



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:16 am BST

PDB ID : 3MV2  
Title : Crystal Structure of a-COP in Complex with e-COP  
Authors : Hoelz, A.; Hsia, K.C.  
Deposited on : 2010-05-03  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

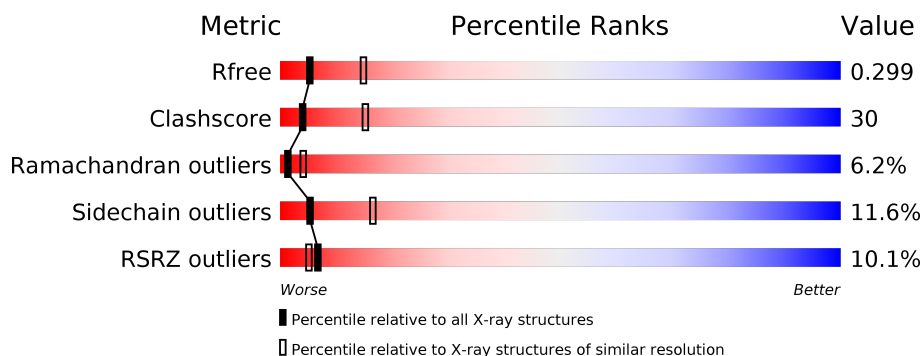
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	<div> <div>2%</div> <div> <div>45%</div> <div>42%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	325	<div> <div>4%</div> <div> <div>49%</div> <div>37%</div> <div>6%</div> <div>7%</div> </div> </div>
1	E	325	<div> <div>14%</div> <div> <div>48%</div> <div>38%</div> <div>7%</div> <div>7%</div> </div> </div>
2	B	310	<div> <div>5%</div> <div> <div>42%</div> <div>43%</div> <div>8%</div> <div>5%</div> </div> </div>
2	D	310	<div> <div>4%</div> <div> <div>39%</div> <div>45%</div> <div>8%</div> <div>5%</div> </div> </div>
2	F	310	<div> <div>28%</div> <div> <div>39%</div> <div>44%</div> <div>9%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14273 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	305	Total	C	N	O	S	0	0	0
			2405	1542	403	449	11			
1	C	303	Total	C	N	O	S	0	0	0
			2388	1531	399	447	11			
1	E	303	Total	C	N	O	S	0	0	0
			2388	1531	399	447	11			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	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	MET	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	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	MET	-	EXPRESSION TAG	UNP P53622
E	-22	MET	-	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	MET	-	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	0	0	0
			2364	1508	371	480	5			
2	D	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			
2	F	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	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	MET	-	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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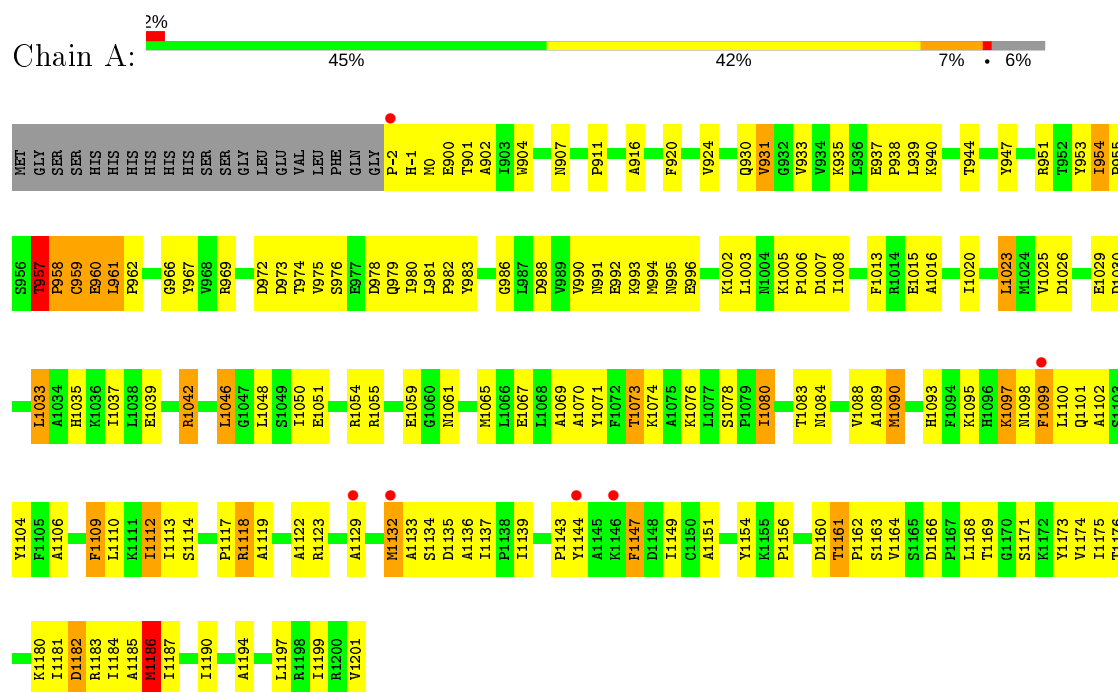
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	-	EXPRESSION TAG	UNP P40509
D	-2	GLN	-	EXPRESSION TAG	UNP P40509
D	-1	ASP	-	EXPRESSION TAG	UNP P40509
D	0	PRO	-	EXPRESSION TAG	UNP P40509
F	-13	MET	-	EXPRESSION TAG	UNP P40509
F	-12	GLY	-	EXPRESSION 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

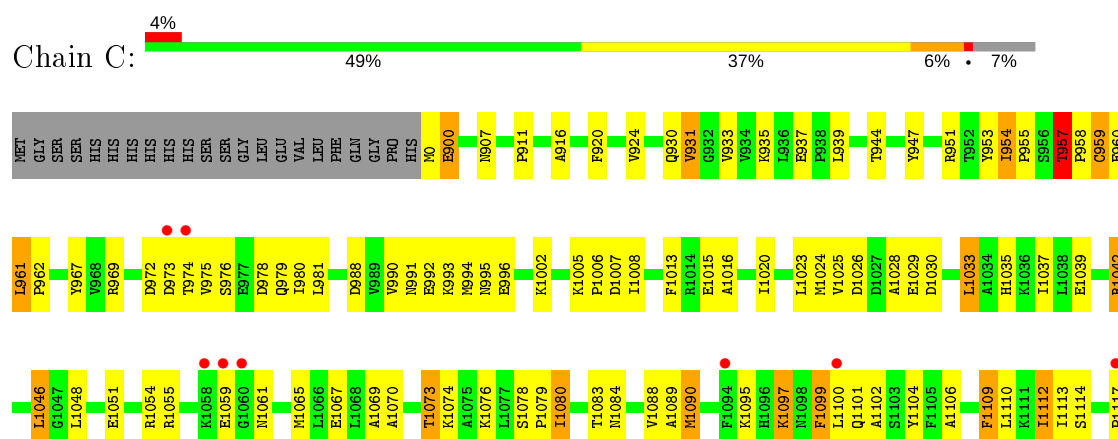
### 3 Residue-property plots [i](#)

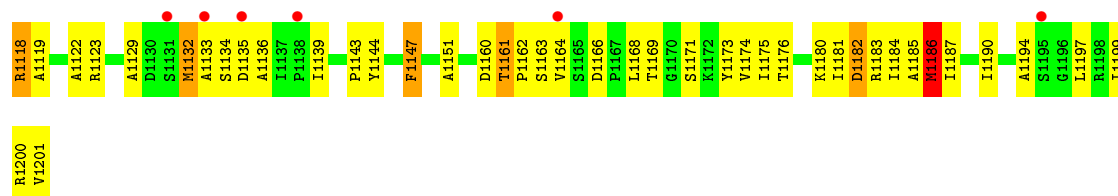
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

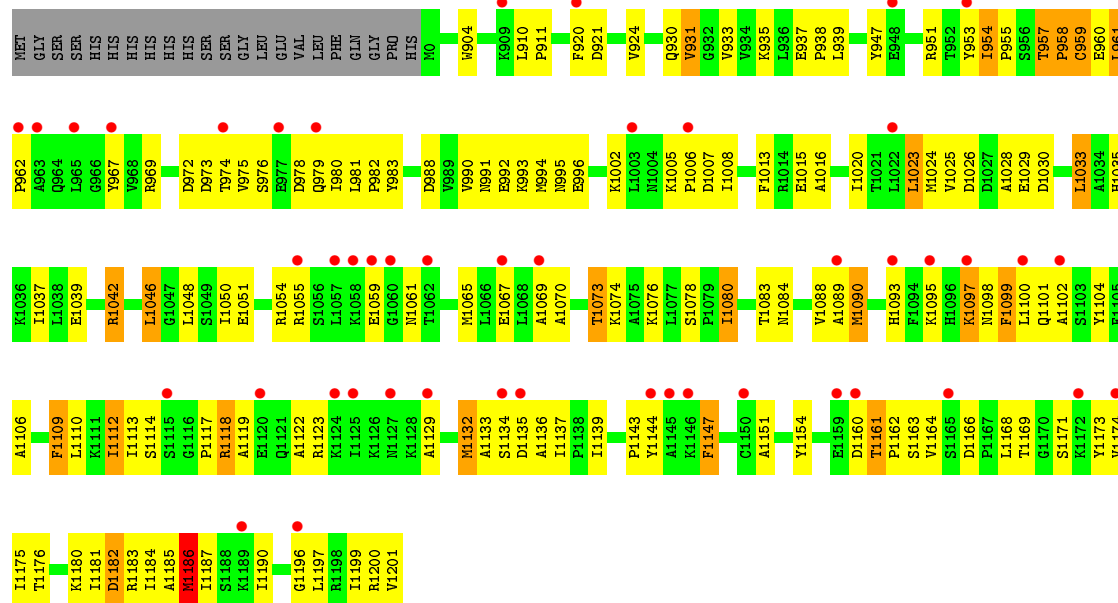


#### • Molecule 1: Coatomer subunit alpha

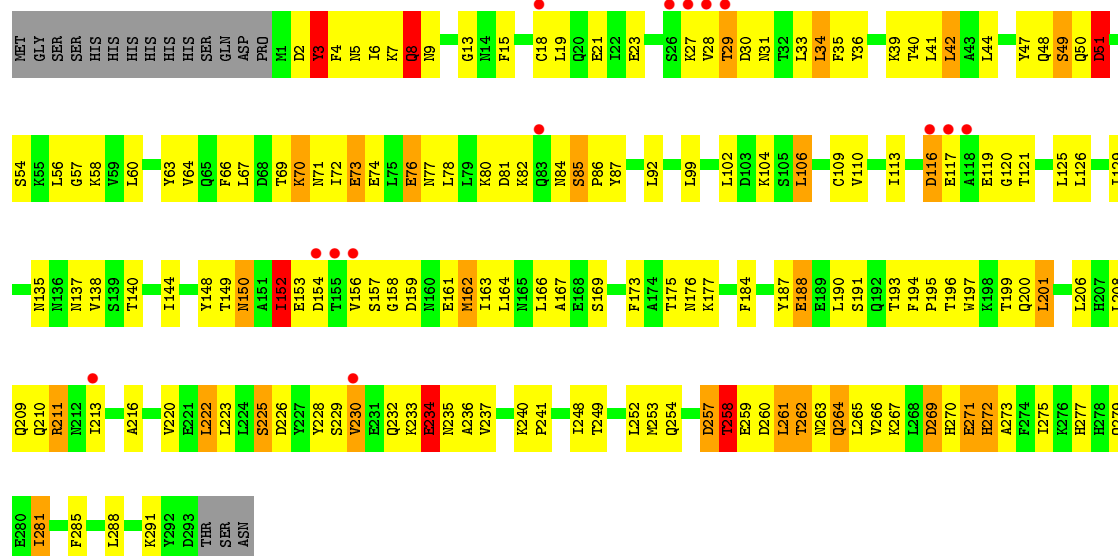
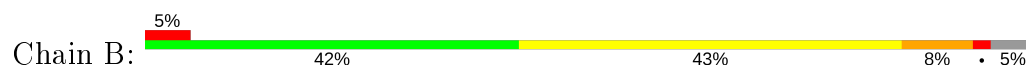




