



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:24 am BST

PDB ID : 3DKB  
Title : Crystal Structure of A20, 2.5 angstrom  
Authors : Lin, S.-C.; Chung, J.Y.; Lo, Y.-C.; Wu, H.  
Deposited on : 2008-06-24  
Resolution : 2.50 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

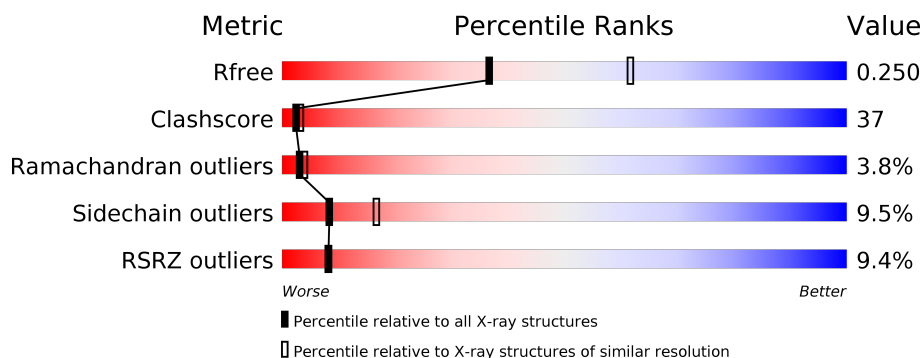
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	390	<div> <div>7%</div> <div> <div></div> <div>33%</div> <div>49%</div> <div>8%</div> <div>10%</div> </div> </div>
1	B	390	<div> <div>8%</div> <div> <div></div> <div>39%</div> <div>42%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	390	<div> <div>11%</div> <div> <div></div> <div>33%</div> <div>50%</div> <div>7%</div> <div>10%</div> </div> </div>
1	D	390	<div> <div>8%</div> <div> <div></div> <div>35%</div> <div>49%</div> <div>6%</div> <div>10%</div> </div> </div>
1	E	390	<div> <div>9%</div> <div> <div></div> <div>39%</div> <div>44%</div> <div>7%</div> <div>10%</div> </div> </div>
1	F	390	<div> <div>8%</div> <div> <div></div> <div>35%</div> <div>48%</div> <div>7%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17550 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 Tumor necrosis factor, alpha-induced protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	B	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	C	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	D	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	E	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	F	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5981	MET	-	EXPRESSION TAG	UNP P21580
A	5982	GLY	-	EXPRESSION TAG	UNP P21580
A	5983	SER	-	EXPRESSION TAG	UNP P21580
A	5984	SER	-	EXPRESSION TAG	UNP P21580
A	5985	HIS	-	EXPRESSION TAG	UNP P21580
A	5986	HIS	-	EXPRESSION TAG	UNP P21580
A	5987	HIS	-	EXPRESSION TAG	UNP P21580
A	5988	HIS	-	EXPRESSION TAG	UNP P21580
A	5989	HIS	-	EXPRESSION TAG	UNP P21580
A	5990	HIS	-	EXPRESSION TAG	UNP P21580
A	5991	SER	-	EXPRESSION TAG	UNP P21580
A	5992	SER	-	EXPRESSION TAG	UNP P21580
A	5993	GLY	-	EXPRESSION TAG	UNP P21580
A	5994	LEU	-	EXPRESSION TAG	UNP P21580
A	5995	VAL	-	EXPRESSION TAG	UNP P21580
A	5996	PRO	-	EXPRESSION TAG	UNP P21580
A	5997	ARG	-	EXPRESSION TAG	UNP P21580

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5998	GLY	-	EXPRESSION TAG	UNP P21580
A	5999	SER	-	EXPRESSION TAG	UNP P21580
A	6000	HIS	-	EXPRESSION TAG	UNP P21580
B	981	MET	-	EXPRESSION TAG	UNP P21580
B	982	GLY	-	EXPRESSION TAG	UNP P21580
B	983	SER	-	EXPRESSION TAG	UNP P21580
B	984	SER	-	EXPRESSION TAG	UNP P21580
B	985	HIS	-	EXPRESSION TAG	UNP P21580
B	986	HIS	-	EXPRESSION TAG	UNP P21580
B	987	HIS	-	EXPRESSION TAG	UNP P21580
B	988	HIS	-	EXPRESSION TAG	UNP P21580
B	989	HIS	-	EXPRESSION TAG	UNP P21580
B	990	HIS	-	EXPRESSION TAG	UNP P21580
B	991	SER	-	EXPRESSION TAG	UNP P21580
B	992	SER	-	EXPRESSION TAG	UNP P21580
B	993	GLY	-	EXPRESSION TAG	UNP P21580
B	994	LEU	-	EXPRESSION TAG	UNP P21580
B	995	VAL	-	EXPRESSION TAG	UNP P21580
B	996	PRO	-	EXPRESSION TAG	UNP P21580
B	997	ARG	-	EXPRESSION TAG	UNP P21580
B	998	GLY	-	EXPRESSION TAG	UNP P21580
B	999	SER	-	EXPRESSION TAG	UNP P21580
B	1000	HIS	-	EXPRESSION TAG	UNP P21580
C	1981	MET	-	EXPRESSION TAG	UNP P21580
C	1982	GLY	-	EXPRESSION TAG	UNP P21580
C	1983	SER	-	EXPRESSION TAG	UNP P21580
C	1984	SER	-	EXPRESSION TAG	UNP P21580
C	1985	HIS	-	EXPRESSION TAG	UNP P21580
C	1986	HIS	-	EXPRESSION TAG	UNP P21580
C	1987	HIS	-	EXPRESSION TAG	UNP P21580
C	1988	HIS	-	EXPRESSION TAG	UNP P21580
C	1989	HIS	-	EXPRESSION TAG	UNP P21580
C	1990	HIS	-	EXPRESSION TAG	UNP P21580
C	1991	SER	-	EXPRESSION TAG	UNP P21580
C	1992	SER	-	EXPRESSION TAG	UNP P21580
C	1993	GLY	-	EXPRESSION TAG	UNP P21580
C	1994	LEU	-	EXPRESSION TAG	UNP P21580
C	1995	VAL	-	EXPRESSION TAG	UNP P21580
C	1996	PRO	-	EXPRESSION TAG	UNP P21580
C	1997	ARG	-	EXPRESSION TAG	UNP P21580
C	1998	GLY	-	EXPRESSION TAG	UNP P21580
C	1999	SER	-	EXPRESSION TAG	UNP P21580

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2000	HIS	-	EXPRESSION TAG	UNP P21580
D	2981	MET	-	EXPRESSION TAG	UNP P21580
D	2982	GLY	-	EXPRESSION TAG	UNP P21580
D	2983	SER	-	EXPRESSION TAG	UNP P21580
D	2984	SER	-	EXPRESSION TAG	UNP P21580
D	2985	HIS	-	EXPRESSION TAG	UNP P21580
D	2986	HIS	-	EXPRESSION TAG	UNP P21580
D	2987	HIS	-	EXPRESSION TAG	UNP P21580
D	2988	HIS	-	EXPRESSION TAG	UNP P21580
D	2989	HIS	-	EXPRESSION TAG	UNP P21580
D	2990	HIS	-	EXPRESSION TAG	UNP P21580
D	2991	SER	-	EXPRESSION TAG	UNP P21580
D	2992	SER	-	EXPRESSION TAG	UNP P21580
D	2993	GLY	-	EXPRESSION TAG	UNP P21580
D	2994	LEU	-	EXPRESSION TAG	UNP P21580
D	2995	VAL	-	EXPRESSION TAG	UNP P21580
D	2996	PRO	-	EXPRESSION TAG	UNP P21580
D	2997	ARG	-	EXPRESSION TAG	UNP P21580
D	2998	GLY	-	EXPRESSION TAG	UNP P21580
D	2999	SER	-	EXPRESSION TAG	UNP P21580
D	3000	HIS	-	EXPRESSION TAG	UNP P21580
E	3981	MET	-	EXPRESSION TAG	UNP P21580
E	3982	GLY	-	EXPRESSION TAG	UNP P21580
E	3983	SER	-	EXPRESSION TAG	UNP P21580
E	3984	SER	-	EXPRESSION TAG	UNP P21580
E	3985	HIS	-	EXPRESSION TAG	UNP P21580
E	3986	HIS	-	EXPRESSION TAG	UNP P21580
E	3987	HIS	-	EXPRESSION TAG	UNP P21580
E	3988	HIS	-	EXPRESSION TAG	UNP P21580
E	3989	HIS	-	EXPRESSION TAG	UNP P21580
E	3990	HIS	-	EXPRESSION TAG	UNP P21580
E	3991	SER	-	EXPRESSION TAG	UNP P21580
E	3992	SER	-	EXPRESSION TAG	UNP P21580
E	3993	GLY	-	EXPRESSION TAG	UNP P21580
E	3994	LEU	-	EXPRESSION TAG	UNP P21580
E	3995	VAL	-	EXPRESSION TAG	UNP P21580
E	3996	PRO	-	EXPRESSION TAG	UNP P21580
E	3997	ARG	-	EXPRESSION TAG	UNP P21580
E	3998	GLY	-	EXPRESSION TAG	UNP P21580
E	3999	SER	-	EXPRESSION TAG	UNP P21580
E	4000	HIS	-	EXPRESSION TAG	UNP P21580
F	4981	MET	-	EXPRESSION TAG	UNP P21580

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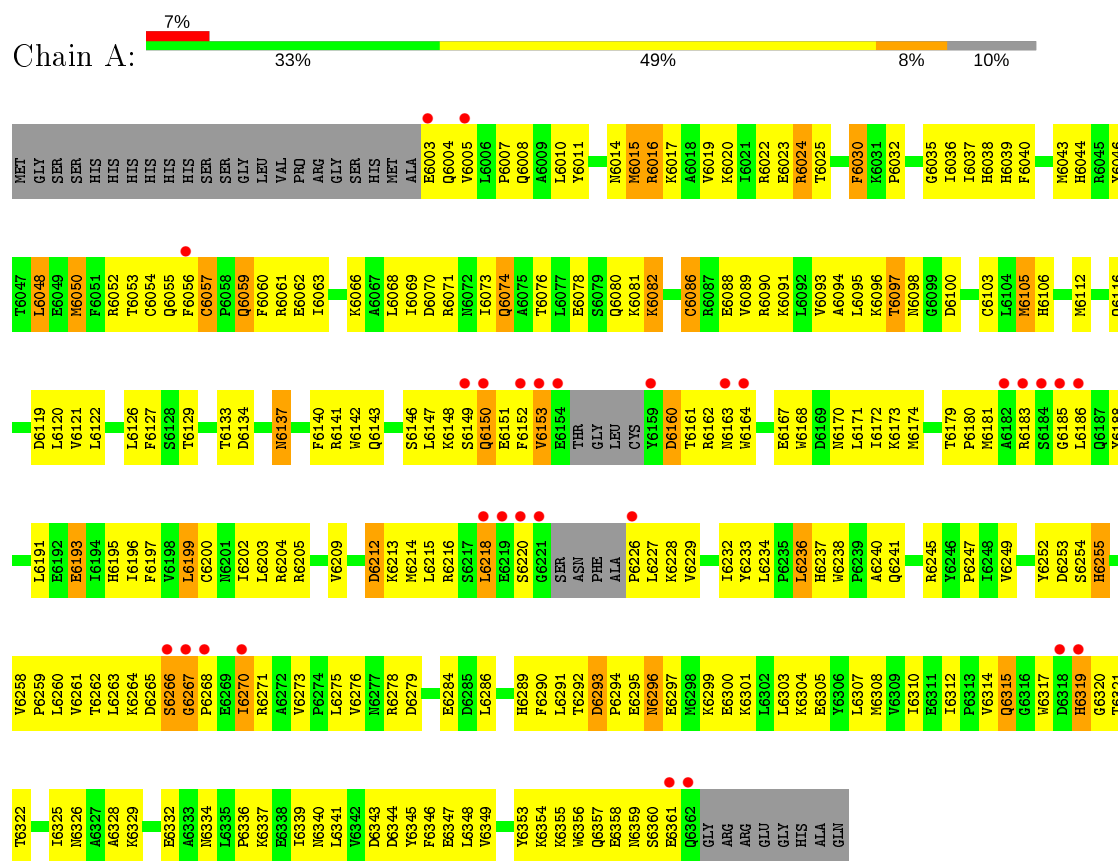
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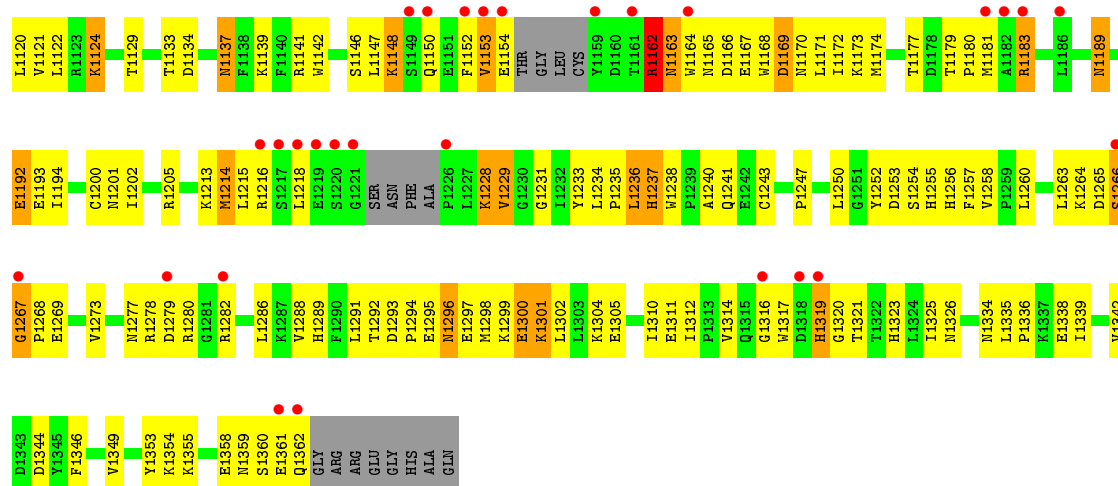
Chain	Residue	Modelled	Actual	Comment	Reference
F	4982	GLY	-	EXPRESSION TAG	UNP P21580
F	4983	SER	-	EXPRESSION TAG	UNP P21580
F	4984	SER	-	EXPRESSION TAG	UNP P21580
F	4985	HIS	-	EXPRESSION TAG	UNP P21580
F	4986	HIS	-	EXPRESSION TAG	UNP P21580
F	4987	HIS	-	EXPRESSION TAG	UNP P21580
F	4988	HIS	-	EXPRESSION TAG	UNP P21580
F	4989	HIS	-	EXPRESSION TAG	UNP P21580
F	4990	HIS	-	EXPRESSION TAG	UNP P21580
F	4991	SER	-	EXPRESSION TAG	UNP P21580
F	4992	SER	-	EXPRESSION TAG	UNP P21580
F	4993	GLY	-	EXPRESSION TAG	UNP P21580
F	4994	LEU	-	EXPRESSION TAG	UNP P21580
F	4995	VAL	-	EXPRESSION TAG	UNP P21580
F	4996	PRO	-	EXPRESSION TAG	UNP P21580
F	4997	ARG	-	EXPRESSION TAG	UNP P21580
F	4998	GLY	-	EXPRESSION TAG	UNP P21580
F	4999	SER	-	EXPRESSION TAG	UNP P21580
F	5000	HIS	-	EXPRESSION TAG	UNP P21580

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

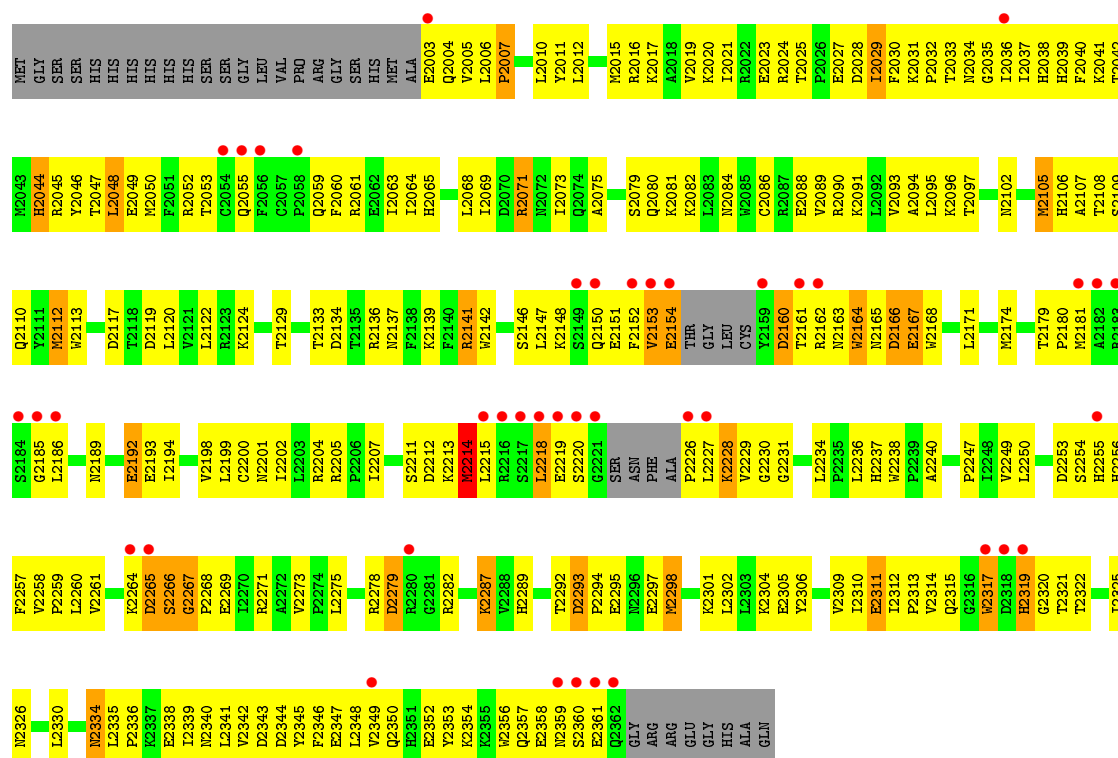
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Tumor necrosis factor, alpha-induced protein 3

