Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:05 pm BST

PDB ID	:	2CJR
Title	:	Crystal structure of oligomerization domain of SARS coronavirus nucleocapsid protein.
Authors	:	Chen, C.-Y.; Hsiao, C.-D.
Deposited on	:	2006-04-06
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

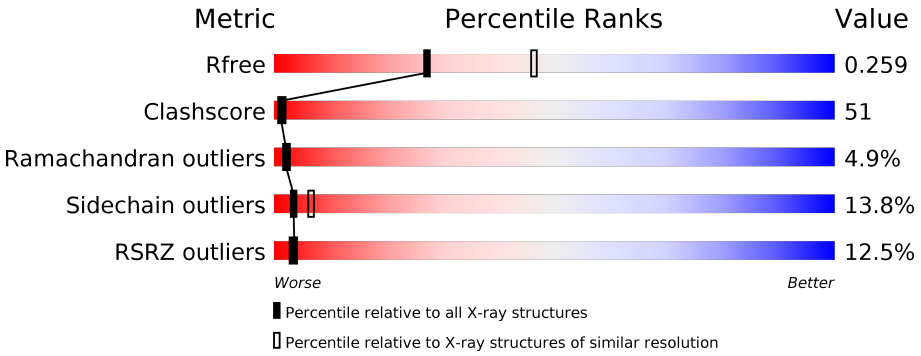
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	128	5% 49% 34% 7% 10%
1	B	128	7% 38% 40% 9% • 12%
1	C	128	2% 47% 34% 8% 12%
1	D	128	3% 43% 39% 8% 10%
1	E	128	20% 24% 46% 15% • 14%
1	F	128	17% 32% 44% 11% • 13%

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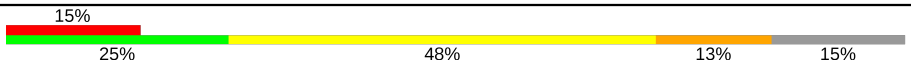
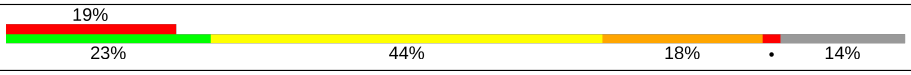
Mol	Chain	Length	Quality of chain
1	G	128	
1	H	128	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7973 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 NUCLEOCAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			912	577	165	168	2			
1	B	113	Total	C	N	O	S	0	0	0
			902	570	162	168	2			
1	C	113	Total	C	N	O	S	0	0	0
			898	568	162	166	2			
1	D	115	Total	C	N	O	S	0	0	0
			909	574	164	169	2			
1	E	110	Total	C	N	O	S	0	0	0
			880	558	159	161	2			
1	F	112	Total	C	N	O	S	0	0	1
			882	556	162	162	2			
1	G	109	Total	C	N	O	S	0	0	1
			867	547	159	159	2			
1	H	110	Total	C	N	O	S	0	0	0
			869	551	155	161	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		
2	B	130	Total	O	0	0
			130	130		
2	C	106	Total	O	0	0
			106	106		
2	D	113	Total	O	0	0
			113	113		
2	E	101	Total	O	0	0
			101	101		
2	F	95	Total	O	0	0
			95	95		

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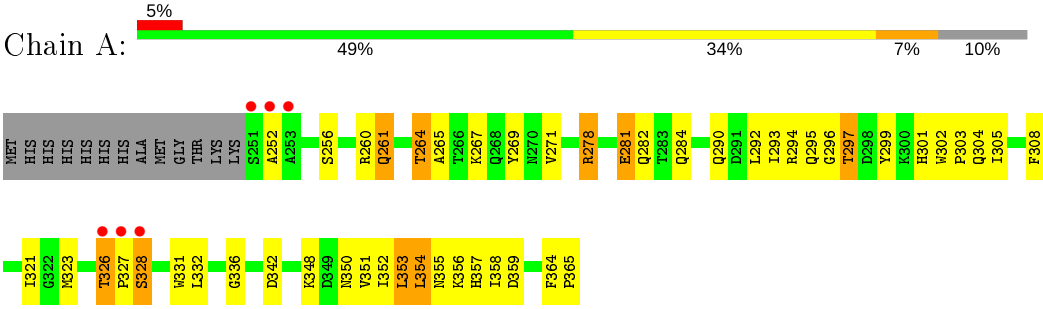
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	89	Total O 89 89	0	0
2	H	98	Total O 98 98	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

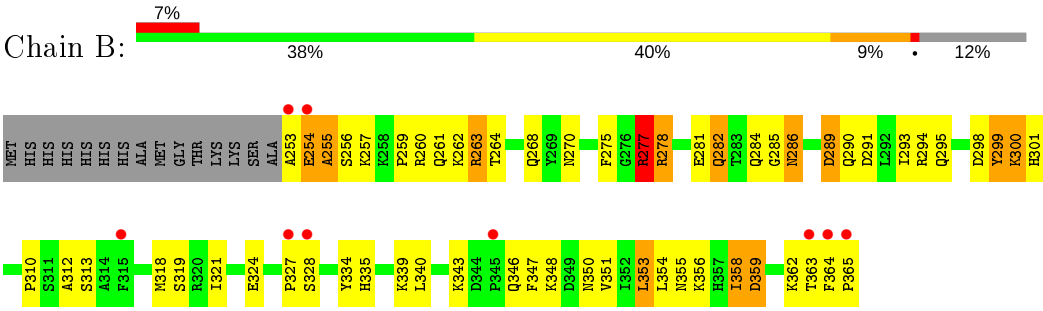
- Molecule 1: NUCLEOCAPSID PROTEIN

Chain A:



