



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:50 AM EST

PDB ID : 7M2Z
EMDB ID : EMD-23638
Title : Monomeric single-particle reconstruction of the Yeast gamma-TuSC
Authors : Brilot, A.F.; Lyon, A.S.; Zelter, A.; Viswanath, S.; Maxwell, A.; MacCoss, M.J.; Muller, E.G.; Sali, A.; Davis, T.N.; Agard, D.A.
Deposited on : 2021-03-17
Resolution : 3.70 Å(reported)

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.dev43
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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

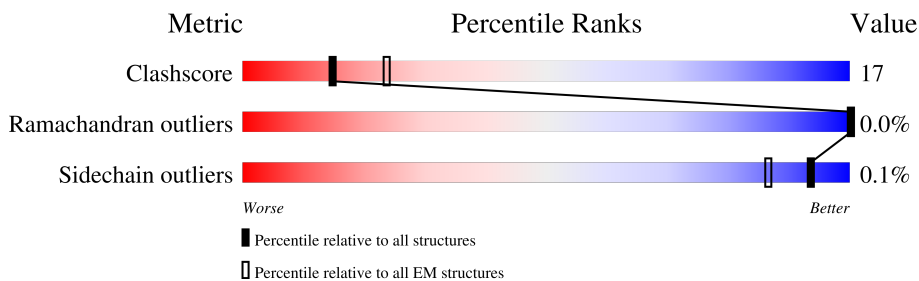
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	473	57% 36% 7%
1	B	473	56% 38% 6%
2	C	846	54% 26% 20%
3	D	823	54% 30% 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18330 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 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	446	Total	C	N	O	S	0	0
			3486	2179	590	700	17		
1	A	440	Total	C	N	O	S	0	0
			3441	2153	584	688	16		

- Molecule 2 is a protein called Spindle pole body component SPC98.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	674	Total	C	N	O	S	0	0
			5569	3601	920	1032	16		

- Molecule 3 is a protein called Spindle pole body component SPC97.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	693	Total	C	N	O	S	0	0
			5778	3716	974	1059	29		

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

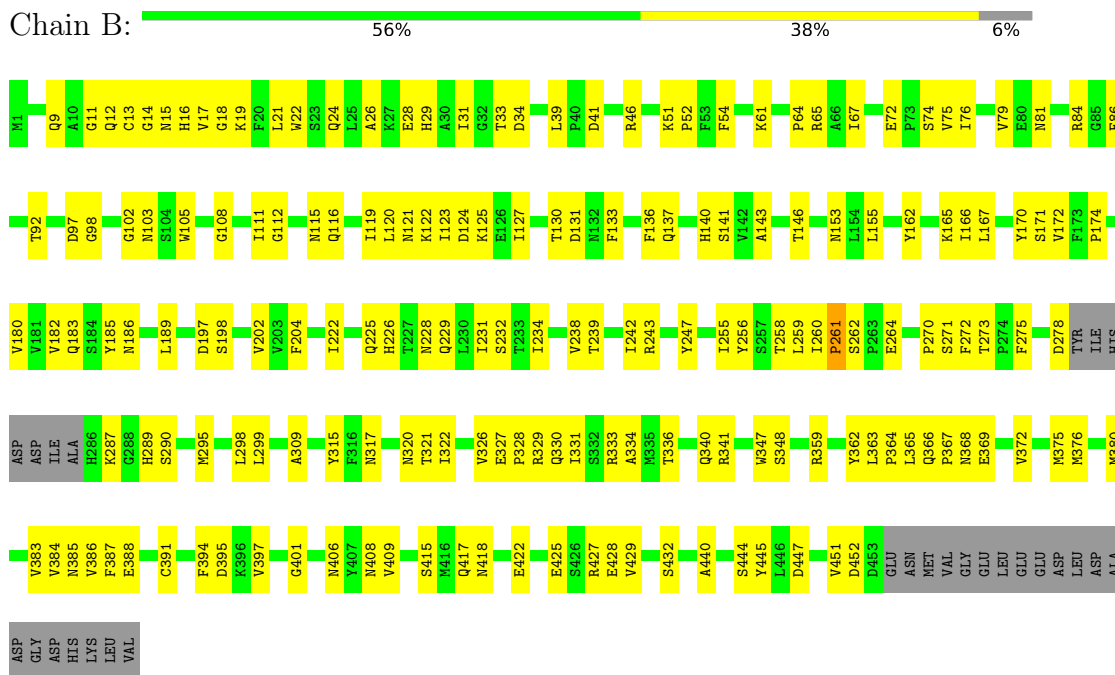


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total 28	C 10	N 5	O 11	P 2	0
4	A	1	Total 28	C 10	N 5	O 11	P 2	0

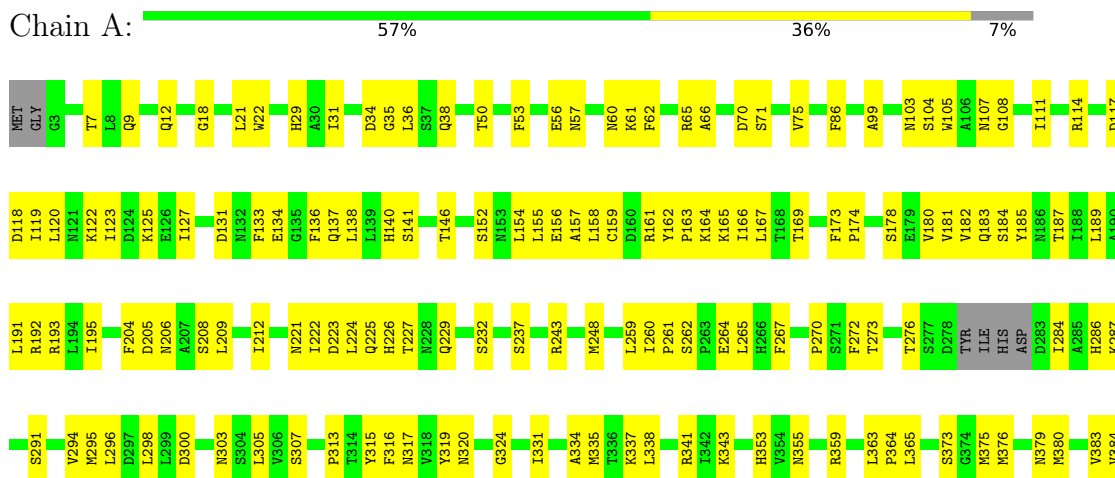
3 Residue-property plots

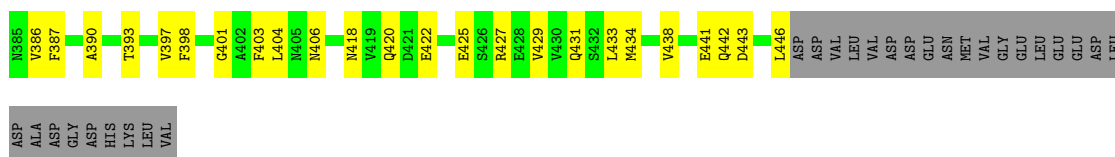
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



