Full wwPDB EM Validation Report (i)

Feb 14, 2024 – 12:55 AM EST

PDB ID	:	3IZ0
EMDB ID	:	EMD-5223
Title	:	Human Ndc80 Bonsai Decorated Microtubule
Authors	:	Alushin, G.M.; Ramey, V.H.; Pasqualato, S.; Ball, D.A.; Grigorieff, N.; Musacchio, A.; Nogales, E.
Deposited on	:	2010-08-09
Resolution	:	8.60 Å(reported)
Based on initial models	:	1JFF, 2VE7

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

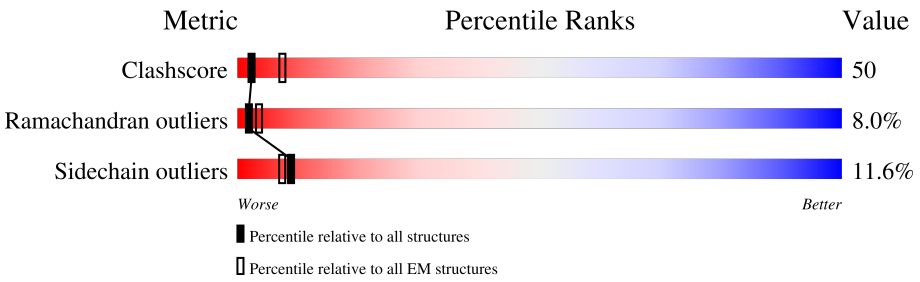
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 8.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	451	38%; 16%, 57%, 17%, •, 9%
2	B	445	38%; 20%, 56%, 18%, •, •
3	C	315	31%; 48%, 9%, •, 42%
3	E	315	32%; 49%, 8%, •, 42%
4	D	250	30%; 44%, 14%, •, 39%
4	F	250	30%; 43%, 15%, •, 39%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12154 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 alpha tubulin, Chain A from PDB 1JFF.

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

- Molecule 2 is a protein called beta tubulin, Chain B from PDB 1JFF.

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

- Molecule 3 is a protein called NDC80-SPC25 chimera protein, Chain B from PDB 2VE7 (Ndc80 bonsai).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	182	1465	950	229	274	12	0	0
3	E	182	1465	950	229	274	12	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	79	MET	-	expression tag	UNP Q05DQ6
C	393	GLN	ASN	conflict	UNP Q9HBM1
E	79	MET	-	expression tag	UNP Q05DQ6
E	393	GLN	ASN	conflict	UNP Q9HBM1

- Molecule 4 is a protein called NUF2-SPC24 chimera protein, Chain D from PDB 2VE7 (Ndc80 bonsai).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	153	1261	818	215	217	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	153	1261	818	215	217	11	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP B1AQT4
D	-3	PRO	-	expression tag	UNP B1AQT4
D	-2	LEU	-	expression tag	UNP B1AQT4
D	-1	GLY	-	expression tag	UNP B1AQT4
D	0	SER	-	expression tag	UNP B1AQT4
D	72	GLY	GLU	engineered mutation	UNP B1AQT4
D	200	GLU	ASP	conflict	UNP C9JGC4
F	-4	GLY	-	expression tag	UNP B1AQT4
F	-3	PRO	-	expression tag	UNP B1AQT4
F	-2	LEU	-	expression tag	UNP B1AQT4
F	-1	GLY	-	expression tag	UNP B1AQT4
F	0	SER	-	expression tag	UNP B1AQT4
F	72	GLY	GLU	engineered mutation	UNP B1AQT4
F	200	GLU	ASP	conflict	UNP C9JGC4

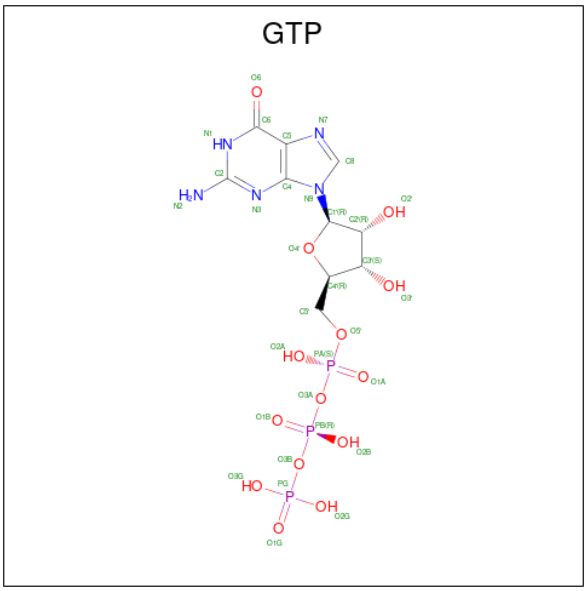
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0

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

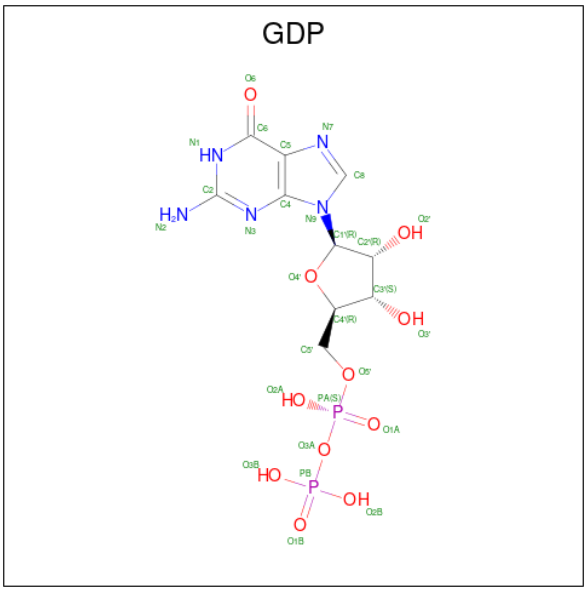
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



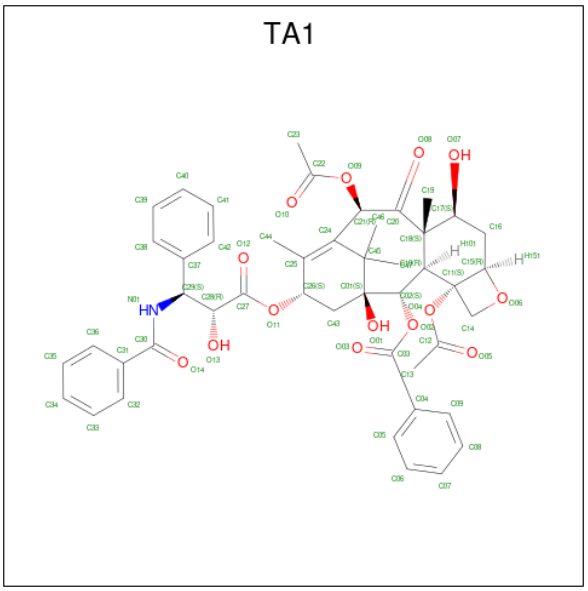
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	32	10	5	14	3	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 9 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



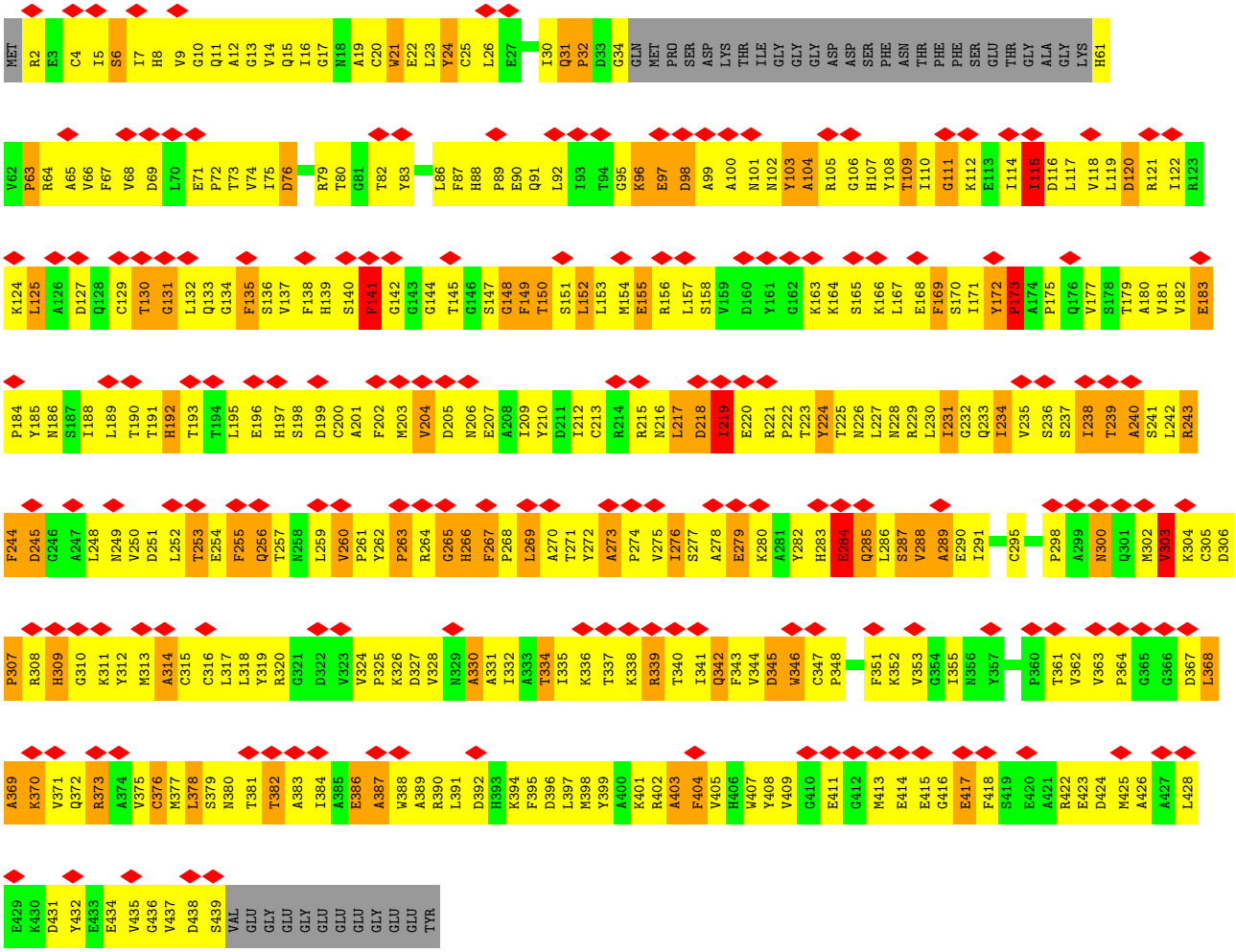
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	62	47	1	14	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

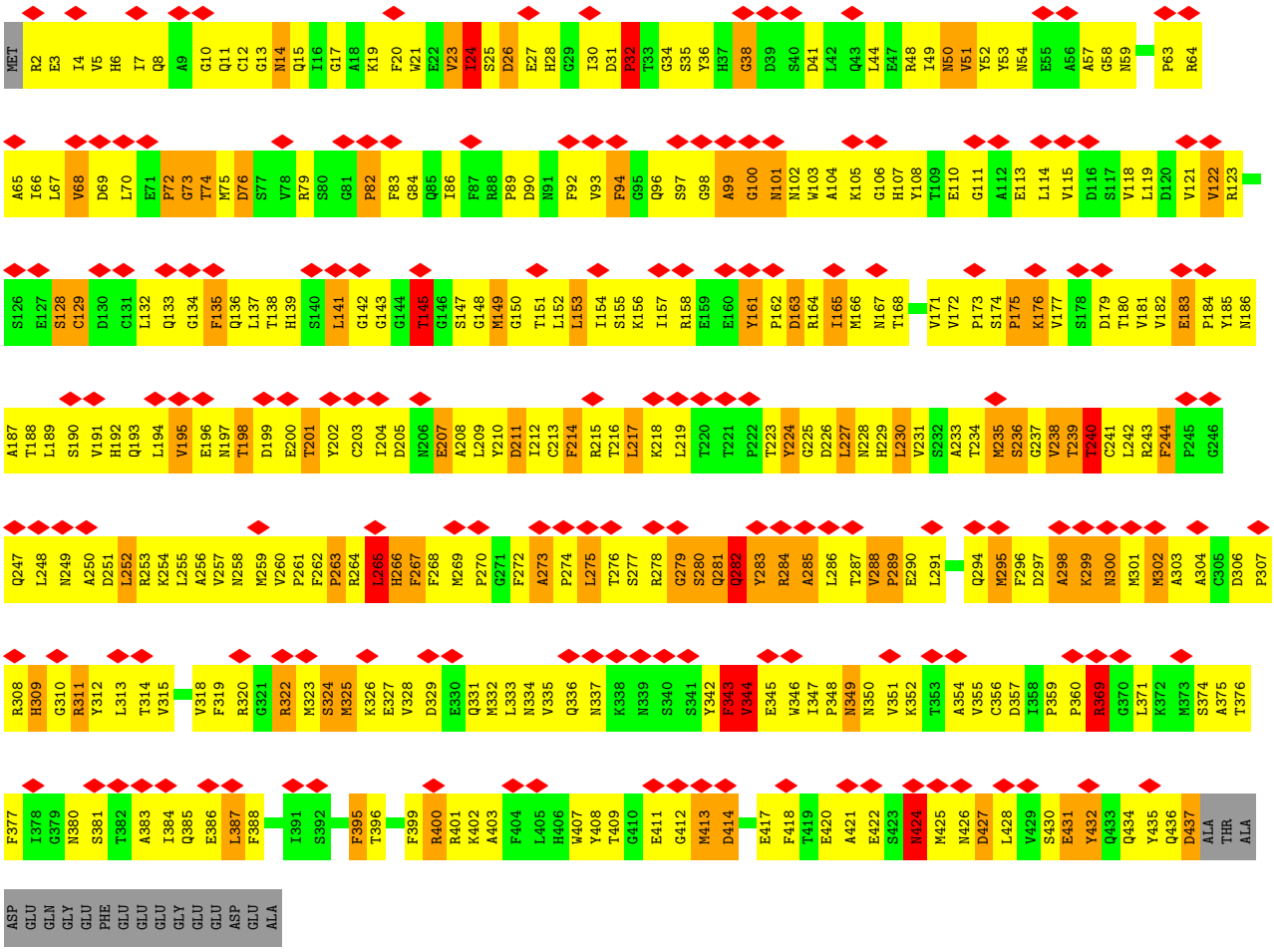
- Molecule 1: alpha tubulin, Chain A from PDB 1JFF

Chain A: 38% 16% 57% 17% • 9%



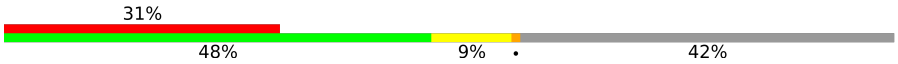
- Molecule 2: beta tubulin, Chain B from PDB 1JFF

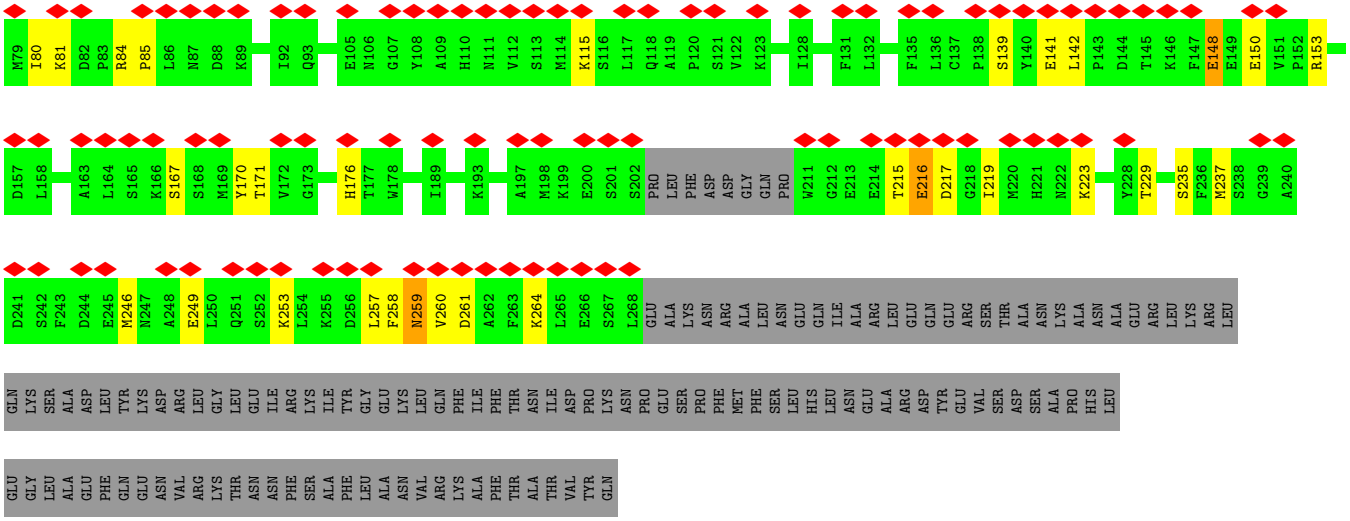
Chain B: 38% 20% 56% 18% • •



• Molecule 3: NDC80-SPC25 chimera protein, Chain B from PDB 2VE7 (Ndc80 bonsai)

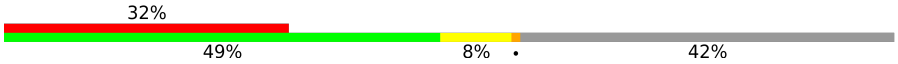
Chain C:

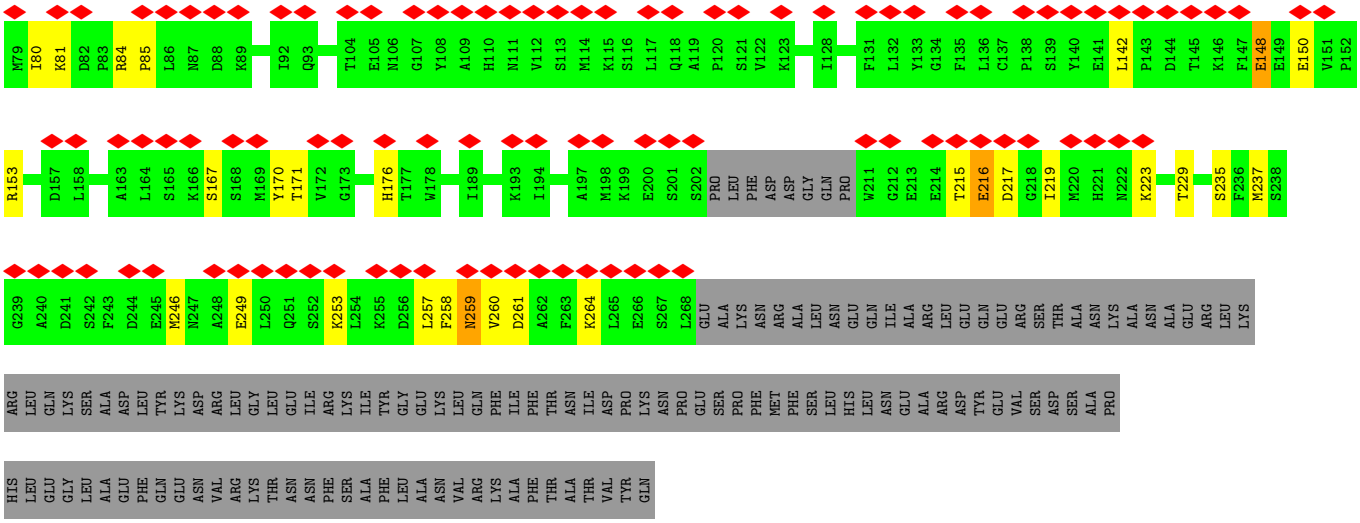




• Molecule 3: NDC80-SPC25 chimera protein, Chain B from PDB 2VE7 (Ndc80 bonsai)

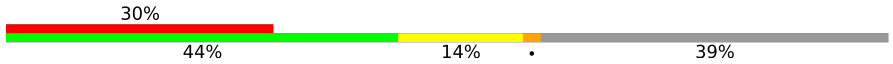
Chain E:

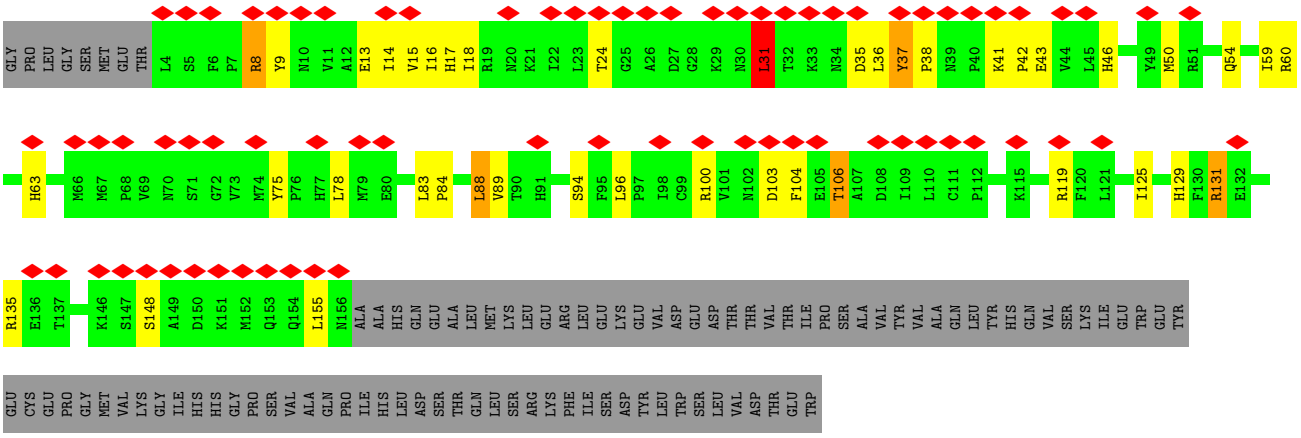




- Molecule 4: NUF2-SPC24 chimera protein, Chain D from PDB 2VE7 (Ndc80 bonsai)

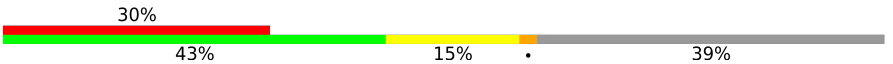
Chain D:

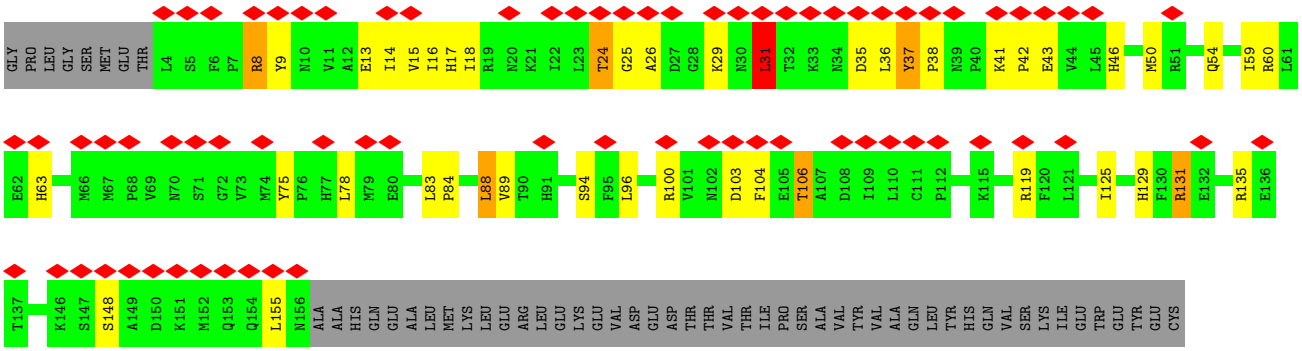




- Molecule 4: NUF2-SPC24 chimera protein, Chain D from PDB 2VE7 (Ndc80 bonsai)

Chain F:





GLU PRO GLY MET VAL LYS GLY ILE HIS HIS GLY PRO SER VAL ALA GLN PRO ILE HIS LEU ASP SER THR GLN LEU SER ARG LYS PHE ILE SER ASP TYR LEU TRP SER LEU VAL ASP THR GLU TRP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	6.146	Depositor
Minimum map value	-4.594	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.9	Depositor
Map size (Å)	545.6, 545.6, 248	wwPDB
Map dimensions	220, 220, 100	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.48, 2.48, 2.48	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: TA1, GDP, MG, ZN, 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	0.50	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
3	C	0.54	0/1502	0.62	0/2027
3	E	0.54	0/1502	0.62	0/2027
4	D	0.61	0/1295	0.68	1/1751 (0.1%)
4	F	0.61	0/1295	0.68	1/1751 (0.1%)
All	All	0.54	0/12320	0.70	4/16680 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	235	MET	CG-SD-CE	6.09	109.95	100.20
2	B	217	LEU	N-CA-C	-5.36	96.53	111.00
4	D	31	LEU	CA-CB-CG	5.24	127.36	115.30
4	F	31	LEU	CA-CB-CG	5.22	127.31	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3227	0	3143	551	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3351	0	3228	553	0
3	C	1465	0	1432	46	0
3	E	1465	0	1432	27	0
4	D	1261	0	1263	33	0
4	F	1261	0	1263	51	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	32	0	12	4	0
8	B	28	0	12	1	0
9	B	62	0	51	5	0
All	All	12154	0	11836	1198	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 50.