### • Molecule 1: Coatomer subunit alpha

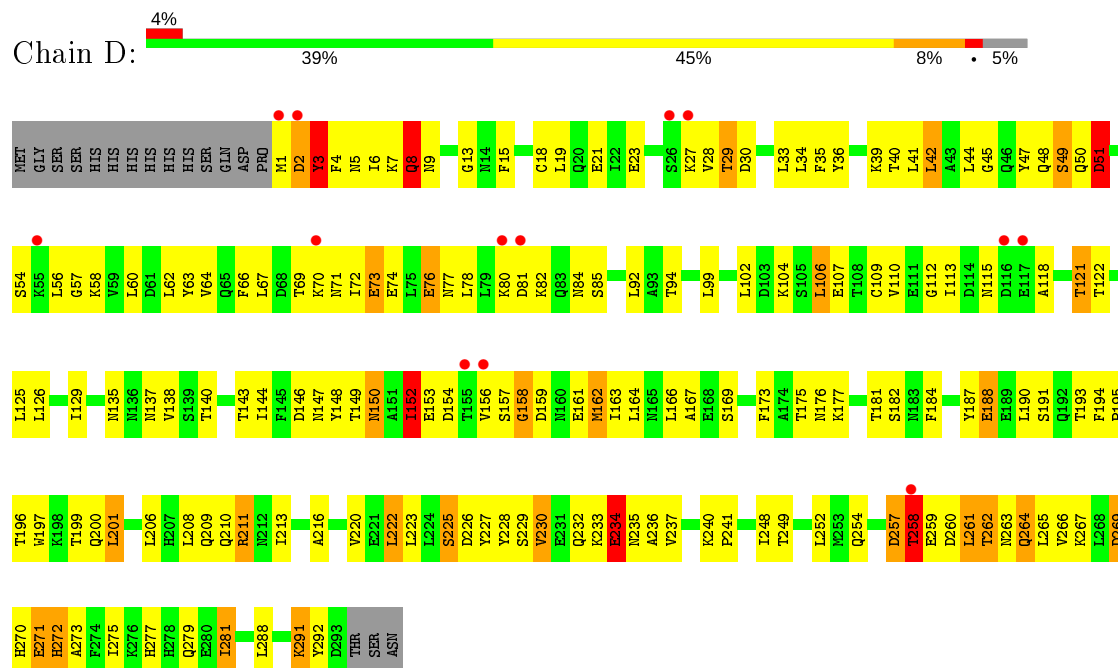


### • Molecule 2: Coatomer subunit epsilon

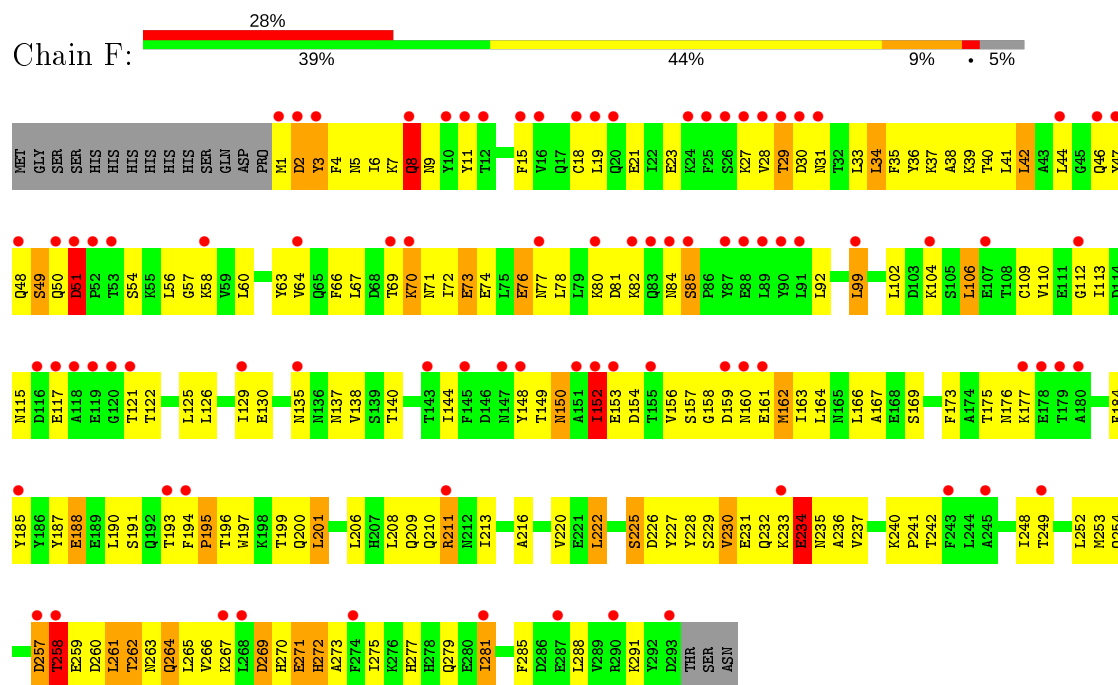




- Molecule 2: Coatomer subunit epsilon



- Molecule 2: Coatomer subunit epsilon



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	329.13Å 74.38Å 97.25Å 90.00° 102.27° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.4 (20.00-2.90) 85.9 (20.02-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.246 , 0.297 0.246 , 0.299	Depositor DCC
$R_{free}$ test set	2080 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 82.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.52	0/2454	0.74	1/3317 (0.0%)
1	C	0.52	0/2435	0.74	1/3291 (0.0%)
1	E	0.49	0/2435	0.73	1/3291 (0.0%)
2	B	0.53	0/2403	0.79	3/3261 (0.1%)
2	D	0.51	0/2403	0.76	1/3261 (0.0%)
2	F	0.49	0/2403	0.76	1/3261 (0.0%)
All	All	0.51	0/14533	0.75	8/19682 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	ASP	CB-CA-C	-5.51	99.39	110.40
2	F	264	GLN	N-CA-C	-5.44	96.31	111.00
2	D	264	GLN	N-CA-C	-5.43	96.34	111.00
2	B	264	GLN	N-CA-C	-5.41	96.40	111.00
1	A	961	LEU	N-CA-C	-5.10	97.23	111.00
1	C	961	LEU	N-CA-C	-5.07	97.31	111.00
1	E	961	LEU	N-CA-C	-5.05	97.37	111.00
2	B	116	ASP	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2405	0	2455	161	0
1	C	2388	0	2441	137	0
1	E	2388	0	2441	148	0
2	B	2364	0	2319	140	0
2	D	2364	0	2319	160	0
2	F	2364	0	2319	165	0
All	All	14273	0	14294	863	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 30.