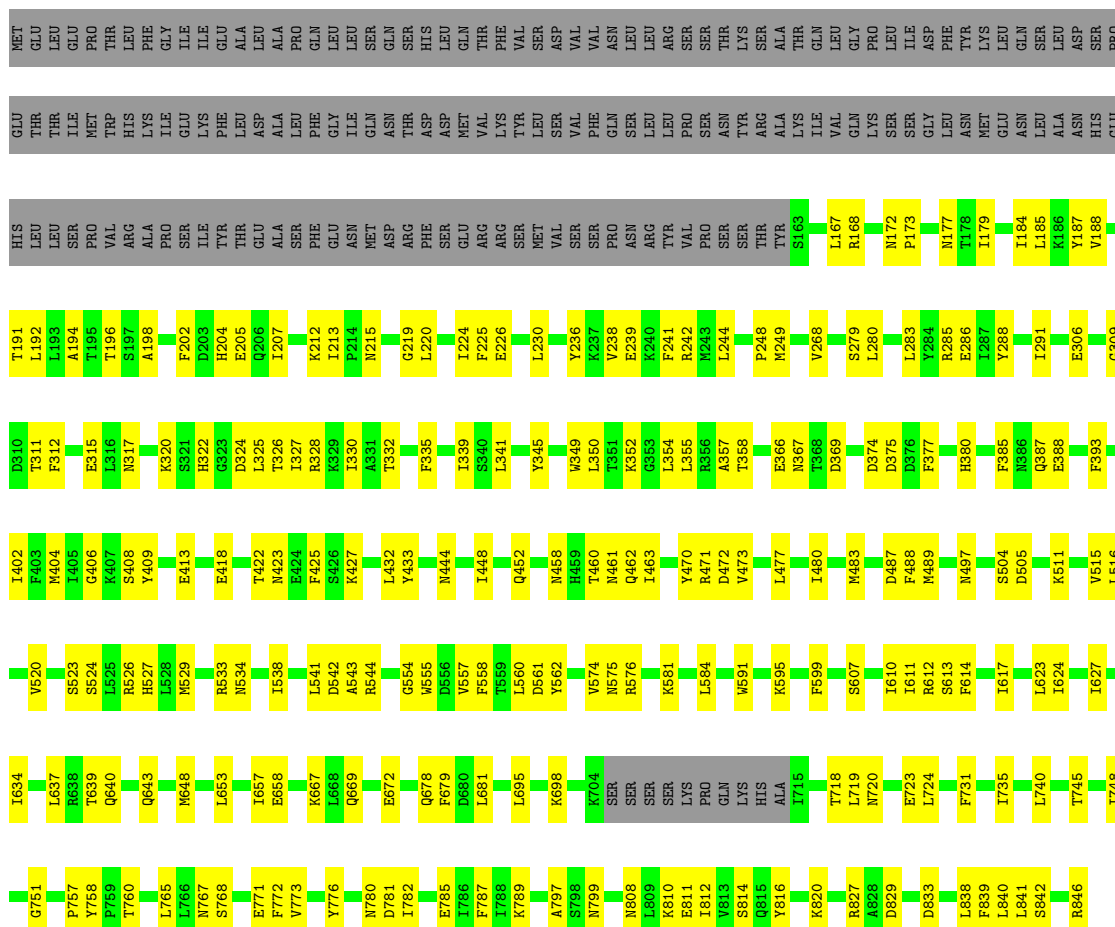
- Molecule 1: Tubulin gamma chain





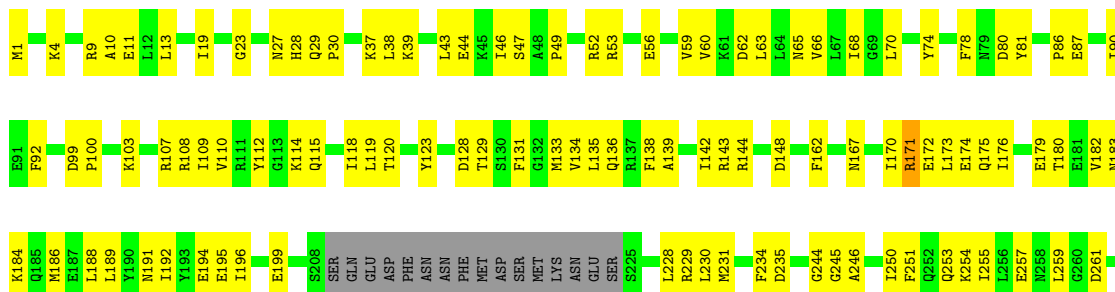
• Molecule 2: Spindle pole body component SPC98

Chain C: 54% 26% 20%



• Molecule 3: Spindle pole body component SPC97

Chain D: 54% 30% 16%



S264	T365	S496	Y558	GLN	E789	LYS	E805	Y809	ARG
V265	I366	Q500	H559	GLU	PHE	PHE	LEU	S810	SER
L268	Q376	ILE	L560	ASP	ASP	TYR	TYR	I811	ALA
K269	E377	PRO	D563	VAL	G751	M713	GLU	P814	ALA
L272	I378	GLU	I566	P666	Y752	K716	LYS	P814	ALA
W286	L384	VAL	P567	L668	Q753	L717	SER	ALA	SER
L287	G387	PRO	Y568	A671	A757	L720	GLY	ALA	SER
T288	S388	GLU	P569	I672	I673	D721	MET	ALA	SER
Q289	N389	ASN	L570	Q673	Q673	P722	LYS	ALA	SER
G290	Y393	ASN	N571	E677	L760	VAL	LYS	GLN	ARG
I291	Y393	SER	T577	I693	K763	A801	SER	ARG	
L292	F410	ALA	I580	P694	S772	ASP	GLY	ALA	
N293	Q411	ASN	K581	L695	S773	ASP	ALA	ALA	
D294	G412	ASP	Y582	I699	R776	ASP	ALA	ALA	
E298	Y413	ASP	I585	F700	L779	ASP	ALA	ALA	
F299	D414	PRO	L586	V703	E789	PHE	ALA	ALA	
M300	L415	LEU	R587	F706	LYS	ASP	ALA	ALA	
T301	I416	MET	Y588	F709	PHE	ASP	ALA	ALA	
Y302	N417	HIS	Q589	S712	TYR	ASP	ALA	ALA	
D303	V418	ALA	L590	M713	ASP	ASP	ALA	ALA	
D304	I425	ASN	V591	K716	L717	ASP	ALA	ALA	
L365	F426	ASN	Y594	L720	D721	ASP	ALA	ALA	
E306	S431	PHE	I598	P722	P722	ASP	ALA	ALA	
GLY	Y434	LYS	L599	VAL	VAL	ASP	ALA	ALA	
THR	N434	MET	L603	LEU	LEU	ASP	ALA	ALA	
ASP	F438	ASN	R615	TYR	TYR	ASP	ALA	ALA	
ASN	N442	ALA	Y614	M713	M713	ASP	ALA	ALA	
ILE	Y445	ALA	S618	K716	L717	ASP	ALA	ALA	
PHE	L446	ILE	V621	L720	D721	ASP	ALA	ALA	
ASP	T447	LEU	K622	P722	P722	ASP	ALA	ALA	
THR	K448	GLU	V626	VAL	VAL	ASP	ALA	ALA	
ARG	Y450	ARG	R627	LEU	LEU	ASP	ALA	ALA	
ASP	R451	THR	V631	LEU	LEU	ASP	ALA	ALA	
R318	L462	GLY	L632	LEU	LEU	ASP	ALA	ALA	
F325	L467	ALA	M636	LEU	LEU	ASP	ALA	ALA	
I326	L467	TYR	N637	LEU	LEU	ASP	ALA	ALA	
R327	L467	GLY	H638	LEU	LEU	ASP	ALA	ALA	
K328	L467	GLY	F639	LEU	LEU	ASP	ALA	ALA	
D329	L467	GLY	I640	LEU	LEU	ASP	ALA	ALA	
V330	L467	GLY	I643	LEU	LEU	ASP	ALA	ALA	
F345	L467	GLY	M644	LEU	LEU	ASP	ALA	ALA	
K346	L467	GLY	E645	LEU	LEU	ASP	ALA	ALA	
M347	L467	GLY	Y646	LEU	LEU	ASP	ALA	ALA	
L348	L467	GLY	N648	LEU	LEU	ASP	ALA	ALA	
R349	L467	GLY	I648	LEU	LEU	ASP	ALA	ALA	
L353	L467	GLY	I648	LEU	LEU	ASP	ALA	ALA	
V357	L467	GLY	I648	LEU	LEU	ASP	ALA	ALA	
R358	L467	GLY	I648	LEU	LEU	ASP	ALA	ALA	
I363	L467	GLY	I648	LEU	LEU	ASP	ALA	ALA	
P364	L467	GLY	I648	LEU	LEU	ASP	ALA	ALA	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	398841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Final reconstruction in cis-TEM	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	39891	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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

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	0.36	0/3513	0.55	0/4769
1	B	0.39	0/3558	0.55	0/4830
2	C	0.39	0/5688	0.51	0/7688
3	D	0.36	0/5890	0.52	0/7949
All	All	0.37	0/18649	0.53	0/25236

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	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	30	PRO	Peptide
3	D	569	PRO	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	3441	0	3304	135	0
1	B	3486	0	3344	133	0
2	C	5569	0	5588	166	0
3	D	5778	0	5841	209	0
4	A	28	0	12	1	0
4	B	28	0	12	1	0
All	All	18330	0	18101	615	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 17.