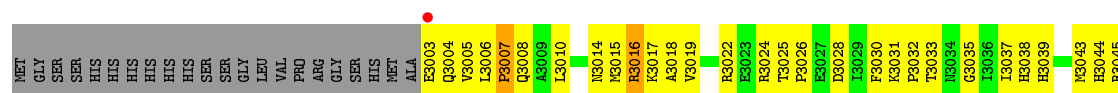


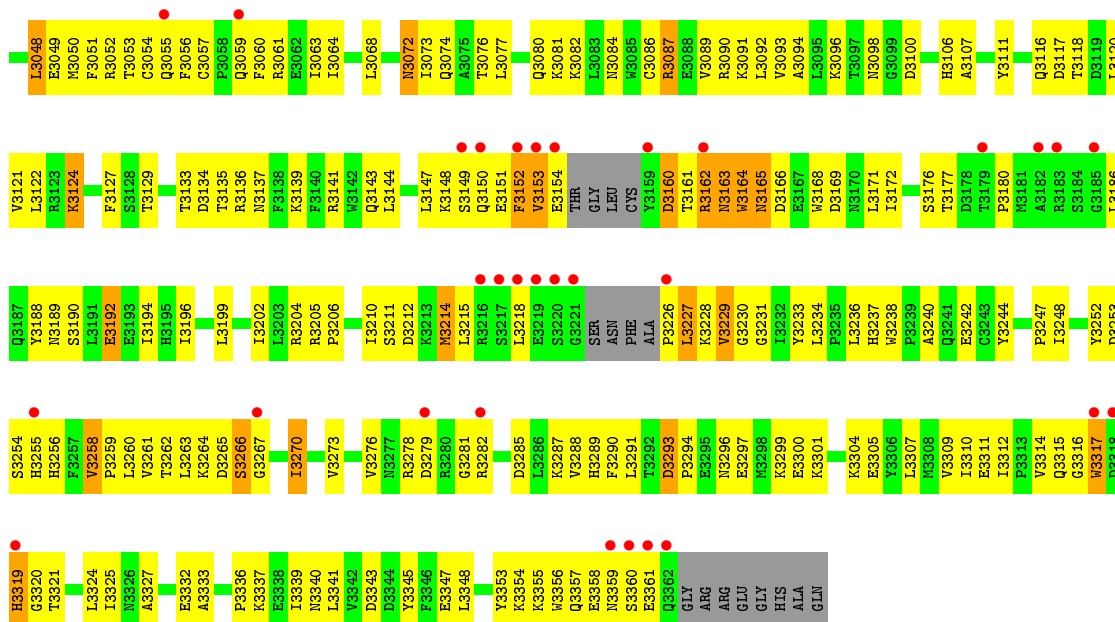


• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

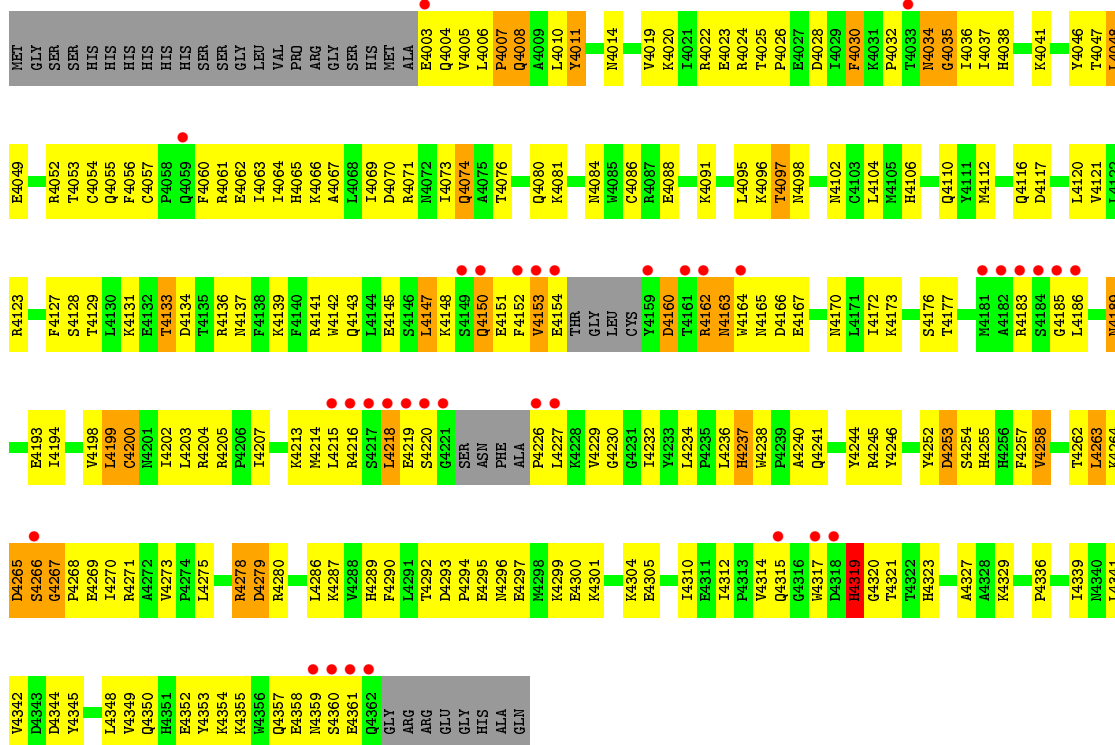


• Molecule 1: Tumor necrosis factor, alpha-induced protein 3



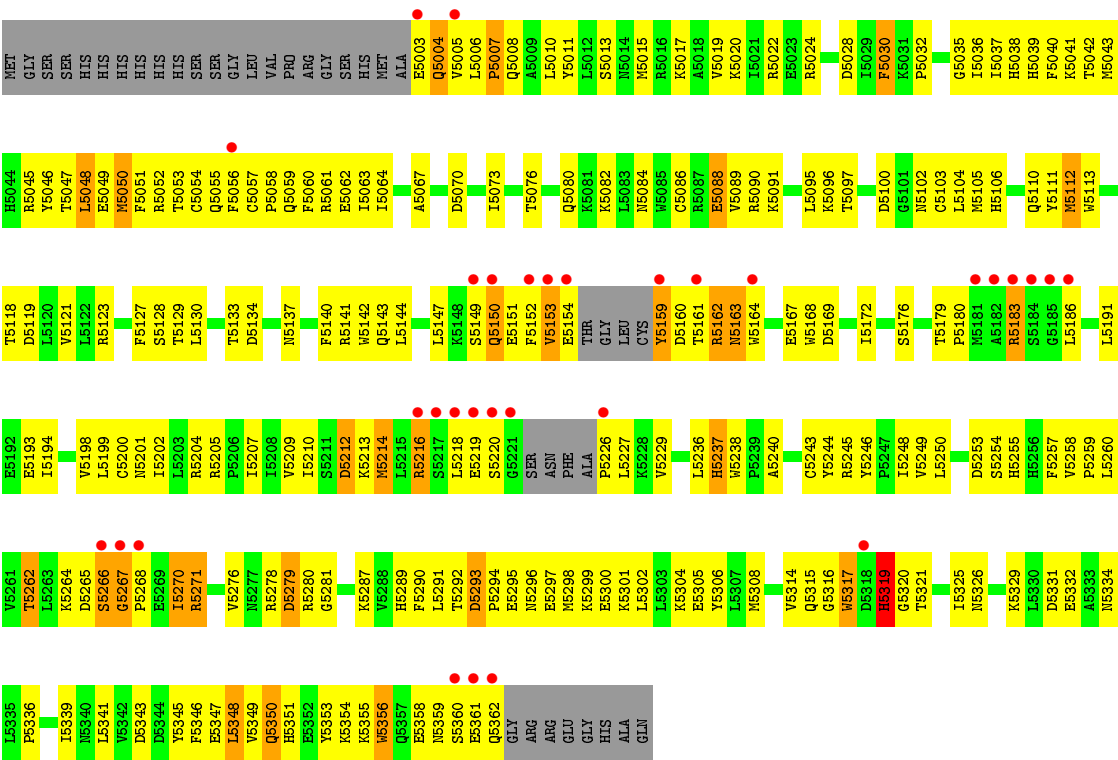


- Molecule 1: Tumor necrosis factor, alpha-induced protein 3



- Molecule 1: Tumor necrosis factor, alpha-induced protein 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.64Å 123.64Å 143.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 29.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (25.00-2.50) 95.8 (29.74-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.246 0.207 , 0.250	Depositor DCC
$R_{free}$ test set	8218 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.039 for h,-h-k,-l 0.488 for -k,-h,-l	Xtriage
Reported twinning fraction	0.476 for h+k,-k,-l	Depositor
Outliers	0 of 84471 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5482e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.43	0/2993	0.65	0/4045
1	B	0.47	0/2993	0.69	1/4045 (0.0%)
1	C	0.40	0/2993	0.65	0/4045
1	D	0.44	0/2993	0.66	0/4045
1	E	0.48	0/2993	0.68	0/4045
1	F	0.42	0/2993	0.66	1/4045 (0.0%)
All	All	0.44	0/17958	0.67	2/24270 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5348	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	1264	LYS	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2925	0	2915	216	0
1	B	2925	0	2915	208	0
1	C	2925	0	2915	227	0
1	D	2925	0	2915	230	0
1	E	2925	0	2915	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2925	0	2915	245	0
All	All	17550	0	17490	1309	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 37.

