



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:19 AM GMT

PDB ID : 3MV3  
Title : Crystal Structure of  $\alpha$ -COP in Complex with e-COP  
Authors : Hoelz, A.; Hsia, K.C.  
Deposited on : 2010-05-03  
Resolution : 3.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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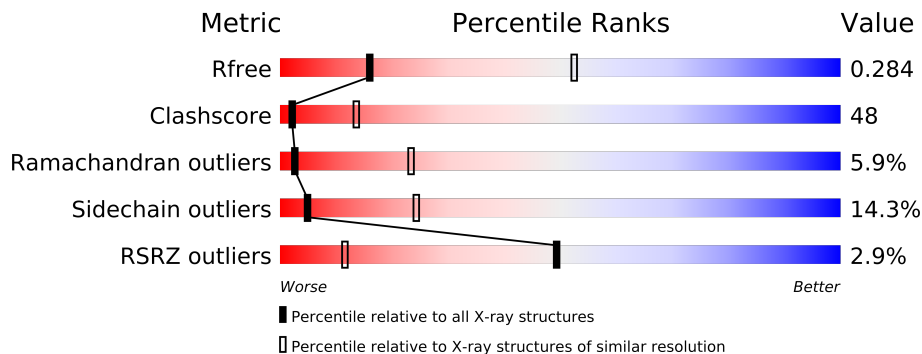
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.25 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	325	
1	C	325	
1	E	325	
2	B	310	
2	D	310	
2	F	310	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14256 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	C	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	E	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP P53622
A	-21	GLY	-	EXPRESSION TAG	UNP P53622
A	-20	SER	-	EXPRESSION TAG	UNP P53622
A	-19	SER	-	EXPRESSION TAG	UNP P53622
A	-18	HIS	-	EXPRESSION TAG	UNP P53622
A	-17	HIS	-	EXPRESSION TAG	UNP P53622
A	-16	HIS	-	EXPRESSION TAG	UNP P53622
A	-15	HIS	-	EXPRESSION TAG	UNP P53622
A	-14	HIS	-	EXPRESSION TAG	UNP P53622
A	-13	HIS	-	EXPRESSION TAG	UNP P53622
A	-12	SER	-	EXPRESSION TAG	UNP P53622
A	-11	SER	-	EXPRESSION TAG	UNP P53622
A	-10	GLY	-	EXPRESSION TAG	UNP P53622
A	-9	LEU	-	EXPRESSION TAG	UNP P53622
A	-8	GLU	-	EXPRESSION TAG	UNP P53622
A	-7	VAL	-	EXPRESSION TAG	UNP P53622
A	-6	LEU	-	EXPRESSION TAG	UNP P53622
A	-5	PHE	-	EXPRESSION TAG	UNP P53622
A	-4	GLN	-	EXPRESSION TAG	UNP P53622
A	-3	GLY	-	EXPRESSION TAG	UNP P53622
A	-2	PRO	-	EXPRESSION TAG	UNP P53622
A	-1	HIS	-	EXPRESSION TAG	UNP P53622
A	0	MSE	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MSE	-	EXPRESSION TAG	UNP P53622
C	-21	GLY	-	EXPRESSION TAG	UNP P53622
C	-20	SER	-	EXPRESSION TAG	UNP P53622
C	-19	SER	-	EXPRESSION TAG	UNP P53622
C	-18	HIS	-	EXPRESSION TAG	UNP P53622
C	-17	HIS	-	EXPRESSION TAG	UNP P53622
C	-16	HIS	-	EXPRESSION TAG	UNP P53622
C	-15	HIS	-	EXPRESSION TAG	UNP P53622
C	-14	HIS	-	EXPRESSION TAG	UNP P53622
C	-13	HIS	-	EXPRESSION TAG	UNP P53622
C	-12	SER	-	EXPRESSION TAG	UNP P53622
C	-11	SER	-	EXPRESSION TAG	UNP P53622
C	-10	GLY	-	EXPRESSION TAG	UNP P53622
C	-9	LEU	-	EXPRESSION TAG	UNP P53622
C	-8	GLU	-	EXPRESSION TAG	UNP P53622
C	-7	VAL	-	EXPRESSION TAG	UNP P53622
C	-6	LEU	-	EXPRESSION TAG	UNP P53622
C	-5	PHE	-	EXPRESSION TAG	UNP P53622
C	-4	GLN	-	EXPRESSION TAG	UNP P53622
C	-3	GLY	-	EXPRESSION TAG	UNP P53622
C	-2	PRO	-	EXPRESSION TAG	UNP P53622
C	-1	HIS	-	EXPRESSION TAG	UNP P53622
C	0	MSE	-	EXPRESSION TAG	UNP P53622
E	-22	MSE	-	EXPRESSION TAG	UNP P53622
E	-21	GLY	-	EXPRESSION TAG	UNP P53622
E	-20	SER	-	EXPRESSION TAG	UNP P53622
E	-19	SER	-	EXPRESSION TAG	UNP P53622
E	-18	HIS	-	EXPRESSION TAG	UNP P53622
E	-17	HIS	-	EXPRESSION TAG	UNP P53622
E	-16	HIS	-	EXPRESSION TAG	UNP P53622
E	-15	HIS	-	EXPRESSION TAG	UNP P53622
E	-14	HIS	-	EXPRESSION TAG	UNP P53622
E	-13	HIS	-	EXPRESSION TAG	UNP P53622
E	-12	SER	-	EXPRESSION TAG	UNP P53622
E	-11	SER	-	EXPRESSION TAG	UNP P53622
E	-10	GLY	-	EXPRESSION TAG	UNP P53622
E	-9	LEU	-	EXPRESSION TAG	UNP P53622
E	-8	GLU	-	EXPRESSION TAG	UNP P53622
E	-7	VAL	-	EXPRESSION TAG	UNP P53622
E	-6	LEU	-	EXPRESSION TAG	UNP P53622
E	-5	PHE	-	EXPRESSION TAG	UNP P53622
E	-4	GLN	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P53622
E	-2	PRO	-	EXPRESSION TAG	UNP P53622
E	-1	HIS	-	EXPRESSION TAG	UNP P53622
E	0	MSE	-	EXPRESSION TAG	UNP P53622

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			
2	D	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			
2	F	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MSE	-	EXPRESSION TAG	UNP P40509
B	-12	GLY	-	EXPRESSION TAG	UNP P40509
B	-11	SER	-	EXPRESSION TAG	UNP P40509
B	-10	SER	-	EXPRESSION TAG	UNP P40509
B	-9	HIS	-	EXPRESSION TAG	UNP P40509
B	-8	HIS	-	EXPRESSION TAG	UNP P40509
B	-7	HIS	-	EXPRESSION TAG	UNP P40509
B	-6	HIS	-	EXPRESSION TAG	UNP P40509
B	-5	HIS	-	EXPRESSION TAG	UNP P40509
B	-4	HIS	-	EXPRESSION TAG	UNP P40509
B	-3	SER	-	EXPRESSION TAG	UNP P40509
B	-2	GLN	-	EXPRESSION TAG	UNP P40509
B	-1	ASP	-	EXPRESSION TAG	UNP P40509
B	0	PRO	-	EXPRESSION TAG	UNP P40509
D	-13	MSE	-	EXPRESSION TAG	UNP P40509
D	-12	GLY	-	EXPRESSION TAG	UNP P40509
D	-11	SER	-	EXPRESSION TAG	UNP P40509
D	-10	SER	-	EXPRESSION TAG	UNP P40509
D	-9	HIS	-	EXPRESSION TAG	UNP P40509
D	-8	HIS	-	EXPRESSION TAG	UNP P40509
D	-7	HIS	-	EXPRESSION TAG	UNP P40509
D	-6	HIS	-	EXPRESSION TAG	UNP P40509
D	-5	HIS	-	EXPRESSION TAG	UNP P40509
D	-4	HIS	-	EXPRESSION TAG	UNP P40509

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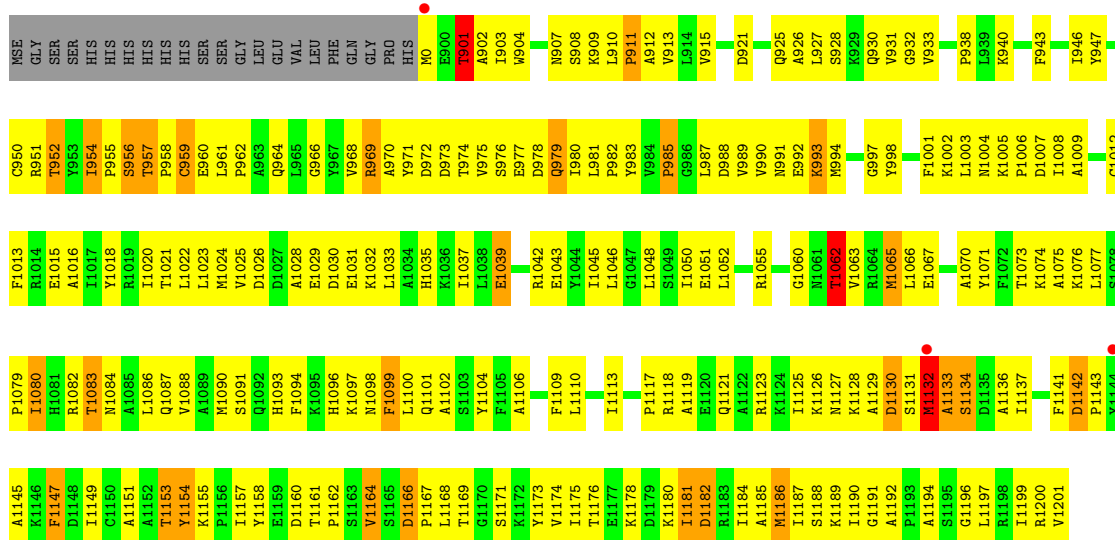
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	-	EXPRESSION TAG	UNP P40509
D	-2	GLN	-	EXPRESSION TAG	UNP P40509
D	-1	ASP	-	EXPRESSION TAG	UNP P40509
D	0	PRO	-	EXPRESSION TAG	UNP P40509
F	-13	MSE	-	EXPRESSION TAG	UNP P40509
F	-12	GLY	-	EXPRESSION TAG	UNP P40509
F	-11	SER	-	EXPRESSION TAG	UNP P40509
F	-10	SER	-	EXPRESSION TAG	UNP P40509
F	-9	HIS	-	EXPRESSION TAG	UNP P40509
F	-8	HIS	-	EXPRESSION TAG	UNP P40509
F	-7	HIS	-	EXPRESSION TAG	UNP P40509
F	-6	HIS	-	EXPRESSION TAG	UNP P40509
F	-5	HIS	-	EXPRESSION TAG	UNP P40509
F	-4	HIS	-	EXPRESSION TAG	UNP P40509
F	-3	SER	-	EXPRESSION TAG	UNP P40509
F	-2	GLN	-	EXPRESSION TAG	UNP P40509
F	-1	ASP	-	EXPRESSION TAG	UNP P40509
F	0	PRO	-	EXPRESSION TAG	UNP P40509

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

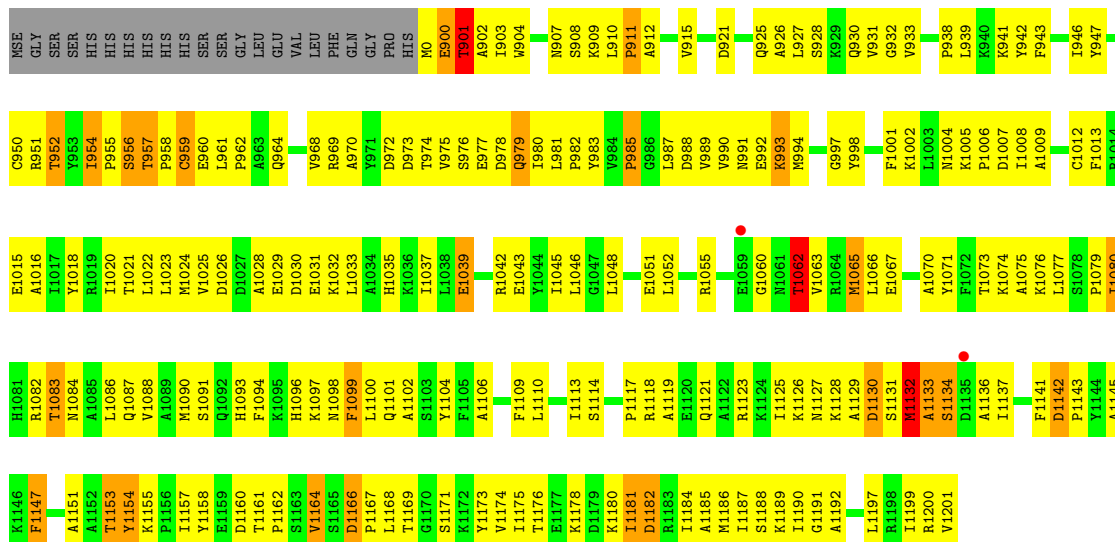
#### • Molecule 1: Coatomer subunit alpha

Chain A: 



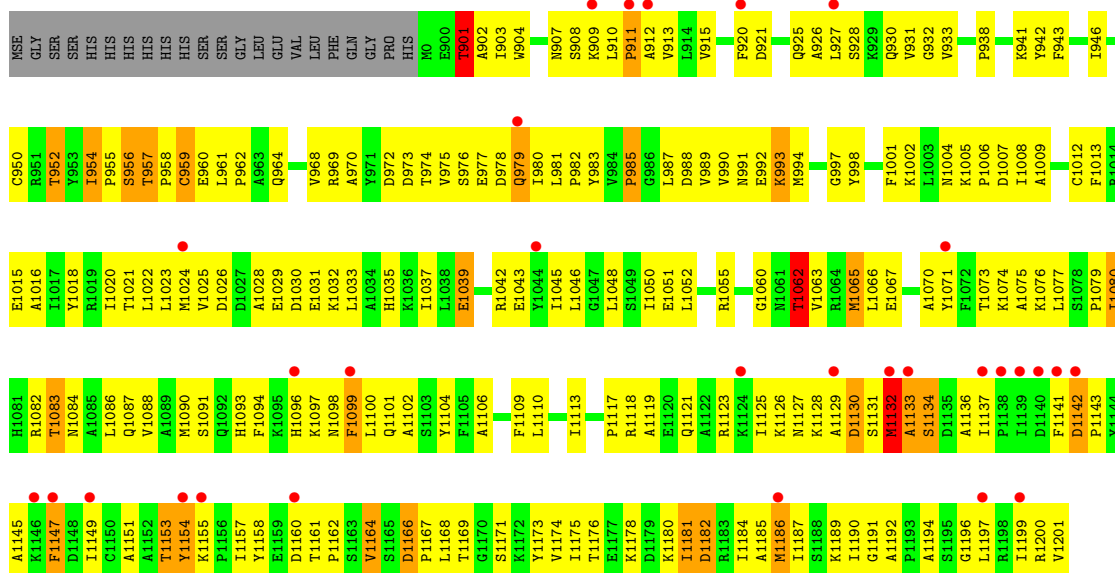
#### • Molecule 1: Coatomer subunit alpha

Chain C: 



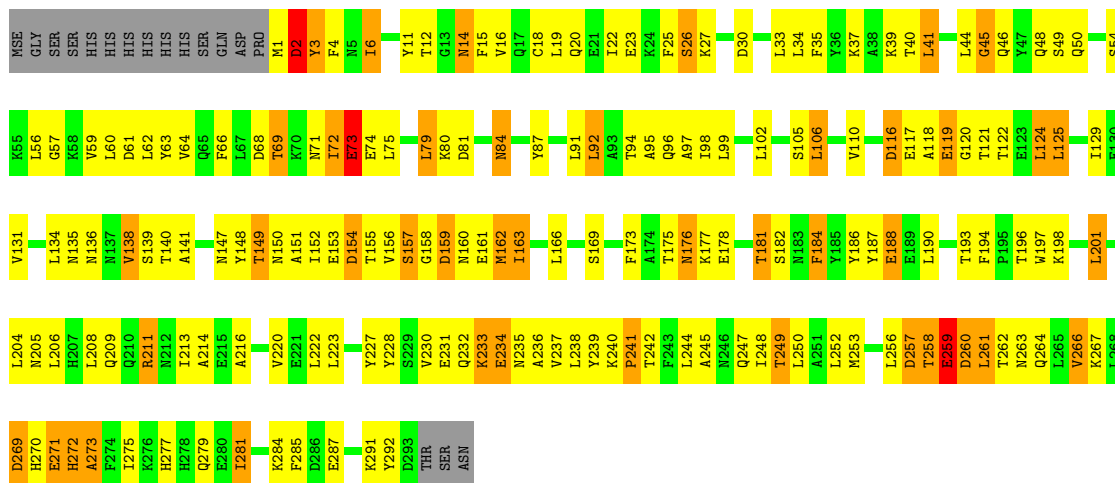
- Molecule 1: Coatomer subunit alpha

Chain E:



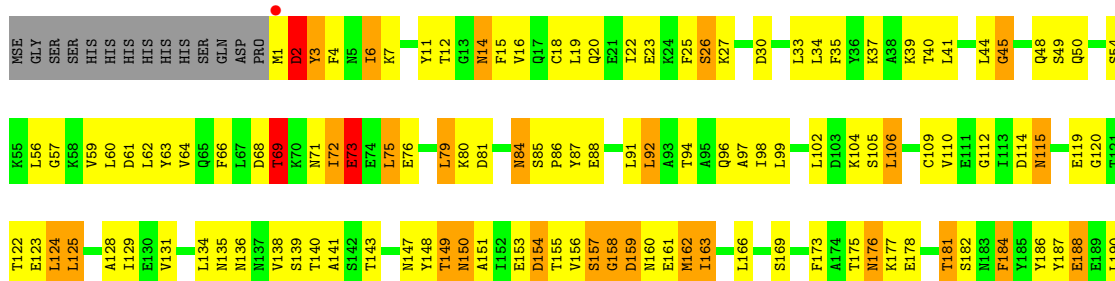
- Molecule 2: Coatomer subunit epsilon

Chain B:

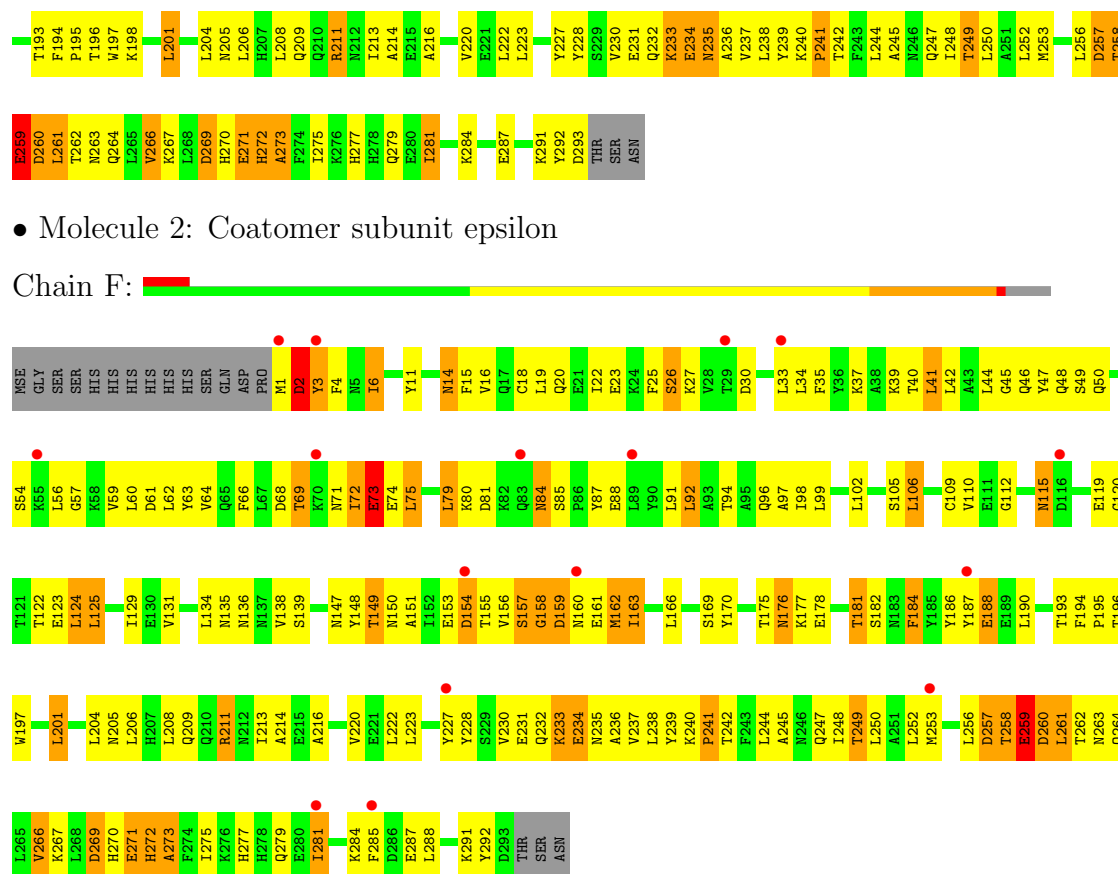


- Molecule 2: Coatomer subunit epsilon

Chain D:







• Molecule 2: Coatomer subunit epsilon

Chain F:

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	328.13Å 74.31Å 96.40Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 48.68 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.7 (50.00-3.25) 96.1 (48.68-3.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.287 0.249 , 0.284	Depositor DCC
$R_{free}$ test set	1705 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 90.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 68519 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	0/2429	0.79	1/3273 (0.0%)
1	C	0.49	0/2429	0.79	1/3273 (0.0%)
1	E	0.47	0/2429	0.78	1/3273 (0.0%)
2	B	0.51	0/2401	0.76	1/3255 (0.0%)
2	D	0.51	0/2401	0.76	1/3255 (0.0%)
2	F	0.49	0/2401	0.75	1/3255 (0.0%)
All	All	0.49	0/14490	0.77	6/19584 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1155	LYS	N-CA-C	-5.69	95.63	111.00
1	A	1155	LYS	N-CA-C	-5.69	95.65	111.00
1	E	1155	LYS	N-CA-C	-5.68	95.67	111.00
2	F	125	LEU	CA-CB-CG	-5.21	103.31	115.30
2	B	125	LEU	CA-CB-CG	-5.18	103.37	115.30
2	D	125	LEU	CA-CB-CG	-5.13	103.49	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2441	281	0
1	C	2388	0	2441	246	0
1	E	2388	0	2441	249	0
2	B	2364	0	2319	214	0
2	D	2364	0	2319	239	0
2	F	2364	0	2319	215	0
All	All	14256	0	14280	1363	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 48.

