

May 27, 2024 – 11:41 AM JST

PDB ID	:	7EFO
EMDB ID	:	EMD-31088
Title	:	LptB2FG-LPS from Klebsiella pneumoniae in nanodiscs
Authors	:	Luo, Q.; Shi, H.
Deposited on	:	2021-03-22
Resolution	:	3.85 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 (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.dev92
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	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.85 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	(# Entries)	$(\# {\rm Entries})$
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				
			26%				
1	A	241	44%		5	51%	••
			26%				
1	В	241	36%		59%		• •
			17%				
2	F	365	30%	28%	•	40%	
			19%				
3	G	360	24%	35%	•	38%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	JSG	F	401	-	-	Х	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7306 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 Lipopolysaccharide export system ATP-binding protein LptB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	235	Total 1833	C 1149	N 335	0 345	$\frac{S}{4}$	0	0
1	В	237	Total 1840	C 1154	N 334	О 347	${ m S}{ m 5}$	0	0

• Molecule 2 is a protein called Lipopolysaccharide export system permease protein LptF.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	F	219	Total 1699	C 1137	N 272	0 277	S 13	0	0

• Molecule 3 is a protein called LPS export ABC transporter permease LptG.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	G	225	Total 1734	C 1154	N 277	0 287	S 16	0	0

• Molecule 4 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[(2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-5-[(2 {S},3 {S},4 {R},5 {R},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-4-[(2 {R},3 {S},4 {R},5 {S},6 {R})-6-[(1 {S})-2-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-1-oxid anyl-ethyl]-3,4-bis(oxidanyl)-5-phosphonooxy-oxan-2-yl]oxy-3-oxidanyl-5-phosphonooxy-oxa n-2-yl]oxy-2-carboxy-2-[[(2 {R},3 {S},4 {R},5 {R},6 {R})-5-[[(3 {R})-3-dodecanoyloxytetra decanoyl]amino]-6-[[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[[(3 {R})-3-oxidanyltet radecanoyl]amino]-6-[[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[[(3 {R})-3-oxidanyltet ndecanoyl]amino]-4-[(3 {R})-3-oxidanyltet radecanoyl]oxy-6-phosphonooxy-oxan-2-yl]methoxy]oxan-4-yl]oxy-4,5-bis(oxidanyl)oxane-2-carboxylic acid (three-letter code: JSG) (formula: C₁₃₁H₂₄₀N₂O₆₃P₄) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				AltConf	
4	Б	1	Total	С	Ν	Ο	Р	0
4	Г	1	200	131	2	63	4	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: Lipopolysaccharide export system ATP-binding protein LptB





• Molecule 2: Lipopolysaccharide export system permease protein LptF





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE $(4k \ge 4k)$	Depositor
Maximum map value	2.763	Depositor
Minimum map value	-1.960	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.612	Depositor
Map size (Å)	199.68, 199.68, 199.68	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: JSG

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.31	0/1858	0.56	0/2512	
1	В	0.33	0/1865	0.59	0/2522	
2	F	0.31	0/1734	0.50	0/2359	
3	G	0.45	0/1772	0.71	0/2396	
All	All	0.35	0/7229	0.59	0/9789	

There are no bond length outliers.

There are no bond angle outliers.

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	А	1833	0	1871	249	0
1	В	1840	0	1874	220	0
2	F	1699	0	1832	201	0
3	G	1734	0	1844	212	0
4	F	200	0	0	22	0
All	All	7306	0	7421	821	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 56.



	A.L. 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:9:LEU:HD12	1:A:48:MET:SD	1.64	1.36
1:A:177:LYS:CE	1:A:203:VAL:HG12	1.61	1.31
4:F:401:JSG:CGH	3:G:317:PHE:HE1	1.43	1.31
1:A:90:PHE:HB2	1:A:98:ASN:ND2	1.47	1.30
1:A:177:LYS:HD2	1:A:203:VAL:CG1	1.62	1.29
2:F:124:SER:O	2:F:128:GLN:HG3	1.30	1.28
3:G:107:MET:CE	3:G:290:LEU:HD23	1.64	1.25
3:G:291:MET:HE2	3:G:291:MET:HA	1.23	1.18
2:F:28:CYS:O	2:F:32:VAL:HG23	1.41	1.17
3:G:356:MET:SD	3:G:357:MET:HG3	1.84	1.16
3:G:107:MET:HE1	3:G:290:LEU:HB2	1.29	1.14
1:A:60:ILE:O	1:A:61:ILE:HD13	1.47	1.14
1:A:177:LYS:HD2	1:A:203:VAL:HG11	1.25	1.13
1:A:177:LYS:CD	1:A:203:VAL:HG12	1.76	1.13
1:B:32:VAL:HG13	1:B:191:LEU:HD12	1.27	1.12
4:F:401:JSG:CGH	3:G:317:PHE:CE1	2.33	1.10
3:G:82:MET:HE2	3:G:86:ARG:NH1	1.67	1.10
3:G:315:PHE:HA	3:G:318:ILE:HD12	1.14	1.09
1:B:159:ILE:HD11	1:B:188:LEU:CD1	1.83	1.08
2:F:2:ILE:HG22	2:F:4:ILE:H	1.13	1.08
2:F:285:PRO:HB2	2:F:345:LEU:CD1	1.84	1.08
1:A:99:LEU:O	1:A:103:LEU:HD12	1.53	1.07
1:B:160:LEU:HD23	1:B:191:LEU:HD23	1.32	1.05
1:A:201:LEU:HD12	1:A:221:PRO:HB3	1.34	1.04
1:A:173:VAL:HG21	1:A:199:GLU:OE1	1.55	1.04
1:B:32:VAL:HG13	1:B:191:LEU:CD1	1.86	1.04
1:A:177:LYS:CD	1:A:203:VAL:CG1	2.32	1.04
1:A:60:ILE:C	1:A:61:ILE:HD13	1.79	1.03
3:G:82:MET:HE3	3:G:86:ARG:CZ	1.88	1.03
3:G:107:MET:HE2	3:G:290:LEU:CD2	1.89	1.02
1:A:229:GLN:O	1:A:233:VAL:HG22	1.60	1.01
2:F:329:ILE:O	2:F:330:TRP:CE3	2.13	1.00
1:B:93:LEU:HG	2:F:6:TYR:CD1	1.97	0.99
1:B:229:GLN:HE22	1:B:232:ARG:HH21	1.05	0.99
1:A:90:PHE:CB	1:A:98:ASN:ND2	2.25	0.99
2:F:2:ILE:HG21	2:F:4:ILE:HD12	1.44	0.99
3:G:315:PHE:CA	3:G:318:ILE:HD12	1.92	0.98
3:G:291:MET:CE	3:G:352:SER:CB	2.42	0.97
2:F:270:PHE:HD1	2:F:270:PHE:O	1.43	0.97
2:F:317:LYS:O	2:F:317:LYS:HG3	1.61	0.97

All (821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:7:LEU:HD23	2:F:101:ALA:CB	1.95	0.97
1:A:177:LYS:HE3	1:A:203:VAL:HG12	1.44	0.97
3:G:82:MET:HE3	3:G:86:ARG:NE	1.80	0.96
1:A:100:MET:HA	1:A:103:LEU:HD12	1.47	0.96
1:B:229:GLN:NE2	1:B:232:ARG:HH21	1.64	0.95
1:A:99:LEU:C	1:A:103:LEU:HD12	1.86	0.95
1:B:32:VAL:CG1	1:B:191:LEU:CD1	2.44	0.95
1:A:9:LEU:CD1	1:A:48:MET:SD	2.55	0.94
3:G:107:MET:HE2	3:G:290:LEU:HD23	0.95	0.94
1:A:100:MET:HE1	1:A:114:ARG:HG2	1.49	0.94
3:G:291:MET:HA	3:G:291:MET:CE	1.98	0.94
3:G:314:SER:O	3:G:318:ILE:HG13	1.68	0.94
3:G:82:MET:CE	3:G:86:ARG:NH1	2.31	0.93
2:F:281:LEU:HD23	2:F:281:LEU:O	1.68	0.93
2:F:329:ILE:O	2:F:330:TRP:HE3	1.49	0.93
3:G:325:ILE:HG22	3:G:329:LEU:HD11	1.51	0.92
1:A:11:LYS:HB2	1:A:56:ASP:OD2	1.70	0.92
2:F:61:GLN:HB3	2:F:272:LEU:CD2	1.99	0.92
2:F:285:PRO:HB2	2:F:345:LEU:HD13	1.51	0.92
1:A:90:PHE:HB2	1:A:98:ASN:HD22	1.27	0.92
1:B:32:VAL:CG1	1:B:191:LEU:HD12	1.99	0.92
3:G:19:ILE:HG21	3:G:113:LEU:HD21	1.51	0.92
3:G:82:MET:CE	3:G:86:ARG:CZ	2.49	0.91
1:B:13:TYR:CE1	1:B:14:LYS:HG2	2.07	0.90
1:B:159:ILE:HD11	1:B:188:LEU:HD13	1.54	0.89
1:A:119:LYS:HA	1:A:122:MET:SD	2.12	0.89
3:G:107:MET:HE1	3:G:290:LEU:CB	2.01	0.89
3:G:315:PHE:HA	3:G:318:ILE:CD1	2.02	0.88
1:A:91:ARG:HH12	3:G:86:ARG:HB3	1.37	0.88
1:A:90:PHE:HB2	1:A:98:ASN:HD21	1.37	0.88
3:G:291:MET:CE	3:G:352:SER:HB2	2.02	0.88
2:F:343:VAL:O	2:F:347:LEU:HD23	1.74	0.88
1:B:91:ARG:HG3	2:F:82:GLU:OE2	1.74	0.87
2:F:285:PRO:CB	2:F:345:LEU:CD1	2.51	0.87
1:A:60:ILE:HG13	1:A:67:ILE:HG13	1.56	0.87
1:B:86:GLU:OE1	1:B:86:GLU:HA	1.72	0.87
2:F:26:PHE:HB3	2:F:59:MET:SD	2.13	0.87
1:A:177:LYS:CE	1:A:203:VAL:CG1	2.52	0.87
3:G:342:LEU:O	3:G:342:LEU:HG	1.73	0.87
1:A:77:ARG:HD3	3:G:96:GLY:O	1.73	0.86
1:B:169:ASP:OD2	1:B:171:ILE:HG22	1.75	0.86



