Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:10 AM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

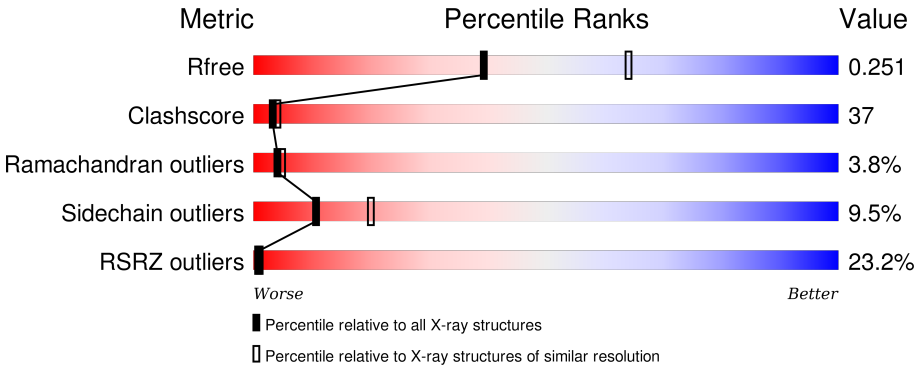
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	19% 33% 49% 8% 10%
1	B	390	18% 39% 42% 8% 10%
1	C	390	25% 33% 50% 7% 10%
1	D	390	22% 35% 49% 6% 10%
1	E	390	19% 39% 44% 7% 10%

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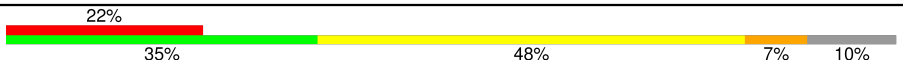
Mol	Chain	Length	Quality of chain
1	F	390	

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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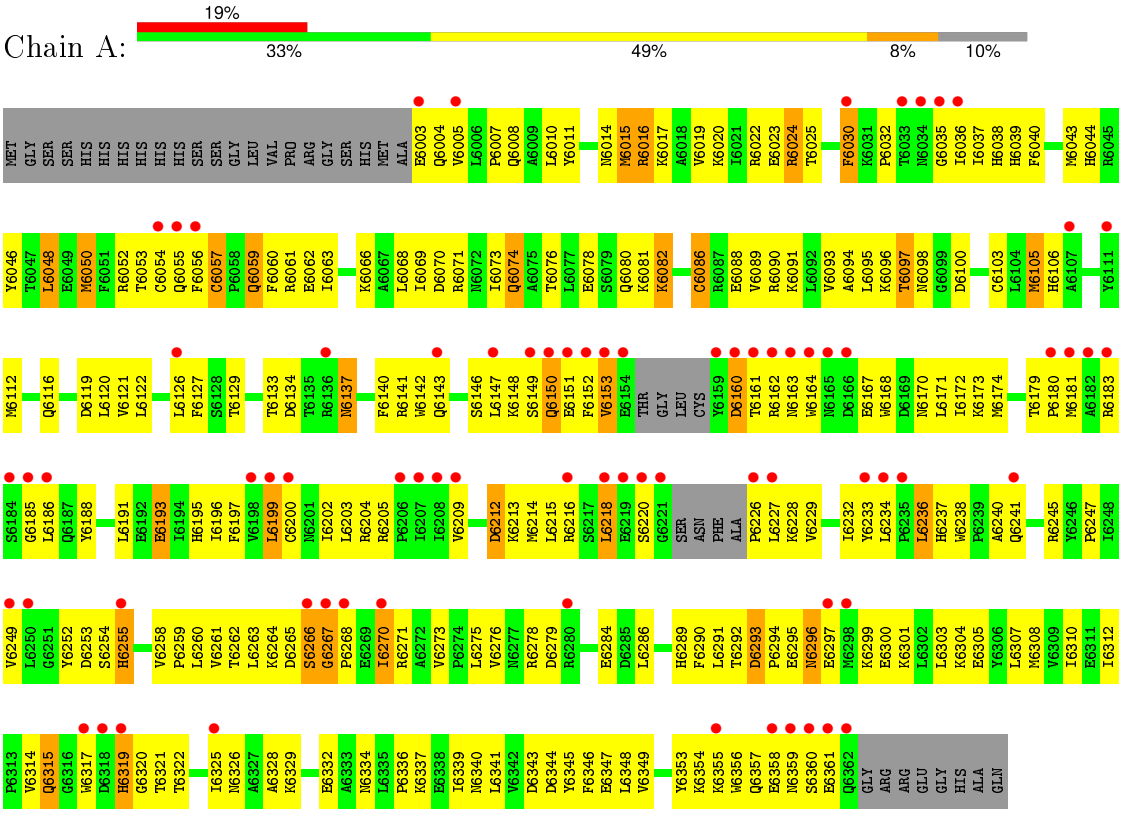
Chain	Residue	Modelled	Actual	Comment	Reference
F	4982	GLY	-	EXPRESSION TAG	UNP P21580
F	4983	SER	-	EXPRESSION TAG	UNP P21580
F	4984	SER	-	EXPRESSION TAG	UNP P21580
F	4985	HIS	-	EXPRESSION TAG	UNP P21580
F	4986	HIS	-	EXPRESSION TAG	UNP P21580
F	4987	HIS	-	EXPRESSION TAG	UNP P21580
F	4988	HIS	-	EXPRESSION 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

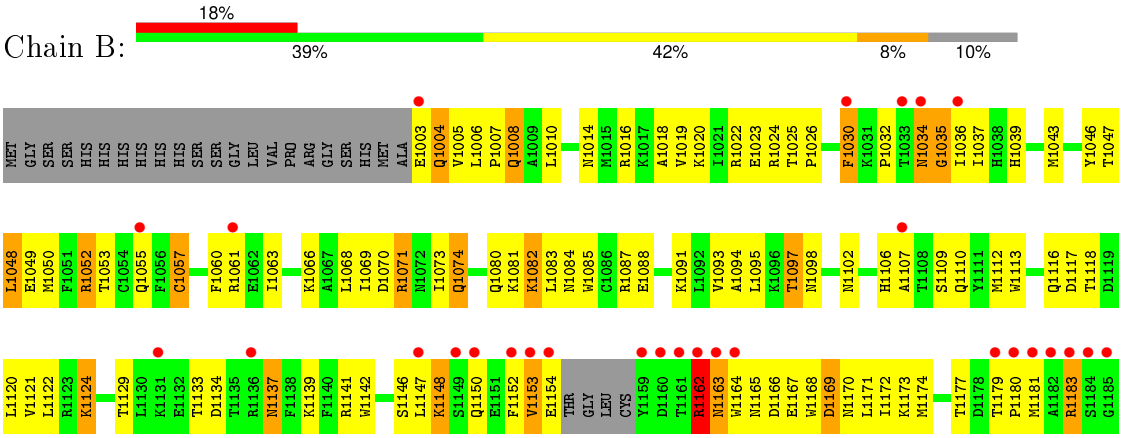
- Molecule 1: Tumor necrosis factor, alpha-induced protein 3

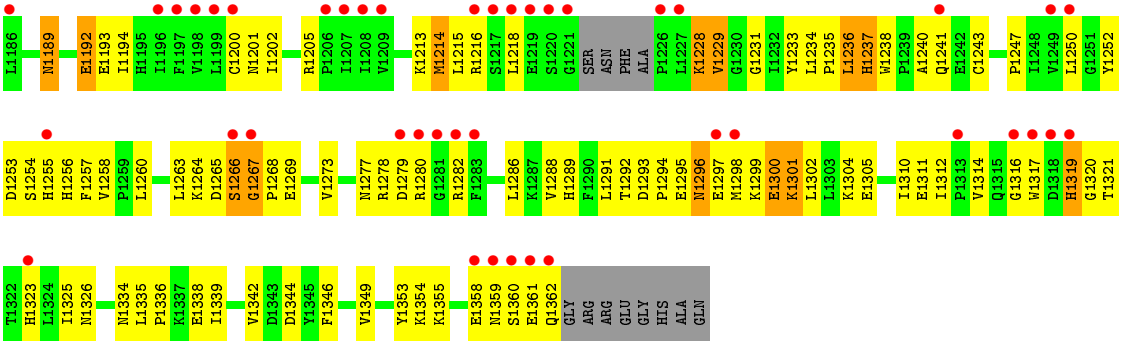
Chain A:



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

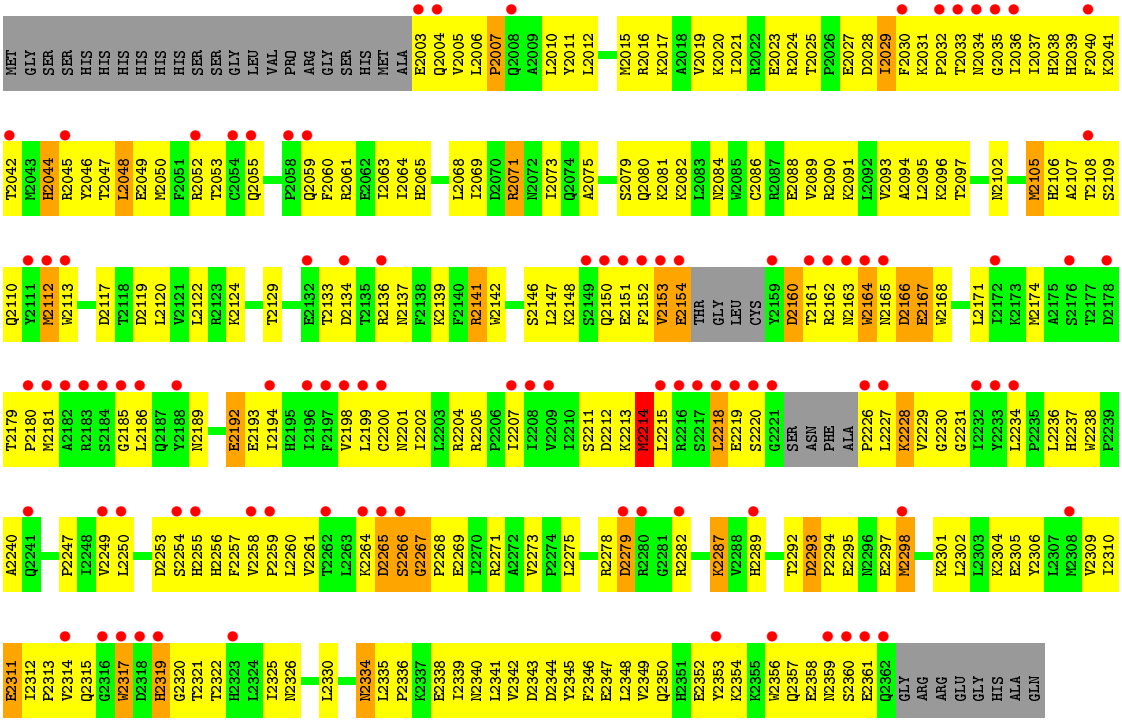
Chain B:





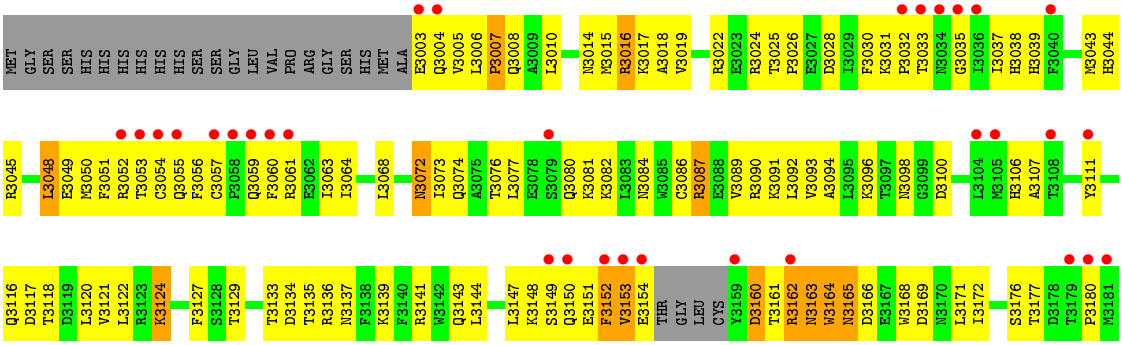
• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

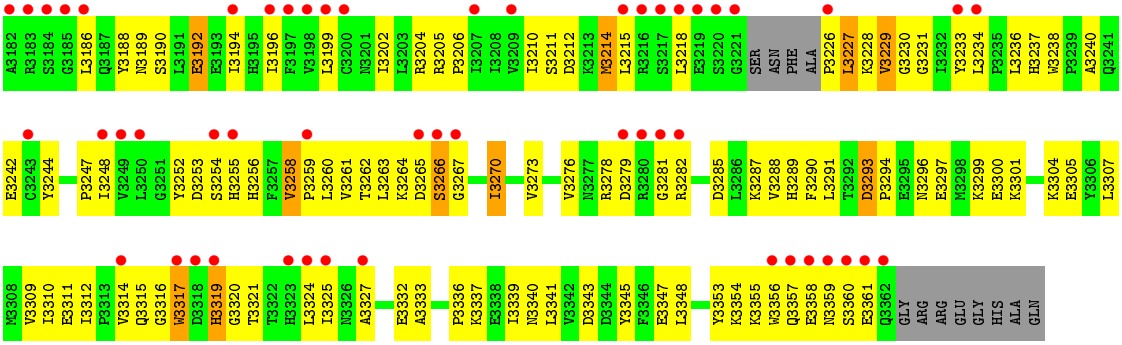
Chain C:



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

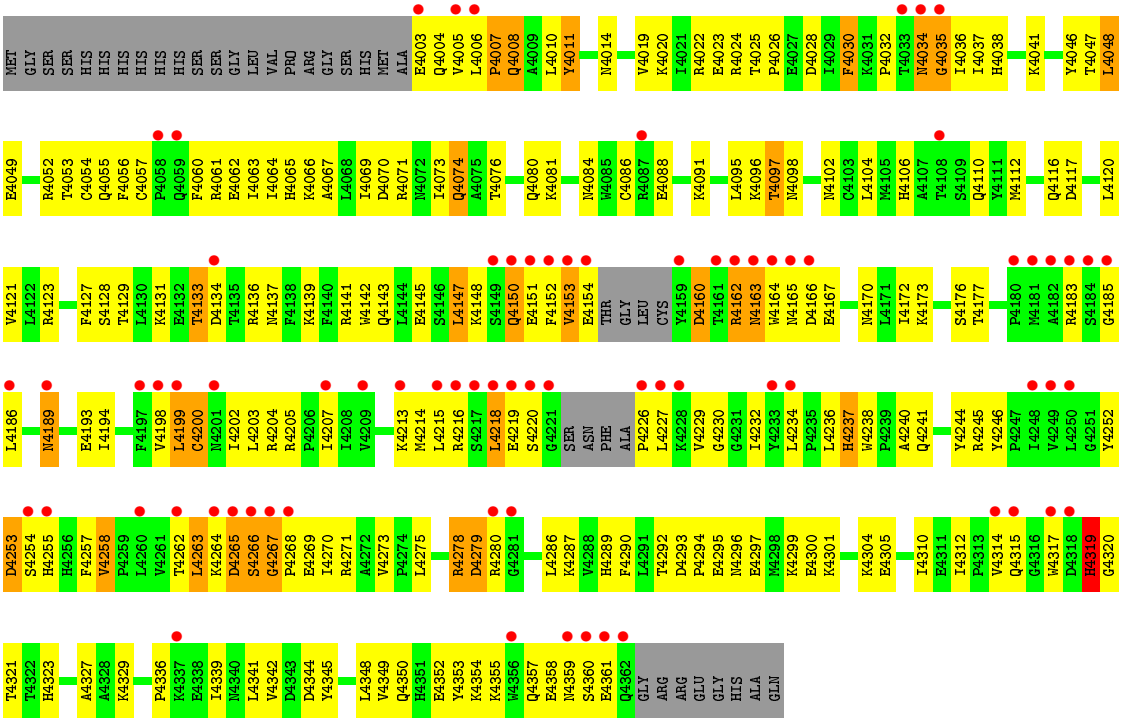
Chain D:





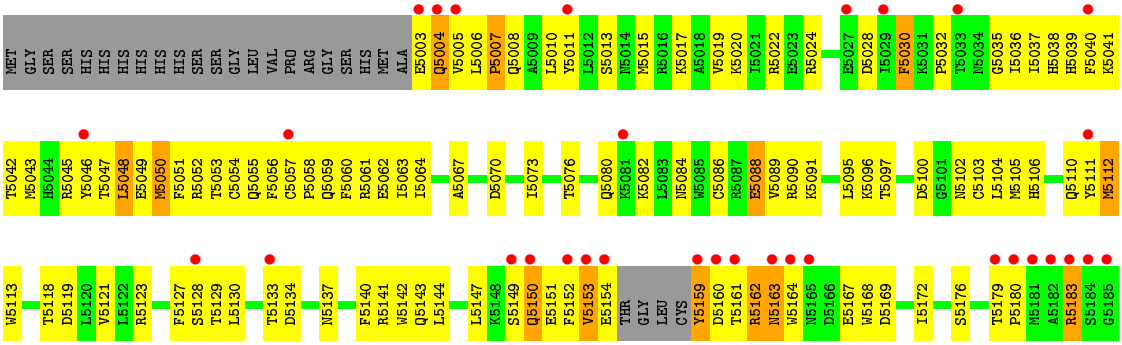
• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

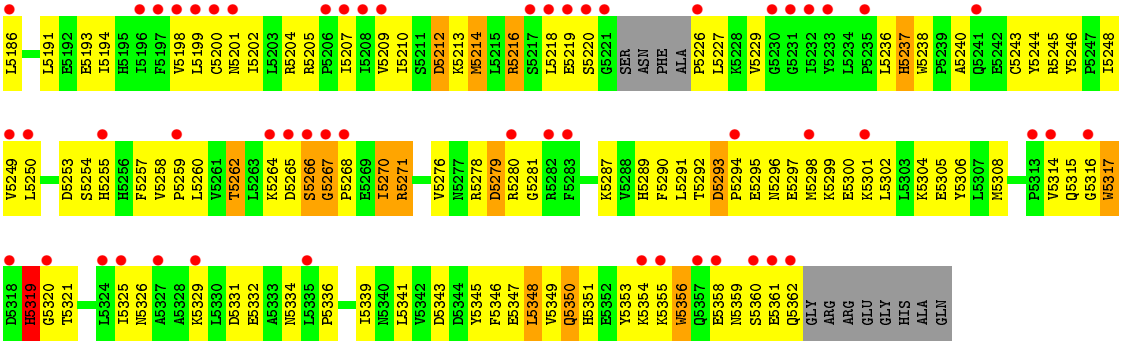
Chain E:



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

Chain F:




L5186 L5191 E5192 E5193 I5194 H5195 I5196 F5197 V5198 L5199 C5200 N5201 I5202 L5203 R5204 R5205 P5206 I5207 I5208 V5209 I5210 S5211 D5212 K5213 M5214 L5215 R5216 S5217 L5218 E5219 S5220 G5221 SER ASN PHE ALA P5226 L5227 K5228 V5229 G5230 G5231 I5232 Y5233 L5234 P5235 L5236 H5237 W5238 P5239 A5240 Q5241 E5242 C5243 Y5244 R5245 Y5246 P5247 I5248
V5249 L5250 D5253 S5254 H5255 H5256 F5257 V5258 P5259 L5260 V5261 T5262 L5263 K5264 D5265 S5266 G5267 P5268 E5269 I5270 R5271 V5276 N5277 R5278 D5279 R5280 G5281 R5282 F5283 K5287 V5288 H5289 F5290 L5291 T5292 D5293 P5294 E5295 N5296 E5297 M5298 K5299 E5300 K5301 L5302 L5303 K5304 E5305 Y5306 L5307 M5308 P5313 V5314 Q5315 G5316 W5317
D5318 H5319 G5320 T5321 L5324 I5325 N5326 A5327 A5328 K5329 L5330 D5331 E5332 A5333 N5334 L5335 P5336 I5339 N5340 L5341 V5342 D5343 D5344 Y5345 F5346 E5347 L5348 V5349 Q5350 H5351 E5352 Y5353 K5354 K5355 W5356 Q5357 E5358 N5359 S5360 E5361 Q5362 GLY ARG ARG GLU GLY HIS ALA GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	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) 95.9 (29.74-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.246 0.206 , 0.251	Depositor DCC
R_{free} test set	7871 reflections (10.75%)	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.3	EDS
Estimated twinning fraction	0.038 for -h,-k,l 0.039 for h,-h-k,-l 0.488 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 84471 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17550	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	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(^{o})	Ideal(^{o})
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