All (615) 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)
1:B:9:GLN:HE22	1:B:18:GLY:HA3	1.33	0.94
3:D:491:LEU:HD13	3:D:587:ARG:HE	1.33	0.91
1:A:111:ILE:HG12	1:A:114:ARG:HH21	1.38	0.88
3:D:647:PHE:O	3:D:651:VAL:HB	1.77	0.84
3:D:446:LEU:HB3	3:D:558:TYR:HE2	1.43	0.83
3:D:489:GLU:O	3:D:559:HIS:NE2	2.15	0.80
2:C:285:ARG:NH1	2:C:286:GLU:OE2	2.16	0.78
1:B:24:GLN:NE2	1:B:28:GLU:OE2	2.15	0.78
3:D:560:LEU:O	3:D:587:ARG:NH1	2.17	0.77
1:A:29:HIS:HD2	1:A:50:THR:HG22	1.50	0.76
3:D:568:TYR:O	3:D:570:LEU:N	2.18	0.76
1:A:182:VAL:O	1:A:185:TYR:HB3	1.85	0.76
2:C:695:LEU:O	3:D:413:TYR:OH	2.01	0.76
3:D:90:ILE:O	3:D:114:LYS:NZ	2.17	0.76
1:A:295:MET:HA	1:A:298:LEU:HD12	1.68	0.75
1:A:259:LEU:O	1:A:317:ASN:ND2	2.20	0.75
1:B:22:TRP:HZ3	1:B:64:PRO:HB3	1.51	0.75
1:A:224:LEU:O	1:A:227:THR:OG1	2.05	0.75
1:B:103:ASN:HD22	1:B:406:ASN:HB2	1.52	0.74
3:D:294:ASP:OD2	3:D:299:PHE:N	2.17	0.74
1:B:22:TRP:CZ3	1:B:64:PRO:HB3	2.22	0.74
2:C:322:HIS:CE1	3:D:136:GLN:HE21	2.05	0.73
2:C:433:TYR:OH	2:C:452:GLN:OE1	2.06	0.73
3:D:228:LEU:HD13	3:D:349:ARG:HH22	1.52	0.73
2:C:776:TYR:O	2:C:780:ASN:ND2	2.21	0.73
2:C:461:ASN:ND2	2:C:718:THR:OG1	2.21	0.73
3:D:123:TYR:OH	3:D:143:ARG:NE	2.23	0.72
2:C:248:PRO:HB2	2:C:341:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:618:SER:H	3:D:622:LYS:NZ	1.87	0.72
1:B:34:ASP:O	1:B:61:LYS:NZ	2.23	0.71
3:D:487:ASP:HB3	3:D:559:HIS:HE1	1.55	0.71
1:B:112:GLY:HA3	1:B:153:ASN:ND2	2.06	0.71
1:A:103:ASN:ND2	1:A:104:SER:O	2.24	0.70
1:A:401:GLY:HA2	1:A:404:LEU:HB2	1.73	0.70
2:C:542:ASP:OD1	2:C:543:ALA:N	2.24	0.70
1:B:295:MET:HE3	1:B:322:ILE:HD11	1.72	0.70
3:D:44:GLU:HA	3:D:47:SER:HB3	1.74	0.70
1:A:12:GLN:HG2	1:A:75:VAL:HG21	1.72	0.70
1:A:192:ARG:HH12	1:A:425:GLU:HG3	1.57	0.70
1:A:57:ASN:HD21	1:A:61:LYS:HB3	1.56	0.70
3:D:559:HIS:HA	3:D:587:ARG:HH22	1.56	0.70
1:A:173:PHE:N	1:A:204:PHE:O	2.21	0.69
1:A:384:VAL:HA	1:A:387:PHE:HD2	1.56	0.69
1:B:327:GLU:OE2	1:B:330:GLN:NE2	2.22	0.69
1:A:380:MET:HB2	1:A:383:VAL:HG13	1.75	0.69
1:B:290:SER:HB3	3:D:467:LEU:HD11	1.75	0.68
2:C:816:TYR:OH	2:C:820:LYS:NZ	2.22	0.68
2:C:224:ILE:HD13	2:C:283:LEU:HD23	1.75	0.68
3:D:487:ASP:OD1	3:D:488:THR:N	2.24	0.68
1:B:417:GLN:NE2	1:B:418:ASN:OD1	2.27	0.68
3:D:618:SER:H	3:D:622:LYS:HZ1	1.42	0.67
1:B:111:ILE:O	1:B:115:ASN:ND2	2.27	0.67
2:C:219:GLY:HA3	3:D:70:LEU:HD11	1.76	0.67
3:D:294:ASP:OD2	3:D:298:GLU:N	2.28	0.67
2:C:765:LEU:O	2:C:768:SER:OG	2.13	0.67
3:D:250:ILE:O	3:D:254:LYS:HG2	1.94	0.67
2:C:207:ILE:HD13	2:C:225:PHE:HD1	1.61	0.66
1:B:394:PHE:HZ	1:B:427:ARG:HD3	1.59	0.66
1:A:122:LYS:HA	1:A:125:LYS:HZ2	1.59	0.66
1:B:46:ARG:NE	1:B:362:TYR:OH	2.25	0.66
1:B:287:LYS:HB3	1:B:289:HIS:CE1	2.31	0.66
3:D:622:LYS:HA	3:D:626:VAL:HG12	1.78	0.66
3:D:78:PHE:HD2	3:D:80:ASP:H	1.44	0.65
3:D:566:ILE:HG22	3:D:567:PRO:HD2	1.78	0.65
1:B:112:GLY:HA3	1:B:153:ASN:HD22	1.62	0.65
1:A:195:ILE:HG23	1:A:433:LEU:HD21	1.79	0.65
3:D:28:HIS:HE1	3:D:29:GLN:HE21	1.45	0.65
1:A:272:PHE:HD1	1:A:375:MET:HB3	1.62	0.65
1:A:70:ASP:OD1	1:A:71:SER:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASN:HB3	1:A:376:MET:HG3	1.79	0.65
2:C:599:PHE:HB3	2:C:773:VAL:HG11	1.79	0.65
1:B:348:SER:HA	2:C:640:GLN:HE22	1.62	0.65
1:B:394:PHE:CZ	1:B:427:ARG:HD3	2.32	0.65
1:B:54:PHE:O	1:B:65:ARG:NH2	2.29	0.64
2:C:444:ASN:O	2:C:448:ILE:HD12	1.96	0.64
1:B:9:GLN:NE2	1:B:18:GLY:HA3	2.08	0.64
2:C:345:TYR:OH	2:C:357:ALA:O	2.13	0.64
2:C:322:HIS:CG	3:D:136:GLN:HE21	2.15	0.64
2:C:695:LEU:HD23	3:D:568:TYR:HB2	1.79	0.64
1:A:183:GLN:O	1:A:187:THR:N	2.29	0.64
3:D:4:LYS:HB2	3:D:37:LYS:HA	1.79	0.64
1:B:272:PHE:HB3	1:B:375:MET:HA	1.80	0.63
2:C:480:ILE:HG21	2:C:541:LEU:HD21	1.80	0.63
1:B:440:ALA:HA	1:B:445:TYR:CD1	2.33	0.63
2:C:350:LEU:HD21	2:C:402:ILE:HG23	1.79	0.63
1:B:397:VAL:O	1:B:401:GLY:N	2.28	0.63
2:C:213:ILE:O	3:D:37:LYS:NZ	2.32	0.63
3:D:772:SER:O	3:D:776:ARG:HG3	1.99	0.63
1:B:81:ASN:HA	1:B:84:ARG:HH11	1.64	0.62
3:D:251:PHE:HB3	3:D:272:LEU:HD21	1.80	0.62
1:A:262:SER:O	1:A:264:GLU:N	2.28	0.62
1:B:137:GLN:NE2	1:B:170:TYR:OH	2.32	0.62
1:B:51:LYS:O	1:B:65:ARG:NH2	2.32	0.62
1:B:299:LEU:HD11	1:B:341:ARG:HG2	1.80	0.62
3:D:115:GLN:HA	3:D:118:ILE:HG22	1.81	0.62
1:B:328:PRO:HA	1:B:331:ILE:HD13	1.82	0.62
2:C:554:GLY:HA2	2:C:557:VAL:HG12	1.81	0.62
1:A:31:ILE:O	1:A:38:GLN:NE2	2.32	0.62
3:D:289:GLN:HE22	3:D:366:ILE:HB	1.64	0.62
2:C:238:VAL:O	2:C:242:ARG:HG3	1.99	0.61
2:C:317:ASN:HD21	2:C:393:PHE:HB3	1.63	0.61
1:B:146:THR:OG1	4:B:501:GDP:O2B	2.15	0.61
2:C:471:ARG:NH1	2:C:672:GLU:OE2	2.33	0.61
1:B:359:ARG:HD3	1:B:365:LEU:HD21	1.82	0.61
3:D:426:PHE:CD2	3:D:582:TYR:HB3	2.36	0.61
1:B:13:CYS:O	1:B:17:VAL:HG23	2.01	0.61
1:A:296:LEU:HD21	1:A:337:LYS:HE3	1.83	0.61
3:D:717:LEU:HD23	3:D:720:LEU:HD12	1.83	0.61
1:A:353:HIS:ND1	3:D:645:GLU:OE2	2.29	0.60
2:C:220:LEU:HD22	3:D:70:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:713:MET:HA	3:D:716:LYS:HB2	1.83	0.60
1:A:316:PHE:HB2	1:A:379:ASN:HB3	1.83	0.60
2:C:526:ARG:HH12	2:C:527:HIS:CE1	2.18	0.60
2:C:610:ILE:O	2:C:613:SER:OG	2.16	0.60
1:B:231:ILE:O	1:B:234:ILE:HG22	2.01	0.60
2:C:352:LYS:HB3	2:C:354:LEU:HD23	1.83	0.60
1:B:17:VAL:HG22	1:B:228:ASN:OD1	2.02	0.60
1:B:108:GLY:O	1:B:111:ILE:HB	2.02	0.60
1:A:205:ASP:OD1	1:A:206:ASN:N	2.34	0.59
2:C:288:TYR:HA	2:C:291:ILE:HD12	1.84	0.59
2:C:529:MET:HB2	2:C:538:ILE:HG13	1.83	0.59
3:D:109:ILE:O	3:D:112:TYR:HB2	2.02	0.59
1:A:192:ARG:HE	1:A:429:VAL:HG21	1.67	0.59
1:A:383:VAL:O	1:A:386:VAL:HG22	2.01	0.59
3:D:303:ASP:OD2	3:D:304:ASP:N	2.32	0.59
2:C:328:ARG:O	2:C:332:THR:HG23	2.02	0.59
2:C:758:TYR:OH	2:C:833:ASP:OD1	2.18	0.58
1:B:415:SER:HB3	1:B:417:GLN:HG3	1.84	0.58
1:A:34:ASP:OD1	1:A:35:GLY:N	2.35	0.58
2:C:320:LYS:HD2	2:C:335:PHE:CD2	2.39	0.58
1:A:313:PRO:HB2	1:A:315:TYR:HE1	1.68	0.58
2:C:511:LYS:O	2:C:515:VAL:HG23	2.04	0.58
2:C:542:ASP:OD1	2:C:544:ARG:NH1	2.37	0.58
1:A:136:PHE:HB2	1:A:167:LEU:HD13	1.85	0.58
1:B:97:ASP:OD1	1:B:98:GLY:N	2.34	0.58
2:C:526:ARG:HG3	2:C:526:ARG:HH11	1.68	0.58
3:D:80:ASP:OD1	3:D:81:TYR:N	2.37	0.58
2:C:617:ILE:HD13	2:C:624:ILE:HG22	1.86	0.57
3:D:134:VAL:HG13	3:D:135:LEU:H	1.69	0.57
1:B:131:ASP:OD1	1:B:131:ASP:N	2.36	0.57
3:D:62:ASP:HA	3:D:65:ASN:HD22	1.69	0.57
1:A:418:ASN:O	1:A:422:GLU:HG3	2.04	0.57
1:B:16:HIS:CG	1:B:225:GLN:HE22	2.23	0.57
1:B:444:SER:HB3	1:B:447:ASP:OD2	2.04	0.57
1:B:198:SER:O	2:C:612:ARG:NH2	2.38	0.57
3:D:587:ARG:O	3:D:591:VAL:HG23	2.05	0.57
1:A:341:ARG:O	1:A:343:LYS:NZ	2.34	0.57
1:B:229:GLN:OE1	1:B:278:ASP:HB3	2.04	0.56
1:A:174:PRO:HA	1:A:206:ASN:OD1	2.05	0.56
2:C:561:ASP:OD1	2:C:575:ASN:ND2	2.34	0.56
1:B:108:GLY:HA2	1:B:111:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:O	1:B:123:ILE:HB	2.06	0.56
1:A:120:LEU:HD23	1:A:161:ARG:HH11	1.70	0.56
1:A:123:ILE:O	1:A:127:ILE:HG13	2.04	0.56
2:C:207:ILE:HB	3:D:10:ALA:HB3	1.87	0.56
2:C:504:SER:OG	2:C:505:ASP:N	2.39	0.56
2:C:785:GLU:O	2:C:789:LYS:HG2	2.05	0.56
3:D:261:ASP:HB3	3:D:264:SER:HB3	1.88	0.56