All (1198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:LYS:NZ	3:E:81:LYS:HZ3	1.04	1.49
3:C:115:LYS:HZ3	3:E:81:LYS:NZ	1.06	1.41
3:C:141:GLU:CD	4:F:29:LYS:HD2	1.03	1.38
3:C:141:GLU:OE1	4:F:29:LYS:CE	1.71	1.38
3:C:141:GLU:OE2	4:F:26:ALA:CA	1.85	1.24
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.17
3:C:115:LYS:NZ	3:E:81:LYS:NZ	1.72	1.17
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.15
3:C:141:GLU:OE2	4:F:26:ALA:HA	0.94	1.10
3:C:141:GLU:OE1	4:F:29:LYS:CG	2.00	1.08
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.30	1.06
3:C:141:GLU:OE1	4:F:29:LYS:CD	0.76	1.06
3:C:141:GLU:OE1	4:F:29:LYS:HD3	1.46	1.05
1:A:109:THR:HG22	1:A:110:ILE:N	1.70	1.02
1:A:243:ARG:HH21	1:A:252:LEU:N	1.57	1.02
2:B:299:LYS:H	2:B:299:LYS:HD3	1.24	1.02
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.37	1.01
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.43	1.00
4:D:35:ASP:HB2	4:D:41:LYS:HD2	1.40	0.99
4:F:35:ASP:HB2	4:F:41:LYS:HD2	1.40	0.99
2:B:236:SER:O	2:B:240:THR:HG23	1.61	0.98
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.47	0.94
1:A:251:ASP:N	1:A:254:GLU:HG3	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:HB2	1:A:105:ARG:HH21	1.31	0.94
1:A:251:ASP:H	1:A:254:GLU:HG3	1.33	0.94
2:B:281:GLN:O	2:B:283:TYR:N	2.00	0.94
1:A:316:CYS:HB3	1:A:378:LEU:HD11	1.48	0.94
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.50	0.93
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.51	0.93
2:B:264:ARG:O	2:B:265:LEU:HB3	1.69	0.93
1:A:237:SER:HB2	1:A:376:CYS:SG	2.08	0.93
3:C:141:GLU:HB3	4:F:26:ALA:HB2	1.49	0.92
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.48	0.92
1:A:151:SER:HB3	1:A:193:THR:HG21	1.51	0.92
2:B:70:LEU:H	2:B:145:THR:HG21	1.33	0.89
1:A:109:THR:HG22	1:A:110:ILE:H	1.33	0.89
2:B:102:ASN:HD21	2:B:408:TYR:HA	1.38	0.89
2:B:147:SER:O	2:B:151:THR:HB	1.71	0.89
2:B:93:VAL:HG11	2:B:118:VAL:CG2	2.03	0.89
1:A:122:ILE:HD12	1:A:157:LEU:HD21	1.54	0.88
1:A:147:SER:HB2	1:A:190:THR:OG1	1.73	0.88
1:A:343:PHE:CZ	1:A:351:PHE:CE1	2.61	0.88
2:B:311:ARG:HD3	2:B:342:TYR:HA	1.56	0.88
2:B:101:ASN:HD21	2:B:143:GLY:HA2	1.38	0.87
2:B:8:GLN:OE1	2:B:67:LEU:HD22	1.72	0.87
2:B:276:THR:HB	2:B:281:GLN:HG3	1.56	0.87
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.53	0.87
1:A:184:PRO:HG2	1:A:398:MET:HE1	1.56	0.87
2:B:264:ARG:HB2	2:B:266:HIS:CD2	2.08	0.87
1:A:110:ILE:HG23	1:A:111:GLY:H	1.38	0.87
2:B:153:LEU:O	2:B:157:ILE:HG12	1.75	0.86
2:B:360:PRO:HG2	2:B:371:LEU:HB3	1.56	0.86
2:B:6:HIS:CE1	2:B:8:GLN:HG2	2.10	0.86
2:B:263:PRO:HG3	3:C:171:THR:HG21	1.56	0.86
1:A:407:TRP:HE1	2:B:260:VAL:HG23	1.38	0.86
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.57	0.86
4:F:35:ASP:CB	4:F:41:LYS:HD2	2.05	0.86
4:D:35:ASP:CB	4:D:41:LYS:HD2	2.05	0.86
2:B:4:ILE:HD13	2:B:136:GLN:HE21	1.42	0.85
2:B:10:GLY:HA2	2:B:145:THR:HB	1.55	0.85
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.57	0.85
1:A:264:ARG:O	1:A:266:HIS:N	2.09	0.84
1:A:234:ILE:HG13	1:A:270:ALA:HB1	1.59	0.84
2:B:242:LEU:HD22	2:B:250:ALA:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.13	0.84
2:B:3:GLU:O	2:B:133:GLN:HB3	1.78	0.84
2:B:20:PHE:CD2	2:B:235:MET:SD	2.71	0.84
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.59	0.83
4:D:37:TYR:C	4:D:37:TYR:CD2	2.51	0.83
4:F:37:TYR:C	4:F:37:TYR:CD2	2.51	0.83
1:A:316:CYS:HB3	1:A:378:LEU:CD1	2.08	0.83
2:B:101:ASN:ND2	2:B:143:GLY:HA2	1.94	0.83
2:B:150:GLY:HA2	2:B:153:LEU:HD22	1.59	0.83
2:B:287:THR:O	2:B:288:VAL:HG23	1.78	0.83
2:B:324:SER:HB3	2:B:327:GLU:HG2	1.60	0.83
1:A:151:SER:CB	1:A:193:THR:HG21	2.09	0.83
2:B:209:LEU:HB3	2:B:227:LEU:HD22	1.59	0.83
1:A:106:GLY:O	1:A:111:GLY:HA3	1.78	0.82
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.60	0.82
2:B:156:LYS:HE2	2:B:156:LYS:HA	1.61	0.82
2:B:234:THR:HG21	2:B:270:PRO:CB	2.06	0.82
2:B:148:GLY:O	2:B:151:THR:HG22	1.79	0.82
2:B:147:SER:HB2	2:B:190:SER:HB3	1.60	0.81
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.60	0.81
1:A:313:MET:HB3	1:A:344:VAL:HG21	1.63	0.81
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.46	0.81
1:A:248:LEU:HD23	1:A:353:VAL:O	1.80	0.81
2:B:20:PHE:CZ	2:B:24:ILE:HD12	2.15	0.81
1:A:6:SER:HB3	1:A:136:SER:OG	1.81	0.80
2:B:264:ARG:HB2	2:B:266:HIS:HD2	1.45	0.80
1:A:7:ILE:HG22	1:A:66:VAL:HG22	1.63	0.80
1:A:109:THR:CG2	1:A:110:ILE:N	2.44	0.80
1:A:132:LEU:HD23	1:A:132:LEU:H	1.46	0.80
4:D:8:ARG:HH11	4:D:8:ARG:HG2	1.45	0.80
4:F:8:ARG:HG2	4:F:8:ARG:HH11	1.45	0.80
2:B:236:SER:O	2:B:240:THR:CG2	2.29	0.79
1:A:220:GLU:C	1:A:222:PRO:HD3	2.02	0.79
2:B:110:GLU:O	2:B:113:GLU:HG2	1.79	0.79
2:B:68:VAL:HG12	2:B:149:MET:SD	2.22	0.79
2:B:259:MET:HA	2:B:314:THR:HG21	1.65	0.79
2:B:265:LEU:HD12	2:B:265:LEU:O	1.83	0.79
1:A:234:ILE:HD13	1:A:234:ILE:O	1.81	0.79
1:A:69:ASP:HA	1:A:145:THR:HG21	1.66	0.78
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.66	0.78
2:B:234:THR:CG2	2:B:270:PRO:HB2	2.11	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:THR:HG23	2:B:422:GLU:OE2	1.83	0.78
2:B:413:MET:HG3	2:B:414:ASP:H	1.47	0.78
1:A:11:GLN:HG3	1:A:74:VAL:CG1	2.13	0.78
1:A:172:TYR:C	1:A:172:TYR:HD1	1.87	0.78
1:A:199:ASP:HB3	1:A:256:GLN:NE2	1.98	0.78
1:A:155:GLU:HA	1:A:197:HIS:ND1	1.99	0.78
1:A:110:ILE:HG23	1:A:111:GLY:N	1.99	0.77
2:B:205:ASP:OD1	2:B:304:ALA:HB2	1.84	0.77
1:A:241:SER:O	1:A:244:PHE:HB3	1.82	0.77
2:B:35:SER:HB3	2:B:59:ASN:HA	1.65	0.77
2:B:198:THR:O	2:B:265:LEU:HD22	1.85	0.77
3:C:141:GLU:CD	4:F:26:ALA:HA	2.03	0.77
2:B:192:HIS:ND1	2:B:424:ASN:OD1	2.18	0.77
2:B:259:MET:HG2	2:B:314:THR:HG21	1.67	0.77
1:A:223:THR:HB	1:A:225:THR:HG22	1.67	0.77
1:A:425:MET:HE2	1:A:428:LEU:HD23	1.66	0.76
1:A:231:ILE:HA	1:A:234:ILE:HG22	1.66	0.76
1:A:267:PHE:N	1:A:267:PHE:CD1	2.49	0.76
1:A:331:ALA:O	1:A:335:ILE:HG12	1.86	0.76
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.21	0.76
1:A:163:LYS:O	1:A:164:LYS:HG2	1.86	0.76
1:A:225:THR:O	1:A:229:ARG:HG3	1.86	0.76
1:A:221:ARG:O	1:A:221:ARG:HD3	1.85	0.75
1:A:243:ARG:HH21	1:A:252:LEU:H	0.79	0.75
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.68	0.75
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.68	0.75
2:B:176:LYS:HE3	2:B:207:GLU:HG3	1.68	0.75
1:A:101:ASN:ND2	2:B:254:LYS:HD2	2.02	0.75
3:C:115:LYS:NZ	3:E:81:LYS:HZ1	1.83	0.75
1:A:205:ASP:CB	1:A:303:VAL:HA	2.17	0.75
3:C:115:LYS:HZ1	3:E:81:LYS:NZ	1.81	0.75
1:A:276:ILE:HG23	1:A:369:ALA:CB	2.16	0.75
2:B:103:TRP:CZ3	2:B:108:TYR:HE1	2.05	0.74
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.27	0.74
1:A:234:ILE:HG21	1:A:302:MET:HE3	1.68	0.74
2:B:168:THR:HB	2:B:201:THR:HG23	1.68	0.74
2:B:250:ALA:HA	2:B:254:LYS:HE2	1.68	0.74
1:A:172:TYR:C	1:A:172:TYR:CD1	2.61	0.74
1:A:362:VAL:HG13	1:A:368:LEU:HD12	1.68	0.74
1:A:104:ALA:CB	1:A:413:MET:HG3	2.18	0.74
1:A:242:LEU:HG	1:A:250:VAL:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:O	1:A:308:ARG:N	2.20	0.74
2:B:209:LEU:HG	2:B:230:LEU:HD22	1.69	0.73
2:B:274:PRO:HG2	2:B:371:LEU:HD21	1.70	0.73
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.18	0.73
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.87	0.73
2:B:19:LYS:HG3	2:B:228:ASN:CB	2.17	0.73
2:B:76:ASP:HA	2:B:79:ARG:HG2	1.71	0.73
1:A:104:ALA:HB2	1:A:413:MET:HG3	1.71	0.73
1:A:112:LYS:O	1:A:115:ILE:HG22	1.89	0.73
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.52	0.73
2:B:217:LEU:O	2:B:219:LEU:N	2.22	0.73
1:A:63:PRO:O	1:A:64:ARG:HG2	1.88	0.73
1:A:105:ARG:O	1:A:110:ILE:HG22	1.89	0.73
2:B:217:LEU:C	2:B:219:LEU:H	1.91	0.73
1:A:264:ARG:C	1:A:266:HIS:H	1.91	0.73
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.19	0.73
2:B:8:GLN:CD	2:B:67:LEU:HD22	2.08	0.73
2:B:242:LEU:HD13	2:B:250:ALA:C	2.08	0.73
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.24	0.72
1:A:7:ILE:HD11	1:A:137:VAL:HG22	1.71	0.72
2:B:356:CYS:SG	2:B:357:ASP:N	2.62	0.72
1:A:25:CYS:HB2	1:A:30:ILE:O	1.89	0.72
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.20	0.72
2:B:111:GLY:O	2:B:115:VAL:HG23	1.89	0.72
1:A:312:TYR:O	1:A:344:VAL:HG23	1.90	0.72
2:B:237:GLY:O	2:B:241:CYS:HB3	1.90	0.71
1:A:166:LYS:HE3	1:A:199:ASP:OD1	1.90	0.71
1:A:259:LEU:HD11	1:A:378:LEU:CD1	2.20	0.71
2:B:6:HIS:HE1	2:B:8:GLN:HG2	1.52	0.71
2:B:243:ARG:NH2	2:B:252:LEU:HG	2.05	0.71
2:B:201:THR:OG1	2:B:265:LEU:HD11	1.90	0.71
1:A:148:GLY:O	1:A:151:SER:HB2	1.91	0.71
1:A:317:LEU:HD12	1:A:351:PHE:HD2	1.56	0.71
1:A:343:PHE:CZ	1:A:351:PHE:HE1	2.08	0.71
2:B:48:ARG:HG2	2:B:243:ARG:O	1.90	0.71
2:B:10:GLY:O	2:B:14:ASN:HB2	1.90	0.71
2:B:255:LEU:O	2:B:259:MET:HG3	1.91	0.71
2:B:70:LEU:HG	2:B:145:THR:CG2	2.20	0.71
2:B:325:MET:HE3	2:B:325:MET:HA	1.73	0.71
1:A:12:ALA:HB3	1:A:140:SER:OG	1.91	0.70
2:B:431:GLU:OE1	2:B:432:TYR:HA	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD21	1:A:250:VAL:HB	1.71	0.70
1:A:381:THR:C	1:A:383:ALA:H	1.95	0.70
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.06	0.70
2:B:175:PRO:HD2	2:B:207:GLU:OE2	1.91	0.70
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.73	0.70
2:B:70:LEU:HG	2:B:145:THR:HG23	1.74	0.70
2:B:291:LEU:O	2:B:295:MET:HG3	1.91	0.70
1:A:63:PRO:C	1:A:64:ARG:HG2	2.12	0.69
2:B:24:ILE:HD11	2:B:52:TYR:CE1	2.28	0.69
2:B:299:LYS:HD3	2:B:299:LYS:N	2.04	0.69
1:A:199:ASP:HB3	1:A:256:GLN:HE21	1.57	0.69
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.74	0.69
1:A:237:SER:CB	1:A:376:CYS:SG	2.80	0.69
1:A:244:PHE:HD2	1:A:245:ASP:N	1.89	0.69
2:B:209:LEU:HD23	2:B:227:LEU:HB3	1.75	0.69
2:B:234:THR:O	2:B:238:VAL:HG23	1.92	0.69
1:A:5:ILE:HG22	1:A:6:SER:N	2.07	0.69
2:B:251:ASP:O	2:B:253:ARG:N	2.26	0.69
1:A:343:PHE:HZ	1:A:351:PHE:CE1	2.10	0.69
1:A:394:LYS:HG2	2:B:348:PRO:HG3	1.75	0.69
1:A:133:GLN:HG2	1:A:243:ARG:HH22	1.57	0.68
1:A:221:ARG:N	1:A:222:PRO:HD3	2.09	0.68
3:C:80:ILE:HG23	3:C:81:LYS:H	1.56	0.68
3:E:80:ILE:HG23	3:E:81:LYS:H	1.56	0.68
1:A:222:PRO:HD2	2:B:326:LYS:HB3	1.74	0.68
1:A:141:PHE:O	1:A:147:SER:HB3	1.94	0.68
2:B:257:VAL:O	2:B:257:VAL:HG12	1.93	0.68
1:A:407:TRP:HE1	2:B:260:VAL:CG2	2.07	0.68
1:A:88:HIS:C	1:A:90:GLU:H	1.95	0.68
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.29	0.68
2:B:44:LEU:HD12	2:B:49:ILE:HD13	1.76	0.68
2:B:242:LEU:CD2	2:B:250:ALA:H	2.06	0.68
2:B:256:ALA:O	2:B:260:VAL:HG22	1.94	0.68
1:A:217:LEU:HD12	1:A:277:SER:HB3	1.75	0.68
1:A:371:VAL:HG12	1:A:372:GLN:H	1.57	0.68
2:B:325:MET:CE	2:B:355:VAL:HG21	2.24	0.68
4:F:103:ASP:OD2	4:F:119:ARG:NH2	2.27	0.68
4:D:103:ASP:OD2	4:D:119:ARG:NH2	2.27	0.67
1:A:152:LEU:HA	1:A:155:GLU:HB2	1.77	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.94	0.67
1:A:251:ASP:O	1:A:254:GLU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:O	1:A:97:GLU:N	2.27	0.67
1:A:243:ARG:NH2	1:A:252:LEU:N	2.28	0.67
1:A:115:ILE:CD1	1:A:119:LEU:HG	2.23	0.67
1:A:175:PRO:HG3	1:A:304:LYS:HG2	1.76	0.67
2:B:107:HIS:CD2	2:B:151:THR:CG2	2.78	0.67
2:B:204:ILE:HD13	2:B:231:VAL:HG22	1.76	0.67
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.67
4:D:8:ARG:HG2	4:D:8:ARG:NH1	2.09	0.67
4:F:8:ARG:HG2	4:F:8:ARG:NH1	2.09	0.67
1:A:7:ILE:HD12	1:A:153:LEU:CD2	2.24	0.67
2:B:230:LEU:HD23	2:B:231:VAL:N	2.10	0.67
2:B:180:THR:HG22	2:B:181:VAL:N	2.07	0.67
2:B:310:GLY:HA3	2:B:436:GLN:HE21	1.59	0.67
4:D:37:TYR:C	4:D:37:TYR:HD2	1.97	0.67
4:F:37:TYR:C	4:F:37:TYR:HD2	1.97	0.67
1:A:100:ALA:CB	1:A:105:ARG:HD3	2.25	0.67
1:A:172:TYR:HD1	1:A:173:PRO:N	1.93	0.67
2:B:250:ALA:HB1	2:B:254:LYS:HB2	1.76	0.67
2:B:103:TRP:HZ3	2:B:108:TYR:HE1	1.42	0.66
1:A:276:ILE:O	1:A:369:ALA:HB2	1.95	0.66
2:B:66:ILE:C	2:B:67:LEU:HD23	2.15	0.66
2:B:276:THR:HB	2:B:281:GLN:CG	2.25	0.66
1:A:71:GLU:HG3	2:B:2:ARG:HH21	1.58	0.66
2:B:4:ILE:HG21	2:B:136:GLN:HG2	1.76	0.66
2:B:281:GLN:O	2:B:283:TYR:HB2	1.96	0.66
1:A:341:ILE:HG12	1:A:341:ILE:O	1.95	0.66
3:E:229:THR:HG21	4:F:131:ARG:HB3	1.76	0.66
3:C:229:THR:HG21	4:D:131:ARG:HB3	1.76	0.66
2:B:66:ILE:CD1	2:B:122:VAL:HG12	2.26	0.66
3:C:148:GLU:HG2	3:C:170:TYR:CZ	2.31	0.66
1:A:217:LEU:HD11	1:A:367:ASP:O	1.97	0.65
2:B:182:VAL:HG23	2:B:186:ASN:HD21	1.60	0.65
4:D:15:VAL:HG13	4:D:31:LEU:HD13	1.77	0.65
3:E:148:GLU:HG2	3:E:170:TYR:CZ	2.31	0.65
4:F:15:VAL:HG13	4:F:31:LEU:HD13	1.77	0.65
1:A:313:MET:HB3	1:A:344:VAL:CG2	2.26	0.65
1:A:68:VAL:HG11	1:A:149:PHE:CZ	2.30	0.65
2:B:242:LEU:CD1	2:B:255:LEU:HD11	2.25	0.65
1:A:206:ASN:OD1	1:A:227:LEU:HD13	1.96	0.65
2:B:35:SER:HB3	2:B:59:ASN:CA	2.26	0.65
1:A:305:CYS:SG	1:A:384:ILE:HD13	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD12	1:A:351:PHE:CD2	2.32	0.65
1:A:344:VAL:HG12	1:A:345:ASP:N	2.12	0.65
2:B:93:VAL:CG1	2:B:118:VAL:HG22	2.19	0.65
2:B:243:ARG:HH22	2:B:252:LEU:HG	1.59	0.65
3:C:115:LYS:NZ	3:E:81:LYS:CE	2.60	0.65
2:B:242:LEU:HD12	2:B:255:LEU:HD11	1.78	0.65
2:B:422:GLU:O	2:B:426:ASN:HB2	1.97	0.65
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.64
1:A:372:GLN:O	1:A:373:ARG:HB3	1.96	0.64
2:B:427:ASP:O	2:B:430:SER:HB3	1.97	0.64
2:B:431:GLU:O	2:B:434:GLN:HG2	1.97	0.64
2:B:265:LEU:HD12	2:B:265:LEU:C	2.16	0.64
2:B:299:LYS:O	2:B:300:ASN:HB2	1.97	0.64
2:B:114:LEU:O	2:B:118:VAL:HG23	1.98	0.64
2:B:158:ARG:NE	2:B:197:ASN:O	2.30	0.64
2:B:243:ARG:HH21	2:B:252:LEU:H	1.45	0.64
2:B:241:CYS:O	2:B:244:PHE:HB2	1.97	0.64
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.79	0.64
2:B:192:HIS:O	2:B:195:VAL:HG12	1.98	0.64
2:B:284:ARG:O	2:B:286:LEU:N	2.31	0.64
1:A:151:SER:O	1:A:155:GLU:HB2	1.98	0.64
1:A:224:TYR:CD1	2:B:325:MET:HG2	2.33	0.64
2:B:267:PHE:N	2:B:267:PHE:CD1	2.62	0.64
1:A:271:THR:HG23	1:A:300:ASN:O	1.97	0.64
2:B:263:PRO:CG	3:C:171:THR:HG21	2.28	0.64
2:B:413:MET:HG2	2:B:418:PHE:HE1	1.61	0.63
1:A:386:GLU:O	1:A:389:ALA:N	2.31	0.63
2:B:137:LEU:HD22	2:B:154:ILE:CG2	2.28	0.63
9:B:820:TA1:H463	9:B:820:TA1:H261	1.80	0.63
2:B:180:THR:CG2	2:B:181:VAL:N	2.61	0.63
1:A:276:ILE:HG23	1:A:369:ALA:HB2	1.80	0.63
1:A:175:PRO:HG2	1:A:207:GLU:OE1	1.98	0.63
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.81	0.63
2:B:105:LYS:O	2:B:110:GLU:HB2	1.97	0.63
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.34	0.63
1:A:315:CYS:HB3	1:A:377:MET:CE	2.29	0.63
1:A:115:ILE:HG23	1:A:116:ASP:N	2.12	0.63
1:A:234:ILE:HD13	1:A:234:ILE:C	2.18	0.63
2:B:318:VAL:HA	2:B:354:ALA:HB3	1.81	0.63
1:A:236:SER:O	1:A:240:ALA:HB3	1.99	0.62
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:9:TYR:HB2	4:D:14:ILE:HG13	1.81	0.62
4:F:9:TYR:HB2	4:F:14:ILE:HG13	1.81	0.62
1:A:23:LEU:HD22	1:A:232:GLY:O	1.99	0.62
1:A:278:ALA:HA	1:A:282:TYR:OH	1.99	0.62
1:A:288:VAL:O	1:A:290:GLU:N	2.33	0.62
1:A:7:ILE:HG22	1:A:66:VAL:CG2	2.28	0.62
2:B:253:ARG:O	2:B:256:ALA:N	2.33	0.62
2:B:282:GLN:O	2:B:282:GLN:HG2	1.97	0.62
1:A:152:LEU:HD12	1:A:153:LEU:N	2.14	0.62
1:A:269:LEU:O	1:A:378:LEU:HA	1.98	0.62
2:B:63:PRO:HD2	2:B:86:ILE:HG12	1.80	0.62
2:B:205:ASP:OD1	2:B:304:ALA:N	2.32	0.62
1:A:267:PHE:HD1	1:A:267:PHE:H	1.47	0.62
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.30	0.62
2:B:263:PRO:HG3	3:C:171:THR:CG2	2.28	0.62
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.81	0.62
1:A:166:LYS:H	1:A:199:ASP:CG	2.03	0.62
2:B:107:HIS:HD2	2:B:151:THR:CG2	2.12	0.62
2:B:133:GLN:HG3	2:B:165:ILE:HD11	1.80	0.62
1:A:179:THR:HG21	2:B:248:LEU:HD21	1.81	0.62
2:B:4:ILE:HA	2:B:134:GLY:O	1.99	0.62
1:A:179:THR:HG21	2:B:248:LEU:CD2	2.30	0.62
1:A:317:LEU:HD11	1:A:351:PHE:HE2	1.63	0.62
1:A:402:ARG:O	1:A:403:ALA:C	2.36	0.62
2:B:114:LEU:HD23	2:B:149:MET:CE	2.30	0.62
1:A:88:HIS:O	1:A:90:GLU:N	2.33	0.61
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.82	0.61
1:A:177:VAL:HG11	2:B:329:ASP:HB3	1.83	0.61
1:A:102:ASN:OD1	1:A:105:ARG:HB3	1.99	0.61
2:B:204:ILE:CD1	2:B:231:VAL:HG13	2.30	0.61
2:B:211:ASP:OD1	2:B:212:ILE:N	2.33	0.61
2:B:230:LEU:O	2:B:233:ALA:HB3	2.00	0.61
1:A:7:ILE:CD1	1:A:137:VAL:HG22	2.29	0.61
1:A:179:THR:HG22	2:B:352:LYS:NZ	2.15	0.61
3:E:219:ILE:HD11	4:F:135:ARG:HG3	1.82	0.61
1:A:115:ILE:HG13	1:A:152:LEU:HD13	1.81	0.61
3:C:219:ILE:HD11	4:D:135:ARG:HG3	1.81	0.61
1:A:177:VAL:CG1	2:B:329:ASP:HB3	2.31	0.61
1:A:362:VAL:HG13	1:A:368:LEU:HB2	1.83	0.61
2:B:108:TYR:CD1	2:B:413:MET:HE1	2.36	0.61
3:C:139:SER:CB	4:F:24:THR:HG23	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG21	2:B:258:ASN:O	2.01	0.61
2:B:324:SER:CB	2:B:327:GLU:HG2	2.30	0.61
1:A:118:VAL:HG11	1:A:149:PHE:HZ	1.65	0.61
2:B:4:ILE:HG23	2:B:134:GLY:O	2.00	0.61
4:F:84:PRO:O	4:F:88:LEU:HB2	2.01	0.61
1:A:191:THR:HG21	1:A:425:MET:SD	2.41	0.60
1:A:345:ASP:C	1:A:347:CYS:H	2.04	0.60
2:B:279:GLY:O	2:B:282:GLN:HB3	2.01	0.60
4:D:84:PRO:O	4:D:88:LEU:HB2	2.01	0.60
1:A:315:CYS:HB3	1:A:377:MET:HE2	1.81	0.60
1:A:311:LYS:HE3	1:A:342:GLN:CD	2.22	0.60
1:A:168:GLU:OE1	1:A:198:SER:HB2	2.01	0.60
2:B:70:LEU:CG	2:B:145:THR:HG23	2.30	0.60
2:B:285:ALA:HB1	2:B:290:GLU:HG2	1.82	0.60
2:B:204:ILE:HG21	2:B:231:VAL:HG22	1.83	0.60
1:A:169:PHE:CE1	1:A:235:VAL:HG22	2.36	0.60
2:B:70:LEU:N	2:B:145:THR:HG21	2.11	0.60
1:A:435:VAL:HG12	1:A:435:VAL:O	2.02	0.60
1:A:11:GLN:HE21	1:A:74:VAL:HG22	1.66	0.60
2:B:324:SER:C	2:B:326:LYS:H	2.03	0.60
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.15	0.60
2:B:229:HIS:HD1	2:B:229:HIS:C	2.05	0.60
3:C:141:GLU:CB	4:F:26:ALA:HB2	2.26	0.60
1:A:248:LEU:CD2	1:A:353:VAL:O	2.49	0.60
1:A:407:TRP:NE1	2:B:260:VAL:HG23	2.14	0.60
2:B:70:LEU:H	2:B:145:THR:CG2	2.10	0.60
2:B:102:ASN:ND2	2:B:407:TRP:O	2.35	0.60
2:B:205:ASP:OD1	2:B:304:ALA:CB	2.50	0.60
2:B:332:MET:CE	2:B:351:VAL:HG11	2.32	0.60
1:A:119:LEU:O	1:A:122:ILE:HG12	2.02	0.59
1:A:167:LEU:HA	1:A:200:CYS:O	2.01	0.59
1:A:229:ARG:NH1	1:A:363:VAL:HG21	2.16	0.59
1:A:344:VAL:HG11	1:A:346:TRP:NE1	2.16	0.59
2:B:49:ILE:O	2:B:51:VAL:N	2.35	0.59
2:B:324:SER:O	2:B:328:VAL:HG23	2.01	0.59
4:D:60:ARG:H	4:D:63:HIS:CD2	2.21	0.59
2:B:68:VAL:CG1	2:B:149:MET:SD	2.90	0.59
2:B:408:TYR:CG	2:B:418:PHE:HZ	2.20	0.59
4:F:60:ARG:H	4:F:63:HIS:CD2	2.21	0.59
2:B:141:LEU:CD1	2:B:141:LEU:N	2.65	0.59
1:A:115:ILE:HD13	1:A:115:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:TYR:C	2:B:163:ASP:H	2.05	0.59
2:B:299:LYS:O	2:B:300:ASN:CB	2.51	0.59
1:A:278:ALA:HB2	1:A:369:ALA:HA	1.85	0.59
1:A:369:ALA:O	1:A:370:LYS:HB3	2.03	0.59
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.29	0.59
1:A:413:MET:O	1:A:414:GLU:HG3	2.02	0.59
2:B:30:ILE:HD13	2:B:53:TYR:CE2	2.37	0.59
2:B:349:ASN:C	2:B:349:ASN:HD22	2.06	0.59
1:A:6:SER:HA	1:A:136:SER:O	2.02	0.58
1:A:284:GLU:O	1:A:286:LEU:N	2.35	0.58
3:C:141:GLU:CD	4:F:29:LYS:CD	1.94	0.58
2:B:115:VAL:HG21	2:B:152:LEU:HD23	1.84	0.58
2:B:198:THR:HG22	2:B:265:LEU:HD22	1.86	0.58
3:C:139:SER:HB2	4:F:24:THR:HG23	1.83	0.58
1:A:2:ARG:N	1:A:131:GLY:O	2.36	0.58
2:B:89:PRO:HA	2:B:92:PHE:CD1	2.38	0.58
2:B:301:MET:HE1	2:B:377:PHE:HE2	1.67	0.58
2:B:253:ARG:O	2:B:257:VAL:N	2.33	0.58
2:B:307:PRO:HB3	2:B:312:TYR:OH	2.04	0.58
1:A:166:LYS:HD2	1:A:197:HIS:O	2.04	0.58
1:A:371:VAL:HG12	1:A:372:GLN:N	2.17	0.58
1:A:407:TRP:O	1:A:411:GLU:HG2	2.02	0.58
2:B:151:THR:OG1	2:B:193:GLN:HB3	2.03	0.58
2:B:253:ARG:O	2:B:254:LYS:C	2.42	0.58
1:A:110:ILE:CG2	1:A:111:GLY:H	2.15	0.58
1:A:202:PHE:CE2	1:A:378:LEU:HD22	2.38	0.58
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.33	0.58
4:D:35:ASP:HB2	4:D:41:LYS:CD	2.26	0.58
2:B:172:VAL:HG11	2:B:387:LEU:CD2	2.22	0.58
4:F:35:ASP:HB2	4:F:41:LYS:CD	2.26	0.58
1:A:264:ARG:HB2	1:A:266:HIS:HD2	1.67	0.58
2:B:180:THR:CG2	2:B:181:VAL:H	2.17	0.58
2:B:270:PRO:HA	2:B:377:PHE:O	2.04	0.58
1:A:63:PRO:HD3	1:A:86:LEU:O	2.04	0.57
1:A:117:LEU:HD11	1:A:121:ARG:HH22	1.69	0.57
1:A:119:LEU:CD2	1:A:122:ILE:HD11	2.28	0.57
2:B:299:LYS:H	2:B:299:LYS:CD	2.07	0.57
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.18	0.57
2:B:70:LEU:C	2:B:99:ALA:HB2	2.24	0.57
1:A:268:PRO:HA	1:A:379:SER:O	2.04	0.57
2:B:283:TYR:C	2:B:284:ARG:HG2	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:C	1:A:90:GLU:N	2.57	0.57
1:A:286:LEU:HD12	1:A:290:GLU:HG2	1.87	0.57
2:B:4:ILE:HD13	2:B:136:GLN:NE2	2.18	0.57
2:B:274:PRO:CG	2:B:371:LEU:HD21	2.34	0.57
2:B:320:ARG:O	2:B:359:PRO:HA	2.04	0.57
2:B:319:PHE:CD2	2:B:375:ALA:HB2	2.40	0.57
1:A:317:LEU:HD11	1:A:351:PHE:CE2	2.38	0.57
1:A:362:VAL:HG11	1:A:368:LEU:O	2.04	0.57
2:B:301:MET:CE	2:B:377:PHE:HE2	2.17	0.57
3:C:141:GLU:OE2	4:F:29:LYS:HD2	1.88	0.57
4:F:46:HIS:HD2	4:F:50:MET:CE	2.17	0.57
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.40	0.57
4:D:46:HIS:HD2	4:D:50:MET:CE	2.18	0.57
1:A:19:ALA:CB	1:A:228:ASN:HB3	2.35	0.57
1:A:152:LEU:HA	1:A:155:GLU:CB	2.35	0.57
1:A:175:PRO:HG3	1:A:304:LYS:CG	2.35	0.57
1:A:394:LYS:HG2	2:B:348:PRO:CG	2.35	0.57
2:B:30:ILE:HA	2:B:35:SER:O	2.04	0.57
1:A:313:MET:O	1:A:314:ALA:HB2	2.04	0.56
2:B:14:ASN:OD1	2:B:75:MET:HG2	2.05	0.56
2:B:19:LYS:CG	2:B:228:ASN:HB3	2.31	0.56
2:B:50:ASN:O	2:B:64:ARG:NH2	2.38	0.56
2:B:149:MET:O	2:B:153:LEU:HD13	2.05	0.56
2:B:217:LEU:C	2:B:219:LEU:N	2.55	0.56
1:A:11:GLN:HE22	2:B:249:ASN:ND2	2.03	0.56
1:A:362:VAL:CG1	1:A:368:LEU:HB2	2.35	0.56
2:B:182:VAL:HG23	2:B:186:ASN:ND2	2.20	0.56
2:B:216:THR:O	2:B:217:LEU:HD12	2.05	0.56
1:A:218:ASP:O	1:A:219:ILE:HG23	2.04	0.56
1:A:331:ALA:O	1:A:334:THR:HG22	2.05	0.56
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.18	0.56
2:B:6:HIS:HB3	2:B:65:ALA:HB2	1.87	0.56
2:B:319:PHE:HA	2:B:375:ALA:HA	1.86	0.56
1:A:11:GLN:CG	1:A:74:VAL:HG11	2.28	0.56
1:A:381:THR:C	1:A:383:ALA:N	2.56	0.56
1:A:436:GLY:C	1:A:438:ASP:H	2.08	0.56
2:B:31:ASP:O	2:B:32:PRO:C	2.44	0.56
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.87	0.56
1:A:165:SER:HA	1:A:199:ASP:OD2	2.04	0.56
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.35	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:O	1:A:347:CYS:N	2.38	0.56
2:B:259:MET:CA	2:B:314:THR:HG21	2.35	0.56
2:B:324:SER:C	2:B:326:LYS:N	2.59	0.56
2:B:312:TYR:O	2:B:344:VAL:HB	2.05	0.56
2:B:19:LYS:O	2:B:23:VAL:HG23	2.06	0.56
2:B:139:HIS:HE1	2:B:168:THR:HG23	1.71	0.56
2:B:128:SER:OG	2:B:129:CYS:N	2.34	0.56
2:B:151:THR:OG1	2:B:193:GLN:CB	2.54	0.56
2:B:147:SER:O	2:B:151:THR:CB	2.52	0.56
2:B:166:MET:HB3	2:B:198:THR:OG1	2.06	0.56
2:B:422:GLU:O	2:B:426:ASN:N	2.37	0.56
4:D:37:TYR:CD2	4:D:38:PRO:N	2.74	0.56
4:F:37:TYR:CD2	4:F:38:PRO:N	2.74	0.56
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.41	0.56
2:B:190:SER:O	2:B:194:LEU:HG	2.06	0.56
2:B:310:GLY:CA	2:B:436:GLN:HE21	2.19	0.55
1:A:172:TYR:OH	1:A:387:ALA:O	2.24	0.55
1:A:210:TYR:CE2	1:A:227:LEU:HD11	2.40	0.55
2:B:223:THR:HG22	2:B:224:TYR:N	2.21	0.55
1:A:216:ASN:O	1:A:217:LEU:HB2	2.05	0.55
1:A:409:VAL:C	1:A:411:GLU:H	2.09	0.55
1:A:5:ILE:CG2	1:A:6:SER:N	2.70	0.55
1:A:408:TYR:CD1	1:A:418:PHE:HZ	2.24	0.55
2:B:70:LEU:CD1	2:B:145:THR:HG23	2.35	0.55
2:B:119:LEU:O	2:B:123:ARG:HG3	2.06	0.55
2:B:210:TYR:HD2	2:B:227:LEU:HD21	1.71	0.55
1:A:231:ILE:HA	1:A:234:ILE:CG2	2.36	0.55
1:A:382:THR:O	1:A:382:THR:HG22	2.05	0.55
2:B:165:ILE:HD13	2:B:165:ILE:H	1.71	0.55
2:B:191:VAL:HA	2:B:194:LEU:HD12	1.88	0.55
2:B:239:THR:HG22	2:B:240:THR:N	2.22	0.55
2:B:250:ALA:CA	2:B:254:LYS:HE2	2.35	0.55
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.42	0.55
2:B:424:ASN:C	2:B:424:ASN:HD22	2.09	0.55
1:A:150:THR:O	1:A:153:LEU:N	2.40	0.55
1:A:242:LEU:C	1:A:244:PHE:H	2.09	0.55
1:A:253:THR:O	1:A:256:GLN:HG2	2.06	0.55
2:B:204:ILE:HG21	2:B:231:VAL:CG2	2.36	0.55
2:B:311:ARG:HG2	2:B:311:ARG:HH11	1.71	0.55
2:B:67:LEU:HD23	2:B:67:LEU:N	2.22	0.54
2:B:272:PHE:HB3	2:B:275:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.42	0.54
3:C:150:GLU:OE2	3:C:153:ARG:NH1	2.39	0.54
3:E:150:GLU:OE2	3:E:153:ARG:NH1	2.39	0.54
1:A:17:GLY:O	1:A:21:TRP:HB2	2.08	0.54
1:A:381:THR:OG1	1:A:383:ALA:HB3	2.07	0.54
2:B:132:LEU:CD2	2:B:164:ARG:HG3	2.32	0.54
2:B:172:VAL:CG1	2:B:387:LEU:HD21	2.24	0.54
2:B:427:ASP:OD1	2:B:428:LEU:N	2.41	0.54
1:A:101:ASN:CG	2:B:254:LYS:HD2	2.28	0.54
1:A:115:ILE:HD13	1:A:115:ILE:C	2.28	0.54
2:B:27:GLU:O	2:B:27:GLU:HG2	2.08	0.54
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.73	0.54
2:B:239:THR:O	2:B:241:CYS:N	2.41	0.54
1:A:5:ILE:O	1:A:136:SER:N	2.40	0.54
2:B:213:CYS:SG	2:B:219:LEU:HD23	2.48	0.54
3:C:141:GLU:OE2	4:F:26:ALA:CB	2.54	0.54
1:A:9:VAL:CG1	1:A:139:HIS:HB3	2.38	0.54
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.43	0.54
2:B:325:MET:CE	2:B:355:VAL:HG11	2.38	0.54
4:F:18:ILE:HG13	4:F:125:ILE:HD11	1.90	0.54
1:A:110:ILE:O	1:A:112:LYS:N	2.41	0.54
1:A:121:ARG:O	1:A:125:LEU:HB2	2.08	0.54
1:A:163:LYS:O	1:A:163:LYS:HG2	2.08	0.54
2:B:311:ARG:HD2	2:B:344:VAL:H	1.71	0.54
3:C:216:GLU:O	3:C:216:GLU:HG2	2.07	0.54
1:A:324:VAL:O	1:A:327:ASP:HB2	2.08	0.54
2:B:20:PHE:CE2	2:B:24:ILE:HD12	2.42	0.54
2:B:68:VAL:HG12	2:B:149:MET:CE	2.38	0.54
2:B:322:ARG:HG3	2:B:322:ARG:HH11	1.73	0.54
2:B:331:GLN:O	2:B:335:VAL:HG23	2.08	0.54
4:D:18:ILE:HG13	4:D:125:ILE:HD11	1.90	0.54
3:E:216:GLU:O	3:E:216:GLU:HG2	2.07	0.54
1:A:6:SER:O	1:A:65:ALA:HB1	2.07	0.53
1:A:215:ARG:C	1:A:216:ASN:HD22	2.12	0.53
2:B:259:MET:CG	2:B:314:THR:HG21	2.36	0.53
2:B:343:PHE:O	2:B:344:VAL:O	2.26	0.53
1:A:182:VAL:O	1:A:184:PRO:N	2.41	0.53
2:B:179:ASP:HB2	8:B:800:GDP:H3'	1.90	0.53
2:B:210:TYR:CD2	2:B:227:LEU:HD21	2.44	0.53
1:A:173:PRO:HB2	1:A:391:LEU:CD1	2.38	0.53
1:A:338:LYS:O	1:A:340:THR:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:O	2:B:49:ILE:HG12	2.07	0.53
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.89	0.53
2:B:323:MET:HG3	2:B:328:VAL:HG21	1.90	0.53
2:B:325:MET:O	2:B:329:ASP:HB2	2.07	0.53
4:F:46:HIS:HD2	4:F:50:MET:HE3	1.73	0.53
2:B:194:LEU:C	2:B:196:GLU:H	2.11	0.53
2:B:332:MET:HE3	2:B:351:VAL:HG11	1.89	0.53
4:D:46:HIS:HD2	4:D:50:MET:HE3	1.73	0.53
2:B:424:ASN:C	2:B:424:ASN:ND2	2.62	0.53
4:D:75:TYR:CB	4:D:78:LEU:HD12	2.39	0.53
4:F:75:TYR:CB	4:F:78:LEU:HD12	2.39	0.53
1:A:23:LEU:HD23	1:A:236:SER:CB	2.37	0.53
1:A:339:ARG:C	1:A:341:ILE:H	2.11	0.53
2:B:107:HIS:HD2	2:B:151:THR:HG22	1.72	0.53
1:A:248:LEU:HB3	1:A:355:ILE:H	1.73	0.53
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.44	0.53
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.89	0.53
2:B:431:GLU:O	2:B:434:GLN:CG	2.56	0.53
1:A:5:ILE:O	1:A:135:PHE:HA	2.09	0.53
1:A:275:VAL:HG21	1:A:300:ASN:OD1	2.09	0.53
2:B:168:THR:CB	2:B:201:THR:HG23	2.38	0.53
4:F:46:HIS:CD2	4:F:50:MET:CE	2.92	0.53
1:A:98:ASP:CB	1:A:105:ARG:HH21	2.14	0.52
1:A:206:ASN:OD1	1:A:227:LEU:CD1	2.57	0.52
1:A:231:ILE:HD13	1:A:231:ILE:N	2.25	0.52
1:A:345:ASP:OD2	1:A:439:SER:HB3	2.10	0.52
2:B:141:LEU:HA	2:B:147:SER:HB3	1.91	0.52
4:D:46:HIS:CD2	4:D:50:MET:CE	2.92	0.52
1:A:150:THR:O	1:A:151:SER:C	2.47	0.52
1:A:283:HIS:O	1:A:284:GLU:C	2.47	0.52
2:B:264:ARG:HE	2:B:264:ARG:HA	1.74	0.52
2:B:425:MET:O	2:B:428:LEU:HB3	2.09	0.52
3:C:259:ASN:HB3	3:C:264:LYS:HE2	1.91	0.52
1:A:362:VAL:HG13	1:A:368:LEU:CD1	2.38	0.52
2:B:4:ILE:CG2	2:B:136:GLN:HG2	2.38	0.52
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.42	0.52
2:B:188:THR:HA	2:B:425:MET:CE	2.40	0.52
2:B:198:THR:HG22	2:B:265:LEU:CD2	2.39	0.52
2:B:212:ILE:O	2:B:216:THR:HB	2.10	0.52