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:F:5020:LYS:HE3	1:F:5024:ARG:HH21	1.22	1.02
1:B:1162:ARG:HB2	1:B:1162:ARG:HH11	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:F:5316:GLY:HA3	1:F:5321:THR:HG23	1.47	0.93
1:C:2037:ILE:HG22	1:C:2133:THR:HG21	1.50	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:HD22	1:E:4189:ASN:H	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:2287:LYS:HE2	1:C:2289:HIS:HA	1.61	0.82
1:C:2097:THR:HG22	1:C:2110:GLN:HE21	1.42	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:2164:TRP:HA	1:C:2164:TRP:HE3	1.46	0.77
1:C:2151:GLU:HG2	1:C:2151:GLU:O	1.82	0.77
1:E:4278:ARG:HD3	1:E:4278:ARG:O	1.83	0.77
1:B:1231:GLY:HA3	1:B:1289:HIS:NE2	1.99	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:C:2228:LYS:N	1:C:2228:LYS:HD3	1.99	0.76
1:B:1171:LEU:HD23	1:B:1174:MET:HE1	1.66	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:D:3139:LYS:O	1:D:3143:GLN:HG3	1.86	0.76
1:B:1008:GLN:HE21	1:B:1008:GLN:N	1.84	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:E:4037:ILE:HG22	1:E:4133:THR:HG21	1.67	0.74
1:A:6220:SER:OG	1:A:6226:PRO:HG3	1.87	0.74
1:F:5039:HIS:CD2	1:F:5204:ARG:NH1	2.53	0.74
1:D:3025:THR:HG22	1:D:3121:VAL:HG11	1.68	0.74
1:F:5271:ARG:CZ	1:F:5332:GLU:HB3	2.18	0.74
1:C:2097:THR:HG21	1:C:2259:PRO:HD3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:4300:GLU:OE2	1:E:4304:LYS:HE3	1.89	0.73
1:D:3087:ARG:NH1	1:F:5162:ARG:HG3	2.03	0.73
1:B:1142:TRP:CE2	1:B:1171:LEU:HD11	2.24	0.73
1:A:6168:TRP:NE1	1:A:6172:ILE:HD11	2.04	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:E:4151:GLU:HB2	1:E:4296:ASN:OD1	1.89	0.72
1:B:1057:CYS:HB3	1:B:1353:TYR:OH	1.90	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: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:A:6039:HIS:HD2	1:A:6204:ARG:NH2	1.88	0.71
1:F:5161:THR:HG22	1:F:5162:ARG:HD2	1.72	0.71
1:D:3150:GLN:HE22	1:D:3291:LEU:HB2	1.54	0.71
1:B:1162:ARG:NH1	1:B:1162:ARG:HB2	2.03	0.71
1:A:6097:THR:HG23	1:A:6258:VAL:HG22	1.72	0.71
1:D:3150:GLN:HE21	1:D:3296:ASN:HB2	1.54	0.71
1:B:1052:ARG:CZ	1:B:1266:SER:HB3	2.20	0.71
1:A:6160:ASP:CG	1:A:6161:THR:H	1.94	0.71
1:B:1071:ARG:H	1:B:1071:ARG:CD	2.03	0.71
1:F:5350:GLN:NE2	1:F:5350:GLN:HA	2.05	0.71
1:D:3150:GLN:NE2	1:D:3296:ASN:HB2	2.06	0.71
1:C:2298:MET:HE1	1:C:2302:LEU:HG	1.72	0.70
1:A:6037:ILE:HG22	1:A:6133:THR:HG21	1.73	0.70
1:F:5292:THR:HG22	1:F:5294:PRO:CD	2.21	0.70
1:B:1124:LYS:HE3	1:B:1177:THR:HG21	1.74	0.70
1:C:2214:MET:HE3	1:C:2214:MET:HA	1.74	0.70
1:E:4097:THR:CG2	1:E:4258:VAL:HG23	2.22	0.70
1:C:2097:THR:HG22	1:C:2110:GLN:NE2	2.06	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:C:2053:THR:OG1	1:C:2061:ARG:HG3	1.92	0.69
1:C:2047:THR:H	1:C:2334:ASN:ND2	1.91	0.69
1:B:1052:ARG:NE	1:B:1266:SER:HB3	2.07	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:F:5292:THR:CG2	1:F:5294:PRO:HD2	2.22	0.69
1:D:3231:GLY:HA3	1:D:3289:HIS:HE1	1.58	0.69
1:F:5052:ARG:NH2	1:F:5054:CYS:HB2	2.08	0.68
1:B:1171:LEU:HA	1:B:1174:MET:HE3	1.75	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:F:5151:GLU:CB	1:F:5296:ASN:HD21	2.06	0.68
1:D:3343:ASP:O	1:D:3347:GLU:HG2	1.93	0.68
1:B:1181:MET:H	1:B:1183:ARG:HH11	1.40	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:C	1:D:3048:LEU:HD12	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: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:A:6008:GLN:HE21	1:A:6096:LYS:HZ2	1.41	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: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:C:2139:LYS:HB2	1:C:2139:LYS:NZ	2.10	0.66
1:B:1052:ARG:HH11	1:B:1265:ASP:N	1.92	0.66
1:F:5336:PRO:HD2	1:F:5339:ILE:CD1	2.20	0.66
1:D:3204:ARG:HD3	1:D:3238:TRP:CE3	2.31	0.66
1:D:3192:GLU:OE1	1:D:3194:ILE:HG22	1.96	0.66
1:C:2029:ILE:HG22	1:C:2031:LYS:HG3	1.77	0.66
1:F:5052:ARG:CD	1:F:5266:SER:H	2.09	0.66
1:E:4353:TYR:O	1:E:4357:GLN:HG3	1.95	0.65
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: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:5271:ARG:HH11	1:F:5271:ARG:HB2	1.61	0.65
1:F:5143:GLN:HG2	1:F:5164:TRP:CE3	2.32	0.65
1:D:3052:ARG:NH1	1:D:3265:ASP:N	2.44	0.65
1:F:5039:HIS:CD2	1:F:5204:ARG:HH11	2.11	0.65
1:A:6141:ARG:HH22	1:A:6236:LEU:HD23	1.60	0.65
1:F:5143:GLN:HG2	1:F:5164:TRP:CZ3	2.31	0.65
1:A:6314:VAL:HG21	1:A:6325:ILE:HD12	1.79	0.65
1:C:2231:GLY:HA3	1:C:2289:HIS:CE1	2.32	0.65
1:C:2240:ALA:CB	1:C:2305:GLU:HG2	2.26	0.65
1:D:3129:THR:O	1:D:3133:THR:HB	1.97	0.65
1:C:2006:LEU:HD21	1:C:2349:VAL:HG12	1.78	0.65
1:E:4348:LEU:O	1:E:4352:GLU:HG2	1.96	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:2030:PHE:HD1	1:C:2032:PRO:HD3	1.62	0.65
1:C:2129:THR:O	1:C:2133:THR:HB	1.97	0.64
1:E:4052:ARG:NE	1:E:4054:CYS:HB2	2.12	0.64
1:D:3031:LYS:HA	1:D:3038:HIS:ND1	2.12	0.64
1:C:2097:THR:CG2	1:C:2259:PRO:HD3	2.27	0.64
1:C:2213:LYS:HE2	1:C:2214:MET:HE3	1.79	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:5160:ASP:CG	1:F:5161:THR:H	2.01	0.64
1:F:5060:PHE:HD2	1:F:5063:ILE:HD12	1.63	0.64
1:F:5036:ILE:HG12	1:F:5238:TRP:CH2	2.33	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:B:1181:MET:H	1:B:1183:ARG:NH1	1.96	0.64
1:B:1139:LYS:HG3	1:B:1168:TRP:CE2	2.32	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:D:3135:THR:O	1:D:3139:LYS:HG3	1.99	0.63
1:B:1106:HIS:ND1	1:B:1116:GLN:HB3	2.13	0.63
1:F:5129:THR:O	1:F:5133:THR:HB	1.98	0.63
1:B:1280:ARG:HG3	1:B:1280:ARG:O	1.97	0.63
1:D:3311:GLU:C	1:D:3312:ILE:HD12	2.18	0.63
1:A:6097:THR:HG21	1:A:6258:VAL:HA	1.80	0.63
1:D:3136:ARG:HH12	1:E:4278:ARG:HH12	1.46	0.63
1:A:6293:ASP:HB2	1:A:6294:PRO:HD3	1.81	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: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: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:B:1030:PHE:O	1:B:1032:PRO:HD2	1.99	0.63
1:A:6086:CYS:HB3	1:A:6089:VAL:HG22	1.81	0.63
1:F:5052:ARG:HH22	1:F:5054:CYS:HB2	1.64	0.62
1:E:4106:HIS:O	1:E:4110:GLN:HG3	1.98	0.62
1:C:2218:LEU:HD23	1:C:2219:GLU:H	1.63	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:F:5298:MET:CA	1:F:5301:LYS:HD3	2.29	0.62
1:D:3231:GLY:HA3	1:D:3289:HIS:CE1	2.35	0.62
1:D:3215:LEU:HD22	1:D:3218:LEU:HD13	1.82	0.62
1:F:5293:ASP:O	1:F:5297:GLU:HG2	2.00	0.62
1:C:2162:ARG:HH22	1:C:2165:ASN:ND2	1.97	0.62
1:D:3314:VAL:HG21	1:D:3325:ILE:HD11	1.82	0.62
1:D:3080:GLN:HE22	1:D:3212:ASP:CG	2.04	0.62
1:D:3018:ALA:O	1:D:3022:ARG:HG3	1.99	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:5141:ARG:HH22	1:F:5295:GLU:CD	2.03	0.61
1:F:5279:ASP:CG	1:F:5280:ARG:H	2.03	0.61
1:F:5210:ILE:HD12	1:F:5260:LEU:HD12	1.82	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: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:4336:PRO:HD2	1:E:4339:ILE:HD11	1.83	0.61
1:E:4269:GLU:OE1	1:E:4269:GLU:N	2.34	0.61
1:F:5052:ARG:HD2	1:F:5266:SER:CB	2.30	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:5298:MET:HA	1:F:5301:LYS:HD3	1.82	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:F:5240:ALA:CB	1:F:5305:GLU:HG2	2.31	0.61
1:C:2293:ASP:HB2	1:C:2294:PRO:HD3	1.81	0.61
1:C:2215:LEU:HD13	1:C:2218:LEU:HG	1.83	0.61
1:B:1147:LEU:HD21	1:B:1164:TRP:HZ2	1.66	0.61
1:F:5213:LYS:HG3	1:F:5214:MET:HE3	1.83	0.61
1:E:4060:PHE:CD2	1:E:4063:ILE:HD12	2.35	0.61
1:B:1310:ILE:HD11	1:B:1312:ILE:HD11	1.82	0.61
1:A:6076:THR:O	1:A:6080:GLN:HG2	2.01	0.61
1:D:3164:TRP:HA	1:D:3164:TRP:CE3	2.35	0.61
1:F:5244:TYR:CE2	1:F:5246:TYR:HB2	2.36	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: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:F:5060:PHE:HE1	1:F:5353:TYR:HB2	1.65	0.60
1:E:4301:LYS:HD2	1:E:4301:LYS:N	2.16	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: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:A:6081:LYS:NZ	1:A:6278:ARG:HH12	1.98	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:E:4074:GLN:HE21	1:E:4074:GLN:CA	2.14	0.60
1:A:6301:LYS:HD2	1:A:6301:LYS:N	2.17	0.60
1:B:1354:LYS:O	1:B:1358:GLU:HG3	2.01	0.60
1:D:3152:PHE:CE1	1:D:3287:LYS:HD2	2.37	0.60
1:D:3045:ARG:HG3	1:D:3244:TYR:CE1	2.36	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:B:1234:LEU:HB2	1:B:1236:LEU:HD13	1.84	0.59
1:B:1046:TYR:CE2	1:B:1336:PRO:HD3	2.37	0.59
1:C:2353:TYR:O	1:C:2357:GLN:HG3	2.02	0.59
1:A:6346:PHE:O	1:A:6349:VAL:HG22	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:E:4162:ARG:NH2	1:E:4164:TRP:H	1.87	0.59
1:E:4025:THR:CG2	1:E:4121:VAL:HG11	2.29	0.59
1:E:4048:LEU:HD21	1:E:4110:GLN:O	2.02	0.59
1:E:4137:ASN:O	1:E:4141:ARG:HG3	2.02	0.59
1:A:6091:LYS:O	1:A:6263:LEU:HD23	2.02	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:F:5245:ARG:HB2	1:F:5308:MET:CE	2.33	0.59
1:B:1109:SER:HG	1:B:1113:TRP:HE3	1.49	0.59
1:F:5325:ILE:HG22	1:F:5326:ASN:N	2.17	0.59
1:B:1319:HIS:CE1	1:B:1321:THR:HG21	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6325:ILE:HG22	1:A:6326:ASN:N	2.17	0.59
1:C:2080:GLN:NE2	1:C:2212:ASP:OD1	2.35	0.59
1:D:3052:ARG:NH1	1:D:3263:LEU:HB3	2.18	0.58
1:D:3008:GLN:HE21	1:D:3096:LYS:HZ2	1.51	0.58
1:A:6039:HIS:HD2	1:A:6204:ARG:HH21	1.51	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:F:5052:ARG:HD2	1:F:5266:SER:N	2.18	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: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:A:6142:TRP:CZ3	1:A:6168:TRP:HB2	2.38	0.58
1:C:2336:PRO:HD2	1:C:2339:ILE:CD1	2.32	0.58
1:C:2048:LEU:HD12	1:C:2049:GLU:N	2.18	0.58
1:F:5209:VAL:HG11	1:F:5229:VAL:HG12	1.85	0.58
1:D:3033:THR:O	1:D:3033:THR:HG22	2.04	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:E:4095:LEU:O	1:E:4258:VAL:HG22	2.03	0.58
1:C:2030:PHE:CD1	1:C:2032:PRO:HD3	2.38	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:B:1034:ASN:CG	1:B:1035:GLY:N	2.57	0.58
1:A:6271:ARG:HB2	1:A:6329:LYS:HE2	1.85	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:F:5053:THR:O	1:F:5061:ARG:HG3	2.05	0.57
1:D:3319:HIS:NE2	1:D:3321:THR:HG21	2.18	0.57
1:D:3141:ARG:NH2	1:D:3236:LEU:HD23	2.20	0.57
1:C:2213:LYS:HG3	1:C:2214:MET:N	2.18	0.57
1:E:4120:LEU:HD13	1:E:4177:THR:HG21	1.86	0.57
1:A:6152:PHE:CE2	1:A:6299:LYS:HD3	2.40	0.57
1:C:2344:ASP:O	1:C:2348:LEU:HD13	2.04	0.57
1:A:6310:ILE:HD11	1:A:6312:ILE:HD11	1.85	0.57
1:D:3060:PHE:HE1	1:D:3064:ILE:HD11	1.70	0.57
1:C:2238:TRP:O	1:C:2306:TYR:OH	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4273:VAL:O	1:E:4273:VAL:HG13	2.04	0.57
1:F:5213:LYS:HE3	1:F:5214:MET:HE3	1.85	0.57
1:C:2021:ILE:O	1:C:2025:THR:HG23	2.04	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:F:5301:LYS:H	1:F:5301:LYS:CD	2.16	0.57
1:E:4345:TYR:O	1:E:4349:VAL:HG23	2.05	0.57
1:D:3230:GLY:O	1:D:3289:HIS:CE1	2.57	0.57
1:D:3060:PHE:CE1	1:D:3064:ILE:HD11	2.39	0.57
1:A:6347:GLU:HA	1:A:6347:GLU:OE2	2.05	0.57
1:B:1291:LEU:HD22	1:B:1295:GLU:HB2	1.87	0.57
1:E:4317:TRP:HE3	1:E:4319:HIS:CE1	2.23	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: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: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:B:1005:VAL:HG13	1:B:1005:VAL:O	2.05	0.56
1:F:5319:HIS:ND1	1:F:5321:THR:HG22	2.20	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:A:6068:LEU:HD21	1:A:6345:TYR:CE1	2.39	0.56
1:E:4186:LEU:HD22	1:E:4186:LEU:N	2.21	0.56
1:D:3082:LYS:HE3	1:D:3211:SER:O	2.04	0.56
1:A:6200:CYS:HB2	1:A:6205:ARG:O	2.06	0.56
1:A:6066:LYS:NZ	1:A:6071:ARG:NH2	2.54	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:C:2107:ALA:O	1:C:2259:PRO:HG3	2.05	0.56
1:B:1336:PRO:HD2	1:B:1339:ILE:CD1	2.31	0.56
1:A:6319:HIS:O	1:A:6321:THR:N	2.39	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:E:4098:ASN:H	1:E:4116:GLN:HE22	1.52	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:D:3150:GLN:NE2	1:D:3291:LEU:HB2	2.19	0.56
1:F:5005:VAL:O	1:F:5005:VAL:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2354:LYS:O	1:C:2358:GLU:HG3	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:CE	1:C:2214:MET:HA	2.34	0.56
1:B:1323:HIS:N	1:B:1323:HIS:CD2	2.73	0.55
1:B:1082:LYS:CD	1:B:1213:LYS:HE3	2.36	0.55
1:E:4319:HIS:O	1:E:4321:THR:N	2.39	0.55
1:C:2319:HIS:O	1:C:2321:THR:N	2.39	0.55
1:F:5080:GLN:HE22	1:F:5212:ASP:HB2	1.71	0.55
1:D:3253:ASP:OD1	1:D:3254:SER:N	2.39	0.55
1:D:3162:ARG:NH2	1:D:3165:ASN:HD21	2.05	0.55
1:D:3028:ASP:OD1	1:D:3043:MET:HG3	2.05	0.55
1:B:1319:HIS:O	1:B:1321:THR:N	2.39	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:D:3310:ILE:HG13	1:D:3312:ILE:CD1	2.28	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: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:3048:LEU:HD12	1:D:3049:GLU:N	2.22	0.55
1:C:2350:GLN:O	1:C:2354:LYS:HG3	2.07	0.55
1:A:6167:GLU:O	1:A:6171:LEU:HD23	2.07	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:F:5043:MET:HG2	1:F:5046:TYR:HE1	1.71	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:5090:ARG:NH2	1:F:5265:ASP:O	2.38	0.55
1:A:6289:HIS:HB3	1:A:6290:PHE:CE1	2.41	0.55
1:B:1180:PRO:HB3	1:B:1183:ARG:HG3	1.88	0.55
1:B:1025:THR:HA	1:B:1043:MET:SD	2.46	0.55
1:E:4056:PHE:HE1	1:E:4349:VAL:HG12	1.72	0.55
1:C:2068:LEU:HD21	1:C:2345:TYR:CE1	2.41	0.55
1:F:5095:LEU:O	1:F:5258:VAL:HG22	2.06	0.55
1:F:5020:LYS:HE3	1:F:5024:ARG:NH2	2.07	0.55
1:D:3147:LEU:HD21	1:D:3164:TRP:HZ2	1.70	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:3052:ARG:NH1	1:D:3263:LEU:C	2.60	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:3164:TRP:HE3	1:D:3164:TRP:HA	1.69	0.55
1:C:2271:ARG:HG3	1:C:2271:ARG:HH11	1.71	0.55
1:D:3107:ALA:HA	1:D:3259:PRO:HG3	1.89	0.55
1:B:1141:ARG:HD2	1:B:1237:HIS:HE1	1.72	0.55
1:F:5319:HIS:O	1:F:5321:THR:N	2.41	0.55
1:C:2046:TYR:CE2	1:C:2336:PRO:HD3	2.42	0.55
1:A:6245:ARG:NE	1:A:6308:MET:SD	2.80	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:5270:ILE:HG22	1:F:5329:LYS:NZ	2.22	0.55
1:F:5052:ARG:NH1	1:F:5054:CYS:HB2	2.22	0.54
1:C:2133:THR:HG22	1:C:2134:ASP:N	2.22	0.54
1:F:5289:HIS:HB3	1:F:5290:PHE:CE1	2.43	0.54
1:E:4030:PHE:HD1	1:E:4032:PRO:HD3	1.70	0.54
1:F:5080:GLN:OE1	1:F:5213:LYS:HG2	2.07	0.54
1:E:4020:LYS:HE2	1:E:4024:ARG:NH2	2.22	0.54
1:A:6133:THR:HG22	1:A:6134:ASP:N	2.22	0.54
1:A:6008:GLN:NE2	1:A:6096:LYS:NZ	2.54	0.54
1:C:2147:LEU:O	1:C:2148:LYS:HB2	2.06	0.54
1:E:4005:VAL:O	1:E:4005:VAL:HG13	2.08	0.54
1:D:3005:VAL:HG13	1:D:3005:VAL:O	2.07	0.54
1:F:5253:ASP:CG	1:F:5254:SER:H	2.09	0.54
1:A:6240:ALA:CB	1:A:6305:GLU:HG2	2.37	0.54
1:F:5161:THR:HG22	1:F:5162:ARG:CD	2.35	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: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:C:2017:LYS:HD2	1:C:2341:LEU:HD23	1.89	0.54
1:C:2011:TYR:HA	1:C:2341:LEU:HD13	1.89	0.54
1:A:6146:SER:O	1:A:6148:LYS:HD3	2.07	0.54
1:E:4131:LYS:NZ	1:E:4173:LYS:NZ	2.56	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:F:5141:ARG:NH1	1:F:5290:PHE:O	2.35	0.54
1:A:6227:LEU:HG	1:A:6229:VAL:HG23	1.90	0.54
1:B:1141:ARG:HH21	1:B:1236:LEU:HD23	1.66	0.54
1:E:4354:LYS:HA	1:E:4357:GLN:NE2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:5276:VAL:CG2	1:F:5325:ILE:HG21	2.38	0.54
1:C:2137:ASN:O	1:C:2141:ARG:HD3	2.07	0.54
1:E:4359:ASN:C	1:E:4361:GLU:H	2.11	0.54
1:A:6080:GLN:HE22	1:A:6212:ASP:HB2	1.72	0.54
1:F:5052:ARG:CZ	1:F:5054:CYS:HB2	2.37	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:HH22	1:F:5054:CYS:CB	2.21	0.53
1:C:2234:LEU:HB2	1:C:2236:LEU:HD13	1.89	0.53
1:A:6050:MET:O	1:A:6264:LYS:HB2	2.07	0.53
1:E:4245:ARG:HG3	1:E:4245:ARG:HH11	1.74	0.53
1:D:3273:VAL:HG13	1:D:3273:VAL:O	2.09	0.53
1:E:4189:ASN:N	1:E:4189:ASN:ND2	2.47	0.53
1:A:6170:ASN:O	1:A:6173:LYS:N	2.40	0.53
1:D:3124:LYS:HD2	1:D:3177:THR:HG21	1.90	0.53
1:C:2229:VAL:HG11	1:C:2257:PHE:HZ	1.72	0.53