3:D:700:PHE:HA	3:D:703:VAL:HG22	1.88	0.56
3:D:144:ARG:NE	3:D:148:ASP:OD2	2.29	0.56
1:B:136:PHE:HB2	1:B:167:LEU:HD22	1.87	0.56
1:B:347:TRP:O	2:C:640:GLN:NE2	2.39	0.56
3:D:490:THR:HA	3:D:559:HIS:CD2	2.41	0.56
1:A:248:MET:HE3	3:D:648:ASN:HB2	1.88	0.56
3:D:451:ARG:HA	3:D:451:ARG:NE	2.21	0.56
1:A:359:ARG:HD3	1:A:365:LEU:HD13	1.87	0.56
3:D:757:ALA:HA	3:D:760:LEU:HB2	1.86	0.56
3:D:65:ASN:O	3:D:68:ILE:HG22	2.05	0.56
1:A:248:MET:CE	3:D:645:GLU:HA	2.36	0.56
1:B:172:VAL:HA	1:B:204:PHE:HB2	1.87	0.55
3:D:713:MET:HE3	3:D:717:LEU:HG	1.88	0.55
1:A:296:LEU:HD11	1:A:337:LYS:HZ1	1.71	0.55
1:A:403:PHE:HA	1:A:406:ASN:ND2	2.21	0.55
1:A:209:LEU:HB3	1:A:227:THR:HG22	1.88	0.55
2:C:797:ALA:O	2:C:799:ASN:ND2	2.39	0.55
1:A:273:THR:HG21	1:A:373:SER:HB2	1.87	0.55
1:A:248:MET:HE1	3:D:645:GLU:HA	1.89	0.55
2:C:574:VAL:O	2:C:576:ARG:N	2.39	0.55
3:D:120:THR:O	3:D:123:TYR:HB3	2.07	0.55
1:B:259:LEU:O	1:B:317:ASN:ND2	2.40	0.55
1:B:408:ASN:OD1	1:B:409:VAL:N	2.40	0.54
1:A:195:ILE:HG12	1:A:433:LEU:HD11	1.89	0.54
2:C:487:ASP:OD1	2:C:488:PHE:N	2.41	0.54
2:C:811:GLU:O	2:C:814:SER:OG	2.23	0.54
3:D:172:GLU:O	3:D:176:ILE:HG12	2.08	0.54
1:B:172:VAL:HG12	1:B:204:PHE:HB2	1.89	0.54
3:D:668:LEU:HG	3:D:671:ALA:H	1.71	0.54
1:A:118:ASP:OD1	1:A:119:ILE:N	2.41	0.54
1:B:366:GLN:HB2	1:B:367:PRO:HD2	1.90	0.54
1:A:184:SER:O	1:A:187:THR:HB	2.08	0.54
1:B:368:ASN:OD1	1:B:369:GLU:N	2.41	0.54
1:B:124:ASP:O	1:B:127:ILE:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:MET:HG2	1:B:334:ALA:HB1	1.89	0.53
3:D:235:ASP:OD2	3:D:302:TYR:OH	2.22	0.53
1:A:313:PRO:HB2	1:A:315:TYR:CE1	2.43	0.53
3:D:43:LEU:HD22	3:D:46:ILE:HD11	1.90	0.53
1:B:298:LEU:HB3	1:B:376:MET:HE2	1.90	0.53
3:D:245:GLY:HA3	3:D:330:VAL:O	2.09	0.53
3:D:760:LEU:HD23	3:D:763:LYS:NZ	2.24	0.53
2:C:191:THR:HG21	2:C:225:PHE:CZ	2.43	0.53
3:D:417:ASN:OD1	3:D:418:VAL:N	2.42	0.53
3:D:491:LEU:HA	3:D:494:VAL:HG22	1.91	0.53
3:D:289:GLN:O	3:D:358:ARG:NE	2.41	0.53
3:D:709:PHE:O	3:D:712:SER:OG	2.22	0.53
1:A:260:ILE:HG22	1:A:261:PRO:O	2.08	0.53
1:A:7:THR:HG22	1:A:137:GLN:HE21	1.74	0.53
1:A:192:ARG:NH1	1:A:425:GLU:HG3	2.24	0.53
3:D:133:MET:O	3:D:136:GLN:HB3	2.09	0.53
3:D:636:MET:SD	3:D:703:VAL:HG12	2.49	0.53
1:B:359:ARG:NH1	1:B:368:ASN:HB3	2.24	0.52
2:C:317:ASN:ND2	2:C:393:PHE:HB3	2.25	0.52
3:D:199:GLU:OE1	3:D:250:ILE:HD11	2.09	0.52
1:B:256:TYR:O	1:B:260:ILE:N	2.38	0.52
1:A:111:ILE:HG12	1:A:114:ARG:NH2	2.17	0.52
2:C:523:SER:O	2:C:526:ARG:HG2	2.09	0.52
3:D:119:LEU:HD22	3:D:142:ILE:HD11	1.91	0.52
3:D:621:VAL:HG13	3:D:622:LYS:HD3	1.91	0.52
2:C:249:MET:HG3	2:C:341:LEU:HD23	1.90	0.52
1:B:428:GLU:OE2	1:B:432:SER:OG	2.28	0.52
3:D:1:MET:H3	3:D:39:LYS:HD3	1.74	0.52
1:A:397:VAL:HG12	1:A:404:LEU:HD11	1.90	0.52
2:C:432:LEU:HG	2:C:448:ILE:HG12	1.91	0.52
1:A:209:LEU:HD13	1:A:227:THR:HB	1.91	0.52
1:A:223:ASP:HA	1:A:225:GLN:NE2	2.25	0.52
2:C:188:VAL:HG23	2:C:225:PHE:HE2	1.74	0.52
3:D:86:PRO:HG2	3:D:87:GLU:OE1	2.10	0.52
3:D:289:GLN:NE2	3:D:366:ILE:HB	2.25	0.52
3:D:329:ASP:OD2	3:D:329:ASP:N	2.42	0.52
3:D:109:ILE:HD12	3:D:109:ILE:H	1.74	0.52
3:D:410:PHE:HE2	3:D:415:LEU:HD13	1.75	0.52
1:A:363:LEU:HD12	1:A:364:PRO:HD2	1.92	0.51
2:C:188:VAL:HA	2:C:191:THR:HG22	1.92	0.51
3:D:294:ASP:CG	3:D:298:GLU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:585:ILE:O	3:D:589:GLN:HG2	2.10	0.51
2:C:385:PHE:CE2	2:C:387:GLN:HG3	2.45	0.51
2:C:385:PHE:HE2	2:C:387:GLN:HG3	1.75	0.51
3:D:246:ALA:O	3:D:250:ILE:HG13	2.10	0.51
1:B:383:VAL:O	1:B:386:VAL:HG12	2.10	0.51
1:B:341:ARG:HG2	1:B:341:ARG:HH11	1.74	0.51
1:A:206:ASN:HD22	1:A:209:LEU:HD12	1.75	0.51
2:C:322:HIS:CD2	3:D:136:GLN:HE21	2.28	0.51
2:C:639:THR:HG22	2:C:643:GLN:NE2	2.26	0.51
3:D:134:VAL:HG13	3:D:135:LEU:N	2.25	0.51
1:A:120:LEU:HA	1:A:123:ILE:HG12	1.91	0.51
3:D:28:HIS:HE1	3:D:29:GLN:NE2	2.09	0.51
1:B:26:ALA:HB1	1:B:31:ILE:HB	1.92	0.51
3:D:286:TRP:HE3	3:D:287:LEU:HD22	1.75	0.51
3:D:445:GLU:N	3:D:445:GLU:OE1	2.43	0.51
1:B:320:ASN:OD1	1:B:321:THR:N	2.43	0.51
1:B:326:VAL:HG22	1:B:372:VAL:HG11	1.92	0.51
1:B:388:GLU:HA	1:B:391:CYS:HB2	1.93	0.51
3:D:491:LEU:O	3:D:495:LEU:HG	2.11	0.51
2:C:167:LEU:HG	3:D:167:ASN:HA	1.93	0.51
2:C:185:LEU:HA	2:C:188:VAL:HG12	1.93	0.51
3:D:1:MET:N	3:D:39:LYS:HD3	2.26	0.51
1:B:329:ARG:O	1:B:333:ARG:HG2	2.11	0.50
1:B:336:THR:O	1:B:340:GLN:HG3	2.11	0.50
2:C:772:PHE:CE1	2:C:812:ILE:HG23	2.46	0.50
2:C:317:ASN:HD22	2:C:393:PHE:HD2	1.59	0.50
2:C:526:ARG:HG3	2:C:526:ARG:NH1	2.25	0.50
3:D:299:PHE:CG	3:D:300:MET:N	2.80	0.50
3:D:4:LYS:H	3:D:38:LEU:HD23	1.76	0.50
1:B:452:ASP:OD2	2:C:810:LYS:NZ	2.44	0.50
3:D:170:ILE:O	3:D:173:LEU:HB3	2.10	0.50
1:B:46:ARG:HB2	2:C:527:HIS:CE1	2.46	0.50
2:C:719:LEU:HB3	2:C:723:GLU:HB2	1.94	0.50
1:B:166:ILE:O	1:B:167:LEU:HD23	2.12	0.50
3:D:559:HIS:HA	3:D:587:ARG:NH2	2.26	0.50
3:D:567:PRO:O	3:D:571:ASN:ND2	2.44	0.50
3:D:228:LEU:HB3	3:D:230:LEU:HD23	1.92	0.50
2:C:241:PHE:CD1	2:C:244:LEU:HD12	2.47	0.50
2:C:740:LEU:HD21	2:C:838:LEU:HD11	1.94	0.50
2:C:782:ILE:HA	2:C:785:GLU:OE1	2.12	0.50
3:D:773:SER:HA	3:D:776:ARG:NE	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASP:OD1	1:B:395:ASP:N	2.41	0.49
2:C:375:ASP:O	2:C:380:HIS:HB3	2.11	0.49
2:C:483:MET:CE	2:C:489:MET:HG3	2.42	0.49
3:D:431:SER:O	3:D:434:ASN:N	2.45	0.49
1:A:53:PHE:O	1:A:65:ARG:HG2	2.12	0.49
3:D:53:ARG:HH11	3:D:167:ASN:HD21	1.61	0.49
1:A:56:GLU:OE2	1:A:60:ASN:HA	2.11	0.49
2:C:309:GLY:O	2:C:312:PHE:N	2.45	0.49
2:C:653:LEU:HD23	2:C:657:ILE:HD12	1.94	0.49
2:C:192:LEU:HD23	2:C:268:VAL:HG13	1.94	0.49
2:C:238:VAL:HG12	2:C:242:ARG:HD3	1.93	0.49
3:D:192:ILE:O	3:D:196:ILE:HG12	2.13	0.49
1:A:267:PHE:HE1	1:A:387:PHE:HZ	1.58	0.49
3:D:487:ASP:HB3	3:D:559:HIS:CE1	2.41	0.49
3:D:599:LEU:HD13	3:D:637:ASN:HA	1.94	0.49
1:B:140:HIS:O	1:B:171:SER:HA	2.13	0.49
1:A:272:PHE:CD1	1:A:375:MET:HB3	2.45	0.49
3:D:229:ARG:HH22	3:D:231:MET:HB3	1.76	0.49
3:D:773:SER:HA	3:D:776:ARG:HE	1.78	0.49
1:B:359:ARG:HH12	1:B:368:ASN:HB3	1.77	0.49
1:A:105:TRP:CZ2	1:A:189:LEU:HD13	2.47	0.49
3:D:175:GLN:O	3:D:179:GLU:HB2	2.13	0.49
1:A:117:ASP:N	1:A:117:ASP:OD1	2.45	0.49
3:D:183:ASN:OD1	3:D:184:LYS:N	2.45	0.49
1:A:119:ILE:HG21	1:A:154:LEU:HD21	1.95	0.49
2:C:179:ILE:HB	2:C:184:ILE:HD11	1.95	0.49
3:D:594:TYR:CZ	3:D:598:LEU:HD11	2.47	0.49
3:D:62:ASP:OD2	3:D:74:TYR:N	2.23	0.49
1:A:270:PRO:HG2	1:A:305:LEU:HB2	1.95	0.48
1:B:418:ASN:O	1:B:422:GLU:HG2	2.14	0.48
1:A:324:GLY:HA2	1:A:359:ARG:HG3	1.94	0.48
2:C:322:HIS:CG	3:D:136:GLN:NE2	2.81	0.48
1:B:11:GLY:O	1:B:15:ASN:N	2.44	0.48
1:B:21:LEU:HA	1:B:232:SER:OG	2.11	0.48
1:B:255:ILE:O	1:B:259:LEU:HD23	2.13	0.48
2:C:772:PHE:HE1	2:C:812:ILE:HG23	1.78	0.48
3:D:438:PHE:HE2	3:D:442:ASN:HD22	1.60	0.48
1:A:29:HIS:CD2	1:A:50:THR:HG22	2.40	0.48
1:B:105:TRP:CE3	1:B:189:LEU:HD13	2.48	0.48
1:A:295:MET:HG2	1:A:334:ALA:HB1	1.95	0.48
3:D:363:ILE:HD12	3:D:364:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:416:ILE:HD12	3:D:663:TYR:CG	2.49	0.48