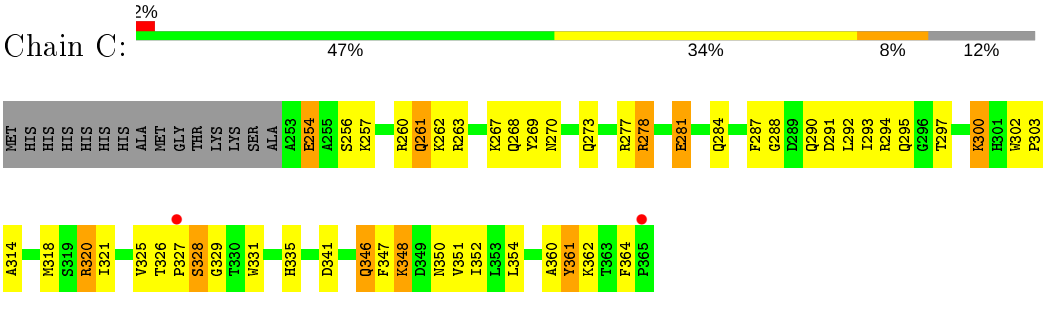
- Molecule 1: NUCLEOCAPSID PROTEIN

Chain B:



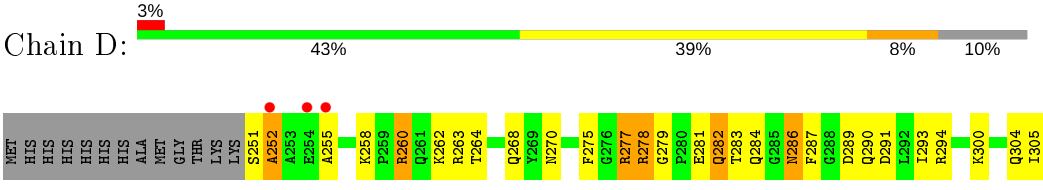
- Molecule 1: NUCLEOCAPSID PROTEIN

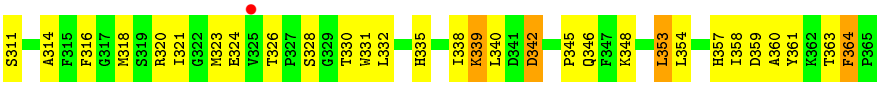
Chain C:



- Molecule 1: NUCLEOCAPSID PROTEIN

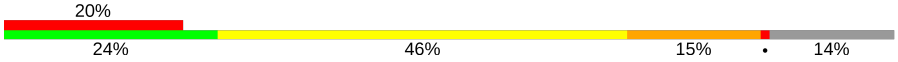
Chain D:

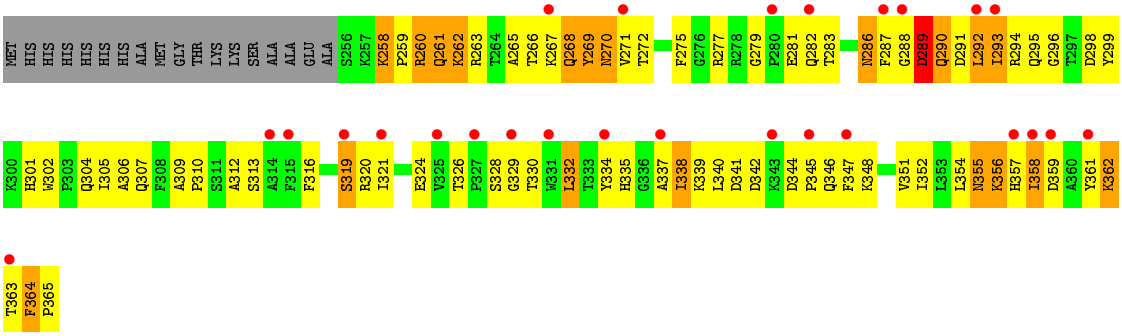




• Molecule 1: NUCLEOCAPSID PROTEIN

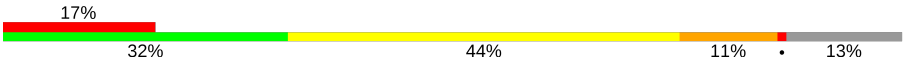
Chain E:

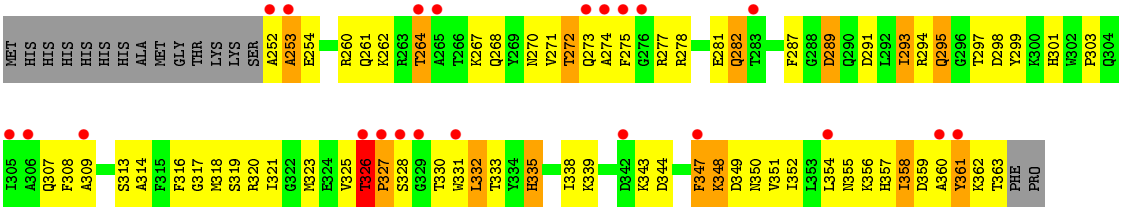




• Molecule 1: NUCLEOCAPSID PROTEIN

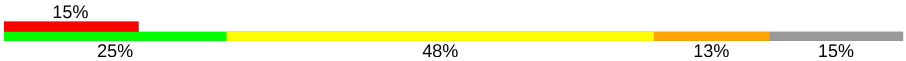
Chain F:

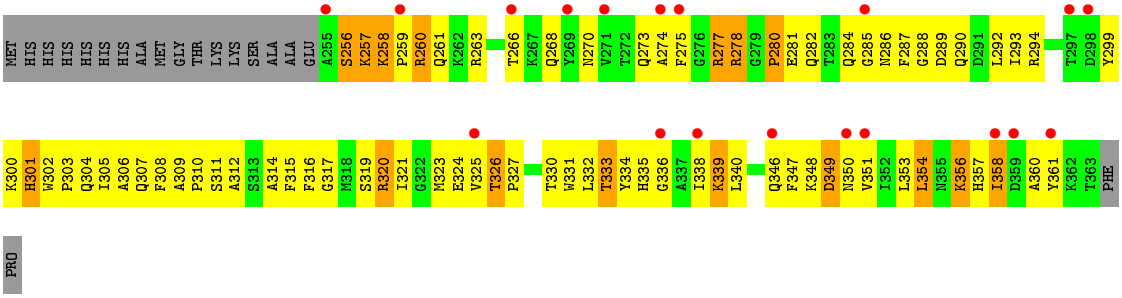




• Molecule 1: NUCLEOCAPSID PROTEIN

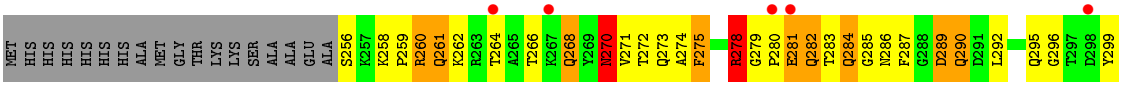
Chain G:

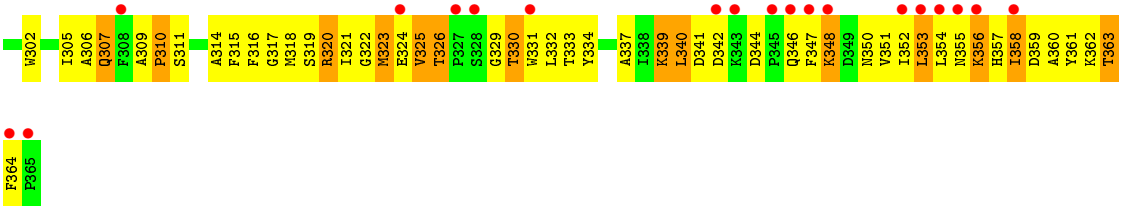




• Molecule 1: NUCLEOCAPSID PROTEIN

Chain H:




W302
I305
A306
Q307
F308
A309
P310
S311
A314
F315
F316
G317
M318
S319
R320
I321
G322
M323
E324
V325
T326
P327
S328
G329
T330
W331
L332
T333
Y334
A337
I338
K339
L340
D341
D342
K343
D344
P345
Q346
F347
K348
D349
N350
V351
I352
L353
L354
N355
K356
H357
I358
D359
A360
Y361
K362
T363
F364
P365

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	159.42Å 84.20Å 105.18Å 90.00° 131.18° 90.00°	Depositor
Resolution (Å)	29.80 – 2.50 29.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.0 (29.80-2.50) 96.9 (29.80-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.12 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.256 , 0.269 0.253 , 0.259	Depositor DCC
R_{free} test set	1800 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7973	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 48.21 % 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 8.8831e-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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.22	1/936 (0.1%)	1.03	0/1263
1	B	1.11	1/926 (0.1%)	1.13	4/1250 (0.3%)
1	C	1.11	0/922	1.02	1/1245 (0.1%)
1	D	1.24	1/933 (0.1%)	1.15	2/1260 (0.2%)
1	E	1.17	1/904 (0.1%)	1.12	1/1220 (0.1%)
1	F	1.06	0/904	1.03	1/1220 (0.1%)
1	G	1.11	2/889 (0.2%)	1.10	2/1199 (0.2%)
1	H	1.15	1/893 (0.1%)	1.13	3/1208 (0.2%)
All	All	1.15	7/7307 (0.1%)	1.09	14/9865 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	314	ALA	CA-CB	6.38	1.65	1.52
1	D	364	PHE	CE1-CZ	5.60	1.48	1.37
1	H	275	PHE	CE2-CZ	5.57	1.48	1.37
1	B	312	ALA	CA-CB	-5.38	1.41	1.52
1	E	269	TYR	CD2-CE2	5.27	1.47	1.39
1	A	271	VAL	CB-CG1	5.23	1.63	1.52
1	G	290	GLN	CB-CG	5.06	1.66	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	278	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	B	277	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	F	289	ASP	CB-CG-OD1	7.21	124.78	118.30
1	D	277	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	E	332	LEU	CA-CB-CG	6.12	129.37	115.30
1	G	354	LEU	CA-CB-CG	6.00	129.10	115.30
1	B	289	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	277	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	H	278	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	263	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	D	263	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	G	258	LYS	N-CA-C	-5.20	96.97	111.00
1	C	277	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	H	340	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	303	PRO	Peptide
1	G	326	THR	Peptide
1	H	310	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	912	0	884	54	0
1	B	902	0	870	80	0
1	C	898	0	866	79	0
1	D	909	0	876	73	0
1	E	880	0	852	134	1
1	F	882	0	859	111	0
1	G	867	0	847	119	0
1	H	869	0	828	152	1
2	A	122	0	0	19	0
2	B	130	0	0	27	1
2	C	106	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	113	0	0	21	1
2	E	101	0	0	38	0
2	F	95	0	0	15	0
2	G	89	0	0	28	0
2	H	98	0	0	35	0
All	All	7973	0	6882	710	2

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 51.