2:B:273:ALA:CB	2:B:274:PRO:HD3	2.30	0.52
3:E:259:ASN:HB3	3:E:264:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:VAL:HG23	2:B:5:VAL:O	2.09	0.52
2:B:360:PRO:HB2	9:B:820:TA1:H281	1.91	0.52
1:A:98:ASP:O	1:A:110:ILE:HD13	2.08	0.52
1:A:173:PRO:HB2	1:A:391:LEU:HD11	1.92	0.52
1:A:239:THR:O	1:A:240:ALA:C	2.48	0.52
1:A:243:ARG:CZ	1:A:252:LEU:HG	2.39	0.52
1:A:101:ASN:ND2	7:A:920:GTP:O3G	2.42	0.52
1:A:179:THR:HG22	2:B:352:LYS:HZ1	1.75	0.52
2:B:49:ILE:O	2:B:50:ASN:C	2.48	0.52
2:B:149:MET:O	2:B:153:LEU:HD22	2.10	0.52
1:A:4:CYS:HA	1:A:134:GLY:O	2.10	0.52
1:A:8:HIS:HB3	1:A:13:GLY:O	2.09	0.52
1:A:231:ILE:CA	1:A:234:ILE:HG22	2.38	0.52
1:A:264:ARG:C	1:A:266:HIS:N	2.60	0.52
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.52
1:A:234:ILE:CG1	1:A:270:ALA:HB1	2.38	0.52
1:A:244:PHE:CD2	1:A:245:ASP:N	2.76	0.52
1:A:263:PRO:HG3	3:E:171:THR:HG21	1.92	0.52
2:B:200:GLU:N	2:B:265:LEU:HD13	2.25	0.52
2:B:226:ASP:O	2:B:227:LEU:C	2.46	0.52
2:B:345:GLU:C	2:B:347:ILE:H	2.13	0.52
2:B:226:ASP:O	2:B:229:HIS:N	2.43	0.52
2:B:314:THR:CG2	2:B:315:VAL:N	2.73	0.52
1:A:196:GLU:C	1:A:197:HIS:CD2	2.82	0.51
1:A:191:THR:HG23	1:A:192:HIS:N	2.25	0.51
2:B:260:VAL:HG23	2:B:260:VAL:O	2.10	0.51
2:B:295:MET:SD	2:B:375:ALA:O	2.68	0.51
2:B:297:ASP:OD1	2:B:298:ALA:N	2.39	0.51
1:A:122:ILE:CD1	1:A:157:LEU:HD21	2.35	0.51
1:A:417:GLU:HA	1:A:417:GLU:OE1	2.10	0.51
2:B:229:HIS:C	2:B:229:HIS:ND1	2.62	0.51
2:B:296:PHE:CZ	2:B:315:VAL:HG11	2.46	0.51
2:B:320:ARG:HA	2:B:356:CYS:HB3	1.92	0.51
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.40	0.51
1:A:243:ARG:NH2	1:A:251:ASP:OD1	2.44	0.51
1:A:251:ASP:OD1	1:A:252:LEU:N	2.43	0.51
2:B:149:MET:O	2:B:149:MET:HG2	2.10	0.51
2:B:242:LEU:HD22	2:B:250:ALA:N	2.19	0.51
2:B:277:SER:OG	2:B:281:GLN:HB2	2.10	0.51
1:A:24:TYR:CE2	1:A:240:ALA:HB2	2.45	0.51
1:A:344:VAL:HG12	1:A:345:ASP:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:HZ2	2:B:65:ALA:HB2	1.76	0.51
2:B:70:LEU:HD12	2:B:145:THR:HG23	1.91	0.51
2:B:240:THR:HG23	2:B:241:CYS:H	1.76	0.51
2:B:431:GLU:OE1	2:B:432:TYR:CA	2.57	0.51
1:A:119:LEU:HA	1:A:122:ILE:HG12	1.93	0.51
1:A:171:ILE:O	1:A:171:ILE:HG22	2.11	0.51
1:A:9:VAL:HG21	1:A:149:PHE:CD1	2.46	0.51
1:A:310:GLY:HA3	1:A:383:ALA:N	2.26	0.51
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.94	0.51
2:B:49:ILE:HG13	2:B:50:ASN:H	1.76	0.51
1:A:67:PHE:HE1	1:A:87:PHE:CE2	2.29	0.51
1:A:133:GLN:HB3	1:A:243:ARG:HH12	1.76	0.51
1:A:16:ILE:HG23	1:A:17:GLY:N	2.26	0.50
1:A:132:LEU:CD2	1:A:164:LYS:HE3	2.41	0.50
1:A:402:ARG:O	1:A:403:ALA:O	2.29	0.50
2:B:113:GLU:HG3	2:B:114:LEU:N	2.26	0.50
2:B:369:ARG:C	2:B:369:ARG:HD2	2.32	0.50
1:A:115:ILE:HD11	1:A:119:LEU:HG	1.92	0.50
1:A:133:GLN:CB	1:A:243:ARG:HH12	2.24	0.50
1:A:140:SER:O	1:A:142:GLY:N	2.44	0.50
2:B:103:TRP:HZ3	2:B:108:TYR:CE1	2.27	0.50
2:B:176:LYS:CE	2:B:207:GLU:HG3	2.39	0.50
1:A:147:SER:CB	1:A:190:THR:OG1	2.52	0.50
1:A:305:CYS:O	1:A:306:ASP:C	2.49	0.50
2:B:103:TRP:CE2	2:B:189:LEU:HB3	2.45	0.50
2:B:156:LYS:HA	2:B:156:LYS:CE	2.38	0.50
1:A:201:ALA:O	1:A:267:PHE:HA	2.10	0.50
2:B:3:GLU:HA	2:B:51:VAL:HA	1.93	0.50
1:A:115:ILE:CG2	1:A:116:ASP:N	2.75	0.50
2:B:265:LEU:O	2:B:266:HIS:O	2.29	0.50
1:A:328:VAL:C	1:A:330:ALA:H	2.16	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.50
2:B:298:ALA:O	2:B:299:LYS:C	2.50	0.50
2:B:345:GLU:O	2:B:347:ILE:N	2.45	0.50
1:A:196:GLU:O	1:A:197:HIS:CD2	2.64	0.49
1:A:238:ILE:O	1:A:242:LEU:HB2	2.11	0.49
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.46	0.49
1:A:414:GLU:OE1	1:A:414:GLU:N	2.46	0.49
2:B:4:ILE:HD12	2:B:239:THR:CG2	2.42	0.49
2:B:431:GLU:HA	2:B:434:GLN:CG	2.42	0.49
3:C:115:LYS:HZ1	3:E:81:LYS:HZ1	1.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:THR:O	2:B:201:THR:HA	2.12	0.49
2:B:336:GLN:HE22	2:B:349:ASN:ND2	2.10	0.49
1:A:11:GLN:O	1:A:14:VAL:HB	2.12	0.49
1:A:408:TYR:O	1:A:411:GLU:N	2.39	0.49
2:B:8:GLN:HB3	2:B:14:ASN:HA	1.94	0.49
2:B:323:MET:HG3	2:B:328:VAL:CG2	2.41	0.49
2:B:333:LEU:O	2:B:336:GLN:N	2.45	0.49
2:B:413:MET:HG3	2:B:414:ASP:N	2.22	0.49
1:A:392:ASP:O	1:A:395:PHE:HB3	2.13	0.49
2:B:107:HIS:CD2	2:B:151:THR:HG22	2.45	0.49
2:B:173:PRO:HB3	2:B:183:GLU:HG2	1.93	0.49
2:B:262:PHE:O	2:B:264:ARG:N	2.45	0.49
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.95	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
1:A:12:ALA:CB	1:A:140:SER:OG	2.59	0.49
2:B:383:ALA:C	2:B:385:GLN:H	2.15	0.49
1:A:5:ILE:HG22	1:A:6:SER:H	1.78	0.49
1:A:149:PHE:HE1	1:A:153:LEU:HD22	1.77	0.49
1:A:283:HIS:O	1:A:285:GLN:N	2.45	0.49
2:B:265:LEU:HD12	2:B:266:HIS:O	2.12	0.49
2:B:296:PHE:HZ	2:B:315:VAL:HG11	1.78	0.49
2:B:431:GLU:OE1	2:B:432:TYR:N	2.46	0.49
1:A:244:PHE:CD2	1:A:244:PHE:C	2.83	0.49
2:B:4:ILE:HG22	2:B:5:VAL:N	2.27	0.49
2:B:173:PRO:HB3	2:B:183:GLU:CG	2.42	0.49
2:B:387:LEU:HD23	2:B:388:PHE:CD2	2.47	0.49
3:E:258:PHE:O	3:E:260:VAL:N	2.46	0.49
1:A:192:HIS:CD2	1:A:424:ASP:OD2	2.66	0.49
1:A:227:LEU:O	1:A:231:ILE:HG12	2.12	0.49
2:B:69:ASP:HA	2:B:145:THR:HG21	1.95	0.49
2:B:137:LEU:HD22	2:B:154:ILE:HG21	1.95	0.49
3:C:258:PHE:O	3:C:260:VAL:N	2.46	0.49
1:A:151:SER:OG	1:A:193:THR:HG21	2.13	0.48
1:A:274:PRO:CB	1:A:371:VAL:HG21	2.43	0.48
2:B:24:ILE:HG22	2:B:25:SER:N	2.27	0.48
2:B:142:GLY:HA3	2:B:183:GLU:OE2	2.13	0.48
2:B:209:LEU:O	2:B:210:TYR:C	2.48	0.48
2:B:199:ASP:O	2:B:200:GLU:HG3	2.13	0.48
2:B:209:LEU:O	2:B:213:CYS:N	2.47	0.48
1:A:163:LYS:C	1:A:164:LYS:HG2	2.33	0.48
1:A:191:THR:CG2	1:A:192:HIS:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:C	1:A:244:PHE:N	2.66	0.48
1:A:369:ALA:O	1:A:370:LYS:CB	2.62	0.48
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.27	0.48
2:B:209:LEU:CD2	2:B:227:LEU:HD13	2.44	0.48
2:B:211:ASP:OD1	2:B:212:ILE:HG13	2.13	0.48
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.48
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.96	0.48
1:A:203:MET:SD	1:A:267:PHE:HB3	2.53	0.48
1:A:328:VAL:O	1:A:330:ALA:N	2.38	0.48
2:B:259:MET:HG2	2:B:314:THR:CG2	2.38	0.48
2:B:269:MET:HB3	2:B:303:ALA:HB2	1.94	0.48
1:A:9:VAL:HG11	1:A:150:THR:OG1	2.13	0.48
1:A:118:VAL:HG21	1:A:149:PHE:CE2	2.48	0.48
1:A:158:SER:OG	1:A:197:HIS:HB3	2.13	0.48
2:B:24:ILE:CD1	2:B:52:TYR:CE1	2.97	0.48
2:B:154:ILE:HG22	2:B:166:MET:CE	2.44	0.48
2:B:287:THR:O	2:B:288:VAL:CG2	2.58	0.48
1:A:96:LYS:O	1:A:97:GLU:O	2.31	0.48
1:A:188:ILE:O	1:A:191:THR:HG22	2.13	0.48
3:E:80:ILE:HG23	3:E:81:LYS:HG2	1.94	0.48
1:A:384:ILE:HG22	1:A:388:TRP:CD1	2.49	0.48
2:B:2:ARG:NH1	2:B:251:ASP:OD2	2.46	0.48
2:B:20:PHE:CG	2:B:235:MET:SD	3.07	0.48
1:A:104:ALA:CB	1:A:408:TYR:HD2	2.26	0.48
1:A:210:TYR:CE2	1:A:227:LEU:HD21	2.49	0.48
2:B:49:ILE:HG13	2:B:50:ASN:N	2.28	0.48
3:C:80:ILE:HG23	3:C:81:LYS:HG2	1.94	0.48
1:A:97:GLU:HB2	1:A:110:ILE:HD11	1.96	0.48
1:A:99:ALA:O	1:A:100:ALA:HB3	2.14	0.48
1:A:132:LEU:HD21	1:A:164:LYS:HE3	1.96	0.48
2:B:264:ARG:HA	2:B:264:ARG:NE	2.29	0.48
1:A:19:ALA:HB2	1:A:228:ASN:HB3	1.96	0.47
1:A:105:ARG:HH11	1:A:105:ARG:HG3	1.78	0.47
1:A:335:ILE:O	1:A:337:THR:N	2.47	0.47
2:B:175:PRO:CD	2:B:207:GLU:OE1	2.61	0.47
2:B:272:PHE:CE1	9:B:820:TA1:H391	2.50	0.47
2:B:307:PRO:HB3	2:B:312:TYR:CZ	2.49	0.47
2:B:308:ARG:HG3	2:B:342:TYR:OH	2.13	0.47
2:B:387:LEU:O	2:B:387:LEU:HG	2.15	0.47
1:A:115:ILE:O	1:A:116:ASP:C	2.51	0.47
1:A:147:SER:O	1:A:190:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:CE	1:A:199:ASP:OD1	2.62	0.47
1:A:175:PRO:HD2	1:A:207:GLU:HB3	1.97	0.47
1:A:253:THR:O	1:A:254:GLU:C	2.52	0.47
1:A:286:LEU:CD1	1:A:290:GLU:HG2	2.44	0.47
1:A:317:LEU:CD1	1:A:351:PHE:CD2	2.97	0.47
2:B:175:PRO:O	2:B:176:LYS:C	2.52	0.47
2:B:176:LYS:HG3	2:B:177:VAL:H	1.78	0.47
2:B:297:ASP:OD2	2:B:299:LYS:HE2	2.14	0.47
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.49	0.47
1:A:255:PHE:O	1:A:256:GLN:C	2.53	0.47
1:A:217:LEU:CD1	1:A:277:SER:HA	2.44	0.47
1:A:316:CYS:HB3	1:A:378:LEU:HD12	1.95	0.47
2:B:185:TYR:HD2	2:B:395:PHE:CE1	2.33	0.47
1:A:104:ALA:HB1	1:A:413:MET:HG3	1.95	0.47
1:A:107:HIS:CE1	1:A:152:LEU:HB3	2.49	0.47
1:A:120:ASP:O	1:A:124:LYS:HB2	2.15	0.47
1:A:148:GLY:O	1:A:151:SER:CB	2.61	0.47
1:A:345:ASP:C	1:A:347:CYS:N	2.68	0.47
1:A:386:GLU:O	1:A:388:TRP:N	2.47	0.47
2:B:191:VAL:HG13	2:B:192:HIS:N	2.28	0.47
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.47
1:A:117:LEU:HD12	1:A:121:ARG:HH12	1.80	0.47
1:A:154:MET:HA	1:A:157:LEU:HD12	1.96	0.47
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.47
1:A:185:TYR:OH	1:A:399:TYR:HA	2.15	0.47
1:A:191:THR:O	1:A:195:LEU:HB2	2.15	0.47
1:A:241:SER:HB3	1:A:320:ARG:NH2	2.29	0.47
2:B:20:PHE:O	2:B:24:ILE:HB	2.14	0.47
2:B:115:VAL:CG2	2:B:152:LEU:HD23	2.44	0.47
2:B:175:PRO:HD2	2:B:207:GLU:CD	2.35	0.47
2:B:198:THR:HG23	2:B:200:GLU:H	1.79	0.47
2:B:226:ASP:O	2:B:229:HIS:HB3	2.14	0.47
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.47
1:A:145:THR:O	1:A:149:PHE:HB3	2.15	0.47
1:A:278:ALA:O	1:A:279:GLU:HG2	2.15	0.47
1:A:384:ILE:HG22	1:A:384:ILE:O	2.15	0.47
2:B:263:PRO:O	2:B:264:ARG:C	2.52	0.47
1:A:6:SER:OG	1:A:65:ALA:HB2	2.14	0.47
1:A:34:GLY:C	1:A:61:HIS:N	2.68	0.47
1:A:224:TYR:CG	2:B:325:MET:HG2	2.50	0.47
1:A:339:ARG:C	1:A:341:ILE:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LEU:O	2:B:99:ALA:HB2	2.15	0.47
2:B:307:PRO:C	2:B:309:HIS:H	2.18	0.47
2:B:332:MET:HE2	2:B:351:VAL:HG11	1.97	0.47
3:C:215:THR:HG22	3:C:217:ASP:H	1.79	0.47
3:E:215:THR:HG22	3:E:217:ASP:H	1.79	0.47
1:A:25:CYS:SG	1:A:83:TYR:HE2	2.38	0.47
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.97	0.47
1:A:226:ASN:O	1:A:229:ARG:N	2.48	0.47
1:A:243:ARG:NH2	1:A:252:LEU:CB	2.78	0.47
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.97	0.47
2:B:134:GLY:HA3	2:B:165:ILE:HG12	1.97	0.47
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.45	0.47
2:B:287:THR:N	2:B:290:GLU:OE1	2.48	0.47
2:B:101:ASN:ND2	2:B:101:ASN:O	2.48	0.46
2:B:137:LEU:HD22	2:B:154:ILE:HG23	1.97	0.46
2:B:242:LEU:HD11	2:B:250:ALA:HB3	1.97	0.46
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.97	0.46
1:A:434:GLU:C	1:A:436:GLY:H	2.18	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
2:B:324:SER:OG	2:B:326:LYS:HB3	2.16	0.46
2:B:360:PRO:O	2:B:369:ARG:C	2.54	0.46
4:D:37:TYR:CG	4:D:38:PRO:HA	2.49	0.46
4:F:37:TYR:CG	4:F:38:PRO:HA	2.49	0.46
1:A:10:GLY:O	1:A:11:GLN:C	2.53	0.46
1:A:22:GLU:O	1:A:23:LEU:C	2.54	0.46
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.30	0.46
2:B:102:ASN:ND2	2:B:408:TYR:HA	2.20	0.46
1:A:99:ALA:H	2:B:2:ARG:HH22	1.63	0.46
1:A:243:ARG:NH2	1:A:252:LEU:HB2	2.31	0.46
1:A:210:TYR:CZ	1:A:227:LEU:HD11	2.51	0.46
1:A:392:ASP:OD2	1:A:422:ARG:NE	2.48	0.46
1:A:436:GLY:O	1:A:438:ASP:N	2.48	0.46
2:B:133:GLN:O	2:B:165:ILE:CD1	2.64	0.46
3:E:237:MET:HG2	4:F:100:ARG:HD2	1.97	0.46
1:A:115:ILE:HG23	1:A:116:ASP:H	1.79	0.46
1:A:119:LEU:HD11	1:A:156:ARG:HD2	1.97	0.46
1:A:172:TYR:CD1	1:A:173:PRO:N	2.80	0.46
1:A:224:TYR:HD1	2:B:247:GLN:HB3	1.80	0.46
1:A:396:ASP:O	1:A:397:LEU:C	2.53	0.46
1:A:404:PHE:CD1	1:A:404:PHE:N	2.83	0.46
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:GLU:O	2:B:197:ASN:OD1	2.34	0.46
2:B:384:ILE:HG23	2:B:384:ILE:O	2.14	0.46
2:B:431:GLU:HA	3:C:176:HIS:HD2	1.81	0.46
1:A:196:GLU:C	1:A:197:HIS:HD2	2.19	0.46
1:A:256:GLN:O	1:A:260:VAL:HG13	2.15	0.46
1:A:286:LEU:O	1:A:287:SER:O	2.34	0.46
1:A:324:VAL:HG12	1:A:326:LYS:H	1.81	0.46
2:B:237:GLY:O	2:B:241:CYS:CB	2.61	0.46
2:B:323:MET:CE	2:B:328:VAL:HG22	2.46	0.46
3:C:237:MET:HG2	4:D:100:ARG:HD2	1.98	0.46
4:D:50:MET:O	4:D:54:GLN:HG3	2.16	0.46
1:A:114:ILE:O	1:A:118:VAL:HG23	2.16	0.46
1:A:317:LEU:CD1	1:A:351:PHE:CE2	2.99	0.46
2:B:224:TYR:O	2:B:225:GLY:C	2.53	0.46
3:C:148:GLU:HG2	3:C:170:TYR:CE2	2.51	0.46
4:F:50:MET:O	4:F:54:GLN:HG3	2.16	0.46
1:A:4:CYS:SG	1:A:252:LEU:CD1	3.02	0.46
1:A:11:GLN:HE21	1:A:74:VAL:CG2	2.29	0.46
1:A:241:SER:C	1:A:244:PHE:HB3	2.36	0.46
1:A:265:GLY:O	1:A:266:HIS:O	2.33	0.46
1:A:423:GLU:O	1:A:426:ALA:HB3	2.16	0.46
2:B:408:TYR:O	2:B:411:GLU:HB2	2.16	0.46
3:E:148:GLU:HG2	3:E:170:TYR:CE2	2.51	0.46
1:A:115:ILE:CG1	1:A:152:LEU:HD13	2.46	0.46
1:A:148:GLY:O	1:A:149:PHE:C	2.55	0.46
1:A:344:VAL:CG1	1:A:345:ASP:N	2.78	0.46
1:A:381:THR:O	1:A:383:ALA:N	2.49	0.46
2:B:113:GLU:CG	2:B:114:LEU:N	2.79	0.46
2:B:208:ALA:O	2:B:212:ILE:HG13	2.16	0.46
1:A:151:SER:HB3	1:A:193:THR:CG2	2.34	0.45
1:A:203:MET:SD	1:A:267:PHE:CB	3.04	0.45
1:A:278:ALA:HB2	1:A:369:ALA:CA	2.45	0.45
1:A:286:LEU:HG	1:A:290:GLU:HB2	1.97	0.45
1:A:334:THR:CG2	1:A:335:ILE:N	2.79	0.45
2:B:168:THR:N	2:B:200:GLU:O	2.43	0.45
2:B:243:ARG:HH21	2:B:252:LEU:N	2.12	0.45
1:A:276:ILE:HG12	1:A:277:SER:N	2.32	0.45
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.81	0.45
2:B:94:PHE:N	2:B:94:PHE:CD2	2.83	0.45
2:B:154:ILE:HD12	2:B:155:SER:N	2.31	0.45
1:A:180:ALA:HA	2:B:352:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HB	1:A:302:MET:HE1	1.98	0.45
1:A:260:VAL:O	1:A:260:VAL:CG2	2.63	0.45
2:B:23:VAL:O	2:B:25:SER:N	2.50	0.45
2:B:242:LEU:C	2:B:244:PHE:H	2.19	0.45
1:A:95:GLY:C	1:A:97:GLU:N	2.69	0.45
1:A:110:ILE:CG2	1:A:111:GLY:N	2.71	0.45
2:B:11:GLN:O	2:B:14:ASN:HB3	2.16	0.45
2:B:67:LEU:HD12	2:B:92:PHE:CD2	2.51	0.45
2:B:313:LEU:O	2:B:347:ILE:HD12	2.16	0.45
2:B:324:SER:O	2:B:326:LYS:N	2.50	0.45
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.92	0.45
1:A:308:ARG:O	1:A:309:HIS:HB3	2.17	0.45
1:A:408:TYR:CG	1:A:418:PHE:HZ	2.34	0.45
1:A:413:MET:C	1:A:414:GLU:HG3	2.36	0.45
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.98	0.45
2:B:274:PRO:HG2	2:B:371:LEU:CD2	2.43	0.45
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.98	0.45
1:A:5:ILE:CG2	1:A:6:SER:H	2.29	0.45
1:A:132:LEU:H	1:A:132:LEU:CD2	2.23	0.45
2:B:209:LEU:HD23	2:B:227:LEU:HD13	1.98	0.45
2:B:288:VAL:N	2:B:289:PRO:CD	2.80	0.45
2:B:288:VAL:N	2:B:289:PRO:HD2	2.32	0.45
3:C:80:ILE:HG23	3:C:81:LYS:N	2.29	0.45
3:E:80:ILE:HG23	3:E:81:LYS:N	2.29	0.45
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.98	0.45
1:A:271:THR:O	1:A:376:CYS:HA	2.17	0.45
1:A:288:VAL:HA	1:A:291:ILE:HG12	1.98	0.45
1:A:407:TRP:O	1:A:411:GLU:CG	2.63	0.45
2:B:6:HIS:HB3	2:B:21:TRP:HZ2	1.81	0.45
2:B:135:PHE:CD1	2:B:135:PHE:N	2.84	0.45
2:B:167:ASN:HA	2:B:200:GLU:O	2.17	0.45
2:B:188:THR:HA	2:B:425:MET:HE3	1.98	0.45
2:B:194:LEU:O	2:B:265:LEU:HD23	2.16	0.45
2:B:310:GLY:HA3	2:B:436:GLN:NE2	2.29	0.45
1:A:204:VAL:CG1	1:A:209:ILE:HD11	2.42	0.45
1:A:392:ASP:OD2	1:A:422:ARG:CZ	2.65	0.45
2:B:210:TYR:CE2	2:B:227:LEU:HD11	2.51	0.45
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.52	0.45
1:A:210:TYR:CD2	1:A:227:LEU:HD21	2.51	0.45
1:A:234:ILE:C	1:A:234:ILE:CD1	2.86	0.45
2:B:175:PRO:HG2	2:B:207:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HD13	1:A:231:ILE:H	1.82	0.45
1:A:278:ALA:CA	1:A:282:TYR:OH	2.65	0.45
1:A:283:HIS:O	1:A:283:HIS:ND1	2.49	0.45
1:A:286:LEU:O	1:A:287:SER:C	2.55	0.45
2:B:150:GLY:HA2	2:B:153:LEU:CD2	2.41	0.45
2:B:204:ILE:HD13	2:B:231:VAL:CG2	2.45	0.45
2:B:230:LEU:HD21	2:B:302:MET:HE2	1.98	0.45
2:B:242:LEU:HD22	2:B:250:ALA:O	2.17	0.45
2:B:250:ALA:HB1	2:B:254:LYS:CB	2.44	0.45
1:A:229:ARG:NH1	1:A:229:ARG:HG2	2.31	0.44
2:B:8:GLN:CG	2:B:67:LEU:HD22	2.47	0.44
1:A:12:ALA:HB2	7:A:920:GTP:C8	2.52	0.44
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.83	0.44
1:A:175:PRO:CG	1:A:304:LYS:HG2	2.47	0.44
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.99	0.44
2:B:24:ILE:CG2	2:B:25:SER:N	2.80	0.44
2:B:82:PRO:C	2:B:84:GLY:H	2.20	0.44
2:B:167:ASN:HD21	2:B:252:LEU:HD22	1.82	0.44
2:B:295:MET:SD	2:B:375:ALA:HB3	2.57	0.44
2:B:409:THR:HA	2:B:413:MET:HB3	1.99	0.44
3:C:249:GLU:HG2	3:C:253:LYS:HE3	1.99	0.44
3:E:249:GLU:HG2	3:E:253:LYS:HE3	1.99	0.44
1:A:23:LEU:O	1:A:26:LEU:HB3	2.17	0.44
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.47	0.44
1:A:230:LEU:O	1:A:233:GLN:N	2.35	0.44
2:B:14:ASN:O	2:B:17:GLY:N	2.50	0.44
2:B:141:LEU:N	2:B:141:LEU:HD12	2.33	0.44
4:D:9:TYR:HB3	4:D:13:GLU:HB2	1.99	0.44
3:E:84:ARG:HA	3:E:85:PRO:HD3	1.78	0.44
4:F:9:TYR:HB3	4:F:13:GLU:HB2	1.99	0.44
1:A:212:ILE:HD11	1:A:302:MET:H	1.82	0.44
1:A:274:PRO:HB2	1:A:371:VAL:HG21	1.99	0.44
2:B:4:ILE:HD12	2:B:239:THR:HG21	1.98	0.44
2:B:72:PRO:O	2:B:74:THR:N	2.50	0.44
2:B:102:ASN:OD1	2:B:408:TYR:CZ	2.70	0.44
2:B:106:GLY:O	2:B:149:MET:HB2	2.17	0.44
2:B:194:LEU:C	2:B:196:GLU:N	2.70	0.44
2:B:307:PRO:C	2:B:309:HIS:N	2.71	0.44
3:C:84:ARG:HA	3:C:85:PRO:HD3	1.78	0.44
1:A:23:LEU:CD2	1:A:232:GLY:O	2.64	0.44
2:B:189:LEU:HD23	2:B:421:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PRO:HG2	2:B:371:LEU:CB	2.38	0.44
2:B:399:PHE:O	2:B:402:LYS:N	2.29	0.44
4:F:35:ASP:HB3	4:F:41:LYS:HD2	1.95	0.44
1:A:9:VAL:HG21	1:A:149:PHE:HD1	1.80	0.44
1:A:182:VAL:O	1:A:184:PRO:CD	2.65	0.44
1:A:204:VAL:HG12	1:A:204:VAL:O	2.17	0.44
1:A:272:TYR:CE2	1:A:274:PRO:HD2	2.53	0.44
1:A:343:PHE:CE1	1:A:351:PHE:HE1	2.36	0.44
2:B:312:TYR:HA	2:B:381:SER:HA	1.99	0.44
1:A:11:GLN:NE2	1:A:74:VAL:HG22	2.30	0.44
1:A:252:LEU:O	1:A:253:THR:C	2.56	0.44
1:A:295:CYS:HB3	1:A:377:MET:HG2	1.99	0.44
2:B:182:VAL:O	2:B:183:GLU:C	2.56	0.44
2:B:288:VAL:C	2:B:290:GLU:N	2.70	0.44
3:E:215:THR:HB	3:E:219:ILE:HB	2.00	0.44
1:A:268:PRO:CA	1:A:379:SER:O	2.65	0.44
1:A:287:SER:N	1:A:290:GLU:OE1	2.51	0.44
1:A:288:VAL:C	1:A:290:GLU:N	2.71	0.44
1:A:434:GLU:CG	3:E:176:HIS:CE1	2.64	0.44
2:B:161:TYR:O	2:B:163:ASP:N	2.51	0.44
2:B:168:THR:CG2	2:B:201:THR:HG23	2.48	0.44
2:B:239:THR:O	2:B:240:THR:C	2.56	0.44
9:B:820:TA1:H463	9:B:820:TA1:C26	2.46	0.44
3:C:215:THR:HB	3:C:219:ILE:HB	2.00	0.44
1:A:149:PHE:O	1:A:150:THR:C	2.56	0.44
1:A:152:LEU:HD12	1:A:152:LEU:C	2.38	0.44
1:A:262:TYR:HB3	1:A:263:PRO:HD2	2.00	0.44
1:A:362:VAL:HG13	1:A:368:LEU:CG	2.48	0.44
2:B:52:TYR:HE1	2:B:240:THR:HB	1.83	0.44
3:C:258:PHE:O	3:C:259:ASN:C	2.56	0.44
3:E:258:PHE:O	3:E:259:ASN:C	2.56	0.44
1:A:72:PRO:HG2	1:A:73:THR:H	1.83	0.43
1:A:255:PHE:O	1:A:259:LEU:N	2.50	0.43
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.79	0.43
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.52	0.43
2:B:68:VAL:HG11	2:B:153:LEU:HD21	2.00	0.43
2:B:180:THR:HG22	2:B:181:VAL:H	1.81	0.43
2:B:282:GLN:HB3	2:B:282:GLN:HE21	1.51	0.43
2:B:301:MET:O	2:B:303:ALA:N	2.51	0.43
4:D:35:ASP:HB3	4:D:41:LYS:NZ	2.32	0.43
4:F:35:ASP:HB3	4:F:41:LYS:NZ	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ALA:O	1:A:102:ASN:N	2.49	0.43
1:A:121:ARG:HG2	1:A:121:ARG:NH1	2.33	0.43
1:A:153:LEU:O	1:A:157:LEU:HG	2.18	0.43
2:B:7:ILE:N	2:B:136:GLN:O	2.51	0.43
1:A:218:ASP:C	1:A:219:ILE:HG12	2.37	0.43
2:B:26:ASP:C	2:B:28:HIS:H	2.21	0.43
2:B:70:LEU:HB2	2:B:99:ALA:CB	2.48	0.43
2:B:212:ILE:O	2:B:212:ILE:HG22	2.18	0.43
4:D:41:LYS:HA	4:D:42:PRO:HD2	1.81	0.43
4:F:41:LYS:HA	4:F:42:PRO:HD2	1.81	0.43
1:A:63:PRO:HG2	1:A:91:GLN:OE1	2.18	0.43
1:A:103:TYR:O	1:A:104:ALA:C	2.57	0.43
1:A:310:GLY:HA3	1:A:383:ALA:CA	2.49	0.43
2:B:409:THR:C	2:B:411:GLU:H	2.22	0.43
1:A:238:ILE:HD11	1:A:378:LEU:HD23	2.01	0.43
1:A:363:VAL:CG1	1:A:364:PRO:HD2	2.48	0.43
2:B:187:ALA:O	2:B:188:THR:C	2.57	0.43
1:A:8:HIS:HA	1:A:138:PHE:HB2	2.00	0.43
1:A:144:GLY:H	7:A:920:GTP:PG	2.41	0.43
1:A:209:ILE:CD1	1:A:231:ILE:CD1	2.97	0.43
1:A:304:LYS:O	1:A:304:LYS:HG3	2.19	0.43
1:A:428:LEU:HD12	1:A:428:LEU:HA	1.79	0.43
1:A:436:GLY:C	1:A:438:ASP:N	2.72	0.43
2:B:161:TYR:CD1	2:B:161:TYR:N	2.86	0.43
2:B:383:ALA:C	2:B:385:GLN:N	2.72	0.43
1:A:154:MET:CE	1:A:166:LYS:HB3	2.48	0.43
1:A:230:LEU:O	1:A:231:ILE:C	2.57	0.43
1:A:238:ILE:O	1:A:242:LEU:CB	2.67	0.43
1:A:263:PRO:O	1:A:264:ARG:C	2.56	0.43
1:A:303:VAL:O	1:A:303:VAL:CG1	2.65	0.43
1:A:377:MET:O	1:A:377:MET:HG3	2.18	0.43
2:B:12:CYS:C	2:B:14:ASN:N	2.71	0.43
2:B:154:ILE:HG22	2:B:166:MET:HE1	2.00	0.43
2:B:311:ARG:HG2	2:B:311:ARG:NH1	2.34	0.43
2:B:422:GLU:O	2:B:426:ASN:CB	2.67	0.43
1:A:25:CYS:SG	1:A:26:LEU:N	2.92	0.43
1:A:409:VAL:C	1:A:411:GLU:N	2.71	0.43
2:B:161:TYR:C	2:B:163:ASP:N	2.72	0.43
2:B:210:TYR:O	2:B:214:PHE:N	2.52	0.43
2:B:240:THR:HG23	2:B:241:CYS:N	2.34	0.43
2:B:333:LEU:O	2:B:334:ASN:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:ND2	2:B:254:LYS:CD	2.75	0.43
1:A:147:SER:HB2	1:A:186:ASN:O	2.19	0.43
1:A:343:PHE:HZ	1:A:351:PHE:CZ	2.36	0.43
2:B:105:LYS:HG2	2:B:110:GLU:CG	2.48	0.43
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.43
2:B:427:ASP:OD1	2:B:427:ASP:C	2.58	0.43
1:A:63:PRO:C	1:A:64:ARG:CG	2.83	0.42
2:B:435:TYR:C	2:B:437:ASP:N	2.72	0.42
4:D:89:VAL:HG21	4:D:106:THR:HG22	2.01	0.42
1:A:6:SER:HB3	1:A:136:SER:HG	1.82	0.42
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.42
1:A:378:LEU:HD12	1:A:378:LEU:O	2.19	0.42
2:B:35:SER:CB	2:B:59:ASN:HA	2.42	0.42
4:F:89:VAL:HG21	4:F:106:THR:HG22	2.01	0.42
1:A:15:GLN:NE2	7:A:920:GTP:N7	2.67	0.42
2:B:6:HIS:HB3	2:B:65:ALA:CB	2.48	0.42
2:B:48:ARG:HG2	2:B:243:ARG:HB3	2.01	0.42
2:B:118:VAL:O	2:B:122:VAL:HG13	2.19	0.42
4:D:96:LEU:CD1	4:D:104:PHE:CD1	3.02	0.42
1:A:7:ILE:HD11	1:A:137:VAL:CG2	2.44	0.42
1:A:13:GLY:C	1:A:16:ILE:HG22	2.38	0.42
1:A:119:LEU:HD11	1:A:156:ARG:HD3	2.01	0.42
1:A:402:ARG:O	1:A:405:VAL:N	2.49	0.42
2:B:11:GLN:O	2:B:15:GLN:N	2.41	0.42
2:B:106:GLY:O	2:B:149:MET:CA	2.68	0.42
2:B:114:LEU:HD23	2:B:149:MET:HE2	2.02	0.42
2:B:210:TYR:O	2:B:211:ASP:C	2.57	0.42
2:B:421:ALA:O	2:B:422:GLU:C	2.58	0.42
4:F:96:LEU:CD1	4:F:104:PHE:CD1	3.02	0.42
1:A:21:TRP:HE1	1:A:63:PRO:HB3	1.83	0.42
1:A:67:PHE:HB2	1:A:92:LEU:HD23	2.02	0.42
1:A:390:ARG:HG3	1:A:390:ARG:HH11	1.83	0.42
2:B:72:PRO:O	2:B:73:GLY:C	2.58	0.42
2:B:72:PRO:HG2	2:B:73:GLY:H	1.83	0.42
2:B:192:HIS:NE2	2:B:420:GLU:HG2	2.34	0.42
1:A:8:HIS:CD2	1:A:138:PHE:CD1	3.07	0.42
1:A:305:CYS:SG	1:A:383:ALA:HB1	2.60	0.42
1:A:363:VAL:HG13	1:A:364:PRO:HD2	2.02	0.42
4:D:75:TYR:HB3	4:D:78:LEU:HD12	2.01	0.42
4:F:75:TYR:HB3	4:F:78:LEU:HD12	2.01	0.42
1:A:95:GLY:C	1:A:97:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:CA	1:A:254:GLU:HG3	2.48	0.42
1:A:335:ILE:C	1:A:337:THR:N	2.73	0.42
2:B:25:SER:O	2:B:28:HIS:N	2.53	0.42
1:A:105:ARG:O	1:A:110:ILE:CG2	2.64	0.42
1:A:213:CYS:O	1:A:219:ILE:HG13	2.20	0.42
2:B:103:TRP:HB2	2:B:186:ASN:HA	2.01	0.42
2:B:138:THR:O	2:B:139:HIS:HB3	2.19	0.42
4:D:103:ASP:CG	4:D:119:ARG:HH22	2.22	0.42
4:F:103:ASP:CG	4:F:119:ARG:HH22	2.22	0.42
1:A:175:PRO:HG3	1:A:304:LYS:CB	2.50	0.42
1:A:255:PHE:O	1:A:257:THR:N	2.53	0.42
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.76	0.42
2:B:307:PRO:O	2:B:309:HIS:N	2.53	0.42
3:C:141:GLU:OE1	4:F:29:LYS:HE3	1.97	0.42
1:A:76:ASP:O	1:A:79:ARG:N	2.52	0.42
1:A:115:ILE:CD1	1:A:115:ILE:C	2.87	0.42
2:B:199:ASP:C	2:B:265:LEU:HD13	2.40	0.42
2:B:343:PHE:CD2	2:B:350:ASN:ND2	2.88	0.42
2:B:399:PHE:O	2:B:401:ARG:N	2.53	0.42
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.50	0.41
1:A:210:TYR:OH	2:B:325:MET:HB3	2.20	0.41
1:A:242:LEU:HD11	1:A:250:VAL:HG23	2.02	0.41
2:B:242:LEU:HB3	2:B:250:ALA:O	2.20	0.41
2:B:250:ALA:CB	2:B:254:LYS:HE2	2.50	0.41
1:A:115:ILE:CG2	1:A:116:ASP:H	2.32	0.41
1:A:152:LEU:C	1:A:152:LEU:CD1	2.89	0.41
1:A:401:LYS:C	1:A:403:ALA:H	2.24	0.41
2:B:2:ARG:NH1	2:B:251:ASP:CG	2.73	0.41
2:B:273:ALA:HB1	2:B:291:LEU:HG	2.01	0.41
1:A:67:PHE:CE1	1:A:87:PHE:CE2	3.08	0.41
2:B:153:LEU:HD13	2:B:153:LEU:N	2.34	0.41
2:B:275:LEU:HD12	2:B:275:LEU:HA	1.78	0.41
1:A:23:LEU:HD11	1:A:361:THR:O	2.21	0.41
1:A:101:ASN:HD21	2:B:254:LYS:NZ	2.19	0.41
1:A:231:ILE:C	1:A:233:GLN:N	2.73	0.41
1:A:289:ALA:HB3	1:A:290:GLU:OE2	2.21	0.41
1:A:328:VAL:C	1:A:330:ALA:N	2.73	0.41
2:B:135:PHE:CD1	2:B:166:MET:SD	3.14	0.41
2:B:175:PRO:O	2:B:177:VAL:N	2.53	0.41
2:B:202:TYR:CE2	2:B:268:PHE:HD1	2.38	0.41
2:B:274:PRO:HD3	2:B:374:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:THR:O	9:B:820:TA1:H192	2.21	0.41
3:C:139:SER:OG	4:F:25:GLY:N	2.54	0.41
1:A:288:VAL:O	1:A:289:ALA:C	2.59	0.41
2:B:147:SER:CB	2:B:190:SER:HB3	2.42	0.41
2:B:192:HIS:HD1	2:B:424:ASN:CG	2.20	0.41
2:B:282:GLN:O	2:B:282:GLN:CG	2.65	0.41
1:A:76:ASP:O	1:A:80:THR:N	2.53	0.41
1:A:384:ILE:C	1:A:386:GLU:N	2.72	0.41
1:A:434:GLU:C	1:A:436:GLY:N	2.74	0.41
2:B:171:VAL:HG12	2:B:171:VAL:O	2.20	0.41
2:B:325:MET:HE2	2:B:355:VAL:CG2	2.51	0.41
1:A:221:ARG:N	1:A:222:PRO:CD	2.83	0.41
1:A:243:ARG:NH2	1:A:252:LEU:HG	2.35	0.41
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.95	0.41
1:A:282:TYR:HD2	1:A:284:GLU:HG3	1.86	0.41
2:B:12:CYS:O	2:B:13:GLY:C	2.59	0.41
2:B:133:GLN:CG	2:B:165:ILE:HD11	2.49	0.41
4:D:17:HIS:ND1	4:D:129:HIS:HE1	2.19	0.41
1:A:104:ALA:HB3	1:A:408:TYR:HD2	1.84	0.41
1:A:130:THR:O	1:A:131:GLY:C	2.59	0.41
1:A:149:PHE:CD1	1:A:150:THR:N	2.89	0.41
1:A:318:LEU:HB2	1:A:376:CYS:SG	2.61	0.41
1:A:332:ILE:CD1	1:A:353:VAL:HG22	2.51	0.41
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.81	0.41
1:A:414:GLU:C	1:A:416:GLY:N	2.74	0.41
1:A:425:MET:O	1:A:426:ALA:C	2.60	0.41
2:B:118:VAL:O	2:B:121:VAL:N	2.54	0.41
2:B:119:LEU:O	2:B:122:VAL:HG22	2.21	0.41
2:B:168:THR:HB	2:B:198:THR:HG21	2.03	0.41
2:B:182:VAL:O	2:B:184:PRO:N	2.54	0.41
2:B:273:ALA:CB	2:B:274:PRO:CD	2.93	0.41
2:B:333:LEU:HD11	2:B:337:ASN:HD21	1.85	0.41
2:B:409:THR:C	2:B:411:GLU:N	2.73	0.41
2:B:417:GLU:O	2:B:420:GLU:HB3	2.20	0.41
4:F:17:HIS:ND1	4:F:129:HIS:HE1	2.19	0.41
1:A:166:LYS:HB2	1:A:199:ASP:OD1	2.20	0.41
1:A:224:TYR:HD2	1:A:224:TYR:HA	1.73	0.41
1:A:362:VAL:HG13	1:A:368:LEU:CB	2.50	0.41
2:B:132:LEU:O	2:B:164:ARG:HD2	2.21	0.41
2:B:188:THR:O	2:B:191:VAL:HG12	2.21	0.41
3:E:260:VAL:HG21	4:F:148:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLU:O	1:A:210:TYR:N	2.51	0.40
1:A:315:CYS:HB3	1:A:377:MET:HE1	2.02	0.40
1:A:320:ARG:O	1:A:373:ARG:HA	2.21	0.40
2:B:11:GLN:HA	2:B:74:THR:HG21	2.03	0.40
2:B:20:PHE:CD2	2:B:235:MET:CG	3.04	0.40
2:B:281:GLN:C	2:B:283:TYR:N	2.67	0.40
3:C:260:VAL:HG21	4:D:148:SER:HB3	2.03	0.40
1:A:401:LYS:O	1:A:402:ARG:HB2	2.21	0.40
2:B:23:VAL:O	2:B:24:ILE:C	2.60	0.40
1:A:98:ASP:OD1	1:A:98:ASP:N	2.55	0.40
1:A:100:ALA:HB2	1:A:105:ARG:HD3	2.02	0.40
1:A:209:ILE:HD13	1:A:231:ILE:HD11	2.04	0.40
1:A:226:ASN:O	1:A:227:LEU:C	2.59	0.40
2:B:98:GLY:C	2:B:100:GLY:H	2.24	0.40
2:B:409:THR:O	2:B:412:GLY:N	2.48	0.40
2:B:413:MET:HE3	2:B:413:MET:HA	2.03	0.40
1:A:181:VAL:HG23	2:B:258:ASN:HB3	2.03	0.40
1:A:313:MET:O	1:A:314:ALA:CB	2.69	0.40
2:B:191:VAL:HG11	2:B:425:MET:CG	2.43	0.40
2:B:243:ARG:N	2:B:243:ARG:HD3	2.26	0.40
2:B:288:VAL:HG22	2:B:323:MET:HE3	2.03	0.40
2:B:301:MET:HE1	2:B:377:PHE:CE2	2.50	0.40
1:A:14:VAL:HG11	1:A:75:ILE:HD13	2.04	0.40
2:B:48:ARG:CG	2:B:243:ARG:O	2.66	0.40
2:B:274:PRO:CB	2:B:371:LEU:HD21	2.52	0.40
4:D:96:LEU:HD23	4:D:96:LEU:HA	1.90	0.40
4:F:96:LEU:HD23	4:F:96:LEU:HA	1.89	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	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	4
2	B	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	5
3	C	178/315 (56%)	167 (94%)	9 (5%)	2 (1%)	14	52
3	E	178/315 (56%)	167 (94%)	9 (5%)	2 (1%)	14	52
4	D	151/250 (60%)	144 (95%)	7 (5%)	0	100	100
4	F	151/250 (60%)	144 (95%)	7 (5%)	0	100	100
All	All	1490/2026 (74%)	1162 (78%)	209 (14%)	119 (8%)	2	12