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		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:164:PRO:HG2	1:A:165:PHE:CE1	2.10	0.86
1:B:34:LEU:HD12	1:B:46:PHE:HD1	1.41	0.85
2:F:2:ILE:HG22	2:F:4:ILE:N	1.91	0.85
1:A:72:LEU:HD21	3:G:94:ALA:HA	1.57	0.85
1:A:100:MET:CA	1:A:103:LEU:HD12	2.06	0.85
1:A:91:ARG:NH1	3:G:86:ARG:HB3	1.90	0.85
1:A:160:LEU:HD23	1:A:191:LEU:HD13	1.57	0.85
1:A:99:LEU:O	1:A:103:LEU:CD1	2.25	0.85
3:G:63:ASP:O	3:G:68:PHE:N	2.07	0.85
1:A:24:LEU:HD21	1:A:49:VAL:HG21	1.56	0.85
1:A:100:MET:HA	1:A:103:LEU:CD1	2.07	0.84
1:B:159:ILE:HD11	1:B:188:LEU:HD12	1.60	0.84
1:B:72:LEU:HD22	2:F:90:ALA:HA	1.58	0.84
1:A:11:LYS:CB	1:A:56:ASP:OD2	2.25	0.83
1:A:72:LEU:CD2	3:G:94:ALA:HA	2.09	0.83
2:F:308:VAL:HG12	2:F:338:TYR:OH	1.78	0.83
1:B:35:LEU:HA	1:B:42:LYS:HD3	1.61	0.83
1:B:160:LEU:HD23	1:B:191:LEU:CD2	2.08	0.83
1:B:119:LYS:O	1:B:123:GLU:HG2	1.79	0.82
1:A:85:GLN:HB2	1:A:162:ASP:OD2	1.79	0.82
1:B:35:LEU:HD11	1:B:200:THR:HG21	1.61	0.82
3:G:107:MET:CE	3:G:290:LEU:CD2	2.50	0.82
3:G:353:LEU:O	3:G:356:MET:SD	2.38	0.82
2:F:61:GLN:HB3	2:F:272:LEU:HD21	1.61	0.82
1:A:22:VAL:HA	1:A:215:LEU:HD22	1.62	0.81
1:A:200:THR:O	1:A:203:VAL:HG22	1.78	0.81
1:B:229:GLN:OE1	1:B:229:GLN:HA	1.80	0.81
1:A:128:GLU:O	1:A:131:ARG:HG3	1.80	0.81
1:B:100:MET:CE	1:B:115:GLU:HA	2.10	0.80
2:F:7:LEU:HD23	2:F:101:ALA:HB2	1.59	0.80
2:F:269:ARG:NH1	2:F:269:ARG:HB2	1.97	0.80
1:B:165:PHE:HD2	1:B:194:ASP:OD2	1.64	0.80
1:A:100:MET:HE1	1:A:114:ARG:CG	2.11	0.80
2:F:61:GLN:CB	2:F:272:LEU:HD21	2.11	0.80
1:A:89:ILE:HG21	1:A:143:ARG:HG3	1.64	0.80
3:G:105:ALA:O	3:G:109:THR:HG23	1.82	0.80
1:A:110:THR:OG1	1:A:113:GLN:HG2	1.81	0.79
2:F:7:LEU:CD2	2:F:101:ALA:CB	2.60	0.79
1:A:59:ASN:OD1	1:A:61:ILE:HD11	1.81	0.79
3:G:82:MET:HE3	3:G:86:ARG:CD	2.13	0.79
1:B:208:TYR:CE1	1:B:215:LEU:HD12	2.17	0.79



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	loub page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:291:MET:HE2	3:G:291:MET:CA	2.03	0.79
1:B:161:LEU:HD12	1:B:180:ILE:HD11	1.64	0.79
3:G:63:ASP:O	3:G:68:PHE:HB2	1.81	0.79
3:G:74:LEU:O	3:G:74:LEU:HD23	1.83	0.78
1:A:26:VAL:HG13	1:A:158:PHE:CE2	2.18	0.78
1:A:171:ILE:O	1:A:174:ILE:HG22	1.83	0.78
1:B:34:LEU:HD13	1:B:46:PHE:HB2	1.66	0.78
3:G:35:PHE:HE1	3:G:51:GLY:HA2	1.46	0.78
3:G:356:MET:HE2	3:G:357:MET:N	1.99	0.78
1:B:93:LEU:HD11	2:F:6:TYR:CB	2.14	0.77
1:B:73:HIS:CE1	2:F:95:LYS:H	2.02	0.77
3:G:356:MET:SD	3:G:357:MET:N	2.58	0.77
3:G:7:LEU:HD22	3:G:97:PHE:CD2	2.20	0.77
1:A:31:ILE:CD1	1:A:184:ARG:HE	1.96	0.77
1:A:106:ARG:CZ	1:A:155:ASN:HB3	2.14	0.77
1:B:13:TYR:CD1	1:B:14:LYS:HG2	2.20	0.77
1:A:62:ILE:HB	1:A:65:GLU:OE2	1.85	0.76
3:G:100:LEU:O	3:G:104:LEU:HD23	1.86	0.76
1:A:17:ARG:NH1	1:A:17:ARG:HB3	2.00	0.76
1:B:35:LEU:CA	1:B:42:LYS:HD3	2.16	0.76
2:F:32:VAL:HG13	3:G:324:GLN:HB2	1.68	0.76
1:A:11:LYS:HA	1:A:56:ASP:OD2	1.85	0.76
1:B:100:MET:HE3	1:B:115:GLU:HA	1.66	0.76
3:G:342:LEU:HG	3:G:345:SER:HB3	1.68	0.76
3:G:110:ALA:O	3:G:114:VAL:HG13	1.86	0.76
3:G:325:ILE:O	3:G:329:LEU:HG	1.85	0.76
1:B:104:GLN:NE2	2:F:2:ILE:HA	2.01	0.76
1:A:100:MET:CE	1:A:114:ARG:HG2	2.16	0.75
3:G:15:ILE:HG21	3:G:106:VAL:HG13	1.69	0.75
1:B:229:GLN:HE22	1:B:232:ARG:NH2	1.82	0.75
1:B:150:ARG:HH21	2:F:87:VAL:HG11	1.51	0.75
2:F:270:PHE:O	2:F:270:PHE:CD1	2.35	0.75
3:G:290:LEU:HD13	3:G:290:LEU:O	1.87	0.75
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.51	0.75
1:A:17:ARG:HB3	1:A:17:ARG:HH11	1.52	0.74
1:B:32:VAL:CG1	1:B:191:LEU:HD13	2.17	0.74
3:G:82:MET:HG3	3:G:86:ARG:NH2	2.01	0.74
1:A:131:ARG:HB3	1:A:131:ARG:NH1	2.02	0.74
1:B:177:LYS:O	1:B:181:GLU:HG2	1.86	0.74
2:F:124:SER:O	2:F:128:GLN:CG	2.25	0.74
1:B:31:ILE:HG23	1:B:190:VAL:CG1	2.17	0.74



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:61:GLN:CA	2:F:272:LEU:HD21	2.17	0.74
2:F:328:ALA:O	2:F:331:MET:CE	2.35	0.74
1:B:99:LEU:CD1	1:B:122:MET:HG3	2.18	0.74
1:A:90:PHE:CG	1:A:98:ASN:ND2	2.56	0.74
2:F:61:GLN:HB3	2:F:272:LEU:HD22	1.69	0.73
1:B:159:ILE:CD1	1:B:183:LEU:HD22	2.17	0.73
1:A:217:ALA:HB1	1:A:224:ILE:HD12	1.71	0.73
3:G:50:LEU:HD22	3:G:54:LEU:HD12	1.69	0.73
2:F:54:LEU:O	2:F:128:GLN:NE2	2.21	0.72
2:F:117:VAL:HG13	2:F:269:ARG:HG3	1.70	0.72
4:F:401:JSG:CEH	3:G:33:ILE:CG2	2.67	0.72
1:A:26:VAL:HG13	1:A:158:PHE:HE2	1.53	0.72
1:A:164:PRO:HG2	1:A:165:PHE:CD1	2.24	0.72
1:A:163:GLU:HG2	1:A:194:ASP:HA	1.71	0.72
2:F:61:GLN:HA	2:F:272:LEU:HD21	1.70	0.71
1:B:101:ALA:HB1	2:F:3:ILE:HB	1.72	0.71
3:G:120:ILE:HG22	3:G:120:ILE:O	1.90	0.71
1:B:229:GLN:OE1	1:B:232:ARG:NE	2.24	0.71
2:F:269:ARG:HB2	2:F:269:ARG:HH11	1.52	0.71
1:A:99:LEU:C	1:A:103:LEU:CD1	2.59	0.71
2:F:116:ASN:HA	2:F:120:ALA:HB3	1.72	0.71
3:G:127:GLN:O	3:G:131:MET:SD	2.49	0.71
2:F:23:LEU:O	2:F:27:PHE:HD2	1.74	0.71
2:F:63:ILE:O	2:F:67:SER:N	2.20	0.71
1:B:25:THR:O	1:B:206:ARG:NH2	2.23	0.71
3:G:325:ILE:O	3:G:328:PRO:HD2	1.90	0.71
2:F:328:ALA:O	2:F:331:MET:HE1	1.89	0.70
2:F:49:LEU:HD12	2:F:49:LEU:O	1.90	0.70
1:A:106:ARG:HG2	1:A:106:ARG:HH11	1.56	0.70
1:B:4:LEU:HB2	1:B:158:PHE:CD2	2.25	0.70
1:A:177:LYS:NZ	1:A:203:VAL:HG12	2.07	0.70
1:A:177:LYS:HE3	1:A:203:VAL:CG1	2.19	0.70
3:G:82:MET:CE	3:G:86:ARG:HD3	2.22	0.70
2:F:317:LYS:O	2:F:317:LYS:CG	2.39	0.70
1:B:163:GLU:OE2	1:B:195:HIS:CE1	2.45	0.70
3:G:60:VAL:HG13	3:G:61:PRO:HD3	1.74	0.70
1:A:118:ALA:O	1:A:122:MET:SD	2.50	0.69
2:F:282:MET:HE2	2:F:342:ALA:HB2	1.73	0.69
1:A:93:LEU:HD11	1:A:97:ASP:CB	2.22	0.69
1:A:35:LEU:HG	1:A:201:LEU:HD21	1.75	0.69
3:G:291:MET:HE1	3:G:352:SER:HA	1.75	0.69



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:G:63:ASP:O	3:G:68:PHE:CB	2.39	0.69
1:A:91:ARG:NH2	3:G:86:ARG:HB3	2.07	0.69
3:G:326:PHE:HA	3:G:329:LEU:HD12	1.74	0.68
2:F:66:LEU:HD13	4:F:401:JSG:CFV	2.24	0.68
1:A:122:MET:CE	1:A:131:ARG:HD3	2.24	0.68
1:B:90:PHE:CE2	2:F:3:ILE:HD11	2.28	0.68
1:B:11:LYS:HG2	1:B:48:MET:HE1	1.76	0.68
3:G:291:MET:HE3	3:G:352:SER:HB2	1.75	0.68
1:A:88:SER:O	1:A:150:ARG:NH2	2.27	0.68
1:A:100:MET:N	1:A:103:LEU:HD12	2.09	0.68
1:B:150:ARG:NH2	2:F:87:VAL:HG11	2.07	0.68
1:A:134:LEU:HD23	1:A:134:LEU:O	1.92	0.68
4:F:401:JSG:CEH	3:G:33:ILE:HG23	2.24	0.68
3:G:82:MET:HE2	3:G:86:ARG:HH11	1.56	0.67
1:A:91:ARG:CZ	3:G:86:ARG:HB3	2.24	0.67
1:A:106:ARG:NH2	1:A:155:ASN:OD1	2.27	0.67
1:B:34:LEU:HD12	1:B:46:PHE:CD1	2.28	0.67
2:F:281:LEU:HD22	2:F:342:ALA:HB1	1.76	0.67
2:F:299:MET:O	2:F:303:MET:HG2	1.94	0.67
1:A:31:ILE:HD12	1:A:184:ARG:HE	1.60	0.67
1:B:122:MET:HE2	1:B:128:GLU:HA	1.77	0.67
1:B:109:LEU:HD12	1:B:110:THR:N	2.10	0.67
2:F:282:MET:HE2	2:F:342:ALA:CB	2.24	0.67
1:A:11:LYS:CA	1:A:56:ASP:OD2	2.42	0.67
2:F:61:GLN:CB	2:F:272:LEU:CD2	2.72	0.67
1:B:22:VAL:HG12	1:B:215:LEU:HB3	1.77	0.67
1:B:35:LEU:HD11	1:B:200:THR:CG2	2.25	0.67
1:B:200:THR:HG23	1:B:201:LEU:HD22	1.76	0.67
1:A:122:MET:CE	1:A:131:ARG:CD	2.73	0.67
1:B:165:PHE:CD2	1:B:194:ASP:OD2	2.48	0.67
2:F:61:GLN:O	2:F:272:LEU:HD11	1.95	0.67
3:G:76:ALA:O	3:G:80:LEU:N	2.27	0.67
3:G:107:MET:HE1	3:G:290:LEU:HD23	1.74	0.66
3:G:97:PHE:HE1	3:G:102:VAL:N	1.93	0.66
1:A:119:LYS:NZ	1:A:122:MET:CE	2.59	0.66
2:F:63:ILE:HA	2:F:66:LEU:HD23	1.78	0.66
1:B:73:HIS:NE2	2:F:95:LYS:HB2	2.11	0.66
1:B:35:LEU:CD1	1:B:200:THR:HG21	2.25	0.65
1:B:73:HIS:CE1	2:F:95:LYS:HB2	2.30	0.65
1:A:91:ARG:HH22	3:G:86:ARG:HB3	1.60	0.65
1:B:13:TYR:HE1	1:B:14:LYS:HG2	1.57	0.65