1:C:2107:ALA:HB1	1:C:2250:LEU:HD22	1.90	0.53
1:F:5097:THR:HG21	1:F:5259:PRO:HD3	1.89	0.53
1:F:5162:ARG:N	1:F:5162:ARG:NE	2.57	0.53
1:D:3355:LYS:O	1:D:3359:ASN:ND2	2.42	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:C:2310:ILE:HG13	1:C:2312:ILE:HD11	1.91	0.53
1:C:2141:ARG:HH22	1:C:2236:LEU:HB3	1.72	0.53
1:E:4047:THR:HG1	1:E:4205:ARG:HH22	1.54	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:A:6355:LYS:O	1:A:6355:LYS:HG2	2.08	0.53
1:C:2042:THR:HA	1:C:2045:ARG:NH1	2.24	0.53
1:B:1048:LEU:HD12	1:B:1048:LEU:C	2.29	0.53
1:E:4048:LEU:CD2	1:E:4110:GLN:O	2.56	0.53
1:B:1293:ASP:O	1:B:1297:GLU:HG2	2.08	0.53
1:A:6098:ASN:HD22	1:A:6098:ASN:N	2.06	0.53
1:B:1095:LEU:O	1:B:1258:VAL:CG2	2.53	0.53
1:B:1346:PHE:O	1:B:1349:VAL:HG22	2.09	0.53
1:B:1201:ASN:OD1	1:B:1235:PRO:HA	2.08	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:E:4136:ARG:HG2	1:E:4136:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3163:ASN:OD1	1:D:3166:ASP:HB2	2.09	0.53
1:F:5046:TYR:HA	1:F:5334:ASN:HD21	1.72	0.53
1:B:1071:ARG:N	1:B:1071:ARG:HD3	2.15	0.53
1:A:6137:ASN:N	1:A:6137:ASN:HD22	2.06	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:A:6126:LEU:HD21	1:A:6195:HIS:HD2	1.74	0.53
1:F:5040:PHE:O	1:F:5204:ARG:NH1	2.42	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:E:4025:THR:HB	1:E:4026:PRO:CD	2.39	0.52
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:F:5052:ARG:HH21	1:F:5055:GLN:NE2	1.92	0.52
1:A:6236:LEU:HD21	1:A:6291:LEU:CD2	2.39	0.52
1:E:4019:VAL:HA	1:E:4022:ARG:HH12	1.74	0.52
1:C:2071:ARG:HH12	1:C:2096:LYS:HE2	1.73	0.52
1:F:5161:THR:CG2	1:F:5162:ARG:HE	2.22	0.52
1:C:2310:ILE:CD1	1:C:2312:ILE:HD11	2.39	0.52
1:A:6024:ARG:HD2	1:A:6024:ARG:N	2.23	0.52
1:C:2359:ASN:C	1:C:2361:GLU:H	2.12	0.52
1:F:5331:ASP:OD2	1:F:5332:GLU:N	2.42	0.52
1:F:5086:CYS:SG	1:F:5088:GLU:HG2	2.49	0.52
1:D:3253:ASP:OD2	1:D:3256:HIS:HB3	2.10	0.52
1:F:5194:ILE:O	1:F:5198:VAL:HG23	2.09	0.52
1:A:6025:THR:CG2	1:A:6121:VAL:HG11	2.35	0.52
1:D:3049:GLU:HG3	1:D:3333:ALA:HB2	1.92	0.52
1:C:2048:LEU:HD12	1:C:2048:LEU:C	2.30	0.52
1:D:3081:LYS:NZ	1:F:5143:GLN:HE22	2.07	0.52
1:A:6120:LEU:HD21	1:A:6188:TYR:CE2	2.44	0.52
1:C:2052:ARG:NH1	1:C:2266:SER:HB3	2.25	0.52
1:F:5287:LYS:HE3	1:F:5289:HIS:CE1	2.45	0.52
1:B:1192:GLU:CD	1:B:1194:ILE:HG22	2.30	0.52
1:D:3084:ASN:CG	1:D:3091:LYS:HG3	2.30	0.52
1:C:2020:LYS:O	1:C:2024:ARG:HG3	2.10	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:E:4215:LEU:HD13	1:E:4218:LEU:HG	1.91	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:4355:LYS:O	1:E:4359:ASN:ND2	2.43	0.52
1:A:6100:ASP:O	1:A:6188:TYR:HD1	1.93	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:C:2073:ILE:HD12	1:C:2258:VAL:HG21	1.91	0.51
1:A:6052:ARG:HG3	1:A:6052:ARG:NH1	2.24	0.51
1:F:5022:ARG:HB3	1:F:5119:ASP:OD1	2.10	0.51
1:B:1110:GLN:NE2	1:B:1116:GLN:NE2	2.58	0.51
1:B:1087:ARG:O	1:B:1087:ARG:HG2	2.11	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:F:5161:THR:O	1:F:5162:ARG:HB2	2.09	0.51
1:D:3077:LEU:HD13	1:D:3210:ILE:HG22	1.92	0.51
1:F:5359:ASN:C	1:F:5361:GLU:H	2.13	0.51
1:F:5319:HIS:ND1	1:F:5321:THR:CG2	2.74	0.51
1:B:1006:LEU:HD11	1:B:1349:VAL:HG12	1.93	0.51
1:A:6073:ILE:N	1:A:6073:ILE:CD1	2.74	0.51
1:C:2137:ASN:HB3	1:C:2237:HIS:NE2	2.25	0.51
1:D:3359:ASN:C	1:D:3361:GLU:H	2.14	0.51
1:D:3144:LEU:CD1	1:D:3149:SER:HB3	2.41	0.51
1:F:5319:HIS:CE1	1:F:5321:THR:HG21	2.45	0.51
1:E:4022:ARG:CG	1:E:4022:ARG:HH11	2.22	0.51
1:D:3194:ILE:HA	1:D:3290:PHE:HE1	1.74	0.51
1:C:2200:CYS:HB2	1:C:2205:ARG:O	2.11	0.51
1:F:5142:TRP:HH2	1:F:5167:GLU:HB3	1.75	0.51
1:A:6314:VAL:HG12	1:A:6315:GLN:N	2.26	0.51
1:D:3226:PRO:HB2	1:D:3228:LYS:NZ	2.26	0.51
1:D:3024:ARG:NH1	1:D:3339:ILE:HD13	2.26	0.51
1:C:2186:LEU:N	1:C:2186:LEU:HD22	2.26	0.51
1:D:3312:ILE:HD13	1:D:3327:ALA:HB3	1.92	0.51
1:B:1094:ALA:HB1	1:B:1258:VAL:HG21	1.92	0.51
1:F:5084:ASN:OD1	1:F:5091:LYS:HG3	2.11	0.51
1:C:2301:LYS:HD2	1:C:2301:LYS:N	2.27	0.50
1:D:3025:THR:CG2	1:D:3121:VAL:HG11	2.40	0.50
1:D:3087:ARG:HD2	1:F:5162:ARG:HH11	1.76	0.50
1:D:3354:LYS:HA	1:D:3357:GLN:HE21	1.76	0.50
1:F:5245:ARG:HB2	1:F:5308:MET:HE3	1.92	0.50
1:C:2273:VAL:O	1:C:2273:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5059:GLN:OE1	1:F:5059:GLN:N	2.42	0.50
1:F:5216:ARG:HH11	1:F:5216:ARG:CB	2.13	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:4173:LYS:N	1:E:4173:LYS:HD2	2.25	0.50
1:F:5249:VAL:HG12	1:F:5260:LEU:HB2	1.93	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:E:4153:VAL:O	1:E:4153:VAL:HG13	2.11	0.50
1:B:1338:GLU:HG2	1:B:1339:ILE:HG23	1.92	0.50
1:A:6036:ILE:HG13	1:A:6037:ILE:N	2.27	0.50
1:D:3120:LEU:O	1:D:3124:LYS:HB2	2.11	0.50
1:C:2185:GLY:C	1:C:2186:LEU:HD22	2.31	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:F:5133:THR:CG2	1:F:5134:ASP:N	2.74	0.50
1:D:3314:VAL:HG13	1:D:3315:GLN:NE2	2.27	0.50
1:C:2139:LYS:HE3	1:C:2168:TRP:NE1	2.26	0.50
1:E:4314:VAL:HG22	1:E:4315:GLN:N	2.25	0.50
1:E:4028:ASP:O	1:E:4041:LYS:HD3	2.10	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:3304:LYS:HA	1:D:3309:VAL:HG23	1.92	0.50
1:D:3240:ALA:CB	1:D:3305:GLU:HG2	2.42	0.50
1:A:6014:ASN:ND2	1:A:6017:LYS:HB2	2.27	0.50
1:C:2164:TRP:C	1:C:2166:ASP:N	2.61	0.50
1:D:3299:LYS:HG3	1:D:3300:GLU:N	2.26	0.50
1:C:2352:GLU:OE2	1:C:2352:GLU:HA	2.11	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:C:2253:ASP:OD1	1:C:2254:SER:N	2.44	0.50
1:E:4244:TYR:CE2	1:E:4246:TYR:HB2	2.46	0.50
1:D:3133:THR:CG2	1:D:3134:ASP:N	2.74	0.50
1:A:6325:ILE:HG22	1:A:6326:ASN:H	1.76	0.50
1:C:2142:TRP:CE2	1:C:2171:LEU:HD11	2.47	0.50
1:D:3060:PHE:HA	1:D:3063:ILE:HD12	1.94	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:F:5219:GLU:HG3	1:F:5219:GLU:O	2.11	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:C:2082:LYS:HE2	1:C:2211:SER:O	2.11	0.50
1:A:6020:LYS:O	1:A:6024:ARG:HD3	2.12	0.50
1:E:4014:ASN:ND2	1:E:4344:ASP:OD2	2.37	0.50
1:F:5279:ASP:CG	1:F:5280:ARG:N	2.65	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:A:6199:LEU:O	1:A:6203:LEU:HG	2.12	0.50
1:F:5153:VAL:O	1:F:5153:VAL:HG13	2.12	0.50
1:D:3297:GLU:HA	1:D:3297:GLU:OE1	2.12	0.50
1:C:2164:TRP:C	1:C:2166:ASP:H	2.13	0.49
1:B:1153:VAL:O	1:B:1153:VAL:HG13	2.12	0.49
1:D:3162:ARG:NH2	1:E:4081:LYS:NZ	2.59	0.49
1:B:1252:TYR:OH	1:B:1255:HIS:HA	2.11	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:B:1240:ALA:CB	1:B:1305:GLU:HG2	2.42	0.49
1:B:1025:THR:HG22	1:B:1026:PRO:N	2.27	0.49
1:A:6149:SER:C	1:A:6150:GLN:HG2	2.32	0.49
1:E:4234:LEU:O	1:E:4236:LEU:HD22	2.13	0.49
1:A:6186:LEU:HD22	1:A:6186:LEU:N	2.27	0.49
1:A:6097:THR:CG2	1:A:6258:VAL:HA	2.43	0.49
1:E:4136:ARG:HG2	1:E:4136:ARG:HH11	1.77	0.49
1:F:5253:ASP:CG	1:F:5254:SER:N	2.65	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:F:5168:TRP:O	1:F:5172:ILE:HG13	2.12	0.49
1:B:1034:ASN:ND2	1:B:1036:ILE:HG22	2.26	0.49
1:B:1003:GLU:OE2	1:B:1003:GLU:N	2.46	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:3355:LYS:HG2	1:D:3355:LYS:O	2.13	0.49
1:D:3227:LEU:CD2	1:D:3229:VAL:HG13	2.43	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:B:1082:LYS:HD3	1:B:1213:LYS:HE3	1.95	0.49
1:E:4354:LYS:O	1:E:4358:GLU:HG3	2.12	0.49
1:A:6204:ARG:HD3	1:A:6238:TRP:CE3	2.47	0.49
1:E:4240:ALA:CB	1:E:4305:GLU:HG2	2.42	0.49
1:C:2060:PHE:CE1	1:C:2064:ILE:HD11	2.47	0.49
1:A:6273:VAL:O	1:A:6273:VAL:HG13	2.12	0.49
1:D:3270:ILE:N	1:D:3270:ILE:HD13	2.21	0.48
1:A:6276:VAL:HG21	1:A:6325:ILE:HG21	1.93	0.48
1:D:3215:LEU:HB3	1:D:3218:LEU:HB2	1.94	0.48
1:F:5355:LYS:O	1:F:5359:ASN:CG	2.51	0.48
1:D:3015:MET:O	1:D:3019:VAL:HG23	2.13	0.48
1:E:4010:LEU:HD13	1:E:4342:VAL:HG22	1.95	0.48
1:F:5265:ASP:O	1:F:5266:SER:O	2.31	0.48
1:D:3052:ARG:CZ	1:D:3263:LEU:HB3	2.42	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:A:6127:PHE:HE1	1:A:6172:ILE:O	1.96	0.48
1:E:4019:VAL:HA	1:E:4022:ARG:NH1	2.29	0.48
1:E:4227:LEU:HG	1:E:4229:VAL:HG22	1.94	0.48
1:D:3227:LEU:HD22	1:D:3229:VAL:HG13	1.94	0.48
1:C:2136:ARG:HG2	1:C:2136:ARG:HH11	1.78	0.48
1:B:1141:ARG:HH22	1:B:1236:LEU:HD23	1.68	0.48
1:E:4069:ILE:O	1:E:4096:LYS:NZ	2.40	0.48
1:D:3162:ARG:O	1:D:3163:ASN:HB2	2.14	0.48
1:B:1133:THR:CG2	1:B:1134:ASP:N	2.76	0.48
1:E:4097:THR:CG2	1:E:4258:VAL:HA	2.39	0.48
1:A:6193:GLU:HB3	1:A:6290:PHE:CZ	2.47	0.48
1:E:4215:LEU:HD13	1:E:4218:LEU:CG	2.43	0.48
1:C:2204:ARG:HD2	1:C:2238:TRP:CH2	2.48	0.48
1:A:6185:GLY:C	1:A:6186:LEU:HD22	2.32	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:A:6070:ASP:CG	1:A:6073:ILE:HD13	2.33	0.48
1:B:1200:CYS:HB2	1:B:1205:ARG:O	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:F:5017:LYS:HD2	1:F:5341:LEU:HD23	1.95	0.48
1:C:2192:GLU:HB2	1:C:2193:GLU:OE1	2.13	0.48
1:A:6270:ILE:H	1:A:6270:ILE:HD12	1.77	0.48
1:B:1082:LYS:HD2	1:B:1213:LYS:HE3	1.95	0.48
1:D:3052:ARG:NH2	1:D:3266:SER:OG	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4066:LYS:O	1:E:4066:LYS:HD3	2.14	0.48
1:B:1277:ASN:HD21	1:B:1286:LEU:CD1	2.27	0.48
1:D:3050:MET:HE2	1:D:3068:LEU:HD13	1.96	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:E:4097:THR:HA	1:E:4116:GLN:HE22	1.78	0.48
1:C:2287:LYS:HD3	1:C:2287:LYS:C	2.34	0.48
1:C:2120:LEU:O	1:C:2124:LYS:HG3	2.14	0.48
1:D:3293:ASP:CB	1:D:3294:PRO:HD3	2.42	0.48
1:C:2010:LEU:HA	1:C:2345:TYR:HD1	1.79	0.48
1:A:6292:THR:HB	1:A:6294:PRO:HD2	1.95	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: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:1179:THR:HG22	1:B:1180:PRO:O	2.13	0.48
1:D:3311:GLU:OE1	1:D:3324:LEU:HD23	2.14	0.47
1:B:1336:PRO:HD2	1:B:1339:ILE:CG1	2.44	0.47
1:D:3087:ARG:CZ	1:F:5162:ARG:HG3	2.44	0.47
1:D:3163:ASN:O	1:D:3163:ASN:OD1	2.32	0.47
1:B:1238:TRP:HB2	1:B:1243:CYS:SG	2.54	0.47
1:F:5281:GLY:HA2	1:F:5317:TRP:CE2	2.48	0.47
1:C:2152:PHE:CD1	1:C:2287:LYS:HG2	2.49	0.47
1:F:5142:TRP:CZ2	1:F:5167:GLU:HG3	2.49	0.47
1:D:3214:MET:HG3	1:F:5140:PHE:CE2	2.49	0.47
1:F:5276:VAL:HG22	1:F:5325:ILE:HG21	1.96	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:F:5346:PHE:O	1:F:5349:VAL:HG23	2.14	0.47
1:A:6022:ARG:NH2	1:A:6119:ASP:OD2	2.46	0.47
1:A:6082:LYS:HA	1:A:6082:LYS:CE	2.40	0.47
1:B:1142:TRP:CH2	1:B:1167:GLU:HG2	2.50	0.47
1:E:4145:GLU:OE1	1:E:4290:PHE:N	2.47	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:B:1010:LEU:HG	1:B:1068:LEU:HD22	1.96	0.47
1:F:5010:LEU:HA	1:F:5345:TYR:CD1	2.49	0.47
1:B:1137:ASN:HB2	1:B:1237:HIS:NE2	2.30	0.47
1:E:4344:ASP:O	1:E:4348:LEU:HD13	2.14	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:A:6015:MET:O	1:A:6019:VAL:HG23	2.14	0.47
1:C:2052:ARG:HB3	1:C:2055:GLN:HE21	1.80	0.47
1:B:1082:LYS:NZ	1:B:1213:LYS:NZ	2.63	0.47
1:D:3050:MET:HE1	1:D:3068:LEU:HD13	1.97	0.47
1:B:1314:VAL:HG21	1:B:1325:ILE:CD1	2.40	0.47
1:F:5314:VAL:HG12	1:F:5315:GLN:N	2.30	0.47
1:F:5218:LEU:HD23	1:F:5219:GLU:H	1.79	0.47
1:F:5010:LEU:HA	1:F:5345:TYR:HD1	1.79	0.47
1:F:5008:GLN:OE1	1:F:5096:LYS:HE2	2.15	0.47
1:A:6337:LYS:HE2	1:A:6343:ASP:CG	2.33	0.47
1:D:3136:ARG:NH1	1:E:4278:ARG:HH12	2.11	0.47
1:E:4064:ILE:HD11	1:E:4349:VAL:HG11	1.97	0.47
1:B:1358:GLU:HA	1:B:1361:GLU:OE2	2.15	0.47
1:A:6271:ARG:NE	1:A:6332:GLU:HB3	2.29	0.47
1:F:5343:ASP:O	1:F:5347:GLU:HG2	2.14	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:E:4254:SER:OG	1:E:4255:HIS:N	2.47	0.47
1:F:5298:MET:C	1:F:5301:LYS:HD3	2.36	0.47
1:D:3281:GLY:HA2	1:D:3317:TRP:CE2	2.49	0.47
1:A:6127:PHE:CE1	1:A:6172:ILE:O	2.67	0.47
1:D:3171:LEU:HD13	1:D:3194:ILE:HG21	1.96	0.47
1:A:6081:LYS:HZ3	1:A:6278:ARG:HH12	1.61	0.47
1:D:3162:ARG:HH21	1:E:4081:LYS:HZ1	1.62	0.47
1:B:1025:THR:HG22	1:B:1121:VAL:HG11	1.96	0.47
1:F:5253:ASP:OD2	1:F:5254:SER:N	2.47	0.47
1:E:4317:TRP:HB2	1:E:4319:HIS:NE2	2.29	0.47
1:B:1046:TYR:HB3	1:B:1335:LEU:HD21	1.97	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:D:3120:LEU:HD11	1:D:3188:TYR:OH	2.15	0.47
1:A:6057:CYS:SG	1:A:6059:GLN:CD	2.94	0.47
1:B:1277:ASN:HD21	1:B:1286:LEU:HD13	1.80	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:F:5271:ARG:HH11	1:F:5271:ARG:CB	2.27	0.47
1:B:1097:THR:HG23	1:B:1256:HIS:NE2	2.29	0.47
1:A:6265:ASP:O	1:A:6266:SER:O	2.32	0.47
1:D:3008:GLN:HE21	1:D:3096:LYS:HZ3	1.57	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:4143:GLN:HA	1:E:4164:TRP:CZ3	2.50	0.46
1:B:1080:GLN:HG3	1:B:1082:LYS:HB2	1.97	0.46
1:C:2164:TRP:CE3	1:C:2164:TRP:CA	2.93	0.46
1:D:3153:VAL:O	1:D:3153:VAL:HG13	2.16	0.46
1:F:5349:VAL:O	1:F:5353:TYR:HB2	2.16	0.46
1:F:5082:LYS:NZ	1:F:5213:LYS:HD3	2.31	0.46
1:E:4312:ILE:HD12	1:E:4327:ALA:CB	2.45	0.46
1:F:5245:ARG:HB2	1:F:5308:MET:HE2	1.97	0.46
1:C:2314:VAL:HG21	1:C:2325:ILE:HD13	1.97	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:A:6152:PHE:HD2	1:A:6299:LYS:NZ	2.02	0.46
1:D:3052:ARG:NH1	1:D:3264:LYS:N	2.62	0.46
1:B:1142:TRP:HH2	1:B:1167:GLU:HG2	1.79	0.46
1:D:3314:VAL:HG12	1:D:3315:GLN:N	2.30	0.46
1:D:3030:PHE:O	1:D:3032:PRO:HD2	2.16	0.46
1:D:3048:LEU:C	1:D:3048:LEU:CD1	2.83	0.46
1:C:2048:LEU:HD13	1:C:2342:VAL:HG21	1.96	0.46
1:A:6191:LEU:HD22	1:A:6195:HIS:CD2	2.51	0.46
1:F:5356:TRP:HA	1:F:5356:TRP:CE3	2.49	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:D:3147:LEU:O	1:D:3148:LYS:HB2	2.15	0.46
1:C:2343:ASP:O	1:C:2346:PHE:HB3	2.16	0.46
1:F:5267:GLY:HA2	1:F:5268:PRO:HD3	1.68	0.46
1:B:1052:ARG:NH1	1:B:1265:ASP:N	2.63	0.46
1:E:4137:ASN:HB2	1:E:4237:HIS:NE2	2.31	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:F:5200:CYS:HB2	1:F:5205:ARG:O	2.15	0.46
1:B:1267:GLY:HA2	1:B:1268:PRO:HD3	1.74	0.46
1:F:5336:PRO:CD	1:F:5339:ILE:HD11	2.28	0.46
1:E:4150:GLN:OE1	1:E:4287:LYS:NZ	2.48	0.46
1:B:1014:ASN:ND2	1:B:1344:ASP:OD2	2.49	0.46
1:E:4030:PHE:O	1:E:4032:PRO:HD2	2.16	0.46
1:A:6227:LEU:HD23	1:A:6252:TYR:OH	2.15	0.46
1:E:4074:GLN:C	1:E:4074:GLN:HE21	2.19	0.46
1:E:4034:ASN:CG	1:E:4035:GLY:N	2.68	0.46
1:F:5090:ARG:HD2	1:F:5271:ARG:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1265:ASP:O	1:B:1266:SER:O	2.33	0.46
1:D:3304:LYS:HA	1:D:3309:VAL:CG2	2.46	0.46
1:C:2240:ALA:HB3	1:C:2305:GLU:HG2	1.97	0.46
1:E:4270:ILE:HD11	1:E:4312:ILE:HD11	1.97	0.46
1:E:4061:ARG:NH1	1:E:4065:HIS:HE1	2.14	0.46
1:F:5053:THR:C	1:F:5055:GLN:H	2.19	0.46
1:C:2265:ASP:O	1:C:2266:SER:O	2.34	0.46
1:B:1008:GLN:HE21	1:B:1008:GLN:CA	2.25	0.46
1:F:5097:THR:HG22	1:F:5110:GLN:NE2	2.25	0.46
1:D:3299:LYS:HG3	1:D:3300:GLU:H	1.81	0.46
1:F:5355:LYS:HG2	1:F:5355:LYS:O	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: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:F:5183:ARG:HH11	1:F:5183:ARG:CG	2.28	0.46
1:A:6059:GLN:O	1:A:6063:ILE:HG13	2.15	0.46
1:C:2349:VAL:O	1:C:2353:TYR:HB2	2.16	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:A:6059:GLN:H	1:A:6059:GLN:CD	2.18	0.45
1:C:2279:ASP:HB3	1:C:2282:ARG:HG2	1.99	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:D:3037:ILE:HB	1:D:3129:THR:HG23	1.98	0.45
1:D:3081:LYS:HZ1	1:F:5143:GLN:NE2	2.14	0.45
1:F:5270:ILE:HG22	1:F:5329:LYS:HZ2	1.80	0.45
1:B:1091:LYS:O	1:B:1263:LEU:HD23	2.16	0.45
1:A:6016:ARG:C	1:A:6016:ARG:HD3	2.37	0.45
1:F:5042:THR:HG22	1:F:5045:ARG:NH2	2.31	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:C:2317:TRP:H	1:C:2319:HIS:CE1	2.34	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: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:E:4193:GLU:HB3	1:E:4290:PHE:CZ	2.51	0.45
1:E:4199:LEU:O	1:E:4203:LEU:HG	2.16	0.45
1:E:4020:LYS:HE2	1:E:4024:ARG:HH21	1.82	0.45
1:A:6215:LEU:HD13	1:A:6218:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2269:GLU:CD	1:C:2269:GLU:H	2.20	0.45
1:B:1020:LYS:O	1:B:1024:ARG:HG3	2.15	0.45
1:C:2230:GLY:O	1:C:2289:HIS:HE1	2.00	0.45
