C:16:ARG:HG2	3:C:17:PRO:HD2	1.63	0.79
1:A:259:MET:HA	1:A:314:THR:HG21	1.65	0.79
2:B:313:MET:HB3	2:B:344:VAL:HG21	1.63	0.79
1:A:54:ASN:HD21	1:A:64:ARG:HD3	1.46	0.79
3:C:86:GLN:HB2	3:C:311:GLU:HG2	1.64	0.79
1:A:396:THR:HG23	1:A:422:GLU:OE2	1.83	0.78
1:A:8:GLN:CD	1:A:67:LEU:HD22	2.08	0.78
1:A:265:LEU:HD12	1:A:265:LEU:O	1.83	0.78
2:B:67:PHE:HE2	2:B:87:PHE:CD2	2.00	0.78
2:B:199:ASP:HB3	2:B:256:GLN:NE2	1.99	0.78
3:C:131:LYS:HG2	3:C:172:PHE:CE1	2.18	0.78
2:B:56:THR:O	2:B:58:ALA:CB	2.30	0.78
2:B:204:VAL:HG13	2:B:209:ILE:HD11	1.66	0.78
1:A:242:LEU:HD13	1:A:250:ALA:C	2.09	0.78
1:A:205:ASP:OD2	1:A:304:ALA:HB2	1.84	0.78
2:B:110:ILE:HG23	2:B:111:GLY:N	1.99	0.78
3:C:3:ASP:HB2	3:C:4:PRO:HD3	1.64	0.78
3:C:71:LYS:O	3:C:71:LYS:HD3	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:CG2	1:A:270:PRO:HB2	2.11	0.78
2:B:52:PHE:CZ	2:B:239:THR:CB	2.67	0.78
2:B:264:ARG:C	2:B:266:HIS:H	1.91	0.78
1:A:35:SER:HB3	1:A:59:ASN:HA	1.65	0.77
1:A:264:ARG:HH11	3:C:278:ARG:CZ	1.97	0.77
2:B:267:PHE:N	2:B:267:PHE:CD1	2.49	0.77
2:B:11:GLN:HE21	2:B:74:VAL:HG22	1.47	0.77
2:B:217:LEU:CD1	2:B:277:SER:HA	2.13	0.77
2:B:223:THR:HB	2:B:225:THR:HG22	1.67	0.77
2:B:11:GLN:HG3	2:B:74:VAL:CG1	2.15	0.77
2:B:52:PHE:CZ	2:B:239:THR:CG2	2.66	0.77
2:B:155:GLU:HA	2:B:197:HIS:ND1	1.99	0.77
3:C:5:ALA:HB3	3:C:8:ASN:OD1	1.83	0.77
3:C:138:TYR:HE1	3:C:203:ARG:HB3	1.48	0.77
3:C:267:ALA:O	3:C:270:GLU:HG2	1.85	0.77
2:B:30:ILE:HD13	2:B:61:HIS:CG	2.20	0.77
2:B:296:PHE:CZ	2:B:335:ILE:HG21	2.18	0.77
2:B:221:ARG:O	2:B:221:ARG:HD3	1.85	0.77
2:B:231:ILE:HA	2:B:234:ILE:HG22	1.66	0.77
2:B:225:THR:O	2:B:229:ARG:HG3	1.86	0.76
1:A:198:THR:O	1:A:265:LEU:HD22	1.85	0.76
2:B:67:PHE:HD2	2:B:92:LEU:HD23	1.49	0.76
2:B:7:ILE:HD12	2:B:153:LEU:HD21	1.68	0.76
3:C:138:TYR:HE1	3:C:203:ARG:CB	1.99	0.76
1:A:217:LEU:C	1:A:219:LEU:H	1.91	0.76
2:B:276:ILE:O	2:B:369:ALA:HB2	1.84	0.76
1:A:325:MET:HE1	1:A:355:VAL:HG11	1.67	0.76
1:A:168:THR:HB	1:A:201:THR:HG23	1.68	0.76
1:A:259:MET:HG2	1:A:314:THR:HG21	1.67	0.75
2:B:331:ALA:O	2:B:335:ILE:HG12	1.86	0.75
2:B:5:ILE:CD1	2:B:64:ARG:NH1	2.38	0.75
2:B:172:TYR:C	2:B:172:TYR:CD1	2.61	0.75
2:B:381:THR:C	2:B:383:ALA:H	1.95	0.75
2:B:62:VAL:CG1	2:B:63:PRO:CD	2.50	0.75
2:B:70:LEU:CD1	2:B:145:THR:CG2	2.64	0.75
1:A:19:LYS:HG3	1:A:228:ASN:CB	2.17	0.75
2:B:296:PHE:CE1	2:B:341:ILE:HD12	2.20	0.75
2:B:167:LEU:HG	2:B:200:CYS:HB3	1.68	0.75
2:B:344:VAL:HG11	2:B:346:TRP:CE2	2.21	0.75
1:A:192:HIS:ND1	1:A:424:ASN:OD1	2.18	0.74
2:B:3:GLU:HG2	2:B:51:THR:HA	0.80	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LYS:O	2:B:164:LYS:HG2	1.86	0.74
1:A:176:LYS:HE3	1:A:207:GLU:HG3	1.68	0.74
2:B:5:ILE:CG1	2:B:64:ARG:CZ	2.56	0.74
2:B:205:ASP:CB	2:B:303:VAL:HA	2.17	0.74
2:B:317:LEU:HB3	2:B:319:TYR:HE1	1.52	0.74
1:A:103:TRP:CZ3	1:A:108:TYR:HE1	2.05	0.74
1:A:6:HIS:HE1	1:A:8:GLN:HG2	1.52	0.73
2:B:104:ALA:CB	2:B:413:MET:HG3	2.18	0.73
2:B:362:VAL:HG13	2:B:368:LEU:HD12	1.68	0.73
2:B:4:CYS:SG	2:B:252:LEU:HD11	2.27	0.73
2:B:172:TYR:OH	2:B:387:ALA:HB1	1.87	0.73
2:B:243:ARG:HH21	2:B:252:LEU:H	0.79	0.73
2:B:103:TYR:CD2	2:B:189:LEU:HD13	2.24	0.73
2:B:104:ALA:HB2	2:B:413:MET:HG3	1.71	0.73
1:A:250:ALA:HA	1:A:254:LYS:HE2	1.68	0.73
1:A:274:PRO:HG2	1:A:371:LEU:HD21	1.70	0.73
2:B:70:LEU:HD11	2:B:145:THR:HG23	1.70	0.73
2:B:112:LYS:O	2:B:115:ILE:HG22	1.89	0.73
2:B:7:ILE:HD11	2:B:137:VAL:HG22	1.71	0.73
1:A:76:ASP:HA	1:A:79:ARG:HG2	1.71	0.73
1:A:111:GLY:O	1:A:115:VAL:HG23	1.89	0.73
1:A:209:LEU:HG	1:A:230:LEU:HD22	1.69	0.73
2:B:306:ASP:O	2:B:308:ARG:N	2.20	0.73
1:A:217:LEU:O	1:A:219:LEU:N	2.22	0.72
1:A:264:ARG:HD3	3:C:278:ARG:HH22	1.48	0.72
2:B:154:MET:HE1	2:B:166:LYS:HB3	1.70	0.72
2:B:242:LEU:HG	2:B:250:VAL:O	1.88	0.72
3:C:98:LYS:CD	3:C:101:ASP:HB2	2.18	0.72
2:B:298:PRO:HB3	2:B:307:PRO:CD	2.15	0.72
1:A:108:TYR:CD1	1:A:413:MET:HE1	2.24	0.72
2:B:105:ARG:O	2:B:110:ILE:HG22	1.89	0.72
2:B:166:LYS:HE3	2:B:199:ASP:OD1	1.90	0.72
1:A:264:ARG:NH1	3:C:278:ARG:HE	1.88	0.72
3:C:269:ALA:HB2	3:C:322:ALA:HA	1.70	0.72
1:A:66:ILE:C	1:A:67:LEU:HD23	2.15	0.72
1:A:264:ARG:CD	3:C:278:ARG:NH2	2.40	0.72
3:C:20:GLU:O	3:C:23:VAL:HG12	1.90	0.72
1:A:325:MET:HE3	1:A:325:MET:HA	1.72	0.72
2:B:7:ILE:CG1	2:B:137:VAL:HG22	2.20	0.72
2:B:312:TYR:O	2:B:344:VAL:HG23	1.90	0.72
1:A:70:LEU:HG	1:A:145:THR:CG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:LEU:HD12	2:B:351:PHE:HD1	1.55	0.71
3:C:119:ILE:HD11	3:C:130:ILE:HD11	1.71	0.71
2:B:3:GLU:HG2	2:B:51:THR:C	2.15	0.71
2:B:259:LEU:HD11	2:B:378:LEU:CD1	2.20	0.71
3:C:4:PRO:HD2	3:C:293:ASN:HA	1.72	0.71
1:A:356:CYS:SG	1:A:357:ASP:N	2.62	0.71
1:A:431:GLU:OE1	1:A:432:TYR:HA	1.91	0.71
1:A:191:VAL:CG1	1:A:425:MET:HG3	2.19	0.71
1:A:201:THR:OG1	1:A:265:LEU:HD11	1.90	0.71
1:A:237:GLY:O	1:A:241:CYS:HB3	1.90	0.71
1:A:243:ARG:NH2	1:A:252:LEU:HG	2.05	0.71
2:B:148:GLY:O	2:B:151:SER:HB2	1.91	0.71
1:A:8:GLN:NE2	1:A:17:GLY:HA3	2.06	0.71
2:B:242:LEU:HD21	2:B:250:VAL:HB	1.71	0.71
2:B:343:PHE:CZ	2:B:351:PHE:HE2	2.08	0.70
1:A:264:ARG:CZ	3:C:278:ARG:CZ	2.69	0.70
2:B:11:GLN:HE21	2:B:74:VAL:CG2	2.03	0.70
3:C:95:MET:HA	3:C:95:MET:HE2	1.73	0.70
1:A:48:ARG:HG2	1:A:243:ARG:O	1.90	0.70
1:A:265:LEU:HD12	1:A:265:LEU:C	2.15	0.70
2:B:12:ALA:HB3	2:B:140:SER:OG	1.91	0.70
3:C:95:MET:HA	3:C:95:MET:CE	2.21	0.70
3:C:156:HIS:HB2	3:C:164:TYR:CZ	2.26	0.70
1:A:255:LEU:O	1:A:259:MET:HG3	1.91	0.70
1:A:269:MET:HE2	1:A:381:SER:OG	1.91	0.70
1:A:260:VAL:HG23	2:B:407:TRP:HE1	1.57	0.70
2:B:199:ASP:HB3	2:B:256:GLN:HE21	1.57	0.70
2:B:5:ILE:HG22	2:B:6:SER:N	2.07	0.70
3:C:134:TYR:CE1	3:C:145:LEU:HD12	2.27	0.70
1:A:70:LEU:HG	1:A:145:THR:HG23	1.74	0.70
1:A:10:GLY:O	1:A:14:ASN:HB2	1.90	0.69
1:A:175:PRO:HD2	1:A:207:GLU:OE2	1.91	0.69
1:A:234:THR:O	1:A:238:VAL:HG23	1.92	0.69
2:B:67:PHE:CD2	2:B:92:LEU:HD23	2.26	0.69
2:B:205:ASP:HB3	2:B:303:VAL:HA	1.73	0.69
2:B:237:SER:CB	2:B:376:CYS:SG	2.80	0.69
2:B:244:PHE:HD1	2:B:245:ASP:N	1.90	0.69
2:B:234:ILE:HG21	2:B:302:MET:HE1	1.72	0.69
1:A:24:ILE:HD11	1:A:52:TYR:CE2	2.28	0.69
2:B:133:GLN:HG2	2:B:243:ARG:HH22	1.57	0.69
2:B:371:VAL:HG12	2:B:372:GLN:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:O	1:A:295:MET:HG3	1.91	0.69
3:C:309:GLU:HB3	3:C:313:LYS:NZ	2.08	0.69
3:C:260:ALA:HB1	3:C:279:ASP:OD1	1.93	0.69
1:A:230:LEU:HD21	1:A:302:MET:HE2	1.74	0.69
1:A:242:LEU:CD2	1:A:250:ALA:H	2.06	0.68
2:B:276:ILE:O	2:B:369:ALA:N	2.25	0.68
2:B:343:PHE:HZ	2:B:351:PHE:CE2	2.10	0.68
2:B:115:ILE:CD1	2:B:119:LEU:HG	2.23	0.68
2:B:234:ILE:HD13	2:B:234:ILE:C	2.18	0.68
1:A:301:MET:HE1	1:A:377:PHE:HE2	1.58	0.68
1:A:209:LEU:HD23	1:A:227:LEU:HB3	1.75	0.68
1:A:251:ASP:O	1:A:253:ARG:N	2.26	0.68
1:A:180:THR:HG22	1:A:181:VAL:N	2.07	0.68
3:C:62:TYR:HB2	3:C:110:ARG:HD3	1.74	0.68
3:C:207:ILE:CD1	3:C:230:VAL:HG22	2.24	0.68
1:A:256:ALA:O	1:A:260:VAL:HG22	1.94	0.68
2:B:102:ASN:HB2	2:B:408:TYR:CE1	2.29	0.68
3:C:81:ILE:HG12	3:C:297:THR:HG22	1.76	0.68
1:A:204:ILE:HD13	1:A:231:VAL:HG22	1.76	0.68
1:A:243:ARG:HH22	1:A:252:LEU:HG	1.59	0.68
2:B:217:LEU:HD12	2:B:277:SER:CA	2.23	0.68
1:A:103:TRP:HZ3	1:A:108:TYR:HE1	1.42	0.67
1:A:328:VAL:O	1:A:332:MET:HG2	1.95	0.67
1:A:359:PRO:HB2	1:A:360:PRO:HD2	1.74	0.67
2:B:70:LEU:HD12	2:B:145:THR:CG2	2.24	0.67
1:A:325:MET:CE	1:A:355:VAL:HG21	2.24	0.67
2:B:141:PHE:O	2:B:147:SER:HB3	1.94	0.67
1:A:310:GLY:HA3	1:A:436:GLN:HE21	1.59	0.67
2:B:402:ARG:O	2:B:403:ALA:C	2.36	0.67
2:B:221:ARG:N	2:B:222:PRO:HD3	2.09	0.67
1:A:250:ALA:HB1	1:A:254:LYS:HB2	1.75	0.67
2:B:49:PHE:CE1	2:B:61:HIS:HE1	2.12	0.67
2:B:95:GLY:O	2:B:97:GLU:N	2.27	0.67
2:B:234:ILE:CB	2:B:302:MET:HE1	2.24	0.67
1:A:276:THR:HB	1:A:281:GLN:CG	2.25	0.67
2:B:278:ALA:O	2:B:279:GLU:CB	2.43	0.67
1:A:4:ILE:HG21	1:A:136:GLN:HG2	1.76	0.67
2:B:251:ASP:O	2:B:254:GLU:HB2	1.94	0.67
1:A:172:VAL:HG11	1:A:387:LEU:CD2	2.22	0.67
1:A:44:LEU:HD12	1:A:49:ILE:HD13	1.76	0.67
2:B:172:TYR:HD1	2:B:173:PRO:N	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:GLU:HG3	2:B:83:TYR:OH	1.95	0.66
1:A:242:LEU:CD1	1:A:255:LEU:HD11	2.25	0.66
2:B:7:ILE:HD12	2:B:153:LEU:CD2	2.24	0.66
2:B:152:LEU:HA	2:B:155:GLU:HB2	1.77	0.66
3:C:191:HIS:HD2	3:C:197:MET:SD	2.18	0.66
1:A:107:HIS:CD2	1:A:151:THR:CG2	2.77	0.66
1:A:257:VAL:HG12	1:A:257:VAL:O	1.93	0.66
2:B:63:PRO:CG	2:B:87:PHE:HA	2.26	0.66
1:A:230:LEU:HD23	1:A:231:VAL:N	2.10	0.66
2:B:68:VAL:HG11	2:B:149:PHE:CZ	2.30	0.66
2:B:345:ASP:C	2:B:347:CYS:H	2.04	0.66
3:C:146:LEU:HD22	3:C:171:ARG:HH12	1.59	0.66
1:A:242:LEU:HD12	1:A:255:LEU:HD11	1.77	0.66
1:A:267:PHE:N	1:A:267:PHE:CD1	2.62	0.66
2:B:341:ILE:HG12	2:B:341:ILE:O	1.95	0.66
3:C:28:LYS:HB2	3:C:306:SER:HB3	1.76	0.66
2:B:67:PHE:CD2	2:B:92:LEU:CD2	2.79	0.66
2:B:166:LYS:H	2:B:199:ASP:CG	2.03	0.66
2:B:175:PRO:HG3	2:B:304:LYS:HG2	1.76	0.66
1:A:281:GLN:O	1:A:283:TYR:HB2	1.96	0.66
1:A:324:SER:C	1:A:326:LYS:H	2.03	0.66
3:C:300:ILE:HB	3:C:315:THR:CG2	2.26	0.66
2:B:100:ALA:CB	2:B:105:ARG:HD3	2.26	0.65
2:B:217:LEU:HD11	2:B:367:ASP:O	1.97	0.65
3:C:48:PHE:HZ	3:C:316:LEU:HD22	1.58	0.65
3:C:95:MET:HE3	3:C:107:ILE:HD12	1.76	0.65
2:B:313:MET:HB3	2:B:344:VAL:CG2	2.26	0.65
2:B:372:GLN:O	2:B:373:ARG:HB3	1.96	0.65
2:B:49:PHE:CE1	2:B:61:HIS:CE1	2.84	0.65
2:B:344:VAL:HG12	2:B:345:ASP:N	2.12	0.65
1:A:66:ILE:HD13	1:A:122:VAL:HG12	1.79	0.65
1:A:158:ARG:NE	1:A:197:ASN:O	2.30	0.65
1:A:161:TYR:C	1:A:163:ASP:H	2.05	0.65
1:A:299:LYS:HD3	1:A:299:LYS:N	2.04	0.65
2:B:206:ASN:OD1	2:B:227:LEU:HD13	1.96	0.65
1:A:431:GLU:O	1:A:434:GLN:HG2	1.97	0.65
2:B:115:ILE:HG23	2:B:116:ASP:N	2.12	0.65
1:A:422:GLU:O	1:A:426:ASN:HB2	1.97	0.65
2:B:311:LYS:HE3	2:B:342:GLN:CD	2.22	0.65
2:B:315:CYS:HB3	2:B:377:MET:HE1	1.78	0.65
2:B:293:ASN:OD1	2:B:338:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:CD1	1:A:122:VAL:HG12	2.26	0.64
1:A:241:CYS:O	1:A:244:PHE:HB2	1.98	0.64
2:B:63:PRO:HG3	2:B:87:PHE:HA	1.79	0.64
2:B:3:GLU:HA	2:B:51:THR:CB	2.28	0.64
2:B:234:ILE:CG2	2:B:302:MET:HE1	2.27	0.64
2:B:388:TRP:CE3	2:B:425:MET:HE1	2.32	0.64
1:A:35:SER:HB3	1:A:59:ASN:CA	2.26	0.64
2:B:5:ILE:HD11	2:B:64:ARG:HH12	1.59	0.64
1:A:180:THR:CG2	1:A:181:VAL:N	2.61	0.64
2:B:317:LEU:HD12	2:B:351:PHE:CD1	2.32	0.64
1:A:182:VAL:HG23	1:A:186:ASN:HD21	1.60	0.64
1:A:284:ARG:O	1:A:286:LEU:N	2.31	0.64
1:A:264:ARG:CZ	3:C:278:ARG:NE	2.59	0.64
1:A:413:MET:HG2	1:A:418:PHE:HE1	1.61	0.64
2:B:209:ILE:HG23	2:B:230:LEU:HD23	1.79	0.64
2:B:271:THR:HG23	2:B:300:ASN:O	1.97	0.64
2:B:386:GLU:O	2:B:389:ALA:N	2.31	0.64
3:C:28:LYS:CB	3:C:306:SER:HB3	2.27	0.64
2:B:25:CYS:HB2	2:B:30:ILE:O	1.98	0.64
2:B:151:SER:O	2:B:155:GLU:HB2	1.98	0.64
1:A:133:GLN:HG3	1:A:165:ILE:HD11	1.80	0.64
2:B:305:CYS:SG	2:B:384:ILE:HD13	2.37	0.64
1:A:105:LYS:O	1:A:110:GLU:HB2	1.97	0.63
2:B:296:PHE:CZ	2:B:341:ILE:HD11	2.22	0.63
3:C:267:ALA:HA	3:C:270:GLU:OE2	1.98	0.63
1:A:114:LEU:O	1:A:118:VAL:HG23	1.97	0.63
1:A:137:LEU:HD22	1:A:154:ILE:CG2	2.28	0.63
1:A:282:GLN:HG2	1:A:282:GLN:O	1.97	0.63
2:B:175:PRO:HG2	2:B:207:GLU:OE1	1.98	0.63
2:B:317:LEU:HD11	2:B:351:PHE:HE1	1.63	0.63
3:C:30:VAL:HG12	3:C:41:ILE:HG12	1.81	0.63
1:A:93:VAL:CG1	1:A:118:VAL:HG22	2.19	0.63
1:A:192:HIS:O	1:A:195:VAL:HG12	1.98	0.63
1:A:315:VAL:HG13	1:A:377:PHE:CE1	2.34	0.63
1:A:318:VAL:HA	1:A:354:ALA:HB3	1.81	0.63
2:B:152:LEU:HD12	2:B:153:LEU:N	2.14	0.63
1:A:253:ARG:O	1:A:254:LYS:C	2.42	0.63
2:B:23:LEU:HD22	2:B:232:GLY:O	1.99	0.63
2:B:155:GLU:HA	2:B:197:HIS:HD1	1.63	0.63
1:A:4:ILE:HA	1:A:134:GLY:O	1.99	0.62
1:A:205:ASP:OD2	1:A:304:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:ALA:HB1	3:C:279:ASP:CG	2.24	0.62
1:A:70:LEU:C	1:A:99:ALA:HB2	2.24	0.62
1:A:299:LYS:O	1:A:300:ASN:HB2	1.98	0.62
2:B:5:ILE:HD13	2:B:64:ARG:HH12	1.59	0.62
1:A:63:PRO:HD2	1:A:86:ILE:HG12	1.80	0.62
1:A:70:LEU:H	1:A:145:THR:CG2	2.10	0.62
2:B:236:SER:O	2:B:240:ALA:HB3	1.99	0.62
2:B:317:LEU:HB3	2:B:319:TYR:CE1	2.33	0.62
3:C:138:TYR:CE2	3:C:139:LEU:HD23	2.35	0.62
1:A:115:VAL:HG21	1:A:152:LEU:CD2	2.30	0.62
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.81	0.62
2:B:315:CYS:HB3	2:B:377:MET:CE	2.29	0.62
1:A:70:LEU:N	1:A:145:THR:HG21	2.11	0.62
1:A:243:ARG:HH21	1:A:252:LEU:H	1.46	0.62
1:A:154:ILE:HG22	1:A:166:MET:HE2	1.81	0.62
1:A:283:TYR:C	1:A:284:ARG:HG2	2.24	0.62
3:C:313:LYS:O	3:C:317:LEU:HG	1.99	0.62
1:A:253:ARG:O	1:A:256:ALA:N	2.33	0.62
1:A:427:ASP:O	1:A:430:SER:HB3	1.97	0.62
2:B:269:LEU:O	2:B:378:LEU:HA	1.99	0.62
2:B:205:ASP:HB2	2:B:303:VAL:HA	1.82	0.62
2:B:276:ILE:CG2	2:B:369:ALA:HB2	2.26	0.62
3:C:207:ILE:HD13	3:C:230:VAL:HG22	1.82	0.62
2:B:7:ILE:HG22	2:B:66:VAL:CG2	2.28	0.61
2:B:30:ILE:HG12	2:B:36:MET:CB	2.12	0.61
2:B:70:LEU:O	2:B:95:GLY:O	2.17	0.61
2:B:118:VAL:HG11	2:B:149:PHE:HZ	1.65	0.61
2:B:7:ILE:CD1	2:B:137:VAL:HG22	2.29	0.61
2:B:102:ASN:OD1	2:B:105:ARG:HB3	1.99	0.61
2:B:277:SER:HA	2:B:367:ASP:O	2.00	0.61
2:B:436:GLY:C	2:B:438:ASP:H	2.08	0.61
3:C:106:GLY:O	3:C:110:ARG:HG3	2.00	0.61
1:A:204:ILE:CD1	1:A:231:VAL:HG13	2.30	0.61
2:B:6:SER:HB3	2:B:136:SER:HG	1.64	0.61
1:A:4:ILE:HG23	1:A:134:GLY:O	2.00	0.61
2:B:115:ILE:HG13	2:B:152:LEU:HD13	1.81	0.61
1:A:70:LEU:CG	1:A:145:THR:HG23	2.30	0.61
1:A:349:ASN:C	1:A:349:ASN:HD22	2.07	0.61
2:B:62:VAL:HG11	2:B:88:HIS:ND1	2.15	0.61
2:B:267:PHE:HD1	2:B:267:PHE:H	1.47	0.61
1:A:31:ASP:O	1:A:32:PRO:C	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:SER:CB	1:A:327:GLU:HG2	2.30	0.61
2:B:168:GLU:OE1	2:B:198:SER:HB2	2.01	0.61
2:B:243:ARG:NH2	2:B:252:LEU:N	2.29	0.61
3:C:209:LEU:HD13	3:C:209:LEU:C	2.25	0.61
1:A:114:LEU:HD23	1:A:149:MET:CE	2.30	0.61
1:A:211:ASP:OD1	1:A:212:ILE:N	2.33	0.61
2:B:5:ILE:HD11	2:B:64:ARG:HH22	1.65	0.61
2:B:381:THR:C	2:B:383:ALA:N	2.56	0.61
1:A:128:SER:OG	1:A:129:CYS:N	2.34	0.60
1:A:188:THR:HA	1:A:425:MET:HE2	1.83	0.60
2:B:169:PHE:CE2	2:B:235:VAL:HG22	2.36	0.60