All (863) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:ASP:OD2	1:A:1169:THR:HB	1.59	1.03
1:E:1166:ASP:OD2	1:E:1169:THR:HB	1.59	1.03
1:C:1166:ASP:OD2	1:C:1169:THR:HB	1.59	1.02
2:D:248:ILE:HD11	2:D:263:ASN:HB3	1.43	0.99
2:F:248:ILE:HD11	2:F:263:ASN:HB3	1.43	0.98
2:D:264:GLN:HA	2:D:264:GLN:OE1	1.65	0.97
2:B:248:ILE:HD11	2:B:263:ASN:HB3	1.44	0.97
1:C:1080:ILE:HB	2:F:227:TYR:CD2	2.02	0.95
2:B:264:GLN:HA	2:B:264:GLN:OE1	1.65	0.94
2:F:264:GLN:HA	2:F:264:GLN:OE1	1.65	0.93
2:F:41:LEU:HB3	2:F:47:TYR:HA	1.49	0.91
1:A:957:THR:HG22	1:A:958:PRO:N	1.82	0.90
2:F:34:LEU:HD11	2:F:57:GLY:CA	2.01	0.90
2:F:277:HIS:O	2:F:281:ILE:HG22	1.72	0.90
1:A:-2:PRO:H3	1:A:901:THR:HG21	1.35	0.90
2:D:277:HIS:O	2:D:281:ILE:HG22	1.72	0.88
2:B:277:HIS:O	2:B:281:ILE:HG22	1.73	0.87
1:C:1080:ILE:HB	2:F:227:TYR:CE2	2.10	0.87
2:F:157:SER:O	2:F:161:GLU:HB2	1.76	0.86
1:C:957:THR:HG22	1:C:958:PRO:N	1.90	0.86
1:E:1074:LYS:HE3	1:E:1147:PHE:HE1	1.40	0.86
1:E:1169:THR:HG22	1:E:1171:SER:H	1.42	0.85
1:C:1169:THR:HG22	1:C:1171:SER:H	1.41	0.85
1:A:1008:ILE:H	1:A:1008:ILE:HD12	1.43	0.84
1:E:1008:ILE:H	1:E:1008:ILE:HD12	1.43	0.83
1:A:-2:PRO:N	1:A:901:THR:HG21	1.93	0.83
1:C:1008:ILE:H	1:C:1008:ILE:HD12	1.43	0.83
1:A:1097:LYS:HG3	1:A:1099:PHE:HE1	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:THR:HG22	1:A:1171:SER:H	1.42	0.83
1:E:1097:LYS:HG3	1:E:1099:PHE:HE1	1.43	0.83
1:E:1074:LYS:HE3	1:E:1147:PHE:CE1	2.15	0.82
2:B:157:SER:O	2:B:161:GLU:HB2	1.80	0.81
2:B:248:ILE:CD1	2:B:263:ASN:HB3	2.10	0.81
2:D:252:LEU:HD21	2:D:259:GLU:HG3	1.62	0.81
1:C:1028:ALA:HB2	1:C:1200:ARG:HH12	1.44	0.81
2:D:216:ALA:O	2:D:220:VAL:HG23	1.81	0.81
2:F:216:ALA:O	2:F:220:VAL:HG23	1.81	0.81
1:E:957:THR:HG22	1:E:958:PRO:N	1.94	0.81
1:A:-2:PRO:CA	1:A:901:THR:HG21	2.10	0.80
1:C:1097:LYS:HG3	1:C:1099:PHE:HE1	1.43	0.80
2:F:248:ILE:CD1	2:F:263:ASN:HB3	2.10	0.80
1:A:1113:ILE:HG23	2:D:150:ASN:ND2	1.97	0.80
2:B:252:LEU:HD21	2:B:259:GLU:HG3	1.63	0.80
2:F:252:LEU:HD21	2:F:259:GLU:HG3	1.62	0.80
2:B:216:ALA:O	2:B:220:VAL:HG23	1.81	0.80
2:D:248:ILE:CD1	2:D:263:ASN:HB3	2.10	0.80
1:E:1100:LEU:HD22	1:E:1135:ASP:OD1	1.81	0.80
1:A:-2:PRO:HA	1:A:901:THR:HG21	1.65	0.79
2:D:60:LEU:O	2:D:64:VAL:HG23	1.83	0.79
1:C:1005:LYS:HB3	1:C:1008:ILE:HD13	1.64	0.78
2:F:60:LEU:O	2:F:64:VAL:HG23	1.83	0.78
1:E:1005:LYS:HB3	1:E:1008:ILE:HD13	1.64	0.78
1:E:931:VAL:HG12	1:E:933:VAL:HG23	1.66	0.78
2:B:60:LEU:O	2:B:64:VAL:HG23	1.84	0.78
1:A:1005:LYS:HB3	1:A:1008:ILE:HD13	1.64	0.78
2:B:50:GLN:O	2:B:51:ASP:HB3	1.83	0.77
1:A:931:VAL:HG12	1:A:933:VAL:HG23	1.66	0.77
1:A:931:VAL:HG13	1:A:1168:LEU:HB2	1.67	0.77
2:F:50:GLN:O	2:F:51:ASP:HB3	1.83	0.77
2:D:227:TYR:HE1	1:E:1113:ILE:CD1	1.98	0.76
1:E:920:PHE:O	1:E:924:VAL:HG23	1.85	0.76
1:C:920:PHE:O	1:C:924:VAL:HG23	1.85	0.76
1:C:1074:LYS:HE3	1:C:1147:PHE:HE1	1.49	0.76
1:A:1118:ARG:HB3	2:D:146:ASP:OD2	1.85	0.76
1:C:931:VAL:HG12	1:C:933:VAL:HG23	1.66	0.76
1:C:1099:PHE:HA	1:C:1102:ALA:HB3	1.69	0.76
1:A:1097:LYS:O	1:A:1136:ALA:HB2	1.86	0.75
2:D:175:THR:HG21	2:D:177:LYS:HD3	1.68	0.75
1:A:920:PHE:O	1:A:924:VAL:HG23	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1074:LYS:HE3	1:C:1147:PHE:CE1	2.20	0.75
2:F:41:LEU:CB	2:F:47:TYR:HA	2.16	0.75
2:B:175:THR:HG21	2:B:177:LYS:HD3	1.68	0.75
2:F:175:THR:HG21	2:F:177:LYS:HD3	1.68	0.75
1:A:944:THR:HA	2:B:281:ILE:HD11	1.68	0.75
2:D:50:GLN:O	2:D:51:ASP:HB3	1.83	0.75
1:E:954:ILE:HD13	1:E:955:PRO:N	2.02	0.75
1:A:954:ILE:HD13	1:A:955:PRO:N	2.02	0.75
1:C:1028:ALA:HB2	1:C:1200:ARG:NH1	2.01	0.75
1:A:1097:LYS:HG3	1:A:1099:PHE:CE1	2.21	0.75
2:B:15:PHE:HB3	2:B:40:THR:HG23	1.69	0.74
1:A:1099:PHE:HA	1:A:1102:ALA:HB3	1.69	0.74
1:E:1097:LYS:HG3	1:E:1099:PHE:CE1	2.21	0.74
2:D:15:PHE:HB3	2:D:40:THR:HG23	1.69	0.74
2:F:38:ALA:HB1	2:F:47:TYR:HE1	1.50	0.74
1:C:954:ILE:HD13	1:C:955:PRO:N	2.02	0.74
1:C:1097:LYS:HG3	1:C:1099:PHE:CE1	2.21	0.74
2:F:15:PHE:HB3	2:F:40:THR:HG23	1.69	0.74
2:F:210:GLN:O	2:F:211:ARG:HB2	1.88	0.73
2:D:57:GLY:HA2	2:D:60:LEU:HD12	1.70	0.73
2:F:57:GLY:HA2	2:F:60:LEU:HD12	1.70	0.73
1:A:1118:ARG:HD2	2:D:146:ASP:OD2	1.87	0.73
2:D:112:GLY:O	2:D:115:ASN:HB2	1.89	0.73
2:B:2:ASP:O	2:B:4:PHE:N	2.20	0.73
2:B:210:GLN:O	2:B:211:ARG:HB2	1.88	0.73
1:E:1099:PHE:HA	1:E:1102:ALA:HB3	1.69	0.73
1:A:1132:MET:O	1:A:1134:SER:N	2.22	0.73
2:B:275:ILE:O	2:B:279:GLN:HG3	1.89	0.73
2:F:112:GLY:O	2:F:115:ASN:HB2	1.88	0.73
2:D:210:GLN:O	2:D:211:ARG:HB2	1.88	0.73
2:D:275:ILE:O	2:D:279:GLN:HG3	1.89	0.73
1:A:-2:PRO:HA	1:A:901:THR:CG2	2.19	0.72
1:E:938:PRO:HG2	1:E:1187:ILE:HD11	1.70	0.72
1:C:972:ASP:O	1:C:974:THR:N	2.22	0.72
1:C:1090:MET:HG3	1:C:1106:ALA:HB2	1.72	0.72
1:A:1181:ILE:O	1:A:1181:ILE:HD12	1.90	0.72
1:C:1181:ILE:O	1:C:1181:ILE:HD12	1.90	0.72
1:E:1097:LYS:O	1:E:1136:ALA:HB2	1.90	0.72
1:A:-1:HIS:H	1:A:901:THR:HB	1.55	0.71
1:A:972:ASP:O	1:A:974:THR:N	2.22	0.71
1:E:947:TYR:CD2	2:F:281:ILE:HD12	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:972:ASP:O	1:E:974:THR:N	2.22	0.71
2:F:275:ILE:O	2:F:279:GLN:HG3	1.89	0.71
1:E:1181:ILE:HD12	1:E:1181:ILE:O	1.90	0.71
1:C:931:VAL:HG13	1:C:1168:LEU:HB2	1.73	0.71
1:A:1090:MET:HG3	1:A:1106:ALA:HB2	1.72	0.71
1:E:1067:GLU:HG3	1:E:1139:ILE:HG22	1.71	0.71
2:B:57:GLY:HA2	2:B:60:LEU:HD12	1.70	0.71
1:A:957:THR:CG2	1:A:958:PRO:N	2.54	0.71
1:E:1090:MET:HG3	1:E:1106:ALA:HB2	1.72	0.71
1:E:1113:ILE:CG2	1:E:1119:ALA:HB2	2.21	0.70
1:C:1113:ILE:CG2	1:C:1119:ALA:HB2	2.21	0.70
1:A:1113:ILE:CG2	1:A:1119:ALA:HB2	2.21	0.70
2:F:196:THR:HG22	2:F:197:TRP:H	1.56	0.70
1:A:1074:LYS:HE3	1:A:1147:PHE:HE1	1.57	0.70
2:B:19:LEU:O	2:B:23:GLU:HG2	1.92	0.69
1:C:1113:ILE:HD12	2:F:231:GLU:HB3	1.74	0.69
1:A:1070:ALA:O	1:A:1073:THR:HB	1.92	0.69
2:B:106:LEU:O	2:B:110:VAL:HG23	1.92	0.69
2:D:19:LEU:O	2:D:23:GLU:HG2	1.92	0.69
2:F:19:LEU:O	2:F:23:GLU:HG2	1.92	0.69
2:B:196:THR:HG22	2:B:197:TRP:H	1.56	0.69
1:C:1070:ALA:O	1:C:1073:THR:HB	1.92	0.69
1:E:1151:ALA:HB3	1:E:1173:TYR:CE2	2.28	0.69
2:F:106:LEU:O	2:F:110:VAL:HG23	1.92	0.69
2:D:196:THR:HG22	2:D:197:TRP:H	1.56	0.69
2:D:106:LEU:O	2:D:110:VAL:HG23	1.92	0.69
2:B:196:THR:HG22	2:B:197:TRP:N	2.08	0.69
1:C:1151:ALA:HB3	1:C:1173:TYR:CE2	2.28	0.69
2:F:28:VAL:HG12	2:F:28:VAL:O	1.93	0.69
1:A:1151:ALA:HB3	1:A:1173:TYR:CE2	2.28	0.68
1:E:1070:ALA:O	1:E:1073:THR:HB	1.92	0.68
2:D:28:VAL:HG12	2:D:28:VAL:O	1.93	0.68
1:C:1132:MET:O	1:C:1134:SER:N	2.27	0.68
2:F:196:THR:HG22	2:F:197:TRP:N	2.08	0.68
2:B:28:VAL:HG12	2:B:28:VAL:O	1.93	0.68
2:D:196:THR:HG22	2:D:197:TRP:N	2.08	0.68
1:C:957:THR:HG22	1:C:958:PRO:CD	2.24	0.68
2:F:1:MET:C	2:F:3:TYR:H	1.95	0.68
2:D:222:LEU:O	2:D:225:SER:HB3	1.94	0.68
2:F:222:LEU:O	2:F:225:SER:HB3	1.94	0.68
2:F:44:LEU:HA	2:F:234:GLU:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:PHE:HD1	1:A:1134:SER:HB3	1.58	0.67
1:C:944:THR:HA	2:D:281:ILE:HD11	1.75	0.67
1:E:957:THR:HB	2:F:130:GLU:OE2	1.95	0.67
2:B:222:LEU:O	2:B:225:SER:HB3	1.95	0.67
1:E:1099:PHE:HD1	1:E:1134:SER:HB3	1.60	0.67
1:A:1006:PRO:HB3	1:A:1048:LEU:HD22	1.77	0.67
1:A:957:THR:HG22	1:A:958:PRO:CD	2.25	0.67
2:F:41:LEU:HB3	2:F:47:TYR:CA	2.25	0.67
2:B:15:PHE:HB2	2:B:44:LEU:HD21	1.77	0.66
1:E:1008:ILE:N	1:E:1008:ILE:HD12	2.10	0.66
1:C:1100:LEU:HD22	1:C:1135:ASP:OD1	1.95	0.66
1:C:1197:LEU:HD21	1:C:1199:ILE:HD11	1.76	0.66
1:E:1006:PRO:HB3	1:E:1048:LEU:HD22	1.77	0.66
1:A:1100:LEU:HD22	1:A:1135:ASP:OD1	1.94	0.66
1:C:1006:PRO:HB3	1:C:1048:LEU:HD22	1.77	0.66
1:C:1008:ILE:HD12	1:C:1008:ILE:N	2.10	0.66
2:D:227:TYR:CE1	1:E:1113:ILE:CD1	2.78	0.66
1:A:1197:LEU:HD21	1:A:1199:ILE:HD11	1.77	0.66
1:E:1132:MET:O	1:E:1134:SER:N	2.29	0.66
1:E:1100:LEU:HB2	1:E:1134:SER:O	1.95	0.65
2:F:190:LEU:HB3	2:F:199:THR:HG22	1.78	0.65
2:F:15:PHE:HB2	2:F:44:LEU:HD21	1.78	0.65
1:E:1197:LEU:HD21	1:E:1199:ILE:HD11	1.77	0.65
2:D:15:PHE:HB2	2:D:44:LEU:HD21	1.77	0.65
1:C:1109:PHE:HZ	1:C:1118:ARG:HD3	1.62	0.65
2:D:190:LEU:HB3	2:D:199:THR:HG22	1.78	0.64
2:F:257:ASP:O	2:F:259:GLU:N	2.31	0.64
1:A:1074:LYS:HE3	1:A:1147:PHE:CE1	2.32	0.64
2:D:227:TYR:CE1	1:E:1113:ILE:HD11	2.32	0.64
1:A:1008:ILE:N	1:A:1008:ILE:HD12	2.10	0.64
2:B:190:LEU:HB3	2:B:199:THR:HG22	1.78	0.64
2:B:257:ASP:O	2:B:259:GLU:N	2.31	0.64
2:F:8:GLN:O	2:F:8:GLN:HG3	1.98	0.64
1:A:1109:PHE:HZ	1:A:1118:ARG:HD3	1.62	0.64
2:D:257:ASP:O	2:D:259:GLU:N	2.31	0.64
2:F:34:LEU:HD11	2:F:57:GLY:HA3	1.80	0.64
2:F:42:LEU:CD2	2:F:64:VAL:HG13	2.28	0.64
1:A:1169:THR:HG22	1:A:1171:SER:N	2.13	0.63
2:D:227:TYR:HE1	1:E:1113:ILE:HD13	1.61	0.63
1:E:1083:THR:HG21	1:E:1118:ARG:NH1	2.14	0.63
1:A:1083:THR:HG21	1:A:1118:ARG:NH1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ASP:C	2:D:269:ASP:OD1	2.37	0.63
1:C:1104:TYR:CE2	1:C:1143:PRO:HB3	2.33	0.63
1:C:1169:THR:HG22	1:C:1171:SER:N	2.13	0.63
2:B:8:GLN:HG3	2:B:8:GLN:O	1.98	0.62
1:E:1109:PHE:HZ	1:E:1118:ARG:HD3	1.62	0.62
2:F:269:ASP:C	2:F:269:ASP:OD1	2.37	0.62
2:B:269:ASP:C	2:B:269:ASP:OD1	2.37	0.62
1:A:957:THR:O	1:A:959:CYS:N	2.32	0.62
1:C:1083:THR:HG21	1:C:1118:ARG:NH1	2.14	0.62
1:C:1109:PHE:CD2	1:C:1109:PHE:C	2.73	0.62
1:C:1042:ARG:HB2	1:C:1184:ILE:HG21	1.80	0.62
1:A:1003:LEU:HD21	2:D:110:VAL:HG21	1.81	0.62
1:A:1109:PHE:CD2	1:A:1109:PHE:C	2.73	0.62
1:C:957:THR:CG2	1:C:958:PRO:N	2.63	0.62
2:D:8:GLN:O	2:D:8:GLN:HG3	1.98	0.62
2:F:261:LEU:O	2:F:261:LEU:HD12	2.00	0.62
2:F:211:ARG:HG2	2:F:211:ARG:HH11	1.65	0.62
2:D:211:ARG:HH11	2:D:211:ARG:HG2	1.65	0.61
1:E:1169:THR:HG22	1:E:1171:SER:N	2.13	0.61
2:B:211:ARG:HH11	2:B:211:ARG:HG2	1.65	0.61
1:C:924:VAL:HG21	2:D:288:LEU:HD13	1.81	0.61
2:F:125:LEU:HD22	2:F:148:TYR:CD2	2.36	0.61
2:D:3:TYR:HB3	2:D:6:ILE:HD13	1.81	0.61
2:D:261:LEU:O	2:D:261:LEU:HD12	2.00	0.61
2:B:3:TYR:HB3	2:B:6:ILE:HD13	1.81	0.61
2:F:3:TYR:HB3	2:F:6:ILE:HD13	1.81	0.61
1:A:1042:ARG:HB2	1:A:1184:ILE:HG21	1.83	0.61
1:E:1109:PHE:C	1:E:1109:PHE:CD2	2.73	0.61
1:A:1113:ILE:HG21	1:A:1119:ALA:HB2	1.83	0.61
1:E:931:VAL:HG13	1:E:1168:LEU:HB2	1.83	0.60
2:D:125:LEU:HD22	2:D:148:TYR:CD2	2.36	0.60
2:B:85:SER:HB2	2:B:117:GLU:HG3	1.82	0.60
2:B:125:LEU:O	2:B:129:ILE:HD13	2.01	0.60
2:B:261:LEU:HD12	2:B:261:LEU:O	2.00	0.60
1:E:1067:GLU:HA	1:E:1139:ILE:HG21	1.83	0.60
1:C:957:THR:O	1:C:959:CYS:N	2.34	0.60
1:E:957:THR:O	1:E:959:CYS:N	2.34	0.60
1:A:1113:ILE:HG23	2:D:150:ASN:HD21	1.66	0.60
1:C:990:VAL:HG11	1:C:1020:ILE:HD11	1.83	0.60
2:F:125:LEU:O	2:F:129:ILE:HD13	2.01	0.60
2:B:262:THR:HG22	2:B:263:ASN:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:LEU:HD22	2:B:148:TYR:CD2	2.36	0.60
2:F:262:THR:HG22	2:F:263:ASN:N	2.17	0.60
1:A:1113:ILE:HG22	1:A:1119:ALA:HB2	1.84	0.60
1:A:990:VAL:HG11	1:A:1020:ILE:HD11	1.83	0.60
1:E:990:VAL:HG11	1:E:1020:ILE:HD11	1.83	0.60
1:C:1113:ILE:HG21	1:C:1119:ALA:HB2	1.84	0.59
2:D:125:LEU:O	2:D:129:ILE:HD13	2.01	0.59
1:A:1008:ILE:CD1	1:A:1008:ILE:H	2.13	0.59
1:A:1067:GLU:HG3	1:A:1139:ILE:HG22	1.84	0.59
1:E:1113:ILE:HG22	1:E:1119:ALA:HB2	1.84	0.59
1:E:1042:ARG:HB2	1:E:1184:ILE:HG21	1.84	0.59
2:D:262:THR:HG22	2:D:263:ASN:N	2.17	0.59
1:E:1113:ILE:HG21	1:E:1119:ALA:HB2	1.83	0.59
2:F:34:LEU:HD11	2:F:57:GLY:HA2	1.82	0.59
2:F:41:LEU:HD13	2:F:46:GLN:O	2.02	0.59
1:C:933:VAL:HG13	1:C:1187:ILE:HG23	1.85	0.58
2:F:72:ILE:HG13	2:F:99:LEU:CD1	2.33	0.58
1:A:940:LYS:HG3	2:B:285:PHE:CD2	2.39	0.58
2:B:184:PHE:O	2:B:188:GLU:HB2	2.03	0.58
2:D:47:TYR:CE2	2:D:64:VAL:HG21	2.39	0.58
2:B:162:MET:HG2	2:B:163:ILE:N	2.18	0.58
2:D:157:SER:O	2:D:161:GLU:HB2	2.04	0.58
2:D:44:LEU:HD23	2:D:234:GLU:OE1	2.03	0.58
1:C:957:THR:HG22	1:C:958:PRO:HD3	1.85	0.58
2:F:162:MET:HG2	2:F:163:ILE:N	2.18	0.58
2:F:184:PHE:O	2:F:188:GLU:HB2	2.03	0.58
2:F:37:LYS:HE2	2:F:50:GLN:OE1	2.03	0.58
2:D:194:PHE:O	2:D:196:THR:N	2.36	0.58
1:E:1008:ILE:H	1:E:1008:ILE:CD1	2.13	0.58
2:F:47:TYR:CE2	2:F:64:VAL:HG21	2.39	0.58
2:B:194:PHE:O	2:B:196:THR:N	2.36	0.58
1:C:1008:ILE:H	1:C:1008:ILE:CD1	2.13	0.58
1:C:1113:ILE:HG22	1:C:1119:ALA:HB2	1.84	0.58
2:B:47:TYR:CE2	2:B:64:VAL:HG21	2.39	0.57
1:C:1007:ASP:HB2	1:C:1008:ILE:HD12	1.86	0.57
1:C:1025:VAL:CG1	1:C:1030:ASP:HB2	2.35	0.57
2:D:184:PHE:O	2:D:188:GLU:HB2	2.03	0.57
1:E:1007:ASP:HB2	1:E:1008:ILE:HD12	1.86	0.57
1:C:961:LEU:HD13	2:D:94:THR:HG23	1.86	0.57
1:E:1025:VAL:CG1	1:E:1030:ASP:HB2	2.35	0.57
2:F:260:ASP:O	2:F:264:GLN:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:LEU:O	2:B:264:GLN:HB2	2.04	0.57
1:C:1099:PHE:HD1	1:C:1134:SER:HB3	1.70	0.57
2:D:166:LEU:O	2:D:169:SER:HB3	2.05	0.57
2:F:194:PHE:O	2:F:196:THR:N	2.36	0.57
2:F:261:LEU:O	2:F:264:GLN:HB2	2.05	0.57
1:A:1097:LYS:HG2	1:A:1097:LYS:O	2.05	0.57
1:A:930:GLN:O	1:A:1194:ALA:HB1	2.05	0.57
1:A:983:TYR:CE2	2:B:253:MET:HG2	2.40	0.57
2:D:162:MET:HG2	2:D:163:ILE:N	2.18	0.57
2:D:222:LEU:C	2:D:222:LEU:CD2	2.73	0.57
1:E:1097:LYS:HG2	1:E:1097:LYS:O	2.05	0.57
2:F:222:LEU:HD23	2:F:222:LEU:O	2.05	0.57
2:D:109:CYS:O	2:D:113:ILE:HG13	2.05	0.57