All (1309) 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:6336:PRO:HD2	1:A:6339:ILE:HD11	1.19	1.17
1:B:1228:LYS:HD2	1:B:1228:LYS:H	1.14	1.11
1:C:2105:MET:HG3	1:C:2122:LEU:HB3	1.29	1.09
1:B:1189:ASN:ND2	1:B:1189:ASN:H	1.43	1.09
1:F:5336:PRO:HD2	1:F:5339:ILE:HD11	1.38	1.06
1:D:3037:ILE:HG22	1:D:3133:THR:HG21	1.39	1.04
1:E:4162:ARG:HH21	1:E:4164:TRP:H	1.03	1.02
1:E:4253:ASP:CG	1:E:4254:SER:H	1.61	1.02
1:B:1162:ARG:HH11	1:B:1162:ARG:HB2	1.22	1.02
1:F:5020:LYS:HE3	1:F:5024:ARG:HH21	1.22	1.02
1:B:1316:GLY:HA3	1:B:1321:THR:HG23	1.42	1.01
1:F:5216:ARG:HH11	1:F:5216:ARG:HB3	1.26	1.00
1:F:5216:ARG:HB3	1:F:5216:ARG:NH1	1.78	0.98
1:B:1141:ARG:NH2	1:B:1236:LEU:HD23	1.79	0.98
1:F:5039:HIS:HD2	1:F:5204:ARG:NH1	1.61	0.98
1:F:5052:ARG:HH21	1:F:5055:GLN:HE21	1.09	0.97
1:F:5350:GLN:HE21	1:F:5350:GLN:HA	1.27	0.96
1:D:3310:ILE:HG13	1:D:3312:ILE:HD11	1.47	0.95
1:A:6337:LYS:HZ3	1:A:6340:ASN:HB3	1.32	0.94
1:B:1189:ASN:HD22	1:B:1189:ASN:N	1.65	0.94
1:C:2037:ILE:HG22	1:C:2133:THR:HG21	1.50	0.93
1:F:5316:GLY:HA3	1:F:5321:THR:HG23	1.47	0.93
1:C:2052:ARG:CZ	1:C:2266:SER:HB3	1.99	0.93
1:B:1080:GLN:NE2	1:B:1213:LYS:HG2	1.83	0.93
1:D:3100:ASP:HA	1:D:3186:LEU:HD12	1.50	0.93
1:B:1080:GLN:HE22	1:B:1213:LYS:H	1.15	0.92
1:B:1301:LYS:HE3	1:B:1301:LYS:N	1.82	0.92
1:B:1037:ILE:HG22	1:B:1133:THR:HG21	1.48	0.92
1:C:2094:ALA:HB1	1:C:2258:VAL:HG11	1.49	0.92
1:E:4189:ASN:H	1:E:4189:ASN:HD22	1.18	0.91
1:E:4354:LYS:HA	1:E:4357:GLN:HE21	1.34	0.91
1:F:5151:GLU:HB2	1:F:5296:ASN:HD21	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1071:ARG:H	1:B:1071:ARG:HD3	1.35	0.90
1:A:6152:PHE:HD2	1:A:6299:LYS:HZ2	1.19	0.90
1:D:3094:ALA:HB1	1:D:3258:VAL:HG11	1.54	0.89
1:C:2298:MET:HE3	1:C:2301:LYS:HB2	1.54	0.89
1:B:1095:LEU:O	1:B:1258:VAL:HG23	1.72	0.88
1:A:6141:ARG:NH2	1:A:6236:LEU:HD23	1.87	0.88
1:E:4025:THR:HG22	1:E:4121:VAL:HG11	1.55	0.88
1:C:2336:PRO:HD2	1:C:2339:ILE:HD11	1.56	0.88
1:C:2228:LYS:H	1:C:2228:LYS:HD3	1.40	0.86
1:A:6025:THR:HG22	1:A:6121:VAL:HG11	1.57	0.86
1:B:1060:PHE:HA	1:B:1063:ILE:HD12	1.55	0.86
1:E:4189:ASN:H	1:E:4189:ASN:ND2	1.72	0.86
1:F:5293:ASP:CG	1:F:5294:PRO:HD3	1.96	0.86
1:F:5292:THR:HG22	1:F:5294:PRO:HD2	1.55	0.86
1:D:3010:LEU:HD11	1:D:3050:MET:SD	2.16	0.85
1:B:1189:ASN:HD22	1:B:1189:ASN:H	0.86	0.85
1:F:5289:HIS:HB3	1:F:5290:PHE:CD1	2.11	0.85
1:B:1301:LYS:HE3	1:B:1301:LYS:H	1.38	0.85
1:D:3270:ILE:HD13	1:D:3270:ILE:H	1.41	0.85
1:A:6137:ASN:O	1:A:6141:ARG:HG3	1.76	0.85
1:E:4319:HIS:CE1	1:E:4321:THR:HB	2.12	0.85
1:A:6094:ALA:HB1	1:A:6258:VAL:HG11	1.58	0.84
1:A:6336:PRO:HD2	1:A:6339:ILE:CD1	2.07	0.84
1:E:4097:THR:HG21	1:E:4258:VAL:HA	1.58	0.83
1:A:6105:MET:HG3	1:A:6122:LEU:HB2	1.61	0.83
1:A:6082:LYS:HA	1:A:6082:LYS:HE3	1.61	0.82
1:C:2097:THR:HG22	1:C:2110:GLN:HE21	1.42	0.82
1:C:2287:LYS:HE2	1:C:2289:HIS:HA	1.61	0.82
1:B:1336:PRO:HD2	1:B:1339:ILE:HD11	1.61	0.82
1:F:5301:LYS:HD2	1:F:5301:LYS:N	1.93	0.82
1:A:6337:LYS:HE2	1:A:6343:ASP:OD1	1.80	0.81
1:B:1228:LYS:N	1:B:1228:LYS:HD2	1.94	0.81
1:B:1189:ASN:ND2	1:B:1189:ASN:N	2.25	0.81
1:D:3316:GLY:HA3	1:D:3321:THR:HG23	1.62	0.81
1:B:1137:ASN:O	1:B:1141:ARG:HG3	1.80	0.81
1:F:5070:ASP:OD1	1:F:5073:ILE:HD13	1.80	0.81
1:C:2298:MET:CE	1:C:2302:LEU:HG	2.10	0.81
1:B:1314:VAL:HG21	1:B:1325:ILE:HD11	1.62	0.80
1:C:2164:TRP:CE3	1:C:2164:TRP:HA	2.14	0.80
1:B:1097:THR:HG21	1:B:1258:VAL:HA	1.63	0.80
1:E:4253:ASP:CG	1:E:4254:SER:N	2.34	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6180:PRO:HB3	1:A:6183:ARG:HD2	1.65	0.79
1:F:5054:CYS:HA	1:F:5061:ARG:HD2	1.63	0.79
1:E:4134:ASP:OD2	1:E:4136:ARG:HG3	1.82	0.79
1:A:6300:GLU:HG2	1:A:6304:LYS:HE3	1.64	0.79
1:B:1048:LEU:HD13	1:B:1342:VAL:HG21	1.65	0.78
1:F:5301:LYS:H	1:F:5301:LYS:HD2	1.48	0.78
1:E:4097:THR:HG22	1:E:4258:VAL:HG23	1.66	0.78
1:E:4162:ARG:HH21	1:E:4164:TRP:N	1.82	0.78
1:C:2151:GLU:HG2	1:C:2151:GLU:O	1.82	0.77
1:C:2164:TRP:HA	1:C:2164:TRP:HE3	1.46	0.77
1:B:1231:GLY:HA3	1:B:1289:HIS:NE2	1.99	0.77
1:E:4278:ARG:HD3	1:E:4278:ARG:O	1.83	0.77
1:A:6082:LYS:HD2	1:A:6213:LYS:HE3	1.64	0.77
1:E:4271:ARG:O	1:E:4329:LYS:HD3	1.84	0.77
1:F:5278:ARG:O	1:F:5278:ARG:HD3	1.85	0.77
1:F:5015:MET:O	1:F:5019:VAL:HG23	1.84	0.77
1:F:5037:ILE:HG22	1:F:5133:THR:HG21	1.67	0.77
1:B:1019:VAL:O	1:B:1023:GLU:HG3	1.85	0.77
1:B:1171:LEU:HD23	1:B:1174:MET:CE	2.15	0.76
1:C:2162:ARG:HH22	1:C:2165:ASN:HD22	1.32	0.76
1:D:3137:ASN:O	1:D:3141:ARG:HG3	1.85	0.76
1:B:1171:LEU:HD23	1:B:1174:MET:HE1	1.66	0.76
1:C:2228:LYS:N	1:C:2228:LYS:HD3	1.99	0.76
1:B:1048:LEU:HD12	1:B:1049:GLU:N	2.01	0.76
1:A:6300:GLU:O	1:A:6304:LYS:HG3	1.84	0.76
1:B:1229:VAL:O	1:B:1233:TYR:OH	2.03	0.76
1:F:5271:ARG:NH2	1:F:5332:GLU:HB3	2.01	0.76
1:E:4030:PHE:CD1	1:E:4032:PRO:HD3	2.20	0.76
1:B:1008:GLN:HE21	1:B:1008:GLN:N	1.84	0.76
1:D:3139:LYS:O	1:D:3143:GLN:HG3	1.86	0.76
1:F:5097:THR:HG22	1:F:5110:GLN:HE21	1.51	0.75
1:B:1228:LYS:CD	1:B:1228:LYS:H	1.96	0.75
1:B:1080:GLN:HE22	1:B:1213:LYS:HG2	1.51	0.74
1:F:5105:MET:HE2	1:F:5123:ARG:HA	1.69	0.74
1:D:3293:ASP:HB2	1:D:3294:PRO:HD3	1.69	0.74
1:A:6220:SER:OG	1:A:6226:PRO:HG3	1.87	0.74
1:E:4037:ILE:HG22	1:E:4133:THR:HG21	1.67	0.74
1:D:3025:THR:HG22	1:D:3121:VAL:HG11	1.68	0.74
1:F:5039:HIS:CD2	1:F:5204:ARG:NH1	2.53	0.74
1:A:6053:THR:O	1:A:6061:ARG:HG2	1.87	0.74
1:C:2019:VAL:O	1:C:2023:GLU:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2097:THR:HG21	1:C:2259:PRO:HD3	1.70	0.74
1:F:5271:ARG:CZ	1:F:5332:GLU:HB3	2.18	0.74
1:C:2231:GLY:HA3	1:C:2289:HIS:HE1	1.52	0.74
1:F:5039:HIS:HD2	1:F:5204:ARG:HH11	1.34	0.73
1:D:3008:GLN:HE21	1:D:3096:LYS:NZ	1.86	0.73
1:A:6193:GLU:OE1	1:A:6229:VAL:HG22	1.86	0.73
1:D:3087:ARG:NH1	1:F:5162:ARG:HG3	2.03	0.73
1:E:4300:GLU:OE2	1:E:4304:LYS:HE3	1.89	0.73
1:A:6168:TRP:NE1	1:A:6172:ILE:HD11	2.04	0.73
1:B:1142:TRP:CE2	1:B:1171:LEU:HD11	2.24	0.73
1:E:4220:SER:OG	1:E:4226:PRO:HG3	1.87	0.73
1:B:1003:GLU:HB2	1:B:1004:GLN:NE2	2.04	0.72
1:C:2311:GLU:C	1:C:2312:ILE:HD12	2.10	0.72
1:B:1057:CYS:HB3	1:B:1353:TYR:OH	1.90	0.72
1:E:4151:GLU:HB2	1:E:4296:ASN:OD1	1.89	0.72
1:F:5045:ARG:HG2	1:F:5244:TYR:CD1	2.25	0.72
1:D:3030:PHE:HD1	1:D:3032:PRO:HD3	1.54	0.72
1:C:2338:GLU:HG2	1:C:2339:ILE:HG23	1.72	0.72
1:E:4289:HIS:HB3	1:E:4290:PHE:CD1	2.25	0.72
1:E:4007:PRO:HG2	1:E:4345:TYR:CE1	2.25	0.72
1:A:6039:HIS:HD2	1:A:6204:ARG:NH2	1.88	0.71
1:A:6056:PHE:O	1:A:6061:ARG:HD2	1.90	0.71
1:F:5152:PHE:CE2	1:F:5299:LYS:HD2	2.25	0.71
1:D:3150:GLN:HE22	1:D:3291:LEU:HB2	1.54	0.71
1:F:5161:THR:HG22	1:F:5162:ARG:HD2	1.72	0.71
1:A:6097:THR:HG23	1:A:6258:VAL:HG22	1.72	0.71
1:B:1162:ARG:NH1	1:B:1162:ARG:HB2	2.03	0.71
1:D:3150:GLN:HE21	1:D:3296:ASN:HB2	1.54	0.71
1:A:6160:ASP:CG	1:A:6161:THR:H	1.94	0.71
1:B:1052:ARG:CZ	1:B:1266:SER:HB3	2.20	0.71
1:B:1071:ARG:H	1:B:1071:ARG:CD	2.03	0.71
1:D:3150:GLN:NE2	1:D:3296:ASN:HB2	2.06	0.71
1:F:5350:GLN:NE2	1:F:5350:GLN:HA	2.05	0.71
1:A:6037:ILE:HG22	1:A:6133:THR:HG21	1.73	0.70
1:C:2298:MET:HE1	1:C:2302:LEU:HG	1.72	0.70
1:B:1124:LYS:HE3	1:B:1177:THR:HG21	1.74	0.70
1:F:5292:THR:HG22	1:F:5294:PRO:CD	2.21	0.70
1:C:2214:MET:HE3	1:C:2214:MET:HA	1.74	0.70
1:C:2097:THR:HG22	1:C:2110:GLN:NE2	2.06	0.70
1:E:4097:THR:CG2	1:E:4258:VAL:HG23	2.22	0.70
1:A:6289:HIS:HB3	1:A:6290:PHE:CD1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6054:CYS:HA	1:A:6061:ARG:HE	1.57	0.69
1:A:6020:LYS:HE2	1:A:6024:ARG:HH12	1.57	0.69
1:F:5052:ARG:NH2	1:F:5055:GLN:HE21	1.88	0.69
1:E:4022:ARG:HG3	1:E:4022:ARG:HH11	1.57	0.69
1:A:6105:MET:HG3	1:A:6122:LEU:CB	2.23	0.69
1:A:6249:VAL:HG12	1:A:6260:LEU:HB2	1.73	0.69
1:B:1052:ARG:NE	1:B:1266:SER:HB3	2.07	0.69
1:C:2047:THR:H	1:C:2334:ASN:ND2	1.91	0.69
1:C:2053:THR:OG1	1:C:2061:ARG:HG3	1.92	0.69
1:A:6008:GLN:HE21	1:A:6096:LYS:NZ	1.91	0.69
1:C:2310:ILE:HG13	1:C:2312:ILE:CD1	2.22	0.69
1:E:4084:ASN:OD1	1:E:4091:LYS:HA	1.93	0.69
1:D:3231:GLY:HA3	1:D:3289:HIS:HE1	1.58	0.69
1:F:5292:THR:CG2	1:F:5294:PRO:HD2	2.22	0.69
1:B:1171:LEU:HA	1:B:1174:MET:HE3	1.75	0.68
1:F:5052:ARG:NH2	1:F:5054:CYS:HB2	2.08	0.68
1:E:4152:PHE:CE2	1:E:4299:LYS:HD3	2.27	0.68
1:B:1359:ASN:O	1:B:1362:GLN:HG2	1.94	0.68
1:C:2220:SER:OG	1:C:2226:PRO:HG3	1.92	0.68
1:B:1181:MET:H	1:B:1183:ARG:HH11	1.40	0.68
1:D:3343:ASP:O	1:D:3347:GLU:HG2	1.93	0.68
1:F:5151:GLU:CB	1:F:5296:ASN:HD21	2.06	0.68
1:A:6253:ASP:CG	1:A:6254:SER:H	1.97	0.68
1:E:4218:LEU:HD23	1:E:4219:GLU:H	1.59	0.68
1:A:6070:ASP:OD1	1:A:6073:ILE:HD13	1.94	0.67
1:C:2298:MET:HE2	1:C:2302:LEU:HG	1.77	0.67
1:B:1048:LEU:HD13	1:B:1342:VAL:CG2	2.25	0.67
1:D:3048:LEU:HD12	1:D:3048:LEU:C	2.14	0.67
1:F:5084:ASN:CG	1:F:5091:LYS:HG3	2.14	0.67
1:C:2146:SER:O	1:C:2148:LYS:HD3	1.95	0.67
1:A:6008:GLN:HE21	1:A:6096:LYS:HZ2	1.41	0.67
1:C:2047:THR:H	1:C:2334:ASN:HD21	1.43	0.67
1:E:4319:HIS:ND1	1:E:4321:THR:HB	2.08	0.67
1:D:3055:GLN:HG3	1:D:3056:PHE:CD1	2.30	0.67
1:B:1181:MET:HB2	1:B:1183:ARG:HH12	1.60	0.67
1:E:4293:ASP:O	1:E:4297:GLU:HG2	1.94	0.67
1:D:3050:MET:HG2	1:D:3261:VAL:HG21	1.77	0.66
1:A:6020:LYS:HE2	1:A:6024:ARG:NH1	2.10	0.66
1:E:4011:TYR:HA	1:E:4341:LEU:HD13	1.75	0.66
1:A:6052:ARG:CZ	1:A:6054:CYS:HB2	2.26	0.66
1:B:1292:THR:OG1	1:B:1295:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5052:ARG:HD2	1:F:5266:SER:H	1.60	0.66
1:E:4317:TRP:H	1:E:4319:HIS:CE1	2.14	0.66
1:B:1069:ILE:O	1:B:1071:ARG:HD3	1.94	0.66
1:C:2139:LYS:HB2	1:C:2139:LYS:NZ	2.10	0.66
1:D:3137:ASN:HB3	1:D:3237:HIS:CE1	2.30	0.66
1:D:3152:PHE:CE2	1:D:3299:LYS:HD2	2.31	0.66
1:B:1052:ARG:HH11	1:B:1265:ASP:N	1.92	0.66
1:D:3204:ARG:HD3	1:D:3238:TRP:CE3	2.31	0.66
1:F:5336:PRO:HD2	1:F:5339:ILE:CD1	2.20	0.66
1:C:2029:ILE:HG22	1:C:2031:LYS:HG3	1.77	0.66
1:D:3192:GLU:OE1	1:D:3194:ILE:HG22	1.96	0.66
1:F:5052:ARG:CD	1:F:5266:SER:H	2.09	0.66
1:C:2007:PRO:HG2	1:C:2345:TYR:CE1	2.29	0.65
1:D:3117:ASP:OD1	1:D:3122:LEU:HB2	1.97	0.65
1:E:4353:TYR:O	1:E:4357:GLN:HG3	1.95	0.65
1:A:6234:LEU:HB2	1:A:6236:LEU:HD13	1.78	0.65
1:E:4060:PHE:HD2	1:E:4063:ILE:HD12	1.61	0.65
1:D:3007:PRO:HG2	1:D:3345:TYR:CE1	2.31	0.65
1:B:1082:LYS:HA	1:B:1082:LYS:HE3	1.78	0.65
1:E:4127:PHE:CE1	1:E:4176:SER:HB3	2.31	0.65
1:F:5030:PHE:HB2	1:F:5041:LYS:HD2	1.77	0.65
1:F:5143:GLN:HG2	1:F:5164:TRP:CE3	2.32	0.65
1:F:5271:ARG:HH11	1:F:5271:ARG:HB2	1.61	0.65
1:D:3052:ARG:NH1	1:D:3265:ASP:N	2.44	0.65
1:A:6141:ARG:HH22	1:A:6236:LEU:HD23	1.60	0.65
1:A:6314:VAL:HG21	1:A:6325:ILE:HD12	1.79	0.65
1:F:5039:HIS:CD2	1:F:5204:ARG:HH11	2.11	0.65
1:F:5143:GLN:HG2	1:F:5164:TRP:CZ3	2.31	0.65
1:C:2240:ALA:CB	1:C:2305:GLU:HG2	2.26	0.65
1:C:2231:GLY:HA3	1:C:2289:HIS:CE1	2.32	0.65
1:C:2006:LEU:HD21	1:C:2349:VAL:HG12	1.78	0.65
1:D:3129:THR:O	1:D:3133:THR:HB	1.97	0.65
1:E:4348:LEU:O	1:E:4352:GLU:HG2	1.96	0.65
1:C:2030:PHE:HD1	1:C:2032:PRO:HD3	1.62	0.65
1:C:2139:LYS:HE3	1:C:2168:TRP:CD1	2.32	0.65
1:C:2319:HIS:CE1	1:C:2321:THR:HB	2.31	0.65
1:C:2129:THR:O	1:C:2133:THR:HB	1.97	0.64
1:D:3031:LYS:HA	1:D:3038:HIS:ND1	2.12	0.64
1:E:4052:ARG:NE	1:E:4054:CYS:HB2	2.12	0.64
1:C:2213:LYS:HE2	1:C:2214:MET:HE3	1.79	0.64
1:C:2097:THR:CG2	1:C:2259:PRO:HD3	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5354:LYS:O	1:F:5358:GLU:HG3	1.96	0.64
1:E:4215:LEU:HD13	1:E:4218:LEU:CD1	2.28	0.64
1:D:3214:MET:HG3	1:F:5140:PHE:CZ	2.32	0.64
1:D:3194:ILE:HA	1:D:3290:PHE:CE1	2.33	0.64
1:F:5270:ILE:HD12	1:F:5270:ILE:H	1.61	0.64
1:E:4008:GLN:OE1	1:E:4096:LYS:HE2	1.98	0.64
1:A:6344:ASP:O	1:A:6348:LEU:HD13	1.96	0.64
1:F:5060:PHE:HD2	1:F:5063:ILE:HD12	1.63	0.64
1:F:5160:ASP:CG	1:F:5161:THR:H	2.01	0.64
1:A:6337:LYS:HE2	1:A:6343:ASP:CB	2.28	0.64
1:C:2150:GLN:HE22	1:C:2287:LYS:HE3	1.63	0.64
1:F:5036:ILE:HG12	1:F:5238:TRP:CH2	2.33	0.64
1:B:1139:LYS:HG3	1:B:1168:TRP:CE2	2.32	0.64
1:B:1181:MET:H	1:B:1183:ARG:NH1	1.96	0.64
1:C:2163:ASN:ND2	1:C:2167:GLU:HB2	2.12	0.64
1:A:6095:LEU:O	1:A:6258:VAL:HG13	1.98	0.63
1:B:1120:LEU:O	1:B:1124:LYS:HB2	1.98	0.63
1:C:2292:THR:OG1	1:C:2295:GLU:HG3	1.97	0.63
1:C:2046:TYR:HA	1:C:2334:ASN:HD21	1.63	0.63
1:D:3150:GLN:HG3	1:D:3151:GLU:H	1.63	0.63
1:B:1106:HIS:ND1	1:B:1116:GLN:HB3	2.13	0.63
1:D:3135:THR:O	1:D:3139:LYS:HG3	1.99	0.63
1:B:1280:ARG:HG3	1:B:1280:ARG:O	1.97	0.63
1:F:5129:THR:O	1:F:5133:THR:HB	1.98	0.63
1:A:6097:THR:HG21	1:A:6258:VAL:HA	1.80	0.63
1:A:6293:ASP:HB2	1:A:6294:PRO:HD3	1.81	0.63
1:D:3311:GLU:C	1:D:3312:ILE:HD12	2.18	0.63
1:D:3136:ARG:HH12	1:E:4278:ARG:HH12	1.46	0.63
1:E:4120:LEU:HD13	1:E:4177:THR:CG2	2.28	0.63
1:B:1298:MET:CA	1:B:1301:LYS:HD2	2.28	0.63
1:E:4046:TYR:CE2	1:E:4336:PRO:HD3	2.33	0.63
1:A:6086:CYS:HB3	1:A:6089:VAL:HG22	1.81	0.63
1:B:1030:PHE:O	1:B:1032:PRO:HD2	1.99	0.63
1:C:2053:THR:HG21	1:C:2065:HIS:NE2	2.13	0.63
1:C:2052:ARG:NH2	1:C:2266:SER:HB3	2.14	0.63
1:D:3310:ILE:CG1	1:D:3312:ILE:HD11	2.27	0.63
1:D:3312:ILE:N	1:D:3312:ILE:HD12	2.14	0.63
1:F:5052:ARG:HH22	1:F:5054:CYS:HB2	1.64	0.62
1:C:2218:LEU:HD23	1:C:2219:GLU:H	1.63	0.62
1:E:4106:HIS:O	1:E:4110:GLN:HG3	1.98	0.62
1:E:4199:LEU:HD22	1:E:4203:LEU:HG	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3230:GLY:O	1:D:3289:HIS:HE1	1.81	0.62
1:D:3215:LEU:HD22	1:D:3218:LEU:HD13	1.82	0.62
1:D:3231:GLY:HA3	1:D:3289:HIS:CE1	2.35	0.62
1:F:5298:MET:CA	1:F:5301:LYS:HD3	2.29	0.62
1:C:2162:ARG:HH22	1:C:2165:ASN:ND2	1.97	0.62
1:F:5293:ASP:O	1:F:5297:GLU:HG2	2.00	0.62
1:D:3018:ALA:O	1:D:3022:ARG:HG3	1.99	0.62
1:D:3080:GLN:HE22	1:D:3212:ASP:CG	2.04	0.62
1:D:3314:VAL:HG21	1:D:3325:ILE:HD11	1.82	0.62
1:F:5293:ASP:OD1	1:F:5294:PRO:HD3	2.00	0.62
1:F:5314:VAL:HG21	1:F:5325:ILE:HD12	1.82	0.62
1:F:5279:ASP:CG	1:F:5280:ARG:H	2.03	0.61
1:F:5141:ARG:HH22	1:F:5295:GLU:CD	2.03	0.61
1:A:6030:PHE:O	1:A:6032:PRO:HD2	2.00	0.61
1:C:2033:THR:HG22	1:C:2033:THR:O	1.99	0.61
1:F:5210:ILE:HD12	1:F:5260:LEU:HD12	1.82	0.61
1:A:6276:VAL:CG2	1:A:6325:ILE:HG21	2.30	0.61
1:A:6168:TRP:HE1	1:A:6172:ILE:HD11	1.62	0.61
1:E:4269:GLU:N	1:E:4269:GLU:OE1	2.34	0.61
1:E:4336:PRO:HD2	1:E:4339:ILE:HD11	1.83	0.61
1:B:1293:ASP:HB2	1:B:1294:PRO:HD3	1.82	0.61
1:D:3054:CYS:SG	1:D:3061:ARG:NH1	2.74	0.61
1:F:5052:ARG:HD2	1:F:5266:SER:CB	2.30	0.61
1:A:6129:THR:O	1:A:6133:THR:HB	1.99	0.61
1:A:6232:ILE:HD11	1:A:6275:LEU:HD22	1.83	0.61
1:C:2293:ASP:HB2	1:C:2294:PRO:HD3	1.81	0.61
1:F:5240:ALA:CB	1:F:5305:GLU:HG2	2.31	0.61
1:F:5298:MET:HA	1:F:5301:LYS:HD3	1.82	0.61
1:B:1147:LEU:HD21	1:B:1164:TRP:HZ2	1.66	0.61
1:C:2215:LEU:HD13	1:C:2218:LEU:HG	1.83	0.61
1:F:5213:LYS:HG3	1:F:5214:MET:HE3	1.83	0.61
1:A:6076:THR:O	1:A:6080:GLN:HG2	2.01	0.61
1:B:1310:ILE:HD11	1:B:1312:ILE:HD11	1.82	0.61
1:D:3164:TRP:HA	1:D:3164:TRP:CE3	2.35	0.61
1:E:4060:PHE:CD2	1:E:4063:ILE:HD12	2.35	0.61
1:D:3030:PHE:CD1	1:D:3032:PRO:HD3	2.33	0.61
1:E:4141:ARG:HH22	1:E:4295:GLU:CD	2.03	0.61
1:F:5244:TYR:CE2	1:F:5246:TYR:HB2	2.36	0.61
1:D:3052:ARG:HD3	1:D:3265:ASP:H	1.65	0.60
1:A:6106:HIS:HB3	1:A:6116:GLN:OE1	2.01	0.60
1:F:5095:LEU:O	1:F:5258:VAL:CG2	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2228:LYS:H	1:C:2228:LYS:CD	2.03	0.60
1:E:4301:LYS:HD2	1:E:4301:LYS:N	2.16	0.60
1:F:5060:PHE:HE1	1:F:5353:TYR:HB2	1.65	0.60
1:D:3050:MET:CE	1:D:3068:LEU:HD13	2.31	0.60
1:E:4230:GLY:O	1:E:4289:HIS:HE1	1.84	0.60
1:F:5144:LEU:CD2	1:F:5149:SER:HB3	2.31	0.60
1:A:6081:LYS:NZ	1:A:6278:ARG:HH12	1.98	0.60
1:B:1171:LEU:HA	1:B:1174:MET:CE	2.32	0.60
1:C:2142:TRP:CZ2	1:C:2171:LEU:HD11	2.36	0.60
1:C:2081:LYS:HB3	1:C:2278:ARG:HD3	1.83	0.60
1:B:1142:TRP:CZ2	1:B:1171:LEU:HD11	2.36	0.60
1:A:6301:LYS:HD2	1:A:6301:LYS:N	2.17	0.60
1:E:4074:GLN:HE21	1:E:4074:GLN:CA	2.14	0.60
1:B:1354:LYS:O	1:B:1358:GLU:HG3	2.01	0.60
1:D:3045:ARG:HG3	1:D:3244:TYR:CE1	2.36	0.60
1:D:3152:PHE:CE1	1:D:3287:LYS:HD2	2.37	0.60
1:B:1129:THR:O	1:B:1133:THR:HB	2.02	0.60
1:B:1052:ARG:NH2	1:B:1266:SER:HB3	2.17	0.60
1:F:5050:MET:O	1:F:5264:LYS:HB2	2.02	0.60
1:F:5281:GLY:HA2	1:F:5317:TRP:NE1	2.17	0.59
1:A:6346:PHE:O	1:A:6349:VAL:HG22	2.02	0.59
1:B:1046:TYR:CE2	1:B:1336:PRO:HD3	2.37	0.59
1:B:1234:LEU:HB2	1:B:1236:LEU:HD13	1.84	0.59
1:C:2353:TYR:O	1:C:2357:GLN:HG3	2.02	0.59
1:E:4076:THR:O	1:E:4080:GLN:HG2	2.01	0.59
1:E:4270:ILE:HD11	1:E:4312:ILE:CD1	2.32	0.59
1:B:1073:ILE:HD11	1:B:1256:HIS:HD2	1.67	0.59
1:B:1110:GLN:NE2	1:B:1116:GLN:HE22	1.99	0.59
1:D:3354:LYS:O	1:D:3358:GLU:HG3	2.01	0.59
1:A:6091:LYS:O	1:A:6263:LEU:HD23	2.02	0.59
1:E:4048:LEU:HD21	1:E:4110:GLN:O	2.02	0.59
1:E:4025:THR:CG2	1:E:4121:VAL:HG11	2.29	0.59
1:E:4137:ASN:O	1:E:4141:ARG:HG3	2.02	0.59
1:E:4162:ARG:NH2	1:E:4164:TRP:H	1.87	0.59
1:A:6052:ARG:HG3	1:A:6052:ARG:HH11	1.66	0.59
1:B:1081:LYS:HG3	1:B:1278:ARG:NH1	2.18	0.59
1:F:5220:SER:OG	1:F:5226:PRO:HG3	2.03	0.59
1:B:1109:SER:HG	1:B:1113:TRP:HE3	1.49	0.59
1:F:5245:ARG:HB2	1:F:5308:MET:CE	2.33	0.59
1:F:5325:ILE:HG22	1:F:5326:ASN:N	2.17	0.59
1:A:6325:ILE:HG22	1:A:6326:ASN:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1319:HIS:CE1	1:B:1321:THR:HG21	2.37	0.59
1:C:2080:GLN:NE2	1:C:2212:ASP:OD1	2.35	0.59
1:A:6039:HIS:HD2	1:A:6204:ARG:HH21	1.51	0.58
1:D:3008:GLN:HE21	1:D:3096:LYS:HZ2	1.51	0.58
1:D:3052:ARG:NH1	1:D:3263:LEU:HB3	2.18	0.58
1:A:6005:VAL:O	1:A:6005:VAL:HG13	2.03	0.58
1:D:3252:TYR:OH	1:D:3255:HIS:HA	2.04	0.58
1:A:6197:PHE:HB2	1:A:6290:PHE:CE1	2.38	0.58
1:A:6068:LEU:HD21	1:A:6345:TYR:CZ	2.38	0.58
1:F:5052:ARG:HD2	1:F:5266:SER:N	2.18	0.58
1:A:6142:TRP:CZ3	1:A:6168:TRP:HB2	2.38	0.58
1:E:4139:LYS:O	1:E:4143:GLN:HG3	2.03	0.58
1:F:5133:THR:HG22	1:F:5134:ASP:N	2.17	0.58
1:D:3087:ARG:HH11	1:F:5162:ARG:NH1	2.01	0.58
1:C:2048:LEU:HD12	1:C:2049:GLU:N	2.18	0.58
1:C:2336:PRO:HD2	1:C:2339:ILE:CD1	2.32	0.58
1:D:3033:THR:HG22	1:D:3033:THR:O	2.04	0.58
1:F:5209:VAL:HG11	1:F:5229:VAL:HG12	1.85	0.58
1:A:6073:ILE:N	1:A:6073:ILE:HD12	2.19	0.58
1:A:6293:ASP:O	1:A:6297:GLU:HG2	2.04	0.58
1:B:1152:PHE:CE2	1:B:1299:LYS:HD2	2.39	0.58
1:B:1298:MET:HB2	1:B:1301:LYS:HD2	1.85	0.58
1:C:2030:PHE:CD1	1:C:2032:PRO:HD3	2.38	0.58
1:E:4095:LEU:O	1:E:4258:VAL:HG22	2.03	0.58
1:C:2046:TYR:O	1:C:2112:MET:HB3	2.04	0.58
1:F:5144:LEU:HD23	1:F:5149:SER:HB3	1.86	0.58
1:A:6271:ARG:HB2	1:A:6329:LYS:HE2	1.85	0.58
1:B:1034:ASN:CG	1:B:1035:GLY:N	2.57	0.58
1:A:6258:VAL:HG13	1:A:6259:PRO:HD2	1.85	0.58
1:B:1052:ARG:HH11	1:B:1265:ASP:H	1.51	0.58
1:D:3337:LYS:O	1:D:3337:LYS:HD2	2.03	0.57
1:C:2213:LYS:HG3	1:C:2214:MET:N	2.18	0.57
1:D:3141:ARG:NH2	1:D:3236:LEU:HD23	2.20	0.57
1:D:3319:HIS:NE2	1:D:3321:THR:HG21	2.18	0.57
1:E:4120:LEU:HD13	1:E:4177:THR:HG21	1.86	0.57
1:F:5053:THR:O	1:F:5061:ARG:HG3	2.05	0.57
1:A:6152:PHE:CE2	1:A:6299:LYS:HD3	2.40	0.57
1:A:6310:ILE:HD11	1:A:6312:ILE:HD11	1.85	0.57
1:C:2344:ASP:O	1:C:2348:LEU:HD13	2.04	0.57
1:C:2238:TRP:O	1:C:2306:TYR:OH	2.14	0.57
1:D:3060:PHE:HE1	1:D:3064:ILE:HD11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4273:VAL:HG13	1:E:4273:VAL:O	2.04	0.57
1:C:2021:ILE:O	1:C:2025:THR:HG23	2.04	0.57
1:F:5213:LYS:HE3	1:F:5214:MET:HE3	1.85	0.57
1:A:6054:CYS:HA	1:A:6061:ARG:NE	2.20	0.57
1:D:3073:ILE:HD11	1:D:3256:HIS:HD2	1.70	0.57
1:D:3052:ARG:HH11	1:D:3265:ASP:N	2.02	0.57
1:A:6347:GLU:HA	1:A:6347:GLU:OE2	2.05	0.57
1:D:3060:PHE:CE1	1:D:3064:ILE:HD11	2.39	0.57
1:D:3230:GLY:O	1:D:3289:HIS:CE1	2.57	0.57
1:E:4345:TYR:O	1:E:4349:VAL:HG23	2.05	0.57
1:F:5301:LYS:H	1:F:5301:LYS:CD	2.16	0.57
1:B:1291:LEU:HD22	1:B:1295:GLU:HB2	1.87	0.57
1:E:4091:LYS:HB2	1:E:4263:LEU:HD12	1.86	0.57
1:E:4240:ALA:HB2	1:E:4305:GLU:HG2	1.87	0.57
1:E:4317:TRP:HE3	1:E:4319:HIS:CE1	2.23	0.57
1:F:5183:ARG:HH11	1:F:5183:ARG:HG2	1.68	0.57
1:D:3052:ARG:HH11	1:D:3265:ASP:H	1.53	0.56
1:D:3314:VAL:HG21	1:D:3325:ILE:CD1	2.35	0.56
1:B:1005:VAL:HG13	1:B:1005:VAL:O	2.05	0.56
1:B:1037:ILE:CG2	1:B:1133:THR:HG21	2.29	0.56
1:D:3319:HIS:O	1:D:3321:THR:N	2.38	0.56
1:A:6068:LEU:HD21	1:A:6345:TYR:CE1	2.39	0.56
1:D:3136:ARG:HH22	1:E:4278:ARG:NH1	2.03	0.56
1:D:3152:PHE:HE2	1:D:3299:LYS:HD2	1.69	0.56
1:F:5319:HIS:ND1	1:F:5321:THR:HG22	2.20	0.56
1:D:3082:LYS:HE3	1:D:3211:SER:O	2.04	0.56
1:E:4186:LEU:HD22	1:E:4186:LEU:N	2.21	0.56
1:A:6066:LYS:NZ	1:A:6071:ARG:NH2	2.54	0.56
1:A:6200:CYS:HB2	1:A:6205:ARG:O	2.06	0.56
1:E:4066:LYS:HE3	1:E:4071:ARG:NH2	2.21	0.56
1:E:4279:ASP:CG	1:E:4280:ARG:H	2.08	0.56
1:A:6319:HIS:O	1:A:6321:THR:N	2.39	0.56
1:B:1336:PRO:HD2	1:B:1339:ILE:CD1	2.31	0.56
1:C:2107:ALA:O	1:C:2259:PRO:HG3	2.05	0.56
1:E:4038:HIS:CD2	1:E:4128:SER:OG	2.59	0.56