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:356:MET:HE2	3:G:356:MET:C	2.15	0.65
3:G:291:MET:HE2	3:G:352:SER:HB2	1.77	0.65
3:G:291:MET:HE2	3:G:352:SER:CB	2.26	0.65
1:A:106:ARG:HD2	1:A:153:ALA:O	1.97	0.65
1:B:24:LEU:HA	1:B:208:TYR:CE2	2.32	0.65
3:G:35:PHE:CE1	3:G:51:GLY:HA2	2.31	0.65
2:F:7:LEU:HG	2:F:101:ALA:HB1	1.80	0.64
2:F:285:PRO:CB	2:F:345:LEU:HD12	2.27	0.64
2:F:270:PHE:HD1	2:F:270:PHE:C	2.00	0.64
3:G:19:ILE:HG13	3:G:75:GLY:HA3	1.79	0.64
3:G:291:MET:HE1	3:G:352:SER:CB	2.27	0.64
1:A:67:ILE:HA	1:A:70:LEU:HD23	1.80	0.64
1:B:60:ILE:H	1:B:68:SER:HB2	1.62	0.64
3:G:356:MET:SD	3:G:357:MET:CG	2.74	0.64
1:B:31:ILE:HG23	1:B:190:VAL:HG12	1.79	0.64
2:F:270:PHE:CD1	2:F:270:PHE:C	2.71	0.64
3:G:120:ILE:HD13	3:G:124:VAL:HG21	1.78	0.64
3:G:291:MET:CE	3:G:352:SER:OG	2.44	0.64
4:F:401:JSG:CEH	3:G:33:ILE:HG21	2.27	0.64
1:A:210:VAL:HA	1:A:215:LEU:HA	1.79	0.64
3:G:310:VAL:HA	3:G:313:ILE:HB	1.80	0.64
1:A:100:MET:HE1	1:A:114:ARG:CB	2.28	0.64
1:A:35:LEU:HD12	1:A:197:VAL:HG12	1.79	0.64
1:A:100:MET:SD	1:A:103:LEU:HD13	2.37	0.63
3:G:275:MET:O	3:G:279:ILE:HG13	1.97	0.63
1:A:93:LEU:HD11	1:A:97:ASP:HB3	1.78	0.63
1:A:173:VAL:CG2	1:A:199:GLU:OE1	2.41	0.63
3:G:29:LEU:O	3:G:33:ILE:HG22	1.97	0.63
1:B:100:MET:HA	1:B:103:LEU:HB3	1.81	0.63
1:B:22:VAL:HA	1:B:215:LEU:HD22	1.80	0.63
1:B:159:ILE:CD1	1:B:188:LEU:CD1	2.71	0.63
1:B:122:MET:CE	1:B:131:ARG:HA	2.29	0.63
2:F:27:PHE:CD1	2:F:52:LEU:HD11	2.32	0.63
1:B:150:ARG:HH21	2:F:87:VAL:CG1	2.11	0.62
1:B:46:PHE:HD2	1:B:47:TYR:CD1	2.17	0.62
1:B:82:TYR:HB3	2:F:90:ALA:HB1	1.81	0.62
2:F:7:LEU:CD2	2:F:101:ALA:HB3	2.29	0.62
3:G:276:TRP:HA	3:G:279:ILE:HD12	1.80	0.62
2:F:26:PHE:CE2	4:F:401:JSG:CGR	2.82	0.62
2:F:266:LEU:HA	2:F:269:ARG:HB3	1.80	0.62
3:G:356:MET:CE	3:G:357:MET:N	2.62	0.62



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Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:330:THR:HG23	3:G:335:ILE:HB	1.80	0.62
1:A:155:ASN:CG	1:A:155:ASN:O	2.35	0.62
1:B:73:HIS:CE1	2:F:95:LYS:N	2.68	0.62
1:A:22:VAL:HG23	1:A:215:LEU:HB3	1.82	0.62
1:A:122:MET:HE3	1:A:131:ARG:CD	2.30	0.62
2:F:281:LEU:O	2:F:281:LEU:CD2	2.46	0.62
2:F:284:VAL:HG23	2:F:285:PRO:HD3	1.81	0.62
3:G:319:PHE:O	3:G:319:PHE:CD1	2.53	0.62
1:B:99:LEU:HD11	1:B:122:MET:HG3	1.82	0.62
1:B:159:ILE:CD1	1:B:188:LEU:HD12	2.29	0.61
1:B:194:ASP:OD2	1:B:196:ASN:ND2	2.33	0.61
2:F:23:LEU:O	2:F:27:PHE:CD2	2.53	0.61
3:G:291:MET:CE	3:G:352:SER:CA	2.77	0.61
2:F:279:MET:HE1	2:F:282:MET:HG2	1.82	0.61
3:G:343:LEU:O	3:G:347:SER:N	2.33	0.61
1:A:157:LYS:O	1:A:158:PHE:HD1	1.84	0.61
3:G:83:LEU:HD22	3:G:88:GLU:HG2	1.81	0.61
1:A:181:GLU:HG3	1:A:184:ARG:HH22	1.66	0.61
3:G:80:LEU:HD23	3:G:296:ILE:HG21	1.83	0.61
2:F:26:PHE:HD2	2:F:59:MET:HG2	1.66	0.60
3:G:7:LEU:HD21	3:G:92:MET:CG	2.31	0.60
1:A:35:LEU:C	1:A:42:LYS:HD3	2.21	0.60
1:A:90:PHE:CB	1:A:98:ASN:HD21	2.02	0.60
2:F:264:ALA:N	2:F:326:ASP:OD1	2.35	0.60
1:B:1:MET:N	1:B:28:SER:OG	2.29	0.60
1:B:124:GLU:HG2	1:B:125:PHE:CE1	2.37	0.60
4:F:401:JSG:CGJ	3:G:317:PHE:CD1	2.84	0.60
1:B:181:GLU:CD	1:B:184:ARG:HH12	2.05	0.60
2:F:27:PHE:HD1	2:F:52:LEU:HD11	1.67	0.60
1:B:200:THR:CG2	1:B:201:LEU:HD22	2.31	0.60
2:F:328:ALA:O	2:F:331:MET:HE3	2.02	0.60
1:B:50:VAL:HG22	1:B:160:LEU:HD13	1.83	0.60
1:B:211:SER:O	1:B:212:GLN:HG2	2.02	0.60
3:G:353:LEU:HA	3:G:356:MET:HG3	1.82	0.60
1:B:96:TYR:HB2	1:B:131:ARG:O	2.02	0.60
2:F:265:GLU:CB	2:F:269:ARG:HH12	2.15	0.60
3:G:356:MET:CE	3:G:357:MET:HB3	2.31	0.60
1:A:80:ILE:HD12	1:A:160:LEU:HD11	1.84	0.59
1:B:93:LEU:CD1	2:F:6:TYR:CG	2.86	0.59
1:A:169:ASP:OD1	1:A:171:ILE:HG23	2.03	0.59
1:B:231:LYS:HZ3	1:B:236:GLY:HA2	1.66	0.59



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		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:119:LYS:HZ3	1:A:122:MET:HE2	1.66	0.59
1:A:122:MET:HE1	1:A:131:ARG:CD	2.33	0.59
1:A:230:VAL:HG13	1:A:234:TYR:CB	2.33	0.59
2:F:279:MET:O	2:F:283:VAL:HG12	2.03	0.59
1:B:100:MET:HE1	1:B:115:GLU:HA	1.84	0.59
1:A:11:LYS:CD	1:A:56:ASP:OD2	2.50	0.59
2:F:28:CYS:O	2:F:32:VAL:CG2	2.35	0.59
1:A:3:THR:CG2	1:A:4:LEU:N	2.66	0.59
3:G:88:GLU:OE2	3:G:92:MET:CE	2.51	0.59
2:F:54:LEU:C	2:F:128:GLN:HE21	2.06	0.58
3:G:13:LYS:O	3:G:17:ASN:HB2	2.02	0.58
3:G:287:VAL:HG12	3:G:288:MET:HE1	1.83	0.58
1:B:55:ARG:C	1:B:55:ARG:HD2	2.24	0.58
2:F:303:MET:CE	4:F:401:JSG:CFX	2.80	0.58
1:A:42:LYS:HA	1:A:210:VAL:HG21	1.83	0.58
1:A:159:ILE:HD13	1:A:183:LEU:HD13	1.86	0.58
1:A:169:ASP:OD1	1:A:171:ILE:CG2	2.52	0.58
1:B:102:VAL:HG11	2:F:91:CYS:HB3	1.86	0.58
3:G:101:GLN:HA	3:G:104:LEU:HB2	1.85	0.58
1:A:26:VAL:O	1:A:158:PHE:HE2	1.87	0.58
3:G:291:MET:CE	3:G:352:SER:HA	2.34	0.58
1:B:208:TYR:HE1	1:B:215:LEU:HD12	1.66	0.57
2:F:57:PRO:HG2	2:F:124:SER:HB3	1.86	0.57
3:G:81:GLY:HA2	3:G:296:ILE:HD11	1.85	0.57
1:A:89:ILE:HG13	1:A:91:ARG:HD3	1.86	0.57
1:B:4:LEU:HA	1:B:62:ILE:HG22	1.86	0.57
1:A:31:ILE:HD11	1:A:184:ARG:NE	2.18	0.57
2:F:102:ALA:HB1	2:F:280:ALA:HB1	1.86	0.57
1:B:13:TYR:HD1	1:B:14:LYS:N	2.02	0.57
1:A:77:ARG:HG3	1:A:77:ARG:NH1	2.19	0.57
2:F:117:VAL:HG13	2:F:269:ARG:CG	2.34	0.57
1:A:119:LYS:HZ1	1:A:131:ARG:HD3	1.69	0.57
1:A:122:MET:HE1	1:A:131:ARG:HD2	1.87	0.57
3:G:50:LEU:HA	3:G:54:LEU:HB2	1.85	0.57
1:A:10:ALA:HA	1:A:19:VAL:HG13	1.86	0.57
1:A:119:LYS:CA	1:A:122:MET:SD	2.92	0.57
1:B:62:ILE:HG23	1:B:67:ILE:HD11	1.86	0.57
1:B:93:LEU:HD21	2:F:6:TYR:HB2	1.85	0.57
2:F:102:ALA:O	2:F:105:LEU:HG	2.04	0.57
1:A:230:VAL:HA	1:A:234:TYR:HB2	1.87	0.57
2:F:53:GLY:HA2	2:F:56:ILE:HD11	1.86	0.57