1:E:938:PRO:HG2	1:E:1187:ILE:CD1	2.35	0.57
1:A:924:VAL:HG21	2:B:288:LEU:HD13	1.87	0.56
1:C:1067:GLU:HG3	1:C:1139:ILE:HG22	1.87	0.56
2:D:197:TRP:O	2:D:201:LEU:HB2	2.05	0.56
2:D:222:LEU:O	2:D:222:LEU:HD23	2.04	0.56
1:A:1025:VAL:CG1	1:A:1030:ASP:HB2	2.35	0.56
2:B:166:LEU:O	2:B:169:SER:HB3	2.05	0.56
1:C:1097:LYS:HG2	1:C:1097:LYS:O	2.05	0.56
2:F:122:THR:HG21	2:F:160:ASN:HB3	1.87	0.56
2:F:197:TRP:O	2:F:201:LEU:HB2	2.05	0.56
1:A:1007:ASP:HB2	1:A:1008:ILE:HD12	1.86	0.56
2:D:261:LEU:O	2:D:264:GLN:HB2	2.04	0.56
2:F:222:LEU:CD2	2:F:222:LEU:C	2.74	0.56
2:D:260:ASP:O	2:D:264:GLN:HG2	2.05	0.56
2:F:166:LEU:O	2:F:169:SER:HB3	2.05	0.56
2:F:109:CYS:O	2:F:113:ILE:HG13	2.05	0.56
2:B:222:LEU:HD23	2:B:222:LEU:O	2.05	0.56
2:B:260:ASP:O	2:B:264:GLN:HG2	2.05	0.56
1:C:1025:VAL:O	1:C:1201:VAL:HG23	2.06	0.56
2:B:109:CYS:O	2:B:113:ILE:HG13	2.06	0.56
2:D:227:TYR:HE1	1:E:1113:ILE:HD11	1.66	0.56
1:A:1117:PRO:CB	2:D:177:LYS:NZ	2.69	0.56
2:B:222:LEU:CD2	2:B:222:LEU:C	2.74	0.56
1:C:1042:ARG:NH1	1:C:1169:THR:O	2.39	0.55
1:A:1113:ILE:HD12	2:D:150:ASN:ND2	2.21	0.55
2:B:197:TRP:O	2:B:201:LEU:HB2	2.05	0.55
1:A:1117:PRO:CB	2:D:177:LYS:HZ1	2.19	0.55
2:D:118:ALA:O	2:D:121:THR:HB	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:994:MET:HE3	1:E:1016:ALA:HB3	1.88	0.55
1:C:994:MET:HE3	1:C:1016:ALA:HB3	1.89	0.55
2:B:28:VAL:O	2:B:30:ASP:N	2.40	0.55
1:C:1079:PRO:HG3	2:F:195:PRO:HG3	1.89	0.55
2:F:28:VAL:O	2:F:30:ASP:N	2.40	0.55
1:C:1117:PRO:HG2	1:C:1118:ARG:H	1.72	0.54
2:D:28:VAL:O	2:D:30:ASP:N	2.40	0.54
1:E:1117:PRO:HG2	1:E:1118:ARG:H	1.72	0.54
1:E:954:ILE:HD13	1:E:955:PRO:CD	2.37	0.54
1:A:1117:PRO:HG2	1:A:1118:ARG:H	1.72	0.54
1:A:1100:LEU:HB2	1:A:1134:SER:O	2.07	0.54
2:F:230:VAL:O	2:F:233:LYS:HG3	2.08	0.54
2:F:173:PHE:CD1	2:F:209:GLN:NE2	2.76	0.54
1:A:954:ILE:HD13	1:A:955:PRO:CD	2.37	0.54
2:D:230:VAL:O	2:D:233:LYS:HG3	2.08	0.54
1:A:940:LYS:HB2	2:B:285:PHE:CE2	2.43	0.54
2:D:122:THR:HG22	2:D:163:ILE:HG21	1.90	0.54
2:B:230:VAL:O	2:B:233:LYS:HG3	2.08	0.54
1:E:930:GLN:HB3	1:E:1196:GLY:O	2.09	0.54
1:C:954:ILE:HD13	1:C:955:PRO:CD	2.37	0.53
2:B:187:TYR:CD1	2:B:206:LEU:HD21	2.43	0.53
1:E:1093:HIS:NE2	1:E:1139:ILE:CD1	2.72	0.53
2:B:270:HIS:CD2	2:B:272:HIS:HB3	2.43	0.53
2:D:248:ILE:HG12	2:D:262:THR:CG2	2.38	0.53
1:E:1104:TYR:CE2	1:E:1143:PRO:HB3	2.43	0.53
2:F:187:TYR:CD1	2:F:206:LEU:HD21	2.44	0.53
2:B:86:PRO:CD	2:B:117:GLU:HB2	2.38	0.53
2:D:270:HIS:CD2	2:D:272:HIS:HB3	2.44	0.53
1:A:1098:ASN:ND2	1:A:1137:ILE:O	2.37	0.53
1:A:1093:HIS:NE2	1:A:1139:ILE:CD1	2.71	0.53
2:F:270:HIS:CD2	2:F:272:HIS:HB3	2.44	0.53
2:F:42:LEU:HD21	2:F:64:VAL:HG13	1.90	0.53
2:F:248:ILE:HG12	2:F:262:THR:CG2	2.38	0.53
2:D:102:LEU:HB3	2:D:135:ASN:HB2	1.91	0.52
2:D:50:GLN:O	2:D:51:ASP:CB	2.56	0.52
1:E:931:VAL:HG23	1:E:1197:LEU:HA	1.90	0.52
2:B:248:ILE:HG12	2:B:262:THR:CG2	2.39	0.52
2:D:4:PHE:C	2:D:4:PHE:CD2	2.82	0.52
1:A:974:THR:HG22	1:A:974:THR:O	2.10	0.52
2:B:50:GLN:O	2:B:51:ASP:CB	2.55	0.52
2:F:85:SER:HB2	2:F:117:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:TYR:CD1	2:D:206:LEU:HD21	2.44	0.52
1:A:957:THR:HG22	1:A:958:PRO:HD3	1.91	0.52
1:A:994:MET:HE3	1:A:1016:ALA:HB3	1.91	0.52
2:B:4:PHE:CD2	2:B:4:PHE:C	2.82	0.52
1:C:1025:VAL:HG11	1:C:1030:ASP:HB2	1.91	0.52
1:A:900:GLU:OE2	1:A:969:ARG:HD3	2.10	0.52
1:C:954:ILE:C	1:C:954:ILE:HD13	2.30	0.52
1:C:974:THR:HG22	1:C:974:THR:O	2.10	0.52
1:A:1113:ILE:HG23	2:D:150:ASN:CG	2.30	0.52
1:E:1197:LEU:HG	1:E:1199:ILE:HG13	1.92	0.52
2:F:38:ALA:HB1	2:F:47:TYR:CE1	2.39	0.52
1:E:910:LEU:HD11	1:E:1024:MET:HG3	1.92	0.52
1:E:954:ILE:C	1:E:954:ILE:HD13	2.30	0.52
2:F:4:PHE:C	2:F:4:PHE:CD2	2.83	0.52
1:A:1025:VAL:HG11	1:A:1030:ASP:HB2	1.91	0.52
1:C:1083:THR:HG23	1:C:1109:PHE:CE1	2.45	0.52
1:E:1025:VAL:HG11	1:E:1030:ASP:HB2	1.91	0.52
2:F:15:PHE:HB2	2:F:44:LEU:CD2	2.40	0.52
1:A:938:PRO:HG2	1:A:1187:ILE:HD11	1.92	0.51
1:C:1197:LEU:HG	1:C:1199:ILE:HG13	1.92	0.51
2:B:15:PHE:HB2	2:B:44:LEU:CD2	2.40	0.51
2:B:72:ILE:HG22	2:B:76:GLU:HB2	1.92	0.51
1:E:993:LYS:HG2	1:E:1015:GLU:HG2	1.93	0.51
2:F:37:LYS:HD3	2:F:50:GLN:OE1	2.10	0.51
2:F:50:GLN:O	2:F:51:ASP:CB	2.55	0.51
2:B:173:PHE:CD1	2:B:209:GLN:NE2	2.76	0.51
1:A:933:VAL:HG13	1:A:1187:ILE:HG23	1.93	0.51
2:D:258:THR:O	2:D:259:GLU:C	2.49	0.51
1:E:1083:THR:HG23	1:E:1109:PHE:CE1	2.45	0.51
2:F:66:PHE:CE1	2:F:72:ILE:HG12	2.45	0.51
2:D:267:LYS:O	2:D:269:ASP:N	2.40	0.51
1:A:980:ILE:C	1:A:981:LEU:HG	2.31	0.51
2:B:149:THR:HG22	2:B:150:ASN:N	2.25	0.51
2:D:173:PHE:CD1	2:D:209:GLN:NE2	2.76	0.51
2:D:248:ILE:HG12	2:D:262:THR:HG22	1.92	0.51
2:F:72:ILE:HG22	2:F:76:GLU:HB2	1.92	0.51
1:A:1002:LYS:NZ	1:A:1080:ILE:HD11	2.26	0.51
1:A:1083:THR:HG23	1:A:1109:PHE:CE1	2.45	0.51
1:C:1002:LYS:NZ	1:C:1080:ILE:HD11	2.26	0.51
1:C:1143:PRO:HG2	1:C:1144:TYR:CD1	2.45	0.51
2:D:149:THR:HG22	2:D:150:ASN:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1143:PRO:HG2	1:E:1144:TYR:CD1	2.45	0.51
1:E:920:PHE:CD2	2:F:285:PHE:HD1	2.29	0.51
1:C:1025:VAL:O	1:C:1200:ARG:HA	2.11	0.51
1:C:980:ILE:C	1:C:981:LEU:HG	2.31	0.51
1:E:1002:LYS:NZ	1:E:1080:ILE:HD11	2.26	0.51
2:F:248:ILE:HG12	2:F:262:THR:HG22	1.93	0.51
1:C:993:LYS:HG2	1:C:1015:GLU:HG2	1.93	0.51
1:E:974:THR:O	1:E:974:THR:HG22	2.10	0.51
1:A:1197:LEU:HG	1:A:1199:ILE:HG13	1.92	0.51
1:C:916:ALA:O	1:C:951:ARG:NH2	2.44	0.51
2:D:15:PHE:HA	2:D:18:CYS:HB3	1.93	0.51
2:D:72:ILE:O	2:D:72:ILE:HG22	2.11	0.51
2:F:6:ILE:H	2:F:6:ILE:HD12	1.76	0.51
2:F:72:ILE:HG22	2:F:72:ILE:O	2.10	0.51
1:A:1143:PRO:HG2	1:A:1144:TYR:CD1	2.45	0.50
2:D:6:ILE:HD12	2:D:6:ILE:H	1.76	0.50
1:A:954:ILE:HD13	1:A:954:ILE:C	2.30	0.50
2:B:42:LEU:HD21	2:B:64:VAL:HG13	1.92	0.50
2:D:235:ASN:O	2:D:235:ASN:ND2	2.44	0.50
1:E:1093:HIS:NE2	1:E:1139:ILE:HD11	2.27	0.50
2:B:72:ILE:HG22	2:B:72:ILE:O	2.11	0.50
1:C:1100:LEU:HB2	1:C:1134:SER:O	2.12	0.50
1:C:1109:PHE:HD2	1:C:1109:PHE:C	2.15	0.50
1:A:1005:LYS:NZ	2:D:107:GLU:OE2	2.44	0.50
1:E:980:ILE:C	1:E:981:LEU:HG	2.31	0.50
2:D:291:LYS:HG2	2:D:292:TYR:CE2	2.47	0.50
1:A:931:VAL:HG11	1:A:1168:LEU:HD13	1.94	0.50
1:A:993:LYS:HG2	1:A:1015:GLU:HG2	1.93	0.50
1:E:1028:ALA:HB2	1:E:1200:ARG:NH1	2.27	0.50
1:E:1025:VAL:HB	1:E:1199:ILE:HG22	1.93	0.50
1:E:957:THR:CG2	1:E:958:PRO:N	2.66	0.50
2:F:15:PHE:HA	2:F:18:CYS:HB3	1.93	0.50
2:F:15:PHE:O	2:F:44:LEU:HD11	2.11	0.50
1:A:1104:TYR:CE2	1:A:1143:PRO:HB3	2.47	0.50
2:B:235:ASN:O	2:B:235:ASN:ND2	2.44	0.50
2:B:248:ILE:HD11	2:B:263:ASN:CB	2.30	0.50
2:D:29:THR:HG22	2:D:29:THR:O	2.12	0.50
2:D:72:ILE:HG22	2:D:76:GLU:HB2	1.92	0.50
2:F:149:THR:HG22	2:F:150:ASN:N	2.26	0.50
2:F:235:ASN:ND2	2:F:235:ASN:O	2.44	0.50
2:B:15:PHE:HA	2:B:18:CYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:THR:O	2:B:259:GLU:C	2.49	0.50
2:F:37:LYS:CE	2:F:50:GLN:OE1	2.59	0.50
1:A:900:GLU:HG2	1:A:967:TYR:CG	2.46	0.50
2:B:191:SER:HA	2:B:199:THR:HB	1.94	0.50
2:D:15:PHE:HB2	2:D:44:LEU:CD2	2.40	0.50
2:B:173:PHE:CE1	2:B:209:GLN:NE2	2.80	0.49
2:B:15:PHE:O	2:B:44:LEU:HD11	2.12	0.49
2:B:6:ILE:H	2:B:6:ILE:HD12	1.77	0.49
1:C:961:LEU:HG	1:C:962:PRO:HD2	1.94	0.49
2:F:29:THR:O	2:F:29:THR:HG22	2.12	0.49
1:A:1069:ALA:O	1:A:1089:ALA:HB2	2.12	0.49
2:B:267:LYS:O	2:B:269:ASP:N	2.40	0.49
2:B:69:THR:O	2:B:70:LYS:C	2.50	0.49
1:C:1069:ALA:O	1:C:1089:ALA:HB2	2.12	0.49
2:D:173:PHE:CE1	2:D:209:GLN:NE2	2.80	0.49
2:F:72:ILE:CG1	2:F:99:LEU:CD1	2.90	0.49
1:C:1097:LYS:O	1:C:1136:ALA:HB2	2.12	0.49
2:F:258:THR:O	2:F:259:GLU:C	2.49	0.49
2:B:248:ILE:HG12	2:B:262:THR:HG22	1.93	0.49
1:C:930:GLN:O	1:C:1194:ALA:HB1	2.12	0.49
2:D:248:ILE:HD11	2:D:263:ASN:CB	2.30	0.49
2:F:1:MET:C	2:F:3:TYR:N	2.64	0.49
2:F:38:ALA:CB	2:F:47:TYR:HE1	2.21	0.49
2:F:72:ILE:HD11	2:F:99:LEU:HD12	1.93	0.49
1:E:1069:ALA:O	1:E:1089:ALA:HB2	2.12	0.49
2:D:15:PHE:O	2:D:44:LEU:HD11	2.12	0.49
1:E:904:TRP:CH2	1:E:982:PRO:HB3	2.47	0.49
2:D:73:GLU:OE1	2:D:73:GLU:HA	2.13	0.49
1:A:1067:GLU:HA	1:A:1139:ILE:HG21	1.95	0.49
2:B:29:THR:O	2:B:29:THR:HG22	2.12	0.49
2:D:13:GLY:HA3	2:D:196:THR:HG21	1.95	0.49
2:F:191:SER:HA	2:F:199:THR:HB	1.95	0.49
1:A:1123:ARG:HG2	1:A:1123:ARG:HH11	1.78	0.48
1:A:1185:ALA:O	1:A:1187:ILE:N	2.46	0.48
1:C:1185:ALA:O	1:C:1187:ILE:N	2.46	0.48
1:E:1185:ALA:O	1:E:1187:ILE:N	2.46	0.48
2:F:104:LYS:HG2	2:F:104:LYS:O	2.13	0.48
1:A:994:MET:HE1	1:A:1013:PHE:HD2	1.78	0.48
1:A:-1:HIS:O	1:A:0:MET:C	2.52	0.48
1:E:961:LEU:HG	1:E:962:PRO:HD2	1.95	0.48
2:F:173:PHE:CE1	2:F:209:GLN:NE2	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:LYS:HG2	2:D:104:LYS:O	2.13	0.48
1:E:931:VAL:HG11	1:E:1168:LEU:HD13	1.95	0.48
1:A:1035:HIS:O	1:A:1039:GLU:HG2	2.14	0.48
2:B:102:LEU:HB3	2:B:135:ASN:HB2	1.95	0.48
1:C:1109:PHE:CZ	1:C:1118:ARG:HD3	2.46	0.48
1:C:1123:ARG:HH11	1:C:1123:ARG:HG2	1.78	0.48
2:D:191:SER:HA	2:D:199:THR:HB	1.95	0.48
1:E:1123:ARG:HG2	1:E:1123:ARG:HH11	1.78	0.48
1:C:1035:HIS:O	1:C:1039:GLU:HG2	2.14	0.48
1:A:1080:ILE:HG13	2:D:147:ASN:OD1	2.14	0.48
2:D:2:ASP:O	2:D:159:ASP:OD2	2.31	0.48
1:E:1098:ASN:ND2	1:E:1137:ILE:H	2.12	0.48
1:A:916:ALA:O	1:A:951:ARG:NH2	2.47	0.48
1:E:1042:ARG:CB	1:E:1184:ILE:HG21	2.43	0.48
2:F:66:PHE:CD2	2:F:67:LEU:HD12	2.49	0.48
2:D:240:LYS:N	2:D:241:PRO:HD2	2.29	0.48
1:C:920:PHE:CZ	2:D:281:ILE:HG13	2.49	0.48
1:E:1035:HIS:O	1:E:1039:GLU:HG2	2.14	0.48
1:E:1109:PHE:C	1:E:1109:PHE:HD2	2.15	0.48
2:D:227:TYR:CE1	1:E:1113:ILE:HD13	2.45	0.48
1:C:1029:GLU:HB3	2:F:185:TYR:OH	2.14	0.48
2:B:270:HIS:ND1	2:B:271:GLU:N	2.60	0.48
1:E:976:SER:C	1:E:978:ASP:N	2.67	0.48
1:A:969:ARG:HD2	1:A:980:ILE:HG23	1.95	0.47
2:F:66:PHE:HD2	2:F:67:LEU:HD12	1.79	0.47
2:F:72:ILE:HD11	2:F:99:LEU:CD1	2.44	0.47
2:F:73:GLU:OE1	2:F:73:GLU:HA	2.13	0.47
1:A:961:LEU:HG	1:A:962:PRO:HD2	1.95	0.47
2:B:2:ASP:C	2:B:4:PHE:H	2.15	0.47
2:D:230:VAL:C	2:D:232:GLN:H	2.18	0.47
2:D:66:PHE:HD2	2:D:67:LEU:HD12	1.79	0.47
2:B:74:GLU:HA	2:B:77:ASN:HB2	1.96	0.47
1:C:1029:GLU:HG3	2:F:185:TYR:OH	2.14	0.47
2:D:1:MET:C	2:D:3:TYR:H	2.16	0.47
1:E:1051:GLU:O	1:E:1055:ARG:HG3	2.15	0.47
2:B:34:LEU:HD11	2:B:57:GLY:CA	2.45	0.47
1:C:1160:ASP:O	1:C:1161:THR:C	2.53	0.47
1:E:955:PRO:HD3	2:F:242:THR:HG21	1.96	0.47
1:A:1160:ASP:O	1:A:1161:THR:C	2.53	0.47
2:B:5:ASN:O	2:B:6:ILE:C	2.53	0.47
1:C:976:SER:C	1:C:978:ASP:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:969:ARG:HD2	1:E:980:ILE:HG23	1.95	0.47
1:E:983:TYR:CE2	2:F:253:MET:HG2	2.49	0.47
2:B:104:LYS:O	2:B:104:LYS:HG2	2.13	0.47
2:B:66:PHE:CD2	2:B:67:LEU:HD12	2.49	0.47
2:D:66:PHE:CD2	2:D:67:LEU:HD12	2.49	0.47
2:B:222:LEU:HD22	2:B:228:TYR:CD1	2.50	0.47
2:B:73:GLU:HA	2:B:73:GLU:OE1	2.13	0.47
1:A:1109:PHE:HD2	1:A:1109:PHE:C	2.15	0.47
1:A:1113:ILE:HG22	1:A:1119:ALA:CB	2.45	0.47
1:A:1118:ARG:NH2	2:D:143:THR:OG1	2.47	0.47
2:B:117:GLU:OE1	2:B:117:GLU:HA	2.15	0.47
2:B:80:LYS:C	2:B:82:LYS:H	2.18	0.47
1:C:969:ARG:HD2	1:C:980:ILE:HG23	1.95	0.47
2:D:6:ILE:CD1	2:D:6:ILE:H	2.28	0.47
2:F:7:LYS:HE2	2:F:36:TYR:OH	2.15	0.47
2:F:5:ASN:O	2:F:6:ILE:C	2.53	0.47
2:D:48:GLN:O	2:D:50:GLN:NE2	2.48	0.47
1:E:1090:MET:HE3	1:E:1106:ALA:HA	1.97	0.47
2:B:240:LYS:N	2:B:241:PRO:HD2	2.29	0.47
1:C:1051:GLU:O	1:C:1055:ARG:HG3	2.15	0.47
2:D:227:TYR:CE2	1:E:1080:ILE:HB	2.50	0.47
2:D:7:LYS:HE2	2:D:36:TYR:OH	2.15	0.47
1:E:1113:ILE:HG22	1:E:1119:ALA:CB	2.45	0.47
1:A:1025:VAL:O	1:A:1201:VAL:HG23	2.14	0.46
1:A:1051:GLU:O	1:A:1055:ARG:HG3	2.15	0.46
1:A:1101:GLN:O	1:A:1104:TYR:N	2.48	0.46
2:B:66:PHE:HD2	2:B:67:LEU:HD12	1.79	0.46
1:C:1101:GLN:O	1:C:1104:TYR:N	2.48	0.46
2:F:230:VAL:C	2:F:232:GLN:H	2.18	0.46
1:A:1174:VAL:HG23	1:A:1176:THR:HB	1.98	0.46
1:C:900:GLU:OE2	1:C:969:ARG:HD3	2.15	0.46
2:D:80:LYS:C	2:D:82:LYS:H	2.18	0.46
2:F:159:ASP:O	2:F:162:MET:HE1	2.14	0.46
2:F:240:LYS:N	2:F:241:PRO:HD2	2.29	0.46
1:A:1109:PHE:CZ	1:A:1118:ARG:HD3	2.47	0.46
2:D:206:LEU:HD22	2:D:206:LEU:N	2.31	0.46
2:D:5:ASN:O	2:D:6:ILE:C	2.53	0.46
1:E:1160:ASP:O	1:E:1161:THR:C	2.53	0.46
2:F:122:THR:HG22	2:F:163:ILE:HG21	1.97	0.46
2:B:42:LEU:CD2	2:B:64:VAL:HG13	2.46	0.46
2:B:6:ILE:H	2:B:6:ILE:CD1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1101:GLN:O	1:E:1104:TYR:N	2.48	0.46
1:E:1025:VAL:O	1:E:1200:ARG:HA	2.15	0.46
1:A:976:SER:C	1:A:978:ASP:N	2.67	0.46
2:D:74:GLU:HA	2:D:77:ASN:HB2	1.96	0.46
2:F:6:ILE:H	2:F:6:ILE:CD1	2.28	0.46
1:A:947:TYR:CE1	1:A:951:ARG:NH2	2.84	0.46
2:B:206:LEU:HD22	2:B:206:LEU:N	2.31	0.46
2:F:222:LEU:HD22	2:F:228:TYR:CD1	2.50	0.46
2:F:74:GLU:HA	2:F:77:ASN:HB2	1.96	0.46
2:F:80:LYS:C	2:F:82:LYS:H	2.18	0.46
2:B:13:GLY:HA3	2:B:196:THR:HG21	1.97	0.46
2:B:230:VAL:C	2:B:232:GLN:H	2.18	0.46
1:C:1174:VAL:HG23	1:C:1176:THR:HB	1.98	0.46
2:D:62:LEU:HD23	2:D:62:LEU:HA	1.73	0.46
1:A:1042:ARG:NH1	1:A:1169:THR:O	2.49	0.46
1:A:904:TRP:CZ3	1:A:982:PRO:HB3	2.51	0.46
2:F:11:TYR:CE1	2:F:163:ILE:HD11	2.51	0.46
2:B:7:LYS:HE2	2:B:36:TYR:OH	2.15	0.46
2:D:126:LEU:HD12	2:D:167:ALA:HB2	1.98	0.46
2:D:222:LEU:HD22	2:D:228:TYR:CD1	2.51	0.46