1:A:6209:VAL:HG11	1:A:6229:VAL:HG12	1.98	0.45
1:E:4152:PHE:CD2	1:E:4299:LYS:HD3	2.51	0.45
1:E:4074:GLN:NE2	1:E:4074:GLN:CA	2.80	0.45
1:C:2060:PHE:HA	1:C:2063:ILE:HD12	1.98	0.45
1:A:6093:VAL:HG12	1:A:6261:VAL:HG23	1.99	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:A:6148:LYS:HE2	1:A:6148:LYS:HB2	1.81	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:F:5345:TYR:O	1:F:5348:LEU:HB3	2.17	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: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:B:1046:TYR:O	1:B:1112:MET:HB3	2.17	0.45
1:A:6196:ILE:HB	1:A:6233:TYR:CE2	2.52	0.45
1:C:2345:TYR:CD2	1:C:2345:TYR:O	2.70	0.45
1:A:6321:THR:HG22	1:A:6322:THR:N	2.31	0.45
1:C:2227:LEU:HG	1:C:2229:VAL:CG2	2.47	0.45
1:A:6019:VAL:O	1:A:6023:GLU:HB2	2.17	0.45
1:C:2084:ASN:OD1	1:C:2091:LYS:HG3	2.16	0.45
1:F:5204:ARG:HG3	1:F:5238:TRP:NE1	2.32	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:C:2015:MET:SD	1:F:5007:PRO:HD3	2.57	0.45
1:C:2006:LEU:HD12	1:C:2006:LEU:HA	1.82	0.45
1:C:2059:GLN:O	1:C:2063:ILE:HG13	2.17	0.45
1:B:1319:HIS:C	1:B:1321:THR:H	2.20	0.45
1:B:1069:ILE:HD11	1:B:1093:VAL:HG21	1.99	0.45
1:F:5161:THR:HG22	1:F:5162:ARG:NE	2.32	0.45
1:B:1147:LEU:CD2	1:B:1164:TRP:HZ2	2.30	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:F:5046:TYR:HD1	1:F:5113:TRP:HE1	1.65	0.45
1:F:5038:HIS:O	1:F:5202:ILE:HG23	2.18	0.44
1:B:1142:TRP:O	1:B:1146:SER:HB2	2.17	0.44
1:A:6053:THR:C	1:A:6055:GLN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6056:PHE:O	1:A:6061:ARG:CD	2.63	0.44
1:E:4064:ILE:CD1	1:E:4349:VAL:HG11	2.46	0.44
1:A:6071:ARG:HG3	1:A:6071:ARG:HH11	1.81	0.44
1:E:4279:ASP:CG	1:E:4280:ARG:N	2.70	0.44
1:B:1286:LEU:HA	1:B:1286:LEU:HD12	1.75	0.44
1:A:6022:ARG:HB3	1:A:6119:ASP:OD1	2.17	0.44
1:C:2086:CYS:SG	1:C:2088:GLU:HG2	2.57	0.44
1:F:5028:ASP:OD1	1:F:5041:LYS:HB2	2.17	0.44
1:B:1036:ILE:HG13	1:B:1037:ILE:N	2.32	0.44
1:A:6249:VAL:CG1	1:A:6260:LEU:HB2	2.46	0.44
1:A:6253:ASP:OD2	1:A:6254:SER:N	2.50	0.44
1:D:3055:GLN:HG3	1:D:3056:PHE:CE1	2.52	0.44
1:A:6232:ILE:HG13	1:A:6286:LEU:HD23	2.00	0.44
1:B:1240:ALA:HB3	1:B:1305:GLU:HG2	1.98	0.44
1:F:5104:LEU:HB2	1:F:5257:PHE:CE1	2.53	0.44
1:C:2334:ASN:C	1:C:2334:ASN:HD22	2.19	0.44
1:D:3265:ASP:O	1:D:3266:SER:O	2.34	0.44
1:D:3087:ARG:HG3	1:D:3315:GLN:OE1	2.16	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:D:3252:TYR:CZ	1:D:3255:HIS:HA	2.52	0.44
1:D:3210:ILE:HD12	1:D:3260:LEU:CD1	2.48	0.44
1:D:3106:HIS:ND1	1:D:3116:GLN:HB3	2.32	0.44
1:F:5137:ASN:HB2	1:F:5237:HIS:CE1	2.52	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:B:1233:TYR:N	1:B:1233:TYR:CD1	2.85	0.44
1:B:1153:VAL:O	1:B:1154:GLU:HB3	2.18	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: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:1228:LYS:N	1:B:1228:LYS:CD	2.67	0.44
1:C:2298:MET:HE3	1:C:2301:LYS:CB	2.37	0.44
1:B:1335:LEU:HA	1:B:1336:PRO:HD3	1.89	0.44
1:E:4011:TYR:CA	1:E:4341:LEU:HD13	2.44	0.44
1:C:2010:LEU:HD13	1:C:2342:VAL:HG22	1.99	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:C:2119:ASP:HA	1:F:5355:LYS:NZ	2.32	0.44
1:C:2052:ARG:CZ	1:C:2266:SER:CB	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2047:THR:N	1:C:2334:ASN:HD21	2.12	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:F:5240:ALA:HB3	1:F:5305:GLU:HG2	1.99	0.44
1:D:3162:ARG:NH2	1:E:4081:LYS:HZ2	2.16	0.44
1:B:1117:ASP:OD1	1:B:1122:LEU:HB2	2.18	0.44
1:E:4102:ASN:ND2	1:E:4117:ASP:OD1	2.40	0.44
1:F:5236:LEU:HA	1:F:5306:TYR:OH	2.17	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:F:5164:TRP:O	1:F:5167:GLU:N	2.50	0.44
1:A:6003:GLU:O	1:A:6005:VAL:N	2.50	0.44
1:D:3111:TYR:CE2	1:D:3248:ILE:HA	2.52	0.44
1:E:4265:ASP:O	1:E:4266:SER:O	2.34	0.44
1:E:4147:LEU:O	1:E:4148:LYS:HB2	2.18	0.44
1:E:4139:LYS:HE3	1:E:4165:ASN:HA	1.99	0.44
1:F:5039:HIS:HA	1:F:5202:ILE:O	2.18	0.44
1:F:5052:ARG:HG2	1:F:5052:ARG:HH11	1.83	0.44
1:B:1046:TYR:HA	1:B:1334:ASN:OD1	2.17	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:3300:GLU:O	1:D:3304:LYS:HG3	2.17	0.44
1:D:3081:LYS:HZ1	1:F:5143:GLN:HE22	1.65	0.44
1:B:1150:GLN:HB2	1:B:1153:VAL:HG12	1.99	0.44
1:E:4003:GLU:O	1:E:4005:VAL:N	2.50	0.44
1:F:5150:GLN:HB3	1:F:5153:VAL:HG12	2.00	0.44
1:D:3168:TRP:CD1	1:D:3169:ASP:N	2.86	0.44
1:E:4317:TRP:HH2	1:E:4323:HIS:HD2	1.66	0.44
1:D:3025:THR:HG22	1:D:3026:PRO:N	2.32	0.44
1:E:4131:LYS:NZ	1:E:4173:LYS:HZ2	2.15	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:F:5162:ARG:O	1:F:5163:ASN:HB2	2.17	0.43
1:A:6314:VAL:CG1	1:A:6315:GLN:N	2.81	0.43
1:D:3162:ARG:CZ	1:E:4081:LYS:HZ2	2.31	0.43
1:A:6150:GLN:HB2	1:A:6153:VAL:HG12	2.00	0.43
1:B:1254:SER:OG	1:B:1255:HIS:N	2.51	0.43
1:F:5130:LEU:HB3	1:F:5172:ILE:HG12	2.00	0.43
1:E:4319:HIS:C	1:E:4321:THR:H	2.21	0.43
1:A:6233:TYR:CE2	1:A:6290:PHE:HE1	2.36	0.43
1:B:1004:GLN:O	1:B:1004:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5043:MET:HB3	1:F:5113:TRP:CZ2	2.53	0.43
1:C:2271:ARG:HG3	1:C:2271:ARG:NH1	2.33	0.43
1:C:2229:VAL:HG11	1:C:2257:PHE:CZ	2.53	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:C:2084:ASN:OD1	1:C:2091:LYS:HA	2.19	0.43
1:C:2028:ASP:OD2	1:C:2041:LYS:HB2	2.18	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:2037:ILE:CG2	1:C:2133:THR:HG21	2.35	0.43
1:F:5073:ILE:N	1:F:5073:ILE:CD1	2.82	0.43
1:E:4136:ARG:HH11	1:E:4136:ARG:CG	2.32	0.43
1:D:3234:LEU:HB2	1:D:3236:LEU:HD13	1.99	0.43
1:F:5102:ASN:HD22	1:F:5106:HIS:CE1	2.37	0.43
1:F:5088:GLU:O	1:F:5270:ILE:HD12	2.18	0.43
1:F:5052:ARG:HH12	1:F:5054:CYS:HB2	1.81	0.43
1:C:2019:VAL:HG13	1:F:5351:HIS:CG	2.52	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:C:2075:ALA:O	1:C:2079:SER:HB2	2.18	0.43
1:A:6069:ILE:HG23	1:A:6094:ALA:O	2.19	0.43
1:C:2110:GLN:HB2	1:C:2259:PRO:HG2	2.01	0.43
1:F:5037:ILE:CD1	1:F:5201:ASN:HB3	2.48	0.43
1:B:1052:ARG:HD3	1:B:1265:ASP:H	1.83	0.43
1:C:2218:LEU:HD23	1:C:2219:GLU:N	2.33	0.43
1:E:4076:THR:HG22	1:E:4080:GLN:NE2	2.33	0.43
1:B:1152:PHE:CZ	1:B:1288:VAL:HB	2.53	0.43
1:E:4143:GLN:HG2	1:E:4164:TRP:CE3	2.54	0.43
1:B:1082:LYS:CA	1:B:1082:LYS:HE3	2.48	0.43
1:C:2334:ASN:ND2	1:C:2334:ASN:C	2.71	0.43
1:F:5161:THR:HG22	1:F:5162:ARG:HE	1.82	0.43
1:A:6143:GLN:HG2	1:A:6164:TRP:CE3	2.54	0.43
1:E:4151:GLU:HB3	1:E:4296:ASN:HD21	1.84	0.43
1:A:6161:THR:O	1:A:6162:ARG:HB3	2.19	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:C:2109:SER:HG	1:C:2113:TRP:HZ3	1.67	0.43
1:D:3150:GLN:CG	1:D:3151:GLU:H	2.31	0.43
1:E:4218:LEU:HD23	1:E:4219:GLU:N	2.28	0.43
1:C:2006:LEU:HG	1:C:2345:TYR:OH	2.18	0.43
1:A:6171:LEU:HD22	1:A:6174:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3196:ILE:HD12	1:D:3233:TYR:CZ	2.53	0.43
1:A:6040:PHE:O	1:A:6204:ARG:NH2	2.47	0.43
1:F:5276:VAL:HG21	1:F:5325:ILE:HG21	2.01	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:C:2012:LEU:HD23	1:C:2012:LEU:HA	1.86	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:D:3133:THR:HG22	1:D:3134:ASP:N	2.33	0.42
1:C:2050:MET:HG2	1:C:2261:VAL:HG21	2.00	0.42
1:E:4317:TRP:N	1:E:4317:TRP:CD2	2.87	0.42
1:D:3059:GLN:O	1:D:3063:ILE:HG13	2.19	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:D:3168:TRP:CD1	1:D:3168:TRP:C	2.92	0.42
1:B:1053:THR:C	1:B:1055:GLN:H	2.20	0.42
1:F:5100:ASP:HA	1:F:5186:LEU:HD12	2.00	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:C:2038:HIS:O	1:C:2202:ILE:HG23	2.19	0.42
1:B:1311:GLU:OE1	1:B:1326:ASN:ND2	2.52	0.42
1:F:5056:PHE:HD1	1:F:5064:ILE:HD11	1.83	0.42
1:B:1273:VAL:O	1:B:1273:VAL:HG13	2.19	0.42
1:B:1018:ALA:O	1:B:1022:ARG:HG3	2.18	0.42
1:F:5052:ARG:HD2	1:F:5266:SER:HB2	2.00	0.42
1:D:3154:GLU:C	1:D:3154:GLU:OE2	2.57	0.42
1:E:4293:ASP:HB2	1:E:4294:PRO:HD3	2.00	0.42
1:C:2319:HIS:C	1:C:2321:THR:H	2.22	0.42
1:E:4038:HIS:O	1:E:4202:ILE:HG23	2.20	0.42
1:A:6098:ASN:ND2	1:A:6098:ASN:N	2.67	0.42
1:D:3014:ASN:ND2	1:D:3017:LYS:HB2	2.33	0.42
1:E:4139:LYS:CE	1:E:4165:ASN:HA	2.49	0.42
1:B:1162:ARG:CB	1:B:1162:ARG:HH11	2.10	0.42
1:F:5317:TRP:O	1:F:5319:HIS:CD2	2.72	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:F:5106:HIS:O	1:F:5110:GLN:HG3	2.18	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:A:6048:LEU:C	1:A:6048:LEU:HD12	2.40	0.42
1:F:5032:PRO:HG3	1:F:5036:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3312:ILE:CD1	1:D:3327:ALA:HB3	2.49	0.42
1:A:6234:LEU:HB2	1:A:6236:LEU:CD1	2.46	0.42
1:D:3052:ARG:NH1	1:D:3265:ASP:H	2.11	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:F:5260:LEU:HD23	1:F:5260:LEU:HA	1.83	0.42
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:E:4204:ARG:HG2	1:E:4238:TRP:CE2	2.54	0.42
1:B:1316:GLY:HA2	1:B:1323:HIS:NE2	2.35	0.42
1:B:1236:LEU:HD21	1:B:1291:LEU:HD23	2.01	0.42
1:A:6137:ASN:HB2	1:A:6237:HIS:NE2	2.34	0.42
1:F:5141:ARG:HB3	1:F:5290:PHE:HB3	2.01	0.42
1:A:6204:ARG:HD3	1:A:6238:TRP:CD2	2.54	0.42
1:D:3353:TYR:O	1:D:3356:TRP:HB3	2.19	0.42
1:C:2200:CYS:HB3	1:C:2207:ILE:HG13	2.00	0.42
1:F:5048:LEU:HD12	1:F:5049:GLU:N	2.35	0.42
1:B:1355:LYS:HE2	1:B:1355:LYS:HB3	1.75	0.42
1:F:5238:TRP:HB2	1:F:5243:CYS:SG	2.60	0.42
1:B:1298:MET:HA	1:B:1301:LYS:NZ	2.34	0.42
1:A:6179:THR:HG22	1:A:6180:PRO:O	2.20	0.42
1:F:5143:GLN:O	1:F:5147:LEU:HG	2.19	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: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:C:2042:THR:HA	1:C:2045:ARG:HH11	1.85	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: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:F:5067:ALA:C	1:F:5096:LYS:HZ3	2.23	0.42
1:E:4253:ASP:OD1	1:E:4254:SER:N	2.52	0.42
1:C:2090:ARG:NH2	1:C:2265:ASP:O	2.53	0.42
1:C:2069:ILE:HG12	1:C:2093:VAL:CG2	2.50	0.42
1:E:4025:THR:HB	1:E:4026:PRO:HD3	2.00	0.42
1:E:4011:TYR:CD1	1:E:4011:TYR:C	2.92	0.42
1:E:4131:LYS:NZ	1:E:4173:LYS:HZ1	2.18	0.42
1:E:4120:LEU:HD22	1:E:4123:ARG:HG2	2.01	0.42
1:C:2293:ASP:O	1:C:2297:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4270:ILE:HD12	1:E:4310:ILE:HD11	2.01	0.42
1:A:6319:HIS:C	1:A:6321:THR:H	2.23	0.42
1:D:3336:PRO:HD2	1:D:3339:ILE:HG13	2.02	0.42
1:E:4350:GLN:O	1:E:4354:LYS:HG3	2.20	0.41
1:D:3317:TRP:O	1:D:3319:HIS:CD2	2.73	0.41
1:D:3141:ARG:HH21	1:D:3236:LEU:HD23	1.85	0.41
1:A:6043:MET:HG2	1:A:6046:TYR:CE1	2.55	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:F:5160:ASP:CG	1:F:5161:THR:N	2.71	0.41
1:F:5051:PHE:HA	1:F:5264:LYS:HE3	2.01	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:C:2060:PHE:HA	1:C:2063:ILE:CD1	2.50	0.41
1:B:1216:ARG:O	1:B:1216:ARG:HG2	2.18	0.41
1:E:4053:THR:OG1	1:E:4065:HIS:NE2	2.52	0.41
1:B:1083:LEU:HD13	1:B:1260:LEU:HD13	2.02	0.41
1:D:3072:ASN:N	1:D:3072:ASN:OD1	2.44	0.41
1:B:1215:LEU:O	1:B:1218:LEU:HB2	2.19	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:C:2032:PRO:HG3	1:C:2036:ILE:HG23	2.02	0.41
1:A:6126:LEU:HD21	1:A:6195:HIS:CD2	2.55	0.41
1:B:1252:TYR:CZ	1:B:1255:HIS:HA	2.56	0.41
1:F:5127:PHE:HE1	1:F:5172:ILE:O	2.03	0.41
1:E:4053:THR:C	1:E:4055:GLN:H	2.23	0.41
1:A:6216:ARG:HG2	1:A:6216:ARG:O	2.20	0.41
1:F:5292:THR:HG22	1:F:5293:ASP:N	2.36	0.41
1:A:6179:THR:HA	1:A:6180:PRO:HD3	1.91	0.41
1:F:5249:VAL:C	1:F:5250:LEU:HD23	2.40	0.41
1:A:6232:ILE:CG1	1:A:6286:LEU:HD23	2.50	0.41
1:D:3120:LEU:HB2	1:D:3124:LYS:HE2	2.02	0.41
1:D:3084:ASN:OD1	1:D:3091:LYS:HA	2.19	0.41
1:D:3039:HIS:HA	1:D:3202:ILE:O	2.20	0.41
1:C:2112:MET:O	1:C:2335:LEU:HD21	2.21	0.41
1:D:3051:PHE:HA	1:D:3264:LYS:HE3	2.03	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:A:6353:TYR:O	1:A:6357:GLN:HG3	2.21	0.41
1:C:2053:THR:C	1:C:2055:GLN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6052:ARG:CZ	1:A:6266:SER:HB2	2.51	0.41
1:A:6233:TYR:CD1	1:A:6233:TYR:N	2.89	0.41
1:F:5152:PHE:CD2	1:F:5299:LYS:HD2	2.56	0.41
1:C:2033:THR:O	1:C:2033:THR:CG2	2.67	0.41
1:B:1163:ASN:ND2	1:B:1163:ASN:O	2.53	0.41
1:D:3147:LEU:HD21	1:D:3164:TRP:CZ2	2.53	0.41
1:A:6090:ARG:HH22	1:A:6271:ARG:CZ	2.33	0.41
1:C:2040:PHE:HB2	1:C:2044:HIS:CD2	2.55	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:F:5359:ASN:O	1:F:5362:GLN:HG3	2.20	0.41
1:A:6057:CYS:SG	1:A:6059:GLN:OE1	2.79	0.41
1:F:5236:LEU:HD11	1:F:5291:LEU:HD23	2.03	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:A:6038:HIS:O	1:A:6202:ILE:HG23	2.21	0.41
1:B:1269:GLU:H	1:B:1269:GLU:CD	2.24	0.41
1:D:3090:ARG:NH2	1:D:3265:ASP:O	2.53	0.41
1:F:5086:CYS:HB3	1:F:5089:VAL:HG22	2.03	0.41
1:A:6293:ASP:N	1:A:6294:PRO:CD	2.84	0.41
1:A:6081:LYS:HZ2	1:A:6278:ARG:HH12	1.67	0.41
1:D:3006:LEU:HD12	1:D:3063:ILE:CG2	2.51	0.41
1:C:2137:ASN:CB	1:C:2237:HIS:NE2	2.83	0.41
1:E:4070:ASP:CG	1:E:4073:ILE:HD13	2.40	0.41
1:C:2037:ILE:HD11	1:C:2201:ASN:HB3	2.03	0.41
1:B:1074:GLN:HB3	1:B:1074:GLN:HE21	1.53	0.41
1:D:3074:GLN:OE1	1:D:3093:VAL:HA	2.21	0.41
1:D:3263:LEU:HA	1:D:3263:LEU:HD23	1.66	0.41
1:A:6082:LYS:HE3	1:A:6082:LYS:CA	2.42	0.41
1:E:4133:THR:CG2	1:E:4134:ASP:N	2.84	0.41
1:B:1289:HIS:H	1:B:1289:HIS:CD2	2.38	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:E:4145:GLU:CD	1:E:4290:PHE:H	2.23	0.41
1:C:2293:ASP:CB	1:C:2294:PRO:HD3	2.49	0.41
1:E:4141:ARG:NH2	1:E:4292:THR:HG23	2.36	0.41
1:E:4280:ARG:O	1:E:4280:ARG:HG3	2.21	0.41
1:B:1025:THR:HG22	1:B:1026:PRO:CD	2.51	0.41
1:A:6063:ILE:HD11	1:A:6356:TRP:CH2	2.56	0.41
1:F:5111:TYR:CD2	1:F:5248:ILE:HG23	2.56	0.41
1:C:2086:CYS:HB3	1:C:2089:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5006:LEU:HA	1:F:5006:LEU:HD23	1.97	0.41
1:F:5030:PHE:O	1:F:5032:PRO:HD2	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: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:E:4200:CYS:HB2	1:E:4205:ARG:O	2.21	0.41
1:C:2194:ILE:O	1:C:2198:VAL:HG23	2.21	0.41
1:C:2069:ILE:HG23	1:C:2094:ALA:O	2.21	0.40
1:F:5141:ARG:NH1	1:F:5295:GLU:OE1	2.41	0.40
1:F:5162:ARG:HG3	1:F:5162:ARG:NH1	2.36	0.40
1:E:4262:THR:HG22	1:E:4263:LEU:N	2.36	0.40
1:E:4218:LEU:CD2	1:E:4219:GLU:N	2.84	0.40
1:C:2010:LEU:HD23	1:C:2345:TYR:CD1	2.56	0.40
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: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:F:5159:TYR:N	1:F:5159:TYR:CD1	2.89	0.40
1:B:1300:GLU:CD	1:B:1304:LYS:HE3	2.41	0.40
1:B:1082:LYS:NZ	1:B:1213:LYS:HZ1	2.19	0.40
1:A:6082:LYS:HD2	1:A:6213:LYS:CE	2.44	0.40
1:F:5346:PHE:HA	1:F:5349:VAL:CG2	2.51	0.40
1:E:4185:GLY:C	1:E:4186:LEU:HD22	2.41	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:F:5302:LEU:HD23	1:F:5302:LEU:HA	1.95	0.40
1:F:5062:GLU:OE2	1:F:5062:GLU:C	2.59	0.40
1:C:2108:THR:CG2	1:C:2122:LEU:HD21	2.52	0.40
1:F:5123:ARG:NH2	1:F:5176:SER:O	2.54	0.40
1:D:3314:VAL:CG1	1:D:3315:GLN:NE2	2.84	0.40
1:B:1003:GLU:HB2	1:B:1004:GLN:HE22	1.82	0.40
1:E:4006:LEU:HA	1:E:4007:PRO:HD2	1.84	0.40
1:A:6066:LYS:NZ	1:A:6071:ARG:HH22	2.19	0.40
1:D:3107:ALA:O	1:D:3259:PRO:HG3	2.22	0.40
1:C:2095:LEU:O	1:C:2258:VAL:HG13	2.21	0.40
1:E:4317:TRP:N	1:E:4317:TRP:CE3	2.89	0.40
1:A:6254:SER:OG	1:A:6255:HIS:N	2.53	0.40
1:D:3081:LYS:CE	1:F:5143:GLN:HE22	2.35	0.40
1:D:3077:LEU:HD11	1:D:3210:ILE:O	2.20	0.40
1:C:2273:VAL:O	1:C:2275:LEU:HD23	2.21	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:F:5153:VAL:O	1:F:5154:GLU:HB3	2.20	0.40
1:C:2153:VAL:O	1:C:2154:GLU:CB	2.69	0.40
1:D:3016:ARG:HG2	1:D:3016:ARG:HH11	1.85	0.40
1:E:4215:LEU:HB3	1:E:4218:LEU:HB2	2.04	0.40
1:C:2249:VAL:HG12	1:C:2260:LEU:HB2	2.03	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%)	4	5
1	B	346/390 (89%)	298 (86%)	33 (10%)	15 (4%)	3	4
1	C	346/390 (89%)	294 (85%)	39 (11%)	13 (4%)	4	5
1	D	346/390 (89%)	298 (86%)	34 (10%)	14 (4%)	4	4
1	E	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	4	6
1	F	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	4	6
All	All	2076/2340 (89%)	1779 (86%)	218 (10%)	79 (4%)	4	5