All (710) 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:D:305:ILE:HD13	1:D:354:LEU:HD23	1.21	1.20
1:C:335:HIS:HE1	1:D:282:GLN:NE2	1.39	1.20
2:F:2016:HOH:O	1:G:277:ARG:HG2	1.44	1.17
1:H:305:ILE:HG12	1:H:353:LEU:HD21	1.20	1.13
1:C:335:HIS:CE1	1:D:282:GLN:HE22	1.64	1.13
1:D:360:ALA:O	1:D:363:THR:HG22	1.48	1.11
1:E:258:LYS:HE2	1:E:263:ARG:HA	1.25	1.10
1:H:353:LEU:HD22	1:H:354:LEU:HD23	1.28	1.07
1:H:353:LEU:CD2	1:H:354:LEU:HD23	1.85	1.05
1:E:289:ASP:O	1:E:293:ILE:HG12	1.56	1.04
1:F:349:ASP:HA	1:F:352:ILE:HG22	1.39	1.01
2:G:2007:HOH:O	1:H:318:MET:HG2	1.60	1.01
1:G:260:ARG:HA	1:G:263:ARG:HD2	1.43	1.00
1:H:256:SER:N	2:H:2005:HOH:O	1.94	1.00
1:C:321:ILE:H	1:D:286:ASN:HD21	1.07	0.99
1:A:321:ILE:H	1:B:286:ASN:HD21	1.11	0.99
1:H:305:ILE:CG1	1:H:353:LEU:HD21	1.91	0.99
1:A:310:PRO:HD3	2:A:2067:HOH:O	1.61	0.99
1:C:326:THR:HG23	1:C:328:SER:H	1.22	0.98
1:G:308:PHE:HD2	2:H:2016:HOH:O	1.43	0.98
1:C:267:LYS:HB3	1:C:268:GLN:OE1	1.65	0.95
1:B:254:GLU:OE1	1:B:254:GLU:HA	1.65	0.94
1:G:311:SER:N	2:G:2048:HOH:O	1.99	0.94
1:H:286:ASN:ND2	1:H:359:ASP:OD2	2.01	0.94
1:E:287:PHE:HA	1:E:358:ILE:O	1.67	0.93
1:G:338:ILE:HG22	1:H:332:LEU:HB3	1.50	0.93
1:H:259:PRO:HD3	2:H:2008:HOH:O	1.66	0.93
1:G:331:TRP:HB3	1:H:337:ALA:HB1	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2007:HOH:O	1:H:318:MET:HA	1.69	0.93
1:E:286:ASN:HD21	1:F:321:ILE:H	0.94	0.92
1:E:259:PRO:HD2	1:E:262:LYS:HZ2	1.36	0.91
1:E:259:PRO:HD2	1:E:262:LYS:NZ	1.85	0.91
1:H:270:ASN:H	1:H:270:ASN:HD22	0.98	0.91
1:C:326:THR:HG22	1:C:329:GLY:O	1.71	0.90
1:C:335:HIS:CE1	1:D:282:GLN:NE2	2.28	0.90
1:A:314:ALA:HB2	2:B:2022:HOH:O	1.71	0.90
1:C:335:HIS:HE1	1:D:282:GLN:HE22	0.95	0.90
1:F:264:THR:HG22	1:F:297:THR:HG21	1.50	0.89
1:F:360:ALA:O	1:F:362:LYS:N	2.05	0.89
1:G:286:ASN:ND2	1:G:358:ILE:HG12	1.88	0.89
1:G:354:LEU:HD12	1:H:323:MET:SD	2.13	0.89
2:E:2067:HOH:O	1:F:339:LYS:HG3	1.72	0.89
1:H:264:THR:HB	2:H:2045:HOH:O	1.72	0.88
1:H:361:TYR:CE1	1:H:362:LYS:HG3	2.09	0.88
1:G:257:LYS:HA	1:G:263:ARG:NH2	1.89	0.87
1:A:310:PRO:HA	1:B:261:GLN:O	1.75	0.86
1:B:293:ILE:HG22	2:B:2045:HOH:O	1.75	0.86
1:H:353:LEU:HD22	1:H:354:LEU:CD2	2.05	0.86
1:E:282:GLN:HG2	2:E:2035:HOH:O	1.76	0.86
1:E:286:ASN:ND2	1:F:321:ILE:H	1.74	0.85
1:H:270:ASN:ND2	1:H:273:GLN:OE1	2.07	0.85
1:G:331:TRP:HE3	1:H:337:ALA:HB3	1.41	0.85
1:C:284:GLN:CB	2:C:2032:HOH:O	2.24	0.85
1:B:257:LYS:HA	2:B:2005:HOH:O	1.76	0.85
1:E:290:GLN:O	1:E:294:ARG:HD2	1.77	0.85
1:H:274:ALA:HB2	2:H:2024:HOH:O	1.76	0.85
1:B:294:ARG:HD3	2:C:2040:HOH:O	1.77	0.85
1:F:326:THR:CG2	1:F:331:TRP:CZ3	2.60	0.85
1:D:363:THR:HB	2:D:2112:HOH:O	1.77	0.85
1:C:284:GLN:CG	2:C:2032:HOH:O	2.25	0.84
1:G:320:ARG:HH22	1:H:280:PRO:HA	1.43	0.84
1:C:346:GLN:NE2	2:C:2088:HOH:O	2.10	0.83
1:E:319:SER:HB2	2:E:2059:HOH:O	1.77	0.83
1:G:304:GLN:O	1:G:307:GLN:HG2	1.78	0.83
1:E:286:ASN:O	1:E:359:ASP:HA	1.78	0.82
1:C:331:TRP:CZ3	1:D:339:LYS:HB2	2.14	0.82
1:D:318:MET:CE	1:D:338:ILE:HD11	2.09	0.82
1:B:300:LYS:NZ	1:B:300:LYS:HB3	1.94	0.82
1:F:348:LYS:HA	2:F:2073:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLN:HE21	1:B:350:ASN:HD22	1.28	0.82
1:D:305:ILE:HD13	1:D:354:LEU:CD2	2.06	0.81
1:C:326:THR:HG23	1:C:328:SER:N	1.95	0.81