2:F:102:LEU:HB3	2:F:135:ASN:HB2	1.99	0.46
2:F:270:HIS:ND1	2:F:271:GLU:N	2.60	0.46
1:A:1093:HIS:NE2	1:A:1139:ILE:HD11	2.31	0.45
2:B:234:GLU:HB3	2:B:235:ASN:H	1.67	0.45
1:E:1180:LYS:O	1:E:1190:ILE:HG13	2.16	0.45
1:E:1028:ALA:HB2	1:E:1200:ARG:HH12	1.80	0.45
2:F:48:GLN:O	2:F:50:GLN:NE2	2.48	0.45
2:F:7:LYS:O	2:F:9:ASN:N	2.49	0.45
2:B:48:GLN:O	2:B:50:GLN:NE2	2.48	0.45
1:C:1113:ILE:HG22	1:C:1119:ALA:CB	2.45	0.45
1:C:1180:LYS:O	1:C:1190:ILE:HG13	2.16	0.45
2:F:267:LYS:O	2:F:269:ASP:N	2.40	0.45
1:C:1084:ASN:O	1:C:1088:VAL:HG23	2.17	0.45
2:F:69:THR:O	2:F:70:LYS:C	2.55	0.45
1:C:0:MET:O	1:C:900:GLU:C	2.54	0.45
1:C:907:ASN:CG	1:C:978:ASP:O	2.54	0.45
2:F:248:ILE:CG1	2:F:262:THR:CG2	2.95	0.45
1:E:920:PHE:HD2	2:F:285:PHE:HD1	1.64	0.45
2:F:3:TYR:CD2	2:F:33:LEU:HD21	2.52	0.45
1:A:1084:ASN:O	1:A:1088:VAL:HG23	2.17	0.45
1:A:907:ASN:CG	1:A:978:ASP:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:ASP:OD1	1:A:972:ASP:N	2.50	0.45
2:B:86:PRO:HD2	2:B:117:GLU:HB2	1.98	0.45
2:B:7:LYS:O	2:B:9:ASN:N	2.49	0.45
2:D:3:TYR:CD2	2:D:33:LEU:HD21	2.52	0.45
1:C:1118:ARG:NH1	2:F:231:GLU:OE2	2.50	0.45
1:A:1180:LYS:O	1:A:1190:ILE:HG13	2.16	0.45
1:A:920:PHE:CZ	2:B:281:ILE:HG13	2.52	0.45
2:B:35:PHE:O	2:B:39:LYS:HB2	2.17	0.45
1:A:951:ARG:NH1	1:A:967:TYR:HE2	2.15	0.45
1:C:1028:ALA:CB	1:C:1200:ARG:NH1	2.76	0.45
2:D:222:LEU:CD2	2:D:222:LEU:O	2.65	0.45
2:D:47:TYR:CZ	2:D:64:VAL:HG21	2.52	0.45
1:E:1067:GLU:HG3	1:E:1139:ILE:CG2	2.42	0.45
1:E:1174:VAL:HG23	1:E:1176:THR:HB	1.97	0.45
2:F:112:GLY:HA2	2:F:115:ASN:HB2	1.99	0.45
2:F:166:LEU:HA	2:F:166:LEU:HD12	1.68	0.45
2:F:63:TYR:O	2:F:66:PHE:HB3	2.17	0.45
2:B:41:LEU:HB3	2:B:47:TYR:HA	1.98	0.45
1:C:1078:SER:OG	1:C:1080:ILE:HG23	2.17	0.45
1:C:1101:GLN:O	1:C:1102:ALA:C	2.55	0.45
2:D:270:HIS:ND1	2:D:271:GLU:N	2.60	0.45
1:E:910:LEU:HD23	1:E:1201:VAL:HA	1.99	0.45
2:B:222:LEU:CD2	2:B:222:LEU:O	2.65	0.45
2:B:3:TYR:CD2	2:B:33:LEU:HD21	2.52	0.45
2:B:63:TYR:O	2:B:66:PHE:HB3	2.17	0.45
2:D:35:PHE:O	2:D:39:LYS:HB2	2.17	0.45
1:E:1084:ASN:O	1:E:1088:VAL:HG23	2.16	0.45
1:E:1109:PHE:CZ	1:E:1118:ARG:HD3	2.46	0.45
1:A:1042:ARG:CB	1:A:1184:ILE:HG21	2.47	0.44
1:A:995:ASN:O	1:A:996:GLU:C	2.56	0.44
1:C:994:MET:HE1	1:C:1013:PHE:HD2	1.82	0.44
1:C:995:ASN:O	1:C:996:GLU:C	2.56	0.44
2:D:159:ASP:O	2:D:162:MET:HE1	2.16	0.44
1:E:1135:ASP:O	1:E:1136:ALA:C	2.56	0.44
1:E:947:TYR:CG	2:F:281:ILE:HD12	2.52	0.44
2:F:54:SER:O	2:F:58:LYS:HB2	2.17	0.44
1:A:-1:HIS:N	1:A:901:THR:HB	2.28	0.44
1:C:972:ASP:N	1:C:972:ASP:OD1	2.50	0.44
2:D:41:LEU:HB3	2:D:47:TYR:HA	1.99	0.44
2:D:54:SER:O	2:D:58:LYS:HB2	2.18	0.44
2:D:7:LYS:O	2:D:9:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:972:ASP:N	1:E:972:ASP:OD1	2.50	0.44
2:F:206:LEU:HD22	2:F:206:LEU:N	2.31	0.44
2:F:35:PHE:O	2:F:39:LYS:HB2	2.17	0.44
2:F:47:TYR:CZ	2:F:64:VAL:HG21	2.53	0.44
1:A:1117:PRO:HB3	2:D:177:LYS:HZ1	1.81	0.44
2:B:248:ILE:CG1	2:B:262:THR:CG2	2.95	0.44
1:C:1090:MET:HE3	1:C:1106:ALA:HA	1.99	0.44
1:E:1078:SER:OG	1:E:1080:ILE:HG23	2.18	0.44
2:F:48:GLN:O	2:F:49:SER:C	2.55	0.44
2:F:6:ILE:HD12	2:F:21:GLU:HB3	2.00	0.44
1:A:1147:PHE:CD1	1:A:1147:PHE:N	2.83	0.44
2:D:248:ILE:CG1	2:D:262:THR:CG2	2.95	0.44
1:E:951:ARG:NH1	1:E:967:TYR:HE2	2.15	0.44
2:F:222:LEU:O	2:F:222:LEU:CD2	2.66	0.44
1:A:1078:SER:OG	1:A:1080:ILE:HG23	2.18	0.44
2:B:126:LEU:HD12	2:B:167:ALA:HB2	2.00	0.44
1:C:1025:VAL:HB	1:C:1199:ILE:HG22	1.99	0.44
2:D:122:THR:HG22	2:D:163:ILE:CG2	2.47	0.44
1:A:1008:ILE:N	1:A:1008:ILE:CD1	2.78	0.44
2:B:47:TYR:CZ	2:B:64:VAL:HG21	2.53	0.44
2:B:54:SER:O	2:B:58:LYS:HB2	2.17	0.44
2:D:63:TYR:O	2:D:66:PHE:HB3	2.17	0.44
1:E:1101:GLN:O	1:E:1102:ALA:C	2.55	0.44
1:A:966:GLY:HA3	2:B:173:PHE:CE2	2.53	0.44
2:B:48:GLN:O	2:B:49:SER:C	2.56	0.44
2:D:181:THR:HB	2:D:182:SER:H	1.52	0.44
1:A:1123:ARG:HG2	1:A:1123:ARG:NH1	2.33	0.44
1:C:1046:LEU:HD22	1:C:1046:LEU:O	2.18	0.44
2:D:265:LEU:O	2:D:269:ASP:HB3	2.18	0.44
2:F:6:ILE:HD12	2:F:6:ILE:N	2.33	0.44
1:C:1135:ASP:O	1:C:1136:ALA:C	2.56	0.43
1:E:994:MET:HE1	1:E:1013:PHE:HD2	1.84	0.43
1:E:1098:ASN:ND2	1:E:1137:ILE:O	2.44	0.43
1:E:1147:PHE:CD1	1:E:1147:PHE:N	2.83	0.43
2:F:152:ILE:HD13	2:F:156:VAL:HG21	2.00	0.43
2:F:31:ASN:OD1	2:F:56:LEU:HD23	2.18	0.43
2:B:152:ILE:CG2	2:B:156:VAL:HB	2.49	0.43
2:B:6:ILE:HD12	2:B:21:GLU:HB3	2.00	0.43
2:D:196:THR:CG2	2:D:197:TRP:N	2.78	0.43
2:D:261:LEU:HD12	2:D:261:LEU:C	2.39	0.43
1:A:1101:GLN:O	1:A:1102:ALA:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:GLY:HA2	1:A:1023:LEU:HD21	1.99	0.43
2:B:140:THR:O	2:B:144:ILE:HG12	2.18	0.43
2:D:166:LEU:HD12	2:D:166:LEU:HA	1.68	0.43
2:D:6:ILE:HD12	2:D:6:ILE:N	2.33	0.43
1:E:1123:ARG:HG2	1:E:1123:ARG:NH1	2.33	0.43
2:F:140:THR:O	2:F:144:ILE:HG12	2.18	0.43
2:F:265:LEU:O	2:F:269:ASP:HB3	2.18	0.43
1:A:1050:ILE:HG12	1:A:1154:TYR:CD2	2.53	0.43
2:B:6:ILE:HD12	2:B:6:ILE:N	2.33	0.43
2:B:72:ILE:O	2:B:73:GLU:C	2.56	0.43
2:D:48:GLN:O	2:D:49:SER:C	2.56	0.43
2:D:6:ILE:HD12	2:D:21:GLU:HB3	2.00	0.43
1:E:910:LEU:CD2	1:E:1201:VAL:HA	2.48	0.43
1:E:991:ASN:O	1:E:992:GLU:C	2.57	0.43
2:F:28:VAL:O	2:F:28:VAL:CG1	2.64	0.43
1:A:1029:GLU:N	1:A:1029:GLU:CD	2.72	0.43
1:A:-2:PRO:CA	1:A:901:THR:CG2	2.84	0.43
2:B:152:ILE:HD13	2:B:156:VAL:HG21	2.00	0.43
1:C:1183:ARG:HD3	1:C:1183:ARG:N	2.34	0.43
2:D:193:THR:HG22	2:D:194:PHE:CE1	2.54	0.43
1:E:1054:ARG:NH2	1:E:1088:VAL:CG1	2.82	0.43
1:E:1183:ARG:N	1:E:1183:ARG:HD3	2.34	0.43
1:E:935:LYS:HE2	1:E:937:GLU:OE1	2.19	0.43
1:A:1099:PHE:HB3	1:A:1129:ALA:HB1	2.00	0.43
1:C:1123:ARG:HG2	1:C:1123:ARG:NH1	2.33	0.43
1:E:1046:LEU:O	1:E:1046:LEU:HD22	2.18	0.43
2:F:261:LEU:C	2:F:261:LEU:HD12	2.39	0.43
1:A:939:LEU:HD12	1:A:939:LEU:HA	1.87	0.43
1:C:1099:PHE:HB3	1:C:1129:ALA:HB1	2.00	0.43
1:E:904:TRP:CZ3	1:E:982:PRO:HB3	2.54	0.43
1:A:1046:LEU:HD22	1:A:1046:LEU:O	2.18	0.43
1:A:1135:ASP:O	1:A:1136:ALA:C	2.56	0.43
1:C:991:ASN:O	1:C:992:GLU:C	2.57	0.43
2:D:42:LEU:HD21	2:D:64:VAL:HG13	2.01	0.43
2:F:193:THR:HG22	2:F:194:PHE:CE1	2.53	0.43
2:F:196:THR:H	2:F:199:THR:HG1	1.67	0.43
2:F:72:ILE:O	2:F:73:GLU:C	2.56	0.43
2:B:31:ASN:HB2	2:B:119:GLU:OE2	2.19	0.43
2:B:166:LEU:HA	2:B:166:LEU:HD12	1.68	0.43
2:B:193:THR:HG22	2:B:194:PHE:CE1	2.53	0.43
1:C:1029:GLU:CG	2:F:185:TYR:OH	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:947:TYR:CE1	1:C:951:ARG:NH2	2.87	0.43
1:C:951:ARG:NH1	1:C:967:TYR:HE2	2.16	0.43
2:D:126:LEU:CD1	2:D:167:ALA:HB2	2.49	0.43
2:D:54:SER:C	2:D:56:LEU:H	2.23	0.43
2:F:152:ILE:CG2	2:F:156:VAL:HB	2.49	0.43
2:F:222:LEU:HD23	2:F:222:LEU:C	2.40	0.43
1:A:1054:ARG:NH2	1:A:1088:VAL:CG1	2.82	0.43
2:B:44:LEU:HA	2:B:234:GLU:OE1	2.19	0.43
2:B:87:TYR:CE2	2:B:120:GLY:HA2	2.54	0.43
1:C:1054:ARG:NH2	1:C:1088:VAL:CG1	2.81	0.43
2:D:140:THR:O	2:D:144:ILE:HG12	2.19	0.43
2:D:72:ILE:O	2:D:73:GLU:C	2.56	0.43
1:A:1112:ILE:HG22	1:A:1112:ILE:O	2.19	0.42
2:B:261:LEU:HD12	2:B:261:LEU:C	2.39	0.42
2:D:152:ILE:CG2	2:D:156:VAL:HB	2.48	0.42
1:E:1029:GLU:CD	1:E:1029:GLU:N	2.72	0.42
2:F:248:ILE:HD11	2:F:263:ASN:CB	2.30	0.42
2:B:196:THR:H	2:B:199:THR:HG1	1.67	0.42
2:D:152:ILE:HD13	2:D:156:VAL:HG21	2.00	0.42
2:D:208:LEU:HA	2:D:208:LEU:HD23	1.82	0.42
1:E:1033:LEU:CD2	1:E:1037:ILE:HG13	2.50	0.42
1:A:1033:LEU:CD2	1:A:1037:ILE:HG13	2.50	0.42
2:B:222:LEU:HD23	2:B:222:LEU:C	2.39	0.42
1:C:1147:PHE:N	1:C:1147:PHE:CD1	2.83	0.42
1:C:931:VAL:HG11	1:C:1168:LEU:HD13	2.02	0.42
2:D:291:LYS:O	2:D:292:TYR:CD2	2.73	0.42
1:E:1008:ILE:N	1:E:1008:ILE:CD1	2.78	0.42
2:F:175:THR:HG22	2:F:177:LYS:HB3	2.02	0.42
1:A:1163:SER:N	1:A:1175:ILE:HD11	2.35	0.42
1:C:935:LYS:HE2	1:C:937:GLU:OE1	2.19	0.42
1:E:1099:PHE:HB3	1:E:1129:ALA:HB1	2.00	0.42
2:F:122:THR:HG22	2:F:163:ILE:CG2	2.50	0.42
2:B:265:LEU:O	2:B:269:ASP:HB3	2.18	0.42
1:C:975:VAL:HG12	1:C:979:GLN:HB3	2.02	0.42
1:E:1033:LEU:O	1:E:1033:LEU:HD23	2.20	0.42
1:E:1182:ASP:OD2	1:E:1184:ILE:HB	2.20	0.42
2:F:54:SER:C	2:F:56:LEU:H	2.23	0.42
1:A:1183:ARG:HD3	1:A:1183:ARG:N	2.34	0.42
2:B:159:ASP:O	2:B:162:MET:HE1	2.20	0.42
1:C:1033:LEU:HD23	1:C:1033:LEU:O	2.20	0.42
1:C:1166:ASP:OD2	1:C:1169:THR:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:933:VAL:HG22	1:C:1187:ILE:CG2	2.49	0.42
2:D:222:LEU:C	2:D:222:LEU:HD23	2.39	0.42
1:A:1033:LEU:HD23	1:A:1033:LEU:O	2.20	0.42
1:A:991:ASN:O	1:A:992:GLU:C	2.57	0.42
1:C:1042:ARG:CB	1:C:1184:ILE:HG21	2.47	0.42
2:D:175:THR:HG22	2:D:177:LYS:HB3	2.02	0.42
1:E:1074:LYS:HG3	1:E:1147:PHE:CE1	2.54	0.42
2:F:2:ASP:C	2:F:3:TYR:CD1	2.93	0.42
1:A:935:LYS:HE2	1:A:937:GLU:OE1	2.19	0.42
1:A:953:TYR:CD1	1:A:953:TYR:N	2.88	0.42
1:A:960:GLU:OE1	2:B:63:TYR:OH	2.35	0.42
2:B:208:LEU:HA	2:B:208:LEU:HD23	1.82	0.42
1:C:1182:ASP:OD2	1:C:1184:ILE:HB	2.20	0.42
1:E:995:ASN:O	1:E:996:GLU:C	2.56	0.42
2:F:37:LYS:CD	2:F:50:GLN:OE1	2.68	0.42
1:A:1162:PRO:C	1:A:1175:ILE:HD11	2.41	0.42
1:A:1166:ASP:OD2	1:A:1169:THR:CB	2.49	0.42
1:C:1112:ILE:O	1:C:1112:ILE:HG22	2.20	0.42
2:D:234:GLU:HB3	2:D:235:ASN:H	1.67	0.42
2:D:44:LEU:O	2:D:45:GLY:C	2.58	0.42
1:A:1110:LEU:HD21	1:A:1122:ALA:HB3	2.02	0.41
1:A:1182:ASP:OD2	1:A:1184:ILE:HB	2.20	0.41
1:E:1185:ALA:O	1:E:1186:MET:C	2.58	0.41
1:C:1185:ALA:O	1:C:1186:MET:C	2.58	0.41
1:E:994:MET:HE3	1:E:1016:ALA:CB	2.50	0.41
1:A:-2:PRO:HA	1:A:901:THR:HG22	1.99	0.41
1:E:1162:PRO:C	1:E:1175:ILE:HD11	2.41	0.41
1:E:975:VAL:HG12	1:E:979:GLN:HB3	2.02	0.41
1:A:1071:TYR:CZ	1:A:1156:PRO:HD3	2.55	0.41
1:A:1090:MET:HE3	1:A:1106:ALA:HA	2.03	0.41
1:A:1185:ALA:O	1:A:1186:MET:C	2.58	0.41
2:B:56:LEU:C	2:B:58:LYS:N	2.73	0.41
1:C:981:LEU:HD13	1:C:1024:MET:HE1	2.02	0.41
1:C:1110:LEU:HD21	1:C:1122:ALA:HB3	2.02	0.41
1:E:1110:LEU:HD21	1:E:1122:ALA:HB3	2.02	0.41
1:E:1163:SER:N	1:E:1175:ILE:HD11	2.35	0.41
1:E:957:THR:HG22	1:E:958:PRO:CD	2.49	0.41
1:C:953:TYR:CD1	1:C:953:TYR:N	2.88	0.41
1:E:1112:ILE:HG22	1:E:1112:ILE:O	2.20	0.41
1:E:1186:MET:SD	1:E:1186:MET:N	2.94	0.41
2:B:197:TRP:NE1	2:B:236:ALA:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:994:MET:HE3	1:C:1016:ALA:CB	2.51	0.41
2:D:197:TRP:NE1	2:D:236:ALA:HB2	2.36	0.41
1:E:953:TYR:CD1	1:E:953:TYR:N	2.88	0.41
2:F:34:LEU:HD11	2:F:57:GLY:N	2.33	0.41
2:B:196:THR:O	2:B:200:GLN:HB2	2.21	0.41
2:B:71:ASN:OD1	2:B:73:GLU:HB2	2.21	0.41
1:C:939:LEU:HD22	1:C:1187:ILE:HD12	2.02	0.41
1:E:980:ILE:HG22	1:E:980:ILE:O	2.19	0.41
2:F:56:LEU:C	2:F:58:LYS:N	2.74	0.41
1:A:920:PHE:N	1:A:920:PHE:CD1	2.89	0.41
1:C:1090:MET:CE	1:C:1106:ALA:HA	2.51	0.41
2:D:223:LEU:HD23	2:D:223:LEU:HA	1.83	0.41
2:D:210:GLN:O	2:D:211:ARG:CB	2.63	0.41
2:D:291:LYS:HG2	2:D:292:TYR:CD2	2.55	0.41
1:E:920:PHE:N	1:E:920:PHE:CD1	2.89	0.41
1:E:939:LEU:HD12	1:E:939:LEU:HA	1.88	0.41
2:F:28:VAL:C	2:F:30:ASP:N	2.74	0.41
2:B:210:GLN:O	2:B:211:ARG:CB	2.63	0.41
2:B:257:ASP:C	2:B:259:GLU:N	2.75	0.41
2:D:71:ASN:OD1	2:D:73:GLU:HB2	2.20	0.41
1:E:1090:MET:CE	1:E:1106:ALA:HA	2.51	0.41
2:F:196:THR:O	2:F:200:GLN:HB2	2.20	0.41
2:B:223:LEU:HD23	2:B:223:LEU:HA	1.83	0.41
2:B:54:SER:C	2:B:56:LEU:H	2.22	0.41
1:A:975:VAL:HG12	1:A:979:GLN:HB3	2.02	0.40
1:A:980:ILE:O	1:A:980:ILE:HG22	2.19	0.40
2:B:222:LEU:HD21	2:B:228:TYR:CE1	2.56	0.40
2:F:222:LEU:HD21	2:F:228:TYR:CE1	2.57	0.40
2:F:71:ASN:OD1	2:F:73:GLU:HB2	2.21	0.40
2:B:206:LEU:HD22	2:B:206:LEU:H	1.86	0.40
1:C:1163:SER:N	1:C:1175:ILE:HD11	2.35	0.40
1:C:1162:PRO:C	1:C:1175:ILE:HD11	2.41	0.40
1:C:920:PHE:N	1:C:920:PHE:CD1	2.89	0.40
2:D:196:THR:O	2:D:200:GLN:HB2	2.20	0.40
2:D:69:THR:O	2:D:70:LYS:C	2.59	0.40
1:E:921:ASP:N	2:F:288:LEU:HD11	2.36	0.40
1:A:901:THR:HG22	1:A:902:ALA:N	2.37	0.40
2:B:175:THR:HG22	2:B:177:LYS:HB3	2.02	0.40
1:C:1029:GLU:N	1:C:1029:GLU:CD	2.72	0.40
1:C:1033:LEU:CD2	1:C:1037:ILE:HG13	2.50	0.40
2:D:56:LEU:C	2:D:58:LYS:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:126:LEU:HD12	2:F:167:ALA:HB2	2.03	0.40
1:A:1090:MET:CE	1:A:1106:ALA:HA	2.51	0.40
1:A:1186:MET:SD	1:A:1186:MET:N	2.94	0.40
1:C:933:VAL:HG22	1:C:1187:ILE:HG22	2.02	0.40
2:D:157:SER:O	2:D:158:GLY:C	2.60	0.40
2:D:206:LEU:HD22	2:D:206:LEU:H	1.86	0.40
2:D:222:LEU:HD21	2:D:228:TYR:CE1	2.56	0.40
1:E:1020:ILE:O	1:E:1023:LEU:HB2	2.22	0.40
1:E:1025:VAL:O	1:E:1201:VAL:HG23	2.21	0.40
1:E:1050:ILE:HG12	1:E:1154:TYR:CD2	2.56	0.40
1:A:1071:TYR:HB3	1:A:1149:ILE:HG12	2.02	0.40
2:D:197:TRP:NE1	2:D:236:ALA:CB	2.85	0.40
1:E:957:THR:O	1:E:958:PRO:C	2.58	0.40
2:F:208:LEU:HD23	2:F:208:LEU:HA	1.82	0.40
2:F:197:TRP:NE1	2:F:236:ALA:HB2	2.36	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 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	303/325 (93%)	256 (84%)	32 (11%)	15 (5%)	2	7
1	C	301/325 (93%)	255 (85%)	31 (10%)	15 (5%)	2	7
1	E	301/325 (93%)	255 (85%)	31 (10%)	15 (5%)	2	7
2	B	291/310 (94%)	227 (78%)	41 (14%)	23 (8%)	1	2
2	D	291/310 (94%)	226 (78%)	44 (15%)	21 (7%)	1	3
2	F	291/310 (94%)	228 (78%)	42 (14%)	21 (7%)	1	3
All	All	1778/1905 (93%)	1447 (81%)	221 (12%)	110 (6%)	1	4