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	97	GLU
1	A	108	TYR
1	A	109	THR
1	A	141	PHE
1	A	183	GLU
1	A	217	LEU
1	A	240	ALA
1	A	249	ASN
1	A	255	PHE
1	A	266	HIS
1	A	280	LYS
1	A	284	GLU
1	A	285	GLN
1	A	289	ALA
1	A	309	HIS
1	A	346	TRP
1	A	370	LYS
1	A	387	ALA
1	A	403	ALA
1	A	437	VAL
2	B	23	VAL
2	B	24	ILE
2	B	32	PRO
2	B	50	ASN
2	B	82	PRO
2	B	97	SER
2	B	128	SER
2	B	176	LYS
2	B	183	GLU

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Mol	Chain	Res	Type
2	B	218	LYS
2	B	238	VAL
2	B	239	THR
2	B	240	THR
2	B	252	LEU
2	B	263	PRO
2	B	266	HIS
2	B	273	ALA
2	B	278	ARG
2	B	280	SER
2	B	281	GLN
2	B	282	GLN
2	B	288	VAL
2	B	294	GLN
2	B	295	MET
2	B	343	PHE
2	B	344	VAL
2	B	346	TRP
2	B	369	ARG
2	B	403	ALA
1	A	24	TYR
1	A	63	PRO
1	A	103	TYR
1	A	111	GLY
1	A	131	GLY
1	A	218	ASP
1	A	219	ILE
1	A	238	ILE
1	A	265	GLY
1	A	287	SER
1	A	314	ALA
1	A	339	ARG
1	A	342	GLN
1	A	373	ARG
1	A	386	GLU
2	B	38	GLY
2	B	73	GLY
2	B	175	PRO
2	B	265	LEU
2	B	279	GLY
2	B	298	ALA
2	B	300	ASN