All (1363) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1090:MSE:HE2	1:C:1106:ALA:HA	1.30	1.12
1:E:1090:MSE:HE2	1:E:1106:ALA:HA	1.29	1.12
1:C:1028:ALA:HB2	1:C:1200:ARG:CZ	1.80	1.10
2:B:211:ARG:HB2	2:B:211:ARG:HH11	1.11	1.10
1:A:1090:MSE:HE2	1:A:1106:ALA:HA	1.30	1.08
2:D:211:ARG:HB2	2:D:211:ARG:HH11	1.11	1.08
1:A:1113:ILE:HG23	2:D:150:ASN:ND2	1.69	1.06
2:F:211:ARG:HB2	2:F:211:ARG:HH11	1.11	1.05
2:D:195:PRO:HG3	1:E:1079:PRO:HG3	1.40	1.03
1:C:957:THR:HB	1:C:958:PRO:CD	1.93	0.99
1:A:957:THR:HB	1:A:958:PRO:CD	1.92	0.99
1:E:957:THR:HB	1:E:958:PRO:CD	1.94	0.98
2:D:1:MSE:HG2	2:D:2:ASP:H	1.29	0.97
1:C:1028:ALA:HB2	1:C:1200:ARG:NH1	1.78	0.97
1:C:990:VAL:HG11	1:C:1020:ILE:HD11	1.46	0.97
1:E:1097:LYS:HG3	1:E:1099:PHE:HE1	1.29	0.97
2:B:1:MSE:HG2	2:B:2:ASP:H	1.29	0.96
1:A:990:VAL:HG11	1:A:1020:ILE:HD11	1.46	0.95
1:E:990:VAL:HG11	1:E:1020:ILE:HD11	1.45	0.95
1:A:1083:THR:HG21	1:A:1118:ARG:NH1	1.84	0.93
1:A:1097:LYS:HG3	1:A:1099:PHE:HE1	1.29	0.93
1:C:1097:LYS:HG3	1:C:1099:PHE:HE1	1.29	0.93
2:F:1:MSE:HG2	2:F:2:ASP:H	1.29	0.92
1:E:1025:VAL:HG11	1:E:1030:ASP:HB2	1.51	0.92
1:C:1025:VAL:HG11	1:C:1030:ASP:HB2	1.51	0.92
1:E:1083:THR:HG21	1:E:1118:ARG:NH1	1.84	0.92
1:A:1080:ILE:HG13	2:D:147:ASN:OD1	1.71	0.91
1:C:1083:THR:HG21	1:C:1118:ARG:NH1	1.84	0.91
2:B:6:ILE:HD12	2:B:6:ILE:H	1.36	0.91
1:A:1003:LEU:HD21	2:D:110:VAL:HG21	1.53	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1079:PRO:HG3	2:F:195:PRO:HG3	1.54	0.90
2:D:6:ILE:HD12	2:D:6:ILE:H	1.36	0.90
2:F:6:ILE:H	2:F:6:ILE:HD12	1.36	0.90
1:A:1025:VAL:HG11	1:A:1030:ASP:HB2	1.51	0.90
1:C:994:MSE:HE3	1:C:1016:ALA:CB	2.02	0.90
2:B:11:TYR:CE1	2:B:163:ILE:HD11	2.08	0.88
2:B:211:ARG:HH11	2:B:211:ARG:CB	1.87	0.88
1:A:994:MSE:HE3	1:A:1016:ALA:CB	2.02	0.88
1:E:994:MSE:HE3	1:E:1016:ALA:CB	2.02	0.88
2:D:211:ARG:CB	2:D:211:ARG:HH11	1.87	0.88
2:F:211:ARG:CB	2:F:211:ARG:HH11	1.87	0.88
1:E:1028:ALA:HB2	1:E:1200:ARG:CZ	2.02	0.87
1:C:1025:VAL:HG23	1:C:1199:ILE:HG22	1.54	0.87
1:E:1166:ASP:OD2	1:E:1169:THR:HB	1.76	0.86
1:A:1028:ALA:HB2	1:A:1200:ARG:CZ	2.05	0.86
1:A:1166:ASP:OD2	1:A:1169:THR:HB	1.76	0.86
1:C:1166:ASP:OD2	1:C:1169:THR:HB	1.76	0.85
2:F:11:TYR:CE1	2:F:163:ILE:HD11	2.10	0.85
2:D:112:GLY:O	2:D:115:ASN:HB2	1.75	0.84
1:C:1174:VAL:HG23	1:C:1176:THR:HB	1.58	0.84
1:A:1174:VAL:HG23	1:A:1176:THR:HB	1.58	0.84
1:E:1174:VAL:HG23	1:E:1176:THR:HB	1.58	0.84
2:D:195:PRO:HG3	1:E:1079:PRO:CG	2.06	0.84
1:A:1113:ILE:HG23	2:D:150:ASN:HD21	1.43	0.83
2:D:87:TYR:HE1	2:D:119:GLU:HG2	1.42	0.83
2:B:72:ILE:HD12	2:B:72:ILE:H	1.43	0.83
1:E:1097:LYS:HG3	1:E:1099:PHE:CE1	2.14	0.83
2:F:211:ARG:HA	2:F:253:MSE:HE1	1.61	0.83
1:C:1097:LYS:HG3	1:C:1099:PHE:CE1	2.14	0.83
2:B:211:ARG:HA	2:B:253:MSE:HE1	1.61	0.82
1:A:976:SER:C	1:A:978:ASP:H	1.82	0.82
1:A:1097:LYS:HG3	1:A:1099:PHE:CE1	2.14	0.82
1:A:1189:LYS:HE3	1:A:1192:ALA:HB2	1.61	0.82
1:A:0:MSE:HE1	2:B:138:VAL:HG11	1.60	0.82
2:F:72:ILE:HD12	2:F:72:ILE:H	1.43	0.82
1:A:1045:ILE:HD12	1:A:1184:ILE:HG23	1.60	0.82
1:C:1189:LYS:HE3	1:C:1192:ALA:HB2	1.61	0.82
2:F:125:LEU:HD22	2:F:148:TYR:CD2	2.15	0.82
2:B:125:LEU:HD22	2:B:148:TYR:CD2	2.15	0.82
2:D:211:ARG:HA	2:D:253:MSE:HE1	1.61	0.82
2:D:72:ILE:H	2:D:72:ILE:HD12	1.43	0.82
2:B:20:GLN:HA	2:B:23:GLU:HG3	1.61	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:264:GLN:HA	2:B:264:GLN:OE1	1.79	0.81
2:F:20:GLN:HA	2:F:23:GLU:HG3	1.61	0.81
2:D:264:GLN:HA	2:D:264:GLN:OE1	1.80	0.81
1:E:1045:ILE:HD12	1:E:1184:ILE:HG23	1.60	0.81
2:B:275:ILE:O	2:B:279:GLN:HG2	1.80	0.81
2:D:20:GLN:HA	2:D:23:GLU:HG3	1.61	0.81
2:F:264:GLN:HA	2:F:264:GLN:OE1	1.80	0.81
2:D:94:THR:O	2:D:98:ILE:HG13	1.81	0.80
2:F:94:THR:O	2:F:98:ILE:HG13	1.80	0.80
2:D:35:PHE:CD1	2:D:87:TYR:HD2	1.99	0.80
2:F:211:ARG:HB2	2:F:211:ARG:NH1	1.96	0.80
1:E:1189:LYS:HE3	1:E:1192:ALA:HB2	1.62	0.80
2:F:275:ILE:O	2:F:279:GLN:HG2	1.80	0.80
1:E:976:SER:C	1:E:978:ASP:H	1.82	0.80
1:C:976:SER:C	1:C:978:ASP:H	1.82	0.80
2:D:125:LEU:HD22	2:D:148:TYR:CD2	2.15	0.80
2:D:275:ILE:O	2:D:279:GLN:HG2	1.80	0.80
2:B:94:THR:O	2:B:98:ILE:HG13	1.81	0.79
1:C:1074:LYS:HE3	1:C:1147:PHE:CE1	2.17	0.79
2:B:181:THR:HG22	2:B:182:SER:N	1.98	0.79
2:B:211:ARG:NH1	2:B:211:ARG:HB2	1.95	0.79
2:D:181:THR:HG22	2:D:182:SER:H	1.48	0.79
1:C:1104:TYR:CE2	1:C:1143:PRO:HB3	2.17	0.79
2:D:181:THR:HG22	2:D:182:SER:N	1.99	0.78
2:B:181:THR:HG22	2:B:182:SER:H	1.48	0.78
1:A:1099:PHE:HD1	1:A:1134:SER:HB3	1.47	0.78
2:F:206:LEU:O	2:F:209:GLN:HB2	1.84	0.78
2:F:71:ASN:HB2	2:F:73:GLU:HG2	1.65	0.78
2:B:71:ASN:HB2	2:B:73:GLU:CG	2.14	0.78
2:D:206:LEU:O	2:D:209:GLN:HB2	1.84	0.78
1:E:983:TYR:CE2	2:F:253:MSE:HG2	2.19	0.78
2:D:71:ASN:HB2	2:D:73:GLU:HG2	1.65	0.78
1:A:983:TYR:CE2	2:B:253:MSE:HG2	2.19	0.77
2:B:206:LEU:O	2:B:209:GLN:HB2	1.84	0.77
2:D:71:ASN:HB2	2:D:73:GLU:CG	2.14	0.77
2:F:181:THR:HG22	2:F:182:SER:H	1.48	0.77
2:D:11:TYR:CE1	2:D:163:ILE:HD11	2.19	0.77
2:D:211:ARG:NH1	2:D:211:ARG:HB2	1.95	0.77
2:F:181:THR:HG22	2:F:182:SER:N	1.99	0.77
2:F:60:LEU:O	2:F:64:VAL:HG23	1.84	0.77
2:D:60:LEU:O	2:D:64:VAL:HG23	1.84	0.77
2:B:71:ASN:HB2	2:B:73:GLU:HG2	1.65	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1099:PHE:HD1	1:E:1134:SER:HB3	1.50	0.76
2:B:6:ILE:CD1	2:B:6:ILE:H	1.98	0.76
1:A:957:THR:HB	1:A:958:PRO:HD2	1.68	0.76
2:F:71:ASN:HB2	2:F:73:GLU:CG	2.14	0.76
1:E:1002:LYS:NZ	1:E:1080:ILE:HD11	2.01	0.76
2:D:6:ILE:HD12	2:D:6:ILE:N	2.01	0.76
1:C:994:MSE:HE3	1:C:1016:ALA:HB3	1.68	0.75
2:F:157:SER:HB2	2:F:161:GLU:HB2	1.67	0.75
2:B:60:LEU:O	2:B:64:VAL:HG23	1.84	0.75
1:C:957:THR:HB	1:C:958:PRO:HD2	1.68	0.75
2:D:6:ILE:CD1	2:D:6:ILE:H	1.98	0.75
2:F:6:ILE:H	2:F:6:ILE:CD1	1.98	0.75
2:D:87:TYR:CE1	2:D:119:GLU:HG2	2.22	0.75
2:F:6:ILE:HD12	2:F:6:ILE:N	2.01	0.74
1:E:994:MSE:HE3	1:E:1016:ALA:HB3	1.68	0.74
1:A:1002:LYS:NZ	1:A:1080:ILE:HD11	2.01	0.74
1:C:1002:LYS:NZ	1:C:1080:ILE:HD11	2.01	0.74
1:A:994:MSE:HE3	1:A:1016:ALA:HB3	1.68	0.74
1:E:957:THR:HB	1:E:958:PRO:HD2	1.68	0.74
1:A:1045:ILE:HB	1:A:1184:ILE:HD12	1.68	0.74
1:A:931:VAL:HG13	1:A:1168:LEU:HB2	1.67	0.74
1:E:954:ILE:HD13	1:E:955:PRO:N	2.03	0.74
1:C:1079:PRO:CG	2:F:195:PRO:HG3	2.18	0.74
1:C:954:ILE:HD13	1:C:955:PRO:N	2.03	0.73
2:F:35:PHE:CD1	2:F:87:TYR:HD2	2.05	0.73
2:F:69:THR:HB	2:F:71:ASN:OD1	1.89	0.73
1:A:954:ILE:HD13	1:A:955:PRO:N	2.03	0.73
2:F:3:TYR:CB	2:F:6:ILE:HD13	2.19	0.73
1:C:933:VAL:HG13	1:C:1187:ILE:HG23	1.69	0.73
2:F:257:ASP:O	2:F:259:GLU:N	2.21	0.73
2:F:63:TYR:O	2:F:66:PHE:HB3	1.89	0.73
2:B:6:ILE:HD12	2:B:6:ILE:N	2.01	0.73
2:B:3:TYR:CB	2:B:6:ILE:HD13	2.19	0.73
2:D:63:TYR:O	2:D:66:PHE:HB3	1.89	0.73
2:B:257:ASP:O	2:B:259:GLU:N	2.21	0.73
2:D:257:ASP:O	2:D:259:GLU:N	2.21	0.72
1:E:1045:ILE:HB	1:E:1184:ILE:HD12	1.71	0.72
2:D:3:TYR:CB	2:D:6:ILE:HD13	2.19	0.72
2:F:159:ASP:O	2:F:162:MSE:HE2	1.89	0.72
2:B:63:TYR:O	2:B:66:PHE:HB3	1.89	0.72
2:B:125:LEU:O	2:B:129:ILE:HD13	1.90	0.72
1:A:1113:ILE:HD12	2:D:150:ASN:HD22	1.52	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:159:ASP:O	2:B:162:MSE:HE2	1.89	0.72
2:D:125:LEU:O	2:D:129:ILE:HD13	1.90	0.72
2:D:159:ASP:O	2:D:162:MSE:HE2	1.89	0.71
1:A:1117:PRO:HB2	2:D:177:LYS:HZ3	1.56	0.71
1:C:978:ASP:O	1:C:980:ILE:N	2.23	0.71
1:E:978:ASP:O	1:E:980:ILE:N	2.23	0.71
2:F:30:ASP:HB3	2:F:33:LEU:HD12	1.73	0.71
2:B:30:ASP:HB3	2:B:33:LEU:HD12	1.73	0.71
1:E:1074:LYS:HE3	1:E:1147:PHE:CE1	2.25	0.71
2:F:125:LEU:O	2:F:129:ILE:HD13	1.90	0.71
1:A:1099:PHE:HA	1:A:1102:ALA:HB3	1.73	0.71
2:F:258:THR:HG22	2:F:262:THR:OG1	1.91	0.70
1:E:1174:VAL:CG2	1:E:1176:THR:HB	2.22	0.70
2:D:156:VAL:C	2:D:158:GLY:H	1.92	0.70
1:E:1099:PHE:HA	1:E:1102:ALA:HB3	1.73	0.70
2:D:30:ASP:HB3	2:D:33:LEU:HD12	1.73	0.70
1:E:1185:ALA:O	1:E:1187:ILE:N	2.25	0.70
2:B:57:GLY:HA2	2:B:60:LEU:HD12	1.73	0.70
2:B:106:LEU:O	2:B:106:LEU:HD23	1.92	0.70
1:E:957:THR:CB	1:E:958:PRO:CD	2.70	0.70
1:A:1185:ALA:O	1:A:1187:ILE:N	2.25	0.70
1:E:1023:LEU:HD23	1:E:1024:MSE:H	1.57	0.70
2:D:106:LEU:HD23	2:D:106:LEU:O	1.92	0.70
1:C:1174:VAL:CG2	1:C:1176:THR:HB	2.22	0.70
2:B:258:THR:HG22	2:B:262:THR:OG1	1.92	0.70
1:A:1074:LYS:HE3	1:A:1147:PHE:CE1	2.27	0.70
1:A:957:THR:CB	1:A:958:PRO:CD	2.69	0.70
1:A:1174:VAL:CG2	1:A:1176:THR:HB	2.22	0.70
1:A:978:ASP:O	1:A:980:ILE:N	2.23	0.70
1:C:957:THR:CB	1:C:958:PRO:CD	2.69	0.69
1:A:1023:LEU:HD23	1:A:1024:MSE:H	1.56	0.69
2:F:57:GLY:HA2	2:F:60:LEU:HD12	1.73	0.69
1:C:1045:ILE:HD12	1:C:1184:ILE:HG23	1.74	0.69
1:E:1090:MSE:HG3	1:E:1106:ALA:HB2	1.75	0.69
1:A:1113:ILE:HD12	2:D:150:ASN:ND2	2.07	0.69
1:A:926:ALA:O	1:A:930:GLN:HG3	1.92	0.69
2:B:222:LEU:HD23	2:B:222:LEU:O	1.92	0.69
1:A:961:LEU:HD21	2:B:134:LEU:HD11	1.72	0.69
1:C:1185:ALA:O	1:C:1187:ILE:N	2.25	0.69
1:E:926:ALA:O	1:E:930:GLN:HG3	1.92	0.69
2:F:112:GLY:O	2:F:115:ASN:HB2	1.92	0.69
1:A:940:LYS:HB2	2:B:285:PHE:CE2	2.28	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1099:PHE:HA	1:C:1102:ALA:HB3	1.73	0.69
1:C:1090:MSE:HG3	1:C:1106:ALA:HB2	1.74	0.69
1:A:1090:MSE:HG3	1:A:1106:ALA:HB2	1.75	0.69
1:C:1023:LEU:HD23	1:C:1024:MSE:H	1.57	0.69
1:E:994:MSE:CE	1:E:1013:PHE:HD2	2.05	0.69
1:A:1002:LYS:NZ	2:D:147:ASN:HB3	2.08	0.69
2:D:57:GLY:HA2	2:D:60:LEU:HD12	1.73	0.69
2:F:106:LEU:O	2:F:106:LEU:HD23	1.92	0.69
2:D:231:GLU:HB3	1:E:1113:ILE:HD12	1.74	0.69
1:A:933:VAL:HG13	1:A:1187:ILE:HG23	1.75	0.69
2:F:222:LEU:HD23	2:F:222:LEU:O	1.92	0.69
1:C:1181:ILE:H	1:C:1181:ILE:HD12	1.58	0.69
2:D:222:LEU:O	2:D:222:LEU:HD23	1.92	0.69
1:C:926:ALA:O	1:C:930:GLN:HG3	1.92	0.69
1:E:1025:VAL:HG23	1:E:1199:ILE:HG22	1.74	0.69
1:E:1181:ILE:H	1:E:1181:ILE:HD12	1.58	0.69
1:A:1117:PRO:CA	2:D:177:LYS:HZ1	2.05	0.69
2:B:175:THR:HG21	2:B:177:LYS:HD3	1.75	0.68
2:F:175:THR:HG21	2:F:177:LYS:HD3	1.75	0.68
2:D:227:TYR:O	2:D:231:GLU:HB2	1.94	0.68
1:A:1099:PHE:CD1	1:A:1134:SER:HB3	2.27	0.68
2:D:258:THR:HG22	2:D:262:THR:OG1	1.92	0.68
2:B:162:MSE:HE3	2:B:163:ILE:CD1	2.24	0.68
2:F:248:ILE:HD11	2:F:263:ASN:HB3	1.76	0.68
1:E:931:VAL:HG13	1:E:1168:LEU:HB2	1.74	0.68
2:F:227:TYR:O	2:F:231:GLU:HB2	1.94	0.68
2:D:162:MSE:HE3	2:D:163:ILE:CD1	2.24	0.68
1:C:994:MSE:CE	1:C:1013:PHE:HD2	2.05	0.68
1:C:1002:LYS:HZ1	1:C:1080:ILE:HD11	1.58	0.68
1:A:1153:THR:O	1:A:1154:TYR:HB2	1.94	0.68
1:C:1153:THR:O	1:C:1154:TYR:HB2	1.94	0.68
2:D:175:THR:HG21	2:D:177:LYS:HD3	1.75	0.67
1:C:911:PRO:HB3	1:C:927:LEU:HD21	1.76	0.67
1:C:1033:LEU:HD23	1:C:1037:ILE:HG13	1.76	0.67
1:C:1025:VAL:HG23	1:C:1199:ILE:CG2	2.24	0.67
2:D:248:ILE:HD11	2:D:263:ASN:HB3	1.76	0.67
1:E:1109:PHE:CZ	1:E:1118:ARG:HD3	2.30	0.67
2:B:157:SER:HB2	2:B:161:GLU:HB2	1.77	0.67
2:F:162:MSE:HE3	2:F:163:ILE:CD1	2.23	0.67
1:E:1153:THR:O	1:E:1154:TYR:HB2	1.95	0.67
1:E:904:TRP:CH2	1:E:982:PRO:HB3	2.29	0.67
1:E:913:VAL:CG2	1:E:1024:MSE:HE3	2.24	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:227:TYR:O	2:B:231:GLU:HB2	1.93	0.67
1:A:994:MSE:CE	1:A:1013:PHE:HD2	2.05	0.67
1:A:1033:LEU:HD23	1:A:1037:ILE:HG13	1.76	0.67
1:A:954:ILE:HD13	1:A:955:PRO:CD	2.25	0.67
1:E:1002:LYS:HZ3	1:E:1080:ILE:HD11	1.60	0.67
1:A:1109:PHE:CZ	1:A:1118:ARG:HD3	2.30	0.67
1:E:911:PRO:HB3	1:E:927:LEU:HD21	1.76	0.67
1:A:1104:TYR:CE2	1:A:1143:PRO:HB3	2.30	0.67
2:B:35:PHE:CD1	2:B:87:TYR:HD2	2.12	0.67
1:C:1109:PHE:CZ	1:C:1118:ARG:HD3	2.30	0.67
2:B:186:TYR:CZ	2:B:190:LEU:HD11	2.30	0.67
1:A:1181:ILE:HD12	1:A:1181:ILE:H	1.58	0.67
2:D:186:TYR:CZ	2:D:190:LEU:HD11	2.30	0.67
2:B:248:ILE:HD11	2:B:263:ASN:HB3	1.76	0.67
1:C:931:VAL:HG13	1:C:1168:LEU:HB2	1.77	0.67
2:F:186:TYR:CZ	2:F:190:LEU:HD11	2.30	0.67
1:A:911:PRO:HB3	1:A:927:LEU:HD21	1.76	0.67
1:E:1162:PRO:O	1:E:1175:ILE:HG12	1.95	0.67
2:D:15:PHE:HB2	2:D:44:LEU:HD21	1.77	0.67
2:F:156:VAL:C	2:F:158:GLY:H	1.99	0.66
2:F:15:PHE:HB2	2:F:44:LEU:HD21	1.77	0.66
1:E:1033:LEU:HD23	1:E:1037:ILE:HG13	1.76	0.66
1:A:976:SER:O	1:A:978:ASP:N	2.29	0.66
2:D:72:ILE:CD1	2:D:72:ILE:H	2.03	0.66
1:C:954:ILE:HD13	1:C:955:PRO:CD	2.26	0.66
1:A:1147:PHE:HD1	1:A:1147:PHE:O	1.79	0.66
1:E:1008:ILE:H	1:E:1008:ILE:HD12	1.61	0.66
1:A:981:LEU:HD13	1:A:1024:MSE:HE2	1.78	0.66
1:C:1008:ILE:H	1:C:1008:ILE:HD12	1.61	0.66
2:B:15:PHE:HB2	2:B:44:LEU:HD21	1.78	0.66
1:C:1147:PHE:HD1	1:C:1147:PHE:O	1.79	0.66
1:A:1162:PRO:O	1:A:1175:ILE:HG12	1.95	0.65
2:D:54:SER:C	2:D:56:LEU:H	2.00	0.65
1:C:1162:PRO:O	1:C:1175:ILE:HG12	1.95	0.65
1:E:961:LEU:HD21	2:F:134:LEU:HD11	1.79	0.65
2:D:19:LEU:O	2:D:23:GLU:HG2	1.97	0.65
1:E:976:SER:O	1:E:978:ASP:N	2.30	0.65
2:B:54:SER:C	2:B:56:LEU:H	1.99	0.65
2:D:80:LYS:O	2:D:81:ASP:HB2	1.96	0.65
1:A:957:THR:HB	1:A:958:PRO:HD3	1.78	0.65
2:B:19:LEU:O	2:B:23:GLU:HG2	1.97	0.65
1:C:976:SER:O	1:C:978:ASP:N	2.29	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:954:ILE:HD13	1:E:955:PRO:CD	2.26	0.65
1:E:1104:TYR:CE2	1:E:1143:PRO:HB3	2.32	0.65
2:F:87:TYR:HE1	2:F:119:GLU:HG2	1.62	0.64
1:E:1147:PHE:O	1:E:1147:PHE:HD1	1.79	0.64
1:A:1008:ILE:HD12	1:A:1008:ILE:H	1.61	0.64
2:F:72:ILE:CD1	2:F:72:ILE:H	2.03	0.64
2:F:80:LYS:O	2:F:81:ASP:HB2	1.97	0.64
2:F:19:LEU:O	2:F:23:GLU:HG2	1.97	0.64
2:D:181:THR:CG2	2:D:182:SER:H	2.07	0.64
2:B:3:TYR:HB2	2:B:6:ILE:HD13	1.80	0.64
1:C:1074:LYS:HE3	1:C:1147:PHE:HE1	1.62	0.64
1:C:1099:PHE:HD1	1:C:1134:SER:HB3	1.62	0.64
1:A:976:SER:C	1:A:978:ASP:N	2.51	0.64
1:E:1099:PHE:CD1	1:E:1134:SER:HB3	2.31	0.64
1:A:0:MSE:HE2	2:B:138:VAL:HG21	1.79	0.64
2:F:54:SER:C	2:F:56:LEU:H	1.99	0.64
1:A:1084:ASN:HD21	2:D:143:THR:HG21	1.62	0.63
1:A:1166:ASP:OD2	1:A:1169:THR:CB	2.46	0.63
2:F:181:THR:CG2	2:F:182:SER:H	2.07	0.63
1:E:957:THR:HB	1:E:958:PRO:HD3	1.79	0.63
1:A:1025:VAL:HG23	1:A:1199:ILE:HG22	1.79	0.63
1:E:1166:ASP:OD2	1:E:1169:THR:CB	2.47	0.63
1:C:1181:ILE:CD1	1:C:1181:ILE:H	2.09	0.63
2:F:63:TYR:HD1	2:F:91:LEU:HB3	1.64	0.63
1:E:1197:LEU:HD21	1:E:1199:ILE:HD11	1.80	0.63
2:D:157:SER:O	2:D:159:ASP:N	2.32	0.63
2:B:80:LYS:O	2:B:81:ASP:HB2	1.96	0.63
2:F:162:MSE:HE3	2:F:163:ILE:HD12	1.81	0.63
1:A:1197:LEU:HD21	1:A:1199:ILE:HD11	1.80	0.63
1:C:957:THR:HB	1:C:958:PRO:HD3	1.78	0.62
1:A:1117:PRO:CB	2:D:177:LYS:NZ	2.62	0.62
1:E:1181:ILE:H	1:E:1181:ILE:CD1	2.09	0.62
2:D:162:MSE:HE3	2:D:163:ILE:HD12	1.81	0.62
2:D:1:MSE:HG2	2:D:2:ASP:N	2.10	0.62
1:C:1074:LYS:HE3	1:C:1147:PHE:CD1	2.34	0.62
2:D:157:SER:HB2	2:D:161:GLU:HB2	1.80	0.62
2:D:208:LEU:HD21	2:D:250:LEU:HB2	1.81	0.62
1:A:1117:PRO:HB2	2:D:177:LYS:NZ	2.14	0.62
2:F:1:MSE:HG2	2:F:2:ASP:N	2.10	0.62
2:B:162:MSE:HE3	2:B:163:ILE:HD12	1.81	0.62
2:F:63:TYR:CD1	2:F:91:LEU:HB3	2.34	0.62
1:C:1197:LEU:HD21	1:C:1199:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:3:TYR:HB2	2:D:6:ILE:HD13	1.80	0.62
1:E:1042:ARG:HG3	1:E:1043:GLU:N	2.15	0.62
1:C:1166:ASP:OD2	1:C:1169:THR:CB	2.47	0.62
1:E:976:SER:C	1:E:978:ASP:N	2.51	0.62
1:C:990:VAL:HG11	1:C:1020:ILE:CD1	2.27	0.62
2:B:20:GLN:HA	2:B:23:GLU:CG	2.30	0.62
2:F:3:TYR:HB2	2:F:6:ILE:HD13	1.80	0.61
2:F:156:VAL:O	2:F:158:GLY:N	2.33	0.61
2:F:20:GLN:HA	2:F:23:GLU:CG	2.30	0.61
1:A:1083:THR:HG21	1:A:1118:ARG:HH12	1.63	0.61
1:A:1002:LYS:HZ1	1:A:1080:ILE:HD11	1.63	0.61
2:F:248:ILE:CD1	2:F:263:ASN:HB3	2.30	0.61
1:A:1042:ARG:HG3	1:A:1043:GLU:N	2.15	0.61
2:F:240:LYS:N	2:F:241:PRO:HD2	2.15	0.61
1:A:1181:ILE:CD1	1:A:1181:ILE:H	2.09	0.61
2:D:240:LYS:N	2:D:241:PRO:HD2	2.15	0.61
2:B:208:LEU:HD21	2:B:250:LEU:HB2	1.81	0.61
1:C:1083:THR:HG21	1:C:1118:ARG:HH12	1.63	0.61
1:C:976:SER:C	1:C:978:ASP:N	2.51	0.61
2:F:197:TRP:CZ3	2:F:223:LEU:HD22	2.36	0.61
2:F:208:LEU:HD21	2:F:250:LEU:HB2	1.81	0.61
1:E:957:THR:O	1:E:959:CYS:N	2.34	0.61
1:E:994:MSE:HE1	1:E:1013:PHE:HD2	1.66	0.61
1:A:971:TYR:CA	2:B:211:ARG:HH21	2.13	0.61
1:C:1042:ARG:HG3	1:C:1043:GLU:N	2.15	0.61
1:E:1083:THR:HG21	1:E:1118:ARG:HH12	1.63	0.61
1:A:961:LEU:HD23	1:A:962:PRO:CD	2.31	0.61
1:C:957:THR:O	1:C:959:CYS:N	2.34	0.61
1:C:1025:VAL:O	1:C:1201:VAL:HG23	2.01	0.60
2:D:248:ILE:CD1	2:D:263:ASN:HB3	2.30	0.60
1:C:954:ILE:HA	2:D:205:ASN:ND2	2.15	0.60
2:F:204:LEU:HD12	2:F:204:LEU:O	2.01	0.60
2:B:79:LEU:HD23	2:B:84:ASN:OD1	2.01	0.60
2:B:248:ILE:CD1	2:B:263:ASN:HB3	2.30	0.60
2:D:197:TRP:CZ3	2:D:223:LEU:HD22	2.36	0.60
1:C:961:LEU:HG	1:C:962:PRO:HD2	1.83	0.60
2:D:72:ILE:HG13	2:D:99:LEU:HD11	1.82	0.60
2:B:240:LYS:N	2:B:241:PRO:HD2	2.15	0.60
1:E:915:VAL:HG11	1:E:943:PHE:HA	1.84	0.60
1:A:957:THR:O	1:A:959:CYS:N	2.34	0.60
1:E:961:LEU:HD23	1:E:962:PRO:CD	2.31	0.60
1:C:915:VAL:HG11	1:C:943:PHE:HA	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:79:LEU:HD23	2:F:84:ASN:OD1	2.01	0.60
1:A:961:LEU:HD23	1:A:961:LEU:C	2.22	0.60
1:C:910:LEU:HB2	1:C:911:PRO:HD2	1.84	0.60
1:C:1005:LYS:HB3	1:C:1008:ILE:HD13	1.84	0.60
1:C:1023:LEU:HD23	1:C:1024:MSE:N	2.17	0.60
1:E:1023:LEU:HD23	1:E:1024:MSE:N	2.17	0.60
2:D:79:LEU:HD23	2:D:84:ASN:OD1	2.01	0.60
2:D:195:PRO:CG	1:E:1079:PRO:HG3	2.25	0.59
1:E:961:LEU:HG	1:E:962:PRO:HD2	1.84	0.59
1:C:994:MSE:HE1	1:C:1013:PHE:HD2	1.66	0.59
1:C:1045:ILE:HB	1:C:1184:ILE:HD12	1.84	0.59
1:E:1071:TYR:HE2	1:E:1141:PHE:HB2	1.67	0.59
1:E:910:LEU:HB2	1:E:911:PRO:HD2	1.84	0.59
2:F:15:PHE:HB3	2:F:40:THR:HG23	1.83	0.59
2:D:20:GLN:HA	2:D:23:GLU:CG	2.30	0.59
1:C:961:LEU:C	1:C:961:LEU:HD23	2.23	0.59
2:B:204:LEU:HD12	2:B:204:LEU:O	2.02	0.59
2:B:197:TRP:CZ3	2:B:223:LEU:HD22	2.36	0.59
1:A:1005:LYS:HB3	1:A:1008:ILE:HD13	1.84	0.59
1:E:990:VAL:HG11	1:E:1020:ILE:CD1	2.27	0.59
1:A:1002:LYS:HZ2	2:D:147:ASN:HB3	1.68	0.59
2:B:15:PHE:HB3	2:B:40:THR:HG23	1.83	0.59
1:A:915:VAL:HG11	1:A:943:PHE:HA	1.84	0.59
1:A:994:MSE:HE1	1:A:1013:PHE:HD2	1.66	0.59
1:A:1132:MSE:O	1:A:1134:SER:N	2.35	0.59
1:A:1018:TYR:HE2	1:A:1187:ILE:CG1	2.15	0.59
1:A:961:LEU:HG	1:A:962:PRO:HD2	1.84	0.59
2:B:63:TYR:CD1	2:B:91:LEU:HB3	2.38	0.59
1:C:1162:PRO:HB2	1:C:1175:ILE:HG13	1.85	0.59
1:E:1162:PRO:HB2	1:E:1175:ILE:HG13	1.85	0.59
1:A:1023:LEU:HD23	1:A:1024:MSE:N	2.17	0.59
1:A:1117:PRO:HA	2:D:177:LYS:HZ1	1.68	0.59
1:C:1084:ASN:O	1:C:1088:VAL:HG23	2.03	0.59
1:A:910:LEU:HB2	1:A:911:PRO:HD2	1.84	0.59
1:E:1005:LYS:HB3	1:E:1008:ILE:HD13	1.84	0.59
1:C:961:LEU:HD21	2:D:134:LEU:HD11	1.84	0.59
2:B:193:THR:HB	2:B:194:PHE:CD1	2.38	0.59
1:A:1084:ASN:O	1:A:1088:VAL:HG23	2.03	0.58
2:D:216:ALA:O	2:D:220:VAL:HG23	2.03	0.58
2:D:193:THR:HB	2:D:194:PHE:CD1	2.38	0.58
2:D:204:LEU:HD12	2:D:204:LEU:O	2.02	0.58
2:D:15:PHE:HB3	2:D:40:THR:HG23	1.83	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1162:PRO:HB2	1:A:1175:ILE:HG13	1.85	0.58
2:F:193:THR:HB	2:F:194:PHE:CD1	2.37	0.58
1:C:961:LEU:CG	1:C:962:PRO:HD2	2.34	0.58
1:A:981:LEU:HB3	1:A:1024:MSE:HE1	1.84	0.58
1:C:1025:VAL:CG1	1:C:1030:ASP:HB2	2.31	0.58
1:C:961:LEU:HD23	1:C:962:PRO:CD	2.32	0.58
1:E:961:LEU:C	1:E:961:LEU:HD23	2.23	0.58
2:B:69:THR:HB	2:B:71:ASN:OD1	2.04	0.58
1:A:1033:LEU:HD23	1:A:1033:LEU:O	2.04	0.58
2:D:35:PHE:CG	2:D:87:TYR:CD2	2.92	0.58
1:C:1028:ALA:CB	1:C:1200:ARG:CZ	2.70	0.58
2:D:149:THR:O	2:D:151:ALA:N	2.37	0.58
1:E:1033:LEU:O	1:E:1033:LEU:HD23	2.04	0.57
1:A:1003:LEU:CD2	2:D:106:LEU:HD22	2.34	0.57
1:E:1025:VAL:CG1	1:E:1030:ASP:HB2	2.31	0.57
2:F:149:THR:O	2:F:151:ALA:N	2.38	0.57
2:D:72:ILE:N	2:D:72:ILE:HD12	2.18	0.57
2:F:59:VAL:O	2:F:62:LEU:HB2	2.05	0.57
1:C:1033:LEU:HD23	1:C:1033:LEU:O	2.04	0.57
2:F:72:ILE:N	2:F:72:ILE:HD12	2.18	0.57
1:E:1084:ASN:O	1:E:1088:VAL:HG23	2.03	0.57
2:B:92:LEU:HD22	2:B:96:GLN:HG3	1.87	0.57
2:B:71:ASN:HB2	2:B:73:GLU:CD	2.25	0.57
2:B:222:LEU:HD21	2:B:228:TYR:HE1	1.68	0.57
2:F:216:ALA:O	2:F:220:VAL:HG23	2.03	0.57
2:B:149:THR:O	2:B:151:ALA:N	2.38	0.57
1:E:921:ASP:OD2	2:F:288:LEU:HD22	2.04	0.57
1:E:1123:ARG:HG2	1:E:1123:ARG:HH11	1.70	0.57
1:E:961:LEU:CG	1:E:962:PRO:HD2	2.34	0.57
2:B:59:VAL:O	2:B:62:LEU:HB2	2.05	0.57
1:A:954:ILE:HD13	1:A:955:PRO:HD2	1.87	0.57
1:A:940:LYS:HA	2:B:285:PHE:CZ	2.40	0.57
1:E:1110:LEU:HD11	1:E:1123:ARG:HA	1.87	0.57
1:C:1131:SER:OG	1:C:1132:MSE:HE2	2.05	0.57
2:D:92:LEU:HD22	2:D:96:GLN:HG3	1.87	0.57
1:C:1110:LEU:HD11	1:C:1123:ARG:HA	1.87	0.57
1:E:1001:PHE:CE1	1:E:1048:LEU:HD21	2.40	0.57
1:E:974:THR:HG22	1:E:974:THR:O	2.04	0.57
2:D:59:VAL:O	2:D:62:LEU:HB2	2.05	0.57
2:B:230:VAL:O	2:B:233:LYS:HG3	2.05	0.57
1:A:990:VAL:HG11	1:A:1020:ILE:CD1	2.27	0.56
1:E:1074:LYS:HE3	1:E:1147:PHE:HE1	1.67	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:222:LEU:HD21	2:D:228:TYR:HE1	1.68	0.56
2:D:230:VAL:O	2:D:233:LYS:HG3	2.05	0.56
1:A:961:LEU:CG	1:A:962:PRO:HD2	2.35	0.56