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Atom-1	Atom-2	distance (Å)	overlap (Å)
3:G:356:MET:HE2	3:G:357:MET:CA	2.34	0.57
1:B:50:VAL:HG21	1:B:82:TYR:HD1	1.69	0.57
2:F:32:VAL:CG1	3:G:324:GLN:HB2	2.34	0.57
2:F:338:TYR:O	2:F:342:ALA:N	2.38	0.57
3:G:31:GLY:O	3:G:35:PHE:N	2.33	0.57
1:A:118:ALA:C	1:A:122:MET:SD	2.83	0.56
1:B:93:LEU:HD11	2:F:6:TYR:CG	2.40	0.56
3:G:291:MET:HE1	3:G:352:SER:CA	2.35	0.56
1:A:31:ILE:CD1	1:A:184:ARG:NE	2.67	0.56
2:F:68:LEU:HG	2:F:72:LEU:HD23	1.87	0.56
2:F:311:LEU:HD13	3:G:36:VAL:HG11	1.86	0.56
1:A:100:MET:CE	1:A:114:ARG:CG	2.81	0.56
1:B:70:LEU:HD23	1:B:74:ALA:HB3	1.88	0.56
1:B:93:LEU:HG	2:F:6:TYR:CG	2.38	0.56
3:G:348:PHE:O	3:G:352:SER:N	2.38	0.56
1:A:89:ILE:CG2	1:A:143:ARG:HG3	2.35	0.56
3:G:26:LEU:HB3	3:G:67:PHE:CE1	2.41	0.56
1:B:83:LEU:HD11	1:B:147:GLU:HB3	1.86	0.56
1:B:159:ILE:CD1	1:B:188:LEU:HD13	2.33	0.56
1:A:34:LEU:HD23	1:A:46:PHE:HB2	1.88	0.56
1:A:118:ALA:O	1:A:122:MET:HG3	2.06	0.56
1:B:124:GLU:HG2	1:B:125:PHE:HE1	1.71	0.56
3:G:356:MET:CE	3:G:357:MET:CB	2.84	0.56
2:F:123:TRP:CD1	2:F:123:TRP:C	2.79	0.56
2:F:265:GLU:HB3	2:F:269:ARG:HH12	1.71	0.56
1:A:60:ILE:HD11	1:A:75:ARG:CZ	2.36	0.56
2:F:81:THR:OG1	2:F:295:ARG:NH1	2.39	0.56
3:G:120:ILE:O	3:G:120:ILE:CG2	2.53	0.56
1:A:46:PHE:HE1	1:A:160:LEU:HB3	1.71	0.55
1:A:106:ARG:HG2	1:A:106:ARG:NH1	2.21	0.55
3:G:77:LEU:O	3:G:308:ARG:HD2	2.05	0.55
3:G:291:MET:HE1	3:G:352:SER:OG	2.05	0.55
1:A:162:ASP:HA	1:A:193:THR:HG22	1.88	0.55
1:B:46:PHE:HD2	1:B:47:TYR:HD1	1.53	0.55
1:B:90:PHE:HE2	2:F:3:ILE:HD11	1.70	0.55
1:B:93:LEU:HD11	2:F:6:TYR:HB2	1.86	0.55
3:G:82:MET:CE	3:G:86:ARG:CD	2.80	0.55
1:A:119:LYS:NZ	1:A:122:MET:HE2	2.21	0.55
2:F:39:VAL:HG11	3:G:328:PRO:HB3	1.89	0.55
2:F:66:LEU:HD13	4:F:401:JSG:CFW	2.37	0.55
2:F:102:ALA:O	2:F:106:ALA:N	2.40	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:F:330:TRP:HA	2:F:333:ALA:HB3	1.88	0.55
2:F:282:MET:CE	2:F:342:ALA:HB2	2.36	0.55
1:B:122:MET:HE3	1:B:127:ILE:O	2.07	0.55
1:B:122:MET:HE3	1:B:131:ARG:HA	1.88	0.55
3:G:323:ASP:OD1	3:G:342:LEU:HD11	2.07	0.55
1:B:10:ALA:HA	1:B:19:VAL:HG13	1.88	0.55
1:B:48:MET:HE3	1:B:54:PRO:O	2.07	0.54
2:F:285:PRO:HG2	2:F:345:LEU:CD1	2.37	0.54
1:A:119:LYS:NZ	1:A:131:ARG:HD3	2.21	0.54
1:B:65:GLU:O	1:B:65:GLU:OE1	2.26	0.54
3:G:319:PHE:CD1	3:G:319:PHE:C	2.80	0.54
1:A:26:VAL:O	1:A:158:PHE:CE2	2.61	0.54
1:A:59:ASN:OD1	1:A:61:ILE:CD1	2.52	0.54
2:F:66:LEU:HD12	2:F:70:LEU:HD23	1.89	0.54
1:A:35:LEU:HG	1:A:201:LEU:CD2	2.37	0.54
3:G:32:ILE:HA	3:G:35:PHE:HB3	1.89	0.54
2:F:32:VAL:HG13	3:G:324:GLN:CB	2.36	0.54
1:A:36:GLY:C	1:A:42:LYS:HE3	2.28	0.54
2:F:26:PHE:HE2	4:F:401:JSG:CGP	2.21	0.54
1:A:72:LEU:HD22	3:G:94:ALA:HA	1.90	0.54
2:F:331:MET:SD	2:F:332:TRP:N	2.80	0.54
1:A:100:MET:HE1	1:A:114:ARG:C	2.29	0.54
2:F:279:MET:CE	2:F:282:MET:HG2	2.38	0.54
2:F:343:VAL:HG13	2:F:347:LEU:HD21	1.90	0.54
1:A:108:ASP:OD1	1:A:109:LEU:CD1	2.56	0.53
1:A:42:LYS:HB3	1:A:42:LYS:HZ2	1.73	0.53
1:A:94:SER:OG	1:A:131:ARG:O	2.22	0.53
1:A:119:LYS:NZ	1:A:122:MET:HE1	2.21	0.53
1:A:119:LYS:HD3	1:A:122:MET:HE2	1.89	0.53
1:A:157:LYS:C	1:A:158:PHE:HD1	2.11	0.53
2:F:290:ASN:O	2:F:293:GLN:NE2	2.40	0.53
1:A:11:LYS:N	1:A:19:VAL:HG13	2.23	0.53
1:B:49:VAL:O	1:B:75:ARG:NH2	2.41	0.53
2:F:282:MET:CE	2:F:342:ALA:HA	2.38	0.53
1:A:101:ALA:HB1	3:G:7:LEU:HB2	1.90	0.53
2:F:66:LEU:HD12	2:F:70:LEU:CD2	2.38	0.53
3:G:288:MET:HE3	3:G:319:PHE:HD2	1.73	0.53
1:A:134:LEU:HD22	1:A:136:GLN:HB2	1.89	0.53
2:F:285:PRO:CG	2:F:345:LEU:CD1	2.87	0.53
3:G:321:VAL:HG23	3:G:325:ILE:HG13	1.90	0.53
1:A:11:LYS:H	1:A:19:VAL:HG13	1.74	0.53



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:65:GLU:CD	1:A:65:GLU:H	2.12	0.53
1:B:229:GLN:CD	1:B:232:ARG:HH21	2.11	0.53
2:F:307:LEU:HG	2:F:311:LEU:HD23	1.91	0.53
1:A:42:LYS:HA	1:A:210:VAL:CG2	2.39	0.53
1:B:35:LEU:C	1:B:42:LYS:HD3	2.30	0.53
1:B:90:PHE:HE1	1:B:150:ARG:HD2	1.72	0.52
1:B:229:GLN:OE1	1:B:229:GLN:CA	2.54	0.52
2:F:26:PHE:CE2	4:F:401:JSG:CGP	2.92	0.52
2:F:285:PRO:HB2	2:F:345:LEU:HD11	1.85	0.52
3:G:353:LEU:HA	3:G:356:MET:CG	2.39	0.52
1:B:94:SER:HA	1:B:134:LEU:HA	1.90	0.52
2:F:286:LEU:HD13	2:F:302:ALA:HA	1.90	0.52
1:A:131:ARG:HB3	1:A:131:ARG:CZ	2.39	0.52
1:B:109:LEU:HD12	1:B:110:THR:H	1.74	0.52
2:F:93:LEU:HD22	2:F:97:VAL:HG21	1.90	0.52
3:G:7:LEU:HD21	3:G:92:MET:HG3	1.90	0.52
1:B:4:LEU:HB3	1:B:26:VAL:HG13	1.89	0.52
2:F:68:LEU:CD1	2:F:105:LEU:CD1	2.87	0.52
1:A:26:VAL:HG13	1:A:158:PHE:CD2	2.45	0.52
1:A:119:LYS:CE	1:A:122:MET:CE	2.88	0.52
1:A:72:LEU:C	1:A:72:LEU:HD23	2.30	0.52
1:A:161:LEU:HD12	1:A:164:PRO:HB3	1.90	0.52
1:B:150:ARG:NH2	2:F:87:VAL:HG21	2.25	0.52
1:A:139:SER:O	1:A:143:ARG:N	2.31	0.52
1:B:120:GLU:HA	1:B:123:GLU:OE2	2.09	0.52
1:B:125:PHE:CD1	1:B:125:PHE:N	2.76	0.52
1:B:11:LYS:HG2	1:B:48:MET:CE	2.38	0.52
1:B:50:VAL:HG21	1:B:82:TYR:CD1	2.45	0.51
1:A:25:THR:O	1:A:206:ARG:NH2	2.40	0.51
1:A:102:VAL:HG21	1:A:150:ARG:HG3	1.92	0.51
1:A:60:ILE:O	1:A:61:ILE:CD1	2.38	0.51
2:F:2:ILE:HG22	2:F:3:ILE:N	2.25	0.51
3:G:109:THR:O	3:G:112:PRO:HD2	2.10	0.51
1:A:31:ILE:HG13	1:A:184:ARG:HD3	1.91	0.51
1:A:201:LEU:HD13	1:A:204:CYS:SG	2.50	0.51
1:B:46:PHE:CD2	1:B:47:TYR:HD1	2.28	0.51
2:F:68:LEU:HD12	2:F:105:LEU:CD1	2.41	0.51
3:G:22:THR:HG22	3:G:71:ALA:HB1	1.93	0.51
1:A:24:LEU:HD21	1:A:49:VAL:CG2	2.36	0.51
1:B:220:THR:HG22	1:B:222:GLN:H	1.76	0.51
2:F:329:ILE:C	2:F:330:TRP:HE3	2.14	0.51