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 (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/354 (92%)	291 (90%)	34 (10%)	8	16
1	B	325/354 (92%)	289 (89%)	36 (11%)	8	14
1	C	325/354 (92%)	296 (91%)	29 (9%)	12	23
1	D	325/354 (92%)	300 (92%)	25 (8%)	16	30
1	E	325/354 (92%)	294 (90%)	31 (10%)	11	20
1	F	325/354 (92%)	294 (90%)	31 (10%)	11	20
All	All	1950/2124 (92%)	1764 (90%)	186 (10%)	11	20

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	352/390 (90%)	1.42	75 (21%)	1	1	20, 62, 150, 195	0
1	B	352/390 (90%)	1.23	71 (20%)	1	1	19, 50, 142, 179	0
1	C	352/390 (90%)	1.75	97 (27%)	1	0	30, 66, 148, 185	0
1	D	352/390 (90%)	1.49	84 (23%)	1	1	23, 59, 145, 188	0
1	E	352/390 (90%)	1.29	75 (21%)	1	1	19, 52, 145, 175	0
1	F	352/390 (90%)	1.54	87 (24%)	1	1	28, 67, 146, 194	0
All	All	2112/2340 (90%)	1.45	489 (23%)	1	1	19, 59, 146, 195	0

All (489) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4153	VAL	22.0
1	C	2318	ASP	20.7
1	A	6153	VAL	16.7
1	F	5153	VAL	16.6
1	A	6159	TYR	15.9
1	A	6150	GLN	15.6
1	D	3318	ASP	14.7
1	C	2218	LEU	13.9
1	B	1220	SER	12.9
1	D	3153	VAL	12.9
1	F	5159	TYR	12.8
1	A	6318	ASP	12.4
1	B	1149	SER	12.2
1	D	3218	LEU	11.6
1	C	2159	TYR	11.5
1	C	2150	GLN	10.7
1	E	4154	GLU	10.6
1	A	6003	GLU	10.6
1	F	5184	SER	10.1