2:B:362:VAL:HG13	2:B:368:LEU:HB2	1.83	0.60
1:A:204:ILE:HG21	1:A:231:VAL:HG22	1.84	0.60
1:A:230:LEU:O	1:A:233:ALA:HB3	2.00	0.60
1:A:279:GLY:O	1:A:282:GLN:HB3	2.01	0.60
2:B:191:THR:HG21	2:B:425:MET:SD	2.41	0.60
1:A:324:SER:C	1:A:326:LYS:N	2.59	0.60
2:B:30:ILE:CD1	2:B:61:HIS:CG	2.82	0.60
2:B:296:PHE:CZ	2:B:341:ILE:CD1	2.79	0.60
3:C:205:HIS:CD2	3:C:282:MET:HE1	2.37	0.60
1:A:107:HIS:HD2	1:A:151:THR:CG2	2.12	0.60
3:C:10:LYS:HG2	3:C:49:ASP:OD2	2.02	0.60
3:C:265:ILE:HD12	3:C:318:PHE:CZ	2.37	0.60
1:A:324:SER:O	1:A:328:VAL:HG23	2.02	0.60
2:B:87:PHE:CD1	2:B:87:PHE:N	2.69	0.60
2:B:167:LEU:HA	2:B:200:CYS:O	2.01	0.60
3:C:17:PRO:CA	3:C:54:SER:HB3	2.29	0.60
3:C:302:CYS:HB3	3:C:312:THR:HG22	1.83	0.60
1:A:49:ILE:O	1:A:51:VAL:N	2.35	0.60
2:B:217:LEU:HD11	2:B:277:SER:HA	1.83	0.60
2:B:296:PHE:CE2	2:B:335:ILE:CG2	2.73	0.60
3:C:208:PHE:CE2	3:C:210:ILE:HD11	2.29	0.60
1:A:141:LEU:CD1	1:A:141:LEU:N	2.65	0.60
2:B:371:VAL:HG12	2:B:372:GLN:N	2.17	0.60
1:A:54:ASN:ND2	1:A:64:ARG:HD3	2.15	0.60
1:A:285:ALA:HB1	1:A:290:GLU:HG2	1.82	0.60
1:A:408:TYR:CG	1:A:418:PHE:HZ	2.20	0.60
3:C:300:ILE:O	3:C:300:ILE:HG13	2.02	0.60
1:A:115:VAL:HG21	1:A:152:LEU:HD23	1.84	0.60
2:B:229:ARG:NH1	2:B:363:VAL:HG21	2.16	0.60
2:B:242:LEU:C	2:B:244:PHE:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:VAL:C	2:B:411:GLU:H	2.09	0.60
3:C:72:ASP:O	3:C:75:GLU:HB3	2.02	0.60
1:A:102:ASN:ND2	1:A:407:TRP:O	2.35	0.59
2:B:413:MET:O	2:B:414:GLU:HG3	2.02	0.59
2:B:435:VAL:HG12	2:B:435:VAL:O	2.02	0.59
1:A:205:ASP:OD2	1:A:304:ALA:CB	2.50	0.59
1:A:30:ILE:HD13	1:A:53:TYR:CE2	2.38	0.59
1:A:114:LEU:HD23	1:A:149:MET:HE1	1.85	0.59
1:A:230:LEU:CD2	1:A:302:MET:HE2	2.32	0.59
2:B:276:ILE:HD11	2:B:280:LYS:HD2	1.85	0.59
3:C:3:ASP:HB2	3:C:293:ASN:OD1	2.02	0.59
1:A:264:ARG:HH11	3:C:278:ARG:NH2	1.99	0.59
3:C:134:TYR:CD2	3:C:208:PHE:HD1	2.20	0.59
1:A:89:PRO:HA	1:A:92:PHE:CD2	2.38	0.59
2:B:61:HIS:C	2:B:62:VAL:HG23	2.28	0.59
2:B:115:ILE:HD13	2:B:115:ILE:O	2.02	0.59
2:B:339:ARG:C	2:B:341:ILE:H	2.11	0.59
3:C:208:PHE:HE2	3:C:210:ILE:CD1	2.14	0.59
2:B:344:VAL:HG11	2:B:346:TRP:NE1	2.16	0.59
1:A:151:THR:OG1	1:A:193:GLN:HB3	2.03	0.59
1:A:424:ASN:C	1:A:424:ASN:HD22	2.09	0.59
2:B:115:ILE:HD13	2:B:115:ILE:C	2.28	0.59
2:B:119:LEU:O	2:B:122:ILE:HG12	2.02	0.59
2:B:317:LEU:HD11	2:B:351:PHE:CE1	2.38	0.58
1:A:19:LYS:CG	1:A:228:ASN:HB3	2.31	0.58
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.33	0.58
2:B:6:SER:HA	2:B:136:SER:O	2.03	0.58
1:A:270:PRO:HA	1:A:377:PHE:O	2.04	0.58
2:B:51:THR:O	2:B:52:PHE:CD1	2.57	0.58
2:B:234:ILE:HB	2:B:302:MET:HE1	1.85	0.58
1:A:194:LEU:C	1:A:196:GLU:H	2.11	0.58
2:B:202:PHE:CE1	2:B:378:LEU:HD22	2.38	0.58
2:B:248:LEU:CD2	2:B:353:VAL:O	2.49	0.58
1:A:198:THR:HG22	1:A:265:LEU:HD22	1.85	0.58
2:B:63:PRO:HG3	2:B:87:PHE:CB	2.34	0.58
2:B:110:ILE:CG2	2:B:111:GLY:H	2.15	0.58
2:B:369:ALA:O	2:B:370:LYS:HB3	2.03	0.58
3:C:62:TYR:CD1	3:C:66:ALA:HB3	2.39	0.58
3:C:316:LEU:O	3:C:320:GLN:HG3	2.04	0.58
1:A:226:ASP:O	1:A:227:LEU:C	2.46	0.58
1:A:307:PRO:HB3	1:A:312:TYR:OH	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:LEU:CD2	2:B:122:ILE:HD11	2.28	0.58
1:A:180:THR:CG2	1:A:181:VAL:H	2.17	0.58
1:A:299:LYS:O	1:A:300:ASN:CB	2.51	0.58
2:B:268:PRO:HA	2:B:379:SER:O	2.04	0.58
2:B:407:TRP:O	2:B:411:GLU:HG2	2.02	0.58
3:C:132:VAL:HG12	3:C:210:ILE:HD13	1.86	0.58
1:A:68:VAL:CG1	1:A:149:MET:SD	2.90	0.58
2:B:165:SER:HA	2:B:199:ASP:OD2	2.04	0.58
2:B:67:PHE:CZ	2:B:87:PHE:CE2	2.92	0.57
2:B:218:ASP:O	2:B:219:ILE:HG23	2.04	0.57
2:B:345:ASP:O	2:B:347:CYS:N	2.37	0.57
3:C:74:LEU:HD13	3:C:118:TYR:CG	2.39	0.57
3:C:180:MET:HE2	3:C:180:MET:CA	2.31	0.57
2:B:196:GLU:C	2:B:197:HIS:CD2	2.82	0.57
2:B:117:LEU:HD11	2:B:121:ARG:HH22	1.69	0.57
2:B:150:THR:O	2:B:151:SER:C	2.47	0.57
2:B:215:ARG:C	2:B:216:ASN:HD22	2.12	0.57
2:B:166:LYS:HD2	2:B:197:HIS:O	2.04	0.57
1:A:6:HIS:HB3	1:A:65:ALA:HB2	1.87	0.57
2:B:2:ARG:N	2:B:131:GLY:O	2.36	0.57
2:B:139:HIS:CE1	2:B:170:SER:HB3	2.40	0.57
2:B:313:MET:O	2:B:314:ALA:HB2	2.04	0.57
1:A:5:VAL:CG2	1:A:135:PHE:HD2	2.18	0.57
2:B:216:ASN:O	2:B:217:LEU:HB2	2.05	0.57
2:B:264:ARG:HB2	2:B:266:HIS:HD2	1.67	0.57
2:B:362:VAL:HG11	2:B:368:LEU:O	2.04	0.57
3:C:309:GLU:O	3:C:313:LYS:HG2	2.05	0.57
1:A:229:HIS:ND1	1:A:229:HIS:C	2.62	0.57
1:A:264:ARG:CD	3:C:278:ARG:NH1	2.68	0.57
2:B:62:VAL:HG13	2:B:63:PRO:HD2	1.78	0.57
1:A:30:ILE:HA	1:A:35:SER:O	2.04	0.57
1:A:149:MET:O	1:A:153:LEU:HD13	2.05	0.57
1:A:273:ALA:CB	1:A:274:PRO:HD3	2.30	0.57
1:A:301:MET:CE	1:A:377:PHE:HE2	2.17	0.57
1:A:14:ASN:OD1	1:A:75:MET:HG2	2.05	0.57
1:A:209:LEU:O	1:A:210:TYR:C	2.48	0.57
1:A:312:TYR:O	1:A:344:VAL:HB	2.05	0.57
2:B:175:PRO:HG3	2:B:304:LYS:CG	2.35	0.57
2:B:362:VAL:CG1	2:B:368:LEU:HB2	2.35	0.57
1:A:274:PRO:CG	1:A:371:LEU:HD21	2.34	0.56
1:A:320:ARG:O	1:A:359:PRO:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:O	1:A:426:ASN:N	2.37	0.56
2:B:57:GLY:HA3	2:B:58:ALA:HB2	0.66	0.56
3:C:138:TYR:CE1	3:C:203:ARG:HB3	2.35	0.56
2:B:209:ILE:CG2	2:B:227:LEU:HD22	2.35	0.56
2:B:210:TYR:CE1	2:B:227:LEU:HD11	2.40	0.56
2:B:239:THR:O	2:B:240:ALA:C	2.48	0.56
2:B:88:HIS:HB2	2:B:91:GLN:NE2	2.06	0.56
2:B:382:THR:HG22	2:B:382:THR:O	2.05	0.56
1:A:50:ASN:O	1:A:64:ARG:NH2	2.38	0.56
1:A:70:LEU:CD1	1:A:145:THR:HG23	2.35	0.56
1:A:182:VAL:HG23	1:A:186:ASN:ND2	2.20	0.56
1:A:259:MET:CA	1:A:314:THR:HG21	2.35	0.56
1:A:272:PHE:HB3	1:A:275:LEU:HD22	1.88	0.56
1:A:319:PHE:HA	1:A:375:ALA:HA	1.86	0.56
2:B:331:ALA:O	2:B:334:THR:HG22	2.05	0.56
1:A:191:VAL:HA	1:A:194:LEU:HD12	1.88	0.56
1:A:216:THR:O	1:A:217:LEU:HD12	2.05	0.56
1:A:250:ALA:CA	1:A:254:LYS:HE2	2.35	0.56
2:B:388:TRP:CE3	2:B:388:TRP:HA	2.41	0.56
3:C:62:TYR:CB	3:C:110:ARG:HD3	2.35	0.56
3:C:300:ILE:HB	3:C:315:THR:HG21	1.88	0.56
1:A:165:ILE:HD13	1:A:165:ILE:H	1.71	0.56
1:A:319:PHE:CD2	1:A:375:ALA:HB2	2.40	0.56
2:B:152:LEU:HA	2:B:155:GLU:CB	2.35	0.56
1:A:251:ASP:O	1:A:252:LEU:C	2.49	0.56
2:B:231:ILE:HA	2:B:234:ILE:CG2	2.36	0.56
2:B:277:SER:O	2:B:280:LYS:HB2	2.06	0.56
1:A:49:ILE:O	1:A:50:ASN:C	2.48	0.56
2:B:16:ILE:HD12	2:B:171:ILE:HD11	1.87	0.56
2:B:209:ILE:HG22	2:B:227:LEU:HD22	1.88	0.56
3:C:116:PHE:HB3	3:C:120:TYR:CE2	2.40	0.56
3:C:146:LEU:CD2	3:C:171:ARG:HH12	2.19	0.56
3:C:229:LEU:N	3:C:229:LEU:HD22	2.21	0.56
1:A:108:TYR:CE1	1:A:413:MET:HE1	2.40	0.56
2:B:408:TYR:CD2	2:B:418:PHE:HZ	2.24	0.56
3:C:81:ILE:HG23	3:C:297:THR:CG2	2.36	0.56
1:A:166:MET:HB3	1:A:198:THR:OG1	2.06	0.56
1:A:204:ILE:HG21	1:A:231:VAL:CG2	2.36	0.56
1:A:424:ASN:C	1:A:424:ASN:ND2	2.62	0.56
1:A:119:LEU:O	1:A:123:ARG:HG3	2.06	0.55
1:A:311:ARG:HG2	1:A:311:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLU:C	1:A:347:ILE:H	2.13	0.55
1:A:19:LYS:O	1:A:23:VAL:HG23	2.06	0.55
1:A:151:THR:OG1	1:A:193:GLN:CB	2.54	0.55
2:B:338:LYS:O	2:B:340:THR:N	2.34	0.55
3:C:98:LYS:HD3	3:C:101:ASP:CB	2.28	0.55
1:A:311:ARG:HD2	1:A:344:VAL:H	1.71	0.55
2:B:150:THR:O	2:B:153:LEU:N	2.40	0.55
1:A:4:ILE:HD13	1:A:136:GLN:NE2	2.18	0.55
1:A:139:HIS:HE1	1:A:168:THR:HG23	1.71	0.55
1:A:147:SER:O	1:A:151:THR:CB	2.51	0.55
1:A:259:MET:CG	1:A:314:THR:HG21	2.36	0.55
1:A:297:ASP:OD1	1:A:298:ALA:N	2.39	0.55
2:B:19:ALA:CB	2:B:228:ASN:HB3	2.35	0.55
3:C:153:LEU:HD12	3:C:166:LYS:O	2.07	0.55
1:A:67:LEU:HD23	1:A:67:LEU:N	2.22	0.55
2:B:64:ARG:O	2:B:64:ARG:HG3	2.07	0.55
3:C:266:SER:OG	3:C:321:ARG:HD3	2.07	0.55
1:A:204:ILE:HD13	1:A:231:VAL:HG13	1.89	0.55
1:A:298:ALA:O	1:A:299:LYS:C	2.50	0.55
3:C:161:ARG:HD2	3:C:161:ARG:O	2.07	0.55
1:A:5:VAL:HG22	1:A:135:PHE:CD2	2.42	0.55
1:A:223:THR:HG22	1:A:224:TYR:N	2.21	0.55
3:C:34:GLN:CG	3:C:40:MET:HE2	2.36	0.55
1:A:310:GLY:CA	1:A:436:GLN:HE21	2.19	0.55
1:A:325:MET:O	1:A:329:ASP:HB2	2.07	0.55
2:B:30:ILE:HG23	2:B:34:GLY:O	2.07	0.55
2:B:253:THR:O	2:B:256:GLN:HG2	2.06	0.55
2:B:276:ILE:O	2:B:369:ALA:CB	2.53	0.55
3:C:16:ARG:HH12	3:C:303:SER:HB2	1.72	0.55
1:A:239:THR:O	1:A:241:CYS:N	2.41	0.54
2:B:244:PHE:CD1	2:B:244:PHE:C	2.84	0.54
2:B:288:VAL:HG22	2:B:373:ARG:NH1	2.23	0.54
1:A:190:SER:O	1:A:194:LEU:HG	2.06	0.54
1:A:210:TYR:HD1	1:A:227:LEU:HD21	1.71	0.54
1:A:239:THR:HG22	1:A:240:THR:N	2.22	0.54
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.29	0.54
2:B:17:GLY:O	2:B:21:TRP:HB2	2.08	0.54
3:C:18:LEU:H	3:C:18:LEU:HD22	1.71	0.54
1:A:133:GLN:HE21	1:A:252:LEU:HB2	1.73	0.54
1:A:369:ARG:HD2	1:A:369:ARG:C	2.32	0.54
2:B:6:SER:O	2:B:65:ALA:HB1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:ARG:NH1	3:C:182:THR:HG23	2.23	0.54
1:A:427:ASP:OD1	1:A:428:LEU:N	2.41	0.54
2:B:381:THR:OG1	2:B:383:ALA:HB3	2.07	0.54
1:A:68:VAL:HG12	1:A:149:MET:CE	2.38	0.54
1:A:253:ARG:O	1:A:257:VAL:N	2.33	0.54
1:A:343:PHE:O	1:A:344:VAL:O	2.26	0.54
2:B:305:CYS:O	2:B:306:ASP:C	2.49	0.54
1:A:20:PHE:CE1	1:A:24:ILE:HD12	2.42	0.54
2:B:118:VAL:HG21	2:B:149:PHE:CZ	2.42	0.54
1:A:172:VAL:CG1	1:A:387:LEU:HD21	2.24	0.54
1:A:323:MET:HG3	1:A:328:VAL:HG21	1.90	0.54
2:B:3:GLU:HG3	2:B:51:THR:HA	1.75	0.54
2:B:24:TYR:OH	2:B:239:THR:OG1	2.24	0.54
2:B:110:ILE:O	2:B:112:LYS:N	2.41	0.54
3:C:95:MET:HE2	3:C:95:MET:CA	2.37	0.54
3:C:303:SER:OG	3:C:305:SER:HB2	2.08	0.54
2:B:55:GLU:O	2:B:56:THR:C	2.50	0.54
2:B:163:LYS:O	2:B:163:LYS:HG2	2.08	0.54
1:A:264:ARG:NH1	3:C:278:ARG:CD	2.70	0.53
1:A:331:GLN:O	1:A:335:VAL:HG23	2.08	0.53
2:B:121:ARG:O	2:B:125:LEU:HB2	2.08	0.53
3:C:265:ILE:HD12	3:C:318:PHE:CE1	2.43	0.53
1:A:4:ILE:CG2	1:A:136:GLN:HG2	2.38	0.53
2:B:23:LEU:HD23	2:B:236:SER:CB	2.37	0.53
2:B:115:ILE:O	2:B:116:ASP:C	2.51	0.53
2:B:172:TYR:OH	2:B:387:ALA:O	2.24	0.53
2:B:264:ARG:C	2:B:266:HIS:N	2.60	0.53
2:B:324:VAL:O	2:B:327:ASP:HB2	2.08	0.53
1:A:36:TYR:CZ	1:A:38:GLY:HA3	2.43	0.53
1:A:168:THR:CB	1:A:201:THR:HG23	2.38	0.53
2:B:5:ILE:CG2	2:B:6:SER:N	2.70	0.53
1:A:44:LEU:O	1:A:49:ILE:HG12	2.07	0.53
1:A:107:HIS:HD2	1:A:151:THR:HG22	1.72	0.53
1:A:191:VAL:HG11	1:A:425:MET:HE2	1.89	0.53
1:A:325:MET:CE	1:A:355:VAL:HG11	2.38	0.53
1:A:431:GLU:O	1:A:434:GLN:CG	2.56	0.53
2:B:5:ILE:O	2:B:136:SER:N	2.40	0.53
2:B:182:VAL:O	2:B:184:PRO:N	2.41	0.53
2:B:248:LEU:HB3	2:B:355:ILE:H	1.73	0.53
3:C:151:THR:HG22	3:C:152:ASN:N	2.23	0.53
1:A:5:VAL:HG23	1:A:5:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ASP:O	2:B:110:ILE:HD13	2.08	0.53
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.44	0.53
1:A:198:THR:HG22	1:A:265:LEU:CD2	2.39	0.53
1:A:288:VAL:HG22	1:A:323:MET:HE3	1.90	0.53
1:A:383:ALA:C	1:A:385:GLN:H	2.15	0.53
2:B:243:ARG:CZ	2:B:252:LEU:HG	2.39	0.53
1:A:141:LEU:HA	1:A:147:SER:HB3	1.91	0.53
2:B:173:PRO:HB2	2:B:391:LEU:CD1	2.39	0.53
1:A:31:ASP:HB3	1:A:32:PRO:HD2	1.89	0.53
2:B:5:ILE:O	2:B:135:PHE:HA	2.09	0.53
2:B:9:VAL:CG1	2:B:139:HIS:HB3	2.38	0.53
2:B:110:ILE:CG2	2:B:111:GLY:N	2.71	0.53
2:B:147:SER:CB	2:B:190:THR:OG1	2.52	0.53
2:B:163:LYS:C	2:B:164:LYS:HG2	2.34	0.53
2:B:231:ILE:CA	2:B:234:ILE:HG22	2.38	0.53
3:C:46:TYR:CG	3:C:316:LEU:HD13	2.44	0.53
3:C:71:LYS:HD3	3:C:71:LYS:C	2.33	0.53
1:A:264:ARG:HE	1:A:264:ARG:HA	1.74	0.53
2:B:253:THR:O	2:B:254:GLU:C	2.52	0.53
1:A:226:ASP:O	1:A:229:HIS:N	2.42	0.53
1:A:322:ARG:HG3	1:A:322:ARG:HH11	1.73	0.53
2:B:101:ASN:ND2	5:B:500:GTP:O3G	2.42	0.53
1:A:8:GLN:OE1	1:A:14:ASN:ND2	2.42	0.52
2:B:345:ASP:OD2	2:B:439:SER:HB3	2.10	0.52
3:C:4:PRO:CD	3:C:293:ASN:HA	2.36	0.52
1:A:210:TYR:CD1	1:A:227:LEU:HD21	2.44	0.52
2:B:67:PHE:CZ	2:B:87:PHE:HE2	2.27	0.52
2:B:231:ILE:N	2:B:231:ILE:HD13	2.25	0.52
1:A:175:PRO:O	1:A:176:LYS:C	2.52	0.52
1:A:213:CYS:SG	1:A:219:LEU:HD23	2.48	0.52
2:B:119:LEU:HD11	2:B:156:ARG:CD	2.40	0.52
2:B:255:PHE:O	2:B:256:GLN:C	2.53	0.52
2:B:345:ASP:C	2:B:347:CYS:N	2.68	0.52
2:B:408:TYR:O	2:B:411:GLU:N	2.39	0.52
1:A:103:TRP:CE2	1:A:189:LEU:HB3	2.45	0.52
1:A:149:MET:O	1:A:149:MET:HG2	2.10	0.52
2:B:24:TYR:CE1	2:B:240:ALA:HB2	2.45	0.52
2:B:328:VAL:C	2:B:330:ALA:H	2.16	0.52
2:B:201:ALA:O	2:B:267:PHE:HA	2.10	0.52
1:A:179:ASP:HB2	4:A:600:GDP:H3'	1.90	0.52
1:A:212:ILE:O	1:A:216:THR:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLN:C	1:A:283:TYR:N	2.67	0.52
1:A:320:ARG:HA	1:A:356:CYS:HB3	1.92	0.52
1:A:399:PHE:O	1:A:400:ARG:C	2.52	0.52
2:B:63:PRO:CG	2:B:91:GLN:CD	2.72	0.52
3:C:202:SER:O	3:C:233:ALA:HA	2.10	0.52
1:A:425:MET:O	1:A:428:LEU:HB3	2.09	0.52
2:B:8:HIS:HB3	2:B:13:GLY:O	2.10	0.52
2:B:63:PRO:HG3	2:B:87:PHE:CA	2.40	0.52
1:A:176:LYS:CE	1:A:207:GLU:HG3	2.39	0.52
1:A:295:MET:SD	1:A:375:ALA:O	2.68	0.52
2:B:173:PRO:HB2	2:B:391:LEU:HD11	1.92	0.52
2:B:344:VAL:HG12	2:B:345:ASP:H	1.75	0.52
1:A:27:GLU:O	1:A:27:GLU:HG2	2.08	0.52
1:A:107:HIS:CD2	1:A:151:THR:HG22	2.45	0.52
1:A:325:MET:HE2	1:A:355:VAL:HG21	1.92	0.52
2:B:11:GLN:NE2	2:B:74:VAL:HG22	2.22	0.52
2:B:67:PHE:CE2	2:B:87:PHE:CD2	2.89	0.52
2:B:122:ILE:CD1	2:B:157:LEU:HD21	2.35	0.51
2:B:144:GLY:H	5:B:500:GTP:PG	2.33	0.51
2:B:434:GLU:C	2:B:436:GLY:H	2.18	0.51
1:A:188:THR:HA	1:A:425:MET:CE	2.40	0.51
1:A:314:THR:CG2	1:A:315:VAL:N	2.73	0.51
2:B:191:THR:HG23	2:B:192:HIS:N	2.25	0.51
1:A:70:LEU:HD12	1:A:145:THR:HG23	1.91	0.51
1:A:224:TYR:O	1:A:225:GLY:C	2.53	0.51
1:A:260:VAL:HG23	1:A:260:VAL:O	2.10	0.51
1:A:346:TRP:H	1:A:346:TRP:CD1	2.27	0.51
2:B:206:ASN:OD1	2:B:227:LEU:CD1	2.57	0.51
2:B:243:ARG:NH2	2:B:251:ASP:OD1	2.44	0.51
3:C:134:TYR:CD2	3:C:208:PHE:CD1	2.98	0.51
1:A:5:VAL:CG2	1:A:135:PHE:CD2	2.94	0.51
1:A:149:MET:O	1:A:153:LEU:HD22	2.10	0.51
1:A:200:GLU:N	1:A:265:LEU:HD13	2.25	0.51
1:A:277:SER:OG	1:A:281:GLN:HB2	2.10	0.51
1:A:259:MET:HG2	1:A:314:THR:CG2	2.38	0.51
2:B:3:GLU:CD	2:B:50:ASN:O	2.54	0.51
2:B:4:CYS:HA	2:B:134:GLY:O	2.10	0.51
2:B:10:GLY:O	2:B:11:GLN:C	2.53	0.51
2:B:22:GLU:O	2:B:23:LEU:C	2.54	0.51
2:B:88:HIS:O	2:B:89:PRO:C	2.52	0.51
2:B:251:ASP:OD1	2:B:252:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:SER:O	2:B:142:GLY:N	2.44	0.51