3:D:577:THR:HA	3:D:580:ILE:HD12	1.95	0.48
1:A:154:LEU:O	1:A:158:LEU:HG	2.14	0.48
1:A:384:VAL:HA	1:A:387:PHE:CD2	2.42	0.48
3:D:289:GLN:HB2	3:D:291:ILE:HG22	1.96	0.48
1:B:182:VAL:O	1:B:185:TYR:HB2	2.14	0.48
1:A:363:LEU:O	1:A:365:LEU:N	2.47	0.48
2:C:205:GLU:O	3:D:11:GLU:HG3	2.14	0.47
1:B:116:GLN:HA	1:B:119:ILE:HB	1.95	0.47
3:D:133:MET:HG3	3:D:298:GLU:OE1	2.13	0.47
3:D:134:VAL:HG11	3:D:244:GLY:HA2	1.95	0.47
3:D:627:ARG:O	3:D:631:VAL:HG23	2.14	0.47
1:A:226:HIS:O	1:A:229:GLN:HB2	2.14	0.47
3:D:128:ASP:HB3	3:D:131:PHE:CD2	2.49	0.47
3:D:228:LEU:HD12	3:D:345:PHE:HD1	1.80	0.47
2:C:404:MET:O	2:C:408:SER:OG	2.22	0.47
2:C:425:PHE:HZ	2:C:452:GLN:HE21	1.62	0.47
3:D:618:SER:O	3:D:621:VAL:HG12	2.13	0.47
1:B:51:LYS:N	1:B:52:PRO:HD2	2.29	0.47
3:D:636:MET:O	3:D:640:ILE:HG12	2.14	0.47
1:A:296:LEU:HD21	1:A:337:LYS:CE	2.45	0.47
2:C:326:THR:O	2:C:330:ILE:HG13	2.15	0.47
1:B:19:LYS:HD3	1:B:79:VAL:HG22	1.97	0.47
1:B:180:VAL:HA	1:B:183:GLN:HB3	1.97	0.47
2:C:591:TRP:O	2:C:595:LYS:HG3	2.15	0.47
3:D:228:LEU:HD13	3:D:349:ARG:NH2	2.27	0.47
3:D:302:TYR:HB3	3:D:327:ARG:HH21	1.80	0.47
1:A:162:TYR:HB3	1:A:165:LYS:HE2	1.96	0.47
2:C:576:ARG:O	2:C:581:LYS:HE2	2.14	0.47
1:B:287:LYS:O	1:B:289:HIS:ND1	2.48	0.47
1:B:425:GLU:O	1:B:429:VAL:HG23	2.15	0.47
3:D:13:LEU:HD21	3:D:27:ASN:HA	1.97	0.47
1:B:384:VAL:O	1:B:387:PHE:HB2	2.14	0.47
1:B:447:ASP:O	1:B:451:VAL:HG22	2.15	0.47
2:C:239:GLU:HG2	2:C:242:ARG:NH2	2.29	0.47
2:C:555:TRP:CD1	2:C:595:LYS:HD2	2.50	0.47
2:C:745:THR:H	2:C:748:ILE:CG1	2.28	0.47
3:D:136:GLN:O	3:D:139:ALA:HB3	2.15	0.47
3:D:446:LEU:HB3	3:D:558:TYR:CE2	2.35	0.47
1:B:130:THR:OG1	1:B:131:ASP:N	2.49	0.46
1:A:21:LEU:HA	1:A:232:SER:OG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:516:LEU:O	2:C:520:VAL:HG22	2.14	0.46
3:D:100:PRO:HA	3:D:103:LYS:HG2	1.98	0.46
1:A:225:GLN:O	1:A:229:GLN:HG3	2.14	0.46
3:D:135:LEU:O	3:D:139:ALA:N	2.47	0.46
3:D:253:GLN:O	3:D:257:GLU:HG3	2.14	0.46
1:A:390:ALA:O	1:A:393:THR:OG1	2.12	0.46
2:C:196:THR:HG22	2:C:202:PHE:HB2	1.97	0.46
2:C:458:ASN:O	2:C:462:GLN:HG2	2.16	0.46
1:A:133:PHE:CE2	1:A:165:LYS:HG2	2.51	0.46
1:A:157:ALA:O	1:A:161:ARG:HG3	2.15	0.46
2:C:325:LEU:O	2:C:328:ARG:HB2	2.14	0.46
3:D:425:ILE:HG21	3:D:482:LEU:HD21	1.98	0.46
1:B:76:ILE:HD13	1:B:92:THR:OG1	2.16	0.46
1:A:434:MET:O	1:A:438:VAL:HG23	2.16	0.46
3:D:62:ASP:O	3:D:65:ASN:HB2	2.15	0.46
1:B:127:ILE:HD11	1:B:133:PHE:CD2	2.51	0.46
1:B:133:PHE:HD2	1:B:165:LYS:HZ2	1.63	0.46
1:A:191:LEU:O	1:A:195:ILE:HG13	2.16	0.46
2:C:533:ARG:NH1	2:C:534:ASN:OD1	2.49	0.46
1:B:247:TYR:OH	2:C:658:GLU:HG2	2.15	0.46
2:C:355:LEU:HD22	2:C:366:GLU:HB2	1.97	0.46
3:D:180:THR:HG23	3:D:182:VAL:HG23	1.97	0.46
3:D:195:GLU:OE1	3:D:254:LYS:HD3	2.16	0.46
3:D:451:ARG:HH12	3:D:556:ALA:N	2.14	0.46
2:C:306:GLU:N	2:C:306:GLU:OE1	2.49	0.46
3:D:632:LEU:HD23	3:D:706:PHE:CE1	2.51	0.46
2:C:204:HIS:HB3	2:C:236:TYR:OH	2.16	0.45
3:D:123:TYR:CE1	3:D:143:ARG:HB2	2.51	0.45
1:B:287:LYS:HB3	1:B:289:HIS:ND1	2.32	0.45
1:A:61:LYS:HD3	1:A:62:PHE:N	2.31	0.45
2:C:623:LEU:HG	2:C:624:ILE:HD12	1.98	0.45
3:D:353:LEU:O	3:D:357:VAL:HG23	2.17	0.45
2:C:581:LYS:HB3	2:C:584:LEU:HD12	1.98	0.45
3:D:108:ARG:NH2	3:D:174:GLU:OE2	2.48	0.45
3:D:387:GLY:O	3:D:388:SER:OG	2.24	0.45
1:B:102:GLY:HA2	1:B:186:ASN:HD21	1.81	0.45
1:A:36:LEU:HD13	1:A:60:ASN:O	2.16	0.45
1:A:438:VAL:O	1:A:442:GLN:N	2.45	0.45
2:C:239:GLU:HA	2:C:242:ARG:CZ	2.46	0.45
2:C:367:ASN:OD1	2:C:369:ASP:HB2	2.16	0.45
2:C:614:PHE:HE1	2:C:787:PHE:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:695:LEU:HD23	3:D:568:TYR:CB	2.45	0.45
3:D:90:ILE:HB	3:D:114:LYS:HZ2	1.81	0.45
1:B:272:PHE:CB	1:B:375:MET:HA	2.45	0.45
1:A:178:SER:O	1:A:181:VAL:HG13	2.17	0.45
2:C:187:TYR:CE2	2:C:198:ALA:HB3	2.51	0.45
1:A:180:VAL:O	1:A:184:SER:N	2.37	0.45
2:C:839:PHE:O	2:C:842:SER:OG	2.25	0.45
1:A:140:HIS:HD2	1:A:141:SER:O	2.00	0.45
2:C:624:ILE:O	2:C:627:ILE:HB	2.16	0.45
3:D:115:GLN:HG3	3:D:186:MET:HE2	1.98	0.45
3:D:490:THR:HA	3:D:559:HIS:HD2	1.81	0.45
3:D:558:TYR:CE1	3:D:594:TYR:CD2	3.05	0.45
1:A:237:SER:HB2	1:A:375:MET:HG2	1.98	0.45
2:C:678:GLN:HG2	2:C:679:PHE:CE2	2.50	0.45
3:D:448:LYS:NZ	3:D:449:HIS:HD2	2.15	0.45
1:B:162:TYR:HB3	1:B:165:LYS:HG3	1.98	0.45
1:A:156:GLU:HA	1:A:159:CYS:SG	2.57	0.45
2:C:483:MET:HE3	2:C:489:MET:HG3	1.99	0.45
2:C:614:PHE:CE1	2:C:787:PHE:HB2	2.52	0.45
2:C:698:LYS:HG2	3:D:412:GLY:O	2.17	0.45
1:A:35:GLY:O	1:A:61:LYS:HA	2.17	0.45
1:A:265:LEU:HD23	1:A:316:PHE:CE2	2.52	0.45
1:B:13:CYS:SG	1:B:14:GLY:N	2.89	0.44
1:B:46:ARG:HB2	2:C:527:HIS:CD2	2.53	0.44
1:B:67:ILE:HG13	1:B:123:ILE:HD11	1.99	0.44
2:C:648:MET:SD	2:C:841:LEU:HD21	2.57	0.44
2:C:667:LYS:HE3	2:C:667:LYS:HB2	1.71	0.44
3:D:191:ASN:HA	3:D:194:GLU:HG2	1.99	0.44
1:B:112:GLY:O	1:B:116:GLN:HG2	2.17	0.44
2:C:471:ARG:HH22	2:C:669:GLN:HG3	1.82	0.44
2:C:808:ASN:O	2:C:812:ILE:HG13	2.17	0.44
2:C:827:ARG:NH2	2:C:846:ARG:HG3	2.32	0.44
3:D:52:ARG:NH2	3:D:99:ASP:OD2	2.50	0.44
3:D:53:ARG:HH11	3:D:167:ASN:ND2	2.14	0.44
3:D:255:ILE:O	3:D:259:LEU:HD23	2.16	0.44
1:A:22:TRP:CZ2	1:A:66:ALA:HB2	2.53	0.44
1:A:163:PRO:HG2	1:A:164:LYS:HG2	1.99	0.44
1:A:291:SER:HB2	1:A:331:ILE:HD11	1.99	0.44
2:C:279:SER:OG	2:C:280:LEU:N	2.50	0.44
2:C:473:VAL:O	2:C:477:LEU:HG	2.17	0.44
3:D:28:HIS:CE1	3:D:29:GLN:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:142:ILE:HG13	3:D:189:LEU:HD23	1.99	0.44
1:A:12:GLN:N	4:A:501:GDP:O1A	2.49	0.44
1:A:331:ILE:HG22	1:A:335:MET:CE	2.47	0.44
2:C:349:TRP:CZ2	2:C:406:GLY:HA3	2.53	0.44
1:A:29:HIS:CE1	1:A:243:ARG:HE	2.36	0.44
2:C:191:THR:O	2:C:194:ALA:N	2.44	0.44
2:C:624:ILE:HD12	2:C:624:ILE:H	1.82	0.44
3:D:19:ILE:HG22	3:D:23:GLY:HA3	1.99	0.44
3:D:184:LYS:O	3:D:188:LEU:HD23	2.17	0.44
3:D:286:TRP:HZ3	3:D:347:MET:HG3	1.82	0.44
1:B:271:SER:O	1:B:272:PHE:HB3	2.16	0.44
1:B:327:GLU:OE2	1:B:329:ARG:HB2	2.18	0.44
1:A:276:THR:OG1	1:A:284:ILE:HD12	2.16	0.44
2:C:168:ARG:HB3	3:D:162:PHE:CE2	2.53	0.44
2:C:607:SER:O	2:C:611:ILE:HD12	2.18	0.44
1:A:208:SER:O	1:A:212:ILE:HG13	2.17	0.44
3:D:805:GLU:HB2	3:D:809:TYR:OH	2.18	0.44
1:B:121:ASN:O	1:B:125:LYS:HG3	2.18	0.44
1:B:341:ARG:HG3	1:B:341:ARG:O	2.17	0.44
3:D:558:TYR:HE1	3:D:594:TYR:CD2	2.36	0.44
1:B:256:TYR:HA	1:B:259:LEU:HB2	1.99	0.44
1:A:35:GLY:HA3	1:A:61:LYS:HE2	2.00	0.44
2:C:374:ASP:HA	2:C:377:PHE:CD2	2.53	0.44
2:C:554:GLY:O	2:C:558:PHE:N	2.51	0.44
3:D:133:MET:HA	3:D:136:GLN:OE1	2.18	0.44
1:B:260:ILE:HG22	1:B:261:PRO:O	2.18	0.43
2:C:335:PHE:O	2:C:339:ILE:HG12	2.17	0.43
1:B:140:HIS:CE1	1:B:141:SER:O	2.70	0.43
2:C:388:GLU:OE2	2:C:388:GLU:N	2.51	0.43
3:D:384:LEU:HD13	3:D:389:ASN:HB3	2.00	0.43
2:C:634:ILE:O	2:C:637:LEU:HB2	2.18	0.43
3:D:639:PHE:O	3:D:643:ILE:HG12	2.18	0.43
3:D:779:LEU:HD13	3:D:811:ILE:HG23	2.00	0.43
3:D:268:LEU:O	3:D:272:LEU:HD23	2.19	0.43
3:D:760:LEU:HD23	3:D:763:LYS:HZ3	1.83	0.43
1:A:180:VAL:HG12	1:A:183:GLN:OE1	2.17	0.43
3:D:92:PHE:HZ	3:D:110:VAL:HB	1.84	0.43
3:D:483:MET:HG2	3:D:563:ASP:O	2.18	0.43