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Mol	Chain	Res	Type	RSRZ
1	D	3152	PHE	9.9
1	C	2220	SER	9.8
1	C	2221	GLY	9.7
1	D	3360	SER	9.2
1	D	3362	GLN	9.1
1	C	2153	VAL	9.1
1	C	2219	GLU	9.0
1	D	3226	PRO	8.9
1	E	4360	SER	8.9
1	D	3217	SER	8.8
1	E	4318	ASP	8.8
1	E	4159	TYR	8.7
1	E	4182	ALA	8.4
1	E	4317	TRP	8.3
1	C	2182	ALA	8.3
1	E	4059	GLN	8.2
1	C	2185	GLY	8.1
1	B	1182	ALA	8.1
1	D	3149	SER	8.1
1	C	2003	GLU	8.1
1	F	5318	ASP	8.1
1	E	4218	LEU	8.1
1	A	6185	GLY	7.8
1	C	2226	PRO	7.8
1	A	6219	GLU	7.7
1	F	5182	ALA	7.7
1	B	1183	ARG	7.7
1	A	6182	ALA	7.7
1	E	4362	GLN	7.6
1	D	3185	GLY	7.6
1	F	5220	SER	7.6
1	E	4003	GLU	7.5
1	B	1154	GLU	7.4
1	F	5152	PHE	7.4
1	F	5226	PRO	7.3
1	C	2152	PHE	7.3
1	F	5003	GLU	7.3
1	A	6220	SER	7.2
1	A	6154	GLU	7.2
1	E	4183	ARG	7.0
1	B	1152	PHE	7.0
1	B	1219	GLU	7.0