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Mol	Chain	Res	Type
2	B	311	ARG
3	C	259	ASN
3	E	259	ASN
1	A	104	ALA
1	A	148	GLY
1	A	149	PHE
1	A	173	PRO
1	A	239	THR
1	A	245	ASP
1	A	263	PRO
1	A	279	GLU
1	A	288	VAL
1	A	330	ALA
1	A	336	LYS
1	A	369	ALA
2	B	83	PHE
2	B	99	ALA
2	B	100	GLY
2	B	302	MET
2	B	386	GLU
1	A	89	PRO
1	A	300	ASN
1	A	348	PRO
2	B	34	GLY
2	B	96	GLN
2	B	395	PHE
3	C	261	ASP
3	E	261	ASP
1	A	129	CYS
1	A	256	GLN
1	A	303	VAL
1	A	307	PRO
1	A	382	THR
2	B	57	ALA
2	B	74	THR
2	B	285	ALA
2	B	424	ASN
1	A	31	GLN
1	A	273	ALA
2	B	51	VAL
2	B	58	GLY
2	B	145	THR

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Mol	Chain	Res	Type
2	B	162	PRO
2	B	400	ARG
2	B	195	VAL
1	A	115	ILE
2	B	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	347/377 (92%)	298 (86%)	49 (14%)	3	16
2	B	367/381 (96%)	307 (84%)	60 (16%)	2	13
3	C	163/279 (58%)	155 (95%)	8 (5%)	25	50
3	E	163/279 (58%)	155 (95%)	8 (5%)	25	50
4	D	140/226 (62%)	126 (90%)	14 (10%)	7	26
4	F	140/226 (62%)	126 (90%)	14 (10%)	7	26
All	All	1320/1768 (75%)	1167 (88%)	153 (12%)	9	21

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	20	CYS
1	A	21	TRP
1	A	32	PRO
1	A	76	ASP
1	A	82	THR
1	A	98	ASP
1	A	115	ILE
1	A	120	ASP
1	A	125	LEU
1	A	127	ASP
1	A	130	THR
1	A	135	PHE

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Mol	Chain	Res	Type
1	A	141	PHE
1	A	150	THR
1	A	152	LEU
1	A	155	GLU
1	A	169	PHE
1	A	172	TYR
1	A	173	PRO
1	A	183	GLU
1	A	192	HIS
1	A	204	VAL
1	A	219	ILE
1	A	224	TYR
1	A	231	ILE
1	A	234	ILE
1	A	243	ARG
1	A	244	PHE
1	A	253	THR
1	A	260	VAL
1	A	267	PHE
1	A	269	LEU
1	A	276	ILE
1	A	284	GLU
1	A	303	VAL
1	A	325	PRO
1	A	334	THR
1	A	345	ASP
1	A	352	LYS
1	A	368	LEU
1	A	376	CYS
1	A	378	LEU
1	A	380	ASN
1	A	404	PHE
1	A	415	GLU
1	A	417	GLU
1	A	431	ASP
1	A	432	TYR
2	B	14	ASN
2	B	24	ILE
2	B	26	ASP
2	B	32	PRO
2	B	41	ASP
2	B	68	VAL