1:A:6141:ARG:NH2	1:A:6295:GLU:OE2	2.37	0.56
1:B:1146:SER:O	1:B:1148:LYS:HD3	2.06	0.56
1:B:1047:THR:HG1	1:B:1205:ARG:HH22	1.53	0.56
1:E:4098:ASN:H	1:E:4116:GLN:HE22	1.52	0.56
1:C:2354:LYS:O	1:C:2358:GLU:HG3	2.06	0.56
1:D:3150:GLN:NE2	1:D:3291:LEU:HB2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5005:VAL:O	1:F:5005:VAL:HG13	2.06	0.56
1:F:5038:HIS:CE1	1:F:5128:SER:HB3	2.41	0.56
1:B:1298:MET:HA	1:B:1301:LYS:HD2	1.86	0.56
1:B:1046:TYR:CD2	1:B:1335:LEU:HD23	2.41	0.56
1:C:2214:MET:HA	1:C:2214:MET:CE	2.34	0.56
1:B:1082:LYS:CD	1:B:1213:LYS:HE3	2.36	0.55
1:B:1323:HIS:N	1:B:1323:HIS:CD2	2.73	0.55
1:C:2319:HIS:O	1:C:2321:THR:N	2.39	0.55
1:D:3028:ASP:OD1	1:D:3043:MET:HG3	2.05	0.55
1:D:3162:ARG:NH2	1:D:3165:ASN:HD21	2.05	0.55
1:D:3253:ASP:OD1	1:D:3254:SER:N	2.39	0.55
1:E:4319:HIS:O	1:E:4321:THR:N	2.39	0.55
1:F:5080:GLN:HE22	1:F:5212:ASP:HB2	1.71	0.55
1:A:6193:GLU:HB3	1:A:6290:PHE:HZ	1.71	0.55
1:A:6354:LYS:O	1:A:6358:GLU:HG3	2.06	0.55
1:B:1319:HIS:O	1:B:1321:THR:N	2.39	0.55
1:A:6010:LEU:HD21	1:A:6068:LEU:HD13	1.88	0.55
1:C:2343:ASP:O	1:C:2347:GLU:HG2	2.07	0.55
1:D:3150:GLN:HE21	1:D:3296:ASN:CB	2.20	0.55
1:D:3205:ARG:HD2	1:D:3244:TYR:HD2	1.72	0.55
1:D:3310:ILE:HG13	1:D:3312:ILE:CD1	2.28	0.55
1:A:6167:GLU:O	1:A:6171:LEU:HD23	2.07	0.55
1:C:2350:GLN:O	1:C:2354:LYS:HG3	2.07	0.55
1:D:3048:LEU:HD12	1:D:3049:GLU:N	2.22	0.55
1:F:5047:THR:N	1:F:5334:ASN:OD1	2.37	0.55
1:C:2298:MET:HE2	1:C:2298:MET:O	2.06	0.55
1:D:3180:PRO:HG3	1:D:3189:ASN:CG	2.27	0.55
1:D:3301:LYS:HD2	1:D:3301:LYS:N	2.21	0.55
1:F:5043:MET:HG2	1:F:5046:TYR:HE1	1.71	0.55
1:A:6289:HIS:HB3	1:A:6290:PHE:CE1	2.41	0.55
1:B:1025:THR:HA	1:B:1043:MET:SD	2.46	0.55
1:B:1180:PRO:HB3	1:B:1183:ARG:HG3	1.88	0.55
1:F:5090:ARG:NH2	1:F:5265:ASP:O	2.38	0.55
1:C:2068:LEU:HD21	1:C:2345:TYR:CE1	2.41	0.55
1:E:4056:PHE:HE1	1:E:4349:VAL:HG12	1.72	0.55
1:F:5095:LEU:O	1:F:5258:VAL:HG22	2.06	0.55
1:B:1296:ASN:O	1:B:1299:LYS:HG2	2.07	0.55
1:C:2180:PRO:HG3	1:C:2189:ASN:OD1	2.05	0.55
1:D:3147:LEU:HD21	1:D:3164:TRP:HZ2	1.70	0.55
1:F:5020:LYS:HE3	1:F:5024:ARG:NH2	2.07	0.55
1:C:2271:ARG:HG3	1:C:2271:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3087:ARG:CD	1:F:5162:ARG:HH11	2.19	0.55
1:D:3107:ALA:HA	1:D:3259:PRO:HG3	1.89	0.55
1:D:3164:TRP:HA	1:D:3164:TRP:HE3	1.69	0.55
1:D:3052:ARG:NH1	1:D:3263:LEU:C	2.60	0.55
1:A:6245:ARG:NE	1:A:6308:MET:SD	2.80	0.55
1:B:1141:ARG:HD2	1:B:1237:HIS:HE1	1.72	0.55
1:C:2046:TYR:CE2	1:C:2336:PRO:HD3	2.42	0.55
1:E:4019:VAL:O	1:E:4023:GLU:HB2	2.06	0.55
1:E:4215:LEU:HD13	1:E:4218:LEU:HD12	1.88	0.55
1:F:5319:HIS:O	1:F:5321:THR:N	2.41	0.55
1:F:5270:ILE:HG22	1:F:5329:LYS:NZ	2.22	0.55
1:C:2133:THR:HG22	1:C:2134:ASP:N	2.22	0.54
1:E:4020:LYS:HE2	1:E:4024:ARG:NH2	2.22	0.54
1:E:4030:PHE:HD1	1:E:4032:PRO:HD3	1.70	0.54
1:F:5052:ARG:NH1	1:F:5054:CYS:HB2	2.22	0.54
1:F:5080:GLN:OE1	1:F:5213:LYS:HG2	2.07	0.54
1:F:5289:HIS:HB3	1:F:5290:PHE:CE1	2.43	0.54
1:A:6008:GLN:NE2	1:A:6096:LYS:NZ	2.54	0.54
1:A:6133:THR:HG22	1:A:6134:ASP:N	2.22	0.54
1:A:6240:ALA:CB	1:A:6305:GLU:HG2	2.37	0.54
1:C:2147:LEU:O	1:C:2148:LYS:HB2	2.06	0.54
1:D:3005:VAL:HG13	1:D:3005:VAL:O	2.07	0.54
1:E:4005:VAL:O	1:E:4005:VAL:HG13	2.08	0.54
1:F:5253:ASP:CG	1:F:5254:SER:H	2.09	0.54
1:A:6253:ASP:CG	1:A:6254:SER:N	2.60	0.54
1:B:1081:LYS:O	1:B:1085:TRP:CD1	2.60	0.54
1:F:5161:THR:HG22	1:F:5162:ARG:CD	2.35	0.54
1:A:6146:SER:O	1:A:6148:LYS:HD3	2.07	0.54
1:C:2011:TYR:HA	1:C:2341:LEU:HD13	1.89	0.54
1:C:2017:LYS:HD2	1:C:2341:LEU:HD23	1.89	0.54
1:D:3050:MET:O	1:D:3264:LYS:HB2	2.07	0.54
1:F:5073:ILE:N	1:F:5073:ILE:HD12	2.23	0.54
1:A:6296:ASN:ND2	1:A:6296:ASN:O	2.40	0.54
1:B:1102:ASN:HD21	1:B:1117:ASP:HB3	1.72	0.54
1:E:4131:LYS:NZ	1:E:4173:LYS:NZ	2.56	0.54
1:A:6227:LEU:HG	1:A:6229:VAL:HG23	1.90	0.54
1:F:5141:ARG:NH1	1:F:5290:PHE:O	2.35	0.54
1:B:1141:ARG:HH21	1:B:1236:LEU:HD23	1.66	0.54
1:C:2015:MET:O	1:C:2019:VAL:HG23	2.08	0.54
1:C:2137:ASN:HB3	1:C:2237:HIS:CE1	2.42	0.54
1:E:4354:LYS:HA	1:E:4357:GLN:NE2	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2137:ASN:O	1:C:2141:ARG:HD3	2.07	0.54
1:C:2311:GLU:O	1:C:2312:ILE:HD12	2.08	0.54
1:E:4199:LEU:HD13	1:E:4207:ILE:HD11	1.90	0.54
1:E:4359:ASN:C	1:E:4361:GLU:H	2.11	0.54
1:F:5276:VAL:CG2	1:F:5325:ILE:HG21	2.38	0.54
1:A:6080:GLN:HE22	1:A:6212:ASP:HB2	1.72	0.54
1:D:3137:ASN:HB3	1:D:3237:HIS:NE2	2.23	0.54
1:E:4071:ARG:HH11	1:E:4071:ARG:HG3	1.73	0.54
1:F:5052:ARG:CZ	1:F:5054:CYS:HB2	2.37	0.54
1:A:6050:MET:O	1:A:6264:LYS:HB2	2.07	0.53
1:C:2234:LEU:HB2	1:C:2236:LEU:HD13	1.89	0.53
1:D:3273:VAL:HG13	1:D:3273:VAL:O	2.09	0.53
1:E:4245:ARG:HG3	1:E:4245:ARG:HH11	1.74	0.53
1:F:5052:ARG:HH22	1:F:5054:CYS:CB	2.21	0.53
1:A:6170:ASN:O	1:A:6173:LYS:N	2.40	0.53
1:C:2229:VAL:HG11	1:C:2257:PHE:HZ	1.72	0.53
1:D:3124:LYS:HD2	1:D:3177:THR:HG21	1.90	0.53
1:E:4189:ASN:N	1:E:4189:ASN:ND2	2.47	0.53
1:C:2107:ALA:HB1	1:C:2250:LEU:HD22	1.90	0.53
1:C:2160:ASP:OD1	1:C:2161:THR:N	2.40	0.53
1:D:3226:PRO:HG2	1:D:3228:LYS:HZ1	1.73	0.53
1:D:3355:LYS:O	1:D:3359:ASN:ND2	2.42	0.53
1:F:5162:ARG:N	1:F:5162:ARG:NE	2.57	0.53
1:F:5097:THR:HG21	1:F:5259:PRO:HD3	1.89	0.53
1:C:2141:ARG:HH22	1:C:2236:LEU:HB3	1.72	0.53
1:C:2310:ILE:HG13	1:C:2312:ILE:HD11	1.91	0.53
1:E:4047:THR:HG1	1:E:4205:ARG:HH22	1.54	0.53
1:A:6355:LYS:O	1:A:6355:LYS:HG2	2.08	0.53
1:B:1084:ASN:OD1	1:B:1091:LYS:HA	2.08	0.53
1:B:1192:GLU:HB2	1:B:1193:GLU:OE1	2.08	0.53
1:C:2042:THR:HA	1:C:2045:ARG:NH1	2.24	0.53
1:A:6098:ASN:HD22	1:A:6098:ASN:N	2.06	0.53
1:B:1048:LEU:HD12	1:B:1048:LEU:C	2.29	0.53
1:B:1293:ASP:O	1:B:1297:GLU:HG2	2.08	0.53
1:E:4048:LEU:CD2	1:E:4110:GLN:O	2.56	0.53
1:B:1095:LEU:O	1:B:1258:VAL:CG2	2.53	0.53
1:B:1201:ASN:OD1	1:B:1235:PRO:HA	2.08	0.53
1:B:1346:PHE:O	1:B:1349:VAL:HG22	2.09	0.53
1:C:2005:VAL:O	1:C:2005:VAL:HG13	2.09	0.53
1:C:2093:VAL:HG13	1:C:2261:VAL:CG2	2.38	0.53
1:D:3163:ASN:OD1	1:D:3166:ASP:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4136:ARG:HG2	1:E:4136:ARG:NH1	2.23	0.53
1:F:5046:TYR:HA	1:F:5334:ASN:HD21	1.72	0.53
1:A:6137:ASN:N	1:A:6137:ASN:HD22	2.06	0.53
1:A:6126:LEU:HD21	1:A:6195:HIS:HD2	1.74	0.53
1:B:1071:ARG:N	1:B:1071:ARG:HD3	2.15	0.53
1:B:1124:LYS:HE3	1:B:1177:THR:CG2	2.39	0.53
1:E:4194:ILE:O	1:E:4198:VAL:HG23	2.08	0.53
1:B:1298:MET:CB	1:B:1301:LYS:HD2	2.39	0.53
1:D:3150:GLN:HG3	1:D:3296:ASN:ND2	2.24	0.53
1:D:3353:TYR:O	1:D:3357:GLN:HG3	2.09	0.53
1:E:4086:CYS:SG	1:E:4088:GLU:HG2	2.49	0.53
1:F:5040:PHE:O	1:F:5204:ARG:NH1	2.42	0.53
1:A:6011:TYR:HA	1:A:6341:LEU:HD13	1.90	0.52
1:A:6359:ASN:C	1:A:6361:GLU:H	2.12	0.52
1:E:4025:THR:HB	1:E:4026:PRO:CD	2.39	0.52
1:A:6236:LEU:HD21	1:A:6291:LEU:CD2	2.39	0.52
1:C:2071:ARG:HH12	1:C:2096:LYS:HE2	1.73	0.52
1:E:4019:VAL:HA	1:E:4022:ARG:HH12	1.74	0.52
1:F:5052:ARG:HH21	1:F:5055:GLN:NE2	1.92	0.52
1:A:6024:ARG:HD2	1:A:6024:ARG:N	2.23	0.52
1:C:2310:ILE:CD1	1:C:2312:ILE:HD11	2.39	0.52
1:C:2359:ASN:C	1:C:2361:GLU:H	2.12	0.52
1:F:5161:THR:CG2	1:F:5162:ARG:HE	2.22	0.52
1:D:3253:ASP:OD2	1:D:3256:HIS:HB3	2.10	0.52
1:F:5086:CYS:SG	1:F:5088:GLU:HG2	2.49	0.52
1:F:5194:ILE:O	1:F:5198:VAL:HG23	2.09	0.52
1:F:5331:ASP:OD2	1:F:5332:GLU:N	2.42	0.52
1:A:6120:LEU:HD21	1:A:6188:TYR:CE2	2.44	0.52
1:A:6025:THR:CG2	1:A:6121:VAL:HG11	2.35	0.52
1:C:2048:LEU:HD12	1:C:2048:LEU:C	2.30	0.52
1:D:3049:GLU:HG3	1:D:3333:ALA:HB2	1.92	0.52
1:D:3081:LYS:NZ	1:F:5143:GLN:HE22	2.07	0.52
1:B:1192:GLU:CD	1:B:1194:ILE:HG22	2.30	0.52
1:C:2020:LYS:O	1:C:2024:ARG:HG3	2.10	0.52
1:C:2052:ARG:NH1	1:C:2266:SER:HB3	2.25	0.52
1:D:3084:ASN:CG	1:D:3091:LYS:HG3	2.30	0.52
1:F:5287:LYS:HE3	1:F:5289:HIS:CE1	2.45	0.52
1:A:6141:ARG:HH22	1:A:6295:GLU:CD	2.12	0.52
1:F:5004:GLN:NE2	1:F:5356:TRP:HH2	2.07	0.52
1:A:6100:ASP:O	1:A:6188:TYR:HD1	1.93	0.52
1:A:6081:LYS:NZ	1:A:6278:ARG:NH1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4215:LEU:HD13	1:E:4218:LEU:HG	1.91	0.52
1:E:4355:LYS:O	1:E:4359:ASN:ND2	2.43	0.52
1:A:6276:VAL:HG22	1:A:6325:ILE:HG21	1.91	0.52
1:E:4199:LEU:HD13	1:E:4207:ILE:CD1	2.40	0.52
1:A:6052:ARG:HG3	1:A:6052:ARG:NH1	2.24	0.51
1:C:2073:ILE:HD12	1:C:2258:VAL:HG21	1.91	0.51
1:F:5022:ARG:HB3	1:F:5119:ASP:OD1	2.10	0.51
1:B:1087:ARG:O	1:B:1087:ARG:HG2	2.11	0.51
1:B:1110:GLN:NE2	1:B:1116:GLN:NE2	2.58	0.51
1:E:4167:GLU:O	1:E:4170:ASN:HB3	2.10	0.51
1:C:2304:LYS:HA	1:C:2309:VAL:HG23	1.91	0.51
1:A:6039:HIS:CD2	1:A:6204:ARG:NH2	2.76	0.51
1:B:1359:ASN:C	1:B:1361:GLU:H	2.14	0.51
1:C:2094:ALA:HB1	1:C:2258:VAL:CG1	2.32	0.51
1:D:3077:LEU:HD13	1:D:3210:ILE:HG22	1.92	0.51
1:F:5161:THR:O	1:F:5162:ARG:HB2	2.09	0.51
1:F:5359:ASN:C	1:F:5361:GLU:H	2.13	0.51
1:A:6073:ILE:N	1:A:6073:ILE:CD1	2.74	0.51
1:B:1006:LEU:HD11	1:B:1349:VAL:HG12	1.93	0.51
1:C:2137:ASN:HB3	1:C:2237:HIS:NE2	2.25	0.51
1:D:3144:LEU:CD1	1:D:3149:SER:HB3	2.41	0.51
1:D:3359:ASN:C	1:D:3361:GLU:H	2.14	0.51
1:F:5319:HIS:ND1	1:F:5321:THR:CG2	2.74	0.51
1:C:2200:CYS:HB2	1:C:2205:ARG:O	2.11	0.51
1:D:3194:ILE:HA	1:D:3290:PHE:HE1	1.74	0.51
1:E:4022:ARG:CG	1:E:4022:ARG:HH11	2.22	0.51
1:F:5319:HIS:CE1	1:F:5321:THR:HG21	2.45	0.51
1:A:6314:VAL:HG12	1:A:6315:GLN:N	2.26	0.51
1:C:2186:LEU:N	1:C:2186:LEU:HD22	2.26	0.51
1:D:3024:ARG:NH1	1:D:3339:ILE:HD13	2.26	0.51
1:D:3226:PRO:HB2	1:D:3228:LYS:NZ	2.26	0.51
1:F:5142:TRP:HH2	1:F:5167:GLU:HB3	1.75	0.51
1:B:1094:ALA:HB1	1:B:1258:VAL:HG21	1.92	0.51
1:D:3312:ILE:HD13	1:D:3327:ALA:HB3	1.92	0.51
1:F:5084:ASN:OD1	1:F:5091:LYS:HG3	2.11	0.51
1:C:2273:VAL:O	1:C:2273:VAL:HG13	2.11	0.50
1:C:2301:LYS:HD2	1:C:2301:LYS:N	2.27	0.50
1:D:3087:ARG:HD2	1:F:5162:ARG:HH11	1.76	0.50
1:D:3025:THR:CG2	1:D:3121:VAL:HG11	2.40	0.50
1:D:3354:LYS:HA	1:D:3357:GLN:HE21	1.76	0.50
1:F:5059:GLN:OE1	1:F:5059:GLN:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5245:ARG:HB2	1:F:5308:MET:HE3	1.92	0.50
1:A:6060:PHE:HA	1:A:6063:ILE:HD12	1.92	0.50
1:A:6153:VAL:HG13	1:A:6153:VAL:O	2.11	0.50
1:A:6193:GLU:HG3	1:A:6233:TYR:OH	2.11	0.50
1:D:3151:GLU:HG2	1:D:3151:GLU:O	2.12	0.50
1:D:3204:ARG:HD2	1:D:3242:GLU:O	2.10	0.50
1:E:4153:VAL:O	1:E:4153:VAL:HG13	2.11	0.50
1:E:4173:LYS:N	1:E:4173:LYS:HD2	2.25	0.50
1:F:5216:ARG:HH11	1:F:5216:ARG:CB	2.13	0.50
1:F:5249:VAL:HG12	1:F:5260:LEU:HB2	1.93	0.50
1:A:6036:ILE:HG13	1:A:6037:ILE:N	2.27	0.50
1:B:1338:GLU:HG2	1:B:1339:ILE:HG23	1.92	0.50
1:C:2185:GLY:C	1:C:2186:LEU:HD22	2.31	0.50
1:D:3120:LEU:O	1:D:3124:LYS:HB2	2.11	0.50
1:D:3276:VAL:HG12	1:D:3285:ASP:HA	1.92	0.50
1:B:1295:GLU:HB3	1:B:1302:LEU:HD11	1.93	0.50
1:C:2139:LYS:HE3	1:C:2168:TRP:NE1	2.26	0.50
1:D:3314:VAL:HG13	1:D:3315:GLN:NE2	2.27	0.50
1:E:4028:ASP:O	1:E:4041:LYS:HD3	2.10	0.50
1:E:4314:VAL:HG22	1:E:4315:GLN:N	2.25	0.50
1:F:5133:THR:CG2	1:F:5134:ASP:N	2.74	0.50
1:A:6014:ASN:ND2	1:A:6017:LYS:HB2	2.27	0.50
1:B:1097:THR:HG21	1:B:1257:PHE:O	2.12	0.50
1:C:2107:ALA:HA	1:C:2259:PRO:HG3	1.92	0.50
1:D:3240:ALA:CB	1:D:3305:GLU:HG2	2.42	0.50
1:D:3304:LYS:HA	1:D:3309:VAL:HG23	1.92	0.50
1:C:2164:TRP:C	1:C:2166:ASP:N	2.61	0.50
1:C:2352:GLU:OE2	1:C:2352:GLU:HA	2.11	0.50
1:D:3299:LYS:HG3	1:D:3300:GLU:N	2.26	0.50
1:C:2253:ASP:OD1	1:C:2254:SER:N	2.44	0.50
1:C:2150:GLN:HE22	1:C:2287:LYS:CE	2.24	0.50
1:D:3086:CYS:SG	1:D:3089:VAL:HG22	2.52	0.50
1:E:4244:TYR:CE2	1:E:4246:TYR:HB2	2.46	0.50
1:A:6325:ILE:HG22	1:A:6326:ASN:H	1.76	0.50
1:B:1107:ALA:HB1	1:B:1250:LEU:HD22	1.93	0.50
1:B:1253:ASP:OD1	1:B:1254:SER:N	2.45	0.50
1:C:2142:TRP:CE2	1:C:2171:LEU:HD11	2.47	0.50
1:C:2082:LYS:HE2	1:C:2211:SER:O	2.11	0.50
1:D:3060:PHE:HA	1:D:3063:ILE:HD12	1.94	0.50
1:D:3133:THR:CG2	1:D:3134:ASP:N	2.74	0.50
1:F:5048:LEU:C	1:F:5048:LEU:HD12	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5219:GLU:O	1:F:5219:GLU:HG3	2.11	0.50
1:A:6020:LYS:O	1:A:6024:ARG:HD3	2.12	0.50
1:A:6199:LEU:O	1:A:6203:LEU:HG	2.12	0.50
1:A:6271:ARG:CZ	1:A:6332:GLU:HB3	2.41	0.50
1:C:2271:ARG:HB3	1:C:2330:LEU:HB2	1.94	0.50
1:D:3297:GLU:OE1	1:D:3297:GLU:HA	2.12	0.50
1:E:4014:ASN:ND2	1:E:4344:ASP:OD2	2.37	0.50
1:F:5153:VAL:O	1:F:5153:VAL:HG13	2.12	0.50
1:F:5279:ASP:CG	1:F:5280:ARG:N	2.65	0.50
1:B:1153:VAL:HG13	1:B:1153:VAL:O	2.12	0.49
1:B:1252:TYR:OH	1:B:1255:HIS:HA	2.11	0.49
1:C:2164:TRP:C	1:C:2166:ASP:H	2.13	0.49
1:D:3162:ARG:NH2	1:E:4081:LYS:NZ	2.59	0.49
1:B:1240:ALA:CB	1:B:1305:GLU:HG2	2.42	0.49
1:F:5070:ASP:CG	1:F:5073:ILE:HD13	2.33	0.49
1:F:5076:THR:O	1:F:5080:GLN:HG2	2.12	0.49
1:A:6149:SER:C	1:A:6150:GLN:HG2	2.32	0.49
1:A:6186:LEU:HD22	1:A:6186:LEU:N	2.27	0.49
1:B:1025:THR:HG22	1:B:1026:PRO:N	2.27	0.49
1:E:4234:LEU:O	1:E:4236:LEU:HD22	2.13	0.49
1:A:6097:THR:CG2	1:A:6258:VAL:HA	2.43	0.49
1:A:6147:LEU:O	1:A:6148:LYS:HB2	2.13	0.49
1:B:1169:ASP:HA	1:B:1172:ILE:HD12	1.93	0.49
1:E:4136:ARG:HG2	1:E:4136:ARG:HH11	1.77	0.49
1:F:5168:TRP:O	1:F:5172:ILE:HG13	2.12	0.49
1:F:5253:ASP:CG	1:F:5254:SER:N	2.65	0.49
1:B:1003:GLU:OE2	1:B:1003:GLU:N	2.46	0.49
1:B:1034:ASN:ND2	1:B:1036:ILE:HG22	2.26	0.49
1:C:2153:VAL:HG13	1:C:2153:VAL:O	2.12	0.49
1:F:5179:THR:HG22	1:F:5180:PRO:O	2.13	0.49
1:D:3094:ALA:HB1	1:D:3258:VAL:CG1	2.35	0.49
1:D:3226:PRO:HB2	1:D:3228:LYS:HZ3	1.76	0.49
1:E:4227:LEU:HD23	1:E:4252:TYR:OH	2.13	0.49
1:B:1074:GLN:OE1	1:B:1093:VAL:HA	2.13	0.49
1:D:3151:GLU:HB3	1:D:3296:ASN:OD1	2.12	0.49
1:D:3227:LEU:CD2	1:D:3229:VAL:HG13	2.43	0.49
1:D:3355:LYS:HG2	1:D:3355:LYS:O	2.13	0.49
1:E:4104:LEU:HB2	1:E:4257:PHE:CE1	2.48	0.49
1:E:4173:LYS:O	1:E:4176:SER:OG	2.23	0.49
1:F:5245:ARG:HH21	1:F:5308:MET:HG2	1.76	0.49
1:F:5090:ARG:HD2	1:F:5271:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6204:ARG:HD3	1:A:6238:TRP:CE3	2.47	0.49
1:A:6273:VAL:O	1:A:6273:VAL:HG13	2.12	0.49
1:B:1082:LYS:HD3	1:B:1213:LYS:HE3	1.95	0.49
1:C:2060:PHE:CE1	1:C:2064:ILE:HD11	2.47	0.49
1:E:4240:ALA:CB	1:E:4305:GLU:HG2	2.42	0.49
1:E:4354:LYS:O	1:E:4358:GLU:HG3	2.12	0.49
1:A:6276:VAL:HG21	1:A:6325:ILE:HG21	1.93	0.48
1:D:3015:MET:O	1:D:3019:VAL:HG23	2.13	0.48
1:D:3215:LEU:HB3	1:D:3218:LEU:HB2	1.94	0.48
1:D:3270:ILE:N	1:D:3270:ILE:HD13	2.21	0.48
1:E:4010:LEU:HD13	1:E:4342:VAL:HG22	1.95	0.48
1:F:5355:LYS:O	1:F:5359:ASN:CG	2.51	0.48
1:A:6127:PHE:HE1	1:A:6172:ILE:O	1.96	0.48
1:C:2136:ARG:HG2	1:C:2136:ARG:HH11	1.78	0.48
1:D:3227:LEU:HD22	1:D:3229:VAL:HG13	1.94	0.48
1:D:3052:ARG:CZ	1:D:3263:LEU:HB3	2.42	0.48
1:E:4019:VAL:HA	1:E:4022:ARG:NH1	2.29	0.48
1:E:4097:THR:HA	1:E:4116:GLN:NE2	2.28	0.48
1:D:3137:ASN:ND2	1:E:4216:ARG:HH11	2.10	0.48
1:E:4227:LEU:HG	1:E:4229:VAL:HG22	1.94	0.48
1:F:5265:ASP:O	1:F:5266:SER:O	2.31	0.48
1:B:1141:ARG:HH22	1:B:1236:LEU:HD23	1.68	0.48
1:D:3162:ARG:O	1:D:3163:ASN:HB2	2.14	0.48
1:E:4069:ILE:O	1:E:4096:LYS:NZ	2.40	0.48
1:A:6185:GLY:C	1:A:6186:LEU:HD22	2.32	0.48
1:A:6193:GLU:HB3	1:A:6290:PHE:CZ	2.47	0.48
1:B:1133:THR:CG2	1:B:1134:ASP:N	2.76	0.48
1:C:2204:ARG:HD2	1:C:2238:TRP:CH2	2.48	0.48
1:E:4215:LEU:HD13	1:E:4218:LEU:CG	2.43	0.48
1:E:4097:THR:CG2	1:E:4258:VAL:HA	2.39	0.48
1:A:6070:ASP:CG	1:A:6073:ILE:HD13	2.33	0.48
1:A:6270:ILE:H	1:A:6270:ILE:HD12	1.77	0.48
1:B:1200:CYS:HB2	1:B:1205:ARG:O	2.13	0.48
1:C:2192:GLU:HB2	1:C:2193:GLU:OE1	2.13	0.48
1:C:2141:ARG:HH22	1:C:2236:LEU:CB	2.25	0.48
1:D:3160:ASP:CG	1:D:3161:THR:H	2.17	0.48
1:D:3317:TRP:C	1:D:3319:HIS:HD2	2.16	0.48
1:E:4215:LEU:HD22	1:E:4218:LEU:HG	1.95	0.48
1:F:5017:LYS:HD2	1:F:5341:LEU:HD23	1.95	0.48
1:B:1082:LYS:HD2	1:B:1213:LYS:HE3	1.95	0.48
1:B:1277:ASN:HD21	1:B:1286:LEU:CD1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3052:ARG:NH2	1:D:3266:SER:OG	2.45	0.48
1:E:4066:LYS:O	1:E:4066:LYS:HD3	2.14	0.48
1:A:6303:LEU:O	1:A:6307:LEU:HB2	2.14	0.48
1:A:6046:TYR:HA	1:A:6334:ASN:OD1	2.13	0.48
1:D:3050:MET:HE2	1:D:3068:LEU:HD13	1.96	0.48
1:C:2120:LEU:O	1:C:2124:LYS:HG3	2.14	0.48
1:C:2287:LYS:HD3	1:C:2287:LYS:C	2.34	0.48
1:E:4097:THR:HA	1:E:4116:GLN:HE22	1.78	0.48
1:A:6292:THR:HB	1:A:6294:PRO:HD2	1.95	0.48
1:C:2010:LEU:HA	1:C:2345:TYR:HD1	1.79	0.48
1:C:2227:LEU:HG	1:C:2229:VAL:HG23	1.96	0.48
1:C:2254:SER:OG	1:C:2255:HIS:N	2.44	0.48
1:D:3293:ASP:CB	1:D:3294:PRO:HD3	2.42	0.48
1:B:1179:THR:HG22	1:B:1180:PRO:O	2.13	0.48
1:D:3052:ARG:HH11	1:D:3264:LYS:N	2.12	0.48
1:E:4097:THR:HG21	1:E:4257:PHE:O	2.13	0.48
1:B:1238:TRP:HB2	1:B:1243:CYS:SG	2.54	0.47
1:B:1336:PRO:HD2	1:B:1339:ILE:CG1	2.44	0.47
1:D:3163:ASN:O	1:D:3163:ASN:OD1	2.32	0.47
1:D:3311:GLU:OE1	1:D:3324:LEU:HD23	2.14	0.47
1:D:3087:ARG:CZ	1:F:5162:ARG:HG3	2.44	0.47
1:C:2152:PHE:CD1	1:C:2287:LYS:HG2	2.49	0.47
1:D:3028:ASP:CG	1:D:3043:MET:HG3	2.34	0.47
1:D:3127:PHE:CE1	1:D:3176:SER:HB2	2.48	0.47
1:D:3214:MET:HG3	1:F:5140:PHE:CE2	2.49	0.47
1:F:5142:TRP:CZ2	1:F:5167:GLU:HG3	2.49	0.47
1:F:5276:VAL:HG22	1:F:5325:ILE:HG21	1.96	0.47
1:F:5281:GLY:HA2	1:F:5317:TRP:CE2	2.48	0.47
1:A:6022:ARG:NH2	1:A:6119:ASP:OD2	2.46	0.47
1:F:5346:PHE:O	1:F:5349:VAL:HG23	2.14	0.47
1:A:6082:LYS:HA	1:A:6082:LYS:CE	2.40	0.47
1:B:1010:LEU:HG	1:B:1068:LEU:HD22	1.96	0.47
1:B:1142:TRP:CH2	1:B:1167:GLU:HG2	2.50	0.47
1:C:2139:LYS:HB2	1:C:2139:LYS:HZ2	1.78	0.47
1:C:2345:TYR:HD2	1:C:2345:TYR:O	1.97	0.47
1:E:4145:GLU:OE1	1:E:4290:PHE:N	2.47	0.47
1:F:5010:LEU:HA	1:F:5345:TYR:CD1	2.49	0.47
1:A:6015:MET:O	1:A:6019:VAL:HG23	2.14	0.47
1:B:1137:ASN:HB2	1:B:1237:HIS:NE2	2.30	0.47
1:B:1169:ASP:O	1:B:1173:LYS:HD3	2.14	0.47
1:C:2060:PHE:CD2	1:C:2063:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4344:ASP:O	1:E:4348:LEU:HD13	2.14	0.47
1:B:1082:LYS:NZ	1:B:1213:LYS:NZ	2.63	0.47
1:B:1314:VAL:HG21	1:B:1325:ILE:CD1	2.40	0.47
1:C:2052:ARG:HB3	1:C:2055:GLN:HE21	1.80	0.47
1:D:3050:MET:HE1	1:D:3068:LEU:HD13	1.97	0.47
1:F:5008:GLN:OE1	1:F:5096:LYS:HE2	2.15	0.47
1:F:5218:LEU:HD23	1:F:5219:GLU:H	1.79	0.47
1:F:5314:VAL:HG12	1:F:5315:GLN:N	2.30	0.47
1:F:5010:LEU:HA	1:F:5345:TYR:HD1	1.79	0.47
1:E:4064:ILE:HD11	1:E:4349:VAL:HG11	1.97	0.47
1:D:3136:ARG:NH1	1:E:4278:ARG:HH12	2.11	0.47
1:F:5343:ASP:O	1:F:5347:GLU:HG2	2.14	0.47
1:A:6271:ARG:NE	1:A:6332:GLU:HB3	2.29	0.47
1:A:6337:LYS:HE2	1:A:6343:ASP:CG	2.33	0.47
1:B:1358:GLU:HA	1:B:1361:GLU:OE2	2.15	0.47
1:C:2102:ASN:HD22	1:C:2106:HIS:CE1	2.33	0.47
1:E:4070:ASP:OD1	1:E:4073:ILE:HD13	2.15	0.47
1:A:6127:PHE:CE1	1:A:6172:ILE:O	2.67	0.47
1:A:6081:LYS:HZ3	1:A:6278:ARG:HH12	1.61	0.47
1:B:1025:THR:HG22	1:B:1121:VAL:HG11	1.96	0.47
1:D:3162:ARG:HH21	1:E:4081:LYS:HZ1	1.62	0.47
1:D:3171:LEU:HD13	1:D:3194:ILE:HG21	1.96	0.47
1:D:3281:GLY:HA2	1:D:3317:TRP:CE2	2.49	0.47
1:E:4254:SER:OG	1:E:4255:HIS:N	2.47	0.47
1:F:5253:ASP:OD2	1:F:5254:SER:N	2.47	0.47
1:F:5298:MET:C	1:F:5301:LYS:HD3	2.36	0.47
1:A:6057:CYS:SG	1:A:6059:GLN:CD	2.94	0.47
1:A:6307:LEU:HD13	1:A:6328:ALA:HB2	1.97	0.47
1:B:1216:ARG:HG3	1:B:1216:ARG:HH11	1.80	0.47
1:B:1277:ASN:HD21	1:B:1286:LEU:HD13	1.80	0.47
1:B:1046:TYR:HB3	1:B:1335:LEU:HD21	1.97	0.47
1:D:3120:LEU:HD11	1:D:3188:TYR:OH	2.15	0.47
1:E:4129:THR:O	1:E:4133:THR:HB	2.15	0.47
1:E:4133:THR:HG23	1:E:4134:ASP:N	2.30	0.47
1:E:4317:TRP:HB2	1:E:4319:HIS:NE2	2.29	0.47
1:A:6265:ASP:O	1:A:6266:SER:O	2.32	0.47
1:B:1097:THR:HG23	1:B:1256:HIS:NE2	2.29	0.47
1:D:3008:GLN:HE21	1:D:3096:LYS:HZ3	1.57	0.47
1:F:5271:ARG:HH11	1:F:5271:ARG:CB	2.27	0.47
1:A:6133:THR:CG2	1:A:6134:ASP:N	2.77	0.46
1:A:6267:GLY:HA2	1:A:6268:PRO:HD3	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:LYS:CE	1:B:1082:LYS:HA	2.45	0.46
1:E:4317:TRP:HH2	1:E:4323:HIS:CD2	2.33	0.46
1:B:1080:GLN:HG3	1:B:1082:LYS:HB2	1.97	0.46
1:C:2164:TRP:CA	1:C:2164:TRP:CE3	2.93	0.46
1:C:2314:VAL:HG21	1:C:2325:ILE:HD13	1.97	0.46
1:D:3153:VAL:O	1:D:3153:VAL:HG13	2.16	0.46
1:E:4143:GLN:HA	1:E:4164:TRP:CZ3	2.50	0.46
1:E:4312:ILE:HD12	1:E:4327:ALA:CB	2.45	0.46
1:F:5082:LYS:NZ	1:F:5213:LYS:HD3	2.31	0.46
1:F:5245:ARG:HB2	1:F:5308:MET:HE2	1.97	0.46
1:F:5349:VAL:O	1:F:5353:TYR:HB2	2.16	0.46
1:A:6057:CYS:SG	1:A:6059:GLN:NE2	2.89	0.46
1:A:6140:PHE:CZ	1:B:1214:MET:HG3	2.51	0.46
1:A:6152:PHE:HD2	1:A:6299:LYS:NZ	2.02	0.46
1:A:6191:LEU:HD22	1:A:6195:HIS:CD2	2.51	0.46
1:B:1142:TRP:HH2	1:B:1167:GLU:HG2	1.79	0.46
1:C:2048:LEU:HD13	1:C:2342:VAL:HG21	1.96	0.46
1:C:2117:ASP:OD2	1:C:2122:LEU:HB2	2.16	0.46
1:C:2133:THR:CG2	1:C:2134:ASP:N	2.78	0.46
1:D:3030:PHE:O	1:D:3032:PRO:HD2	2.16	0.46
1:D:3048:LEU:CD1	1:D:3048:LEU:C	2.83	0.46
1:D:3052:ARG:NH1	1:D:3264:LYS:N	2.62	0.46
1:D:3314:VAL:HG12	1:D:3315:GLN:N	2.30	0.46
1:F:5356:TRP:HA	1:F:5356:TRP:CE3	2.49	0.46