1:E:1065:MSE:HG3	1:E:1066:LEU:N	2.19	0.56
1:E:1131:SER:OG	1:E:1132:MSE:HE2	2.05	0.56
2:D:71:ASN:HB2	2:D:73:GLU:CD	2.25	0.56
1:A:930:GLN:HB3	1:A:1196:GLY:O	2.05	0.56
2:B:216:ALA:O	2:B:220:VAL:HG23	2.03	0.56
2:B:1:MSE:HG2	2:B:2:ASP:N	2.10	0.56
2:D:106:LEU:O	2:D:110:VAL:HG23	2.06	0.56
2:B:72:ILE:HD12	2:B:72:ILE:N	2.18	0.56
2:F:92:LEU:HD22	2:F:96:GLN:HG3	1.87	0.56
2:D:252:LEU:HD21	2:D:259:GLU:HG3	1.87	0.56
2:F:252:LEU:HD21	2:F:259:GLU:HG3	1.87	0.56
2:F:35:PHE:CG	2:F:87:TYR:CD2	2.94	0.56
1:A:1074:LYS:HE3	1:A:1147:PHE:HE1	1.70	0.56
1:A:1001:PHE:CE1	1:A:1048:LEU:HD21	2.40	0.56
1:E:930:GLN:C	1:E:1194:ALA:HB1	2.26	0.56
1:C:1123:ARG:HH11	1:C:1123:ARG:HG2	1.70	0.56
1:C:983:TYR:CE2	2:D:253:MSE:HG2	2.40	0.56
1:C:1099:PHE:CD1	1:C:1134:SER:HB3	2.40	0.56
2:B:252:LEU:HD21	2:B:259:GLU:HG3	1.87	0.56
2:F:230:VAL:O	2:F:233:LYS:HG3	2.05	0.56
1:E:1083:THR:HG23	1:E:1109:PHE:CE1	2.41	0.56
2:D:181:THR:CG2	2:D:182:SER:N	2.64	0.56
1:A:1002:LYS:HZ3	1:A:1080:ILE:HD11	1.70	0.56
2:D:156:VAL:O	2:D:158:GLY:N	2.38	0.56
2:F:222:LEU:HD21	2:F:228:TYR:HE1	1.69	0.56
1:A:1123:ARG:HG2	1:A:1123:ARG:HH11	1.70	0.56
1:C:1001:PHE:CE1	1:C:1048:LEU:HD21	2.40	0.56
1:A:981:LEU:HD13	1:A:1024:MSE:CE	2.36	0.56
1:A:1083:THR:HG23	1:A:1109:PHE:CE1	2.41	0.56
1:C:1083:THR:HG23	1:C:1109:PHE:CE1	2.41	0.56
1:E:1018:TYR:HE2	1:E:1187:ILE:CG1	2.18	0.56
1:C:974:THR:HG22	1:C:974:THR:O	2.04	0.56
2:D:149:THR:C	2:D:151:ALA:H	2.09	0.56
1:A:1131:SER:OG	1:A:1132:MSE:HE2	2.05	0.56
1:C:1113:ILE:HD12	2:F:231:GLU:HB3	1.88	0.56
2:F:71:ASN:HB2	2:F:73:GLU:CD	2.25	0.56
2:F:37:LYS:HE2	2:F:50:GLN:HE22	1.71	0.56
2:B:63:TYR:HD1	2:B:91:LEU:HB3	1.70	0.56
1:A:974:THR:HG22	1:A:974:THR:O	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:954:ILE:HD13	1:C:955:PRO:HD2	1.88	0.56
2:B:106:LEU:O	2:B:110:VAL:HG23	2.05	0.56
1:C:1151:ALA:HB3	1:C:1173:TYR:CE2	2.41	0.56
2:B:270:HIS:CD2	2:B:272:HIS:HB3	2.41	0.56
1:A:932:GLY:O	1:A:1188:SER:HB2	2.06	0.55
2:D:270:HIS:CD2	2:D:272:HIS:HB3	2.41	0.55
1:E:1151:ALA:HB3	1:E:1173:TYR:CE2	2.41	0.55
1:C:1065:MSE:HG3	1:C:1066:LEU:N	2.19	0.55
2:B:148:TYR:O	2:B:151:ALA:HB3	2.07	0.55
1:E:954:ILE:HD13	1:E:955:PRO:HD2	1.88	0.55
2:F:106:LEU:O	2:F:110:VAL:HG23	2.06	0.55
1:E:1094:PHE:C	1:E:1096:HIS:H	2.10	0.55
2:B:1:MSE:CG	2:B:2:ASP:H	2.10	0.55
2:D:35:PHE:CG	2:D:87:TYR:HD2	2.23	0.55
1:E:930:GLN:O	1:E:1194:ALA:HB1	2.07	0.55
1:A:1065:MSE:HG3	1:A:1066:LEU:N	2.20	0.55
1:E:946:ILE:HD11	1:E:1022:LEU:HB3	1.88	0.55
1:A:1110:LEU:HD11	1:A:1123:ARG:HA	1.87	0.55
2:B:270:HIS:CG	2:B:271:GLU:H	2.25	0.55
2:B:6:ILE:CD1	2:B:6:ILE:N	2.67	0.55
1:A:954:ILE:HA	2:B:205:ASN:ND2	2.22	0.55
1:A:1153:THR:O	1:A:1154:TYR:CB	2.55	0.55
1:C:1028:ALA:HA	1:C:1200:ARG:HD2	1.88	0.55
2:B:35:PHE:CG	2:B:87:TYR:HD2	2.24	0.55
1:A:961:LEU:HD23	1:A:962:PRO:N	2.22	0.54
1:A:931:VAL:HG11	1:A:1168:LEU:HD13	1.89	0.54
2:F:149:THR:C	2:F:151:ALA:H	2.09	0.54
2:F:270:HIS:CD2	2:F:272:HIS:HB3	2.41	0.54
2:F:270:HIS:CG	2:F:271:GLU:H	2.25	0.54
2:D:149:THR:C	2:D:151:ALA:N	2.59	0.54
2:F:148:TYR:O	2:F:151:ALA:HB3	2.07	0.54
1:E:1153:THR:O	1:E:1154:TYR:CB	2.55	0.54
2:F:162:MSE:HE3	2:F:163:ILE:HD13	1.90	0.54
2:D:148:TYR:O	2:D:151:ALA:HB3	2.07	0.54
1:A:1151:ALA:HB3	1:A:1173:TYR:CE2	2.41	0.54
1:A:1117:PRO:CB	2:D:177:LYS:HZ1	2.18	0.54
1:C:975:VAL:O	1:C:976:SER:C	2.46	0.54
1:C:981:LEU:HD13	1:C:1024:MSE:CE	2.38	0.54
1:A:1066:LEU:HB3	1:A:1093:HIS:CE1	2.43	0.54
2:B:4:PHE:HD1	2:B:159:ASP:HB2	1.71	0.54
2:B:149:THR:C	2:B:151:ALA:H	2.09	0.54
1:E:933:VAL:HG13	1:E:1187:ILE:HG23	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:930:GLN:HB3	1:E:1196:GLY:O	2.07	0.54
1:E:1181:ILE:N	1:E:1181:ILE:HD12	2.22	0.54
2:D:76:GLU:OE2	2:D:104:LYS:NZ	2.40	0.54
1:E:1066:LEU:HB3	1:E:1093:HIS:CE1	2.43	0.54
1:E:938:PRO:HG2	1:E:1187:ILE:HD11	1.89	0.54
1:C:1153:THR:O	1:C:1154:TYR:CB	2.55	0.54
2:D:270:HIS:CG	2:D:271:GLU:H	2.25	0.54
1:E:1006:PRO:HG2	1:E:1007:ASP:H	1.73	0.54
2:D:291:LYS:HD2	2:D:292:TYR:CE1	2.43	0.54
2:D:291:LYS:HG2	2:D:291:LYS:O	2.08	0.54
1:A:1065:MSE:SE	1:A:1066:LEU:HD23	2.58	0.54
1:A:1136:ALA:C	1:A:1137:ILE:HG13	2.28	0.54
1:A:1003:LEU:HD21	2:D:110:VAL:CG2	2.33	0.54
1:C:1071:TYR:HE2	1:C:1141:PHE:HB2	1.71	0.54
1:C:1181:ILE:HD12	1:C:1181:ILE:N	2.22	0.54
1:E:1035:HIS:O	1:E:1039:GLU:HG2	2.08	0.54
1:A:1006:PRO:HG2	1:A:1007:ASP:H	1.73	0.54
2:B:291:LYS:O	2:B:291:LYS:HG2	2.07	0.54
1:E:952:THR:HA	2:F:249:THR:HG21	1.89	0.54
1:A:981:LEU:HB3	1:A:982:PRO:HD2	1.90	0.54
1:C:1094:PHE:C	1:C:1096:HIS:H	2.10	0.54
2:F:149:THR:C	2:F:151:ALA:N	2.60	0.54
2:F:69:THR:CB	2:F:71:ASN:OD1	2.56	0.54
2:B:30:ASP:CB	2:B:33:LEU:HD12	2.38	0.54
1:E:961:LEU:HD23	1:E:962:PRO:N	2.23	0.54
2:D:30:ASP:CB	2:D:33:LEU:HD12	2.37	0.54
1:C:1035:HIS:O	1:C:1039:GLU:HG2	2.08	0.54
2:D:166:LEU:O	2:D:169:SER:HB3	2.08	0.54
2:D:37:LYS:HE2	2:D:50:GLN:HE22	1.73	0.54
1:C:1066:LEU:HB3	1:C:1093:HIS:CE1	2.43	0.53
1:C:1113:ILE:HD11	2:F:227:TYR:CD1	2.43	0.53
1:A:1025:VAL:CG1	1:A:1030:ASP:HB2	2.31	0.53
2:F:35:PHE:CG	2:F:87:TYR:HD2	2.24	0.53
1:A:1071:TYR:HE2	1:A:1141:PHE:HB2	1.73	0.53
1:E:981:LEU:HB3	1:E:982:PRO:HD2	1.90	0.53
1:A:1094:PHE:C	1:A:1096:HIS:H	2.10	0.53
2:B:162:MSE:HE3	2:B:163:ILE:HD13	1.90	0.53
1:C:1006:PRO:HG2	1:C:1007:ASP:H	1.73	0.53
1:E:1025:VAL:HG23	1:E:1199:ILE:CG2	2.39	0.53
1:E:1189:LYS:CE	1:E:1192:ALA:HB2	2.36	0.53
1:E:975:VAL:O	1:E:976:SER:C	2.45	0.53
2:F:166:LEU:O	2:F:169:SER:HB3	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:162:MSE:HE3	2:D:163:ILE:HD13	1.90	0.53
2:D:222:LEU:CD2	2:D:228:TYR:CE1	2.92	0.53
1:A:966:GLY:HA3	2:B:173:PHE:CZ	2.43	0.53
1:A:1035:HIS:O	1:A:1039:GLU:HG2	2.08	0.53
1:E:1065:MSE:SE	1:E:1066:LEU:HD23	2.58	0.53
1:E:994:MSE:HE2	1:E:1013:PHE:HD2	1.73	0.53
1:E:1018:TYR:HE2	1:E:1187:ILE:HG12	1.73	0.53
1:E:974:THR:O	1:E:975:VAL:HG23	2.08	0.53
2:D:4:PHE:HD1	2:D:159:ASP:HB2	1.73	0.53
2:B:222:LEU:CD2	2:B:228:TYR:CE1	2.92	0.53
2:D:44:LEU:O	2:D:45:GLY:C	2.46	0.53
2:D:102:LEU:HD13	2:D:135:ASN:HB2	1.91	0.53
1:A:962:PRO:HG2	2:B:134:LEU:CD1	2.38	0.53
1:E:1099:PHE:HB3	1:E:1129:ALA:HB1	1.91	0.53
1:A:974:THR:O	1:A:975:VAL:HG23	2.08	0.53
1:C:974:THR:O	1:C:975:VAL:HG23	2.08	0.53
1:C:1123:ARG:NH1	1:C:1123:ARG:HG2	2.24	0.53
1:C:998:TYR:HD1	1:C:998:TYR:N	2.07	0.53
1:A:971:TYR:HA	2:B:211:ARG:HH21	1.71	0.53
1:C:961:LEU:HD23	1:C:962:PRO:N	2.23	0.53
1:A:962:PRO:HG2	2:B:134:LEU:HD11	1.89	0.53
1:A:1189:LYS:CE	1:A:1192:ALA:HB2	2.36	0.53
2:B:149:THR:C	2:B:151:ALA:N	2.60	0.53
2:F:14:ASN:O	2:F:14:ASN:ND2	2.37	0.53
2:F:291:LYS:O	2:F:291:LYS:HG2	2.08	0.53
1:C:1099:PHE:HB3	1:C:1129:ALA:HB1	1.91	0.53
1:E:1045:ILE:CD1	1:E:1184:ILE:HG23	2.37	0.53
2:D:157:SER:C	2:D:159:ASP:H	2.13	0.53
2:B:227:TYR:HA	2:B:231:GLU:HG3	1.91	0.53
1:E:998:TYR:HD1	1:E:998:TYR:N	2.07	0.53
1:A:904:TRP:CH2	1:A:982:PRO:HB3	2.44	0.53
2:F:227:TYR:HA	2:F:231:GLU:HG3	1.91	0.53
1:A:975:VAL:O	1:A:976:SER:C	2.45	0.53
1:A:1090:MSE:CE	1:A:1106:ALA:HA	2.21	0.53
1:A:1025:VAL:HG12	1:A:1026:ASP:N	2.24	0.53
1:C:1147:PHE:CD1	1:C:1147:PHE:C	2.82	0.53
1:E:1002:LYS:HZ1	1:E:1080:ILE:HD11	1.73	0.52
1:E:1132:MSE:O	1:E:1134:SER:N	2.42	0.52
1:A:931:VAL:HG12	1:A:933:VAL:HG23	1.91	0.52
1:A:1181:ILE:HD12	1:A:1181:ILE:N	2.22	0.52
1:C:1136:ALA:C	1:C:1137:ILE:HG13	2.28	0.52
2:F:135:ASN:O	2:F:136:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:998:TYR:N	1:A:998:TYR:CD1	2.77	0.52
2:D:231:GLU:HB3	1:E:1113:ILE:CD1	2.38	0.52
1:C:1065:MSE:SE	1:C:1066:LEU:HD23	2.59	0.52
2:B:35:PHE:CG	2:B:87:TYR:CD2	2.97	0.52
1:E:1075:ALA:O	1:E:1077:LEU:HG	2.09	0.52
1:E:961:LEU:CD2	1:E:962:PRO:HD2	2.39	0.52
1:C:1025:VAL:HG12	1:C:1026:ASP:N	2.24	0.52
2:D:178:GLU:OE1	2:D:182:SER:HB3	2.10	0.52
1:C:1101:GLN:O	1:C:1104:TYR:HB3	2.10	0.52
1:A:1101:GLN:O	1:A:1104:TYR:HB3	2.09	0.52
1:A:998:TYR:N	1:A:998:TYR:HD1	2.07	0.52
1:A:961:LEU:CD2	1:A:962:PRO:HD2	2.39	0.52
1:C:1042:ARG:HD3	1:C:1169:THR:HG22	1.90	0.52
2:D:157:SER:C	2:D:159:ASP:N	2.63	0.52
1:E:1029:GLU:O	1:E:1032:LYS:HB3	2.10	0.52
1:E:1136:ALA:C	1:E:1137:ILE:HG13	2.28	0.52
1:C:961:LEU:CD2	1:C:962:PRO:HD2	2.39	0.52
1:C:1147:PHE:HD1	1:C:1147:PHE:C	2.13	0.52
2:F:222:LEU:CD2	2:F:228:TYR:HE1	2.23	0.52
2:D:222:LEU:CD2	2:D:228:TYR:HE1	2.22	0.52
1:E:1008:ILE:N	1:E:1008:ILE:HD12	2.25	0.52
1:C:998:TYR:N	1:C:998:TYR:CD1	2.77	0.52
1:A:1075:ALA:O	1:A:1077:LEU:HG	2.10	0.52
2:F:178:GLU:OE1	2:F:182:SER:HB3	2.10	0.52
1:E:1147:PHE:C	1:E:1147:PHE:CD1	2.83	0.52
1:A:1073:THR:HG23	1:A:1086:LEU:CD2	2.40	0.52
1:C:1073:THR:HG23	1:C:1086:LEU:CD2	2.40	0.52
2:D:112:GLY:HA2	2:D:115:ASN:OD1	2.09	0.52
2:D:87:TYR:CE1	2:D:120:GLY:CA	2.92	0.52
1:A:938:PRO:HG2	1:A:1187:ILE:HD11	1.92	0.52
2:B:260:ASP:O	2:B:262:THR:N	2.43	0.52
1:C:974:THR:O	1:C:975:VAL:CG2	2.58	0.52
2:B:181:THR:CG2	2:B:182:SER:H	2.07	0.52
2:D:158:GLY:O	2:D:159:ASP:HB3	2.10	0.52
2:F:222:LEU:CD2	2:F:228:TYR:CE1	2.92	0.52
1:E:920:PHE:CD2	2:F:285:PHE:HD1	2.28	0.52
2:D:135:ASN:O	2:D:136:ASN:HB2	2.10	0.52
2:B:166:LEU:O	2:B:169:SER:HB3	2.08	0.52
1:C:1075:ALA:O	1:C:1077:LEU:HG	2.09	0.52
2:D:227:TYR:CE2	1:E:1080:ILE:HB	2.45	0.52
1:E:1094:PHE:HE1	1:E:1129:ALA:HB2	1.75	0.52
1:A:994:MSE:HE2	1:A:1013:PHE:HD2	1.73	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1118:ARG:NH2	2:D:143:THR:HA	2.25	0.52
2:F:158:GLY:O	2:F:159:ASP:HB3	2.10	0.52
1:A:1147:PHE:CD1	1:A:1147:PHE:C	2.82	0.52
1:A:1123:ARG:HG2	1:A:1123:ARG:NH1	2.24	0.52
2:D:227:TYR:HA	2:D:231:GLU:HG3	1.91	0.52
1:E:1109:PHE:HZ	1:E:1118:ARG:HD3	1.75	0.52
1:C:1132:MSE:O	1:C:1134:SER:N	2.43	0.52
1:A:974:THR:O	1:A:975:VAL:CG2	2.58	0.52
1:E:974:THR:O	1:E:975:VAL:CG2	2.58	0.52
2:F:56:LEU:O	2:F:59:VAL:HB	2.10	0.52
1:C:981:LEU:HB3	1:C:982:PRO:HD2	1.90	0.52
1:A:989:VAL:O	1:A:990:VAL:C	2.48	0.52
2:F:30:ASP:CB	2:F:33:LEU:HD12	2.38	0.52
2:B:135:ASN:O	2:B:136:ASN:HB2	2.09	0.52
1:C:987:LEU:HD23	1:C:1033:LEU:HD22	1.92	0.51
1:A:1094:PHE:HE1	1:A:1129:ALA:HB2	1.75	0.51
1:A:1099:PHE:HB3	1:A:1129:ALA:HB1	1.91	0.51
1:C:1094:PHE:HE1	1:C:1129:ALA:HB2	1.75	0.51
2:D:260:ASP:O	2:D:262:THR:N	2.43	0.51
1:A:1018:TYR:HE2	1:A:1187:ILE:HG12	1.74	0.51
2:B:241:PRO:HG2	2:B:242:THR:H	1.75	0.51
2:D:56:LEU:O	2:D:59:VAL:HB	2.10	0.51
1:C:931:VAL:HG12	1:C:933:VAL:HG23	1.91	0.51
2:B:222:LEU:CD2	2:B:228:TYR:HE1	2.23	0.51
1:E:904:TRP:CZ2	1:E:982:PRO:HB3	2.45	0.51
1:E:1073:THR:HG23	1:E:1086:LEU:CD2	2.39	0.51
1:A:1029:GLU:O	1:A:1032:LYS:HB3	2.10	0.51
2:D:54:SER:O	2:D:56:LEU:N	2.37	0.51
1:C:994:MSE:HE2	1:C:1013:PHE:HD2	1.74	0.51
1:E:1097:LYS:HG2	1:E:1097:LYS:O	2.10	0.51
1:A:987:LEU:HD23	1:A:1033:LEU:HD22	1.92	0.51
1:A:994:MSE:HE1	1:A:1013:PHE:CD2	2.45	0.51
1:A:1097:LYS:HG2	1:A:1097:LYS:O	2.10	0.51
1:C:1097:LYS:HG2	1:C:1097:LYS:O	2.10	0.51
2:B:96:GLN:O	2:B:99:LEU:HB2	2.10	0.51
2:F:241:PRO:HG2	2:F:242:THR:H	1.75	0.51
2:B:178:GLU:OE1	2:B:182:SER:HB3	2.10	0.51
1:E:998:TYR:CD1	1:E:998:TYR:N	2.77	0.51
1:A:1008:ILE:N	1:A:1008:ILE:HD12	2.25	0.51
1:E:1020:ILE:O	1:E:1023:LEU:HB2	2.11	0.51
1:A:1109:PHE:HZ	1:A:1118:ARG:HD3	1.75	0.51
2:F:1:MSE:CG	2:F:2:ASP:H	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1025:VAL:HG12	1:E:1026:ASP:N	2.25	0.51
1:A:1045:ILE:CD1	1:A:1184:ILE:HG23	2.36	0.51
2:D:96:GLN:O	2:D:99:LEU:HB2	2.11	0.51
2:F:260:ASP:O	2:F:262:THR:N	2.43	0.51
2:D:86:PRO:HG2	2:D:119:GLU:O	2.10	0.51
1:E:1147:PHE:C	1:E:1147:PHE:HD1	2.13	0.51
2:B:222:LEU:HD23	2:B:222:LEU:C	2.30	0.51
2:D:222:LEU:C	2:D:222:LEU:HD23	2.31	0.51
1:E:1101:GLN:O	1:E:1104:TYR:HB3	2.09	0.51
2:B:291:LYS:HD2	2:B:292:TYR:CE1	2.46	0.51
1:A:983:TYR:HE2	2:B:253:MSE:HG2	1.72	0.51
2:D:231:GLU:OE2	1:E:1118:ARG:NH1	2.44	0.51
1:C:994:MSE:HE1	1:C:1013:PHE:CD2	2.45	0.51
2:B:54:SER:C	2:B:56:LEU:N	2.64	0.51
2:F:222:LEU:HD23	2:F:222:LEU:C	2.31	0.51
1:C:950:CYS:O	1:C:968:VAL:HG23	2.11	0.51
1:C:928:SER:O	1:C:932:GLY:HA2	2.11	0.51
1:A:1113:ILE:CD1	2:D:150:ASN:ND2	2.73	0.51
1:A:1020:ILE:HD13	1:A:1023:LEU:HD12	1.93	0.51
2:B:56:LEU:O	2:B:59:VAL:HB	2.10	0.51
1:E:987:LEU:HD23	1:E:1033:LEU:HD22	1.92	0.51
1:E:989:VAL:O	1:E:990:VAL:C	2.48	0.51
1:E:931:VAL:HG12	1:E:933:VAL:HG23	1.91	0.51
2:D:25:PHE:O	2:D:26:SER:C	2.50	0.51
1:E:928:SER:O	1:E:932:GLY:HA2	2.11	0.51
1:E:993:LYS:HG2	1:E:1015:GLU:HG2	1.93	0.51
1:C:1020:ILE:O	1:C:1023:LEU:HB2	2.12	0.50
1:C:1020:ILE:HD13	1:C:1023:LEU:HD12	1.94	0.50
1:C:987:LEU:O	1:C:988:ASP:C	2.49	0.50
2:F:197:TRP:O	2:F:201:LEU:HB2	2.10	0.50
1:E:1123:ARG:HG2	1:E:1123:ARG:NH1	2.24	0.50
1:A:993:LYS:HG2	1:A:1015:GLU:HG2	1.93	0.50
1:A:947:TYR:CE1	1:A:951:ARG:NH2	2.79	0.50
2:D:97:ALA:HB2	2:D:105:SER:OG	2.11	0.50
2:D:241:PRO:HG2	2:D:242:THR:H	1.75	0.50
2:B:197:TRP:O	2:B:201:LEU:HB2	2.10	0.50
1:A:928:SER:O	1:A:932:GLY:HA2	2.11	0.50
2:F:41:LEU:HD13	2:F:46:GLN:O	2.11	0.50
1:A:971:TYR:HA	2:B:211:ARG:NH2	2.25	0.50
1:C:989:VAL:O	1:C:990:VAL:C	2.48	0.50
1:E:994:MSE:HE1	1:E:1013:PHE:CD2	2.45	0.50
1:A:0:MSE:CE	2:B:138:VAL:HG21	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:42:LEU:HD21	2:F:64:VAL:HG13	1.94	0.50
1:C:932:GLY:O	1:C:1188:SER:HB2	2.10	0.50
1:A:950:CYS:O	1:A:968:VAL:HG23	2.11	0.50
1:A:952:THR:HA	2:B:249:THR:HG21	1.94	0.50
1:E:950:CYS:O	1:E:968:VAL:HG23	2.11	0.50
1:E:983:TYR:HE2	2:F:253:MSE:HG2	1.70	0.50
2:F:159:ASP:OD1	2:F:160:ASN:N	2.45	0.50
1:C:1180:LYS:O	1:C:1190:ILE:HG13	2.11	0.50
1:E:961:LEU:HD23	1:E:962:PRO:HD2	1.94	0.50
1:C:1079:PRO:O	1:C:1082:ARG:N	2.45	0.50
1:A:1147:PHE:HD1	1:A:1147:PHE:C	2.13	0.50
2:D:197:TRP:O	2:D:201:LEU:HB2	2.11	0.50
1:C:1029:GLU:O	1:C:1032:LYS:HB3	2.10	0.50
1:A:987:LEU:O	1:A:988:ASP:C	2.49	0.50
1:A:1003:LEU:HD21	2:D:106:LEU:HD22	1.94	0.50
2:B:158:GLY:O	2:B:159:ASP:HB3	2.10	0.50
2:F:157:SER:O	2:F:159:ASP:N	2.45	0.50
2:F:96:GLN:O	2:F:99:LEU:HB2	2.11	0.50
1:C:931:VAL:HG11	1:C:1168:LEU:HD13	1.94	0.50
2:D:227:TYR:CD1	1:E:1113:ILE:HD11	2.47	0.50
1:A:961:LEU:HD23	1:A:962:PRO:HD2	1.94	0.50
1:E:987:LEU:O	1:E:988:ASP:C	2.49	0.50
2:B:72:ILE:H	2:B:72:ILE:CD1	2.03	0.50
1:C:993:LYS:HG2	1:C:1015:GLU:HG2	1.93	0.50
1:A:1079:PRO:O	1:A:1082:ARG:N	2.45	0.50
1:C:1109:PHE:HZ	1:C:1118:ARG:HD3	1.75	0.50
1:C:1083:THR:CG2	1:C:1118:ARG:NH1	2.67	0.50
2:D:184:PHE:CE2	2:D:188:GLU:HG3	2.47	0.50
1:C:1008:ILE:HD12	1:C:1008:ILE:N	2.25	0.50
2:D:213:ILE:HG13	2:D:214:ALA:N	2.26	0.50
2:F:213:ILE:HG13	2:F:214:ALA:N	2.27	0.50
1:A:1126:LYS:O	1:A:1130:ASP:HB2	2.12	0.50
1:C:1090:MSE:CE	1:C:1106:ALA:HA	2.21	0.49
2:B:97:ALA:HB2	2:B:105:SER:OG	2.11	0.49
2:F:97:ALA:HB2	2:F:105:SER:OG	2.11	0.49
2:B:263:ASN:OD1	2:B:263:ASN:C	2.50	0.49
2:F:258:THR:O	2:F:259:GLU:C	2.50	0.49
1:C:939:LEU:HD13	1:C:1187:ILE:CD1	2.41	0.49
1:E:1126:LYS:O	1:E:1130:ASP:HB2	2.12	0.49
1:A:1045:ILE:HB	1:A:1184:ILE:CD1	2.41	0.49
2:D:159:ASP:OD1	2:D:160:ASN:N	2.45	0.49
2:F:54:SER:C	2:F:56:LEU:N	2.64	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:25:PHE:O	2:B:26:SER:C	2.50	0.49
2:D:277:HIS:O	2:D:281:ILE:HG22	2.13	0.49
1:A:1020:ILE:O	1:A:1023:LEU:HB2	2.11	0.49
2:B:156:VAL:HG12	2:B:156:VAL:O	2.13	0.49
1:C:938:PRO:HG2	1:C:1187:ILE:HD11	1.93	0.49
1:C:1126:LYS:O	1:C:1130:ASP:HB2	2.12	0.49
1:A:1180:LYS:O	1:A:1190:ILE:HG13	2.12	0.49
1:E:1079:PRO:O	1:E:1082:ARG:N	2.45	0.49
2:F:242:THR:O	2:F:245:ALA:HB3	2.12	0.49
2:F:184:PHE:CE2	2:F:188:GLU:HG3	2.47	0.49
1:C:1093:HIS:O	1:C:1102:ALA:HB2	2.13	0.49
1:C:1002:LYS:HZ3	1:C:1080:ILE:HD11	1.76	0.49
2:F:263:ASN:C	2:F:263:ASN:OD1	2.51	0.49
2:D:263:ASN:OD1	2:D:263:ASN:C	2.51	0.49
2:B:102:LEU:HD13	2:B:135:ASN:HB2	1.95	0.49
1:E:1060:GLY:C	1:E:1062:THR:H	2.16	0.49
1:C:947:TYR:CE1	1:C:951:ARG:CZ	2.96	0.49
1:E:1180:LYS:O	1:E:1190:ILE:HG13	2.12	0.49
2:D:54:SER:C	2:D:56:LEU:N	2.65	0.49
1:E:1051:GLU:O	1:E:1055:ARG:HG3	2.13	0.49
1:A:1060:GLY:C	1:A:1062:THR:H	2.16	0.49
1:E:1020:ILE:HD13	1:E:1023:LEU:HD12	1.93	0.49
1:E:1025:VAL:O	1:E:1201:VAL:HG23	2.12	0.49
2:D:72:ILE:CG1	2:D:99:LEU:HD11	2.43	0.49
2:B:184:PHE:CE2	2:B:188:GLU:HG3	2.47	0.49
2:B:184:PHE:HD2	2:B:184:PHE:O	1.95	0.49
2:D:156:VAL:O	2:D:156:VAL:HG12	2.13	0.49
1:A:1074:LYS:HE3	1:A:1147:PHE:CD1	2.48	0.49
2:B:277:HIS:O	2:B:281:ILE:HG22	2.13	0.49
2:B:37:LYS:HE2	2:B:50:GLN:HE22	1.77	0.49
1:E:1083:THR:HG22	1:E:1084:ASN:N	2.28	0.49
2:B:159:ASP:OD1	2:B:160:ASN:N	2.46	0.49
2:B:258:THR:O	2:B:259:GLU:C	2.50	0.49
1:E:1071:TYR:CE2	1:E:1141:PHE:HB2	2.47	0.49
1:A:947:TYR:CE1	1:A:951:ARG:CZ	2.96	0.49
2:B:213:ILE:HG13	2:B:214:ALA:N	2.26	0.49
1:A:1109:PHE:HZ	1:A:1118:ARG:CD	2.26	0.49
1:E:1028:ALA:HB2	1:E:1200:ARG:NH1	2.26	0.49
1:C:1189:LYS:CE	1:C:1192:ALA:HB2	2.36	0.49
1:C:954:ILE:HA	2:D:205:ASN:HD21	1.76	0.49
1:A:954:ILE:HA	2:B:205:ASN:HD21	1.78	0.49
1:A:1051:GLU:O	1:A:1055:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:184:PHE:O	2:F:184:PHE:HD2	1.95	0.48
2:F:54:SER:O	2:F:56:LEU:N	2.37	0.48
1:A:1161:THR:HG23	1:A:1162:PRO:HD2	1.95	0.48
1:C:1161:THR:HG23	1:C:1162:PRO:HD2	1.95	0.48
1:C:904:TRP:CH2	1:C:982:PRO:HB3	2.48	0.48
1:E:1093:HIS:O	1:E:1102:ALA:HB2	2.12	0.48
1:A:1083:THR:HG22	1:A:1084:ASN:N	2.28	0.48
2:F:15:PHE:HB3	2:F:40:THR:CG2	2.43	0.48
2:B:242:THR:O	2:B:245:ALA:HB3	2.13	0.48
2:D:184:PHE:HD2	2:D:184:PHE:O	1.95	0.48
1:E:1074:LYS:HE3	1:E:1147:PHE:CD1	2.48	0.48
2:F:102:LEU:HD13	2:F:135:ASN:HB2	1.94	0.48
2:B:117:GLU:O	2:B:119:GLU:N	2.33	0.48
2:B:18:CYS:O	2:B:22:ILE:HG13	2.13	0.48
2:B:15:PHE:HB3	2:B:40:THR:CG2	2.43	0.48
2:F:156:VAL:C	2:F:158:GLY:N	2.66	0.48
2:D:242:THR:O	2:D:245:ALA:HB3	2.12	0.48
1:E:920:PHE:HB3	2:F:288:LEU:HD12	1.95	0.48
2:B:272:HIS:O	2:B:273:ALA:C	2.52	0.48
1:C:1028:ALA:CB	1:C:1200:ARG:NH1	2.65	0.48
1:A:940:LYS:CB	2:B:285:PHE:CE2	2.96	0.48
2:F:277:HIS:O	2:F:281:ILE:HG22	2.13	0.48
1:E:1109:PHE:HZ	1:E:1118:ARG:CD	2.26	0.48
2:D:258:THR:O	2:D:259:GLU:C	2.50	0.48
1:E:1164:VAL:HG22	1:E:1175:ILE:HD13	1.96	0.48
2:F:272:HIS:O	2:F:273:ALA:C	2.52	0.48
1:E:1073:THR:HG23	1:E:1086:LEU:HD23	1.95	0.48
1:C:947:TYR:CE1	1:C:951:ARG:NH2	2.81	0.48
2:B:284:LYS:O	2:B:287:GLU:HB3	2.14	0.48
2:F:269:ASP:C	2:F:269:ASP:OD1	2.52	0.48
1:E:1109:PHE:C	1:E:1109:PHE:CD2	2.87	0.48
1:C:1083:THR:HG22	1:C:1084:ASN:N	2.28	0.48
2:D:15:PHE:HB3	2:D:40:THR:CG2	2.43	0.48
1:C:1004:ASN:CG	1:C:1004:ASN:O	2.52	0.48
2:D:269:ASP:C	2:D:269:ASP:OD1	2.52	0.48
2:F:25:PHE:O	2:F:26:SER:C	2.50	0.48
1:A:1109:PHE:CD2	1:A:1109:PHE:C	2.87	0.48
2:B:72:ILE:HG13	2:B:99:LEU:HD11	1.94	0.48
2:D:156:VAL:C	2:D:158:GLY:N	2.64	0.48
2:D:85:SER:HB3	2:D:88:GLU:OE2	2.14	0.48
2:D:14:ASN:O	2:D:14:ASN:ND2	2.37	0.48
1:A:1093:HIS:O	1:A:1102:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1109:PHE:CD2	1:C:1109:PHE:C	2.87	0.48
2:B:73:GLU:HB2	2:B:74:GLU:H	1.56	0.48
1:C:952:THR:HA	2:D:249:THR:HG21	1.96	0.48
1:C:1109:PHE:HZ	1:C:1118:ARG:CD	2.26	0.48
2:F:72:ILE:HG13	2:F:99:LEU:HD11	1.96	0.48
2:F:18:CYS:O	2:F:22:ILE:HG13	2.13	0.47
1:C:1104:TYR:CZ	1:C:1143:PRO:HB3	2.48	0.47
1:A:1164:VAL:HG22	1:A:1175:ILE:HD13	1.96	0.47
2:D:272:HIS:O	2:D:273:ALA:C	2.52	0.47
1:E:1004:ASN:CG	1:E:1004:ASN:O	2.52	0.47
2:F:232:GLN:O	2:F:234:GLU:N	2.47	0.47
1:C:1067:GLU:HG2	1:C:1071:TYR:CE1	2.50	0.47
1:E:970:ALA:HB2	1:E:982:PRO:O	2.14	0.47
1:C:1164:VAL:HG22	1:C:1175:ILE:HD13	1.96	0.47
1:A:1070:ALA:O	1:A:1073:THR:HB	2.14	0.47
1:C:1073:THR:HG23	1:C:1086:LEU:HD23	1.95	0.47
2:B:232:GLN:O	2:B:234:GLU:N	2.47	0.47
2:F:206:LEU:HD13	2:F:206:LEU:HA	1.67	0.47
1:A:1067:GLU:HG2	1:A:1071:TYR:CE1	2.49	0.47
1:E:904:TRP:CD2	1:E:982:PRO:HD3	2.50	0.47
1:E:946:ILE:CD1	1:E:1022:LEU:HB3	2.44	0.47
1:C:1051:GLU:O	1:C:1055:ARG:HG3	2.13	0.47
1:A:1083:THR:CG2	1:A:1118:ARG:NH1	2.68	0.47
2:F:187:TYR:O	2:F:188:GLU:C	2.53	0.47
2:F:284:LYS:O	2:F:287:GLU:HB3	2.14	0.47
1:A:1004:ASN:O	1:A:1004:ASN:CG	2.51	0.47
1:A:1018:TYR:CE2	1:A:1187:ILE:CG1	2.95	0.47
2:B:54:SER:O	2:B:56:LEU:N	2.36	0.47
2:F:288:LEU:O	2:F:292:TYR:HD1	1.98	0.47
1:A:969:ARG:O	2:B:211:ARG:NE	2.42	0.47
1:A:1113:ILE:CG2	1:A:1119:ALA:HB2	2.45	0.47
1:E:1087:GLN:OE1	1:E:1118:ARG:HG3	2.15	0.47
1:C:1109:PHE:CE1	1:C:1118:ARG:HD3	2.49	0.47
1:C:1087:GLN:OE1	1:C:1118:ARG:HG3	2.15	0.47
2:F:156:VAL:HG12	2:F:156:VAL:O	2.13	0.47
1:E:1070:ALA:O	1:E:1073:THR:HB	2.14	0.47
2:F:267:LYS:O	2:F:269:ASP:N	2.45	0.47
1:C:994:MSE:CE	1:C:1013:PHE:HA	2.45	0.47
1:C:970:ALA:HB2	1:C:982:PRO:O	2.14	0.47
1:A:970:ALA:HB2	1:A:982:PRO:O	2.14	0.47
1:A:1025:VAL:O	1:A:1201:VAL:HG23	2.15	0.47