Atom-1	Atom-2	Interatomic	Clash overlap (Å)
1.A.150.ARC.HH21	$3 \cdot C \cdot 91 \cdot V\Delta L \cdot HC 21$	1 75	$\frac{0.51}{0.51}$
1.R.91.ARC.HD2	2.F.82.GLU.OE1	2 11	0.51
2·F·347·LEU·CD2	$2 \cdot F \cdot 347 \cdot L E I \cdot N$	2.11	0.51
1.A.108.ASP.OD1	1.A.109.LEU.HD12	2.14	0.51
1.A.159.ILE.HG22	1.A.188.LEU.HD12	1.92	0.51
1.B.32.VAL.O	$1 \cdot \text{R} \cdot 191 \cdot \text{LEU} \cdot \text{HD} 12$	2.11	0.51
1.A.91.ARG.HH12	3·G·86·ARG·CB	2.11	0.51
1.A.122.MET.HE3	1·A·131·ARG·HD3	1 90	0.51
1:A:131:ABG:CZ	1:A:131:ABG:CB	2.89	0.51
1:A:165:PHE:CD1	1:A:165:PHE:N	2.79	0.51
1:B:117:ARG:O	1:B:121:LEU:N	2.35	0.51
1:B:90:PHE:HA	2:F:84:GLU:OE1	2.10	0.50
3:G:269:GLY:O	3:G:273:LEU:HD23	2.10	0.50
3:G:323:ASP:OD2	3:G:324:GLN:NE2	2.45	0.50
1:A:42:LYS:CB	1:A:42:LYS:NZ	2.74	0.50
1:A:72:LEU:O	1:A:76:ALA:N	2.38	0.50
1:B:85:GLN:HB3	1:B:163:GLU:HB2	1.93	0.50
1:A:119:LYS:HZ3	1:A:122:MET:CE	2.20	0.50
2:F:311:LEU:O	2:F:315:SER:N	2.41	0.50
1:B:122:MET:CE	1:B:127:ILE:O	2.60	0.50
3:G:60:VAL:HG13	3:G:61:PRO:CD	2.40	0.50
2:F:72:LEU:HB3	2:F:283:VAL:HG21	1.94	0.50
1:A:91:ARG:NH1	3:G:86:ARG:CB	2.70	0.50
2:F:19:LEU:HD12	2:F:19:LEU:O	2.11	0.50
3:G:82:MET:HG3	3:G:86:ARG:CZ	2.41	0.50
3:G:356:MET:HE1	3:G:357:MET:HB3	1.92	0.50
1:B:88:SER:HB2	2:F:87:VAL:HG11	1.93	0.50
3:G:291:MET:O	3:G:291:MET:SD	2.70	0.50
1:A:122:MET:CE	1:A:131:ARG:HD2	2.41	0.49
2:F:2:ILE:CG2	2:F:3:ILE:N	2.74	0.49
2:F:26:PHE:CD2	2:F:59:MET:HG2	2.47	0.49
2:F:279:MET:HE3	2:F:282:MET:HB3	1.93	0.49
2:F:282:MET:HE2	2:F:342:ALA:CA	2.42	0.49
3:G:77:LEU:HD21	3:G:295:PHE:CD2	2.47	0.49
1:A:118:ALA:O	1:A:122:MET:CG	2.61	0.49
1:B:65:GLU:OE1	1:B:67:ILE:HG23	2.12	0.49
3:G:291:MET:HE2	3:G:352:SER:OG	2.10	0.49
4:F:401:JSG:OAS	3:G:37:ASP:OD2	2.29	0.49
3:G:107:MET:HE1	3:G:290:LEU:CD2	2.33	0.49
3:G:49:ALA:HB1	3:G:135:TYR:OH	2.12	0.49
3:G:73:LEU:HD12	3:G:288:MET:SD	2.52	0.49



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:89:ILE:HG21	1:A:143:ARG:CG	2.39	0.49
1:B:11:LYS:HA	1:B:56:ASP:HB3	1.95	0.49
1:B:31:ILE:HG12	1:B:190:VAL:HB	1.94	0.49
1:A:109:LEU:O	1:A:114:ARG:NH2	2.46	0.49
3:G:88:GLU:CG	3:G:92:MET:HE1	2.41	0.49
1:A:106:ARG:NH1	1:A:154:ALA:O	2.45	0.49
1:A:35:LEU:O	1:A:42:LYS:HD3	2.13	0.49
1:A:119:LYS:CE	1:A:122:MET:HE2	2.42	0.49
1:B:18:VAL:HG11	1:B:44:THR:HG21	1.95	0.49
2:F:68:LEU:CD1	2:F:105:LEU:HD12	2.42	0.49
2:F:99:ILE:O	2:F:103:MET:HG2	2.11	0.49
2:F:282:MET:HE2	2:F:342:ALA:HA	1.95	0.49
3:G:77:LEU:HD21	3:G:295:PHE:HD2	1.77	0.49
1:A:35:LEU:O	1:A:209:ILE:HA	2.12	0.48
3:G:315:PHE:CG	3:G:318:ILE:HD12	2.48	0.48
1:B:23:SER:O	1:B:208:TYR:CZ	2.65	0.48
1:A:49:VAL:O	1:A:75:ARG:NH1	2.36	0.48
2:F:99:ILE:HD11	2:F:346:ASN:ND2	2.29	0.48
1:A:85:GLN:O	1:A:144:ARG:NH2	2.42	0.48
1:B:36:GLY:O	1:B:42:LYS:NZ	2.45	0.48
3:G:88:GLU:O	3:G:91:VAL:HG12	2.13	0.48
3:G:8:ASP:OD1	3:G:8:ASP:O	2.32	0.48
1:B:100:MET:CE	1:B:114:ARG:O	2.61	0.48
1:B:150:ARG:HH21	2:F:87:VAL:HG21	1.78	0.48
2:F:31:LEU:HB3	3:G:325:ILE:CD1	2.43	0.48
4:F:401:JSG:CEQ	3:G:313:ILE:HD12	2.43	0.48
3:G:291:MET:HE3	3:G:352:SER:CB	2.32	0.48
2:F:73:LEU:HD11	2:F:302:ALA:HB3	1.96	0.48
2:F:282:MET:CE	2:F:342:ALA:CA	2.92	0.48
1:B:118:ALA:O	1:B:122:MET:HB2	2.14	0.48
1:A:17:ARG:NH1	1:A:17:ARG:CB	2.74	0.47
1:A:150:ARG:HE	3:G:91:VAL:HG21	1.79	0.47
1:B:9:LEU:HD23	1:B:10:ALA:N	2.29	0.47
1:B:182:HIS:O	1:B:186:SER:N	2.48	0.47
1:B:3:THR:C	1:B:158:PHE:CZ	2.88	0.47
2:F:76:LEU:HG	2:F:85:ILE:HD11	1.96	0.47
3:G:268:PRO:O	3:G:272:GLN:HB3	2.14	0.47
1:B:3:THR:N	1:B:158:PHE:HZ	2.12	0.47
1:B:194:ASP:OD1	1:B:195:HIS:N	2.47	0.47
3:G:271:TYR:CD1	3:G:271:TYR:N	2.83	0.47
1:A:72:LEU:HD23	1:A:72:LEU:O	2.15	0.47



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Atom-1	Atom-2	Interatomic	Clash
110111-1	1100111-2	distance (Å)	overlap (Å)
1:A:155:ASN:OD1	1:A:155:ASN:O	2.31	0.47
1:B:174:ILE:CG2	1:B:178:ARG:NH2	2.78	0.47
1:B:212:GLN:O	1:B:212:GLN:CG	2.63	0.47
1:A:3:THR:HG22	1:A:4:LEU:N	2.27	0.47
1:A:89:ILE:CG2	1:A:143:ARG:CG	2.92	0.47
1:A:106:ARG:NE	1:A:155:ASN:HB3	2.30	0.47
1:B:65:GLU:OE2	1:B:67:ILE:HG23	2.15	0.47
1:B:201:LEU:HD12	1:B:221:PRO:HG3	1.97	0.47
4:F:401:JSG:CDW	3:G:70:MET:SD	3.02	0.47
3:G:276:TRP:HA	3:G:279:ILE:CD1	2.45	0.47
1:B:121:LEU:HD11	1:B:152:LEU:HD23	1.96	0.47
1:B:209:ILE:HB	1:B:217:ALA:HB3	1.96	0.47
2:F:62:LEU:HD12	2:F:62:LEU:N	2.29	0.47
1:A:32:VAL:HA	1:A:206:ARG:O	2.15	0.47
1:A:65:GLU:N	1:A:65:GLU:OE1	2.46	0.47
2:F:60:ALA:HA	2:F:63:ILE:HG12	1.97	0.47
1:B:20:GLU:HG2	1:B:21:ASP:H	1.80	0.47
1:A:42:LYS:HB3	1:A:42:LYS:NZ	2.30	0.46
2:F:285:PRO:CG	2:F:345:LEU:HD12	2.44	0.46
3:G:291:MET:HE3	3:G:352:SER:CA	2.45	0.46
2:F:278:ILE:HG12	2:F:339:PHE:HD2	1.80	0.46
3:G:356:MET:C	3:G:356:MET:CE	2.83	0.46
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.78	0.46
2:F:7:LEU:CG	2:F:101:ALA:HB1	2.45	0.46
2:F:99:ILE:HG12	2:F:284:VAL:HG21	1.98	0.46
3:G:113:LEU:HD23	3:G:289:MET:CE	2.45	0.46
3:G:352:SER:O	3:G:356:MET:HG3	2.15	0.46
1:B:102:VAL:CG1	1:B:102:VAL:O	2.63	0.46
2:F:2:ILE:HG21	2:F:4:ILE:CD1	2.32	0.46
2:F:285:PRO:HG2	2:F:345:LEU:HD12	1.97	0.46
3:G:46:SER:O	3:G:50:LEU:HG	2.16	0.46
2:F:281:LEU:HD23	2:F:281:LEU:C	2.34	0.46
3:G:288:MET:HE3	3:G:319:PHE:CD2	2.51	0.46
3:G:356:MET:HE2	3:G:357:MET:CB	2.45	0.46
1:B:43:THR:O	1:B:43:THR:HG22	2.16	0.46
1:B:90:PHE:CE1	1:B:150:ARG:HD2	2.51	0.46
1:B:229:GLN:OE1	1:B:232:ARG:CZ	2.63	0.46
1:B:231:LYS:O	1:B:236:GLY:N	2.46	0.46
1:A:75:ARG:HG2	1:A:80:ILE:HG13	1.98	0.46
1:B:34:LEU:N	1:B:192:ILE:O	2.44	0.46
2:F:279:MET:HA	2:F:282:MET:HB3	1.97	0.46