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Mol	Chain	Res	Type
2	B	76	ASP
2	B	90	ASP
2	B	94	PHE
2	B	101	ASN
2	B	122	VAL
2	B	129	CYS
2	B	135	PHE
2	B	141	LEU
2	B	145	THR
2	B	149	MET
2	B	153	LEU
2	B	161	TYR
2	B	163	ASP
2	B	165	ILE
2	B	174	SER
2	B	198	THR
2	B	201	THR
2	B	203	CYS
2	B	207	GLU
2	B	211	ASP
2	B	214	PHE
2	B	215	ARG
2	B	224	TYR
2	B	227	LEU
2	B	230	LEU
2	B	236	SER
2	B	240	THR
2	B	244	PHE
2	B	265	LEU
2	B	267	PHE
2	B	275	LEU
2	B	282	GLN
2	B	283	TYR
2	B	284	ARG
2	B	289	PRO
2	B	299	LYS
2	B	306	ASP
2	B	309	HIS
2	B	322	ARG
2	B	324	SER
2	B	325	MET
2	B	343	PHE

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Mol	Chain	Res	Type
2	B	344	VAL
2	B	349	ASN
2	B	369	ARG
2	B	380	ASN
2	B	387	LEU
2	B	413	MET
2	B	414	ASP
2	B	424	ASN
2	B	427	ASP
2	B	431	GLU
2	B	432	TYR
2	B	437	ASP
3	C	142	LEU
3	C	148	GLU
3	C	167	SER
3	C	216	GLU
3	C	223	LYS
3	C	235	SER
3	C	246	MET
3	C	257	LEU
4	D	8	ARG
4	D	16	ILE
4	D	24	THR
4	D	31	LEU
4	D	36	LEU
4	D	37	TYR
4	D	43	GLU
4	D	59	ILE
4	D	83	LEU
4	D	88	LEU
4	D	94	SER
4	D	106	THR
4	D	131	ARG
4	D	155	LEU
3	E	142	LEU
3	E	148	GLU
3	E	167	SER
3	E	216	GLU
3	E	223	LYS
3	E	235	SER
3	E	246	MET
3	E	257	LEU

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Mol	Chain	Res	Type
4	F	8	ARG
4	F	16	ILE
4	F	24	THR
4	F	31	LEU
4	F	36	LEU
4	F	37	TYR
4	F	43	GLU
4	F	59	ILE
4	F	83	LEU
4	F	88	LEU
4	F	94	SER
4	F	106	THR
4	F	131	ARG
4	F	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	28	HIS
1	A	128	GLN
1	A	133	GLN
1	A	139	HIS
1	A	197	HIS
1	A	216	ASN
1	A	226	ASN
1	A	256	GLN
1	A	309	HIS
1	A	380	ASN
2	B	14	ASN
2	B	91	ASN
2	B	101	ASN
2	B	102	ASN
2	B	107	HIS
2	B	136	GLN
2	B	139	HIS
2	B	282	GLN
2	B	331	GLN
2	B	334	ASN
2	B	337	ASN
2	B	349	ASN

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Mol	Chain	Res	Type
2	B	380	ASN
2	B	406	HIS
2	B	436	GLN
3	C	98	GLN
3	C	106	ASN
3	C	118	GLN
4	D	46	HIS
4	D	63	HIS
4	D	129	HIS
4	D	144	GLN
4	D	153	GLN
4	D	154	GLN
3	E	98	GLN
3	E	106	ASN
3	E	118	GLN
4	F	46	HIS
4	F	63	HIS
4	F	129	HIS
4	F	144	GLN
4	F	153	GLN
4	F	154	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GTP	A	920	6	26,34,34	1.29	4 (15%)	32,54,54	1.10	3 (9%)
8	GDP	B	800	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)
9	TA1	B	820	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)

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
7	GTP	A	920	6	-	3/18/38/38	0/3/3/3
8	GDP	B	800	-	-	4/12/32/32	0/3/3/3
9	TA1	B	820	-	-	9/41/127/127	0/7/7/7

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	800	GDP	O4'-C1'	6.28	1.49	1.41
8	B	800	GDP	O6-C6	5.67	1.34	1.23
9	B	820	TA1	C06-C05	5.29	1.50	1.38
9	B	820	TA1	C18-C10	5.14	1.69	1.57
8	B	800	GDP	C2-N1	4.67	1.49	1.37
9	B	820	TA1	C08-C07	-4.60	1.25	1.38
9	B	820	TA1	C05-C04	4.36	1.46	1.39
9	B	820	TA1	C45-C24	4.00	1.61	1.54
8	B	800	GDP	PB-O2B	-3.76	1.40	1.54
7	A	920	GTP	C5-C6	-3.73	1.39	1.47
8	B	800	GDP	C8-N7	3.57	1.41	1.35
9	B	820	TA1	O02-C03	3.53	1.41	1.34
9	B	820	TA1	C36-C31	3.36	1.45	1.39
9	B	820	TA1	C25-C24	3.23	1.39	1.34
9	B	820	TA1	C46-C45	3.15	1.60	1.53
9	B	820	TA1	C43-C01	3.08	1.60	1.54
9	B	820	TA1	C11-C10	3.04	1.61	1.54
8	B	800	GDP	C5-C6	-2.85	1.41	1.47
9	B	820	TA1	C43-C26	2.79	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	920	GTP	C6-N1	2.61	1.41	1.37
9	B	820	TA1	C26-C25	2.51	1.56	1.51
7	A	920	GTP	C8-N7	-2.42	1.30	1.35
8	B	800	GDP	C2-N3	-2.40	1.27	1.33
9	B	820	TA1	C18-C20	2.40	1.62	1.55
8	B	800	GDP	PB-O3B	2.35	1.63	1.54
9	B	820	TA1	C01-C45	2.35	1.66	1.56
9	B	820	TA1	C04-C03	-2.34	1.44	1.50
9	B	820	TA1	C16-C15	2.25	1.56	1.52
7	A	920	GTP	O4'-C1'	2.13	1.44	1.41
9	B	820	TA1	C37-C29	2.11	1.54	1.52
9	B	820	TA1	C10-C02	2.08	1.62	1.57
8	B	800	GDP	O3'-C3'	2.07	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	800	GDP	C8-N7-C5	9.28	120.66	102.99
8	B	800	GDP	N2-C2-N3	6.25	131.90	119.74
8	B	800	GDP	C5-C6-N1	6.10	124.72	113.95
9	B	820	TA1	C06-C05-C04	-4.87	114.58	120.34
9	B	820	TA1	C07-C08-C09	4.72	127.38	120.19
8	B	800	GDP	O6-C6-C5	-4.24	116.09	124.37
8	B	800	GDP	N2-C2-N1	-4.18	107.81	116.71
9	B	820	TA1	C05-C04-C03	-3.95	111.48	120.40
8	B	800	GDP	C2-N1-C6	-3.75	118.19	125.10
9	B	820	TA1	C09-C04-C03	3.51	128.33	120.40
8	B	800	GDP	C2'-C3'-C4'	3.39	109.23	102.64
9	B	820	TA1	C17-C18-C20	3.13	109.82	102.59
9	B	820	TA1	C45-C01-C02	3.04	115.24	111.91
9	B	820	TA1	O04-C11-C14	-2.88	101.78	108.09
7	A	920	GTP	O2G-PG-O3B	2.65	113.51	104.64
9	B	820	TA1	O01-C01-C43	2.53	113.36	107.03
8	B	800	GDP	O2'-C2'-C3'	2.26	119.14	111.82
9	B	820	TA1	C10-C18-C17	-2.19	102.28	106.54
9	B	820	TA1	C14-C11-C15	-2.17	83.09	85.40
9	B	820	TA1	O06-C15-C11	2.11	92.96	90.58
7	A	920	GTP	O5'-C5'-C4'	2.05	116.06	108.99
7	A	920	GTP	O3G-PG-O3B	2.01	111.38	104.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	800	GDP	PA-O3A-PB-O2B
8	B	800	GDP	C5'-O5'-PA-O3A
8	B	800	GDP	C5'-O5'-PA-O1A
9	B	820	TA1	O02-C03-C04-C05
9	B	820	TA1	O02-C03-C04-C09
9	B	820	TA1	O03-C03-C04-C09
9	B	820	TA1	O03-C03-C04-C05
9	B	820	TA1	N01-C30-C31-C36
9	B	820	TA1	O14-C30-C31-C36
9	B	820	TA1	N01-C30-C31-C32
9	B	820	TA1	O14-C30-C31-C32
7	A	920	GTP	C3'-C4'-C5'-O5'
7	A	920	GTP	O4'-C4'-C5'-O5'
8	B	800	GDP	PA-O3A-PB-O3B
9	B	820	TA1	C15-C11-O04-C12
7	A	920	GTP	C5'-O5'-PA-O1A

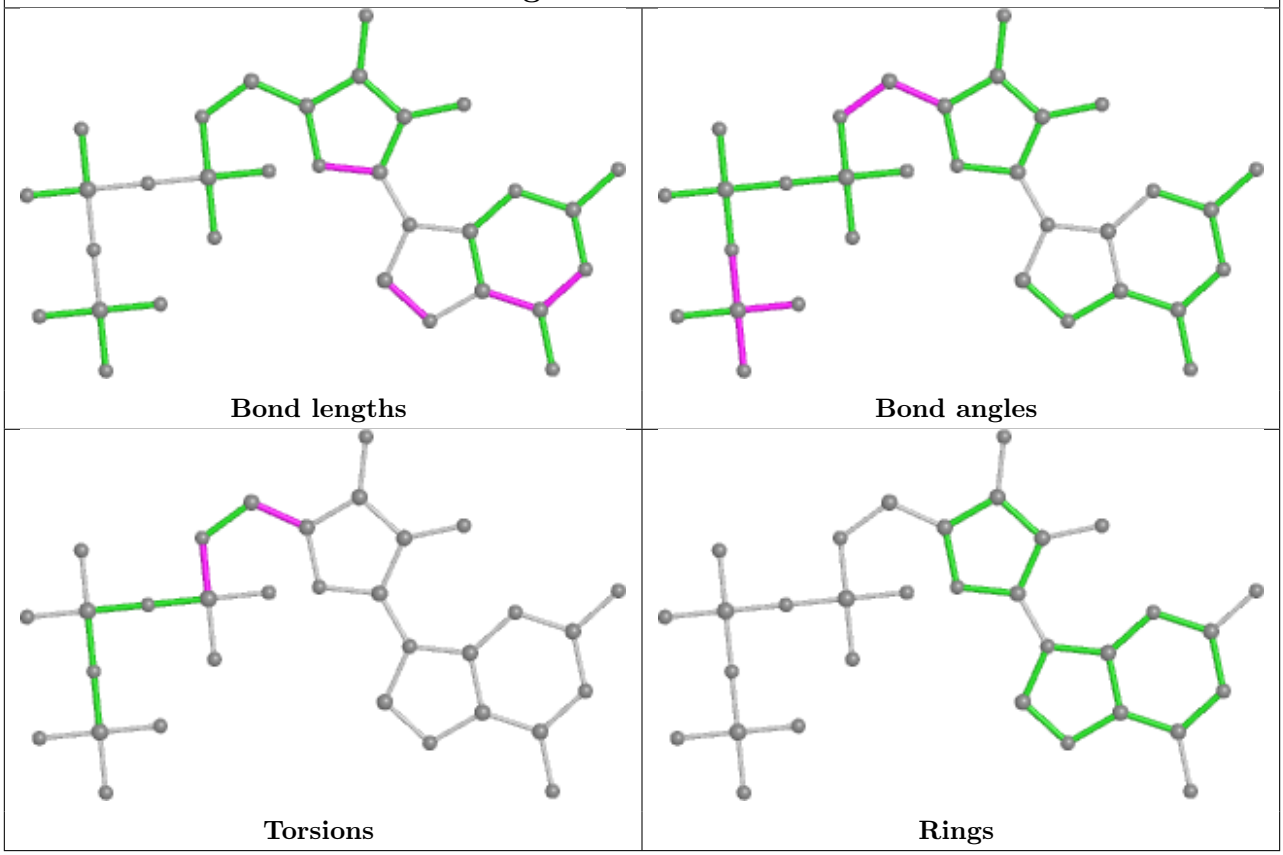
There are no ring outliers.

3 monomers are involved in 10 short contacts:

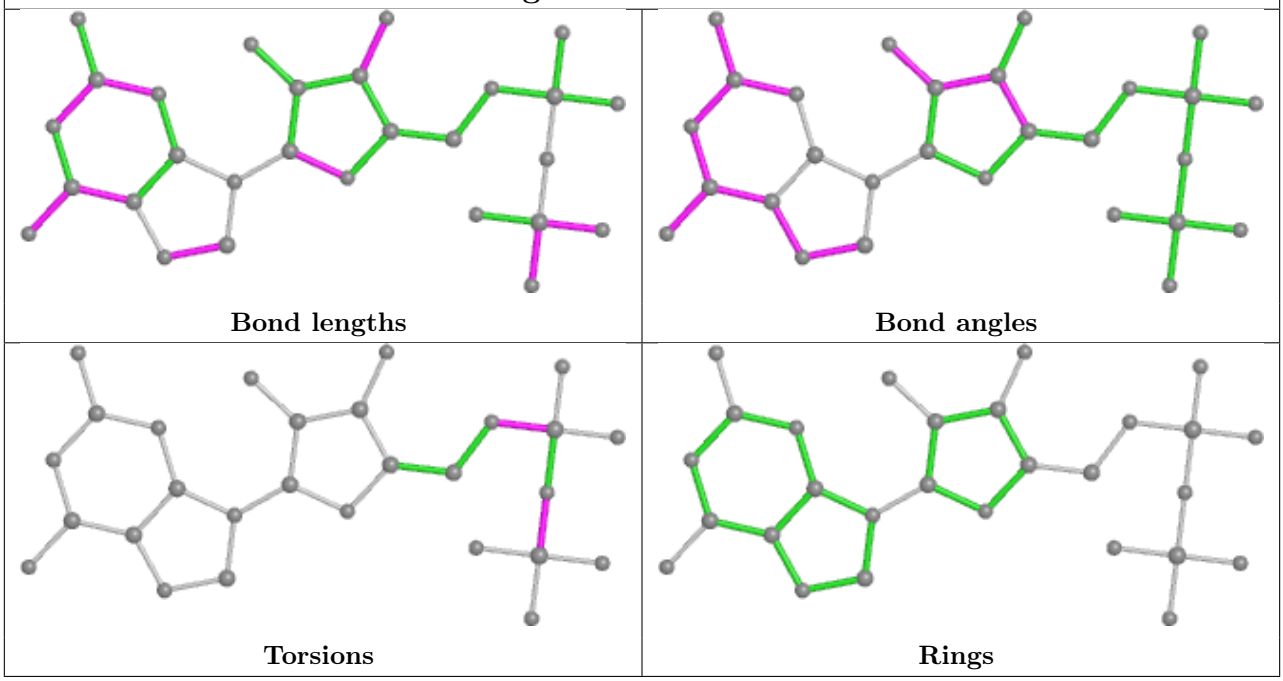
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	920	GTP	4	0
8	B	800	GDP	1	0
9	B	820	TA1	5	0

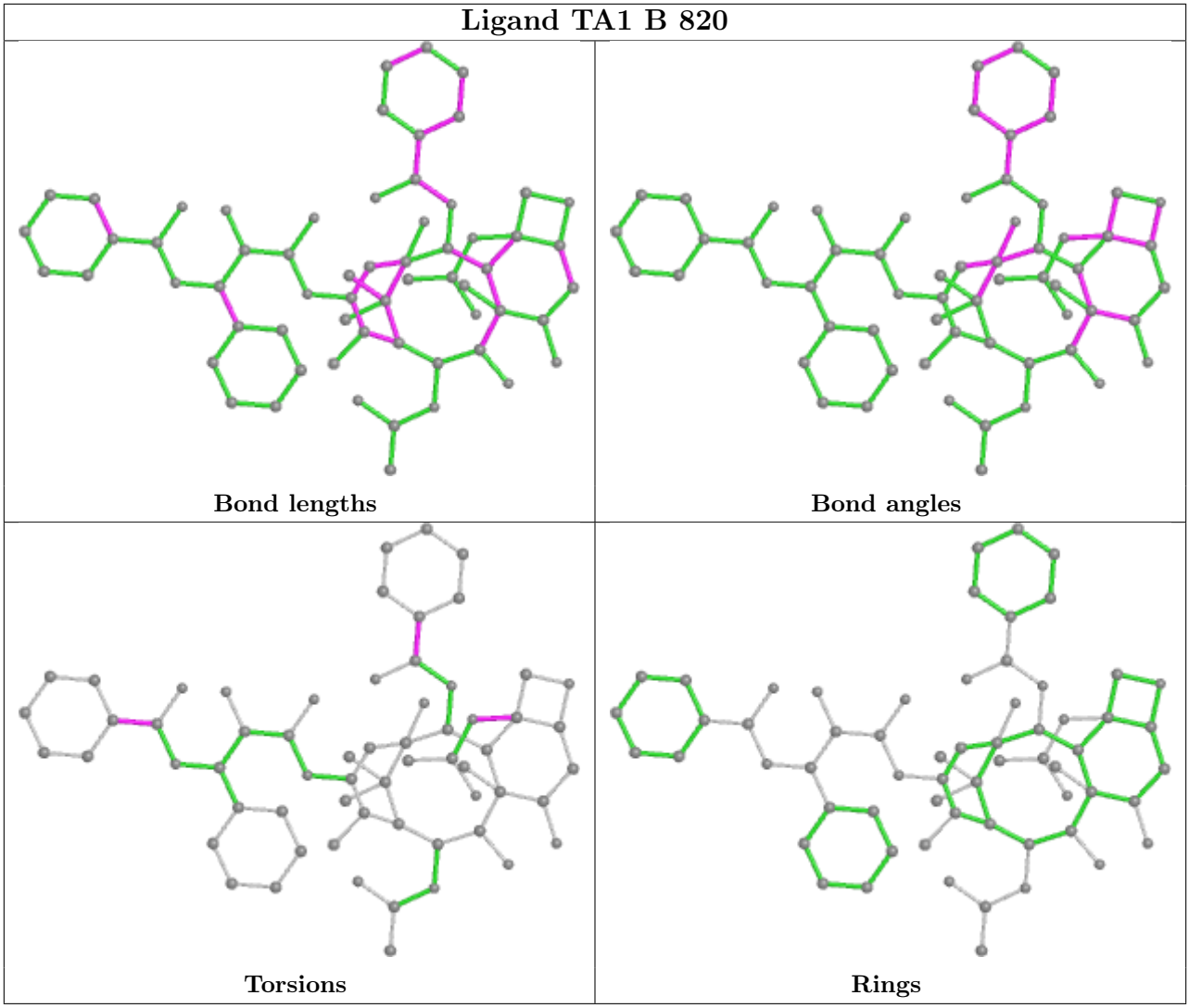
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GTP A 920



Ligand GDP B 800





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

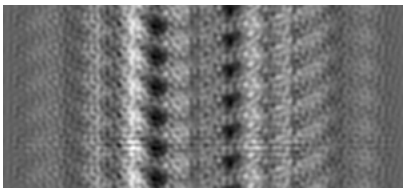
6 Map visualisation (i)

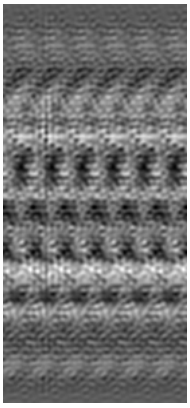
This section contains visualisations of the EMDB entry EMD-5223. These allow visual inspection of the internal detail of the map and identification of artifacts.