3:C:236:GLU:CD	3:C:236:GLU:H	2.19	0.51
1:A:263:PRO:O	1:A:264:ARG:C	2.52	0.51
1:A:307:PRO:C	1:A:309:HIS:H	2.18	0.51
1:A:323:MET:HG3	1:A:328:VAL:CG2	2.41	0.51
2:B:70:LEU:CD1	2:B:145:THR:CB	2.89	0.51
1:A:103:TRP:HZ3	1:A:108:TYR:CE1	2.27	0.51
2:B:242:LEU:C	2:B:244:PHE:N	2.66	0.51
3:C:18:LEU:HD13	3:C:18:LEU:N	2.24	0.51
1:A:288:VAL:CG2	1:A:323:MET:HE3	2.40	0.51
1:A:360:PRO:O	1:A:369:ARG:C	2.54	0.51
2:B:133:GLN:CB	2:B:243:ARG:HH12	2.24	0.51
1:A:260:VAL:HG23	2:B:407:TRP:NE1	2.24	0.51
2:B:9:VAL:HG21	2:B:149:PHE:CD1	2.46	0.51
2:B:87:PHE:HD1	2:B:87:PHE:H	1.59	0.51
2:B:119:LEU:HA	2:B:122:ILE:HG12	1.93	0.51
3:C:122:MET:O	3:C:124:GLU:HG3	2.10	0.51
1:A:264:ARG:HH12	3:C:278:ARG:NE	2.00	0.50
2:B:196:GLU:O	2:B:197:HIS:CD2	2.64	0.50
2:B:244:PHE:CD1	2:B:245:ASP:N	2.76	0.50
2:B:396:ASP:O	2:B:397:LEU:C	2.53	0.50
3:C:131:LYS:CE	3:C:213:LYS:HD2	2.41	0.50
2:B:14:VAL:HG11	2:B:75:ILE:HD13	1.93	0.50
2:B:133:GLN:HB3	2:B:243:ARG:HH12	1.76	0.50
2:B:171:ILE:HG22	2:B:171:ILE:O	2.10	0.50
2:B:362:VAL:HG13	2:B:368:LEU:CD1	2.38	0.50
2:B:413:MET:C	2:B:414:GLU:HG3	2.36	0.50
1:A:431:GLU:OE1	1:A:432:TYR:CA	2.57	0.50
2:B:261:PRO:HB2	2:B:262:TYR:CD2	2.46	0.50
3:C:101:ASP:CG	3:C:102:PRO:HD2	2.36	0.50
1:A:242:LEU:C	1:A:244:PHE:H	2.20	0.50
1:A:296:PHE:CZ	1:A:315:VAL:HG11	2.46	0.50
2:B:132:LEU:CD2	2:B:164:LYS:HE3	2.42	0.50
3:C:62:TYR:CE1	3:C:66:ALA:HB3	2.46	0.50
1:A:175:PRO:HD2	1:A:207:GLU:CD	2.36	0.50
1:A:333:LEU:O	1:A:336:GLN:N	2.45	0.50
2:B:241:SER:C	2:B:244:PHE:HB3	2.36	0.50
2:B:310:GLY:HA3	2:B:383:ALA:N	2.26	0.50
1:A:431:GLU:HA	1:A:434:GLN:CG	2.42	0.50
2:B:95:GLY:C	2:B:97:GLU:N	2.69	0.50
3:C:191:HIS:O	3:C:194:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:HG3	1:A:114:LEU:N	2.26	0.50
1:A:345:GLU:O	1:A:347:ILE:N	2.45	0.50
2:B:62:VAL:HG12	2:B:63:PRO:N	2.25	0.50
3:C:138:TYR:CE2	3:C:139:LEU:CD2	2.95	0.50
1:A:21:TRP:HZ2	1:A:65:ALA:HB2	1.76	0.50
1:A:262:PHE:O	1:A:264:ARG:N	2.45	0.50
1:A:265:LEU:HD12	1:A:266:HIS:O	2.12	0.50
2:B:196:GLU:C	2:B:197:HIS:HD2	2.19	0.50
2:B:402:ARG:O	2:B:403:ALA:O	2.29	0.50
1:A:49:ILE:HG13	1:A:50:ASN:H	1.76	0.50
1:A:173:PRO:HB3	1:A:183:GLU:HG2	1.93	0.50
1:A:265:LEU:O	1:A:266:HIS:O	2.29	0.50
2:B:11:GLN:O	2:B:14:VAL:HB	2.12	0.50
2:B:115:ILE:HD11	2:B:119:LEU:HG	1.92	0.50
2:B:227:LEU:O	2:B:231:ILE:HG12	2.12	0.50
2:B:238:ILE:O	2:B:242:LEU:HB2	2.11	0.50
3:C:207:ILE:HD12	3:C:230:VAL:HG22	1.91	0.50
1:A:82:PRO:C	1:A:84:GLY:H	2.20	0.49
1:A:156:LYS:HA	1:A:156:LYS:CE	2.38	0.49
1:A:269:MET:HB3	1:A:303:ALA:HB2	1.94	0.49
1:A:336:GLN:HE22	1:A:349:ASN:ND2	2.10	0.49
1:A:399:PHE:O	1:A:402:LYS:N	2.29	0.49
2:B:148:GLY:O	2:B:149:PHE:C	2.55	0.49
2:B:414:GLU:N	2:B:414:GLU:OE1	2.45	0.49
2:B:417:GLU:OE1	2:B:417:GLU:HA	2.10	0.49
3:C:28:LYS:HB2	3:C:306:SER:CB	2.41	0.49
3:C:270:GLU:HG3	3:C:272:SER:HB3	1.94	0.49
3:C:275:VAL:HB	3:C:277:TYR:CE2	2.47	0.49
1:A:24:ILE:HG22	1:A:25:SER:N	2.27	0.49
1:A:194:LEU:C	1:A:196:GLU:N	2.70	0.49
1:A:280:SER:O	1:A:282:GLN:N	2.45	0.49
1:A:3:GLU:HA	1:A:51:VAL:HA	1.93	0.49
1:A:264:ARG:CZ	3:C:278:ARG:CD	2.90	0.49
1:A:387:LEU:HD23	1:A:388:PHE:CD1	2.47	0.49
2:B:63:PRO:HD3	2:B:86:LEU:O	2.11	0.49
2:B:231:ILE:O	2:B:235:VAL:HG23	2.12	0.49
2:B:5:ILE:CG1	2:B:64:ARG:NH2	2.75	0.49
2:B:16:ILE:HG23	2:B:17:GLY:N	2.26	0.49
2:B:149:PHE:HE1	2:B:153:LEU:HD22	1.77	0.49
2:B:234:ILE:C	2:B:234:ILE:CD1	2.86	0.49
3:C:142:ILE:O	3:C:153:LEU:HD23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:HZ	1:A:315:VAL:HG11	1.78	0.49
2:B:192:HIS:CD2	2:B:424:ASP:OD2	2.66	0.49
3:C:71:LYS:HE3	3:C:75:GLU:OE1	2.12	0.49
1:A:4:ILE:HD12	1:A:239:THR:CG2	2.42	0.49
1:A:240:THR:HG23	1:A:241:CYS:H	1.76	0.49
2:B:2:ARG:NH1	2:B:47:ASP:CB	2.76	0.49
2:B:12:ALA:CB	2:B:140:SER:OG	2.59	0.49
2:B:115:ILE:CG2	2:B:116:ASP:N	2.75	0.49
2:B:118:VAL:HG21	2:B:149:PHE:CE2	2.48	0.49
2:B:234:ILE:CG1	2:B:270:ALA:HB1	2.38	0.49
1:A:8:GLN:HB3	1:A:14:ASN:HA	1.94	0.49
1:A:168:THR:O	1:A:201:THR:HA	2.12	0.49
1:A:242:LEU:HD22	1:A:250:ALA:N	2.19	0.49
3:C:265:ILE:CD1	3:C:318:PHE:CE1	2.95	0.49
1:A:431:GLU:OE1	1:A:432:TYR:N	2.46	0.49
2:B:188:ILE:O	2:B:191:THR:HG22	2.13	0.49
2:B:30:ILE:HD12	2:B:61:HIS:ND1	2.22	0.49
2:B:96:LYS:O	2:B:97:GLU:O	2.31	0.49
2:B:105:ARG:HG3	2:B:105:ARG:HH11	1.78	0.49
2:B:152:LEU:HD12	2:B:152:LEU:C	2.38	0.49
2:B:155:GLU:OE1	2:B:197:HIS:HE1	1.96	0.49
2:B:191:THR:CG2	2:B:192:HIS:N	2.76	0.49
1:A:49:ILE:HG13	1:A:50:ASN:N	2.28	0.49
1:A:173:PRO:HB3	1:A:183:GLU:CG	2.42	0.49
1:A:199:ASP:O	1:A:200:GLU:HG3	2.13	0.49
1:A:239:THR:O	1:A:240:THR:C	2.56	0.49
1:A:288:VAL:C	1:A:290:GLU:N	2.70	0.49
2:B:104:ALA:CB	2:B:408:TYR:HD1	2.26	0.49
2:B:218:ASP:C	2:B:219:ILE:HG12	2.37	0.49
2:B:293:ASN:HD21	2:B:338:LYS:NZ	2.11	0.49
2:B:297:GLU:HG3	2:B:299:ALA:N	2.28	0.49
2:B:392:ASP:O	2:B:395:PHE:HB3	2.13	0.49
3:C:230:VAL:CG1	3:C:232:LEU:HD23	2.42	0.49
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.13	0.48
1:A:175:PRO:CD	1:A:207:GLU:OE1	2.61	0.48
2:B:98:ASP:CB	2:B:105:ARG:HH21	2.14	0.48
1:A:161:TYR:C	1:A:163:ASP:N	2.71	0.48
1:A:182:VAL:O	1:A:183:GLU:C	2.56	0.48
2:B:203:MET:SD	2:B:267:PHE:HB3	2.53	0.48
1:A:69:ASP:HA	1:A:145:THR:HG21	1.95	0.48
1:A:192:HIS:HD1	1:A:424:ASN:CG	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:HD12	2:B:70:LEU:N	2.28	0.48
3:C:216:ASN:HB3	3:C:219:THR:HB	1.96	0.48
1:A:409:THR:C	1:A:411:GLU:H	2.22	0.48
2:B:50:ASN:ND2	2:B:53:PHE:O	2.46	0.48
2:B:409:VAL:C	2:B:411:GLU:N	2.71	0.48
3:C:261:LEU:O	3:C:265:ILE:HG13	2.13	0.48
1:A:2:ARG:NH1	1:A:251:ASP:OD2	2.46	0.48
1:A:102:ASN:HB3	1:A:105:LYS:HB2	1.95	0.48
1:A:133:GLN:NE2	1:A:252:LEU:HB2	2.27	0.48
1:A:154:ILE:HG22	1:A:166:MET:CE	2.44	0.48
1:A:308:ARG:HG3	1:A:342:TYR:OH	2.13	0.48
2:B:6:SER:OG	2:B:65:ALA:HB2	2.14	0.48
2:B:9:VAL:HG11	2:B:150:THR:OG1	2.13	0.48
2:B:99:ALA:O	2:B:100:ALA:HB3	2.14	0.48
3:C:138:TYR:HE1	3:C:203:ARG:HB2	1.76	0.48
1:A:301:MET:HE1	1:A:377:PHE:CE2	2.43	0.48
2:B:252:LEU:O	2:B:253:THR:C	2.56	0.48
2:B:436:GLY:C	2:B:438:ASP:N	2.72	0.48
3:C:34:GLN:HG3	3:C:40:MET:HE2	1.95	0.48
1:A:209:LEU:O	1:A:213:CYS:N	2.47	0.48
1:A:243:ARG:N	1:A:243:ARG:HD3	2.26	0.48
1:A:307:PRO:HB3	1:A:312:TYR:CZ	2.49	0.48
2:B:103:TYR:O	2:B:104:ALA:C	2.57	0.48
2:B:263:PRO:O	2:B:264:ARG:C	2.56	0.48
2:B:274:PRO:CB	2:B:371:VAL:HG21	2.43	0.48
3:C:148:VAL:O	3:C:148:VAL:HG22	2.13	0.48
1:A:20:PHE:CG	1:A:235:MET:SD	3.06	0.48
2:B:13:GLY:C	2:B:16:ILE:HG22	2.38	0.48
2:B:107:HIS:CE1	2:B:152:LEU:HB3	2.49	0.48
2:B:369:ALA:O	2:B:370:LYS:CB	2.62	0.48
3:C:3:ASP:CB	3:C:4:PRO:HD3	2.39	0.48
2:B:230:LEU:O	2:B:233:GLN:N	2.35	0.48
3:C:30:VAL:CG1	3:C:41:ILE:HG12	2.42	0.48
1:A:24:ILE:CD1	1:A:52:TYR:CE2	2.97	0.47
1:A:26:ASP:C	1:A:28:HIS:H	2.21	0.47
1:A:137:LEU:HD22	1:A:154:ILE:HG21	1.95	0.47
1:A:191:VAL:HG13	1:A:192:HIS:N	2.28	0.47
1:A:211:ASP:OD1	1:A:212:ILE:HG13	2.13	0.47
1:A:383:ALA:C	1:A:385:GLN:N	2.72	0.47
2:B:11:GLN:NE2	2:B:74:VAL:CG2	2.76	0.47
2:B:110:ILE:O	2:B:111:GLY:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:PRO:HD2	2:B:207:GLU:HB3	1.96	0.47
2:B:339:ARG:C	2:B:341:ILE:N	2.68	0.47
3:C:119:ILE:CD1	3:C:130:ILE:HD11	2.41	0.47
1:A:70:LEU:O	1:A:99:ALA:HB2	2.14	0.47
1:A:217:LEU:C	1:A:219:LEU:N	2.55	0.47
1:A:413:MET:HG3	1:A:414:ASP:N	2.22	0.47
2:B:115:ILE:HG23	2:B:116:ASP:H	1.79	0.47
1:A:20:PHE:O	1:A:24:ILE:HB	2.14	0.47
1:A:132:LEU:CD2	1:A:164:ARG:HG3	2.32	0.47
1:A:209:LEU:CD2	1:A:227:LEU:HD13	2.44	0.47
1:A:274:PRO:HG2	1:A:371:LEU:CD2	2.43	0.47
1:A:333:LEU:O	1:A:334:ASN:C	2.58	0.47
2:B:158:SER:OG	2:B:197:HIS:HB3	2.13	0.47
2:B:241:SER:HB3	2:B:320:ARG:NH2	2.29	0.47
3:C:146:LEU:HA	3:C:185:GLU:OE2	2.14	0.47
1:A:198:THR:HG23	1:A:200:GLU:H	1.79	0.47
2:B:97:GLU:HB2	2:B:110:ILE:HD11	1.96	0.47
2:B:115:ILE:CD1	2:B:115:ILE:C	2.87	0.47
2:B:117:LEU:HD12	2:B:121:ARG:HH12	1.80	0.47
2:B:335:ILE:O	2:B:337:THR:N	2.47	0.47
2:B:384:ILE:HG22	2:B:388:TRP:CD1	2.49	0.47
1:A:176:LYS:HG3	1:A:177:VAL:H	1.78	0.47
2:B:145:THR:H	5:B:500:GTP:PG	2.37	0.47
2:B:147:SER:O	2:B:190:THR:HG23	2.14	0.47
2:B:149:PHE:O	2:B:150:THR:C	2.56	0.47
2:B:154:MET:HA	2:B:157:LEU:HD12	1.96	0.47
2:B:210:TYR:CE1	2:B:227:LEU:HD21	2.49	0.47
1:A:187:ALA:O	1:A:188:THR:C	2.57	0.47
1:A:237:GLY:O	1:A:241:CYS:CB	2.61	0.47
2:B:11:GLN:O	2:B:15:GLN:HG3	2.15	0.47
2:B:155:GLU:HA	2:B:197:HIS:CE1	2.49	0.47
2:B:185:TYR:OH	2:B:399:TYR:HA	2.15	0.47
2:B:386:GLU:O	2:B:388:TRP:N	2.47	0.47
3:C:261:LEU:HA	3:C:264:VAL:HG22	1.96	0.47
1:A:12:CYS:C	1:A:14:ASN:N	2.71	0.47
1:A:168:THR:N	1:A:200:GLU:O	2.43	0.47
1:A:226:ASP:O	1:A:229:HIS:HB3	2.14	0.47
1:A:264:ARG:NE	3:C:278:ARG:CZ	2.77	0.47
1:A:346:TRP:CD1	2:B:401:LYS:HZ2	2.33	0.47
1:A:384:ILE:O	1:A:384:ILE:HG23	2.14	0.47
2:B:132:LEU:HD21	2:B:164:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:THR:O	2:B:195:LEU:HB2	2.15	0.47
2:B:260:VAL:O	2:B:260:VAL:CG2	2.62	0.47
3:C:84:TYR:CD1	3:C:315:THR:HG23	2.50	0.47
3:C:191:HIS:HA	3:C:197:MET:SD	2.54	0.47
1:A:103:TRP:CE3	1:A:189:LEU:HD13	2.50	0.47
1:A:237:GLY:HA3	1:A:376:THR:OG1	2.15	0.47
1:A:260:VAL:HG21	2:B:407:TRP:HZ2	1.80	0.47
2:B:62:VAL:HA	2:B:86:LEU:O	2.15	0.47
2:B:155:GLU:HG2	2:B:197:HIS:CE1	2.49	0.47
2:B:231:ILE:C	2:B:233:GLN:N	2.73	0.47
3:C:156:HIS:HB2	3:C:164:TYR:CE1	2.50	0.47
1:A:4:ILE:HG22	1:A:5:VAL:N	2.27	0.47
1:A:101:ASN:ND2	1:A:101:ASN:O	2.48	0.47
1:A:242:LEU:CD1	1:A:250:ALA:HB3	2.45	0.47
2:B:404:PHE:CD1	2:B:404:PHE:N	2.83	0.47
1:A:72:PRO:O	1:A:73:GLY:C	2.58	0.47
2:B:104:ALA:HB1	2:B:413:MET:HG3	1.95	0.47
2:B:151:SER:OG	2:B:193:THR:HG21	2.13	0.47
2:B:226:ASN:O	2:B:229:ARG:N	2.48	0.47
2:B:335:ILE:C	2:B:337:THR:N	2.73	0.47
1:A:115:VAL:CG2	1:A:152:LEU:HD23	2.44	0.46
1:A:199:ASP:C	1:A:265:LEU:HD13	2.40	0.46
1:A:307:PRO:C	1:A:309:HIS:N	2.71	0.46
2:B:148:GLY:O	2:B:151:SER:CB	2.61	0.46
2:B:328:VAL:C	2:B:330:ALA:N	2.73	0.46
2:B:388:TRP:HA	2:B:388:TRP:HE3	1.79	0.46
2:B:436:GLY:O	2:B:438:ASP:N	2.48	0.46
1:A:2:ARG:NH1	1:A:251:ASP:CG	2.73	0.46
2:B:63:PRO:HG3	2:B:87:PHE:CG	2.50	0.46
2:B:316:CYS:HB3	2:B:378:LEU:HD12	1.95	0.46
2:B:317:LEU:CD1	2:B:351:PHE:CD1	2.97	0.46
3:C:300:ILE:CD1	3:C:316:LEU:HD23	2.45	0.46
1:A:297:ASP:OD2	1:A:299:LYS:HE2	2.14	0.46
1:A:421:ALA:O	1:A:422:GLU:C	2.58	0.46
2:B:119:LEU:HD11	2:B:156:ARG:HD2	1.97	0.46
2:B:120:ASP:O	2:B:124:LYS:HB2	2.15	0.46
2:B:256:GLN:HA	2:B:260:VAL:HG13	1.97	0.46
2:B:384:ILE:HG22	2:B:384:ILE:O	2.15	0.46
1:A:242:LEU:HD11	1:A:250:ALA:HB3	1.97	0.46
2:B:7:ILE:HD11	2:B:137:VAL:CG2	2.44	0.46
2:B:23:LEU:CD2	2:B:232:GLY:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ARG:NH2	2:B:252:LEU:CB	2.78	0.46
2:B:256:GLN:O	2:B:260:VAL:HG13	2.15	0.46
2:B:407:TRP:O	2:B:411:GLU:CG	2.63	0.46
1:A:262:PHE:HA	1:A:263:PRO:HD2	1.65	0.46
2:B:81:GLY:O	2:B:82:THR:C	2.59	0.46
2:B:145:THR:O	2:B:149:PHE:HB3	2.15	0.46
1:A:208:ALA:O	1:A:212:ILE:HG13	2.16	0.46
1:A:324:SER:OG	1:A:326:LYS:HB3	2.15	0.46
1:A:431:GLU:HA	1:A:434:GLN:HG3	1.97	0.46
3:C:37:ASP:O	3:C:51:VAL:HG23	2.15	0.46
3:C:38:THR:HG22	3:C:39:VAL:N	2.30	0.46
3:C:300:ILE:HD12	3:C:316:LEU:HD23	1.98	0.46
1:A:185:TYR:HD1	1:A:395:PHE:CE1	2.33	0.46
1:A:287:THR:N	1:A:290:GLU:OE1	2.48	0.46
1:A:380:ASN:C	1:A:380:ASN:HD22	2.24	0.46
1:A:409:THR:C	1:A:411:GLU:N	2.73	0.46
1:A:67:LEU:HD12	1:A:92:PHE:CD1	2.51	0.46
1:A:94:PHE:CD1	1:A:94:PHE:N	2.84	0.46
1:A:137:LEU:HD22	1:A:154:ILE:HG23	1.97	0.46
1:A:259:MET:HE1	1:A:378:ILE:CG2	2.45	0.46
1:A:435:TYR:C	1:A:437:ASP:N	2.72	0.46
2:B:5:ILE:CG2	2:B:6:SER:H	2.29	0.46
2:B:203:MET:SD	2:B:267:PHE:CB	3.04	0.46
2:B:210:TYR:CZ	2:B:227:LEU:HD11	2.51	0.46
2:B:265:GLY:O	2:B:266:HIS:O	2.33	0.46
1:A:387:LEU:O	1:A:387:LEU:HG	2.15	0.46
2:B:19:ALA:HB2	2:B:228:ASN:HB3	1.96	0.46
2:B:95:GLY:C	2:B:97:GLU:H	2.23	0.46
2:B:324:VAL:HG12	2:B:326:LYS:H	1.81	0.46
2:B:346:TRP:HZ2	2:B:435:VAL:HG12	1.81	0.46
2:B:392:ASP:OD1	2:B:422:ARG:NE	2.48	0.46
3:C:131:LYS:HG2	3:C:172:PHE:CD1	2.51	0.46
3:C:209:LEU:HD21	3:C:226:LYS:HB3	1.98	0.46
3:C:309:GLU:HB3	3:C:313:LYS:HZ1	1.79	0.46
1:A:102:ASN:ND2	1:A:104:ALA:HB3	2.31	0.46
1:A:115:VAL:HG21	1:A:152:LEU:HD21	1.98	0.46
1:A:133:GLN:O	1:A:165:ILE:CD1	2.64	0.46
1:A:134:GLY:HA3	1:A:165:ILE:HG12	1.97	0.46
1:A:360:PRO:HG2	1:A:371:LEU:CB	2.38	0.46
1:A:427:ASP:OD1	1:A:427:ASP:C	2.57	0.46
2:B:130:THR:O	2:B:131:GLY:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LEU:C	2:B:152:LEU:CD1	2.89	0.46
2:B:392:ASP:OD1	2:B:422:ARG:CZ	2.65	0.46
2:B:401:LYS:C	2:B:403:ALA:H	2.24	0.46
2:B:434:GLU:C	2:B:436:GLY:N	2.74	0.46
3:C:86:GLN:HA	3:C:236:GLU:OE1	2.15	0.46
1:A:210:TYR:O	1:A:211:ASP:C	2.57	0.45
1:A:230:LEU:CG	1:A:302:MET:HE2	2.46	0.45
1:A:243:ARG:HD3	1:A:243:ARG:HA	1.62	0.45
2:B:308:ARG:O	2:B:309:HIS:HB3	2.16	0.45
2:B:317:LEU:CD1	2:B:351:PHE:CE1	2.99	0.45
2:B:381:THR:O	2:B:383:ALA:N	2.49	0.45
3:C:262:GLY:O	3:C:321:ARG:HD3	2.15	0.45
1:A:210:TYR:CE1	1:A:227:LEU:HD11	2.52	0.45
1:A:408:TYR:O	1:A:411:GLU:HB2	2.15	0.45
1:A:409:THR:HA	1:A:413:MET:HB3	1.98	0.45
2:B:9:VAL:HG21	2:B:149:PHE:HD1	1.80	0.45
2:B:210:TYR:CD1	2:B:227:LEU:HD21	2.51	0.45
2:B:243:ARG:NH2	2:B:252:LEU:HB2	2.30	0.45
1:A:72:PRO:O	1:A:74:THR:N	2.49	0.45
1:A:259:MET:HE1	1:A:378:ILE:HG21	1.98	0.45
2:B:132:LEU:H	2:B:132:LEU:CD2	2.23	0.45
2:B:204:VAL:HG21	2:B:231:ILE:HG23	1.97	0.45
2:B:230:LEU:O	2:B:231:ILE:C	2.57	0.45
3:C:98:LYS:O	3:C:105:MET:HA	2.16	0.45
3:C:264:VAL:O	3:C:268:LEU:HG	2.16	0.45
1:A:6:HIS:HB3	1:A:21:TRP:HZ2	1.81	0.45
1:A:135:PHE:CD1	1:A:135:PHE:N	2.85	0.45
1:A:196:GLU:O	1:A:197:ASN:OD1	2.34	0.45
1:A:264:ARG:HA	1:A:264:ARG:NE	2.29	0.45
1:A:423:SER:O	1:A:424:ASN:C	2.60	0.45
2:B:5:ILE:HG22	2:B:6:SER:H	1.78	0.45
2:B:5:ILE:HD11	2:B:64:ARG:NH2	2.31	0.45
2:B:212:ILE:HD11	2:B:302:MET:H	1.82	0.45
2:B:274:PRO:HB2	2:B:371:VAL:HG21	1.98	0.45
2:B:70:LEU:HD12	2:B:145:THR:HG21	1.95	0.45