2:F:159:ASP:O	2:F:162:MSE:CE	2.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:87:TYR:CE1	2:D:120:GLY:HA3	2.50	0.47
2:B:66:PHE:CE1	2:B:72:ILE:HG23	2.50	0.47
1:A:954:ILE:HG22	1:A:964:GLN:HB2	1.97	0.47
1:C:910:LEU:HB2	1:C:911:PRO:CD	2.45	0.47
1:E:1161:THR:HG23	1:E:1162:PRO:HD2	1.95	0.47
1:C:1070:ALA:O	1:C:1073:THR:HB	2.14	0.47
2:D:267:LYS:O	2:D:269:ASP:N	2.45	0.47
1:A:1109:PHE:CE1	1:A:1118:ARG:HD3	2.50	0.47
1:C:1060:GLY:C	1:C:1062:THR:H	2.16	0.47
1:E:1109:PHE:CE1	1:E:1118:ARG:HD3	2.50	0.47
1:C:954:ILE:HG22	1:C:964:GLN:HB2	1.96	0.47
1:E:1067:GLU:HG2	1:E:1071:TYR:CE1	2.49	0.47
2:D:232:GLN:O	2:D:234:GLU:N	2.47	0.47
2:B:269:ASP:C	2:B:269:ASP:OD1	2.52	0.47
2:D:284:LYS:O	2:D:287:GLU:HB3	2.14	0.47
1:A:994:MSE:CE	1:A:1013:PHE:HA	2.45	0.47
1:E:994:MSE:CE	1:E:1013:PHE:HA	2.45	0.47
1:E:1018:TYR:CE2	1:E:1187:ILE:CG1	2.98	0.47
2:D:18:CYS:O	2:D:22:ILE:HG13	2.13	0.46
2:D:187:TYR:O	2:D:188:GLU:C	2.53	0.46
2:B:187:TYR:O	2:B:188:GLU:C	2.53	0.46
1:A:1100:LEU:HD11	1:A:1133:ALA:HB1	1.97	0.46
1:C:1128:LYS:O	1:C:1132:MSE:HE3	2.16	0.46
2:F:157:SER:C	2:F:159:ASP:H	2.19	0.46
1:C:911:PRO:O	1:C:915:VAL:HG23	2.15	0.46
1:E:921:ASP:HA	2:F:288:LEU:HD13	1.97	0.46
1:A:1073:THR:HG23	1:A:1086:LEU:HD23	1.95	0.46
1:A:1087:GLN:OE1	1:A:1118:ARG:HG3	2.15	0.46
2:D:76:GLU:CD	2:D:104:LYS:NZ	2.68	0.46
1:E:1121:GLN:O	1:E:1125:ILE:HG12	2.15	0.46
2:B:14:ASN:ND2	2:B:14:ASN:O	2.37	0.46
1:A:904:TRP:CZ3	1:A:982:PRO:HB3	2.50	0.46
1:C:1113:ILE:CG2	1:C:1119:ALA:HB2	2.45	0.46
1:C:1113:ILE:HD11	2:F:227:TYR:HD1	1.81	0.46
1:E:1042:ARG:HB3	1:E:1169:THR:HG23	1.98	0.46
2:B:117:GLU:C	2:B:119:GLU:H	2.17	0.46
2:D:49:SER:HB2	2:D:61:ASP:OD2	2.15	0.46
1:E:1113:ILE:CG2	1:E:1119:ALA:HB2	2.45	0.46
1:E:1128:LYS:O	1:E:1132:MSE:HE3	2.16	0.46
1:E:987:LEU:HA	1:E:990:VAL:HG23	1.98	0.46
2:B:156:VAL:C	2:B:158:GLY:H	2.19	0.46
1:C:911:PRO:O	1:C:912:ALA:C	2.54	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:911:PRO:O	1:A:912:ALA:C	2.54	0.46
1:A:911:PRO:O	1:A:915:VAL:HG23	2.15	0.46
2:B:211:ARG:CG	2:B:211:ARG:HH11	2.29	0.46
1:C:981:LEU:HD13	1:C:1024:MSE:HE2	1.98	0.46
1:E:1045:ILE:HB	1:E:1184:ILE:CD1	2.42	0.46
1:E:911:PRO:O	1:E:915:VAL:HG23	2.15	0.46
2:B:267:LYS:O	2:B:269:ASP:N	2.45	0.46
1:E:1083:THR:CG2	1:E:1118:ARG:NH1	2.67	0.46
2:D:69:THR:HB	2:D:71:ASN:OD1	2.15	0.46
1:A:930:GLN:C	1:A:1194:ALA:HB1	2.36	0.46
2:B:48:GLN:O	2:B:49:SER:C	2.54	0.46
1:A:1050:ILE:HD11	1:A:1149:ILE:HG21	1.97	0.46
1:E:1033:LEU:CD2	1:E:1037:ILE:HG13	2.44	0.46
1:A:1128:LYS:O	1:A:1132:MSE:HE3	2.16	0.46
1:C:1121:GLN:O	1:C:1125:ILE:HG12	2.16	0.46
1:E:1100:LEU:HD11	1:E:1133:ALA:HB1	1.97	0.46
1:A:987:LEU:HA	1:A:990:VAL:HG23	1.98	0.46
1:A:1025:VAL:HG23	1:A:1199:ILE:CG2	2.45	0.46
1:C:1042:ARG:HB3	1:C:1169:THR:HG23	1.98	0.46
1:A:1162:PRO:HB2	1:A:1175:ILE:CG1	2.45	0.46
1:C:1162:PRO:HB2	1:C:1175:ILE:CG1	2.45	0.46
2:B:49:SER:HB2	2:B:61:ASP:OD2	2.16	0.46
2:F:48:GLN:O	2:F:49:SER:C	2.54	0.46
1:C:1142:ASP:OD1	1:C:1145:ALA:HB3	2.16	0.46
1:C:903:ILE:O	1:C:907:ASN:HB2	2.16	0.46
2:D:124:LEU:HD23	2:D:124:LEU:HA	1.77	0.46
1:E:903:ILE:O	1:E:907:ASN:HB2	2.16	0.46
1:C:1033:LEU:CD2	1:C:1037:ILE:HG13	2.44	0.46
1:A:1084:ASN:HD21	2:D:143:THR:CG2	2.28	0.46
2:B:260:ASP:C	2:B:262:THR:N	2.70	0.46
1:A:903:ILE:O	1:A:907:ASN:HB2	2.16	0.45
2:D:260:ASP:C	2:D:262:THR:N	2.70	0.45
1:E:954:ILE:HG22	1:E:964:GLN:HB2	1.97	0.45
1:A:1142:ASP:OD1	1:A:1145:ALA:HB3	2.16	0.45
1:E:1166:ASP:HA	1:E:1167:PRO:HD2	1.78	0.45
2:F:197:TRP:CH2	2:F:223:LEU:HD22	2.51	0.45
2:D:197:TRP:CH2	2:D:223:LEU:HD22	2.52	0.45
2:D:1:MSE:O	2:D:2:ASP:HB2	2.17	0.45
1:C:1113:ILE:CD1	2:F:231:GLU:HB3	2.47	0.45
1:E:1191:GLY:O	1:E:1192:ALA:C	2.55	0.45
1:E:910:LEU:HB2	1:E:911:PRO:CD	2.45	0.45
2:F:109:CYS:O	2:F:124:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1142:ASP:OD1	1:E:1145:ALA:HB3	2.16	0.45
1:A:1042:ARG:HB3	1:A:1169:THR:HG23	1.97	0.45
1:A:1191:GLY:O	1:A:1192:ALA:C	2.55	0.45
2:F:129:ILE:N	2:F:129:ILE:HD12	2.32	0.45
2:F:260:ASP:O	2:F:264:GLN:HG2	2.17	0.45
2:F:62:LEU:HB3	2:F:75:LEU:HG	1.98	0.45
1:A:1121:GLN:O	1:A:1125:ILE:HG12	2.15	0.45
1:C:961:LEU:HD23	1:C:962:PRO:HD2	1.94	0.45
2:D:1:MSE:CG	2:D:2:ASP:H	2.11	0.45
1:A:974:THR:C	1:A:975:VAL:HG23	2.37	0.45
2:B:129:ILE:N	2:B:129:ILE:HD12	2.31	0.45
2:F:62:LEU:HD13	2:F:75:LEU:HA	1.99	0.45
1:E:1075:ALA:O	1:E:1077:LEU:N	2.50	0.45
2:B:117:GLU:OE2	2:B:152:ILE:CD1	2.65	0.45
2:F:1:MSE:O	2:F:2:ASP:HB2	2.16	0.45
1:A:1002:LYS:NZ	2:D:147:ASN:CB	2.79	0.45
2:B:159:ASP:O	2:B:162:MSE:CE	2.62	0.45
1:A:1028:ALA:HB2	1:A:1200:ARG:NH1	2.31	0.45
2:D:244:LEU:O	2:D:245:ALA:C	2.55	0.45
1:A:910:LEU:HB2	1:A:911:PRO:CD	2.45	0.45
1:C:1100:LEU:HD11	1:C:1133:ALA:HB1	1.98	0.45
2:D:211:ARG:HH11	2:D:211:ARG:CG	2.29	0.45
2:B:44:LEU:O	2:B:45:GLY:C	2.55	0.45
1:A:1028:ALA:HB2	1:A:1200:ARG:NH2	2.28	0.45
1:C:972:ASP:O	1:C:974:THR:N	2.50	0.45
1:C:1184:ILE:HG22	1:C:1185:ALA:N	2.32	0.45
1:C:1075:ALA:O	1:C:1077:LEU:N	2.50	0.45
2:B:44:LEU:O	2:B:46:GLN:N	2.50	0.45
2:F:11:TYR:CZ	2:F:163:ILE:HD11	2.48	0.45
2:D:129:ILE:N	2:D:129:ILE:HD12	2.31	0.45
1:E:954:ILE:HA	2:F:205:ASN:ND2	2.31	0.45
1:E:1162:PRO:HB2	1:E:1175:ILE:CG1	2.45	0.45
2:F:49:SER:HB2	2:F:61:ASP:OD2	2.16	0.45
2:B:1:MSE:O	2:B:2:ASP:HB2	2.16	0.45
2:F:157:SER:C	2:F:159:ASP:N	2.70	0.45
1:A:1184:ILE:HG22	1:A:1185:ALA:N	2.32	0.45
2:B:54:SER:HB2	2:B:57:GLY:H	1.82	0.45
2:D:48:GLN:O	2:D:49:SER:C	2.54	0.45
1:E:979:GLN:O	1:E:979:GLN:HG2	2.17	0.45
1:C:1016:ALA:O	1:C:1020:ILE:HG12	2.17	0.45
1:A:0:MSE:SE	2:B:138:VAL:HB	2.67	0.45
2:F:184:PHE:C	2:F:184:PHE:CD2	2.90	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:56:LEU:HG	2:D:57:GLY:N	2.32	0.45
1:C:1161:THR:CG2	1:C:1162:PRO:HD2	2.47	0.45
2:B:66:PHE:HE2	2:B:98:ILE:HD12	1.83	0.44
1:A:972:ASP:O	1:A:974:THR:N	2.50	0.44
2:F:244:LEU:HB2	2:F:266:VAL:HG23	2.00	0.44
2:D:244:LEU:HB2	2:D:266:VAL:HG23	1.99	0.44
2:F:120:GLY:HA2	2:F:123:GLU:OE1	2.17	0.44
2:F:211:ARG:HH11	2:F:211:ARG:CG	2.30	0.44
1:C:954:ILE:HB	2:D:173:PHE:CE2	2.52	0.44
1:E:911:PRO:O	1:E:912:ALA:C	2.54	0.44
1:A:1161:THR:CG2	1:A:1162:PRO:HD2	2.47	0.44
1:E:1050:ILE:HD11	1:E:1149:ILE:HG21	1.99	0.44
1:A:913:VAL:CG2	1:A:1024:MSE:HE3	2.48	0.44
1:E:1016:ALA:O	1:E:1020:ILE:HG12	2.17	0.44
1:A:1018:TYR:CE2	1:A:1187:ILE:HG13	2.53	0.44
1:C:1191:GLY:O	1:C:1192:ALA:C	2.55	0.44
2:B:125:LEU:O	2:B:129:ILE:CD1	2.63	0.44
2:F:260:ASP:C	2:F:262:THR:N	2.70	0.44
2:F:73:GLU:HB2	2:F:74:GLU:H	1.57	0.44
2:F:222:LEU:CD2	2:F:222:LEU:C	2.86	0.44
2:D:222:LEU:C	2:D:222:LEU:CD2	2.86	0.44
2:B:197:TRP:CH2	2:B:223:LEU:HD22	2.51	0.44
1:A:1033:LEU:CD2	1:A:1037:ILE:HG13	2.45	0.44
1:E:974:THR:C	1:E:975:VAL:HG23	2.37	0.44
2:F:54:SER:HB2	2:F:57:GLY:H	1.82	0.44
2:F:56:LEU:HG	2:F:57:GLY:N	2.32	0.44
1:A:1074:LYS:HG3	1:A:1147:PHE:HE1	1.83	0.44
1:A:946:ILE:HD11	1:A:1022:LEU:HB3	1.99	0.44
1:C:979:GLN:HG2	1:C:979:GLN:O	2.18	0.44
1:E:956:SER:O	1:E:957:THR:C	2.56	0.44
1:C:987:LEU:HA	1:C:990:VAL:HG23	1.99	0.44
1:C:1094:PHE:C	1:C:1096:HIS:N	2.70	0.44
2:D:260:ASP:O	2:D:264:GLN:HG2	2.16	0.44
1:E:972:ASP:O	1:E:974:THR:N	2.50	0.44
1:C:974:THR:C	1:C:975:VAL:HG23	2.37	0.44
1:A:997:GLY:HA3	1:A:1013:PHE:CE2	2.53	0.44
2:F:6:ILE:CG2	2:F:22:ILE:HG12	2.48	0.44
2:F:41:LEU:HB3	2:F:47:TYR:HA	1.99	0.44
2:F:85:SER:HB3	2:F:88:GLU:OE2	2.18	0.44
1:E:1042:ARG:HD3	1:E:1169:THR:HG22	2.00	0.44
2:B:96:GLN:OE1	2:B:105:SER:HA	2.18	0.44
1:A:907:ASN:ND2	1:A:978:ASP:O	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:260:ASP:O	2:B:264:GLN:HG2	2.17	0.44
2:B:184:PHE:O	2:B:188:GLU:HB2	2.18	0.44
1:A:1002:LYS:HZ2	2:D:147:ASN:CB	2.31	0.44
2:F:96:GLN:OE1	2:F:105:SER:HA	2.18	0.44
1:A:1018:TYR:HE2	1:A:1187:ILE:HG13	1.81	0.44
2:F:248:ILE:HD11	2:F:263:ASN:CB	2.46	0.44
1:C:933:VAL:HG13	1:C:1187:ILE:CG2	2.43	0.44
2:D:193:THR:O	2:D:193:THR:HG22	2.18	0.44
1:E:997:GLY:HA3	1:E:1013:PHE:CE2	2.53	0.44
1:E:1074:LYS:HG3	1:E:1147:PHE:HE1	1.83	0.44
2:D:35:PHE:CD1	2:D:87:TYR:CD2	2.91	0.43
2:D:184:PHE:C	2:D:184:PHE:CD2	2.90	0.43
2:B:270:HIS:CG	2:B:271:GLU:N	2.86	0.43
1:E:1090:MSE:CE	1:E:1106:ALA:HA	2.21	0.43
1:C:997:GLY:HA3	1:C:1013:PHE:CE2	2.54	0.43
2:F:244:LEU:O	2:F:245:ALA:C	2.56	0.43
1:C:939:LEU:HD13	1:C:1187:ILE:HD12	2.00	0.43
1:A:1071:TYR:CE2	1:A:1141:PHE:HB2	2.51	0.43
1:E:1161:THR:CG2	1:E:1162:PRO:HD2	2.47	0.43
1:A:1075:ALA:O	1:A:1077:LEU:N	2.50	0.43
2:D:96:GLN:OE1	2:D:105:SER:HA	2.18	0.43
2:D:248:ILE:HD11	2:D:263:ASN:CB	2.47	0.43
2:D:184:PHE:O	2:D:188:GLU:HB2	2.18	0.43
2:D:159:ASP:O	2:D:162:MSE:CE	2.62	0.43
1:A:979:GLN:O	1:A:979:GLN:HG2	2.18	0.43
1:A:956:SER:O	1:A:957:THR:C	2.56	0.43
2:F:112:GLY:O	2:F:115:ASN:N	2.51	0.43
1:A:1097:LYS:O	1:A:1136:ALA:CB	2.67	0.43
2:B:6:ILE:CG2	2:B:22:ILE:HG12	2.48	0.43
2:B:256:LEU:O	2:B:257:ASP:C	2.56	0.43
1:E:1184:ILE:HG22	1:E:1185:ALA:N	2.32	0.43
2:B:248:ILE:HD11	2:B:263:ASN:CB	2.47	0.43
2:F:187:TYR:CD1	2:F:206:LEU:HD21	2.54	0.43
2:F:184:PHE:O	2:F:188:GLU:HB2	2.18	0.43
2:D:54:SER:HB2	2:D:57:GLY:H	1.82	0.43
2:B:222:LEU:CD2	2:B:222:LEU:C	2.85	0.43
1:E:1009:ALA:O	1:E:1012:CYS:HB2	2.18	0.43
1:A:1016:ALA:O	1:A:1020:ILE:HG12	2.18	0.43
2:F:244:LEU:O	2:F:247:GLN:HB2	2.19	0.43
2:B:175:THR:O	2:B:176:ASN:CB	2.67	0.43
2:F:193:THR:HG22	2:F:193:THR:O	2.18	0.43
2:D:270:HIS:CG	2:D:271:GLU:N	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:117:GLU:HA	2:B:121:THR:HB	1.99	0.43
1:A:1186:MSE:HG3	1:A:1186:MSE:H	1.64	0.43
2:B:66:PHE:CE2	2:B:95:ALA:HA	2.53	0.43
2:B:244:LEU:O	2:B:245:ALA:C	2.55	0.43
2:F:66:PHE:HE2	2:F:98:ILE:HD12	1.82	0.43
2:D:125:LEU:O	2:D:129:ILE:CD1	2.63	0.43
2:B:187:TYR:CD1	2:B:206:LEU:HD21	2.54	0.43
1:E:908:SER:OG	1:E:910:LEU:HD23	2.19	0.43
2:B:193:THR:O	2:B:193:THR:HG22	2.17	0.43
1:C:1009:ALA:O	1:C:1012:CYS:HB2	2.18	0.43
1:C:981:LEU:HD22	1:C:1024:MSE:HE1	2.00	0.43
1:E:994:MSE:HA	1:E:994:MSE:HE2	2.01	0.43
1:A:1094:PHE:C	1:A:1096:HIS:N	2.70	0.43
2:B:156:VAL:O	2:B:158:GLY:N	2.43	0.43
2:B:94:THR:HG22	2:B:98:ILE:HD11	2.01	0.43
1:C:908:SER:OG	1:C:910:LEU:HD23	2.18	0.43
1:C:1008:ILE:H	1:C:1008:ILE:CD1	2.31	0.43
2:D:197:TRP:CE3	2:D:223:LEU:HD22	2.54	0.43
1:C:1079:PRO:HG2	1:C:1080:ILE:H	1.84	0.43
1:E:1028:ALA:HB2	1:E:1200:ARG:NH2	2.31	0.43
1:A:931:VAL:CG1	1:A:931:VAL:O	2.67	0.43
2:D:244:LEU:O	2:D:247:GLN:HB2	2.19	0.43
1:E:931:VAL:CG1	1:E:931:VAL:O	2.67	0.43
2:F:256:LEU:O	2:F:257:ASP:C	2.57	0.43
2:D:94:THR:HG22	2:D:98:ILE:HD11	2.01	0.43
1:A:908:SER:OG	1:A:910:LEU:HD23	2.18	0.43
2:D:197:TRP:O	2:D:198:LYS:C	2.58	0.43
1:A:994:MSE:HA	1:A:994:MSE:HE2	2.01	0.42
1:E:987:LEU:HA	1:E:990:VAL:CG2	2.49	0.42
2:F:44:LEU:HA	2:F:234:GLU:OE1	2.19	0.42
2:F:71:ASN:HB2	2:F:73:GLU:OE1	2.19	0.42
2:B:106:LEU:C	2:B:106:LEU:HD23	2.39	0.42
2:F:106:LEU:C	2:F:106:LEU:HD23	2.39	0.42
1:E:1157:ILE:HG23	1:E:1161:THR:HB	2.01	0.42
1:E:921:ASP:N	2:F:288:LEU:HD11	2.34	0.42
1:C:994:MSE:CE	1:C:1013:PHE:CD2	2.96	0.42
1:A:1127:ASN:C	1:A:1129:ALA:N	2.73	0.42
2:D:106:LEU:C	2:D:106:LEU:HD23	2.39	0.42
2:B:244:LEU:HB2	2:B:266:VAL:HG23	2.00	0.42
2:D:187:TYR:CD1	2:D:206:LEU:HD21	2.54	0.42
2:D:49:SER:HB2	2:D:61:ASP:CG	2.40	0.42
1:A:1009:ALA:O	1:A:1012:CYS:HB2	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:1094:PHE:C	1:E:1096:HIS:N	2.70	0.42
1:E:913:VAL:HG22	1:E:1024:MSE:HE3	2.00	0.42
2:B:184:PHE:CD2	2:B:184:PHE:C	2.90	0.42
1:A:1142:ASP:CG	1:A:1142:ASP:O	2.58	0.42
1:A:1157:ILE:HG23	1:A:1161:THR:HB	2.01	0.42
2:F:197:TRP:CE3	2:F:223:LEU:HD22	2.54	0.42
2:F:270:HIS:CG	2:F:271:GLU:N	2.86	0.42
1:E:1079:PRO:HG2	1:E:1080:ILE:H	1.84	0.42
1:C:956:SER:O	1:C:957:THR:C	2.56	0.42
2:D:134:LEU:HD23	2:D:134:LEU:HA	1.90	0.42
1:C:981:LEU:HD13	1:C:1024:MSE:HE1	2.00	0.42
2:B:244:LEU:O	2:B:247:GLN:HB2	2.19	0.42
2:B:245:ALA:O	2:B:248:ILE:HB	2.20	0.42
2:B:56:LEU:HG	2:B:57:GLY:N	2.32	0.42
1:C:931:VAL:CG1	1:C:931:VAL:O	2.67	0.42
1:E:1100:LEU:HA	1:E:1100:LEU:HD12	1.72	0.42
1:E:1186:MSE:HG3	1:E:1186:MSE:H	1.63	0.42
2:D:235:ASN:O	2:D:235:ASN:ND2	2.46	0.42
1:C:987:LEU:HA	1:C:990:VAL:CG2	2.49	0.42
2:D:6:ILE:CG2	2:D:22:ILE:HG12	2.48	0.42
2:D:92:LEU:O	2:D:96:GLN:HG3	2.20	0.42
2:B:258:THR:O	2:B:260:ASP:N	2.53	0.42
2:B:12:THR:C	2:B:198:LYS:HD3	2.39	0.42
2:B:116:ASP:O	2:B:117:GLU:HB2	2.19	0.42
1:C:1100:LEU:HA	1:C:1100:LEU:HD12	1.72	0.42
2:D:238:LEU:HD23	2:D:239:TYR:CE1	2.55	0.42
1:C:1028:ALA:O	1:C:1031:GLU:HB3	2.19	0.42
1:E:1127:ASN:C	1:E:1129:ALA:H	2.23	0.42
2:D:175:THR:O	2:D:176:ASN:CB	2.67	0.42
1:A:1166:ASP:HA	1:A:1167:PRO:HD2	1.78	0.42
2:D:256:LEU:O	2:D:257:ASP:C	2.57	0.42
2:D:245:ALA:O	2:D:248:ILE:HB	2.20	0.42
2:F:175:THR:O	2:F:176:ASN:CB	2.67	0.42
2:B:197:TRP:CE3	2:B:223:LEU:HD22	2.54	0.42
2:B:49:SER:HB2	2:B:61:ASP:CG	2.40	0.42
1:E:1142:ASP:O	1:E:1142:ASP:CG	2.57	0.42
2:B:154:ASP:O	2:B:155:THR:C	2.58	0.42
2:D:109:CYS:HB3	2:D:128:ALA:HB2	2.01	0.42
2:B:124:LEU:HA	2:B:124:LEU:HD23	1.76	0.42
1:A:987:LEU:HA	1:A:990:VAL:CG2	2.49	0.42
2:F:45:GLY:HA2	2:F:234:GLU:OE2	2.20	0.42
1:E:1028:ALA:O	1:E:1031:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:262:THR:C	2:F:264:GLN:H	2.23	0.42
1:C:1071:TYR:CE2	1:C:1141:PHE:HB2	2.53	0.42
1:C:1074:LYS:HG3	1:C:1147:PHE:HE1	1.83	0.42
2:D:62:LEU:HD23	2:D:62:LEU:HA	1.82	0.42
1:C:946:ILE:HD11	1:C:1022:LEU:HB3	2.02	0.42
2:D:262:THR:C	2:D:264:GLN:H	2.23	0.42
2:D:63:TYR:CD1	2:D:91:LEU:HB3	2.55	0.42
2:D:44:LEU:HA	2:D:234:GLU:OE1	2.19	0.42
1:C:1157:ILE:HG23	1:C:1161:THR:HB	2.01	0.42
2:B:238:LEU:HD23	2:B:239:TYR:CE1	2.55	0.42
2:F:154:ASP:O	2:F:155:THR:C	2.58	0.42
1:C:901:THR:HG22	1:C:902:ALA:N	2.35	0.42
1:A:1131:SER:O	1:A:1132:MSE:CB	2.68	0.42
1:C:1114:SER:HB3	2:F:232:GLN:HA	2.01	0.42
1:A:1042:ARG:HD3	1:A:1169:THR:HG22	2.00	0.42
2:F:94:THR:HG22	2:F:98:ILE:HD11	2.01	0.42
2:F:238:LEU:HD23	2:F:239:TYR:CE1	2.55	0.42
2:D:154:ASP:O	2:D:155:THR:C	2.58	0.42
1:C:994:MSE:HE2	1:C:994:MSE:HA	2.01	0.42
2:B:157:SER:O	2:B:159:ASP:N	2.53	0.42
2:B:275:ILE:HA	2:B:275:ILE:HD13	1.95	0.42
2:D:62:LEU:HB3	2:D:75:LEU:HG	2.02	0.42
1:C:1142:ASP:CG	1:C:1142:ASP:O	2.57	0.42
1:E:1113:ILE:HG22	1:E:1119:ALA:HB2	2.01	0.41
1:A:1127:ASN:C	1:A:1129:ALA:H	2.23	0.41
1:A:1079:PRO:HG2	1:A:1080:ILE:H	1.84	0.41
1:C:1113:ILE:HG22	1:C:1119:ALA:HB2	2.01	0.41
2:D:71:ASN:HB2	2:D:73:GLU:OE1	2.19	0.41
1:C:1022:LEU:HA	1:C:1022:LEU:HD23	1.83	0.41
1:C:921:ASP:O	1:C:925:GLN:HG3	2.20	0.41
1:E:1158:TYR:N	1:E:1158:TYR:CD1	2.88	0.41
1:C:989:VAL:O	1:C:992:GLU:N	2.54	0.41
2:B:15:PHE:HB2	2:B:44:LEU:CD2	2.47	0.41
2:F:156:VAL:CG1	2:F:156:VAL:O	2.69	0.41
2:F:244:LEU:HD12	2:F:266:VAL:HG23	2.01	0.41
2:D:244:LEU:HD12	2:D:266:VAL:HG23	2.01	0.41
2:B:71:ASN:HB2	2:B:73:GLU:OE1	2.19	0.41
2:D:234:GLU:C	2:D:236:ALA:H	2.23	0.41
2:B:197:TRP:O	2:B:198:LYS:C	2.57	0.41
1:C:991:ASN:O	1:C:992:GLU:C	2.59	0.41
1:E:989:VAL:O	1:E:992:GLU:N	2.53	0.41
1:C:1127:ASN:C	1:C:1129:ALA:H	2.23	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1127:ASN:C	1:C:1129:ALA:N	2.73	0.41
1:A:1028:ALA:O	1:A:1031:GLU:HB3	2.19	0.41
2:F:4:PHE:HD1	2:F:159:ASP:HB2	1.85	0.41
2:D:258:THR:O	2:D:260:ASP:N	2.53	0.41
2:F:245:ALA:O	2:F:248:ILE:HB	2.20	0.41
2:F:87:TYR:CE1	2:F:119:GLU:HG2	2.49	0.41
1:E:1071:TYR:O	1:E:1074:LYS:HB2	2.20	0.41
2:D:15:PHE:HB2	2:D:44:LEU:CD2	2.47	0.41
2:D:193:THR:CG2	2:D:194:PHE:CE1	3.03	0.41
1:C:1158:TYR:N	1:C:1158:TYR:CD1	2.88	0.41
2:B:1:MSE:O	2:B:2:ASP:CB	2.68	0.41
1:A:991:ASN:O	1:A:992:GLU:C	2.59	0.41
1:A:1178:LYS:HE3	1:A:1191:GLY:HA3	2.02	0.41
1:E:1018:TYR:O	1:E:1021:THR:HB	2.20	0.41
2:D:206:LEU:HA	2:D:206:LEU:HD13	1.67	0.41
1:A:1071:TYR:O	1:A:1074:LYS:HB2	2.20	0.41
2:B:166:LEU:HA	2:B:166:LEU:HD12	1.60	0.41
2:F:49:SER:HB2	2:F:61:ASP:CG	2.40	0.41
1:A:1158:TYR:N	1:A:1158:TYR:CD1	2.88	0.41
2:D:1:MSE:O	2:D:2:ASP:CB	2.68	0.41
1:C:1131:SER:O	1:C:1132:MSE:CB	2.68	0.41
1:A:1018:TYR:O	1:A:1021:THR:HB	2.21	0.41
2:D:260:ASP:O	2:D:261:LEU:C	2.59	0.41
2:D:156:VAL:CG1	2:D:156:VAL:O	2.68	0.41
1:A:1142:ASP:HA	1:A:1143:PRO:HD2	1.91	0.41
2:F:41:LEU:CD1	2:F:46:GLN:O	2.67	0.41
2:B:117:GLU:OE2	2:B:152:ILE:HD12	2.20	0.41
1:E:1117:PRO:HG2	1:E:1118:ARG:H	1.86	0.41
1:E:1127:ASN:C	1:E:1129:ALA:N	2.73	0.41
1:E:991:ASN:O	1:E:992:GLU:C	2.58	0.41
2:F:1:MSE:O	2:F:2:ASP:CB	2.68	0.41
2:B:41:LEU:HD13	2:B:46:GLN:O	2.21	0.41
2:F:92:LEU:O	2:F:96:GLN:HG3	2.20	0.41
2:D:7:LYS:HE2	2:D:123:GLU:OE2	2.20	0.41
1:A:959:CYS:C	1:A:961:LEU:H	2.24	0.41
1:E:987:LEU:HD12	1:E:987:LEU:N	2.35	0.41
2:F:11:TYR:CD1	2:F:163:ILE:HD11	2.55	0.41
2:B:244:LEU:HD12	2:B:266:VAL:HG23	2.01	0.41
1:E:1178:LYS:HE3	1:E:1191:GLY:HA3	2.02	0.41
1:A:1182:ASP:HA	1:A:1190:ILE:HD11	2.02	0.41
1:A:987:LEU:HD12	1:A:987:LEU:N	2.36	0.41
2:F:234:GLU:C	2:F:236:ALA:H	2.23	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1166:ASP:HA	1:C:1167:PRO:HD2	1.78	0.41
2:F:258:THR:O	2:F:260:ASP:N	2.53	0.41
2:F:260:ASP:O	2:F:261:LEU:C	2.59	0.41
1:C:1071:TYR:O	1:C:1074:LYS:HB2	2.20	0.41
2:D:12:THR:C	2:D:198:LYS:HD3	2.41	0.41
1:C:1182:ASP:HA	1:C:1190:ILE:HD11	2.02	0.41
1:A:921:ASP:O	1:A:925:GLN:HG3	2.20	0.41
1:E:1131:SER:O	1:E:1132:MSE:CB	2.68	0.41
1:A:989:VAL:O	1:A:992:GLU:N	2.53	0.41
1:C:1109:PHE:CZ	1:C:1118:ARG:CD	3.01	0.41
2:D:106:LEU:C	2:D:106:LEU:CD2	2.89	0.41
1:A:1003:LEU:CD2	2:D:110:VAL:HG21	2.38	0.41
1:C:1080:ILE:HB	2:F:227:TYR:CE2	2.56	0.41
1:C:1178:LYS:HE3	1:C:1191:GLY:HA3	2.02	0.41
2:D:266:VAL:CG1	2:D:275:ILE:HG12	2.51	0.41
2:F:106:LEU:C	2:F:106:LEU:CD2	2.90	0.41
1:E:1100:LEU:CD1	1:E:1133:ALA:HB1	2.51	0.41
1:E:959:CYS:C	1:E:961:LEU:H	2.24	0.41
1:A:904:TRP:CD2	1:A:982:PRO:HD3	2.56	0.41
1:C:1117:PRO:HG2	1:C:1118:ARG:H	1.86	0.41
1:E:931:VAL:HG11	1:E:1168:LEU:HD13	2.02	0.41
2:B:266:VAL:CG1	2:B:275:ILE:HG12	2.51	0.41
2:F:266:VAL:CG1	2:F:275:ILE:HG12	2.51	0.41
1:E:904:TRP:CG	1:E:982:PRO:HD3	2.56	0.41
1:A:1100:LEU:HB3	1:A:1101:GLN:NE2	2.36	0.41
1:E:921:ASP:O	1:E:925:GLN:HG3	2.20	0.41
1:C:1100:LEU:CD1	1:C:1133:ALA:HB1	2.51	0.41
1:C:0:MSE:O	1:C:900:GLU:C	2.59	0.41
1:A:1113:ILE:HG22	1:A:1119:ALA:HB2	2.01	0.40
2:B:134:LEU:HD23	2:B:134:LEU:HA	1.90	0.40
1:C:901:THR:O	1:C:904:TRP:HB2	2.21	0.40
1:A:901:THR:HG22	1:A:902:ALA:N	2.35	0.40
2:B:92:LEU:O	2:B:96:GLN:HG3	2.21	0.40
2:B:260:ASP:O	2:B:261:LEU:C	2.59	0.40
1:E:1045:ILE:HD12	1:E:1184:ILE:CG2	2.43	0.40
1:E:954:ILE:HD12	2:F:170:TYR:HE2	1.87	0.40
2:B:106:LEU:C	2:B:106:LEU:CD2	2.89	0.40
1:A:940:LYS:HA	2:B:285:PHE:CE2	2.55	0.40
2:B:193:THR:CG2	2:B:194:PHE:CE1	3.04	0.40
2:F:193:THR:CG2	2:F:194:PHE:CE1	3.04	0.40
2:B:234:GLU:C	2:B:236:ALA:H	2.23	0.40
1:E:1100:LEU:HD13	1:E:1133:ALA:CA	2.52	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:983:TYR:HE2	2:D:253:MSE:HG2	1.86	0.40
1:C:957:THR:CB	1:C:958:PRO:HD3	2.48	0.40
1:C:959:CYS:C	1:C:961:LEU:H	2.24	0.40
1:A:904:TRP:CG	1:A:982:PRO:HD3	2.56	0.40
2:B:87:TYR:CE1	2:B:120:GLY:CA	3.04	0.40
2:D:140:THR:O	2:D:141:ALA:C	2.59	0.40
1:C:1018:TYR:O	1:C:1021:THR:HB	2.20	0.40
1:A:901:THR:O	1:A:904:TRP:HB2	2.21	0.40
2:F:15:PHE:HB2	2:F:44:LEU:CD2	2.47	0.40
2:D:35:PHE:CG	2:D:87:TYR:CE2	3.09	0.40
1:C:954:ILE:CG2	1:C:964:GLN:HB2	2.51	0.40
1:A:954:ILE:CG2	1:A:964:GLN:HB2	2.51	0.40
1:E:941:LYS:HE2	1:E:942:TYR:CZ	2.56	0.40
1:C:941:LYS:HE2	1:C:942:TYR:CZ	2.56	0.40
1:C:904:TRP:CG	1:C:982:PRO:HD3	2.57	0.40
1:A:1117:PRO:HG2	1:A:1118:ARG:H	1.86	0.40
1:A:1097:LYS:O	1:A:1136:ALA:HB3	2.21	0.40
1:A:1080:ILE:CG1	2:D:147:ASN:OD1	2.55	0.40
2:B:15:PHE:HA	2:B:18:CYS:HB3	2.03	0.40
2:F:15:PHE:HA	2:F:18:CYS:HB3	2.04	0.40
2:B:156:VAL:CG1	2:B:156:VAL:O	2.68	0.40
2:B:125:LEU:HD22	2:B:148:TYR:CE2	2.56	0.40
1:E:954:ILE:HA	2:F:205:ASN:HD21	1.86	0.40
2:D:63:TYR:CD2	2:D:63:TYR:C	2.95	0.40
2:F:201:LEU:O	2:F:204:LEU:HB3	2.22	0.40
2:B:140:THR:O	2:B:141:ALA:C	2.59	0.40
1:E:1131:SER:C	1:E:1132:MSE:HG2	2.42	0.40
2:F:147:ASN:O	2:F:151:ALA:HB2	2.22	0.40
2:B:147:ASN:O	2:B:151:ALA:HB2	2.22	0.40
1:E:1182:ASP:HA	1:E:1190:ILE:HD11	2.02	0.40
1:E:901:THR:HG22	1:E:902:ALA:N	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	301/325 (93%)	233 (77%)	53 (18%)	15 (5%)	3	29
1	C	301/325 (93%)	232 (77%)	53 (18%)	16 (5%)	3	26
1	E	301/325 (93%)	233 (77%)	53 (18%)	15 (5%)	3	29
2	B	291/310 (94%)	211 (72%)	59 (20%)	21 (7%)	2	16
2	D	291/310 (94%)	215 (74%)	56 (19%)	20 (7%)	2	17
2	F	291/310 (94%)	212 (73%)	61 (21%)	18 (6%)	2	21
All	All	1776/1905 (93%)	1336 (75%)	335 (19%)	105 (6%)	2	23