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Mol	Chain	Res	Type	RSRZ
1	F	5154	GLU	7.0
1	D	3183	ARG	7.0
1	B	1033	THR	6.9
1	C	2217	SER	6.9
1	B	1218	LEU	6.9
1	D	3034	ASN	6.9
1	C	2361	GLU	6.8
1	D	3359	ASN	6.7
1	E	4361	GLU	6.7
1	E	4181	MET	6.7
1	D	3221	GLY	6.7
1	C	2162	ARG	6.6
1	C	2183	ARG	6.6
1	B	1150	GLN	6.5
1	B	1318	ASP	6.3
1	B	1226	PRO	6.3
1	E	4221	GLY	6.3
1	D	3219	GLU	6.2
1	E	4150	GLN	6.2
1	D	3179	THR	6.2
1	F	5362	GLN	6.2
1	B	1361	GLU	6.1
1	F	5161	THR	6.0
1	D	3317	TRP	6.0
1	A	6183	ARG	6.0
1	B	1221	GLY	5.9
1	C	2362	GLN	5.9
1	F	5149	SER	5.9
1	C	2181	MET	5.8
1	E	4220	SER	5.8
1	B	1267	GLY	5.7
1	A	6184	SER	5.7
1	D	3184	SER	5.7
1	F	5218	LEU	5.7
1	E	4162	ARG	5.6
1	A	6152	PHE	5.6
1	B	1153	VAL	5.6
1	A	6186	LEU	5.6
1	C	2317	TRP	5.6
1	E	4184	SER	5.6
1	F	5181	MET	5.5
1	B	1316	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	3159	TYR	5.5
1	C	2186	LEU	5.5
1	B	1159	TYR	5.4
1	D	3150	GLN	5.4
1	D	3003	GLU	5.4
1	C	2149	SER	5.3
1	F	5360	SER	5.3
1	B	1362	GLN	5.3
1	C	2036	ILE	5.3
1	C	2058	PRO	5.3
1	F	5207	ILE	5.3
1	A	6149	SER	5.3
1	F	5183	ARG	5.2
1	C	2154	GLU	5.2
1	C	2280	ARG	5.2
1	E	4359	ASN	5.2
1	C	2184	SER	5.2
1	C	2032	PRO	5.2
1	B	1359	ASN	5.2
1	C	2054	CYS	5.1
1	A	6218	LEU	5.1
1	A	6221	GLY	5.0
1	D	3036	ILE	5.0
1	D	3186	LEU	5.0
1	D	3220	SER	5.0
1	F	5196	ILE	4.9
1	D	3361	GLU	4.9
1	E	4151	GLU	4.9
1	F	5005	VAL	4.8
1	D	3162	ARG	4.8
1	A	6268	PRO	4.8
1	A	6161	THR	4.8
1	E	4226	PRO	4.7
1	B	1216	ARG	4.7
1	E	4217	SER	4.7
1	B	1161	THR	4.7
1	C	2319	HIS	4.7
1	C	2360	SER	4.7
1	A	6207	ILE	4.7
1	A	6361	GLU	4.6
1	A	6181	MET	4.6
1	A	6226	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	3282	ARG	4.6
1	D	3319	HIS	4.6
1	E	4356	TRP	4.6
1	F	5185	GLY	4.5
1	B	1186	LEU	4.5
1	E	4185	GLY	4.5
1	E	4152	PHE	4.5
1	F	5221	GLY	4.5
1	F	5361	GLU	4.4
1	B	1282	ARG	4.4
1	D	3281	GLY	4.4
1	B	1279	ASP	4.4
1	A	6163	ASN	4.4
1	E	4161	THR	4.4
1	F	5165	ASN	4.4
1	D	3154	GLU	4.3
1	C	2207	ILE	4.3
1	B	1319	HIS	4.3
1	E	4034	ASN	4.3
1	E	4227	LEU	4.3
1	A	6266	SER	4.3
1	D	3057	CYS	4.3
1	D	3058	PRO	4.3
1	B	1184	SER	4.3
1	D	3180	PRO	4.2
1	B	1217	SER	4.2
1	B	1164	TRP	4.2
1	C	2356	TRP	4.2
1	A	6208	ILE	4.2
1	D	3182	ALA	4.2
1	E	4033	THR	4.2
1	C	2199	LEU	4.1
1	B	1003	GLU	4.1
1	B	1360	SER	4.1
1	A	6360	SER	4.1
1	B	1280	ARG	4.1
1	D	3356	TRP	4.1
1	E	4219	GLU	4.1
1	C	2353	TYR	4.1
1	C	2282	ARG	4.0
1	A	6270	ILE	4.0
1	F	5268	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	3181	MET	4.0
1	C	2198	VAL	4.0
1	D	3033	THR	4.0
1	C	2033	THR	3.9
1	A	6200	CYS	3.9
1	E	4254	SER	3.9
1	A	6199	LEU	3.9
1	A	6325	ILE	3.9
1	A	6280	ARG	3.8
1	D	3199	LEU	3.8
1	F	5217	SER	3.8
1	C	2359	ASN	3.8
1	C	2215	LEU	3.8
1	F	5250	LEU	3.8
1	C	2216	ARG	3.8
1	A	6005	VAL	3.8
1	C	2209	VAL	3.8
1	C	2059	GLN	3.8
1	F	5316	GLY	3.8
1	C	2264	LYS	3.8
1	E	4164	TRP	3.8
1	F	5298	MET	3.7
1	A	6164	TRP	3.7
1	F	5150	GLN	3.7
1	F	5241	GLN	3.7
1	F	5029	ILE	3.7
1	E	4267	GLY	3.7
1	F	5163	ASN	3.7
1	C	2197	PHE	3.7
1	D	3216	ARG	3.7
1	B	1180	PRO	3.7
1	C	2227	LEU	3.6
1	C	2165	ASN	3.6
1	C	2255	HIS	3.6
1	A	6216	ARG	3.6
1	F	5282	ARG	3.6
1	D	3209	VAL	3.6
1	F	5186	LEU	3.5
1	C	2241	GLN	3.5
1	F	5219	GLU	3.5
1	F	5358	GLU	3.5
1	A	6033	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1181	MET	3.5
1	B	1208	ILE	3.5
1	A	6162	ARG	3.5
1	C	2196	ILE	3.5
1	B	1200	CYS	3.5
1	C	2030	PHE	3.4
1	D	3104	LEU	3.4
1	F	5160	ASP	3.4
1	E	4207	ILE	3.4
1	D	3004	GLN	3.4
1	B	1317	TRP	3.4
1	D	3266	SER	3.4
1	F	5027	GLU	3.4
1	D	3059	GLN	3.4
1	D	3061	ARG	3.4
1	B	1209	VAL	3.3
1	D	3108	THR	3.3
1	F	5033	THR	3.3
1	F	5164	TRP	3.3
1	F	5004	GLN	3.3
1	E	4198	VAL	3.3
1	C	2266	SER	3.3
1	D	3250	LEU	3.3
1	D	3198	VAL	3.3
1	E	4149	SER	3.3
1	C	2163	ASN	3.3
1	E	4165	ASN	3.3
1	B	1196	ILE	3.2
1	A	6317	TRP	3.2
1	C	2108	THR	3.2
1	F	5206	PRO	3.2
1	B	1160	ASP	3.2
1	B	1281	GLY	3.2
1	A	6362	GLN	3.2
1	E	4186	LEU	3.2
1	E	4255	HIS	3.2
1	C	2164	TRP	3.2
1	C	2200	CYS	3.1
1	A	6160	ASP	3.1
1	F	5198	VAL	3.1
1	C	2172	ILE	3.1
1	F	5233	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1266	SER	3.1
1	C	2249	VAL	3.1
1	F	5266	SER	3.0
1	E	4005	VAL	3.0
1	D	3040	PHE	3.0
1	F	5180	PRO	3.0
1	F	5249	VAL	3.0
1	F	5057	CYS	3.0
1	F	5354	LYS	3.0
1	F	5199	LEU	3.0
1	E	4315	GLN	2.9
1	A	6233	TYR	2.9
1	A	6235	PRO	2.9
1	D	3032	PRO	2.9
1	E	4166	ASP	2.9
1	D	3233	TYR	2.9
1	A	6054	CYS	2.9
1	D	3054	CYS	2.9
1	E	4233	TYR	2.9
1	C	2279	ASP	2.9
1	C	2034	ASN	2.9
1	D	3248	ILE	2.9
1	C	2176	SER	2.8
1	C	2250	LEU	2.8
1	E	4163	ASN	2.8
1	F	5081	LYS	2.8
1	B	1136	ARG	2.8
1	F	5046	TYR	2.8
1	C	2323	HIS	2.8
1	D	3323	HIS	2.8
1	F	5301	LYS	2.8
1	B	1185	GLY	2.8
1	C	2035	GLY	2.8
1	F	5329	LYS	2.8
1	D	3207	ILE	2.8
1	A	6249	VAL	2.8
1	B	1241	GLN	2.8
1	C	2004	GLN	2.8
1	D	3197	PHE	2.8
1	A	6255	HIS	2.8
1	D	3196	ILE	2.8
1	A	6234	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1298	MET	2.8
1	E	4134	ASP	2.8
1	D	3357	GLN	2.8
1	C	2316	GLY	2.8
1	C	2045	ARG	2.8
1	C	2008	GLN	2.7
1	F	5208	ILE	2.7
1	F	5209	VAL	2.7
1	A	6355	LYS	2.7
1	E	4035	GLY	2.7
1	B	1358	GLU	2.7
1	B	1207	ILE	2.7
1	B	1297	GLU	2.7
1	E	4199	LEU	2.7
1	A	6056	PHE	2.7
1	A	6136	ARG	2.7
1	E	4189	ASN	2.7
1	D	3234	LEU	2.7
1	A	6319	HIS	2.7
1	D	3254	SER	2.7
1	E	4266	SER	2.7
1	A	6126	LEU	2.6
1	D	3194	ILE	2.6
1	D	3200	CYS	2.6
1	A	6180	PRO	2.6
1	B	1283	PHE	2.6
1	B	1313	PRO	2.6
1	B	1107	ALA	2.6
1	F	5283	PHE	2.6
1	A	6297	GLU	2.6
1	B	1055	GLN	2.6
1	A	6250	LEU	2.6
1	B	1199	LEU	2.6
1	E	4265	ASP	2.6
1	B	1179	THR	2.6
1	F	5179	THR	2.6
1	C	2151	GLU	2.6
1	A	6209	VAL	2.5
1	C	2134	ASP	2.5
1	A	6241	GLN	2.5
1	F	5231	GLY	2.5
1	B	1250	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	3324	LEU	2.5
1	F	5335	LEU	2.5
1	C	2112	MET	2.5
1	C	2298	MET	2.5
1	B	1034	ASN	2.5
1	E	4268	PRO	2.5
1	D	3265	ASP	2.5
1	F	5255	HIS	2.5
1	F	5232	ILE	2.5
1	D	3055	GLN	2.5
1	F	5197	PHE	2.5
1	F	5324	LEU	2.5
1	D	3279	ASP	2.4
1	E	4249	VAL	2.4
1	F	5201	ASN	2.4
1	C	2314	VAL	2.4
1	C	2136	ARG	2.4
1	E	4209	VAL	2.4
1	A	6165	ASN	2.4
1	C	2132	GLU	2.4
1	A	6030	PHE	2.4
1	D	3267	GLY	2.4
1	A	6147	LEU	2.4
1	E	4215	LEU	2.4
1	C	2265	ASP	2.4
1	D	3358	GLU	2.4
1	D	3215	LEU	2.4
1	C	2180	PRO	2.4
1	F	5294	PRO	2.4
1	F	5313	PRO	2.4
1	B	1197	PHE	2.4
1	D	3052	ARG	2.4
1	A	6227	LEU	2.4
1	B	1036	ILE	2.4
1	A	6107	ALA	2.4
1	B	1323	HIS	2.4
1	C	2233	TYR	2.3
1	A	6151	GLU	2.3
1	A	6036	ILE	2.3
1	E	4213	LYS	2.3
1	F	5264	LYS	2.3
1	F	5327	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	4280	ARG	2.3
1	A	6166	ASP	2.3
1	F	5357	GLN	2.3
1	A	6358	GLU	2.3
1	C	2208	ILE	2.3
1	D	3325	ILE	2.3
1	E	4260	LEU	2.3
1	C	2055	GLN	2.3
1	D	3243	CYS	2.3
1	F	5111	TYR	2.3
1	D	3079	SER	2.3
1	B	1227	LEU	2.3
1	B	1061	ARG	2.3
1	B	1162	ARG	2.3
1	C	2052	ARG	2.3
1	C	2178	ASP	2.2
1	E	4250	LEU	2.2
1	D	3053	THR	2.2
1	E	4216	ARG	2.2
1	A	6034	ASN	2.2
1	D	3035	GLY	2.2
1	E	4087	ARG	2.2
1	F	5200	CYS	2.2
1	E	4108	THR	2.2
1	B	1131	LYS	2.2
1	E	4180	PRO	2.2
1	F	5259	PRO	2.2
1	A	6298	MET	2.2
1	C	2254	SER	2.2
1	F	5267	GLY	2.2
1	A	6055	GLN	2.2
1	D	3255	HIS	2.2
1	D	3280	ARG	2.2
1	A	6267	GLY	2.2
1	D	3249	VAL	2.2
1	F	5280	ARG	2.2
1	C	2308	MET	2.2
1	F	5355	LYS	2.2
1	F	5320	GLY	2.2
1	C	2040	PHE	2.2
1	E	4197	PHE	2.2
1	C	2042	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	2262	THR	2.2
1	D	3259	PRO	2.2
1	B	1249	VAL	2.2
1	F	5314	VAL	2.2
1	C	2232	ILE	2.2
1	A	6143	GLN	2.2
1	A	6206	PRO	2.2
1	B	1206	PRO	2.2
1	B	1198	VAL	2.1
1	C	2188	TYR	2.1
1	D	3105	MET	2.1
1	F	5011	TYR	2.1
1	D	3314	VAL	2.1
1	D	3327	ALA	2.1
1	B	1030	PHE	2.1
1	B	1255	HIS	2.1
1	F	5230	GLY	2.1
1	C	2194	ILE	2.1
1	B	1163	ASN	2.1
1	E	4337	LYS	2.1
1	F	5040	PHE	2.1
1	C	2161	THR	2.1
1	A	6198	VAL	2.1
1	C	2258	VAL	2.1
1	F	5265	ASP	2.1
1	C	2111	TYR	2.1
1	E	4201	ASN	2.1
1	A	6111	TYR	2.1
1	D	3111	TYR	2.1
1	F	5325	ILE	2.1
1	B	1147	LEU	2.1
1	E	4058	PRO	2.1
1	E	4281	GLY	2.1
1	A	6359	ASN	2.1
1	E	4314	VAL	2.1
1	C	2234	LEU	2.1
1	E	4006	LEU	2.1
1	F	5235	PRO	2.1
1	F	5128	SER	2.1
1	E	4262	THR	2.0
1	A	6035	GLY	2.0
1	C	2289	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	4234	LEU	2.0
1	F	5133	THR	2.0
1	E	4228	LYS	2.0
1	C	2259	PRO	2.0
1	E	4248	ILE	2.0
1	C	2113	TRP	2.0
1	D	3060	PHE	2.0
1	E	4264	LYS	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.