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	957	THR
1	A	973	ASP
1	A	1114	SER
1	A	1133	ALA
1	A	1186	MET
2	B	29	THR
2	B	51	ASP
2	B	73	GLU
2	B	234	GLU
2	B	258	THR
1	C	973	ASP
1	C	1114	SER
1	C	1133	ALA
1	C	1186	MET
2	D	29	THR
2	D	51	ASP
2	D	73	GLU
2	D	234	GLU
2	D	258	THR
1	E	973	ASP
1	E	1114	SER
1	E	1133	ALA
1	E	1186	MET
2	F	29	THR
2	F	51	ASP
2	F	73	GLU
2	F	234	GLU
2	F	258	THR
1	A	1076	LYS
1	A	1097	LYS
2	B	3	TYR
2	B	8	GLN
2	B	154	ASP
2	B	195	PRO
2	B	273	ALA
1	C	957	THR
1	C	1076	LYS
1	C	1097	LYS
2	D	8	GLN
2	D	154	ASP
2	D	195	PRO
2	D	273	ALA
1	E	1076	LYS

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Mol	Chain	Res	Type
1	E	1097	LYS
2	F	8	GLN
2	F	70	LYS
2	F	154	ASP
2	F	195	PRO
2	F	273	ALA
1	A	959	CYS
1	A	1095	LYS
1	A	1099	PHE
1	A	1132	MET
2	B	27	LYS
2	B	78	LEU
2	B	116	ASP
2	B	150	ASN
2	B	226	ASP
1	C	959	CYS
1	C	1095	LYS
1	C	1099	PHE
1	C	1132	MET
2	D	27	LYS
2	D	78	LEU
2	D	150	ASN
2	D	158	GLY
2	D	226	ASP
2	D	291	LYS
1	E	957	THR
1	E	959	CYS
1	E	1095	LYS
1	E	1099	PHE
1	E	1132	MET
2	F	27	LYS
2	F	78	LEU
2	F	150	ASN
2	F	226	ASP
2	F	291	LYS
2	B	49	SER
2	B	70	LYS
2	B	269	ASP
2	B	291	LYS
2	D	3	TYR
2	D	49	SER
2	D	152	ILE