1:G:266:THR:HG22	1:G:268:GLN:H	1.44	0.81
1:E:340:LEU:HD12	2:E:2086:HOH:O	1.81	0.81
1:D:326:THR:HG23	1:D:328:SER:H	1.46	0.81
1:E:361:TYR:HA	1:E:364:PHE:CE2	2.16	0.81
1:C:261:GLN:HB3	1:D:338:ILE:HD12	1.62	0.80
1:G:270:ASN:ND2	1:G:294:ARG:HA	1.95	0.80
1:G:358:ILE:HG13	1:H:321:ILE:O	1.80	0.80
1:F:314:ALA:O	1:F:318:MET:HG2	1.80	0.80
1:H:290:GLN:NE2	2:H:2041:HOH:O	2.14	0.80
2:G:2012:HOH:O	1:H:311:SER:HB2	1.82	0.80
1:H:305:ILE:HG12	1:H:353:LEU:CD2	2.08	0.80
1:C:327:PRO:O	2:C:2064:HOH:O	1.98	0.80
1:G:286:ASN:HD21	1:G:358:ILE:HG12	1.43	0.80
1:B:304:GLN:HE21	1:B:350:ASN:ND2	1.80	0.80
2:F:2015:HOH:O	1:G:273:GLN:HG3	1.81	0.80
2:E:2070:HOH:O	1:F:331:TRP:HB3	1.82	0.79
1:E:260:ARG:HH12	1:F:318:MET:HB3	1.45	0.79
1:B:278:ARG:HD2	1:B:293:ILE:HD11	1.63	0.79
1:E:351:VAL:HG12	1:F:323:MET:HE3	1.65	0.79
1:C:278:ARG:CD	1:C:293:ILE:HD11	2.12	0.79
1:D:260:ARG:O	2:D:2017:HOH:O	2.01	0.79
1:E:258:LYS:CE	1:E:263:ARG:HA	2.09	0.79
1:E:338:ILE:HG21	2:E:2051:HOH:O	1.83	0.79
1:A:353:LEU:HG	2:A:2110:HOH:O	1.82	0.79
1:H:270:ASN:ND2	1:H:270:ASN:H	1.79	0.78
1:E:319:SER:O	2:E:2062:HOH:O	2.02	0.78
1:H:309:ALA:HB3	2:H:2051:HOH:O	1.83	0.78
1:C:254:GLU:HA	2:C:2004:HOH:O	1.82	0.78
1:D:305:ILE:CD1	1:D:354:LEU:HD23	2.10	0.78
1:H:330:THR:HG21	2:H:2065:HOH:O	1.83	0.78
1:G:336:GLY:HA3	1:H:334:TYR:CZ	2.18	0.77
1:F:349:ASP:HA	1:F:352:ILE:CG2	2.12	0.77
1:B:281:GLU:HB2	1:B:284:GLN:HE21	1.50	0.76
1:F:282:GLN:NE2	1:F:282:GLN:HA	1.98	0.76
1:H:284:GLN:NE2	2:H:2037:HOH:O	2.19	0.76
1:B:300:LYS:HZ3	1:B:300:LYS:HB3	1.52	0.75
1:B:278:ARG:CD	1:B:293:ILE:HD11	2.15	0.75
1:C:284:GLN:HB2	2:C:2032:HOH:O	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:310:PRO:HB2	1:H:315:PHE:HB2	1.69	0.75
1:F:360:ALA:C	1:F:362:LYS:H	1.89	0.75
1:E:324:GLU:O	1:E:330:THR:OG1	2.04	0.75
1:E:316:PHE:HA	1:E:321:ILE:HD11	1.69	0.75
1:F:326:THR:HG21	1:F:331:TRP:CH2	2.23	0.74
1:H:279:GLY:N	1:H:284:GLN:HG2	2.02	0.74
1:A:261:GLN:HE21	1:A:261:GLN:H	1.36	0.74
1:B:362:LYS:HD2	2:B:2121:HOH:O	1.87	0.74
1:D:318:MET:HE3	1:D:338:ILE:HD11	1.69	0.74
1:E:361:TYR:HA	1:E:364:PHE:CD2	2.21	0.74
1:G:320:ARG:NH2	1:H:279:GLY:O	2.21	0.74
1:H:278:ARG:HA	1:H:285:GLY:O	1.88	0.73
1:F:267:LYS:HD3	1:F:298:ASP:HB2	1.70	0.73
1:E:260:ARG:NH1	1:F:318:MET:HB3	2.02	0.73
1:G:260:ARG:HD2	1:H:339:LYS:HE3	1.70	0.73
1:H:354:LEU:O	1:H:358:ILE:HG12	1.89	0.73
1:E:259:PRO:CD	1:E:262:LYS:NZ	2.52	0.73
1:H:321:ILE:HG23	1:H:332:LEU:HD11	1.71	0.72
1:E:319:SER:CB	2:E:2059:HOH:O	2.35	0.72
1:G:320:ARG:HB3	1:G:335:HIS:HB3	1.70	0.72
1:G:340:LEU:CB	1:G:347:PHE:HE1	2.02	0.72
1:H:351:VAL:HB	2:H:2087:HOH:O	1.88	0.72
1:A:296:GLY:N	2:A:2059:HOH:O	2.23	0.72
1:A:308:PHE:O	2:A:2067:HOH:O	2.07	0.72
1:C:290:GLN:O	1:C:294:ARG:HG2	1.88	0.72
1:C:278:ARG:HD3	1:C:293:ILE:HD11	1.70	0.72
1:G:338:ILE:HD11	1:H:261:GLN:HB3	1.71	0.72
1:H:361:TYR:HA	1:H:364:PHE:CD2	2.25	0.72
1:A:355:ASN:O	1:A:356:LYS:C	2.27	0.72
1:B:254:GLU:OE1	1:B:254:GLU:CA	2.38	0.72
1:B:343:LYS:CE	2:B:2092:HOH:O	2.38	0.72
1:D:287:PHE:HZ	1:D:305:ILE:HD12	1.53	0.72
1:C:351:VAL:HG23	1:D:323:MET:CE	2.20	0.71
1:G:338:ILE:CG2	1:H:332:LEU:HB3	2.20	0.71
1:F:355:ASN:O	2:F:2083:HOH:O	2.07	0.71
1:F:272:THR:CG2	1:F:273:GLN:N	2.53	0.71