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	957	THR
1	A	973	ASP
1	A	977	GLU
1	A	979	GLN
1	A	985	PRO
1	A	1132	MSE
1	A	1133	ALA
1	A	1186	MSE
2	B	2	ASP
2	B	73	GLU
2	B	159	ASP
2	B	181	THR
2	B	258	THR
2	B	273	ALA
1	C	957	THR
1	C	973	ASP
1	C	977	GLU
1	C	979	GLN
1	C	985	PRO
1	C	1132	MSE
1	C	1133	ALA
1	C	1186	MSE
2	D	2	ASP
2	D	73	GLU
2	D	159	ASP
2	D	181	THR
2	D	258	THR
2	D	273	ALA
1	E	957	THR
1	E	973	ASP

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Mol	Chain	Res	Type
1	E	977	GLU
1	E	979	GLN
1	E	985	PRO
1	E	1132	MSE
1	E	1133	ALA
1	E	1186	MSE
2	F	2	ASP
2	F	73	GLU
2	F	159	ASP
2	F	181	THR
2	F	258	THR
2	F	273	ALA
1	A	1076	LYS
1	A	1154	TYR
2	B	119	GLU
2	B	157	SER
2	B	233	LYS
2	B	234	GLU
2	B	261	LEU
1	C	900	GLU
1	C	1076	LYS
1	C	1154	TYR
2	D	157	SER
2	D	158	GLY
2	D	233	LYS
2	D	234	GLU
2	D	261	LEU
1	E	1076	LYS
1	E	1154	TYR
2	F	157	SER
2	F	158	GLY
2	F	233	LYS
2	F	234	GLU
2	F	261	LEU
1	A	901	THR
1	A	959	CYS
1	A	1062	THR
2	B	26	SER
2	B	27	LYS
2	B	45	GLY
2	B	116	ASP
2	B	118	ALA