1:B:155:LEU:HB3	1:B:197:ASP:HB3	1.99	0.43
1:A:319:TYR:OH	1:A:355:ASN:ND2	2.51	0.43
1:B:33:THR:O	1:B:86:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLY:CA	1:B:186:ASN:HD21	2.31	0.43
1:B:331:ILE:HD12	1:B:331:ILE:H	1.83	0.43
1:A:152:SER:HB3	1:A:193:ARG:HG3	2.00	0.43
1:A:276:THR:O	1:A:284:ILE:HD11	2.19	0.43
1:A:398:PHE:CZ	1:A:420:GLN:HG2	2.53	0.43
2:C:409:TYR:O	2:C:413:GLU:HG2	2.19	0.43
3:D:49:PRO:O	3:D:52:ARG:HB2	2.19	0.43
3:D:265:VAL:O	3:D:269:LYS:HG2	2.18	0.43
3:D:566:ILE:CG2	3:D:567:PRO:HD2	2.48	0.43
3:D:673:GLN:O	3:D:677:GLU:HG2	2.19	0.43
1:B:12:GLN:HB3	1:B:75:VAL:HG21	2.00	0.43
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.92	0.43
1:A:108:GLY:HA3	1:A:146:THR:HA	2.00	0.43
1:A:443:ASP:O	1:A:446:LEU:HB2	2.18	0.43
2:C:311:THR:O	2:C:315:GLU:HG2	2.19	0.43
2:C:335:PHE:CE2	2:C:339:ILE:HD13	2.54	0.43
3:D:135:LEU:O	3:D:138:PHE:HB3	2.18	0.43
3:D:487:ASP:CB	3:D:559:HIS:HE1	2.28	0.43
1:B:41:ASP:OD1	1:B:41:ASP:N	2.52	0.43
1:A:99:ALA:HB2	1:A:107:ASN:HB3	2.00	0.43
2:C:516:LEU:HD11	2:C:560:LEU:HD11	2.01	0.43
1:B:238:VAL:HG12	1:B:239:THR:HG23	2.00	0.42
1:A:61:LYS:NZ	1:A:86:PHE:HA	2.33	0.42
2:C:470:TYR:OH	2:C:724:LEU:HD12	2.19	0.42
2:C:541:LEU:HD23	2:C:562:TYR:HD1	1.84	0.42
3:D:39:LYS:HA	3:D:39:LYS:HD2	1.83	0.42
1:B:102:GLY:HA2	1:B:186:ASN:ND2	2.34	0.42
2:C:215:ASN:OD1	2:C:215:ASN:N	2.51	0.42
3:D:66:VAL:HA	3:D:70:LEU:O	2.19	0.42
1:B:17:VAL:N	1:B:228:ASN:HD21	2.17	0.42
1:A:35:GLY:O	1:A:36:LEU:HD22	2.20	0.42
2:C:239:GLU:HG2	2:C:242:ARG:CZ	2.49	0.42
2:C:607:SER:O	2:C:610:ILE:N	2.53	0.42
2:C:720:ASN:O	2:C:724:LEU:HD23	2.20	0.42
3:D:289:GLN:OE1	3:D:366:ILE:N	2.48	0.42
3:D:292:LEU:H	3:D:292:LEU:HD23	1.85	0.42
2:C:767:ASN:O	2:C:771:GLU:OE1	2.38	0.42
1:B:143:ALA:HB2	1:B:174:PRO:HG3	2.01	0.42
1:B:309:ALA:HA	1:B:385:ASN:HD22	1.84	0.42
1:A:9:GLN:NE2	1:A:18:GLY:HA3	2.33	0.42
2:C:242:ARG:HE	2:C:242:ARG:HB2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:229:ARG:HH11	3:D:229:ARG:C	2.23	0.42
1:A:57:ASN:HD21	1:A:61:LYS:CB	2.30	0.42
2:C:757:PRO:HB2	2:C:760:THR:HG23	2.02	0.42
3:D:349:ARG:O	3:D:353:LEU:HG	2.20	0.42
3:D:410:PHE:HE1	3:D:666:PRO:HG3	1.84	0.42
3:D:489:GLU:O	3:D:559:HIS:CD2	2.72	0.42
1:B:359:ARG:HD3	1:B:365:LEU:CD2	2.48	0.42
1:A:131:ASP:OD1	1:A:131:ASP:N	2.50	0.42
2:C:418:GLU:O	2:C:422:THR:HG22	2.20	0.42
3:D:632:LEU:O	3:D:636:MET:HG3	2.19	0.42
1:A:248:MET:HE2	3:D:644:MET:O	2.20	0.42
3:D:133:MET:SD	3:D:134:VAL:N	2.93	0.42
1:B:111:ILE:O	1:B:115:ASN:N	2.53	0.42
1:A:294:VAL:O	1:A:298:LEU:HG	2.20	0.42
2:C:497:ASN:OD1	2:C:497:ASN:N	2.53	0.42
3:D:416:ILE:HD12	3:D:663:TYR:CD2	2.55	0.42
3:D:618:SER:H	3:D:622:LYS:HZ3	1.66	0.42
3:D:757:ALA:HA	3:D:760:LEU:HD12	2.02	0.42
1:A:300:ASP:HB3	1:A:303:ASN:OD1	2.20	0.41
1:A:427:ARG:O	1:A:431:GLN:HG2	2.20	0.41
1:A:438:VAL:O	1:A:441:GLU:HB3	2.19	0.41
3:D:693:ILE:N	3:D:694:PRO:HD2	2.35	0.41
1:B:239:THR:HA	1:B:242:ILE:HG12	2.02	0.41
1:A:223:ASP:HB3	1:A:226:HIS:HB2	2.02	0.41
2:C:177:ASN:HD21	2:C:212:LYS:HE2	1.84	0.41
3:D:229:ARG:HA	3:D:229:ARG:HD2	1.85	0.41
3:D:613:LYS:HB3	3:D:615:ARG:CZ	2.50	0.41
1:A:334:ALA:O	1:A:338:LEU:HD13	2.20	0.41
3:D:53:ARG:O	3:D:56:GLU:HG3	2.19	0.41
3:D:107:ARG:HA	3:D:110:VAL:HG22	2.01	0.41
3:D:195:GLU:OE1	3:D:250:ILE:HG23	2.21	0.41
1:B:72:GLU:HG2	1:B:74:SER:H	1.84	0.41
1:A:118:ASP:OD1	1:A:119:ILE:HG13	2.20	0.41
1:A:164:LYS:C	1:A:165:LYS:HD3	2.40	0.41
3:D:462:LEU:HD23	3:D:484:ILE:HB	2.02	0.41
1:A:208:SER:OG	1:A:307:SER:N	2.53	0.41
2:C:460:THR:O	2:C:463:ILE:HG22	2.21	0.41
2:C:681:LEU:HD12	2:C:681:LEU:HA	1.90	0.41
2:C:840:LEU:HA	2:C:840:LEU:HD13	1.79	0.41
3:D:170:ILE:HG22	3:D:171:ARG:NH1	2.35	0.41
1:A:221:ASN:OD1	1:A:222:ILE:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:SER:O	1:B:264:GLU:N	2.53	0.41
1:B:273:THR:HB	1:B:275:PHE:CE2	2.55	0.41
2:C:172:ASN:HB2	2:C:173:PRO:HD3	2.03	0.41
3:D:376:GLN:O	3:D:393:TYR:OH	2.16	0.41
3:D:378:ILE:HG23	3:D:384:LEU:HG	2.03	0.41
3:D:613:LYS:HB3	3:D:615:ARG:NH1	2.35	0.41
3:D:695:LEU:O	3:D:699:ILE:HG12	2.21	0.41
1:A:443:ASP:HB3	1:A:446:LEU:HD12	2.01	0.41
2:C:354:LEU:C	2:C:355:LEU:HD12	2.41	0.41
1:B:202:VAL:HG13	1:B:270:PRO:HD3	2.02	0.41
1:A:138:LEU:HB3	1:A:169:THR:HG22	2.03	0.41
1:A:155:LEU:HD23	1:A:193:ARG:HB3	2.02	0.41
1:A:182:VAL:HG13	1:A:183:GLN:N	2.36	0.41
2:C:335:PHE:CZ	2:C:339:ILE:HG21	2.56	0.41
2:C:607:SER:O	2:C:610:ILE:HG22	2.21	0.41
2:C:827:ARG:HH21	2:C:846:ARG:HG3	1.85	0.41
3:D:59:VAL:HG12	3:D:63:LEU:HD23	2.03	0.41
3:D:235:ASP:HB2	3:D:325:PHE:HB3	2.03	0.41
3:D:487:ASP:C	3:D:559:HIS:CE1	2.94	0.41
3:D:496:SER:O	3:D:500:GLN:HA	2.20	0.41
3:D:586:LEU:O	3:D:590:LEU:HD23	2.21	0.41
3:D:752:TYR:C	3:D:754:GLU:HG3	2.41	0.41
1:B:255:ILE:O	1:B:258:THR:HG22	2.21	0.41
1:B:315:TYR:HA	1:B:380:MET:HA	2.02	0.41
1:A:29:HIS:CE1	1:A:243:ARG:NE	2.89	0.41
1:A:61:LYS:HZ3	1:A:86:PHE:HD1	1.67	0.41
2:C:345:TYR:OH	2:C:358:THR:HA	2.21	0.41
2:C:487:ASP:OD1	2:C:523:SER:OG	2.35	0.41
2:C:781:ASP:O	2:C:785:GLU:OE1	2.38	0.41
1:B:222:ILE:HD11	1:B:226:HIS:ND1	2.36	0.40
1:A:166:ILE:O	1:A:167:LEU:HD22	2.20	0.40
2:C:196:THR:HG22	2:C:202:PHE:N	2.36	0.40
2:C:423:ASN:O	2:C:427:LYS:HG2	2.20	0.40
2:C:768:SER:HA	2:C:771:GLU:OE1	2.20	0.40
3:D:234:PHE:CD2	3:D:326:ILE:HD13	2.56	0.40
1:B:119:ILE:O	1:B:122:LYS:HB2	2.22	0.40
2:C:226:GLU:O	2:C:230:LEU:HD23	2.22	0.40
2:C:470:TYR:C	2:C:472:ASP:H	2.25	0.40
3:D:60:VAL:O	3:D:63:LEU:HG	2.21	0.40
1:B:120:LEU:O	1:B:124:ASP:N	2.41	0.40
1:B:321:THR:CG2	1:B:375:MET:HB3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:751:GLY:HA3	2:C:829:ASP:OD1	2.21	0.40
1:B:29:HIS:NE2	1:B:243:ARG:HD2	2.36	0.40
1:B:34:ASP:N	1:B:34:ASP:OD1	2.53	0.40
1:A:205:ASP:O	1:A:209:LEU:HG	2.20	0.40
2:C:324:ASP:HB3	2:C:327:ILE:HB	2.04	0.40
2:C:523:SER:OG	2:C:524:SER:N	2.55	0.40
2:C:541:LEU:HD23	2:C:541:LEU:HA	1.71	0.40
2:C:731:PHE:CE1	2:C:735:ILE:HD11	2.56	0.40
3:D:639:PHE:CE1	3:D:643:ILE:HD11	2.56	0.40
1:B:363:LEU:HG	1:B:364:PRO:HD2	2.02	0.40
1:A:134:GLU:HA	1:A:134:GLU:OE1	2.21	0.40
1:A:286:HIS:C	1:A:287:LYS:HG2	2.42	0.40
3:D:128:ASP:OD1	3:D:129:THR:N	2.54	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	436/473 (92%)	399 (92%)	37 (8%)	0	100	100
1	B	442/473 (93%)	403 (91%)	38 (9%)	1 (0%)	47	78
2	C	670/846 (79%)	623 (93%)	47 (7%)	0	100	100
3	D	681/823 (83%)	631 (93%)	50 (7%)	0	100	100
All	All	2229/2615 (85%)	2056 (92%)	172 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/420 (93%)	391 (100%)	0	100	100
1	B	397/420 (94%)	397 (100%)	0	100	100
2	C	628/787 (80%)	628 (100%)	0	100	100
3	D	649/766 (85%)	647 (100%)	2 (0%)	92	96
All	All	2065/2393 (86%)	2063 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	9	ARG
3	D	171	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	GLN
1	B	12	GLN
1	B	103	ASN
1	B	137	GLN
1	B	153	ASN
1	B	183	GLN
1	B	186	ASN
1	B	225	GLN
1	B	417	GLN
1	A	29	HIS
1	A	103	ASN
1	A	137	GLN
1	A	140	HIS
1	A	153	ASN
1	A	186	ASN
1	A	228	ASN
1	A	289	HIS