2:B:114:ILE:O	2:B:118:VAL:HG23	2.15	0.45
2:B:204:VAL:O	2:B:204:VAL:HG12	2.17	0.45
2:B:271:THR:O	2:B:376:CYS:HA	2.17	0.45
1:A:11:GLN:O	1:A:14:ASN:HB3	2.16	0.45
1:A:209:LEU:HD23	1:A:227:LEU:HD13	1.98	0.45
1:A:319:PHE:CD2	1:A:323:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MET:HE1	1:A:355:VAL:HG21	1.99	0.45
2:B:54:SER:O	2:B:61:HIS:O	2.35	0.45
2:B:100:ALA:C	2:B:102:ASN:H	2.24	0.45
2:B:393:HIS:O	2:B:394:LYS:C	2.59	0.45
2:B:413:MET:C	2:B:414:GLU:CG	2.90	0.45
3:C:208:PHE:CE2	3:C:210:ILE:CD1	2.95	0.45
1:A:12:CYS:O	1:A:13:GLY:C	2.59	0.45
1:A:245:PRO:HA	2:B:73:THR:CG2	2.46	0.45
1:A:250:ALA:HB1	1:A:254:LYS:CB	2.43	0.45
1:A:324:SER:O	1:A:326:LYS:N	2.50	0.45
2:B:115:ILE:CG1	2:B:152:LEU:HD13	2.46	0.45
2:B:425:MET:O	2:B:426:ALA:C	2.60	0.45
3:C:4:PRO:HD3	3:C:293:ASN:OD1	2.17	0.45
1:A:98:GLY:C	1:A:100:GLY:H	2.24	0.45
1:A:154:ILE:HD12	1:A:155:SER:N	2.31	0.45
1:A:175:PRO:HG2	1:A:207:GLU:OE1	2.17	0.45
1:A:282:GLN:O	1:A:282:GLN:CG	2.65	0.45
2:B:231:ILE:HD13	2:B:231:ILE:H	1.82	0.45
2:B:295:CYS:SG	2:B:375:VAL:HG11	2.57	0.45
1:A:113:GLU:CG	1:A:114:LEU:N	2.79	0.45
1:A:189:LEU:HD23	1:A:421:ALA:CB	2.47	0.45
1:A:242:LEU:HD22	1:A:250:ALA:O	2.17	0.45
1:A:312:TYR:HA	1:A:381:SER:HA	1.99	0.45
2:B:334:THR:CG2	2:B:335:ILE:N	2.79	0.45
2:B:423:GLU:O	2:B:426:ALA:HB3	2.16	0.45
3:C:211:ASN:OD1	3:C:213:LYS:HE3	2.16	0.45
3:C:221:GLN:OE1	3:C:221:GLN:HA	2.17	0.45
1:A:194:LEU:O	1:A:265:LEU:HD23	2.16	0.45
1:A:313:LEU:O	1:A:347:ILE:HD12	2.16	0.45
2:B:182:VAL:O	2:B:183:GLU:C	2.60	0.44
2:B:408:TYR:CG	2:B:418:PHE:HZ	2.34	0.44
3:C:69:ILE:HD12	3:C:295:ARG:HB2	1.99	0.44
3:C:153:LEU:N	3:C:153:LEU:HD22	2.32	0.44
1:A:23:VAL:O	1:A:25:SER:N	2.50	0.44
1:A:23:VAL:O	1:A:24:ILE:C	2.60	0.44
1:A:67:LEU:HD12	1:A:92:PHE:CE1	2.52	0.44
1:A:70:LEU:HD21	1:A:149:MET:HE3	1.98	0.44
1:A:243:ARG:HH21	1:A:252:LEU:N	2.13	0.44
1:A:280:SER:OG	1:A:281:GLN:N	2.49	0.44
1:A:295:MET:SD	1:A:375:ALA:HB3	2.58	0.44
2:B:103:TYR:CD1	2:B:148:GLY:HA2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD12	1:A:239:THR:HG21	1.98	0.44
1:A:14:ASN:O	1:A:17:GLY:N	2.50	0.44
1:A:106:GLY:O	1:A:149:MET:HB2	2.16	0.44
1:A:167:ASN:HA	1:A:200:GLU:O	2.17	0.44
1:A:288:VAL:N	1:A:289:PRO:CD	2.79	0.44
2:B:12:ALA:HB2	5:B:500:GTP:C8	2.52	0.44
2:B:121:ARG:HG2	2:B:121:ARG:HH11	1.83	0.44
2:B:182:VAL:O	2:B:184:PRO:CD	2.65	0.44
1:A:167:ASN:HD21	1:A:252:LEU:HD22	1.82	0.44
2:B:84:ARG:HE	2:B:84:ARG:HB3	1.51	0.44
2:B:121:ARG:HG2	2:B:121:ARG:NH1	2.33	0.44
2:B:272:TYR:CE2	2:B:274:PRO:HD2	2.53	0.44
2:B:276:ILE:CG2	2:B:369:ALA:CB	2.91	0.44
2:B:301:GLN:O	2:B:302:MET:C	2.61	0.44
2:B:402:ARG:O	2:B:405:VAL:N	2.49	0.44
3:C:134:TYR:HD1	3:C:145:LEU:HD12	1.69	0.44
1:A:8:GLN:CG	1:A:67:LEU:HD22	2.47	0.44
1:A:141:LEU:N	1:A:141:LEU:HD12	2.32	0.44
2:B:226:ASN:O	2:B:227:LEU:C	2.59	0.44
2:B:229:ARG:NH1	2:B:229:ARG:HG2	2.31	0.44
2:B:296:PHE:HZ	2:B:351:PHE:HZ	1.66	0.44
1:A:147:SER:HB2	1:A:190:SER:CB	2.41	0.44
1:A:188:THR:HG23	1:A:425:MET:HE3	1.98	0.44
1:A:332:MET:CE	1:A:351:VAL:HG11	2.32	0.44
2:B:88:HIS:C	2:B:90:GLU:N	2.74	0.44
2:B:117:LEU:HD11	2:B:121:ARG:NH2	2.30	0.44
2:B:175:PRO:CG	2:B:304:LYS:HG2	2.47	0.44
2:B:344:VAL:CG1	2:B:345:ASP:N	2.78	0.44
1:A:82:PRO:HB2	1:A:83:PHE:H	1.56	0.44
1:A:402:LYS:O	1:A:403:ALA:C	2.61	0.44
2:B:49:PHE:HE1	2:B:61:HIS:CE1	2.34	0.44
3:C:115:ILE:O	3:C:119:ILE:HG13	2.17	0.44
1:A:99:ALA:O	1:A:100:GLY:C	2.60	0.44
1:A:273:ALA:CB	1:A:274:PRO:CD	2.93	0.44
2:B:23:LEU:O	2:B:26:LEU:HB3	2.17	0.44
2:B:64:ARG:HD2	2:B:125:LEU:HD22	1.99	0.44
3:C:16:ARG:HD3	3:C:89:SER:O	2.18	0.44
2:B:217:LEU:HD13	2:B:277:SER:N	2.33	0.44
2:B:262:TYR:HB3	2:B:263:PRO:HD2	2.00	0.44
2:B:304:LYS:HG3	2:B:304:LYS:O	2.18	0.44
2:B:328:VAL:O	2:B:330:ALA:N	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:LYS:HB3	3:C:306:SER:HB3	2.00	0.44
3:C:80:THR:OG1	3:C:296:THR:HG23	2.18	0.44
3:C:107:ILE:O	3:C:111:ILE:HG13	2.18	0.44
1:A:352:LYS:HD3	1:A:352:LYS:C	2.43	0.43
2:B:119:LEU:O	2:B:120:ASP:C	2.61	0.43
2:B:363:VAL:CG1	2:B:364:PRO:HD2	2.48	0.43
1:A:42:LEU:C	1:A:44:LEU:H	2.26	0.43
1:A:70:LEU:HB2	1:A:99:ALA:CB	2.49	0.43
1:A:288:VAL:N	1:A:289:PRO:HD2	2.32	0.43
2:B:151:SER:HB3	2:B:193:THR:CG2	2.34	0.43
2:B:268:PRO:CA	2:B:379:SER:O	2.65	0.43
1:A:7:ILE:N	1:A:136:GLN:O	2.51	0.43
1:A:95:GLY:C	1:A:97:SER:H	2.25	0.43
1:A:103:TRP:HB2	1:A:186:ASN:HA	2.01	0.43
1:A:161:TYR:O	1:A:163:ASP:N	2.51	0.43
2:B:166:LYS:CE	2:B:199:ASP:OD1	2.62	0.43
2:B:209:ILE:CD1	2:B:231:ILE:HD11	2.47	0.43
2:B:276:ILE:O	2:B:369:ALA:CA	2.66	0.43
2:B:303:VAL:O	2:B:303:VAL:CG1	2.64	0.43
2:B:388:TRP:CD2	2:B:425:MET:HE1	2.52	0.43
3:C:143:ARG:HH22	3:C:190:ARG:HA	1.84	0.43
1:A:105:LYS:HG2	1:A:110:GLU:CG	2.48	0.43
1:A:269:MET:HB2	1:A:301:MET:HE3	2.00	0.43
1:A:299:LYS:H	1:A:299:LYS:CD	2.07	0.43
1:A:345:GLU:C	1:A:347:ILE:N	2.77	0.43
2:B:105:ARG:O	2:B:110:ILE:CG2	2.64	0.43
2:B:362:VAL:HG13	2:B:368:LEU:CG	2.48	0.43
2:B:384:ILE:O	2:B:385:ALA:C	2.59	0.43
2:B:390:ARG:HG3	2:B:390:ARG:HH11	1.83	0.43
1:A:72:PRO:HG2	1:A:73:GLY:H	1.83	0.43
1:A:102:ASN:OD1	1:A:408:TYR:CZ	2.70	0.43
2:B:8:HIS:HA	2:B:138:PHE:HB2	2.00	0.43
2:B:108:TYR:O	2:B:109:THR:C	2.61	0.43
2:B:153:LEU:O	2:B:157:LEU:HG	2.18	0.43
3:C:127:GLU:O	3:C:214:GLN:HA	2.19	0.43
1:A:37:HIS:O	1:A:38:GLY:C	2.61	0.43
2:B:377:MET:HG3	2:B:377:MET:O	2.18	0.43
2:B:398:MET:HE3	2:B:398:MET:HB2	1.78	0.43
3:C:219:THR:HG21	3:C:221:GLN:HG2	1.93	0.43
3:C:274:TYR:CD1	3:C:274:TYR:C	2.96	0.43
2:B:310:GLY:HA3	2:B:383:ALA:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:LEU:HD12	2:B:378:LEU:O	2.19	0.43
3:C:108:ILE:CB	3:C:109:PRO:HD3	2.38	0.43
1:A:68:VAL:HG11	1:A:153:LEU:HD21	2.00	0.43
1:A:330:GLU:O	1:A:331:GLN:C	2.61	0.43
1:A:409:THR:O	1:A:412:GLY:N	2.48	0.43
1:A:435:TYR:C	1:A:437:ASP:H	2.27	0.43
2:B:4:CYS:SG	2:B:252:LEU:CD1	3.02	0.43
2:B:8:HIS:CD2	2:B:138:PHE:CD2	3.07	0.43
2:B:343:PHE:CE1	2:B:351:PHE:HE2	2.36	0.43
3:C:318:PHE:CD1	3:C:318:PHE:C	2.96	0.43
1:A:52:TYR:HE2	1:A:240:THR:HB	1.82	0.43
1:A:168:THR:CG2	1:A:201:THR:HG23	2.48	0.43
3:C:74:LEU:HD13	3:C:118:TYR:CD1	2.53	0.43
3:C:87:THR:HA	3:C:91:LYS:HZ1	1.84	0.43
3:C:138:TYR:HB2	3:C:204:SER:OG	2.18	0.43
1:A:118:VAL:O	1:A:119:LEU:C	2.62	0.43
1:A:118:VAL:O	1:A:122:VAL:HG13	2.19	0.43
1:A:389:LYS:O	1:A:390:ARG:C	2.62	0.43
2:B:140:SER:O	2:B:141:PHE:C	2.62	0.43
2:B:293:ASN:HD21	2:B:338:LYS:HZ1	1.67	0.43
2:B:384:ILE:C	2:B:386:GLU:N	2.72	0.43
1:A:192:HIS:NE2	1:A:420:GLU:HG2	2.34	0.42
1:A:240:THR:HG23	1:A:241:CYS:N	2.33	0.42
1:A:249:ASN:OD1	2:B:71:GLU:OE1	2.36	0.42
1:A:250:ALA:CB	1:A:254:LYS:HE2	2.49	0.42
2:B:7:ILE:HG13	2:B:137:VAL:HG22	1.97	0.42
2:B:16:ILE:CG2	2:B:17:GLY:N	2.82	0.42
2:B:119:LEU:HD11	2:B:156:ARG:HD3	2.01	0.42
2:B:147:SER:HB2	2:B:186:ASN:O	2.19	0.42
1:A:6:HIS:HB3	1:A:65:ALA:CB	2.49	0.42
1:A:153:LEU:HD13	1:A:153:LEU:N	2.34	0.42
1:A:161:TYR:CD1	1:A:161:TYR:N	2.86	0.42
1:A:210:TYR:O	1:A:214:PHE:N	2.52	0.42
1:A:282:GLN:HB3	1:A:282:GLN:HE21	1.50	0.42
1:A:301:MET:O	1:A:303:ALA:N	2.51	0.42
2:B:12:ALA:C	2:B:14:VAL:N	2.75	0.42
2:B:184:PRO:HG2	2:B:398:MET:CE	2.40	0.42
3:C:37:ASP:C	3:C:51:VAL:HG23	2.44	0.42
3:C:326:LYS:HD3	3:C:326:LYS:HA	1.90	0.42
1:A:138:THR:O	1:A:139:HIS:HB3	2.19	0.42
1:A:178:SER:C	1:A:180:THR:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ILE:O	1:A:212:ILE:HG22	2.18	0.42
2:B:63:PRO:HG3	2:B:87:PHE:CD2	2.54	0.42
2:B:268:PRO:C	2:B:269:LEU:HD23	2.44	0.42
2:B:292:THR:O	2:B:295:CYS:HB2	2.18	0.42
2:B:363:VAL:HG13	2:B:364:PRO:HD2	2.02	0.42
2:B:399:TYR:C	2:B:401:LYS:N	2.77	0.42
3:C:80:THR:HG23	3:C:289:SER:HB3	2.01	0.42
1:A:121:VAL:C	1:A:123:ARG:N	2.77	0.42
1:A:332:MET:HE3	1:A:351:VAL:CG1	2.32	0.42
2:B:25:CYS:SG	2:B:26:LEU:N	2.92	0.42
2:B:209:ILE:CD1	2:B:231:ILE:CD1	2.97	0.42
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.77	0.42
1:A:390:ARG:O	1:A:391:ILE:C	2.61	0.42
2:B:104:ALA:HB3	2:B:408:TYR:HD1	1.84	0.42
3:C:38:THR:CG2	3:C:39:VAL:N	2.82	0.42
3:C:46:TYR:CD1	3:C:316:LEU:HD13	2.54	0.42
1:A:106:GLY:O	1:A:149:MET:CA	2.68	0.42
1:A:413:MET:CG	1:A:414:ASP:H	2.26	0.42
1:A:82:PRO:C	1:A:84:GLY:N	2.78	0.42
2:B:173:PRO:HG3	2:B:183:GLU:CD	2.45	0.42
2:B:175:PRO:HG3	2:B:304:LYS:CB	2.50	0.42
2:B:204:VAL:CG1	2:B:231:ILE:HD12	2.42	0.42
1:A:175:PRO:O	1:A:177:VAL:N	2.53	0.42
1:A:204:ILE:HD13	1:A:231:VAL:CG2	2.45	0.42
2:B:15:GLN:NE2	5:B:500:GTP:N7	2.67	0.42
2:B:213:CYS:O	2:B:219:ILE:HG13	2.20	0.42
3:C:73:VAL:HA	3:C:77:TYR:O	2.19	0.42
1:A:310:GLY:HA3	1:A:436:GLN:NE2	2.29	0.42
2:B:13:GLY:HA2	2:B:16:ILE:CG2	2.50	0.42
2:B:24:TYR:O	2:B:25:CYS:C	2.63	0.42
2:B:199:ASP:OD2	2:B:256:GLN:NE2	2.46	0.42
2:B:238:ILE:O	2:B:242:LEU:CB	2.67	0.42
2:B:238:ILE:HD11	2:B:378:LEU:HD23	2.01	0.42
2:B:280:LYS:O	2:B:282:TYR:N	2.52	0.42
3:C:281:LYS:O	3:C:285:ILE:HG13	2.20	0.42
2:B:274:PRO:C	2:B:275:VAL:CA	2.89	0.42
2:B:335:ILE:C	2:B:337:THR:H	2.28	0.42
2:B:414:GLU:C	2:B:416:GLY:N	2.74	0.42
1:A:261:PRO:HB2	1:A:262:PHE:CD2	2.54	0.41
1:A:297:ASP:CG	1:A:299:LYS:HE2	2.45	0.41
1:A:422:GLU:O	1:A:426:ASN:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ARG:NH2	2:B:252:LEU:HG	2.35	0.41
2:B:255:PHE:O	2:B:257:THR:N	2.53	0.41
2:B:292:THR:HG21	2:B:331:ALA:HB1	2.02	0.41
1:A:62:VAL:HA	1:A:63:PRO:HD2	1.92	0.41
1:A:147:SER:CB	1:A:190:SER:HB3	2.42	0.41
1:A:171:VAL:O	1:A:171:VAL:HG12	2.20	0.41
1:A:343:PHE:CD1	1:A:350:ASN:ND2	2.88	0.41
1:A:359:PRO:CB	1:A:360:PRO:HD2	2.45	0.41
2:B:265:GLY:O	2:B:266:HIS:C	2.63	0.41
2:B:383:ALA:C	2:B:385:ALA:N	2.78	0.41
3:C:105:MET:HB2	3:C:109:PRO:HB2	2.01	0.41
1:A:48:ARG:HG2	1:A:243:ARG:HB3	2.01	0.41
3:C:62:TYR:OH	3:C:70:VAL:HG21	2.19	0.41
3:C:139:LEU:N	3:C:139:LEU:HD22	2.34	0.41
1:A:399:PHE:O	1:A:401:ARG:N	2.53	0.41
1:A:417:GLU:O	1:A:420:GLU:HB3	2.21	0.41
2:B:231:ILE:C	2:B:233:GLN:H	2.28	0.41
2:B:244:PHE:HD1	2:B:244:PHE:C	2.24	0.41
2:B:296:PHE:CG	2:B:341:ILE:HD12	2.53	0.41
2:B:386:GLU:O	2:B:387:ALA:C	2.63	0.41
3:C:20:GLU:HA	3:C:23:VAL:HG12	2.03	0.41
3:C:207:ILE:HD13	3:C:230:VAL:HG13	2.02	0.41
1:A:301:MET:C	1:A:303:ALA:N	2.77	0.41
1:A:307:PRO:O	1:A:309:HIS:N	2.53	0.41
1:A:395:PHE:HB3	1:A:396:THR:H	1.73	0.41
2:B:199:ASP:CB	2:B:256:GLN:NE2	2.77	0.41
3:C:34:GLN:HE21	3:C:34:GLN:HB3	1.64	0.41
1:A:24:ILE:CG2	1:A:25:SER:N	2.80	0.41
1:A:52:TYR:C	1:A:53:TYR:CD1	2.99	0.41
1:A:242:LEU:HB3	1:A:250:ALA:O	2.20	0.41
1:A:259:MET:HE3	1:A:268:PHE:CZ	2.56	0.41
1:A:333:LEU:HD11	1:A:337:ASN:HD21	1.85	0.41
2:B:161:TYR:C	2:B:163:LYS:N	2.77	0.41
2:B:242:LEU:HD11	2:B:250:VAL:HG23	2.02	0.41
2:B:408:TYR:O	2:B:409:VAL:C	2.63	0.41
3:C:23:VAL:HG13	3:C:24:ASN:N	2.34	0.41
3:C:87:THR:O	3:C:88:SER:HB2	2.21	0.41
3:C:105:MET:HE3	3:C:110:ARG:HG2	2.03	0.41
3:C:150:LYS:HB3	3:C:153:LEU:HD11	2.02	0.41
3:C:255:ASN:HB3	3:C:258:LEU:HG	2.02	0.41
1:A:119:LEU:O	1:A:122:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:CD1	1:A:166:MET:SD	3.14	0.41
2:B:95:GLY:O	2:B:96:LYS:C	2.64	0.41
2:B:343:PHE:HZ	2:B:351:PHE:CZ	2.36	0.41
2:B:397:LEU:HA	2:B:397:LEU:HD23	1.81	0.41
3:C:219:THR:O	3:C:220:GLU:HB2	2.21	0.41
1:A:150:GLY:HA2	1:A:153:LEU:CD2	2.42	0.41
1:A:182:VAL:O	1:A:184:PRO:N	2.54	0.41
1:A:11:GLN:O	1:A:15:GLN:N	2.41	0.41
1:A:25:SER:O	1:A:28:HIS:N	2.53	0.41
1:A:26:ASP:C	1:A:26:ASP:OD1	2.64	0.41
1:A:133:GLN:CG	1:A:165:ILE:HD11	2.49	0.41
1:A:168:THR:HB	1:A:198:THR:HG21	2.03	0.41
1:A:273:ALA:HB1	1:A:291:LEU:HG	2.02	0.41
1:A:311:ARG:HG2	1:A:311:ARG:NH1	2.34	0.41
2:B:11:GLN:CG	2:B:74:VAL:HG21	2.50	0.41
2:B:23:LEU:HD11	2:B:361:THR:O	2.21	0.41
2:B:115:ILE:CG2	2:B:116:ASP:H	2.32	0.41
2:B:248:LEU:HD12	2:B:248:LEU:HA	1.93	0.41
2:B:305:CYS:SG	2:B:383:ALA:HB1	2.60	0.41
2:B:332:ILE:CD1	2:B:353:VAL:HG22	2.51	0.41
3:C:275:VAL:HA	3:C:276:PRO:HD3	1.66	0.41
1:A:114:LEU:HD12	1:A:117:SER:OG	2.21	0.41
1:A:405:LEU:HD23	1:A:405:LEU:O	2.21	0.41
2:B:207:GLU:C	2:B:209:ILE:H	2.29	0.41
2:B:251:ASP:CA	2:B:254:GLU:HG3	2.48	0.41
3:C:173:VAL:HG23	3:C:173:VAL:O	2.20	0.41
3:C:270:GLU:CG	3:C:272:SER:HB3	2.51	0.41
1:A:20:PHE:CD1	1:A:235:MET:CG	3.04	0.40
1:A:202:TYR:CE2	1:A:268:PHE:HD2	2.38	0.40
1:A:287:THR:O	1:A:288:VAL:CG2	2.58	0.40
2:B:34:GLY:O	2:B:61:HIS:HB2	2.20	0.40
2:B:260:VAL:HA	2:B:261:PRO:HD3	1.95	0.40
3:C:57:SER:OG	3:C:60:GLN:HG3	2.22	0.40
1:A:78:VAL:O	1:A:84:GLY:HA3	2.22	0.40
1:A:105:LYS:HG2	1:A:110:GLU:HG3	2.03	0.40
1:A:187:ALA:O	1:A:190:SER:N	2.54	0.40
2:B:166:LYS:HB2	2:B:199:ASP:OD1	2.20	0.40
2:B:272:TYR:O	2:B:300:ASN:ND2	2.54	0.40
2:B:362:VAL:HG13	2:B:368:LEU:CB	2.50	0.40
3:C:95:MET:HA	3:C:95:MET:HE3	2.02	0.40
1:A:11:GLN:HA	1:A:74:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HB2	1:A:99:ALA:HB2	2.03	0.40
1:A:239:THR:CG2	1:A:240:THR:H	2.34	0.40
2:B:11:GLN:HG3	2:B:74:VAL:HG21	2.04	0.40
2:B:172:TYR:OH	2:B:387:ALA:C	2.64	0.40
2:B:209:ILE:HD13	2:B:231:ILE:HD11	2.04	0.40
2:B:405:VAL:C	2:B:407:TRP:N	2.79	0.40
3:C:23:VAL:CG1	3:C:24:ASN:N	2.84	0.40
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.78	0.40
2:B:30:ILE:HG23	2:B:34:GLY:C	2.47	0.40
2:B:71:GLU:HA	2:B:72:PRO:HD3	1.89	0.40
2:B:147:SER:OG	2:B:148:GLY:N	2.54	0.40
2:B:184:PRO:O	2:B:185:TYR:C	2.62	0.40
2:B:293:ASN:ND2	2:B:338:LYS:NZ	2.69	0.40
1:A:12:CYS:O	1:A:14:ASN:N	2.55	0.40
1:A:14:ASN:O	1:A:15:GLN:C	2.64	0.40
1:A:125:GLU:O	1:A:128:SER:HB3	2.22	0.40
1:A:291:LEU:HD21	1:A:373:MET:HG2	2.03	0.40
1:A:326:LYS:HB3	2:B:222:PRO:HD2	2.03	0.40
1:A:380:ASN:C	1:A:380:ASN:ND2	2.79	0.40
2:B:149:PHE:CD1	2:B:150:THR:N	2.89	0.40
2:B:287:SER:O	2:B:291:ILE:HG12	2.21	0.40
2:B:425:MET:O	2:B:428:LEU:N	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	4
2	B	423/452 (94%)	279 (66%)	87 (21%)	57 (14%)	0	4
3	C	306/340 (90%)	295 (96%)	8 (3%)	3 (1%)	12	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1153/1237 (93%)	848 (74%)	189 (16%)	116 (10%)	1 7