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Mol	Chain	Res	Type
2	B	149	THR
2	B	150	ASN
2	B	269	ASP
1	C	901	THR
1	C	959	CYS
1	C	1062	THR
2	D	26	SER
2	D	27	LYS
2	D	149	THR
2	D	150	ASN
2	D	269	ASP
1	E	901	THR
1	E	959	CYS
1	E	1062	THR
2	F	26	SER
2	F	27	LYS
2	F	149	THR
2	F	150	ASN
2	F	269	ASP
1	A	1039	GLU
2	B	241	PRO
2	B	259	GLU
1	C	1039	GLU
2	D	69	THR
2	D	241	PRO
1	E	1039	GLU
2	F	241	PRO
1	A	911	PRO
1	C	911	PRO
2	D	259	GLU
1	E	911	PRO
2	F	259	GLU
2	D	45	GLY

### 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 X-ray entries followed by that with respect to entries of similar resolution. 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	257/268 (96%)	226 (88%)	31 (12%)	7	34
1	C	257/268 (96%)	226 (88%)	31 (12%)	7	34
1	E	257/268 (96%)	226 (88%)	31 (12%)	7	34
2	B	263/275 (96%)	221 (84%)	42 (16%)	3	18
2	D	263/275 (96%)	218 (83%)	45 (17%)	3	16
2	F	263/275 (96%)	220 (84%)	43 (16%)	3	17
All	All	1560/1629 (96%)	1337 (86%)	223 (14%)	5	24