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Mol	Chain	Res	Type
1	A	355	ASN
2	C	169	GLN
2	C	245	ASN
2	C	317	ASN
2	C	461	ASN
2	C	469	HIS
2	C	673	ASN
2	C	767	ASN
2	C	780	ASN
2	C	799	ASN
3	D	29	GLN
3	D	65	ASN
3	D	115	GLN
3	D	136	GLN
3	D	227	HIS
3	D	449	HIS
3	D	497	HIS

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](#)

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	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
4	GDP	B	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	4 (13%)

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	501	-	-	4/12/32/32	0/3/3/3
4	GDP	B	501	-	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GDP	C6-N1	-2.73	1.33	1.37
4	B	501	GDP	C6-N1	-2.53	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	GDP	PA-O3A-PB	-4.17	118.51	132.83
4	A	501	GDP	PA-O3A-PB	-3.95	119.27	132.83
4	B	501	GDP	C3'-C2'-C1'	2.89	105.32	100.98
4	A	501	GDP	C8-N7-C5	2.52	107.78	102.99
4	A	501	GDP	C5-C6-N1	2.46	118.30	113.95
4	B	501	GDP	C5-C6-N1	2.39	118.17	113.95
4	B	501	GDP	C8-N7-C5	2.33	107.43	102.99
4	A	501	GDP	C3'-C2'-C1'	2.06	104.08	100.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