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	24	ILE
1	A	32	PRO
1	A	50	ASN
1	A	82	PRO
1	A	97	SER
1	A	128	SER
1	A	176	LYS
1	A	183	GLU
1	A	218	LYS
1	A	238	VAL
1	A	239	THR
1	A	240	THR
1	A	252	LEU
1	A	263	PRO
1	A	266	HIS
1	A	273	ALA
1	A	278	ARG
1	A	280	SER
1	A	281	GLN
1	A	282	GLN
1	A	288	VAL
1	A	294	GLN
1	A	295	MET
1	A	343	PHE
1	A	344	VAL
1	A	346	TRP
1	A	369	ARG
1	A	403	ALA
2	B	56	THR
2	B	58	ALA
2	B	96	LYS
2	B	97	GLU
2	B	108	TYR
2	B	109	THR
2	B	141	PHE
2	B	183	GLU

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Mol	Chain	Res	Type
2	B	217	LEU
2	B	240	ALA
2	B	249	ASN
2	B	255	PHE
2	B	266	HIS
2	B	309	HIS
2	B	346	TRP
2	B	370	LYS
2	B	387	ALA
2	B	403	ALA
2	B	437	VAL
3	C	4	PRO
1	A	38	GLY
1	A	73	GLY
1	A	175	PRO
1	A	265	LEU
1	A	279	GLY
1	A	298	ALA
1	A	300	ASN
1	A	311	ARG
2	B	24	TYR
2	B	73	THR
2	B	83	TYR
2	B	103	TYR
2	B	111	GLY
2	B	131	GLY
2	B	218	ASP
2	B	219	ILE
2	B	238	ILE
2	B	265	GLY
2	B	281	ALA
2	B	314	ALA
2	B	339	ARG
2	B	342	GLN
2	B	373	ARG
2	B	386	GLU
3	C	123	ASP
1	A	34	GLY
1	A	83	PHE
1	A	99	ALA
1	A	100	GLY
1	A	302	MET