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:G:82:MET:CG	3:G:86:ARG:NH2	2.75	0.46	
1:A:6:ALA:HB1	1:A:9:LEU:HD23	1.98	0.46	
1:A:9:LEU:HA	1:A:58:GLY:HA3	1.98	0.46	
1:B:90:PHE:CE2	2:F:3:ILE:CD1	2.97	0.46	
1:B:221:PRO:HA	1:B:224:ILE:HD12	1.98	0.46	
3:G:294:SER:OG	3:G:356:MET:HB3	2.16	0.46	
2:F:309:PHE:HB2	2:F:338:TYR:CE2	2.50	0.45	
3:G:26:LEU:HB3	3:G:67:PHE:CD1	2.50	0.45	
1:B:31:ILE:HG23	1:B:190:VAL:HG11	1.95	0.45	
2:F:105:LEU:HD12	2:F:105:LEU:C	2.36	0.45	
1:B:106:ARG:NH1	1:B:155:ASN:HB2	2.31	0.45	
2:F:27:PHE:HD1	2:F:52:LEU:HD21	1.80	0.45	
3:G:12:GLY:O	3:G:16:PHE:HB3	2.17	0.45	
3:G:72:ALA:CB	3:G:285:VAL:HG23	2.47	0.45	
1:A:46:PHE:CE1	1:A:160:LEU:HB3	2.49	0.45	
1:A:91:ARG:HH22	3:G:86:ARG:CB	2.29	0.45	
3:G:7:LEU:HD21	3:G:92:MET:SD	2.56	0.45	
1:B:140:GLY:HA2	1:B:143:ARG:HB2	1.98	0.45	
2:F:84:GLU:O	2:F:87:VAL:HG12	2.17	0.45	
1:A:93:LEU:CD1	1:A:97:ASP:HB2	2.47	0.45	
2:F:29:GLN:HG2	4:F:401:JSG:CGE	2.46	0.45	
3:G:314:SER:O	3:G:318:ILE:N	2.41	0.45	
1:A:72:LEU:HD23	1:A:76:ALA:HB2	1.99	0.45	
1:A:170:PRO:HD2	1:B:234:TYR:CE1	2.51	0.45	
1:B:32:VAL:HG13	1:B:32:VAL:O	2.17	0.45	
2:F:271:THR:OG1	2:F:335:ASN:ND2	2.50	0.45	
1:B:83:LEU:HD13	1:B:148:ILE:HG12	1.99	0.45	
1:B:86:GLU:OE1	1:B:86:GLU:CA	2.50	0.45	
1:B:100:MET:O	1:B:104:GLN:N	2.45	0.45	
2:F:82:GLU:CG	2:F:82:GLU:O	2.65	0.45	
1:A:26:VAL:HB	1:A:32:VAL:HG11	1.98	0.45	
1:A:122:MET:HE1	1:A:131:ARG:HD3	1.97	0.45	
2:F:303:MET:HE3	4:F:401:JSG:CFX	2.46	0.45	
1:A:35:LEU:HD21	1:A:200:THR:HG21	2.00	0.44	
1:A:157:LYS:O	1:A:158:PHE:CD1	2.67	0.44	
1:A:161:LEU:HG	1:A:180:ILE:HD11	1.99	0.44	
1:A:34:LEU:O	1:A:42:LYS:HD2	2.17	0.44	
1:B:32:VAL:O	1:B:191:LEU:HA	2.17	0.44	
1:A:148:ILE:HG13	1:A:179:ILE:HG21	1.97	0.44	
4:F:401:JSG:CEL	3:G:67:PHE:HZ	2.30	0.44	
3:G:98:THR:HG22	3:G:100:LEU:H	1.82	0.44	



	to us page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:32:VAL:HG11	1:B:191:LEU:HD13	1.97	0.44	
1:B:90:PHE:HA	2:F:84:GLU:CD	2.38	0.44	
1:B:113:GLN:HA	1:B:116:ASP:HB2	2.00	0.44	
3:G:107:MET:HE1	3:G:290:LEU:CG	2.47	0.44	
3:G:88:GLU:HG3	3:G:92:MET:HE1	1.99	0.44	
1:A:93:LEU:HD11	1:A:97:ASP:HB2	1.98	0.44	
1:A:150:ARG:HE	3:G:91:VAL:CG2	2.31	0.44	
1:B:23:SER:H	1:B:215:LEU:HD13	1.83	0.44	
3:G:70:MET:HG2	3:G:316:GLY:O	2.17	0.44	
1:A:35:LEU:HA	1:A:42:LYS:HD2	1.99	0.44	
1:B:200:THR:CG2	1:B:201:LEU:N	2.81	0.44	
2:F:23:LEU:HD23	2:F:23:LEU:HA	1.86	0.44	
2:F:285:PRO:HG2	2:F:345:LEU:HD11	1.99	0.44	
1:A:76:ALA:HA	1:A:80:ILE:HB	2.00	0.44	
1:A:227:ASP:OD2	1:A:229:GLN:HB2	2.17	0.44	
1:B:7:LYS:NZ	1:B:59:ASN:O	2.50	0.44	
1:B:125:PHE:HZ	1:B:152:LEU:CD2	2.30	0.44	
3:G:109:THR:C	3:G:112:PRO:HD2	2.38	0.44	
3:G:291:MET:CE	3:G:291:MET:CA	2.77	0.44	
1:A:100:MET:HA	1:A:103:LEU:HD13	1.95	0.43	
1:B:55:ARG:HD2	1:B:55:ARG:O	2.17	0.43	
1:B:83:LEU:HD22	1:B:161:LEU:HD22	2.00	0.43	
2:F:281:LEU:CD2	2:F:281:LEU:C	2.87	0.43	
3:G:113:LEU:CD2	3:G:289:MET:HE3	2.48	0.43	
1:A:91:ARG:CZ	3:G:86:ARG:HD2	2.48	0.43	
1:A:108:ASP:OD1	1:A:108:ASP:N	2.50	0.43	
1:B:93:LEU:CG	2:F:6:TYR:CG	3.01	0.43	
2:F:49:LEU:HD12	2:F:49:LEU:C	2.39	0.43	
3:G:12:GLY:O	3:G:16:PHE:N	2.35	0.43	
3:G:77:LEU:HD12	3:G:77:LEU:HA	1.72	0.43	
3:G:271:TYR:H	3:G:271:TYR:HD1	1.65	0.43	
1:A:35:LEU:C	1:A:209:ILE:HG23	2.38	0.43	
1:A:131:ARG:HB3	1:A:131:ARG:HH11	1.81	0.43	
1:A:147:GLU:HG2	1:A:150:ARG:HH22	1.84	0.43	
1:B:174:ILE:HG21	1:B:178:ARG:NH2	2.34	0.43	
1:B:177:LYS:HB3	1:B:177:LYS:HE3	1.77	0.43	
3:G:279:ILE:HG13	3:G:279:ILE:H	1.63	0.43	
2:F:11:THR:O	2:F:15:GLN:N	2.35	0.43	
3:G:293:LEU:HA	3:G:296:ILE:HG22	2.00	0.43	
1:A:184:ARG:CZ	1:A:184:ARG:HB3	2.48	0.43	
1:A:230:VAL:HG13	1:A:234:TYR:HB3	1.99	0.43	



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	Clash			
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:151:ALA:O	1:B:156:PRO:HG3	2.17	0.43	
1:B:197:VAL:O	1:B:201:LEU:HD23	2.19	0.43	
1:A:119:LYS:HZ1	1:A:131:ARG:CD	2.31	0.43	
1:A:171:ILE:O	1:A:171:ILE:HD12	2.18	0.43	
2:F:26:PHE:CD2	4:F:401:JSG:CGR	3.02	0.43	
3:G:81:GLY:O	3:G:308:ARG:NH2	2.52	0.43	
1:A:7:LYS:N	1:A:59:ASN:O	2.51	0.43	
1:A:148:ILE:HD11	1:A:161:LEU:HD11	2.01	0.43	
1:B:80:ILE:HD12	1:B:160:LEU:HD11	2.01	0.43	
2:F:68:LEU:HD11	2:F:105:LEU:CD1	2.49	0.43	
2:F:278:ILE:HG12	2:F:339:PHE:CD2	2.53	0.43	
1:A:80:ILE:HD13	1:A:80:ILE:HA	1.88	0.43	
1:B:162:ASP:HA	1:B:193:THR:HG22	1.99	0.43	
2:F:87:VAL:HA	2:F:90:ALA:HB3	2.01	0.43	
1:B:13:TYR:CD1	1:B:14:LYS:N	2.85	0.43	
1:B:67:ILE:HD12	1:B:75:ARG:HD2	2.00	0.43	
2:F:82:GLU:O	2:F:82:GLU:HG2	2.19	0.43	
1:A:220:THR:O	1:A:224:ILE:HG12	2.19	0.43	
1:B:122:MET:CE	1:B:128:GLU:HA	2.48	0.43	
2:F:32:VAL:CG1	3:G:324:GLN:CB	2.96	0.43	
1:B:150:ARG:HH21	2:F:87:VAL:CG2	2.32	0.42	
1:B:159:ILE:CD1	1:B:183:LEU:HD13	2.49	0.42	
1:B:212:GLN:O	1:B:212:GLN:HG3	2.18	0.42	
2:F:121:GLY:O	2:F:124:SER:OG	2.32	0.42	
2:F:265:GLU:O	2:F:269:ARG:N	2.45	0.42	
2:F:303:MET:HE1	4:F:401:JSG:CFX	2.49	0.42	
1:A:31:ILE:HG23	1:A:190:VAL:HB	2.01	0.42	
1:B:47:TYR:CD1	1:B:47:TYR:N	2.87	0.42	
1:A:50:VAL:HG22	1:A:160:LEU:HD13	2.00	0.42	
1:B:34:LEU:CD1	1:B:46:PHE:HB2	2.44	0.42	
1:B:48:MET:CE	1:B:54:PRO:O	2.67	0.42	
1:B:116:ASP:O	1:B:120:GLU:HG2	2.19	0.42	
1:A:109:LEU:HD12	1:A:109:LEU:N	2.34	0.42	
2:F:265:GLU:HB2	2:F:269:ARG:HH12	1.83	0.42	
3:G:97:PHE:HE1	3:G:101:GLN:C	2.22	0.42	
1:A:148:ILE:HG13	1:A:179:ILE:CG2	2.49	0.42	
1:B:159:ILE:HD12	1:B:183:LEU:HD13	2.00	0.42	
2:F:114:ALA:O	2:F:118:MET:N	2.29	0.42	
3:G:64:ILE:O	3:G:281:GLN:NE2	2.52	0.42	
3:G:80:LEU:HD22	3:G:106:VAL:HG21	2.00	0.42	
3:G:317:PHE:O	3:G:321:VAL:HG12	2.19	0.42	



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Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:36:GLY:C	1:A:234:TYR:OH	2.58	0.42	
1:A:89:ILE:CG1	1:A:91:ARG:HD3	2.49	0.42	
1:B:13:TYR:HB3	1:B:16:ARG:HH21	1.84	0.42	
1:B:74:ALA:O	1:B:78:ARG:HG3	2.20	0.42	
2:F:73:LEU:HD23	2:F:73:LEU:HA	1.85	0.42	
3:G:29:LEU:HD22	3:G:29:LEU:HA	1.75	0.42	
3:G:340:GLY:O	3:G:343:LEU:HG	2.19	0.42	
3:G:344:PRO:HA	3:G:347:SER:HB2	2.01	0.42	
1:A:83:LEU:HD22	1:A:83:LEU:HA	1.68	0.42	
1:B:127:ILE:HG22	1:B:130:LEU:HB2	2.01	0.42	
2:F:13:LYS:HA	2:F:13:LYS:HE2	2.02	0.42	
2:F:27:PHE:CD1	2:F:52:LEU:HD21	2.53	0.42	
3:G:309:VAL:O	3:G:313:ILE:N	2.47	0.42	
1:B:62:ILE:HG12	1:B:67:ILE:HD13	2.02	0.42	
1:B:70:LEU:HD23	1:B:74:ALA:CB	2.48	0.42	
1:B:90:PHE:CD2	2:F:84:GLU:OE2	2.73	0.42	
2:F:62:LEU:N	2:F:62:LEU:CD1	2.83	0.42	
1:A:72:LEU:CD2	1:A:72:LEU:C	2.88	0.42	
1:B:95:VAL:HA	1:B:98:ASN:OD1	2.20	0.42	
2:F:66:LEU:HD22	4:F:401:JSG:CFU	2.49	0.42	
2:F:284:VAL:CG2	2:F:285:PRO:HD3	2.48	0.42	
3:G:15:ILE:HD11	3:G:80:LEU:HD13	2.01	0.42	
3:G:23:LEU:O	3:G:27:VAL:HG23	2.20	0.42	
3:G:310:VAL:O	3:G:314:SER:N	2.53	0.42	
1:B:13:TYR:CD1	1:B:13:TYR:C	2.94	0.41	
1:B:34:LEU:HD23	1:B:34:LEU:HA	1.90	0.41	
1:B:46:PHE:CD2	1:B:47:TYR:CD1	3.02	0.41	
2:F:347:LEU:N	2:F:347:LEU:HD22	2.34	0.41	
3:G:63:ASP:OD1	3:G:63:ASP:N	2.51	0.41	
1:A:72:LEU:HD21	3:G:94:ALA:CA	2.41	0.41	
1:A:148:ILE:HD13	1:A:148:ILE:HA	1.78	0.41	
1:B:169:ASP:O	1:B:172:SER:N	2.53	0.41	
1:B:111:SER:HA	1:B:114:ARG:HB3	2.01	0.41	
1:B:229:GLN:OE1	1:B:232:ARG:NH2	2.53	0.41	
1:A:144:ARG:NH1	1:A:147:GLU:OE1	2.53	0.41	
1:B:9:LEU:HD11	1:B:48:MET:HB3	2.02	0.41	
1:B:147:GLU:HA	1:B:150:ARG:HH12	1.84	0.41	
2:F:68:LEU:HD12	2:F:105:LEU:HD12	2.03	0.41	
1:B:55:ARG:HH11	1:B:57:ALA:HA	1.86	0.41	
2:F:23:LEU:C	2:F:27:PHE:HD2	2.23	0.41	
1:A:17:ARG:CB	1:A:17:ARG:CZ	2.99	0.41	