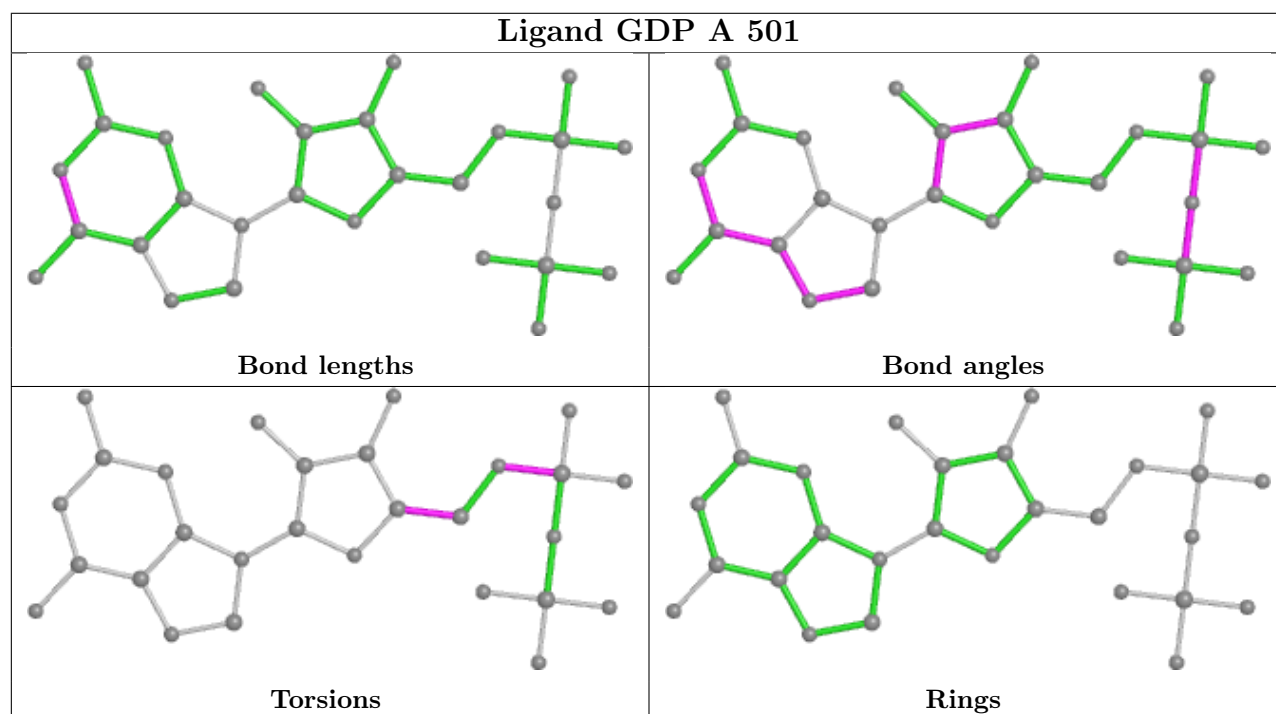
Mol	Chain	Res	Type	Atoms
4	B	501	GDP	C5'-O5'-PA-O3A
4	B	501	GDP	C5'-O5'-PA-O1A
4	A	501	GDP	C5'-O5'-PA-O1A
4	A	501	GDP	C5'-O5'-PA-O3A
4	A	501	GDP	C5'-O5'-PA-O2A
4	A	501	GDP	O4'-C4'-C5'-O5'

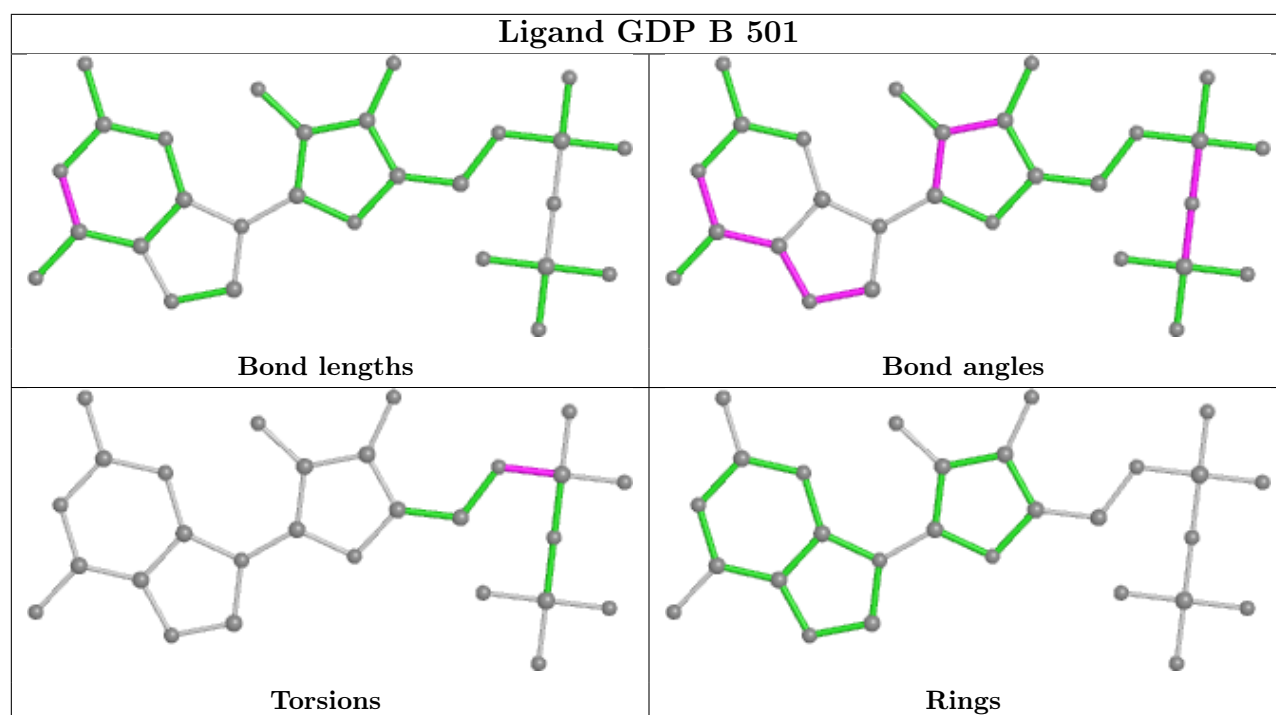
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GDP	1	0
4	B	501	GDP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23638. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.