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Mol	Chain	Res	Type
1	A	386	GLU
2	B	48	SER
2	B	104	ALA
2	B	148	GLY
2	B	149	PHE
2	B	173	PRO
2	B	239	THR
2	B	245	ASP
2	B	263	PRO
2	B	279	GLU
2	B	330	ALA
2	B	336	LYS
2	B	369	ALA
1	A	96	GLN
1	A	395	PHE
2	B	129	CYS
2	B	300	ASN
2	B	348	PRO
1	A	57	ALA
1	A	74	THR
1	A	285	ALA
1	A	424	ASN
2	B	256	GLN
2	B	303	VAL
2	B	382	THR
3	C	6	GLU
1	A	51	VAL
1	A	58	GLY
1	A	145	THR
1	A	162	PRO
1	A	400	ARG
2	B	62	VAL
2	B	273	ALA
2	B	307	PRO
1	A	195	VAL
2	B	115	ILE
1	A	72	PRO

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/381 (96%)	307 (84%)	60 (16%)	2	10
2	B	354/378 (94%)	288 (81%)	66 (19%)	1	8
3	C	279/303 (92%)	263 (94%)	16 (6%)	18	40
All	All	1000/1062 (94%)	858 (86%)	142 (14%)	5	13

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	26	ASP
1	A	32	PRO
1	A	41	ASP
1	A	67	LEU
1	A	68	VAL
1	A	90	ASP
1	A	94	PHE
1	A	121	VAL
1	A	122	VAL
1	A	129	CYS
1	A	135	PHE
1	A	141	LEU
1	A	145	THR
1	A	149	MET
1	A	151	THR
1	A	153	LEU
1	A	161	TYR
1	A	163	ASP
1	A	165	ILE
1	A	174	SER
1	A	193	GLN
1	A	198	THR
1	A	201	THR
1	A	203	CYS
1	A	207	GLU
1	A	211	ASP
1	A	214	PHE
1	A	227	LEU
1	A	229	HIS