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	901	THR
1	A	909	LYS
1	A	952	THR
1	A	954	ILE
1	A	956	SER
1	A	960	GLU
1	A	969	ARG
1	A	985	PRO
1	A	993	LYS
1	A	1046	LEU
1	A	1052	LEU
1	A	1062	THR
1	A	1063	VAL
1	A	1065	MSE
1	A	1080	ILE
1	A	1083	THR
1	A	1091	SER
1	A	1098	ASN
1	A	1099	PHE
1	A	1130	ASP
1	A	1132	MSE
1	A	1134	SER
1	A	1142	ASP
1	A	1147	PHE
1	A	1153	THR
1	A	1160	ASP
1	A	1164	VAL
1	A	1166	ASP
1	A	1171	SER
1	A	1181	ILE

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Mol	Chain	Res	Type
1	A	1182	ASP
2	B	2	ASP
2	B	3	TYR
2	B	6	ILE
2	B	14	ASN
2	B	16	VAL
2	B	34	LEU
2	B	39	LYS
2	B	41	LEU
2	B	68	ASP
2	B	69	THR
2	B	72	ILE
2	B	73	GLU
2	B	75	LEU
2	B	79	LEU
2	B	84	ASN
2	B	92	LEU
2	B	106	LEU
2	B	122	THR
2	B	124	LEU
2	B	131	VAL
2	B	138	VAL
2	B	139	SER
2	B	153	GLU
2	B	154	ASP
2	B	162	MSE
2	B	163	ILE
2	B	176	ASN
2	B	184	PHE
2	B	188	GLU
2	B	196	THR
2	B	201	LEU
2	B	211	ARG
2	B	235	ASN
2	B	237	VAL
2	B	249	THR
2	B	257	ASP
2	B	259	GLU
2	B	260	ASP
2	B	266	VAL
2	B	271	GLU
2	B	272	HIS

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Mol	Chain	Res	Type
2	B	281	ILE
1	C	901	THR
1	C	909	LYS
1	C	952	THR
1	C	954	ILE
1	C	956	SER
1	C	960	GLU
1	C	969	ARG
1	C	985	PRO
1	C	993	LYS
1	C	1046	LEU
1	C	1052	LEU
1	C	1062	THR
1	C	1063	VAL
1	C	1065	MSE
1	C	1080	ILE
1	C	1083	THR
1	C	1091	SER
1	C	1098	ASN
1	C	1099	PHE
1	C	1130	ASP
1	C	1132	MSE
1	C	1134	SER
1	C	1142	ASP
1	C	1147	PHE
1	C	1153	THR
1	C	1160	ASP
1	C	1164	VAL
1	C	1166	ASP
1	C	1171	SER
1	C	1181	ILE
1	C	1182	ASP
2	D	2	ASP
2	D	3	TYR
2	D	6	ILE
2	D	14	ASN
2	D	16	VAL
2	D	34	LEU
2	D	39	LYS
2	D	41	LEU
2	D	68	ASP
2	D	69	THR

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Mol	Chain	Res	Type
2	D	72	ILE
2	D	73	GLU
2	D	75	LEU
2	D	79	LEU
2	D	84	ASN
2	D	92	LEU
2	D	106	LEU
2	D	114	ASP
2	D	115	ASN
2	D	122	THR
2	D	124	LEU
2	D	131	VAL
2	D	138	VAL
2	D	139	SER
2	D	153	GLU
2	D	154	ASP
2	D	162	MSE
2	D	163	ILE
2	D	176	ASN
2	D	184	PHE
2	D	188	GLU
2	D	196	THR
2	D	201	LEU
2	D	211	ARG
2	D	235	ASN
2	D	237	VAL
2	D	249	THR
2	D	257	ASP
2	D	259	GLU
2	D	260	ASP
2	D	266	VAL
2	D	271	GLU
2	D	272	HIS
2	D	281	ILE
2	D	293	ASP
1	E	901	THR
1	E	909	LYS
1	E	952	THR
1	E	954	ILE
1	E	956	SER
1	E	960	GLU
1	E	969	ARG

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Mol	Chain	Res	Type
1	E	985	PRO
1	E	993	LYS
1	E	1046	LEU
1	E	1052	LEU
1	E	1062	THR
1	E	1063	VAL
1	E	1065	MSE
1	E	1080	ILE
1	E	1083	THR
1	E	1091	SER
1	E	1098	ASN
1	E	1099	PHE
1	E	1130	ASP
1	E	1132	MSE
1	E	1134	SER
1	E	1142	ASP
1	E	1147	PHE
1	E	1153	THR
1	E	1160	ASP
1	E	1164	VAL
1	E	1166	ASP
1	E	1171	SER
1	E	1181	ILE
1	E	1182	ASP
2	F	2	ASP
2	F	3	TYR
2	F	6	ILE
2	F	14	ASN
2	F	16	VAL
2	F	34	LEU
2	F	39	LYS
2	F	41	LEU
2	F	68	ASP
2	F	69	THR
2	F	72	ILE
2	F	73	GLU
2	F	75	LEU
2	F	79	LEU
2	F	84	ASN
2	F	92	LEU
2	F	106	LEU
2	F	115	ASN

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Mol	Chain	Res	Type
2	F	122	THR
2	F	124	LEU
2	F	131	VAL
2	F	138	VAL
2	F	139	SER
2	F	153	GLU
2	F	154	ASP
2	F	162	MSE
2	F	163	ILE
2	F	176	ASN
2	F	184	PHE
2	F	188	GLU
2	F	196	THR
2	F	201	LEU
2	F	211	ARG
2	F	235	ASN
2	F	237	VAL
2	F	249	THR
2	F	257	ASP
2	F	259	GLU
2	F	260	ASP
2	F	266	VAL
2	F	271	GLU
2	F	272	HIS
2	F	281	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	GLN
1	C	1093	HIS
1	C	1101	GLN
2	D	50	GLN
2	F	50	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	303/325 (93%)	-0.02	3 (0%) 79 32	47, 89, 149, 193	0
1	C	303/325 (93%)	0.03	2 (0%) 84 40	56, 111, 177, 201	0
1	E	303/325 (93%)	0.67	30 (9%) 8 2	113, 171, 201, 201	0
2	B	293/310 (94%)	-0.04	0 100 100	44, 96, 169, 188	0
2	D	293/310 (94%)	0.01	1 (0%) 91 60	59, 110, 174, 201	0
2	F	293/310 (94%)	0.41	16 (5%) 24 5	92, 177, 201, 201	0
All	All	1788/1905 (93%)	0.18	52 (2%) 49 11	44, 127, 196, 201	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1197	LEU	5.8
1	A	0	MSE	5.6
1	E	1141	PHE	5.5
2	D	1	MSE	4.4
1	E	1024	MSE	4.1
1	E	1132	MSE	3.7
1	E	1139	ILE	3.6
2	F	70	LYS	3.6
1	E	1129	ALA	3.6
1	E	909	LYS	3.5
2	F	55	LYS	3.4
1	C	1135	ASP	3.2
1	C	1059	GLU	3.2
1	E	1155	LYS	3.1
2	F	89	LEU	3.0
1	E	927	LEU	3.0
1	E	911	PRO	2.9
2	F	1	MSE	2.9
1	E	1149	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	253	MSE	2.9
1	E	1133	ALA	2.8
2	F	227	TYR	2.8
1	E	1099	PHE	2.7
1	E	1199	ILE	2.6
1	E	1138	PRO	2.6
1	E	1140	ASP	2.6
1	E	1146	LYS	2.6
1	A	1132	MSE	2.4
1	E	1044	TYR	2.4
2	F	33	LEU	2.4
2	F	83	GLN	2.4
2	F	160	ASN	2.4
2	F	116	ASP	2.4
1	A	1144	TYR	2.3
2	F	29	THR	2.3
1	E	1147	PHE	2.3
2	F	154	ASP	2.3
1	E	1124	LYS	2.3
1	E	1154	TYR	2.2
1	E	1142	ASP	2.2
1	E	1137	ILE	2.2
2	F	281	ILE	2.2
1	E	920	PHE	2.2
1	E	912	ALA	2.2
2	F	3	TYR	2.2
1	E	1071	TYR	2.1
1	E	1186	MSE	2.1
1	E	1096	HIS	2.1
2	F	187	TYR	2.0
1	E	1160	ASP	2.0
2	F	285	PHE	2.0
1	E	979	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.