1:H:324:GLU:O	1:H:330:THR:HA	1.90	0.71
2:E:2070:HOH:O	1:F:331:TRP:CD1	2.43	0.70
1:H:270:ASN:N	1:H:270:ASN:HD22	1.79	0.70
1:B:277:ARG:NH1	1:C:267:LYS:O	2.23	0.70
1:G:310:PRO:HG2	1:G:315:PHE:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:270:ASN:O	2:H:2024:HOH:O	2.09	0.70
1:G:331:TRP:HE3	1:H:337:ALA:CB	2.04	0.70
1:B:364:PHE:HB2	1:B:365:PRO:HD3	1.73	0.70
1:E:355:ASN:O	1:E:357:HIS:N	2.24	0.69
1:B:256:SER:O	2:B:2005:HOH:O	2.10	0.69
1:E:289:ASP:HB2	1:E:357:HIS:CE1	2.26	0.69
1:G:320:ARG:NH2	1:H:280:PRO:HA	2.08	0.69
1:D:255:ALA:HB1	2:D:2011:HOH:O	1.93	0.69
1:E:362:LYS:HE2	1:E:362:LYS:HA	1.74	0.69
1:F:326:THR:HG22	1:F:331:TRP:HZ3	1.58	0.68
1:C:288:GLY:HA2	1:C:292:LEU:HD23	1.75	0.68
1:H:353:LEU:HD23	1:H:354:LEU:N	2.08	0.68
1:G:331:TRP:CH2	2:H:2001:HOH:O	2.46	0.68
1:G:354:LEU:CD1	1:H:323:MET:SD	2.80	0.68
1:C:341:ASP:OD1	2:C:2079:HOH:O	2.10	0.68
1:D:308:PHE:CE1	1:D:340:LEU:HD22	2.29	0.68
1:H:354:LEU:O	1:H:358:ILE:CG1	2.42	0.68
1:A:260:ARG:NH2	2:A:2013:HOH:O	2.27	0.68
1:H:351:VAL:HG21	2:H:2010:HOH:O	1.93	0.68
1:H:306:ALA:O	2:H:2051:HOH:O	2.11	0.68
1:A:261:GLN:NE2	1:A:261:GLN:H	1.92	0.68
1:H:287:PHE:HE2	1:H:292:LEU:CD1	2.06	0.68
1:F:361:TYR:O	1:F:361:TYR:CD1	2.47	0.67
1:H:333:THR:O	2:H:2067:HOH:O	2.12	0.67
1:G:331:TRP:CE3	1:H:337:ALA:HB3	2.29	0.67
1:E:304:GLN:NE2	2:E:2047:HOH:O	2.15	0.67
1:G:327:PRO:O	2:G:2058:HOH:O	2.12	0.67
1:E:320:ARG:NH2	1:F:281:GLU:O	2.28	0.67
1:F:326:THR:HG22	1:F:331:TRP:CZ3	2.29	0.67
1:G:257:LYS:O	2:G:2005:HOH:O	2.12	0.67
1:E:290:GLN:O	1:E:293:ILE:HB	1.94	0.67
1:C:297:THR:HG22	1:C:302:TRP:NE1	2.10	0.66
1:G:308:PHE:CD2	2:H:2016:HOH:O	2.27	0.66
1:H:309:ALA:O	2:H:2053:HOH:O	2.13	0.66
1:F:272:THR:HG22	1:F:273:GLN:N	2.11	0.66
1:F:326:THR:HB	1:F:331:TRP:CZ3	2.31	0.66
1:H:305:ILE:HG13	1:H:353:LEU:HD11	1.78	0.66
1:E:279:GLY:HA2	1:E:361:TYR:CE2	2.30	0.66
1:E:292:LEU:HD13	1:E:299:TYR:CD2	2.30	0.66
1:D:289:ASP:OD2	2:D:2042:HOH:O	2.13	0.66
1:G:361:TYR:CD2	2:G:2081:HOH:O	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HA	2:A:2059:HOH:O	1.95	0.66
1:G:312:ALA:HB2	2:G:2049:HOH:O	1.94	0.66
1:D:342:ASP:OD1	2:D:2087:HOH:O	2.14	0.65
1:D:289:ASP:H	1:D:357:HIS:HD2	1.43	0.65
1:E:332:LEU:HD23	1:F:308:PHE:HB3	1.78	0.65
1:D:277:ARG:HB2	2:D:2095:HOH:O	1.96	0.65
1:G:319:SER:HB2	1:G:321:ILE:HD11	1.78	0.65
1:H:289:ASP:HB3	1:H:357:HIS:ND1	2.11	0.65
1:G:358:ILE:HD13	1:G:358:ILE:O	1.96	0.65
1:E:283:THR:HG22	2:E:2039:HOH:O	1.97	0.65
1:G:260:ARG:HG2	1:H:318:MET:SD	2.37	0.65
1:A:326:THR:OG1	1:A:328:SER:HB2	1.97	0.65
1:G:326:THR:HG22	2:G:2057:HOH:O	1.96	0.65
1:E:319:SER:CA	2:E:2059:HOH:O	2.45	0.64
1:D:289:ASP:O	1:D:293:ILE:HG12	1.98	0.64
1:E:286:ASN:HD21	1:F:321:ILE:N	1.80	0.64
1:A:282:GLN:HG2	2:A:2045:HOH:O	1.98	0.64
1:E:334:TYR:HH	1:F:319:SER:HG	1.43	0.64
1:C:270:ASN:HB2	1:C:293:ILE:O	1.97	0.64
1:G:270:ASN:HD21	1:G:294:ARG:HA	1.59	0.64
1:H:325:VAL:O	1:H:326:THR:OG1	2.14	0.64
1:F:349:ASP:CA	1:F:352:ILE:HG22	2.24	0.64
1:G:332:LEU:O	1:H:337:ALA:HA	1.98	0.64
1:H:299:TYR:HB3	1:H:302:TRP:HB2	1.79	0.63
1:E:290:GLN:HG3	1:E:294:ARG:NE	2.14	0.63
1:F:282:GLN:CA	1:F:282:GLN:NE2	2.61	0.63
1:F:271:VAL:HB	1:F:293:ILE:HG12	1.80	0.63
1:B:358:ILE:HG22	1:B:359:ASP:N	2.13	0.63