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Mol	Chain	Res	Type
1	A	230	LEU
1	A	232	SER
1	A	236	SER
1	A	240	THR
1	A	265	LEU
1	A	267	PHE
1	A	275	LEU
1	A	282	GLN
1	A	284	ARG
1	A	299	LYS
1	A	306	ASP
1	A	309	HIS
1	A	314	THR
1	A	322	ARG
1	A	324	SER
1	A	325	MET
1	A	331	GLN
1	A	343	PHE
1	A	344	VAL
1	A	352	LYS
1	A	353	THR
1	A	369	ARG
1	A	387	LEU
1	A	413	MET
1	A	414	ASP
1	A	424	ASN
1	A	427	ASP
1	A	431	GLU
1	A	432	TYR
1	A	437	ASP
2	B	6	SER
2	B	7	ILE
2	B	16	ILE
2	B	20	CYS
2	B	31	GLN
2	B	36	MET
2	B	48	SER
2	B	50	ASN
2	B	60	LYS
2	B	61	HIS
2	B	62	VAL
2	B	73	THR

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Mol	Chain	Res	Type
2	B	74	VAL
2	B	79	ARG
2	B	82	THR
2	B	84	ARG
2	B	87	PHE
2	B	88	HIS
2	B	90	GLU
2	B	98	ASP
2	B	109	THR
2	B	115	ILE
2	B	120	ASP
2	B	125	LEU
2	B	130	THR
2	B	135	PHE
2	B	141	PHE
2	B	150	THR
2	B	152	LEU
2	B	154	MET
2	B	155	GLU
2	B	172	TYR
2	B	173	PRO
2	B	183	GLU
2	B	192	HIS
2	B	204	VAL
2	B	219	ILE
2	B	224	TYR
2	B	231	ILE
2	B	234	ILE
2	B	243	ARG
2	B	244	PHE
2	B	253	THR
2	B	260	VAL
2	B	267	PHE
2	B	269	LEU
2	B	279	GLU
2	B	280	LYS
2	B	288	VAL
2	B	290	GLU
2	B	303	VAL
2	B	325	PRO
2	B	328	VAL
2	B	334	THR

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Mol	Chain	Res	Type
2	B	345	ASP
2	B	352	LYS
2	B	368	LEU
2	B	376	CYS
2	B	377	MET
2	B	378	LEU
2	B	415	GLU
2	B	417	GLU
2	B	420	GLU
2	B	431	ASP
2	B	432	TYR
2	B	433	GLU
3	C	18	LEU
3	C	28	LYS
3	C	29	TYR
3	C	95	MET
3	C	127	GLU
3	C	153	LEU
3	C	204	SER
3	C	229	LEU
3	C	236	GLU
3	C	306	SER
3	C	308	ASN
3	C	323	LYS
3	C	324	THR
3	C	325	ILE
3	C	326	LYS
3	C	328	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	43	GLN
1	A	91	ASN
1	A	101	ASN
1	A	102	ASN
1	A	107	HIS
1	A	133	GLN
1	A	136	GLN
1	A	139	HIS
1	A	186	ASN

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Mol	Chain	Res	Type
1	A	282	GLN
1	A	331	GLN
1	A	334	ASN
1	A	336	GLN
1	A	337	ASN
1	A	349	ASN
1	A	380	ASN
1	A	385	GLN
1	A	406	HIS
1	A	434	GLN
1	A	436	GLN
2	B	11	GLN
2	B	15	GLN
2	B	50	ASN
2	B	61	HIS
2	B	91	GLN
2	B	101	ASN
2	B	133	GLN
2	B	139	HIS
2	B	197	HIS
2	B	216	ASN
2	B	226	ASN
2	B	256	GLN
2	B	309	HIS
3	C	34	GLN
3	C	58	GLN
3	C	125	ASN
3	C	156	HIS
3	C	189	ASN
3	C	191	HIS
3	C	198	ASN
3	C	214	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
4	GDP	A	600	-	29,30,30	2.85	11 (37%)	45,47,47	3.48	16 (35%)
5	GTP	B	500	-	33,34,34	2.05	5 (15%)	50,54,54	1.37	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	A	600	-	-	4/16/32/32	0/3/3/3
5	GTP	B	500	-	-	3/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GDP	PA-O3A	7.47	1.67	1.59
5	B	500	GTP	PA-O3A	-5.95	1.53	1.59
4	A	600	GDP	O6-C6	5.93	1.34	1.23
4	A	600	GDP	C8-N9	5.88	1.50	1.37
5	B	500	GTP	PB-O3A	-5.80	1.53	1.59
5	B	500	GTP	PB-O3B	5.52	1.65	1.59
4	A	600	GDP	C2-N1	4.77	1.49	1.37
4	A	600	GDP	PB-O2B	-3.93	1.40	1.54
5	B	500	GTP	PG-O1G	3.78	1.62	1.50
4	A	600	GDP	O4'-C1'	3.38	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GDP	C8-N7	3.03	1.41	1.32
4	A	600	GDP	C5-N7	-2.88	1.33	1.39
4	A	600	GDP	C5-C4	2.65	1.46	1.38
4	A	600	GDP	PB-O3B	2.44	1.63	1.54
4	A	600	GDP	C2-N3	-2.42	1.27	1.33
5	B	500	GTP	PB-O2B	-2.00	1.46	1.55

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	GDP	N9-C8-N7	-10.79	93.39	113.40
4	A	600	GDP	C8-N7-C5	9.24	120.72	104.26
4	A	600	GDP	C6-C5-N7	8.60	145.94	130.29
4	A	600	GDP	N2-C2-N3	6.29	131.94	119.67
4	A	600	GDP	C6-C5-C4	-6.21	109.49	118.83
4	A	600	GDP	C8-N9-C4	5.90	117.08	106.03
5	B	500	GTP	O2G-PG-O3B	5.04	121.52	104.64
4	A	600	GDP	C5-C6-N1	4.50	124.72	113.25
5	B	500	GTP	O3G-PG-O3B	4.41	119.44	104.64
4	A	600	GDP	N2-C2-N1	-4.25	107.80	116.76
4	A	600	GDP	C2-N3-C4	4.07	119.31	112.30
4	A	600	GDP	O6-C6-C5	-3.95	116.11	126.53
4	A	600	GDP	C4-C5-N7	-3.85	104.57	110.67
4	A	600	GDP	C2-N1-C6	-3.79	118.23	125.11
4	A	600	GDP	C2'-C3'-C4'	3.41	109.19	102.61
4	A	600	GDP	C1'-N9-C8	-2.69	119.09	126.73
5	B	500	GTP	O3G-PG-O2G	-2.67	97.77	107.80
5	B	500	GTP	O3A-PB-O1B	-2.43	103.39	110.70
4	A	600	GDP	O2'-C2'-C3'	2.27	119.10	111.82
5	B	500	GTP	O2B-PB-O3A	2.20	113.22	107.27
4	A	600	GDP	C4'-O4'-C1'	2.08	114.05	109.47
5	B	500	GTP	O5'-C5'-C4'	2.06	116.02	108.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GDP	PA-O3A-PB-O2B
4	A	600	GDP	C5'-O5'-PA-O3A
4	A	600	GDP	C5'-O5'-PA-O1A
5	B	500	GTP	C3'-C4'-C5'-O5'
5	B	500	GTP	O4'-C4'-C5'-O5'

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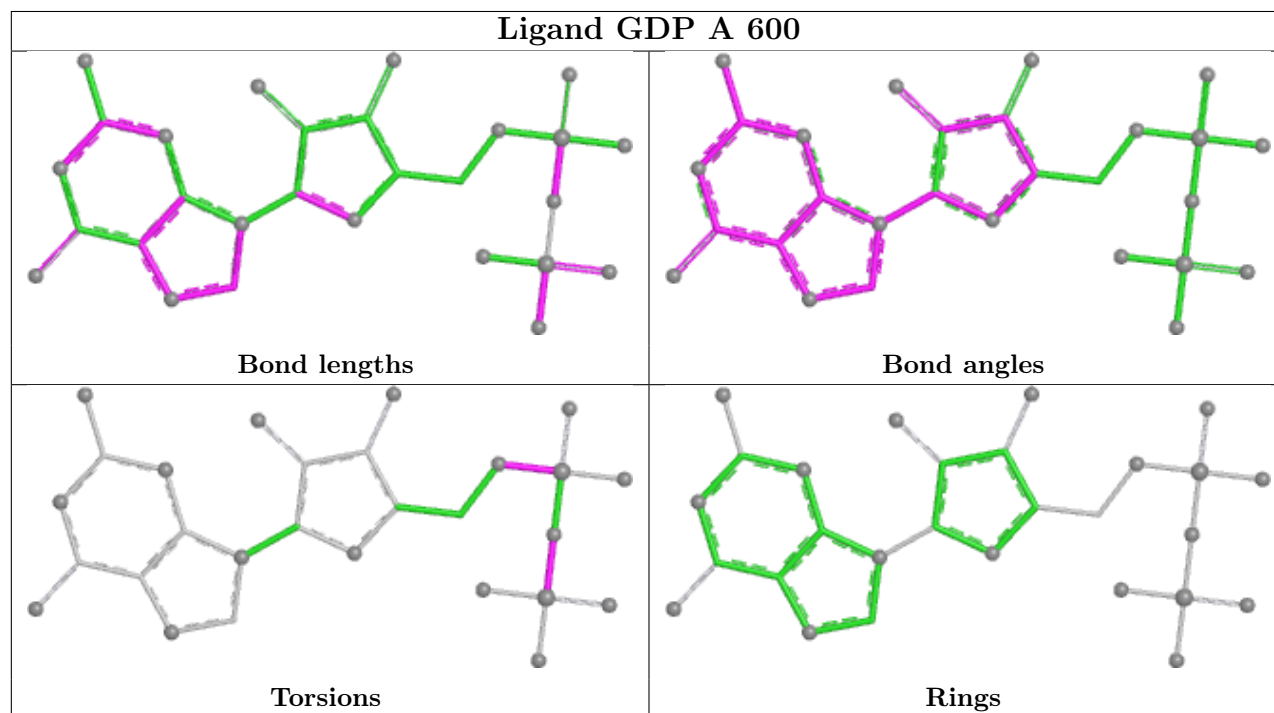
Mol	Chain	Res	Type	Atoms
4	A	600	GDP	PA-O3A-PB-O3B
5	B	500	GTP	PG-O3B-PB-O1B

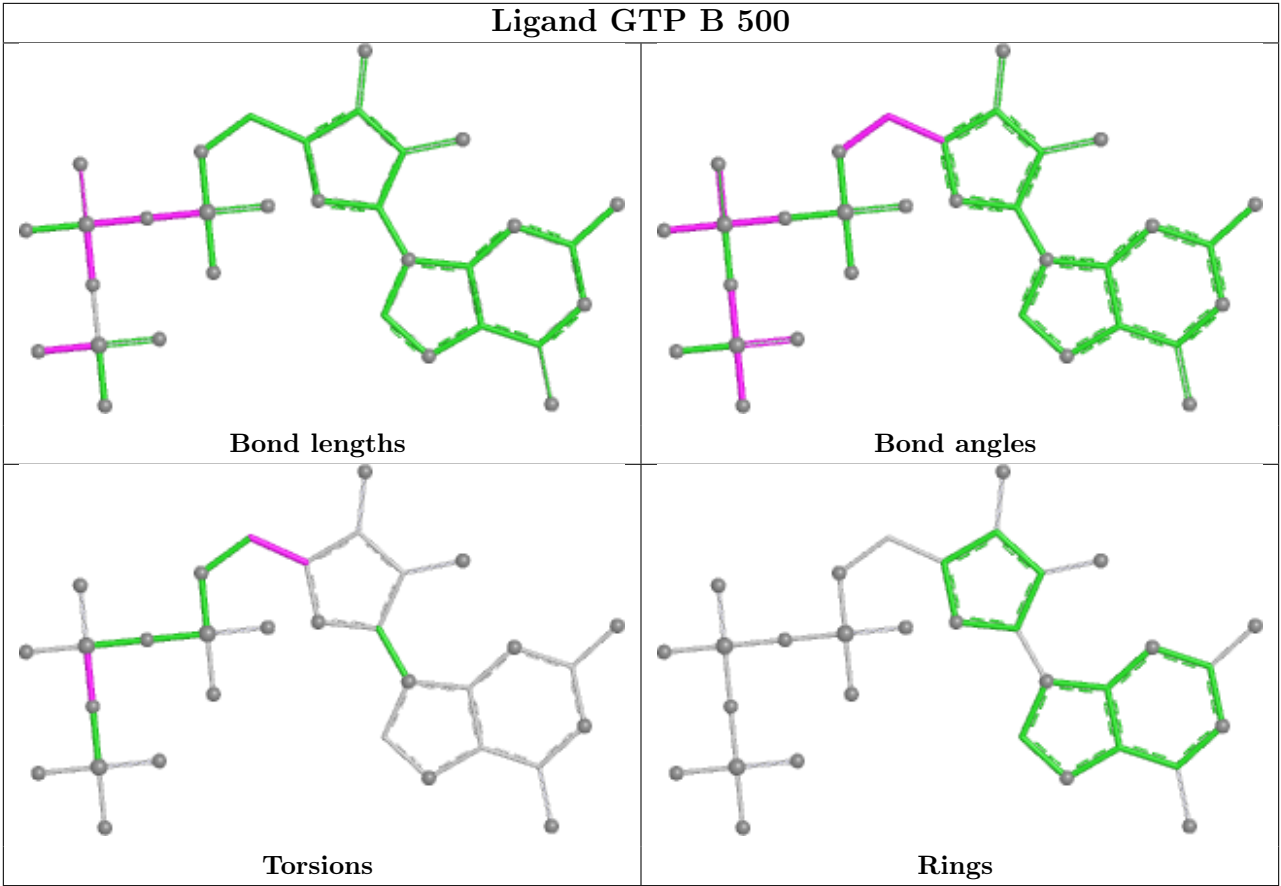
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GDP	1	0
5	B	500	GTP	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	274:PRO	C	275:VAL	N	2.09
1	B	92:LEU	C	93:ILE	N	1.98
1	B	298:PRO	C	299:ALA	N	1.73
1	B	68:VAL	C	69:ASP	N	1.67

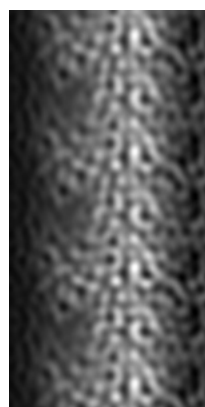
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2098. These allow visual inspection of the internal detail of the map and identification of artifacts.

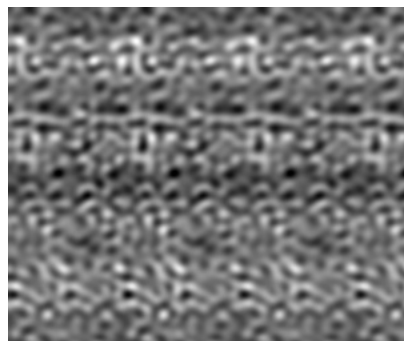
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

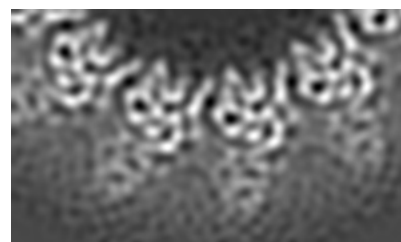
6.1.1 Primary map



X



Y



Z

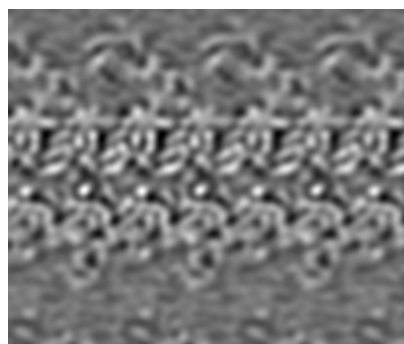
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

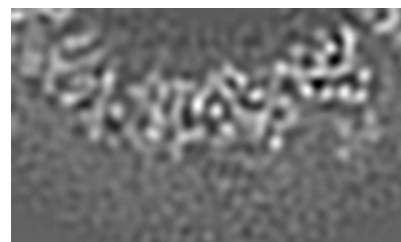
6.2.1 Primary map



X Index: 42



Y Index: 25



Z Index: 50

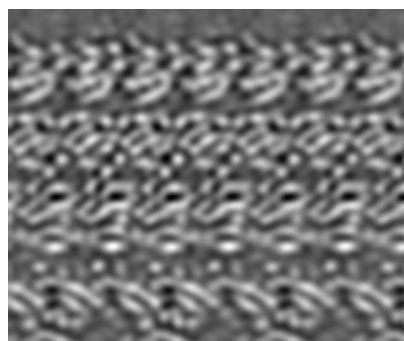
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

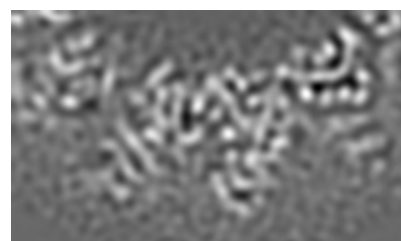
6.3.1 Primary map



X Index: 46



Y Index: 31

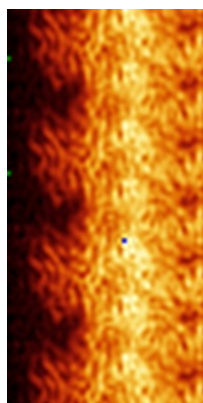


Z Index: 35

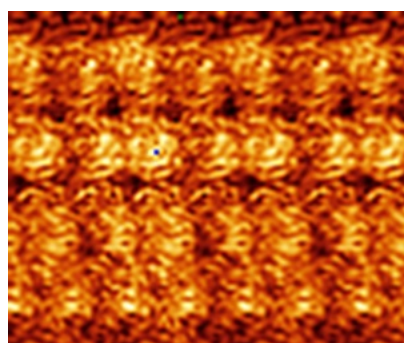
The images above show the largest variance slices of the map in three orthogonal directions.