1:C:2343:ASP:O	1:C:2346:PHE:HB3	2.16	0.46
1:D:3147:LEU:O	1:D:3148:LYS:HB2	2.15	0.46
1:F:5267:GLY:HA2	1:F:5268:PRO:HD3	1.68	0.46
1:A:6066:LYS:HZ1	1:A:6071:ARG:NH2	2.12	0.46
1:A:6151:GLU:HB3	1:A:6296:ASN:HD21	1.80	0.46
1:B:1052:ARG:NH1	1:B:1265:ASP:N	2.63	0.46
1:B:1267:GLY:HA2	1:B:1268:PRO:HD3	1.74	0.46
1:E:4137:ASN:HB2	1:E:4237:HIS:NE2	2.31	0.46
1:F:5200:CYS:HB2	1:F:5205:ARG:O	2.15	0.46
1:B:1014:ASN:ND2	1:B:1344:ASP:OD2	2.49	0.46
1:E:4150:GLN:OE1	1:E:4287:LYS:NZ	2.48	0.46
1:F:5336:PRO:CD	1:F:5339:ILE:HD11	2.28	0.46
1:A:6227:LEU:HD23	1:A:6252:TYR:OH	2.15	0.46
1:E:4030:PHE:O	1:E:4032:PRO:HD2	2.16	0.46
1:E:4034:ASN:CG	1:E:4035:GLY:N	2.68	0.46
1:E:4074:GLN:HE21	1:E:4074:GLN:C	2.19	0.46
1:B:1265:ASP:O	1:B:1266:SER:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2240:ALA:HB3	1:C:2305:GLU:HG2	1.97	0.46
1:D:3304:LYS:HA	1:D:3309:VAL:CG2	2.46	0.46
1:E:4061:ARG:NH1	1:E:4065:HIS:HE1	2.14	0.46
1:E:4270:ILE:HD11	1:E:4312:ILE:HD11	1.97	0.46
1:F:5090:ARG:HD2	1:F:5271:ARG:CG	2.45	0.46
1:B:1008:GLN:HE21	1:B:1008:GLN:CA	2.25	0.46
1:C:2265:ASP:O	1:C:2266:SER:O	2.34	0.46
1:D:3299:LYS:HG3	1:D:3300:GLU:H	1.81	0.46
1:F:5053:THR:C	1:F:5055:GLN:H	2.19	0.46
1:F:5097:THR:HG22	1:F:5110:GLN:NE2	2.25	0.46
1:F:5355:LYS:HG2	1:F:5355:LYS:O	2.16	0.46
1:A:6059:GLN:O	1:A:6063:ILE:HG13	2.15	0.46
1:D:3150:GLN:HB3	1:D:3153:VAL:HG12	1.98	0.46
1:D:3153:VAL:O	1:D:3154:GLU:HB3	2.16	0.46
1:E:4104:LEU:HB2	1:E:4257:PHE:CD1	2.51	0.46
1:F:5162:ARG:HH11	1:F:5162:ARG:HG3	1.81	0.46
1:F:5183:ARG:HH11	1:F:5183:ARG:CG	2.28	0.46
1:A:6059:GLN:H	1:A:6059:GLN:CD	2.18	0.45
1:C:2003:GLU:O	1:C:2005:VAL:N	2.49	0.45
1:C:2275:LEU:HD23	1:C:2275:LEU:N	2.31	0.45
1:C:2279:ASP:HB3	1:C:2282:ARG:HG2	1.99	0.45
1:C:2349:VAL:O	1:C:2353:TYR:HB2	2.16	0.45
1:D:3206:PRO:HG3	1:D:3307:LEU:HD23	1.96	0.45
1:F:5207:ILE:HG12	1:F:5248:ILE:HB	1.99	0.45
1:A:6016:ARG:C	1:A:6016:ARG:HD3	2.37	0.45
1:B:1091:LYS:O	1:B:1263:LEU:HD23	2.16	0.45
1:D:3081:LYS:HZ1	1:F:5143:GLN:NE2	2.14	0.45
1:D:3037:ILE:HB	1:D:3129:THR:HG23	1.98	0.45
1:F:5270:ILE:HG22	1:F:5329:LYS:HZ2	1.80	0.45
1:C:2253:ASP:OD2	1:C:2256:HIS:HB3	2.17	0.45
1:C:2314:VAL:HG12	1:C:2315:GLN:N	2.31	0.45
1:C:2317:TRP:H	1:C:2319:HIS:CE1	2.34	0.45
1:D:3152:PHE:CZ	1:D:3288:VAL:HB	2.51	0.45
1:E:4127:PHE:HE1	1:E:4172:ILE:O	1.99	0.45
1:F:5042:THR:HG22	1:F:5045:ARG:NH2	2.31	0.45
1:A:6215:LEU:HD13	1:A:6218:LEU:CD1	2.46	0.45
1:A:6245:ARG:NH1	1:A:6304:LYS:O	2.41	0.45
1:B:1003:GLU:O	1:B:1005:VAL:N	2.49	0.45
1:B:1020:LYS:O	1:B:1024:ARG:HG3	2.15	0.45
1:C:2269:GLU:CD	1:C:2269:GLU:H	2.20	0.45
1:E:4020:LYS:HE2	1:E:4024:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4199:LEU:O	1:E:4203:LEU:HG	2.16	0.45
1:E:4193:GLU:HB3	1:E:4290:PHE:CZ	2.51	0.45
1:A:6093:VAL:HG12	1:A:6261:VAL:HG23	1.99	0.45
1:A:6209:VAL:HG11	1:A:6229:VAL:HG12	1.98	0.45
1:C:2060:PHE:HA	1:C:2063:ILE:HD12	1.98	0.45
1:C:2230:GLY:O	1:C:2289:HIS:HE1	2.00	0.45
1:E:4074:GLN:NE2	1:E:4074:GLN:CA	2.80	0.45
1:E:4152:PHE:CD2	1:E:4299:LYS:HD3	2.51	0.45
1:A:6148:LYS:HE2	1:A:6148:LYS:HB2	1.81	0.45
1:B:1048:LEU:HD12	1:B:1049:GLU:CA	2.46	0.45
1:E:4127:PHE:CE1	1:E:4172:ILE:O	2.69	0.45
1:F:5057:CYS:SG	1:F:5058:PRO:HD2	2.57	0.45
1:C:2230:GLY:O	1:C:2289:HIS:CE1	2.70	0.45
1:E:4049:GLU:O	1:E:4264:LYS:HE3	2.17	0.45
1:E:4267:GLY:HA2	1:E:4268:PRO:HD3	1.68	0.45
1:F:5345:TYR:O	1:F:5348:LEU:HB3	2.17	0.45
1:A:6019:VAL:O	1:A:6023:GLU:HB2	2.17	0.45
1:A:6196:ILE:HB	1:A:6233:TYR:CE2	2.52	0.45
1:A:6321:THR:HG22	1:A:6322:THR:N	2.31	0.45
1:B:1046:TYR:O	1:B:1112:MET:HB3	2.17	0.45
1:C:2084:ASN:OD1	1:C:2091:LYS:HG3	2.16	0.45
1:C:2227:LEU:HG	1:C:2229:VAL:CG2	2.47	0.45
1:C:2345:TYR:CD2	1:C:2345:TYR:O	2.70	0.45
1:F:5038:HIS:HE1	1:F:5128:SER:HB3	1.81	0.45
1:F:5262:THR:HG21	1:F:5271:ARG:HG2	1.99	0.45
1:C:2006:LEU:HA	1:C:2006:LEU:HD12	1.82	0.45
1:C:2015:MET:SD	1:F:5007:PRO:HD3	2.57	0.45
1:C:2059:GLN:O	1:C:2063:ILE:HG13	2.17	0.45
1:C:2152:PHE:CE1	1:C:2287:LYS:HG2	2.51	0.45
1:D:3319:HIS:C	1:D:3321:THR:H	2.19	0.45
1:F:5204:ARG:HG3	1:F:5238:TRP:NE1	2.32	0.45
1:B:1069:ILE:HD11	1:B:1093:VAL:HG21	1.99	0.45
1:B:1150:GLN:NE2	1:B:1152:PHE:CE1	2.85	0.45
1:B:1152:PHE:CE2	1:B:1296:ASN:ND2	2.85	0.45
1:B:1147:LEU:CD2	1:B:1164:TRP:HZ2	2.30	0.45
1:B:1319:HIS:C	1:B:1321:THR:H	2.20	0.45
1:F:5046:TYR:HD1	1:F:5113:TRP:HE1	1.65	0.45
1:F:5161:THR:HG22	1:F:5162:ARG:NE	2.32	0.45
1:A:6053:THR:C	1:A:6055:GLN:H	2.20	0.44
1:A:6056:PHE:O	1:A:6061:ARG:CD	2.63	0.44
1:A:6071:ARG:HG3	1:A:6071:ARG:HH11	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6022:ARG:HB3	1:A:6119:ASP:OD1	2.17	0.44
1:B:1142:TRP:O	1:B:1146:SER:HB2	2.17	0.44
1:B:1286:LEU:HA	1:B:1286:LEU:HD12	1.75	0.44
1:C:2086:CYS:SG	1:C:2088:GLU:HG2	2.57	0.44
1:E:4279:ASP:CG	1:E:4280:ARG:N	2.70	0.44
1:E:4064:ILE:CD1	1:E:4349:VAL:HG11	2.46	0.44
1:F:5038:HIS:O	1:F:5202:ILE:HG23	2.18	0.44
1:A:6253:ASP:OD2	1:A:6254:SER:N	2.50	0.44
1:A:6249:VAL:CG1	1:A:6260:LEU:HB2	2.46	0.44
1:A:6232:ILE:HG13	1:A:6286:LEU:HD23	2.00	0.44
1:B:1036:ILE:HG13	1:B:1037:ILE:N	2.32	0.44
1:B:1240:ALA:HB3	1:B:1305:GLU:HG2	1.98	0.44
1:D:3055:GLN:HG3	1:D:3056:PHE:CE1	2.52	0.44
1:F:5028:ASP:OD1	1:F:5041:LYS:HB2	2.17	0.44
1:F:5104:LEU:HB2	1:F:5257:PHE:CE1	2.53	0.44
1:A:6160:ASP:CG	1:A:6161:THR:N	2.64	0.44
1:B:1180:PRO:CB	1:B:1183:ARG:HG3	2.48	0.44
1:C:2334:ASN:C	1:C:2334:ASN:HD22	2.19	0.44
1:D:3087:ARG:HG3	1:D:3315:GLN:OE1	2.16	0.44
1:D:3106:HIS:ND1	1:D:3116:GLN:HB3	2.32	0.44
1:D:3210:ILE:HD12	1:D:3260:LEU:CD1	2.48	0.44
1:D:3252:TYR:CZ	1:D:3255:HIS:HA	2.52	0.44
1:D:3265:ASP:O	1:D:3266:SER:O	2.34	0.44
1:F:5137:ASN:HB2	1:F:5237:HIS:CE1	2.52	0.44
1:A:6074:GLN:HE22	1:A:6078:GLU:CD	2.21	0.44
1:A:6181:MET:HA	1:A:6181:MET:CE	2.48	0.44
1:B:1153:VAL:O	1:B:1154:GLU:HB3	2.18	0.44
1:B:1233:TYR:CD1	1:B:1233:TYR:N	2.85	0.44
1:E:4142:TRP:CZ3	1:E:4164:TRP:HE3	2.35	0.44
1:E:4164:TRP:C	1:E:4166:ASP:H	2.21	0.44
1:F:5046:TYR:O	1:F:5112:MET:HB3	2.17	0.44
1:F:5127:PHE:CE1	1:F:5172:ILE:O	2.70	0.44
1:B:1228:LYS:N	1:B:1228:LYS:CD	2.67	0.44
1:B:1335:LEU:HA	1:B:1336:PRO:HD3	1.89	0.44
1:C:2010:LEU:HD13	1:C:2342:VAL:HG22	1.99	0.44
1:C:2298:MET:HE3	1:C:2301:LYS:CB	2.37	0.44
1:D:3003:GLU:O	1:D:3005:VAL:N	2.51	0.44
1:D:3092:LEU:HD22	1:D:3260:LEU:O	2.17	0.44
1:E:4011:TYR:CA	1:E:4341:LEU:HD13	2.44	0.44
1:C:2119:ASP:HA	1:F:5355:LYS:NZ	2.32	0.44
1:B:1117:ASP:OD1	1:B:1122:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2052:ARG:CZ	1:C:2266:SER:CB	2.84	0.44
1:C:2047:THR:N	1:C:2334:ASN:HD21	2.12	0.44
1:D:3162:ARG:NH2	1:E:4081:LYS:HZ2	2.16	0.44
1:D:3317:TRP:O	1:D:3319:HIS:HD2	2.01	0.44
1:E:4036:ILE:HG13	1:E:4037:ILE:N	2.33	0.44
1:E:4102:ASN:ND2	1:E:4117:ASP:OD1	2.40	0.44
1:F:5240:ALA:HB3	1:F:5305:GLU:HG2	1.99	0.44
1:F:5236:LEU:HA	1:F:5306:TYR:OH	2.17	0.44
1:A:6003:GLU:O	1:A:6005:VAL:N	2.50	0.44
1:A:6337:LYS:NZ	1:A:6340:ASN:HB3	2.17	0.44
1:D:3074:GLN:HG2	1:D:3094:ALA:HB3	1.99	0.44
1:D:3111:TYR:CE2	1:D:3248:ILE:HA	2.52	0.44
1:E:4147:LEU:O	1:E:4148:LYS:HB2	2.18	0.44
1:E:4265:ASP:O	1:E:4266:SER:O	2.34	0.44
1:F:5164:TRP:O	1:F:5167:GLU:N	2.50	0.44
1:B:1046:TYR:HA	1:B:1334:ASN:OD1	2.17	0.44
1:B:1150:GLN:HB2	1:B:1153:VAL:HG12	1.99	0.44
1:D:3049:GLU:OE2	1:D:3332:GLU:HG3	2.18	0.44
1:D:3053:THR:C	1:D:3055:GLN:H	2.20	0.44
1:D:3168:TRP:CD1	1:D:3169:ASP:N	2.86	0.44
1:D:3300:GLU:O	1:D:3304:LYS:HG3	2.17	0.44
1:E:4003:GLU:O	1:E:4005:VAL:N	2.50	0.44
1:E:4139:LYS:HE3	1:E:4165:ASN:HA	1.99	0.44
1:F:5052:ARG:HG2	1:F:5052:ARG:HH11	1.83	0.44
1:D:3081:LYS:HZ1	1:F:5143:GLN:HE22	1.65	0.44
1:F:5150:GLN:HB3	1:F:5153:VAL:HG12	2.00	0.44
1:F:5039:HIS:HA	1:F:5202:ILE:O	2.18	0.44
1:D:3025:THR:HG22	1:D:3026:PRO:N	2.32	0.44
1:D:3081:LYS:HB3	1:D:3278:ARG:HD3	2.00	0.44
1:D:3168:TRP:HE1	1:D:3172:ILE:HD11	1.83	0.44
1:E:4131:LYS:NZ	1:E:4173:LYS:HZ2	2.15	0.44
1:E:4317:TRP:HH2	1:E:4323:HIS:HD2	1.66	0.44
1:A:6150:GLN:HB2	1:A:6153:VAL:HG12	2.00	0.43
1:A:6314:VAL:CG1	1:A:6315:GLN:N	2.81	0.43
1:B:1254:SER:OG	1:B:1255:HIS:N	2.51	0.43
1:D:3162:ARG:CZ	1:E:4081:LYS:HZ2	2.31	0.43
1:F:5162:ARG:O	1:F:5163:ASN:HB2	2.17	0.43
1:F:5130:LEU:HB3	1:F:5172:ILE:HG12	2.00	0.43
1:A:6233:TYR:CE2	1:A:6290:PHE:HE1	2.36	0.43
1:B:1004:GLN:HG2	1:B:1004:GLN:O	2.18	0.43
1:C:2028:ASP:OD2	1:C:2041:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2084:ASN:OD1	1:C:2091:LYS:HA	2.19	0.43
1:C:2229:VAL:HG11	1:C:2257:PHE:CZ	2.53	0.43
1:C:2271:ARG:HG3	1:C:2271:ARG:NH1	2.33	0.43
1:D:3144:LEU:HD11	1:D:3149:SER:HB3	1.99	0.43
1:E:4234:LEU:HB2	1:E:4236:LEU:CD2	2.48	0.43
1:E:4319:HIS:C	1:E:4321:THR:H	2.21	0.43
1:F:5043:MET:HB3	1:F:5113:TRP:CZ2	2.53	0.43
1:C:2037:ILE:CG2	1:C:2133:THR:HG21	2.35	0.43
1:D:3234:LEU:HB2	1:D:3236:LEU:HD13	1.99	0.43
1:E:4136:ARG:HH11	1:E:4136:ARG:CG	2.32	0.43
1:F:5073:ILE:N	1:F:5073:ILE:CD1	2.82	0.43
1:F:5088:GLU:O	1:F:5270:ILE:HD12	2.18	0.43
1:F:5102:ASN:HD22	1:F:5106:HIS:CE1	2.37	0.43
1:F:5246:TYR:CD2	1:F:5331:ASP:N	2.85	0.43
1:F:5319:HIS:C	1:F:5321:THR:H	2.21	0.43
1:C:2019:VAL:HG13	1:F:5351:HIS:CG	2.52	0.43
1:C:2075:ALA:O	1:C:2079:SER:HB2	2.18	0.43
1:E:4193:GLU:HB3	1:E:4290:PHE:HZ	1.83	0.43
1:F:5003:GLU:O	1:F:5005:VAL:N	2.51	0.43
1:F:5052:ARG:HH12	1:F:5054:CYS:HB2	1.81	0.43
1:A:6069:ILE:HG23	1:A:6094:ALA:O	2.19	0.43
1:B:1052:ARG:HD3	1:B:1265:ASP:H	1.83	0.43
1:B:1152:PHE:CZ	1:B:1288:VAL:HB	2.53	0.43
1:C:2218:LEU:HD23	1:C:2219:GLU:N	2.33	0.43
1:C:2110:GLN:HB2	1:C:2259:PRO:HG2	2.01	0.43
1:E:4076:THR:HG22	1:E:4080:GLN:NE2	2.33	0.43
1:F:5037:ILE:CD1	1:F:5201:ASN:HB3	2.48	0.43
1:A:6161:THR:O	1:A:6162:ARG:HB3	2.19	0.43
1:A:6143:GLN:HG2	1:A:6164:TRP:CE3	2.54	0.43
1:B:1082:LYS:CA	1:B:1082:LYS:HE3	2.48	0.43
1:C:2109:SER:HG	1:C:2113:TRP:HZ3	1.67	0.43
1:C:2334:ASN:ND2	1:C:2334:ASN:C	2.71	0.43
1:D:3076:THR:O	1:D:3080:GLN:HG2	2.19	0.43
1:D:3063:ILE:HD11	1:D:3356:TRP:CZ3	2.53	0.43
1:E:4143:GLN:HG2	1:E:4164:TRP:CE3	2.54	0.43
1:E:4151:GLU:HB3	1:E:4296:ASN:HD21	1.84	0.43
1:F:5161:THR:HG22	1:F:5162:ARG:HE	1.82	0.43
1:A:6171:LEU:HD22	1:A:6174:MET:HE3	2.00	0.43
1:C:2006:LEU:HG	1:C:2345:TYR:OH	2.18	0.43
1:D:3150:GLN:CG	1:D:3151:GLU:H	2.31	0.43
1:D:3196:ILE:HD12	1:D:3233:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4218:LEU:HD23	1:E:4219:GLU:N	2.28	0.43
1:A:6040:PHE:O	1:A:6204:ARG:NH2	2.47	0.43
1:C:2012:LEU:HD23	1:C:2012:LEU:HA	1.86	0.43
1:C:2171:LEU:HD23	1:C:2174:MET:HE2	2.01	0.43
1:C:2181:MET:O	1:C:2181:MET:HG3	2.19	0.43
1:F:5276:VAL:HG21	1:F:5325:ILE:HG21	2.01	0.43
1:C:2312:ILE:HA	1:C:2313:PRO:HD3	1.88	0.43
1:F:5300:GLU:O	1:F:5304:LYS:HG3	2.19	0.43
1:B:1053:THR:C	1:B:1055:GLN:H	2.20	0.42
1:C:2039:HIS:CD2	1:C:2238:TRP:HH2	2.37	0.42
1:C:2084:ASN:CG	1:C:2091:LYS:HG3	2.40	0.42
1:C:2050:MET:HG2	1:C:2261:VAL:HG21	2.00	0.42
1:D:3059:GLN:O	1:D:3063:ILE:HG13	2.19	0.42
1:D:3133:THR:HG22	1:D:3134:ASP:N	2.33	0.42
1:D:3168:TRP:CD1	1:D:3168:TRP:C	2.92	0.42
1:E:4317:TRP:N	1:E:4317:TRP:CD2	2.87	0.42
1:F:5100:ASP:HA	1:F:5186:LEU:HD12	2.00	0.42
1:B:1018:ALA:O	1:B:1022:ARG:HG3	2.18	0.42
1:B:1273:VAL:O	1:B:1273:VAL:HG13	2.19	0.42
1:B:1311:GLU:OE1	1:B:1326:ASN:ND2	2.52	0.42
1:C:2038:HIS:O	1:C:2202:ILE:HG23	2.19	0.42
1:C:2298:MET:CE	1:C:2298:MET:O	2.67	0.42
1:D:3006:LEU:HD12	1:D:3063:ILE:HG22	2.00	0.42
1:F:5056:PHE:HD1	1:F:5064:ILE:HD11	1.83	0.42
1:A:6098:ASN:ND2	1:A:6098:ASN:N	2.67	0.42
1:C:2319:HIS:C	1:C:2321:THR:H	2.22	0.42
1:D:3014:ASN:ND2	1:D:3017:LYS:HB2	2.33	0.42
1:D:3154:GLU:C	1:D:3154:GLU:OE2	2.57	0.42
1:E:4038:HIS:O	1:E:4202:ILE:HG23	2.20	0.42
1:E:4293:ASP:HB2	1:E:4294:PRO:HD3	2.00	0.42
1:F:5052:ARG:HD2	1:F:5266:SER:HB2	2.00	0.42
1:A:6048:LEU:C	1:A:6048:LEU:HD12	2.40	0.42
1:B:1162:ARG:HH11	1:B:1162:ARG:CB	2.10	0.42
1:C:2050:MET:O	1:C:2264:LYS:HB2	2.20	0.42
1:C:2164:TRP:O	1:C:2166:ASP:N	2.52	0.42
1:C:2215:LEU:HB3	1:C:2218:LEU:HB2	2.00	0.42
1:C:2314:VAL:HG21	1:C:2325:ILE:CD1	2.49	0.42
1:E:4139:LYS:CE	1:E:4165:ASN:HA	2.49	0.42
1:F:5106:HIS:O	1:F:5110:GLN:HG3	2.18	0.42
1:F:5317:TRP:O	1:F:5319:HIS:CD2	2.72	0.42
1:A:6234:LEU:HB2	1:A:6236:LEU:CD1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1163:ASN:O	1:B:1164:TRP:C	2.58	0.42
1:C:2179:THR:HA	1:C:2180:PRO:HD3	1.93	0.42
1:D:3052:ARG:NH1	1:D:3265:ASP:H	2.11	0.42
1:D:3312:ILE:CD1	1:D:3327:ALA:HB3	2.49	0.42
1:E:4022:ARG:CG	1:E:4022:ARG:NH1	2.81	0.42
1:E:4067:ALA:O	1:E:4096:LYS:HD2	2.18	0.42
1:E:4204:ARG:HG2	1:E:4238:TRP:CE2	2.54	0.42
1:F:5032:PRO:HG3	1:F:5036:ILE:HG23	2.02	0.42
1:F:5260:LEU:HD23	1:F:5260:LEU:HA	1.83	0.42
1:A:6204:ARG:HD3	1:A:6238:TRP:CD2	2.54	0.42
1:A:6137:ASN:HB2	1:A:6237:HIS:NE2	2.34	0.42
1:B:1236:LEU:HD21	1:B:1291:LEU:HD23	2.01	0.42
1:B:1316:GLY:HA2	1:B:1323:HIS:NE2	2.35	0.42
1:B:1355:LYS:HE2	1:B:1355:LYS:HB3	1.75	0.42
1:C:2200:CYS:HB3	1:C:2207:ILE:HG13	2.00	0.42
1:D:3353:TYR:O	1:D:3356:TRP:HB3	2.19	0.42
1:F:5048:LEU:HD12	1:F:5049:GLU:N	2.35	0.42
1:F:5141:ARG:HB3	1:F:5290:PHE:HB3	2.01	0.42
1:A:6179:THR:HG22	1:A:6180:PRO:O	2.20	0.42
1:B:1050:MET:HE1	1:B:1068:LEU:CD1	2.49	0.42
1:B:1039:HIS:HA	1:B:1202:ILE:O	2.19	0.42
1:B:1298:MET:HA	1:B:1301:LYS:NZ	2.34	0.42
1:C:2040:PHE:O	1:C:2204:ARG:NH1	2.53	0.42
1:D:3162:ARG:HH21	1:E:4081:LYS:NZ	2.18	0.42
1:F:5043:MET:HA	1:F:5046:TYR:CD1	2.55	0.42
1:F:5143:GLN:O	1:F:5147:LEU:HG	2.19	0.42
1:F:5238:TRP:HB2	1:F:5243:CYS:SG	2.60	0.42
1:C:2042:THR:HA	1:C:2045:ARG:HH11	1.85	0.42
1:A:6040:PHE:HB2	1:A:6044:HIS:HD2	1.84	0.42
1:A:6314:VAL:CG2	1:A:6325:ILE:HD12	2.49	0.42
1:B:1070:ASP:HA	1:B:1071:ARG:HH11	1.84	0.42
1:C:2150:GLN:HE22	1:C:2287:LYS:NZ	2.18	0.42
1:F:5067:ALA:C	1:F:5096:LYS:HZ3	2.23	0.42
1:A:6319:HIS:C	1:A:6321:THR:H	2.23	0.42
1:C:2069:ILE:HG12	1:C:2093:VAL:CG2	2.50	0.42
1:C:2090:ARG:NH2	1:C:2265:ASP:O	2.53	0.42
1:C:2293:ASP:O	1:C:2297:GLU:HG2	2.20	0.42
1:D:3336:PRO:HD2	1:D:3339:ILE:HG13	2.02	0.42
1:E:4011:TYR:CD1	1:E:4011:TYR:C	2.92	0.42
1:E:4025:THR:HB	1:E:4026:PRO:HD3	2.00	0.42
1:E:4120:LEU:HD22	1:E:4123:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4131:LYS:NZ	1:E:4173:LYS:HZ1	2.18	0.42
1:E:4253:ASP:OD1	1:E:4254:SER:N	2.52	0.42
1:E:4270:ILE:HD12	1:E:4310:ILE:HD11	2.01	0.42
1:A:6043:MET:HG2	1:A:6046:TYR:CE1	2.55	0.41
1:D:3141:ARG:HH21	1:D:3236:LEU:HD23	1.85	0.41
1:D:3317:TRP:O	1:D:3319:HIS:CD2	2.73	0.41
1:E:4350:GLN:O	1:E:4354:LYS:HG3	2.20	0.41
1:A:6271:ARG:HB2	1:A:6329:LYS:CE	2.50	0.41
1:B:1025:THR:HG22	1:B:1026:PRO:HD3	2.02	0.41
1:B:1037:ILE:HG22	1:B:1129:THR:HG23	2.02	0.41
1:B:1097:THR:CG2	1:B:1257:PHE:O	2.68	0.41
1:B:1215:LEU:O	1:B:1218:LEU:HB2	2.19	0.41
1:B:1216:ARG:O	1:B:1216:ARG:HG2	2.18	0.41
1:B:1083:LEU:HD13	1:B:1260:LEU:HD13	2.02	0.41
1:C:2060:PHE:HA	1:C:2063:ILE:CD1	2.50	0.41
1:D:3072:ASN:N	1:D:3072:ASN:OD1	2.44	0.41
1:E:4053:THR:OG1	1:E:4065:HIS:NE2	2.52	0.41
1:F:5051:PHE:HA	1:F:5264:LYS:HE3	2.01	0.41
1:F:5160:ASP:CG	1:F:5161:THR:N	2.71	0.41
1:A:6094:ALA:HB1	1:A:6258:VAL:CG1	2.39	0.41
1:C:2139:LYS:HZ3	1:C:2139:LYS:HB2	1.83	0.41
1:C:2352:GLU:O	1:C:2356:TRP:HB2	2.20	0.41
1:A:6126:LEU:HD21	1:A:6195:HIS:CD2	2.55	0.41
1:A:6216:ARG:HG2	1:A:6216:ARG:O	2.20	0.41
1:B:1252:TYR:CZ	1:B:1255:HIS:HA	2.56	0.41
1:C:2032:PRO:HG3	1:C:2036:ILE:HG23	2.02	0.41
1:E:4053:THR:C	1:E:4055:GLN:H	2.23	0.41
1:F:5127:PHE:HE1	1:F:5172:ILE:O	2.03	0.41
1:A:6179:THR:HA	1:A:6180:PRO:HD3	1.91	0.41
1:A:6232:ILE:CG1	1:A:6286:LEU:HD23	2.50	0.41
1:D:3084:ASN:OD1	1:D:3091:LYS:HA	2.19	0.41
1:D:3120:LEU:HB2	1:D:3124:LYS:HE2	2.02	0.41
1:D:3039:HIS:HA	1:D:3202:ILE:O	2.20	0.41
1:F:5249:VAL:C	1:F:5250:LEU:HD23	2.40	0.41
1:F:5292:THR:HG22	1:F:5293:ASP:N	2.36	0.41
1:A:6353:TYR:O	1:A:6357:GLN:HG3	2.21	0.41
1:C:2112:MET:O	1:C:2335:LEU:HD21	2.21	0.41
1:C:2039:HIS:HA	1:C:2202:ILE:O	2.21	0.41
1:C:2304:LYS:HA	1:C:2309:VAL:CG2	2.50	0.41
1:D:3051:PHE:HA	1:D:3264:LYS:HE3	2.03	0.41
1:A:6057:CYS:SG	1:A:6059:GLN:OE1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6090:ARG:HH22	1:A:6271:ARG:CZ	2.33	0.41
1:A:6038:HIS:O	1:A:6202:ILE:HG23	2.21	0.41
1:A:6233:TYR:N	1:A:6233:TYR:CD1	2.89	0.41
1:A:6052:ARG:CZ	1:A:6266:SER:HB2	2.51	0.41
1:B:1163:ASN:ND2	1:B:1163:ASN:O	2.53	0.41
1:B:1269:GLU:H	1:B:1269:GLU:CD	2.24	0.41
1:C:2033:THR:O	1:C:2033:THR:CG2	2.67	0.41
1:C:2040:PHE:HB2	1:C:2044:HIS:CD2	2.55	0.41
1:C:2053:THR:C	1:C:2055:GLN:H	2.24	0.41
1:D:3147:LEU:HD21	1:D:3164:TRP:CZ2	2.53	0.41
1:D:3180:PRO:HG3	1:D:3189:ASN:OD1	2.21	0.41
1:D:3092:LEU:HD23	1:D:3262:THR:HA	2.02	0.41
1:D:3017:LYS:HD2	1:D:3341:LEU:HD23	2.02	0.41
1:E:4232:ILE:HD11	1:E:4275:LEU:HD22	2.03	0.41
1:F:5236:LEU:HD11	1:F:5291:LEU:HD23	2.03	0.41
1:F:5152:PHE:CD2	1:F:5299:LYS:HD2	2.56	0.41
1:F:5359:ASN:O	1:F:5362:GLN:HG3	2.20	0.41
1:A:6081:LYS:HZ2	1:A:6278:ARG:HH12	1.67	0.41
1:A:6293:ASP:N	1:A:6294:PRO:CD	2.84	0.41
1:C:2137:ASN:CB	1:C:2237:HIS:NE2	2.83	0.41
1:D:3006:LEU:HD12	1:D:3063:ILE:CG2	2.51	0.41
1:D:3090:ARG:NH2	1:D:3265:ASP:O	2.53	0.41
1:E:4070:ASP:CG	1:E:4073:ILE:HD13	2.40	0.41
1:F:5086:CYS:HB3	1:F:5089:VAL:HG22	2.03	0.41
1:A:6142:TRP:CH2	1:A:6164:TRP:HE3	2.39	0.41
1:B:1349:VAL:O	1:B:1353:TYR:HB2	2.21	0.41
1:C:2037:ILE:HD11	1:C:2201:ASN:HB3	2.03	0.41
1:C:2086:CYS:HB3	1:C:2089:VAL:HG22	2.02	0.41
1:D:3074:GLN:OE1	1:D:3093:VAL:HA	2.21	0.41
1:E:4133:THR:CG2	1:E:4134:ASP:N	2.84	0.41
1:E:4280:ARG:HG3	1:E:4280:ARG:O	2.21	0.41
1:E:4145:GLU:CD	1:E:4290:PHE:H	2.23	0.41
1:E:4141:ARG:NH2	1:E:4292:THR:HG23	2.36	0.41
1:F:5006:LEU:HA	1:F:5006:LEU:HD23	1.97	0.41
1:A:6082:LYS:HE3	1:A:6082:LYS:CA	2.42	0.41
1:A:6063:ILE:HD11	1:A:6356:TRP:CH2	2.56	0.41
1:B:1025:THR:HG22	1:B:1026:PRO:CD	2.51	0.41
1:B:1074:GLN:HB3	1:B:1074:GLN:HE21	1.53	0.41
1:B:1289:HIS:H	1:B:1289:HIS:CD2	2.38	0.41
1:C:2293:ASP:CB	1:C:2294:PRO:HD3	2.49	0.41
1:D:3263:LEU:HA	1:D:3263:LEU:HD23	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5111:TYR:CD2	1:F:5248:ILE:HG23	2.56	0.41
1:A:6052:ARG:HD3	1:A:6055:GLN:OE1	2.20	0.41
1:A:6066:LYS:HZ3	1:A:6071:ARG:NH2	2.18	0.41
1:C:2194:ILE:O	1:C:2198:VAL:HG23	2.21	0.41
1:D:3052:ARG:HH12	1:D:3263:LEU:C	2.24	0.41
1:E:4095:LEU:O	1:E:4258:VAL:CG2	2.67	0.41
1:E:4200:CYS:HB2	1:E:4205:ARG:O	2.21	0.41
1:F:5030:PHE:O	1:F:5032:PRO:HD2	2.21	0.41
1:A:6088:GLU:OE1	1:A:6314:VAL:HA	2.20	0.40
1:B:1201:ASN:O	1:B:1238:TRP:NE1	2.53	0.40
1:B:1300:GLU:CD	1:B:1304:LYS:HE3	2.41	0.40
1:C:2069:ILE:HG23	1:C:2094:ALA:O	2.21	0.40
1:C:2010:LEU:HD23	1:C:2345:TYR:CD1	2.56	0.40
1:D:3336:PRO:HD2	1:D:3339:ILE:CD1	2.51	0.40
1:E:4163:ASN:C	1:E:4163:ASN:ND2	2.73	0.40
1:E:4218:LEU:CD2	1:E:4219:GLU:N	2.84	0.40
1:E:4262:THR:HG22	1:E:4263:LEU:N	2.36	0.40
1:F:5159:TYR:N	1:F:5159:TYR:CD1	2.89	0.40
1:F:5162:ARG:HG3	1:F:5162:ARG:NH1	2.36	0.40
1:F:5141:ARG:NH1	1:F:5295:GLU:OE1	2.41	0.40
1:A:6082:LYS:HD2	1:A:6213:LYS:CE	2.44	0.40
1:B:1082:LYS:NZ	1:B:1213:LYS:HZ1	2.19	0.40
1:C:2141:ARG:HE	1:C:2237:HIS:HE1	1.70	0.40
1:C:2267:GLY:HA2	1:C:2268:PRO:HD3	1.68	0.40
1:E:4185:GLY:C	1:E:4186:LEU:HD22	2.41	0.40
1:F:5062:GLU:OE2	1:F:5062:GLU:C	2.59	0.40
1:F:5302:LEU:HD23	1:F:5302:LEU:HA	1.95	0.40
1:F:5346:PHE:HA	1:F:5349:VAL:CG2	2.51	0.40
1:A:6066:LYS:NZ	1:A:6071:ARG:HH22	2.19	0.40
1:B:1003:GLU:HB2	1:B:1004:GLN:HE22	1.82	0.40
1:C:2108:THR:CG2	1:C:2122:LEU:HD21	2.52	0.40
1:D:3107:ALA:O	1:D:3259:PRO:HG3	2.22	0.40
1:D:3314:VAL:CG1	1:D:3315:GLN:NE2	2.84	0.40
1:E:4006:LEU:HA	1:E:4007:PRO:HD2	1.84	0.40
1:F:5123:ARG:NH2	1:F:5176:SER:O	2.54	0.40
1:A:6254:SER:OG	1:A:6255:HIS:N	2.53	0.40
1:C:2153:VAL:O	1:C:2154:GLU:CB	2.69	0.40
1:C:2095:LEU:O	1:C:2258:VAL:HG13	2.21	0.40
1:C:2273:VAL:O	1:C:2275:LEU:HD23	2.21	0.40
1:D:3016:ARG:HG2	1:D:3016:ARG:HH11	1.85	0.40
1:D:3077:LEU:HD11	1:D:3210:ILE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4153:VAL:O	1:E:4154:GLU:HB3	2.22	0.40
1:E:4317:TRP:N	1:E:4317:TRP:CE3	2.89	0.40
1:D:3081:LYS:CE	1:F:5143:GLN:HE22	2.35	0.40
1:F:5153:VAL:O	1:F:5154:GLU:HB3	2.20	0.40
1:C:2249:VAL:HG12	1:C:2260:LEU:HB2	2.03	0.40
1:E:4215:LEU:HB3	1:E:4218:LEU:HB2	2.04	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	346/390 (89%)	297 (86%)	36 (10%)	13 (4%)	3	4
1	B	346/390 (89%)	298 (86%)	33 (10%)	15 (4%)	2	3
1	C	346/390 (89%)	294 (85%)	39 (11%)	13 (4%)	3	4
1	D	346/390 (89%)	298 (86%)	34 (10%)	14 (4%)	3	3
1	E	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	3	4
1	F	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	3	4
All	All	2076/2340 (89%)	1779 (86%)	218 (10%)	79 (4%)	3	4