	to ao pageini	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:91:ARG:NH2	3:G:86:ARG:HG2	2.35	0.41	
1:A:119:LYS:CD	1:A:122:MET:HE2	2.51	0.41	
1:B:6:ALA:HB3	1:B:24:LEU:HG	2.03	0.41	
1:B:46:PHE:CE1	1:B:160:LEU:HB3	2.55	0.41	
3:G:113:LEU:HA	3:G:113:LEU:HD12	1.85	0.41	
1:A:26:VAL:HG22	1:A:158:PHE:CE2	2.55	0.41	
1:A:62:ILE:HG12	1:A:67:ILE:HD13	2.01	0.41	
3:G:34:LYS:HG3	3:G:58:LEU:HD11	2.03	0.41	
1:A:34:LEU:HA	1:A:34:LEU:HD12	1.83	0.41	
1:A:82:TYR:HB3	3:G:94:ALA:HB1	2.02	0.41	
1:A:99:LEU:HD21	1:A:149:ALA:CB	2.51	0.41	
1:A:122:MET:HB3	1:A:128:GLU:HA	2.02	0.41	
1:B:34:LEU:O	1:B:42:LYS:CD	2.69	0.41	
2:F:31:LEU:HB3	3:G:325:ILE:HD13	2.02	0.41	
1:A:19:VAL:HG11	1:A:48:MET:HE1	2.02	0.41	
1:A:55:ARG:HD2	1:A:56:ASP:N	2.36	0.41	
1:B:50:VAL:O	1:B:75:ARG:HG2	2.21	0.41	
1:B:196:ASN:OD1	1:B:199:GLU:HB2	2.19	0.41	
1:B:199:GLU:OE1	1:B:199:GLU:HA	2.21	0.41	
4:F:401:JSG:CEQ	3:G:313:ILE:CD1	2.99	0.41	
3:G:63:ASP:O	3:G:68:PHE:CA	2.68	0.41	
3:G:135:TYR:CD2	3:G:135:TYR:O	2.73	0.41	
1:A:85:GLN:CB	1:A:162:ASP:OD2	2.62	0.41	
1:A:119:LYS:CE	1:A:122:MET:HE1	2.50	0.41	
1:B:148:ILE:HD12	1:B:179:ILE:HD12	2.03	0.41	
3:G:83:LEU:O	3:G:88:GLU:N	2.52	0.41	
1:B:65:GLU:CD	1:B:67:ILE:HG23	2.41	0.40	
1:B:220:THR:O	1:B:224:ILE:HG13	2.21	0.40	
1:B:226:GLU:H	1:B:226:GLU:HG3	1.71	0.40	
2:F:2:ILE:CG2	2:F:4:ILE:H	2.04	0.40	
3:G:61:PRO:HB3	3:G:129:GLU:HB2	2.03	0.40	
3:G:74:LEU:HD12	3:G:313:ILE:HD13	2.03	0.40	
1:A:55:ARG:HE	1:A:68:SER:HB2	1.86	0.40	
2:F:7:LEU:CG	2:F:101:ALA:CB	2.98	0.40	
2:F:120:ALA:HA	2:F:123:TRP:HB3	2.03	0.40	
3:G:270:ARG:N	3:G:270:ARG:HD2	2.36	0.40	
2:F:62:LEU:O	2:F:66:LEU:HB3	2.21	0.40	
3:G:60:VAL:N	3:G:61:PRO:HD2	2.36	0.40	
1:A:95:VAL:HB	1:A:130:LEU:O	2.21	0.40	
1:A:119:LYS:HZ1	1:A:122:MET:HE1	1.84	0.40	
1:B:161:LEU:HD12	1:B:180:ILE:CD1	2.44	0.40	



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:B:169:ASP:OD2	1:B:171:ILE:CG2	2.58	0.40	
3:G:121:GLY:HA2	3:G:125:ALA:HB3	2.02	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	Perce	ntiles
1	А	233/241~(97%)	216~(93%)	17~(7%)	0	100	100
1	В	235/241~(98%)	211 (90%)	24 (10%)	0	100	100
2	F	215/365~(59%)	204~(95%)	11 (5%)	0	100	100
3	G	221/360~(61%)	208 (94%)	12~(5%)	1 (0%)	29	66
All	All	904/1207~(75%)	839 (93%)	64 (7%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	45	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	196/202~(97%)	186~(95%)	10~(5%)	24 53	



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	196/202~(97%)	184 (94%)	12~(6%)	18 48
2	F	183/301~(61%)	172 (94%)	11 (6%)	19 49
3	G	185/300~(62%)	153~(83%)	32~(17%)	2 13
All	All	760/1005~(76%)	695~(91%)	65~(9%)	14 38

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All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	16	ARG
1	А	28	SER
1	А	47	TYR
1	А	48	MET
1	А	83	LEU
1	А	115	GLU
1	А	130	LEU
1	А	165	PHE
1	А	196	ASN
1	А	234	TYR
1	В	7	LYS
1	В	13	TYR
1	В	45	THR
1	В	62	ILE
1	В	85	GLN
1	В	89	ILE
1	В	110	THR
1	В	143	ARG
1	В	208	TYR
1	В	226	GLU
1	В	229	GLN
1	В	234	TYR
2	F	33	ARG
2	F	50	SER
2	F	66	LEU
2	F	123	TRP
2	F	127	HIS
2	F	131	VAL
2	F	270	PHE
2	F	310	PHE
2	F	315	SER
2	F	317	LYS
2	F	332	TRP



Mol	Chain	Res	Type
3	G	9	ARG
3	G	15	ILE
3	G	17	ASN
3	G	19	ILE
3	G	21	MET
3	G	22	THR
3	G	25	MET
3	G	29	LEU
3	G	30	SER
3	G	34	LYS
3	G	37	ASP
3	G	41	LYS
3	G	44	GLN
3	G	47	TYR
3	G	48	ASP
3	G	54	LEU
3	G	56	THR
3	G	57	ILE
3	G	58	LEU
3	G	66	ILE
3	G	67	PHE
3	G	122	GLU
3	G	273	LEU
3	G	280	PHE
3	G	283	LEU
3	G	288	MET
3	G	291	MET
3	G	294	SER
3	G	322	LEU
3	G	338	ILE
3	G	349	PHE
3	G	356	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	73	HIS
1	В	104	GLN
2	F	128	GLN
2	F	335	ASN
2	F	346	ASN
3	G	272	GLN



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Mol	Chain	\mathbf{Res}	Type
3	G	281	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)

1 ligand is 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).

Mal	Type	Chain	Dog	Link	Bon	nd lengtl	ns	Bo	nd angle	es
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	JSG	F	401	-	203,206,206	0.97	10 (4%)	257,278,278	1.48	35 (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	JSG	F	401	-	-	62/195/333/333	1/7/7/7

All (10) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	F	401	JSG	O1-C1	3.81	1.46	1.40
4	F	401	JSG	CBG-CBE	3.69	1.59	1.52
4	F	401	JSG	OBH-CBA	3.55	1.47	1.42
4	F	401	JSG	OBH-CBG	2.91	1.48	1.44
4	F	401	JSG	ODA-CDB	2.89	1.45	1.40
4	F	401	JSG	C1-C2	2.47	1.57	1.53
4	F	401	JSG	PHO-OHR	-2.03	1.47	1.54
4	F	401	JSG	PHG-OHJ	-2.02	1.47	1.54
4	F	401	JSG	PHK-OHM	-2.01	1.47	1.54
4	F	401	JSG	OBF-CCB	2.01	1.47	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	F	401	JSG	O5-C5-C6	6.33	119.44	106.67
4	F	401	JSG	O3-C3-C2	5.16	117.55	107.91
4	F	401	JSG	C3-O3-CFK	4.68	125.31	117.53
4	F	401	JSG	CAP-OAQ-CEE	-4.64	109.80	117.53
4	F	401	JSG	CBB-CBC-CBE	-4.34	103.49	111.06
4	F	401	JSG	OFJ-CEW-C8	4.16	114.83	106.65
4	F	401	JSG	OFZ-CFM-CFL	4.14	114.79	106.65
4	F	401	JSG	CAV-CAT-CAR	-4.01	103.71	112.09
4	F	401	JSG	CAV-O1-C1	3.48	120.54	113.74
4	F	401	JSG	CAN-NAO-CDO	-3.43	117.84	122.90
4	F	401	JSG	O6-CBA-OBH	-3.04	101.62	110.07
4	F	401	JSG	C4-C3-C2	-2.85	105.27	110.57
4	F	401	JSG	C1-C2-C3	-2.83	104.68	109.88
4	F	401	JSG	OAQ-CEE-CEF	2.68	116.38	111.46
4	F	401	JSG	C3-C2-N2	2.64	115.30	110.91
4	F	401	JSG	C1-O5-C5	2.62	118.82	113.69
4	F	401	JSG	CBQ-CBR-CBT	-2.61	108.28	110.84
4	F	401	JSG	OBF-CBE-CBG	2.60	114.09	107.48
4	F	401	JSG	C2-N2-C7	-2.57	119.11	122.90
4	F	401	JSG	CCO-OCJ-CCD	-2.57	111.59	117.96
4	F	401	JSG	CBA-OBH-CBG	2.55	120.14	114.20
4	F	401	JSG	ODL-CDF-CDE	2.46	111.33	107.87
4	F	401	JSG	CEW-OFJ-CGB	2.46	123.85	117.79
4	F	401	JSG	CDB-ODL-CDF	2.42	116.96	113.06
4	F	401	JSG	O6-C6-C5	2.29	112.73	107.68
4	F	401	JSG	OCK-PHO-OHQ	-2.19	100.95	109.39
4	F	401	JSG	CCT-CCS-CCR	-2.19	110.34	114.18
4	F	401	JSG	OHN-PHK-OHM	2.18	115.96	107.64
4	F	401	JSG	CBI-CBG-CBE	2.14	117.92	114.18



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	F	401	JSG	OES-CEE-CEF	-2.10	120.09	124.73
4	F	401	JSG	CCU-ODA-CDB	-2.08	109.68	113.74
4	F	401	JSG	OAU-CAL-CAN	-2.07	106.54	110.58
4	F	401	JSG	OBD-CBC-CBE	2.02	115.44	108.73
4	F	401	JSG	CDG-CDF-CDE	-2.02	110.68	114.03
4	F	401	JSG	OAZ-CAX-CBA	-2.00	117.25	123.70

There are no chirality outliers.