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

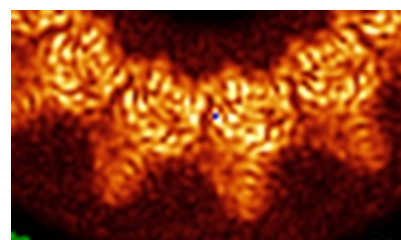
6.4.1 Primary map



X



Y

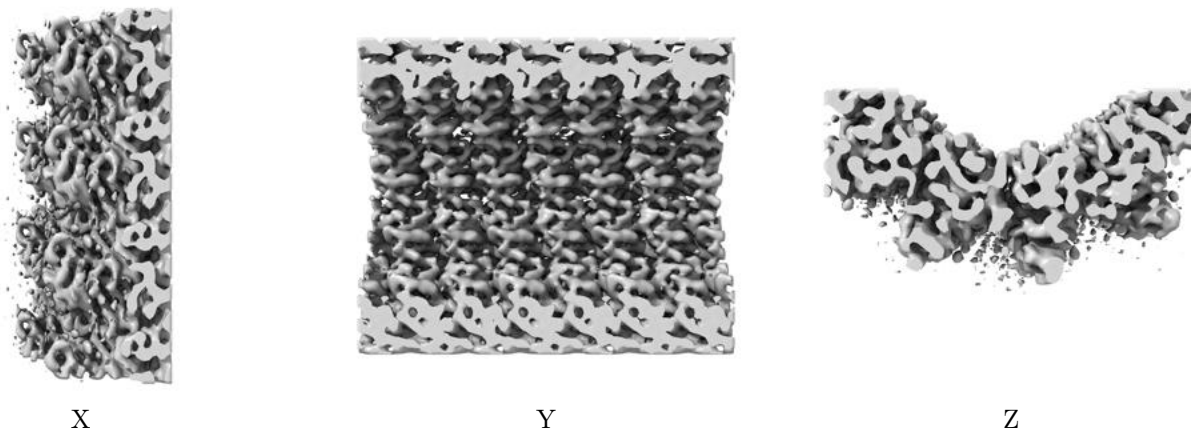


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

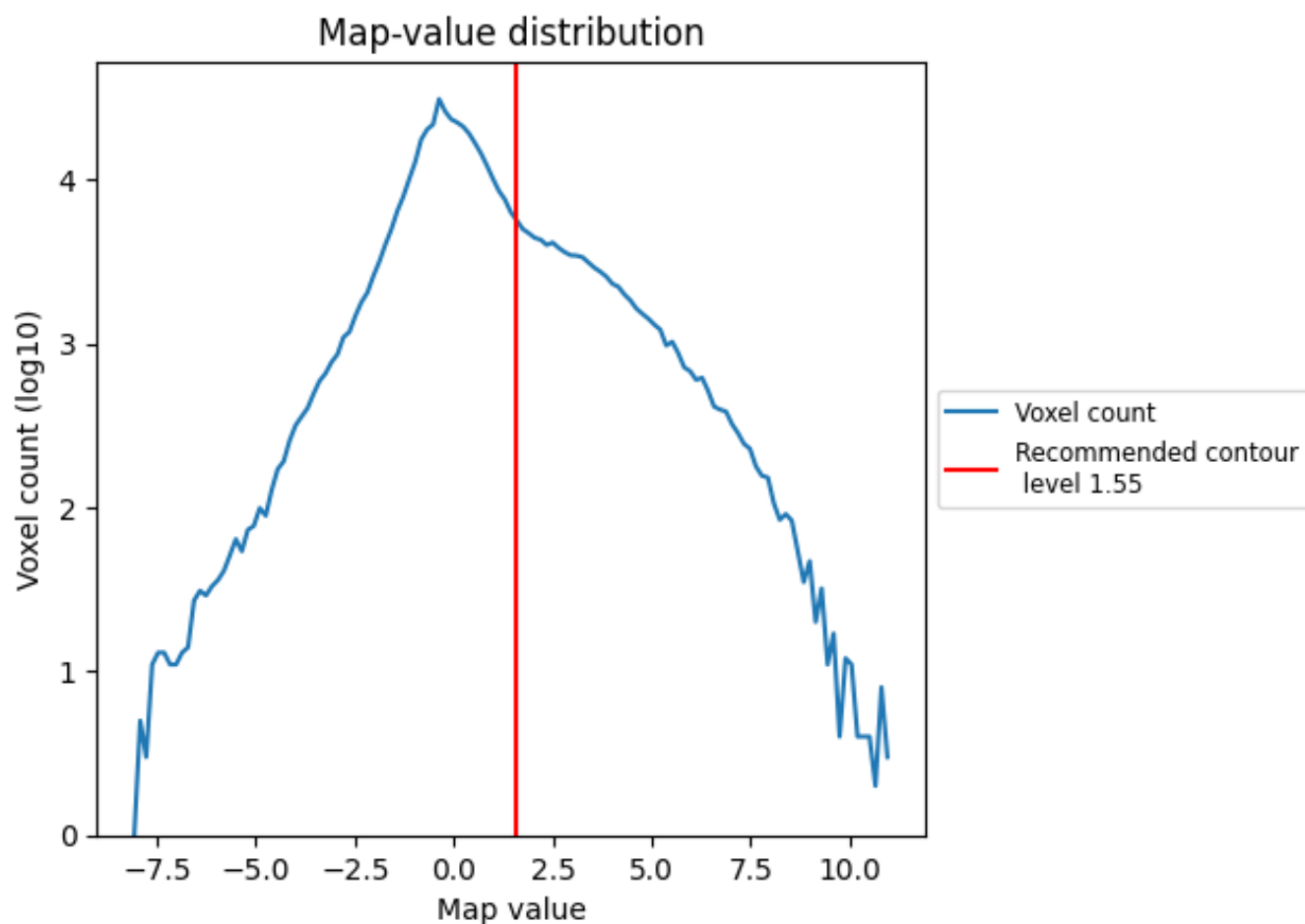
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

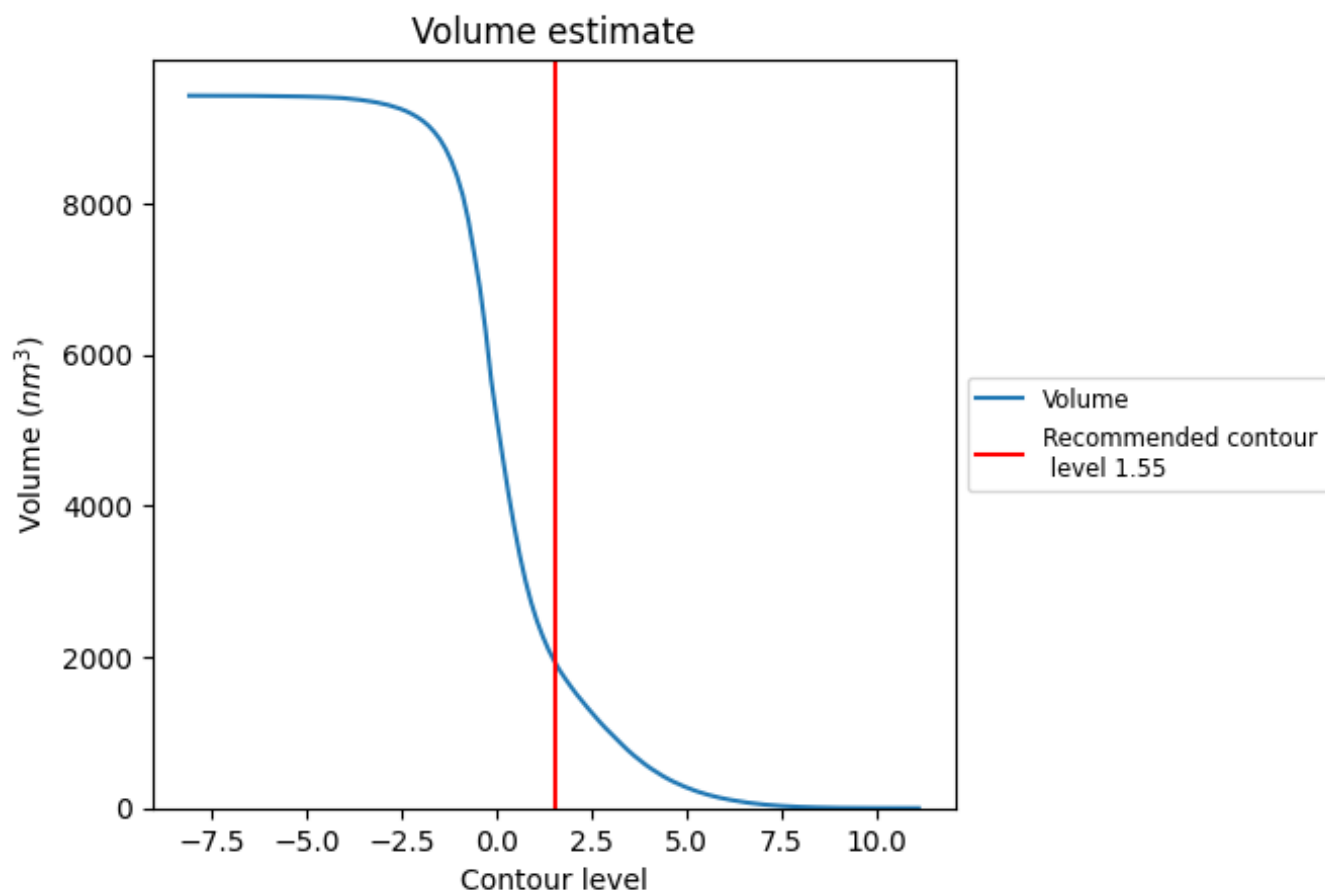
This section contains the results of statistical analysis of the map.

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 1924 nm^3 ; this corresponds to an approximate mass of 1738 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

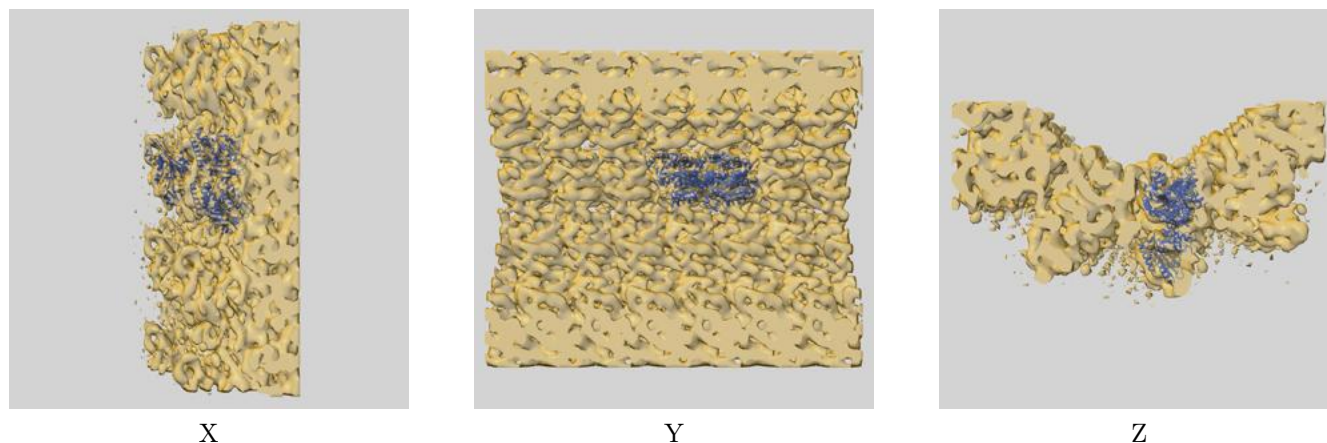
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

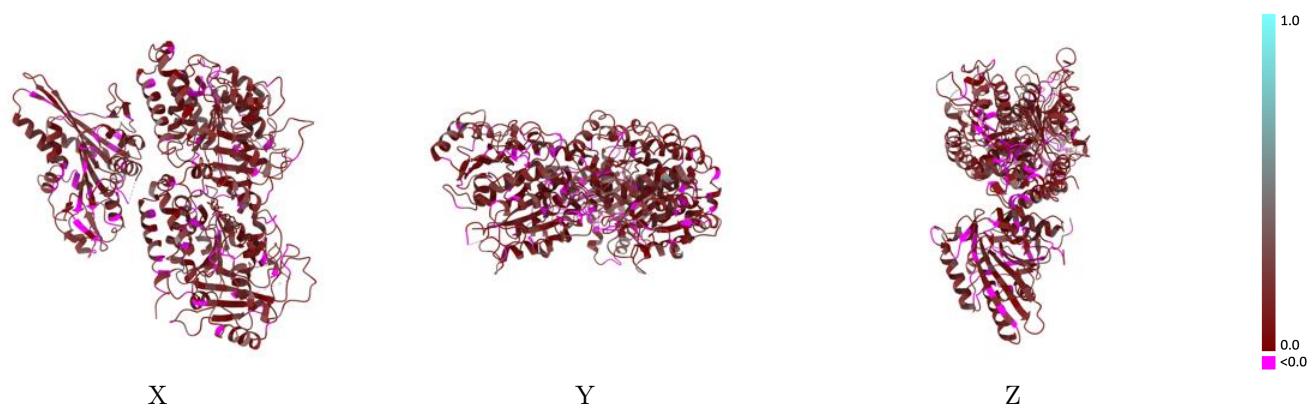
This section contains information regarding the fit between EMDB map EMD-2098 and PDB model 4ATX. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

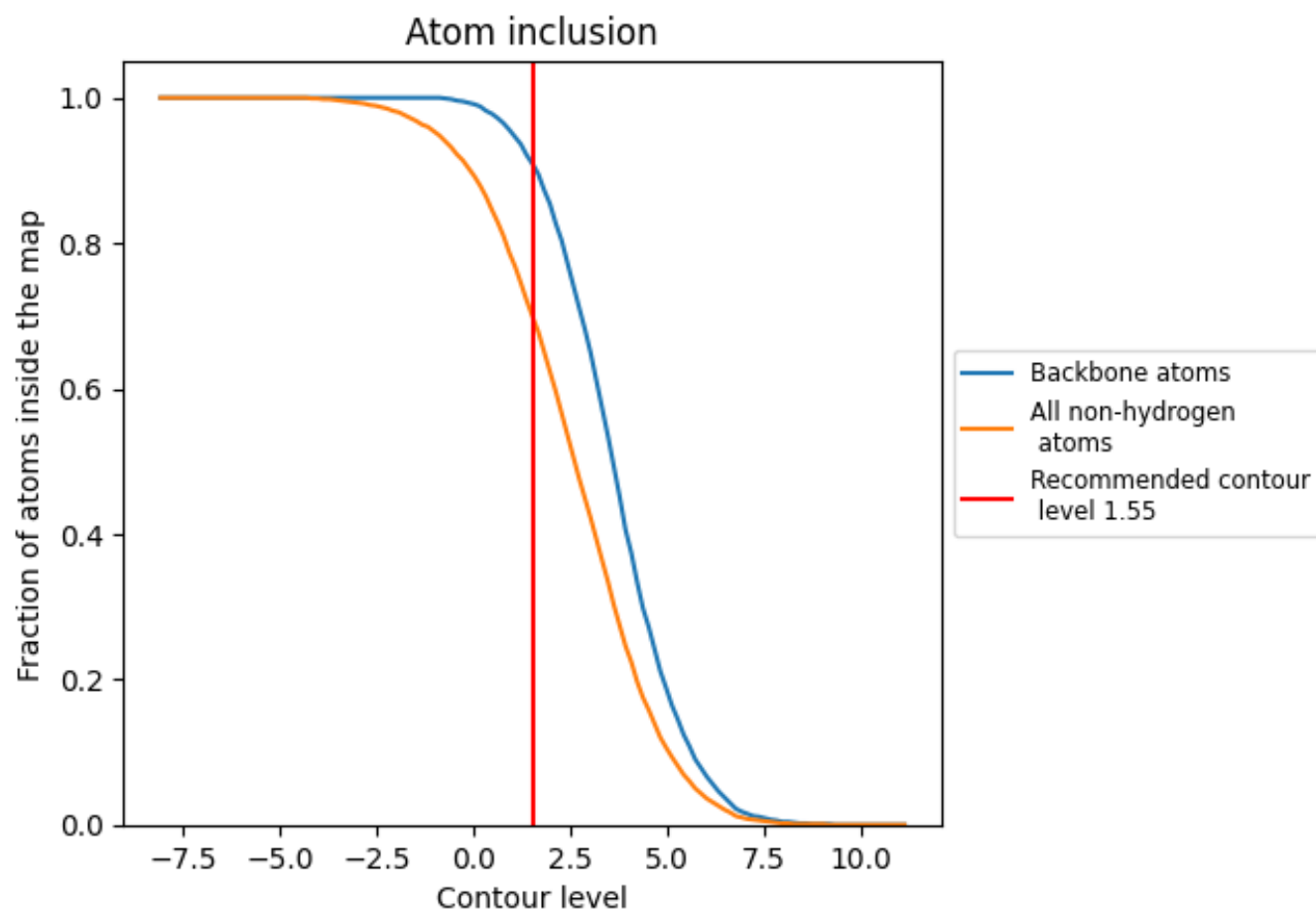


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 69% 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 (1.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.1280
A	0.7160	0.1310
B	0.6960	0.1250
C	0.6610	0.1270