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6004	GLN
1	A	6266	SER
1	A	6279	ASP
1	B	1004	GLN
1	B	1163	ASN
1	B	1266	SER

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Mol	Chain	Res	Type
1	C	2004	GLN
1	C	2266	SER
1	D	3163	ASN
1	D	3266	SER
1	D	3279	ASP
1	E	4004	GLN
1	E	4266	SER
1	F	5004	GLN
1	F	5163	ASN
1	F	5266	SER
1	F	5279	ASP
1	A	6153	VAL
1	A	6160	ASP
1	A	6214	MET
1	A	6320	GLY
1	B	1153	VAL
1	B	1214	MET
1	B	1279	ASP
1	B	1320	GLY
1	C	2153	VAL
1	C	2160	ASP
1	C	2214	MET
1	C	2279	ASP
1	C	2320	GLY
1	D	3004	GLN
1	D	3153	VAL
1	D	3160	ASP
1	D	3162	ARG
1	D	3214	MET
1	D	3320	GLY
1	E	4153	VAL
1	E	4214	MET
1	E	4279	ASP
1	E	4320	GLY
1	F	5153	VAL
1	F	5214	MET
1	F	5320	GLY
1	A	6163	ASN
1	A	6360	SER
1	B	1165	ASN
1	B	1267	GLY
1	B	1360	SER