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Mol	Chain	Res	Type
2	D	269	ASP
2	F	49	SER
2	F	269	ASP
1	A	958	PRO
2	B	81	ASP
2	B	152	ILE
1	C	900	GLU
2	D	81	ASP
2	F	81	ASP
2	F	152	ILE
1	A	911	PRO
1	C	911	PRO
1	E	911	PRO
2	B	158	GLY
1	A	1161	THR
2	B	230	VAL
1	C	1161	THR
2	D	230	VAL
1	E	1161	THR
2	F	230	VAL
1	A	1112	ILE
1	C	1112	ILE
1	E	1112	ILE
2	F	158	GLY
1	E	958	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	259/276 (94%)	237 (92%)	22 (8%)	10	31
1	C	257/276 (93%)	235 (91%)	22 (9%)	10	30
1	E	257/276 (93%)	236 (92%)	21 (8%)	11	32
2	B	263/279 (94%)	225 (86%)	38 (14%)	3	9
2	D	263/279 (94%)	224 (85%)	39 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	263/279 (94%)	224 (85%)	39 (15%)	<b>3</b> <b>9</b>
All	All	1562/1665 (94%)	1381 (88%)	181 (12%)	<b>5</b> <b>16</b>

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	931	VAL
1	A	954	ILE
1	A	957	THR
1	A	960	GLU
1	A	988	ASP
1	A	1023	LEU
1	A	1026	ASP
1	A	1033	LEU
1	A	1042	ARG
1	A	1046	LEU
1	A	1059	GLU
1	A	1061	ASN
1	A	1065	MET
1	A	1073	THR
1	A	1080	ILE
1	A	1090	MET
1	A	1109	PHE
1	A	1118	ARG
1	A	1147	PHE
1	A	1164	VAL
1	A	1182	ASP
1	A	1186	MET
2	B	3	TYR
2	B	8	GLN
2	B	34	LEU
2	B	42	LEU
2	B	51	ASP
2	B	76	GLU
2	B	84	ASN
2	B	85	SER
2	B	92	LEU
2	B	99	LEU
2	B	106	LEU
2	B	121	THR
2	B	137	ASN
2	B	138	VAL