\mathbf{Mol}	Chain	\mathbf{Res}	Type	Atoms
4	F	401	JSG	C2-C1-O1-CAV
4	F	401	JSG	O5-C1-O1-CAV
4	F	401	JSG	OAY-CAX-CBA-O6
4	F	401	JSG	CAX-CBA-O6-C6
4	F	401	JSG	CBB-CBA-O6-C6
4	F	401	JSG	OBH-CBA-O6-C6
4	F	401	JSG	OBN-CBM-CBP-OBD
4	F	401	JSG	OBW-CBP-OBD-CBC
4	F	401	JSG	CCF-CCE-OCK-PHO
4	F	401	JSG	CCE-CCF-CCG-CCH
4	F	401	JSG	CCR-CCS-CCT-CCU
4	F	401	JSG	CCR-CCS-CCT-OCZ
4	F	401	JSG	OCY-CCS-CCT-CCU
4	F	401	JSG	OCY-CCS-CCT-OCZ
4	F	401	JSG	CCS-CCT-CCU-ODA
4	F	401	JSG	OCZ-CCT-CCU-ODA
4	F	401	JSG	ODL-CDB-ODA-CCU
4	F	401	JSG	C8-CEW-OFJ-CGB
4	F	401	JSG	OFY-CFK-O3-C3
4	F	401	JSG	CFL-CFM-CFN-CFO
4	F	401	JSG	OFZ-CFM-CFN-CFO
4	F	401	JSG	CFN-CFM-OFZ-CGN
4	F	401	JSG	CCE-OCK-PHO-OHQ
4	F	401	JSG	OCL-CCB-OBF-CBE
4	F	401	JSG	OAU-CAT-CAV-O1
4	F	401	JSG	CFL-CFK-O3-C3
4	F	401	JSG	OGO-CGN-OFZ-CFM
4	F	401	JSG	CAR-CAT-CAV-O1
4	F	401	JSG	CGP-CGN-OFZ-CFM
4	F	401	JSG	C2-C3-O3-CFK
4	F	401	JSG	CDC-CDB-ODA-CCU

All (62) torsion outliers are listed below:



4 F 401 JSG CGN-CGP-CGQ-CGR 4 F 401 JSG CGV-CGW-CGX-CGY 4 F 401 JSG OBJ-CBI-CBK-OBL 4 F 401 JSG CGD-CGE-CGF-CGG 4 F 401 JSG CGD-CFP-CFQ-CFR 4 F 401 JSG CGP-CGS-CGT-CGU 4 F 401 JSG CGP-CFP-CFQ-CFR 4 F 401 JSG CGP-CGS-CGT-CGU 4 F 401 JSG CGP-CFR-CFS-CFT 4 F 401 JSG CGY-CGZ-CHA-CHB 4 F 401 JSG CGY-CGZ-CHA-CHB 4 F 401 JSG CGU-CGV-CGW-CGX 4 F 401 JSG CGU-CGV-CGW-CGX 4 F 401 JSG CDU-CDV-CDW-CDX 4 F 401 JSG CCGY-CGY-CGZ-CHA 4 F 401	Mol	Chain	\mathbf{Res}	Type	Atoms	
4 F 401 JSG CGV-CGW-CGX-CGY 4 F 401 JSG OBJ-CBI-CBK-OBL 4 F 401 JSG CGD-CGE-CGF-CGG 4 F 401 JSG CFO-CFP-CFQ-CFR 4 F 401 JSG CEH-CEI-CEJ-CEK 4 F 401 JSG CGR-CGS-CGT-CGU 4 F 401 JSG CGY-CGZ-CHA-CHB 4 F 401 JSG CFQ-CFR-CFS-CFT 4 F 401 JSG CGU-CGV-CGW-CGX 4 F 401 JSG CGU-COV-CDW-CDX 4 F 401 JSG CCGC-CEH-CEI-CEJ 4 F 401 JSG CCGX-CGY-CGZ-CHA 4 F 401 JSG CCGY-CCO-OCJ-CCD 4 F 401 JSG CCGY-CCO-OCJ-CCD 4 F 401 JSG CCP-CCO-OCJ-CCD 4 F 401 JSG CCP-CCO-OCJ-CCD 4 F 401 JSG </td <td>4</td> <td>F</td> <td>401</td> <td>JSG</td> <td>CGN-CGP-CGQ-CGR</td>	4	F	401	JSG	CGN-CGP-CGQ-CGR	
4 F 401 JSG OBJ-CBI-CBK-OBL 4 F 401 JSG CGD-CGE-CGF-CGG 4 F 401 JSG CFO-CFP-CFQ-CFR 4 F 401 JSG CEH-CEI-CEJ-CEK 4 F 401 JSG CGR-CGS-CGT-CGU 4 F 401 JSG CGY-CGZ-CHA-CHB 4 F 401 JSG CFQ-CFR-CFS-CFT 4 F 401 JSG CGY-CGZ-CHA-CHB 4 F 401 JSG CCGY-CGZ-CHA-CHB 4 F 401 JSG CCGY-CGZ-CHA-CHB 4 F 401 JSG CCGU-CGV-CGW-CGX 4 F 401 JSG CDU-CDV-CDW-CDX 4 F 401 JSG CCGY-CGY-CGZ-CHA 4 F 401 JSG CCGY-CCO-OCJ-CCD 4 F 401 JSG CCDY-CCO-OCJ-CCD 4 F <t< td=""><td>4</td><td>F</td><td>401</td><td>JSG</td><td colspan="2">CGV-CGW-CGX-CGY</td></t<>	4	F	401	JSG	CGV-CGW-CGX-CGY	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	OBJ-CBI-CBK-OBL	
4 F 401 JSG CFO-CFP-CFQ-CFR 4 F 401 JSG CEH-CEI-CEJ-CEK 4 F 401 JSG CGR-CGS-CGT-CGU 4 F 401 JSG CGY-CGZ-CHA-CHB 4 F 401 JSG CFQ-CFR-CFS-CFT 4 F 401 JSG CGU-CGV-CGW-CGX 4 F 401 JSG CBH-CBG-CBI-CBK 4 F 401 JSG CDU-CDV-CDW-CDX 4 F 401 JSG CCGX-CGY-CGZ-CHA 4 F 401 JSG CCGX-CGY-CGZ-CHA 4 F 401 JSG CCGX-CGY-CGZ-CHA 4 F 401 JSG CCTO-CCO-OCJ-CCD 4 F 401 JSG CCP-CCO-OCJ-CCD 4 F 401 JSG CCD-CCP-CCQ-OCJ-CCD 4 F 401 JSG CCD-CCP-CCQ-OCJ-CCD 4 F	4	F	401	JSG	CGD-CGE-CGF-CGG	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CFO-CFP-CFQ-CFR	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CEH-CEI-CEJ-CEK	
4 F 401 JSG CGY-CGZ-CHA-CHB 4 F 401 JSG CFQ-CFR-CFS-CFT 4 F 401 JSG CS-C6-06-CBA 4 F 401 JSG CGU-CGV-CGW-CGX 4 F 401 JSG CBH-CBG-CBI-CBK 4 F 401 JSG CDU-CDV-CDW-CDX 4 F 401 JSG CCGX-CGY-CGZ-CHA 4 F 401 JSG CGX-CGY-CGZ-CHA 4 F 401 JSG CCGX-CGY-CGZ-CHA 4 F 401 JSG CCTD-CFE-CFF-CFG 4 F 401 JSG CCY-CCO-OCJ-CCD 4 F 401 JSG CCP-CCO-OCJ-CCD 4 F 401 JSG	4	F	401	JSG	CGR-CGS-CGT-CGU	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CGY-CGZ-CHA-CHB	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CFQ-CFR-CFS-CFT	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	C5-C6-O6-CBA	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CGU-CGV-CGW-CGX	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	OBH-CBG-CBI-CBK	
4 F 401 JSG C4-C3-O3-CFK 4 F 401 JSG CEG-CEH-CEI-CEJ 4 F 401 JSG CGX-CGY-CGZ-CHA 4 F 401 JSG CFD-CFE-CFF-CFG 4 F 401 JSG OCY-CCO-OCJ-CCD 4 F 401 JSG CDW-CDX-CDY-CDZ 4 F 401 JSG CCP-CCO-OCJ-CCD 4 F 401 JSG CCD-CEP-CEQ-CER 4 F 401 JSG CCE-CCF-CCG-OCM 4 F 401 JSG CEF-CEF-OAQ-CAP 4 F 401 JSG CEF-CEG-CEH-CEI 4 F 401 JSG CEF-CEG-CEH-CEI 4 F 401 JSG	4	F	401	JSG	CDU-CDV-CDW-CDX	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	C4-C3-O3-CFK	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CEG-CEH-CEI-CEJ	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CGX-CGY-CGZ-CHA	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CFD-CFE-CFF-CFG	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	OCY-CCO-OCJ-CCD	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CDW-CDX-CDY-CDZ	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CCP-CCO-OCJ-CCD	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CEO-CEP-CEQ-CER	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CCD-CCE-OCK-PHO	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CCE-CCF-CCG-OCM	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	F	401	JSG	CDE-CDF-CDG-ODM	
4F401JSGCEF-CEE-OAQ-CAP4F401JSGCEF-CEG-CEH-CEI4F401JSGCBE-CBG-CBI-CBK4F401JSGCDS-CDT-CDU-CDV4F401JSGCEX-CEW-OFJ-CGB4F401JSGOET-CEG-CEH-CEI	4	F	401	JSG	CFB-CFC-CFD-CFE	
4F401JSGCEF-CEG-CEH-CEI4F401JSGCBE-CBG-CBI-CBK4F401JSGCDS-CDT-CDU-CDV4F401JSGCEX-CEW-OFJ-CGB4F401JSGOET-CEG-CEH-CEI	4	F	401	JSG	CEF-CEE-OAQ-CAP	
4F401JSGCBE-CBG-CBI-CBK4F401JSGCDS-CDT-CDU-CDV4F401JSGCEX-CEW-OFJ-CGB4F401JSGOET-CEG-CEH-CEI	4	F	401	JSG	CEF-CEG-CEH-CEI	
4F401JSGCDS-CDT-CDU-CDV4F401JSGCEX-CEW-OFJ-CGB4F401JSGOET-CEG-CEH-CEI	4	F	401	JSG	CBE-CBG-CBI-CBK	
4F401JSGCEX-CEW-OFJ-CGB4F401JSGOET-CEG-CEH-CEI	4	F	401	JSG	CDS-CDT-CDU-CDV	
4 F 401 JSG OET-CEG-CEH-CEI	4	F	401	JSG	CEX-CEW-OFJ-CGB	
	4	F	401	JSG	OET-CEG-CEH-CEI	

Continued from previ	ious page
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All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	401	JSG	CDB-CDC-CDD-CDE-CDF-ODL

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	401	JSG	22	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 similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31088. 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



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 96

Y Index: 96



Z Index: 96

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

Largest variance slices (i) 6.3

6.3.1Primary map



X Index: 93

Y Index: 93

Z Index: 93

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

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

6.4.1**Primary map**



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.612. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_31088_msk_1.map (i)





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 31 nm^3 ; this corresponds to an approximate mass of 28 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)



*Reported resolution corresponds to spatial frequency of 0.260 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.260 \AA^{-1}



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	3.85	4.44	3.91
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31088 and PDB model 7EFO. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.612 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.612).



9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.612) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5190	0.3930
А	0.5360	0.4020
В	0.5540	0.4170
F	0.4930	0.3770
G	0.4910	0.3740