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Mol	Chain	Res	Type
1	C	2360	SER
1	D	3360	SER
1	E	4360	SER
1	F	5360	SER
1	A	6035	GLY
1	A	6319	HIS
1	B	1035	GLY
1	B	1319	HIS
1	C	2035	GLY
1	C	2319	HIS
1	D	3035	GLY
1	E	4035	GLY
1	F	5035	GLY
1	F	5267	GLY
1	F	5319	HIS
1	A	6267	GLY
1	B	1162	ARG
1	C	2007	PRO
1	D	3319	HIS
1	E	4160	ASP
1	E	4267	GLY
1	E	4319	HIS
1	A	6007	PRO
1	B	1007	PRO
1	B	1148	LYS
1	C	2167	GLU
1	C	2267	GLY
1	D	3267	GLY
1	D	3007	PRO
1	E	4007	PRO
1	F	5007	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/354 (92%)	291 (90%)	34 (10%)	7	13
1	B	325/354 (92%)	289 (89%)	36 (11%)	6	11
1	C	325/354 (92%)	296 (91%)	29 (9%)	9	19
1	D	325/354 (92%)	300 (92%)	25 (8%)	13	25
1	E	325/354 (92%)	294 (90%)	31 (10%)	8	17
1	F	325/354 (92%)	294 (90%)	31 (10%)	8	17
All	All	1950/2124 (92%)	1764 (90%)	186 (10%)	8	17