1:G:302:TRP:O	1:G:305:ILE:HB	1.99	0.63
1:G:287:PHE:HE2	1:G:354:LEU:HD22	1.64	0.63
1:G:307:GLN:O	1:H:262:LYS:HD3	1.97	0.63
1:G:331:TRP:HH2	2:H:2001:HOH:O	1.78	0.63
1:A:301:HIS:HD2	2:A:2064:HOH:O	1.82	0.62
1:A:321:ILE:H	1:B:286:ASN:ND2	1.90	0.62
1:F:272:THR:N	1:F:293:ILE:HD11	2.15	0.62
1:C:260:ARG:HA	1:C:263:ARG:HD2	1.81	0.62
1:H:287:PHE:HE2	1:H:292:LEU:HD11	1.63	0.62
1:B:343:LYS:HE2	2:B:2092:HOH:O	1.98	0.62
1:C:326:THR:HB	2:C:2061:HOH:O	1.99	0.62
1:G:340:LEU:HB2	1:G:347:PHE:HE1	1.63	0.62
1:H:342:ASP:OD2	2:H:2078:HOH:O	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:TYR:HB2	2:A:2059:HOH:O	1.99	0.62
1:G:340:LEU:HB3	1:G:347:PHE:HE1	1.65	0.62
1:A:256:SER:HB2	2:A:2007:HOH:O	1.98	0.62
1:E:259:PRO:CD	1:E:262:LYS:HZ2	2.09	0.62
1:H:261:GLN:NE2	1:H:261:GLN:H	1.98	0.62
1:H:290:GLN:HB2	2:H:2040:HOH:O	1.99	0.62
1:C:302:TRP:HB3	1:C:303:PRO:HD3	1.80	0.62
1:H:347:PHE:O	1:H:351:VAL:HG23	1.98	0.62
1:E:265:ALA:HB2	1:E:275:PHE:CE1	2.35	0.61
1:C:320:ARG:NH2	1:D:279:GLY:O	2.33	0.61
1:C:321:ILE:H	1:D:286:ASN:ND2	1.88	0.61
1:E:354:LEU:O	1:E:355:ASN:O	2.18	0.61
1:G:346:GLN:HA	1:G:349:ASP:OD1	2.00	0.61
1:H:281:GLU:HB2	1:H:284:GLN:NE2	2.15	0.61
1:E:265:ALA:HB2	1:E:275:PHE:HE1	1.65	0.61
1:F:359:ASP:O	1:F:362:LYS:HG3	2.00	0.61
1:D:287:PHE:CZ	1:D:305:ILE:HD12	2.35	0.61
1:E:295:GLN:O	1:E:298:ASP:HB2	2.01	0.61
1:E:290:GLN:HG3	1:E:294:ARG:CZ	2.30	0.61
1:F:332:LEU:C	1:F:332:LEU:HD23	2.21	0.61
1:G:324:GLU:N	1:G:331:TRP:O	2.34	0.61
1:H:360:ALA:HB3	2:H:2094:HOH:O	2.01	0.61
1:D:270:ASN:OD1	1:D:270:ASN:C	2.39	0.61
1:H:289:ASP:O	1:H:292:LEU:N	2.34	0.61
1:C:360:ALA:O	1:C:362:LYS:N	2.34	0.60
1:D:320:ARG:HG3	1:D:335:HIS:NE2	2.16	0.60
1:G:320:ARG:O	1:G:334:TYR:HA	2.01	0.60
1:E:355:ASN:O	1:E:356:LYS:C	2.40	0.60
1:E:364:PHE:HD1	2:E:2041:HOH:O	1.84	0.60
1:F:291:ASP:O	1:F:295:GLN:HB2	2.01	0.60
1:C:331:TRP:CE3	1:D:339:LYS:HB2	2.37	0.60
1:F:271:VAL:HB	1:F:293:ILE:CD1	2.32	0.60
1:E:313:SER:HB3	2:E:2054:HOH:O	2.02	0.60
1:H:334:TYR:HB3	2:H:2067:HOH:O	2.01	0.60
1:C:278:ARG:HD2	1:C:293:ILE:HD11	1.84	0.60
1:E:342:ASP:HA	1:E:347:PHE:CD2	2.37	0.60
1:E:363:THR:O	1:E:364:PHE:C	2.38	0.60
1:G:256:SER:HB3	2:G:2002:HOH:O	2.02	0.60
1:H:355:ASN:O	1:H:357:HIS:N	2.34	0.59
1:F:363:THR:N	2:F:2093:HOH:O	2.34	0.59
1:D:260:ARG:HG3	2:D:2017:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:HIS:HD2	2:E:2047:HOH:O	1.83	0.59
1:F:272:THR:HG22	1:F:273:GLN:H	1.66	0.59
1:H:281:GLU:HB2	1:H:284:GLN:HE21	1.65	0.59
1:C:325:VAL:O	2:C:2059:HOH:O	2.16	0.59
1:C:351:VAL:HG23	1:D:323:MET:HE3	1.84	0.59
1:F:348:LYS:HD2	2:F:2072:HOH:O	2.02	0.59
1:D:314:ALA:HB1	1:D:318:MET:HE2	1.84	0.58
1:G:320:ARG:O	1:G:335:HIS:N	2.26	0.58
1:B:281:GLU:HB2	1:B:284:GLN:NE2	2.16	0.58
1:E:358:ILE:HD12	1:F:321:ILE:HG22	1.85	0.58
2:E:2070:HOH:O	1:F:331:TRP:HD1	1.81	0.58
1:E:290:GLN:CG	1:E:294:ARG:CZ	2.81	0.58
1:G:286:ASN:HB3	1:H:320:ARG:HH11	1.68	0.58
1:B:350:ASN:O	1:B:354:LEU:HG	2.04	0.57
1:F:354:LEU:HD11	2:F:2041:HOH:O	2.03	0.57
1:A:265:ALA:HA	1:A:269:TYR:O	2.04	0.57
1:G:334:TYR:OH	1:H:319:SER:HB3	2.04	0.57
1:E:259:PRO:CD	1:E:262:LYS:HZ3	2.17	0.57
1:F:313:SER:O	1:F:317:GLY:N	2.37	0.57
1:A:364:PHE:O	1:A:365:PRO:C	2.40	0.57
1:C:352:ILE:HD13	2:C:2095:HOH:O	2.04	0.57