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Mol	Chain	Res	Type
2	B	152	ILE
2	B	153	GLU
2	B	162	MET
2	B	164	LEU
2	B	176	ASN
2	B	188	GLU
2	B	201	LEU
2	B	211	ARG
2	B	213	ILE
2	B	222	LEU
2	B	225	SER
2	B	229	SER
2	B	234	GLU
2	B	237	VAL
2	B	249	THR
2	B	254	GLN
2	B	257	ASP
2	B	258	THR
2	B	261	LEU
2	B	262	THR
2	B	266	VAL
2	B	271	GLU
2	B	272	HIS
2	B	281	ILE
1	C	931	VAL
1	C	954	ILE
1	C	957	THR
1	C	960	GLU
1	C	988	ASP
1	C	1023	LEU
1	C	1026	ASP
1	C	1033	LEU
1	C	1042	ARG
1	C	1046	LEU
1	C	1059	GLU
1	C	1061	ASN
1	C	1065	MET
1	C	1073	THR
1	C	1080	ILE
1	C	1090	MET
1	C	1109	PHE
1	C	1118	ARG

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Mol	Chain	Res	Type
1	C	1147	PHE
1	C	1164	VAL
1	C	1182	ASP
1	C	1186	MET
2	D	2	ASP
2	D	3	TYR
2	D	8	GLN
2	D	34	LEU
2	D	42	LEU
2	D	51	ASP
2	D	76	GLU
2	D	84	ASN
2	D	85	SER
2	D	92	LEU
2	D	99	LEU
2	D	106	LEU
2	D	121	THR
2	D	137	ASN
2	D	138	VAL
2	D	152	ILE
2	D	153	GLU
2	D	162	MET
2	D	164	LEU
2	D	176	ASN
2	D	188	GLU
2	D	201	LEU
2	D	211	ARG
2	D	213	ILE
2	D	222	LEU
2	D	225	SER
2	D	229	SER
2	D	234	GLU
2	D	237	VAL
2	D	249	THR
2	D	254	GLN
2	D	257	ASP
2	D	258	THR
2	D	261	LEU
2	D	262	THR
2	D	266	VAL
2	D	271	GLU
2	D	272	HIS

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Mol	Chain	Res	Type
2	D	281	ILE
1	E	931	VAL
1	E	954	ILE
1	E	960	GLU
1	E	988	ASP
1	E	1023	LEU
1	E	1026	ASP
1	E	1033	LEU
1	E	1042	ARG
1	E	1046	LEU
1	E	1059	GLU
1	E	1061	ASN
1	E	1065	MET
1	E	1073	THR
1	E	1080	ILE
1	E	1090	MET
1	E	1109	PHE
1	E	1118	ARG
1	E	1147	PHE
1	E	1164	VAL
1	E	1182	ASP
1	E	1186	MET
2	F	2	ASP
2	F	3	TYR
2	F	8	GLN
2	F	34	LEU
2	F	42	LEU
2	F	51	ASP
2	F	76	GLU
2	F	84	ASN
2	F	85	SER
2	F	92	LEU
2	F	99	LEU
2	F	106	LEU
2	F	121	THR
2	F	137	ASN
2	F	138	VAL
2	F	152	ILE
2	F	153	GLU
2	F	162	MET
2	F	164	LEU
2	F	176	ASN

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Mol	Chain	Res	Type
2	F	188	GLU
2	F	201	LEU
2	F	211	ARG
2	F	213	ILE
2	F	222	LEU
2	F	225	SER
2	F	229	SER
2	F	234	GLU
2	F	237	VAL
2	F	249	THR
2	F	254	GLN
2	F	257	ASP
2	F	258	THR
2	F	261	LEU
2	F	262	THR
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	907	ASN
1	A	930	GLN
1	A	1087	GLN
2	B	235	ASN
1	C	907	ASN
1	C	930	GLN
1	C	1087	GLN
2	D	150	ASN
2	D	176	ASN
2	D	235	ASN
1	E	930	GLN
1	E	1087	GLN
1	E	1098	ASN
2	F	160	ASN
2	F	176	ASN
2	F	235	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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 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	305/325 (93%)	-0.17	6 (1%) 65 63	55, 89, 144, 199	0
1	C	303/325 (93%)	0.07	14 (4%) 32 29	57, 97, 167, 201	0
1	E	303/325 (93%)	0.85	47 (15%) 2 1	98, 157, 196, 201	0
2	B	293/310 (94%)	-0.00	14 (4%) 30 27	59, 99, 166, 201	0
2	D	293/310 (94%)	0.11	13 (4%) 34 30	64, 104, 172, 201	0
2	F	293/310 (94%)	1.52	87 (29%) 0 0	106, 179, 201, 201	0
All	All	1790/1905 (93%)	0.39	181 (10%) 7 5	55, 119, 197, 201	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	160	ASN	9.1
2	F	29	THR	8.9
2	F	153	GLU	8.7
2	F	51	ASP	8.6
1	C	1135	ASP	7.6
2	F	70	LYS	7.4
2	F	50	GLN	7.3
2	D	155	THR	7.2
2	F	83	GLN	7.0
1	C	1133	ALA	6.6
2	F	180	ALA	6.2
2	F	178	GLU	6.2
2	F	118	ALA	6.1
2	F	257	ASP	6.1
2	F	20	GLN	6.0
2	F	1	MET	6.0
2	F	58	LYS	5.8
2	F	116	ASP	5.8
2	F	47	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
2	D	258	THR	5.7
1	E	979	GLN	5.7
2	F	48	GLN	5.5
1	A	1144	TYR	5.4
2	B	29	THR	5.4
2	F	151	ALA	5.3
2	F	84	ASN	5.1
2	B	156	VAL	4.9
1	E	1165	SER	4.9
1	E	977	GLU	4.9
2	F	30	ASP	4.8
1	E	1057	LEU	4.8
2	F	31	ASN	4.7
2	F	143	THR	4.7
2	F	27	LYS	4.7
1	E	1135	ASP	4.7
1	E	1093	HIS	4.6
2	F	152	ILE	4.6
1	C	1060	GLY	4.5
2	B	154	ASP	4.4
1	E	1058	LYS	4.4
2	D	81	ASP	4.3
2	F	26	SER	4.3
1	E	1124	LYS	4.2
2	B	155	THR	4.2
2	F	3	TYR	4.2
2	F	2	ASP	4.1
1	E	1144	TYR	4.1
1	E	1196	GLY	4.0
2	F	107	GLU	4.0
2	B	117	GLU	4.0
1	E	1055	ARG	3.8
2	F	161	GLU	3.8
2	D	1	MET	3.8
2	F	15	PHE	3.8
2	F	147	ASN	3.8
1	C	1138	PRO	3.8
1	A	1099	PHE	3.7
2	F	44	LEU	3.7
2	F	53	THR	3.7
2	F	104	LYS	3.6
1	E	1115	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	1097	LYS	3.6
2	F	233	LYS	3.6
1	C	1058	LYS	3.6
1	E	1174	VAL	3.6
2	F	99	LEU	3.5
1	A	-2	PRO	3.5
1	C	1117	PRO	3.5
1	E	1089	ALA	3.5
1	C	1059	GLU	3.4
2	F	28	VAL	3.4
1	E	974	THR	3.4
2	D	26	SER	3.4
2	F	52	PRO	3.4
2	F	179	THR	3.4
2	F	11	TYR	3.3
2	F	177	LYS	3.3
2	F	24	LYS	3.3
2	F	117	GLU	3.3
1	E	962	PRO	3.3
1	E	965	LEU	3.3
1	C	973	ASP	3.2
2	B	116	ASP	3.2
1	E	1146	LYS	3.2
2	F	91	LEU	3.2
2	D	27	LYS	3.1
2	F	121	THR	3.1
1	E	1022	LEU	3.0
1	E	909	LYS	3.0
2	F	10	TYR	3.0
2	F	194	PHE	3.0
1	E	963	ALA	3.0
1	E	1067	GLU	3.0
2	F	258	THR	3.0
2	F	46	GLN	3.0
2	F	281	ILE	3.0
1	E	1059	GLU	2.9
2	F	185	TYR	2.9
2	F	16	VAL	2.9
1	E	1100	LEU	2.9
1	E	967	TYR	2.9
2	B	27	LYS	2.8
1	E	1060	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	1127	ASN	2.8
2	F	18	CYS	2.8
2	F	64	VAL	2.8
2	F	155	THR	2.8
1	E	1003	LEU	2.8
2	B	26	SER	2.8
2	F	159	ASP	2.7
2	D	156	VAL	2.7
2	F	25	PHE	2.7
2	F	112	GLY	2.7
2	F	267	LYS	2.7
2	B	18	CYS	2.6
2	F	287	GLU	2.6
1	C	1094	PHE	2.6
2	F	129	ILE	2.6
2	B	118	ALA	2.6
2	D	2	ASP	2.6
1	E	1160	ASP	2.6
1	E	1129	ALA	2.6
2	F	135	ASN	2.6
2	D	80	LYS	2.5
2	F	293	ASP	2.5
2	F	12	THR	2.5
2	F	268	LEU	2.5
1	E	1125	ILE	2.5
2	F	19	LEU	2.5
2	F	120	GLY	2.5
1	A	1146	LYS	2.5
1	E	1150	CYS	2.5
2	F	148	TYR	2.5
1	C	974	THR	2.4
2	F	89	LEU	2.4
2	F	77	ASN	2.4
2	F	243	PHE	2.4
2	F	88	GLU	2.3
2	F	193	THR	2.3
1	E	1172	LYS	2.3
2	D	70	LYS	2.3
2	F	249	THR	2.3
1	C	1131	SER	2.3
1	E	920	PHE	2.3
2	D	55	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	211	ARG	2.2
1	E	1095	LYS	2.2
2	D	116	ASP	2.2
1	E	1120	GLU	2.2
2	F	85	SER	2.2
1	E	1134	SER	2.2
2	F	145	PHE	2.2
2	F	274	PHE	2.2
2	F	290	ARG	2.2
1	E	1159	GLU	2.2
1	C	1195	SER	2.2
2	B	213	ILE	2.2
1	A	1132	MET	2.2
2	B	28	VAL	2.2
2	B	230	VAL	2.1
1	E	1102	ALA	2.1
1	C	1100	LEU	2.1
1	E	953	TYR	2.1
2	F	69	THR	2.1
1	A	1129	ALA	2.1
1	C	1164	VAL	2.1
2	F	8	GLN	2.1
1	E	1189	LYS	2.1
2	F	87	TYR	2.1
1	E	1062	THR	2.0
1	E	948	GLU	2.0
2	F	80	LYS	2.0
2	F	119	GLU	2.0
2	B	83	GLN	2.0
2	F	82	LYS	2.0
1	E	1069	ALA	2.0
2	D	117	GLU	2.0
1	E	1006	PRO	2.0
1	E	1145	ALA	2.0
2	F	245	ALA	2.0
2	F	90	TYR	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.