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6015	MET
1	A	6016	ARG
1	A	6024	ARG
1	A	6030	PHE
1	A	6048	LEU
1	A	6050	MET
1	A	6057	CYS
1	A	6059	GLN
1	A	6062	GLU
1	A	6074	GLN
1	A	6082	LYS
1	A	6086	CYS
1	A	6097	THR
1	A	6103	CYS
1	A	6105	MET
1	A	6112	MET
1	A	6137	ASN
1	A	6150	GLN
1	A	6193	GLU
1	A	6199	LEU
1	A	6212	ASP
1	A	6218	LEU
1	A	6228	LYS
1	A	6236	LEU
1	A	6241	GLN
1	A	6247	PRO
1	A	6255	HIS

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Mol	Chain	Res	Type
1	A	6262	THR
1	A	6270	ILE
1	A	6284	GLU
1	A	6293	ASP
1	A	6296	ASN
1	A	6315	GLN
1	A	6317	TRP
1	B	1008	GLN
1	B	1016	ARG
1	B	1030	PHE
1	B	1034	ASN
1	B	1048	LEU
1	B	1052	ARG
1	B	1057	CYS
1	B	1061	ARG
1	B	1066	LYS
1	B	1071	ARG
1	B	1074	GLN
1	B	1082	LYS
1	B	1088	GLU
1	B	1097	THR
1	B	1098	ASN
1	B	1118	THR
1	B	1124	LYS
1	B	1137	ASN
1	B	1162	ARG
1	B	1166	ASP
1	B	1169	ASP
1	B	1170	ASN
1	B	1183	ARG
1	B	1189	ASN
1	B	1192	GLU
1	B	1228	LYS
1	B	1229	VAL
1	B	1236	LEU
1	B	1237	HIS
1	B	1241	GLN
1	B	1247	PRO
1	B	1282	ARG
1	B	1296	ASN
1	B	1300	GLU
1	B	1301	LYS

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Mol	Chain	Res	Type
1	B	1317	TRP
1	C	2016	ARG
1	C	2027	GLU
1	C	2029	ILE
1	C	2034	ASN
1	C	2044	HIS
1	C	2048	LEU
1	C	2071	ARG
1	C	2105	MET
1	C	2112	MET
1	C	2141	ARG
1	C	2154	GLU
1	C	2164	TRP
1	C	2166	ASP
1	C	2192	GLU
1	C	2199	LEU
1	C	2214	MET
1	C	2218	LEU
1	C	2228	LYS
1	C	2247	PRO
1	C	2265	ASP
1	C	2287	LYS
1	C	2293	ASP
1	C	2298	MET
1	C	2311	GLU
1	C	2317	TRP
1	C	2322	THR
1	C	2326	ASN
1	C	2334	ASN
1	C	2340	ASN
1	D	3016	ARG
1	D	3044	HIS
1	D	3048	LEU
1	D	3057	CYS
1	D	3072	ASN
1	D	3087	ARG
1	D	3098	ASN
1	D	3118	THR
1	D	3124	LYS
1	D	3152	PHE
1	D	3164	TRP
1	D	3165	ASN

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Mol	Chain	Res	Type
1	D	3190	SER
1	D	3192	GLU
1	D	3199	LEU
1	D	3227	LEU
1	D	3229	VAL
1	D	3247	PRO
1	D	3258	VAL
1	D	3270	ILE
1	D	3282	ARG
1	D	3293	ASP
1	D	3317	TRP
1	D	3340	ASN
1	D	3348	LEU
1	E	4008	GLN
1	E	4011	TYR
1	E	4030	PHE
1	E	4034	ASN
1	E	4048	LEU
1	E	4057	CYS
1	E	4062	GLU
1	E	4074	GLN
1	E	4097	THR
1	E	4112	MET
1	E	4133	THR
1	E	4147	LEU
1	E	4150	GLN
1	E	4160	ASP
1	E	4162	ARG
1	E	4163	ASN
1	E	4183	ARG
1	E	4189	ASN
1	E	4199	LEU
1	E	4200	CYS
1	E	4213	LYS
1	E	4218	LEU
1	E	4237	HIS
1	E	4241	GLN
1	E	4253	ASP
1	E	4258	VAL
1	E	4263	LEU
1	E	4265	ASP
1	E	4278	ARG

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Mol	Chain	Res	Type
1	E	4286	LEU
1	E	4319	HIS
1	F	5011	TYR
1	F	5013	SER
1	F	5030	PHE
1	F	5048	LEU
1	F	5050	MET
1	F	5088	GLU
1	F	5103	CYS
1	F	5112	MET
1	F	5118	THR
1	F	5121	VAL
1	F	5150	GLN
1	F	5159	TYR
1	F	5162	ARG
1	F	5169	ASP
1	F	5183	ARG
1	F	5191	LEU
1	F	5193	GLU
1	F	5199	LEU
1	F	5212	ASP
1	F	5216	ARG
1	F	5227	LEU
1	F	5237	HIS
1	F	5255	HIS
1	F	5262	THR
1	F	5270	ILE
1	F	5271	ARG
1	F	5293	ASP
1	F	5317	TRP
1	F	5319	HIS
1	F	5350	GLN
1	F	5356	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6008	GLN
1	A	6039	HIS
1	A	6044	HIS
1	A	6074	GLN
1	A	6098	ASN

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Mol	Chain	Res	Type
1	A	6137	ASN
1	A	6170	ASN
1	A	6187	GLN
1	A	6241	GLN
1	A	6277	ASN
1	A	6326	ASN
1	A	6351	HIS
1	B	1004	GLN
1	B	1008	GLN
1	B	1080	GLN
1	B	1110	GLN
1	B	1116	GLN
1	B	1137	ASN
1	B	1150	GLN
1	B	1163	ASN
1	B	1170	ASN
1	B	1187	GLN
1	B	1189	ASN
1	B	1241	GLN
1	B	1256	HIS
1	B	1277	ASN
1	B	1323	HIS
1	B	1326	ASN
1	B	1357	GLN
1	C	2008	GLN
1	C	2038	HIS
1	C	2055	GLN
1	C	2110	GLN
1	C	2143	GLN
1	C	2150	GLN
1	C	2163	ASN
1	C	2165	ASN
1	C	2289	HIS
1	C	2296	ASN
1	C	2315	GLN
1	C	2323	HIS
1	C	2326	ASN
1	C	2334	ASN
1	C	2340	ASN
1	C	2351	HIS
1	C	2357	GLN
1	D	3004	GLN

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Mol	Chain	Res	Type
1	D	3008	GLN
1	D	3110	GLN
1	D	3116	GLN
1	D	3150	GLN
1	D	3256	HIS
1	D	3289	HIS
1	D	3319	HIS
1	D	3326	ASN
1	D	3340	ASN
1	D	3357	GLN
1	E	4004	GLN
1	E	4038	HIS
1	E	4044	HIS
1	E	4074	GLN
1	E	4098	ASN
1	E	4116	GLN
1	E	4163	ASN
1	E	4189	ASN
1	E	4256	HIS
1	E	4289	HIS
1	E	4319	HIS
1	E	4357	GLN
1	F	5004	GLN
1	F	5038	HIS
1	F	5039	HIS
1	F	5055	GLN
1	F	5098	ASN
1	F	5110	GLN
1	F	5143	GLN
1	F	5165	ASN
1	F	5170	ASN
1	F	5187	GLN
1	F	5241	GLN
1	F	5296	ASN
1	F	5350	GLN
1	F	5357	GLN

### 5.3.3 RNA ⓘ

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	352/390 (90%)	0.32	29 (8%)	11 11	20, 62, 150, 195	0
1	B	352/390 (90%)	0.21	30 (8%)	10 10	19, 50, 142, 179	0
1	C	352/390 (90%)	0.52	41 (11%)	4 4	30, 66, 148, 185	0
1	D	352/390 (90%)	0.29	32 (9%)	9 9	23, 59, 145, 188	0
1	E	352/390 (90%)	0.24	35 (9%)	7 7	19, 52, 145, 175	0
1	F	352/390 (90%)	0.40	31 (8%)	10 10	28, 67, 146, 194	0
All	All	2112/2340 (90%)	0.33	198 (9%)	8 8	19, 59, 146, 195	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5153	VAL	22.8
1	C	2318	ASP	19.4
1	E	4153	VAL	18.3
1	D	3153	VAL	16.5
1	A	6150	GLN	15.2
1	A	6153	VAL	15.1
1	C	2159	TYR	11.8
1	A	6159	TYR	10.5
1	D	3218	LEU	10.2
1	C	2218	LEU	10.0
1	D	3152	PHE	9.5
1	B	1153	VAL	8.9
1	F	5154	GLU	8.8
1	B	1220	SER	8.6
1	C	2220	SER	8.5
1	C	2150	GLN	8.4
1	C	2221	GLY	8.4
1	A	6219	GLU	8.3
1	A	6318	ASP	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	6185	GLY	8.2
1	E	4218	LEU	7.8
1	D	3226	PRO	7.8
1	D	3362	GLN	7.6
1	A	6154	GLU	7.5
1	E	4154	GLU	7.5
1	F	5318	ASP	7.5
1	A	6218	LEU	7.5
1	C	2153	VAL	7.4
1	A	6220	SER	7.4
1	A	6149	SER	7.0
1	C	2219	GLU	6.8
1	F	5220	SER	6.7
1	F	5152	PHE	6.5
1	D	3149	SER	6.5
1	A	6152	PHE	6.5
1	B	1149	SER	6.5
1	F	5149	SER	6.5
1	B	1152	PHE	6.4
1	C	2361	GLU	6.3
1	D	3217	SER	6.2
1	E	4221	GLY	6.1
1	A	6003	GLU	6.0
1	B	1159	TYR	5.9
1	C	2182	ALA	5.9
1	C	2217	SER	5.8
1	E	4318	ASP	5.8
1	A	6268	PRO	5.8
1	C	2152	PHE	5.7
1	E	4150	GLN	5.7
1	F	5184	SER	5.7
1	E	4152	PHE	5.7
1	D	3318	ASP	5.5
1	E	4226	PRO	5.4
1	B	1219	GLU	5.2
1	B	1361	GLU	5.2
1	B	1154	GLU	5.1
1	B	1218	LEU	5.1
1	C	2185	GLY	5.0
1	C	2003	GLU	5.0
1	C	2181	MET	5.0
1	F	5217	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	3150	GLN	4.9
1	F	5361	GLU	4.9
1	B	1150	GLN	4.8
1	D	3003	GLU	4.8
1	E	4361	GLU	4.8
1	C	2149	SER	4.8
1	E	4059	GLN	4.7
1	F	5268	PRO	4.7
1	D	3183	ARG	4.7
1	F	5005	VAL	4.6
1	E	4359	ASN	4.6
1	F	5362	GLN	4.5
1	E	4184	SER	4.5
1	A	6186	LEU	4.5
1	E	4159	TYR	4.4
1	E	4182	ALA	4.4
1	D	3360	SER	4.4
1	E	4149	SER	4.4
1	B	1221	GLY	4.3
1	C	2359	ASN	4.3
1	C	2362	GLN	4.3
1	E	4217	SER	4.2
1	D	3220	SER	4.2
1	E	4227	LEU	4.1
1	F	5159	TYR	4.0
1	B	1362	GLN	3.9
1	B	1033	THR	3.9
1	D	3361	GLU	3.9
1	A	6221	GLY	3.8
1	D	3162	ARG	3.8
1	D	3154	GLU	3.8
1	E	4219	GLU	3.7
1	E	4360	SER	3.6
1	A	6182	ALA	3.6
1	A	6226	PRO	3.6
1	B	1316	GLY	3.5
1	D	3282	ARG	3.5
1	E	4162	ARG	3.4
1	F	5221	GLY	3.4
1	B	1182	ALA	3.4
1	E	4220	SER	3.4
1	E	4181	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	4185	GLY	3.3
1	F	5360	SER	3.3
1	C	2161	THR	3.3
1	F	5226	PRO	3.3
1	C	2264	LYS	3.3
1	F	5003	GLU	3.3
1	B	1161	THR	3.3
1	A	6267	GLY	3.3
1	A	6266	SER	3.2
1	D	3182	ALA	3.2
1	E	4033	THR	3.2
1	C	2216	ARG	3.2
1	A	6319	HIS	3.1
1	C	2184	SER	3.1
1	B	1226	PRO	3.1
1	B	1318	ASP	3.1
1	D	3159	TYR	3.1
1	C	2154	GLU	3.1
1	E	4362	GLN	3.1
1	A	6183	ARG	3.1
1	B	1267	GLY	3.1
1	B	1319	HIS	3.1
1	F	5219	GLU	3.0
1	E	4183	ARG	3.0
1	C	2360	SER	3.0
1	D	3216	ARG	3.0
1	C	2055	GLN	3.0
1	C	2036	ILE	3.0
1	C	2280	ARG	2.9
1	F	5218	LEU	2.9
1	B	1183	ARG	2.9
1	F	5150	GLN	2.9
1	C	2162	ARG	2.8
1	F	5186	LEU	2.8
1	E	4266	SER	2.8
1	A	6056	PHE	2.8
1	E	4003	GLU	2.8
1	A	6362	GLN	2.8
1	E	4216	ARG	2.8
1	D	3221	GLY	2.7
1	C	2186	LEU	2.7
1	D	3359	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	5267	GLY	2.7
1	C	2255	HIS	2.6
1	B	1216	ARG	2.6
1	D	3179	THR	2.6
1	C	2227	LEU	2.6
1	A	6184	SER	2.6
1	A	6361	GLU	2.6
1	F	5185	GLY	2.6
1	B	1164	TRP	2.6
1	B	1217	SER	2.5
1	E	4317	TRP	2.5
1	C	2054	CYS	2.5
1	D	3317	TRP	2.5
1	E	4161	THR	2.5
1	B	1003	GLU	2.4
1	F	5216	ARG	2.4
1	D	3279	ASP	2.4
1	F	5266	SER	2.4
1	A	6005	VAL	2.4
1	B	1266	SER	2.4
1	C	2317	TRP	2.4
1	E	4215	LEU	2.3
1	C	2183	ARG	2.3
1	B	1186	LEU	2.3
1	C	2226	PRO	2.3
1	D	3255	HIS	2.3
1	D	3267	GLY	2.3
1	C	2265	ASP	2.3
1	F	5056	PHE	2.3
1	C	2058	PRO	2.2
1	F	5182	ALA	2.2
1	F	5161	THR	2.2
1	E	4164	TRP	2.2
1	B	1181	MET	2.2
1	D	3319	HIS	2.1
1	A	6163	ASN	2.1
1	B	1282	ARG	2.1
1	D	3219	GLU	2.1
1	F	5181	MET	2.1
1	A	6270	ILE	2.1
1	D	3059	GLN	2.1
1	E	4315	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	4186	LEU	2.1
1	C	2319	HIS	2.1
1	F	5183	ARG	2.1
1	F	5164	TRP	2.1
1	C	2215	LEU	2.0
1	A	6164	TRP	2.0
1	C	2349	VAL	2.0
1	C	2056	PHE	2.0
1	D	3185	GLY	2.0
1	B	1279	ASP	2.0
1	D	3055	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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.