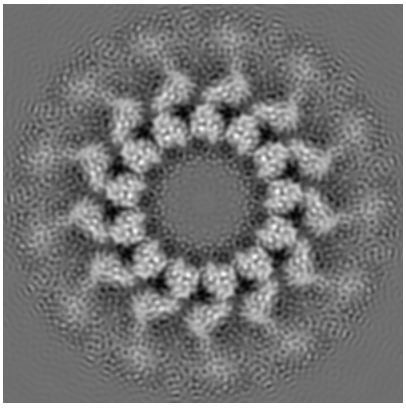
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

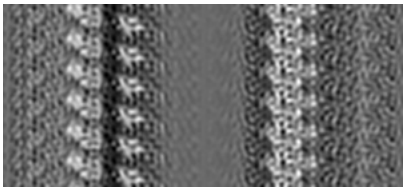

Y

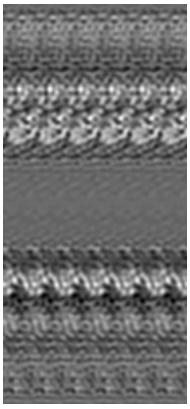

Z

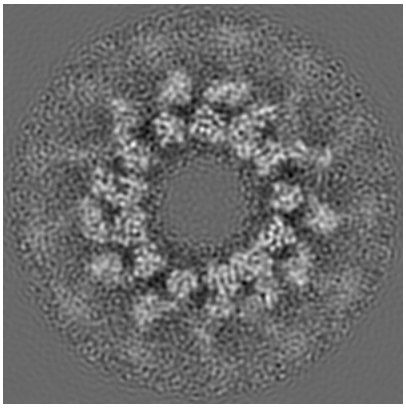
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 110

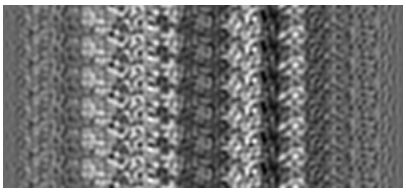

Y Index: 110


Z Index: 50

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

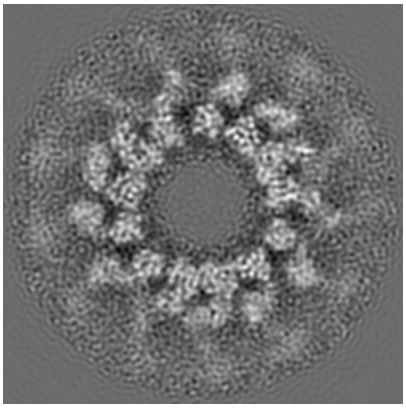
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 142

Y Index: 147

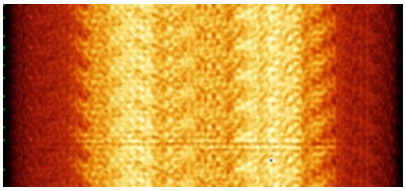


Z Index: 21

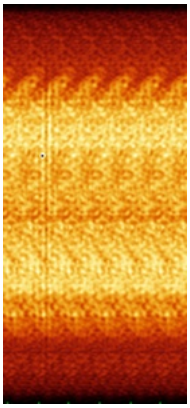
The images above show the largest variance slices of the map in three orthogonal directions.

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

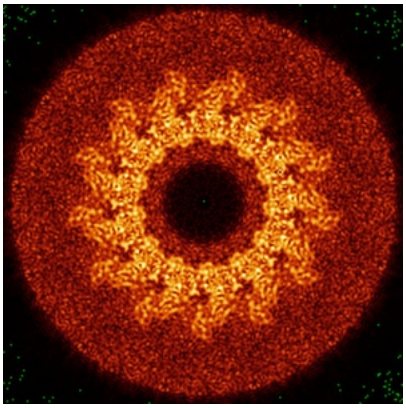
6.4.1 Primary map



X



Y

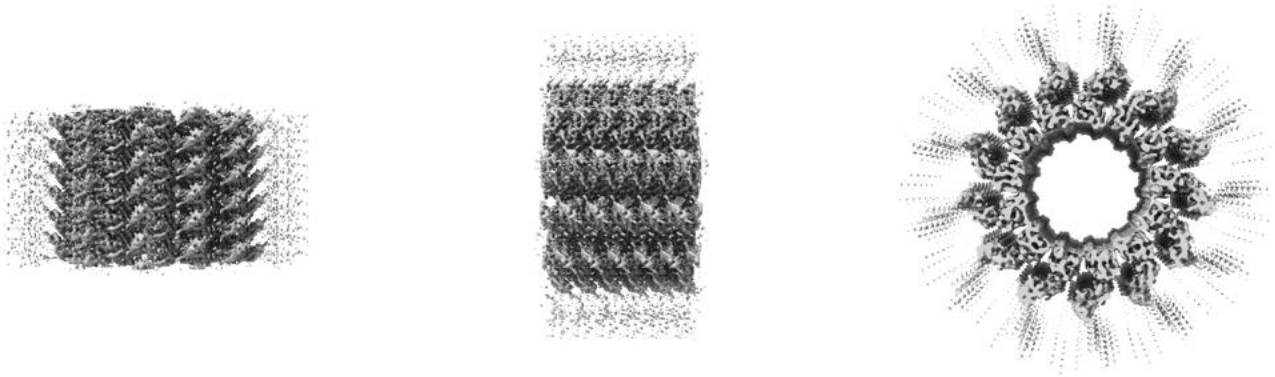


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

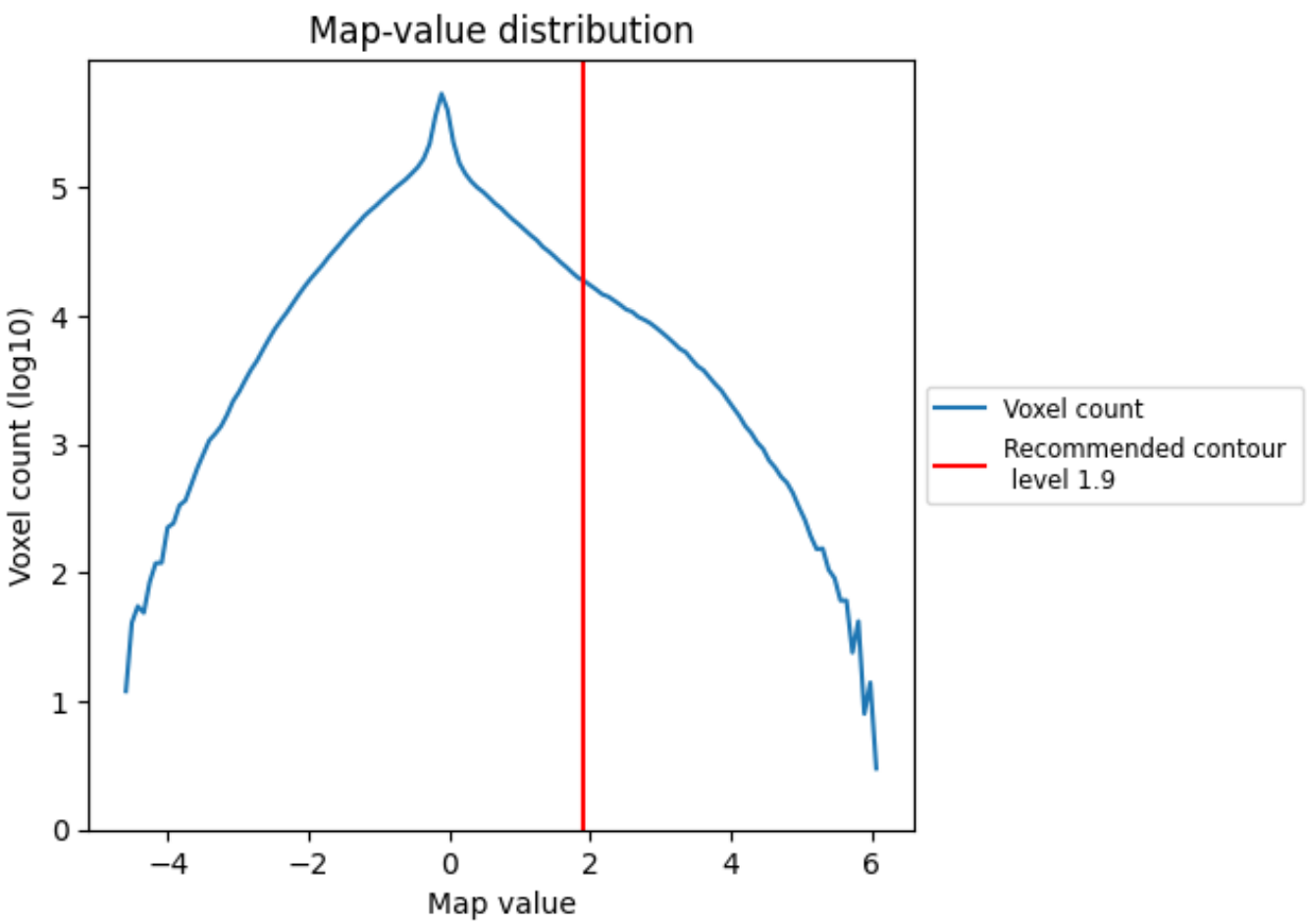
6.6 Mask visualisation (i)

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

7 Map analysis (i)

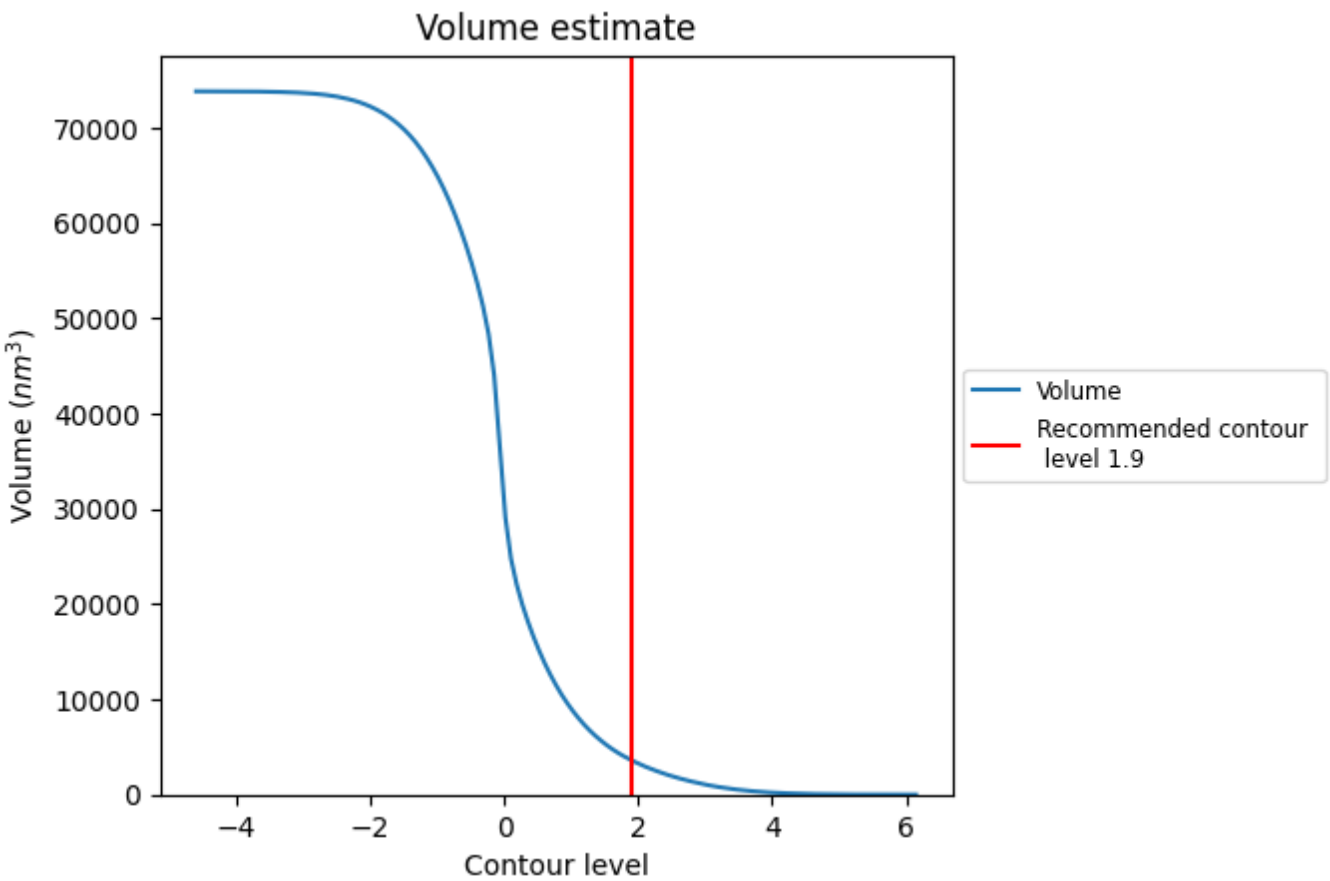
This section contains the results of statistical analysis of the map.

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 3609 nm^3; this corresponds to an approximate mass of 3260 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.

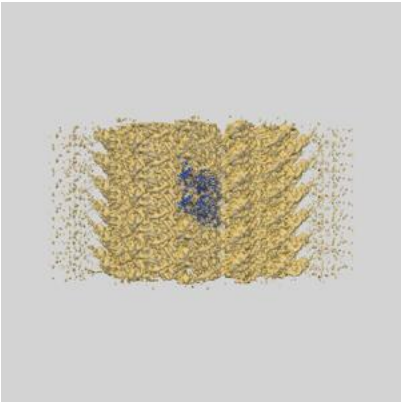
8 Fourier-Shell correlation (i)

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

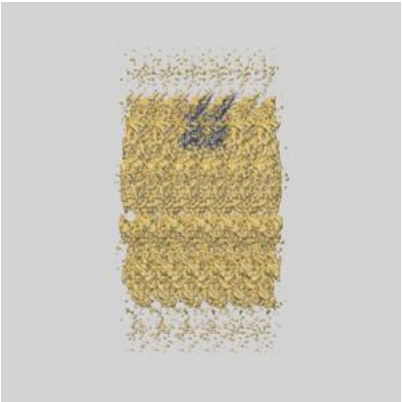
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5223 and PDB model 3IZ0. Per-residue inclusion information can be found in section 3 on page 7.

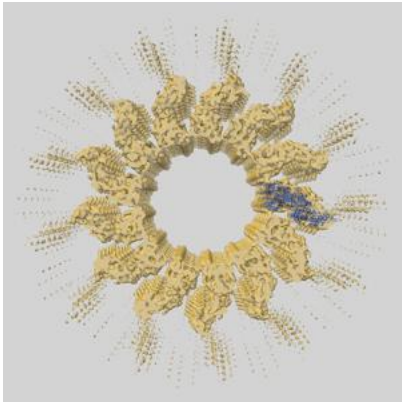
9.1 Map-model overlay (i)



X



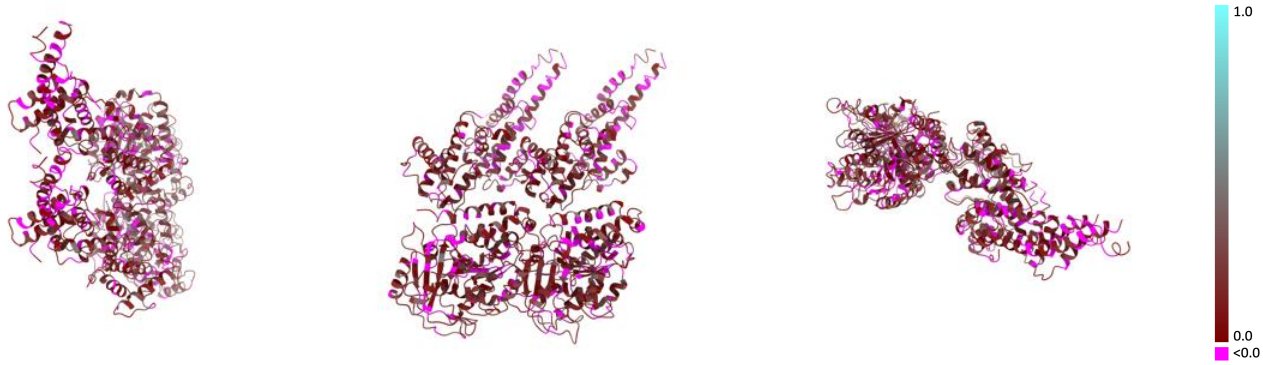
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

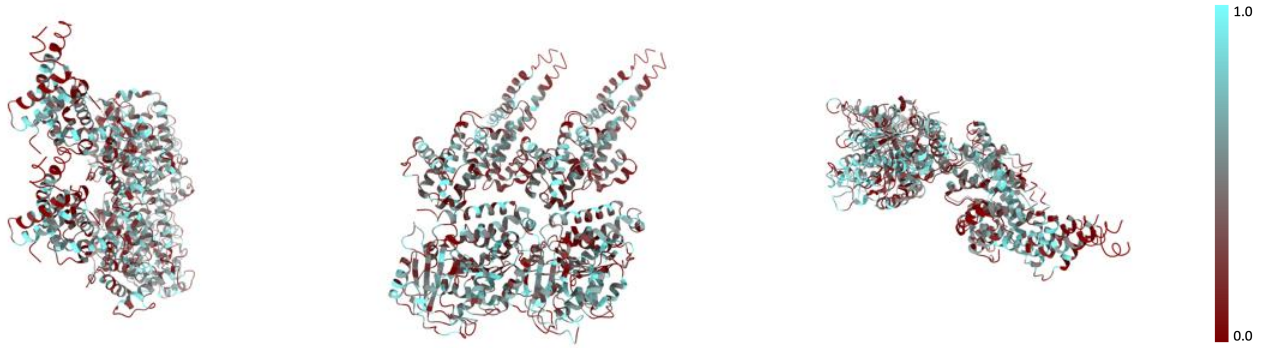
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

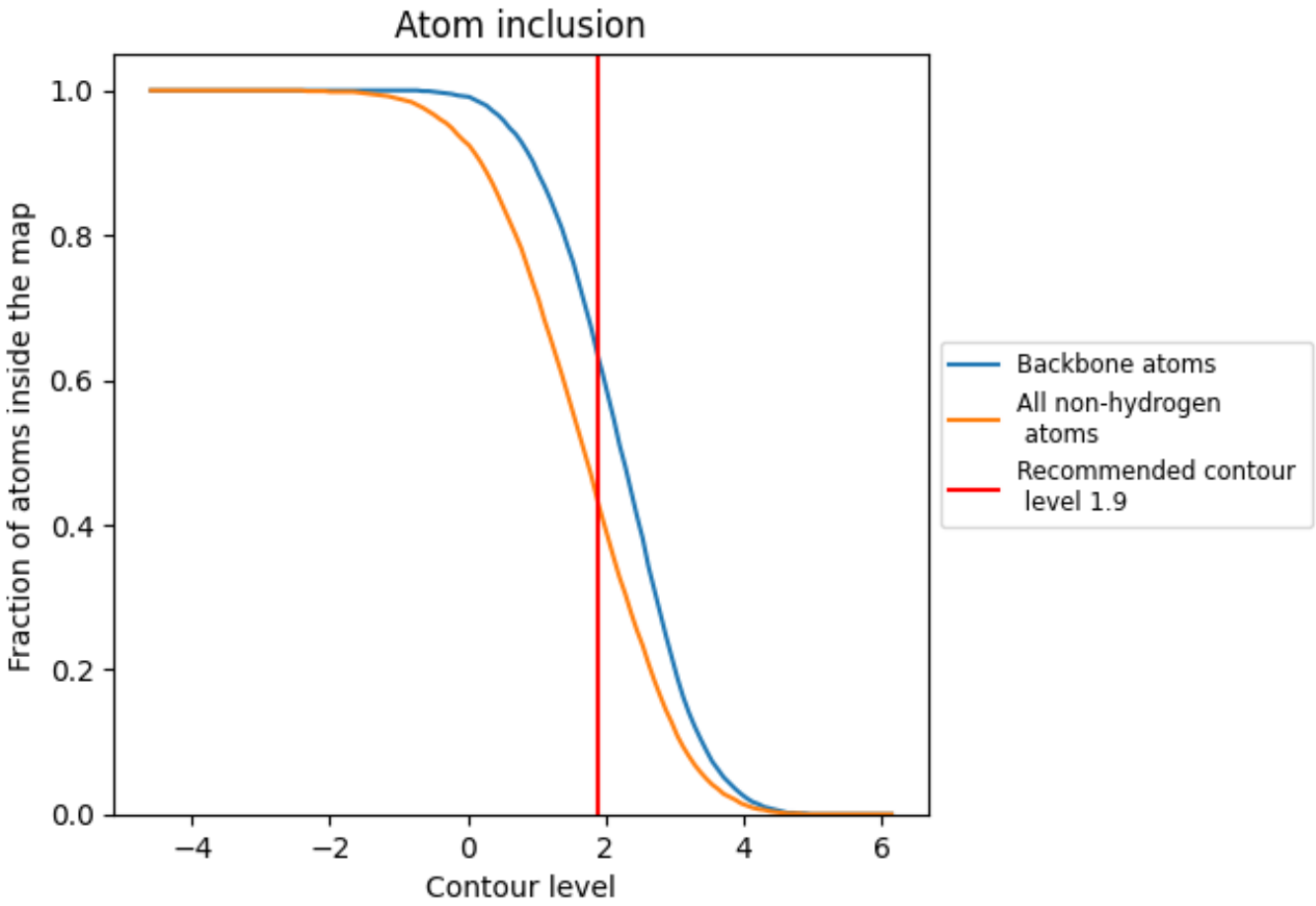
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.9).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4270	0.1100
A	0.4600	0.1190
B	0.4590	0.1170
C	0.3860	0.1050
D	0.3930	0.0940
E	0.3810	0.1050
F	0.3930	0.0960