1:D:305:ILE:HG12	1:D:353:LEU:HD13	1.86	0.57
1:C:278:ARG:NH1	1:C:287:PHE:O	2.33	0.57
1:E:313:SER:CB	2:E:2054:HOH:O	2.53	0.57
1:H:279:GLY:H	1:H:284:GLN:HG2	1.70	0.57
1:B:286:ASN:O	1:B:358:ILE:O	2.23	0.57
1:G:338:ILE:O	1:H:332:LEU:N	2.33	0.57
1:G:340:LEU:HB3	1:G:347:PHE:CE1	2.39	0.57
1:H:282:GLN:HG2	1:H:283:THR:H	1.70	0.57
1:B:346:GLN:HA	2:B:2098:HOH:O	2.03	0.57
1:G:284:GLN:NE2	2:G:2028:HOH:O	2.37	0.57
1:H:347:PHE:HA	2:H:2090:HOH:O	2.05	0.57
1:G:308:PHE:O	2:G:2044:HOH:O	2.17	0.56
1:C:281:GLU:CD	1:C:281:GLU:H	2.07	0.56
1:F:316:PHE:CD2	1:F:321:ILE:HD13	2.40	0.56
1:B:282:GLN:HA	1:B:282:GLN:OE1	2.06	0.56
1:G:310:PRO:N	2:G:2044:HOH:O	2.38	0.56
1:G:346:GLN:O	1:G:350:ASN:HB2	2.06	0.56
1:E:352:ILE:O	1:E:355:ASN:HB2	2.05	0.56
1:F:325:VAL:HG22	1:F:330:THR:HG23	1.87	0.56
2:E:2070:HOH:O	1:F:331:TRP:CB	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:341:ASP:HB3	2:H:2081:HOH:O	2.04	0.56
1:A:332:LEU:C	1:A:332:LEU:HD23	2.24	0.56
1:A:321:ILE:HG23	1:A:332:LEU:HD21	1.87	0.56
1:C:326:THR:CG2	1:C:329:GLY:H	2.19	0.56
1:C:361:TYR:HA	1:C:364:PHE:CD1	2.41	0.56
1:F:271:VAL:HB	1:F:293:ILE:CG1	2.36	0.56
1:G:260:ARG:O	1:G:263:ARG:HB2	2.06	0.56
1:G:287:PHE:CB	1:H:321:ILE:HD12	2.36	0.56
1:H:337:ALA:N	2:H:2069:HOH:O	2.35	0.56
1:E:338:ILE:CG2	2:E:2051:HOH:O	2.48	0.56
1:H:283:THR:O	2:H:2035:HOH:O	2.17	0.56
1:C:326:THR:HG21	1:C:331:TRP:HE1	1.71	0.56
1:D:252:ALA:CB	2:D:2081:HOH:O	2.54	0.56
1:F:281:GLU:HG2	1:F:282:GLN:H	1.71	0.56
1:G:320:ARG:CB	1:G:335:HIS:HB3	2.36	0.56
1:H:322:GLY:O	1:H:332:LEU:HD12	2.06	0.56
1:H:279:GLY:CA	1:H:284:GLN:HG2	2.36	0.55
1:G:258:LYS:O	1:G:259:PRO:C	2.43	0.55
1:G:274:ALA:O	1:G:275:PHE:CD1	2.59	0.55
1:H:341:ASP:CB	2:H:2081:HOH:O	2.54	0.55
1:H:361:TYR:CZ	1:H:362:LYS:HD2	2.41	0.55
1:B:362:LYS:CD	2:B:2121:HOH:O	2.50	0.55
1:F:360:ALA:C	1:F:362:LYS:N	2.52	0.55
1:G:278:ARG:HH12	1:H:317:GLY:HA2	1.70	0.55
1:H:355:ASN:O	1:H:356:LYS:C	2.45	0.55
1:H:353:LEU:C	1:H:353:LEU:HD23	2.26	0.55
1:H:344:ASP:OD1	1:H:346:GLN:HB3	2.07	0.55
1:B:343:LYS:HE3	2:B:2092:HOH:O	2.02	0.54
2:G:2045:HOH:O	1:H:316:PHE:HE2	1.88	0.54
1:H:309:ALA:HB2	2:H:2054:HOH:O	2.08	0.54
1:F:326:THR:HG21	1:F:331:TRP:CZ3	2.39	0.54
1:G:361:TYR:HD2	2:G:2081:HOH:O	1.88	0.54
1:E:282:GLN:N	2:E:2033:HOH:O	2.41	0.54
1:F:326:THR:CB	1:F:331:TRP:CZ3	2.90	0.54
1:G:280:PRO:HD2	2:G:2029:HOH:O	2.07	0.54
1:F:344:ASP:O	1:F:347:PHE:HB2	2.07	0.54
1:C:347:PHE:HZ	1:D:330:THR:HG1	1.54	0.54
1:E:259:PRO:HB3	2:E:2009:HOH:O	2.06	0.54
1:E:361:TYR:CA	1:E:364:PHE:CE2	2.89	0.54
1:H:355:ASN:HA	1:H:358:ILE:HG13	1.90	0.54
1:H:361:TYR:HA	1:H:364:PHE:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:SER:HB3	1:C:269:TYR:OH	2.08	0.54
1:C:321:ILE:N	1:D:286:ASN:HD21	1.90	0.54
1:E:261:GLN:O	1:F:314:ALA:HB3	2.08	0.54
1:F:289:ASP:CG	1:F:357:HIS:CE1	2.82	0.54
1:G:315:PHE:HE2	1:G:316:PHE:CZ	2.26	0.54
1:G:286:ASN:HD21	1:G:358:ILE:CG1	2.16	0.54
1:G:321:ILE:HD13	1:H:287:PHE:HB2	1.90	0.54
1:B:278:ARG:HA	1:B:285:GLY:O	2.06	0.53
1:B:335:HIS:ND1	2:B:2082:HOH:O	2.34	0.53
1:F:289:ASP:OD1	1:F:291:ASP:HB2	2.08	0.53
1:A:326:THR:HB	1:A:327:PRO:CD	2.38	0.53
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.73	0.53
1:F:326:THR:HG23	1:F:327:PRO:N	2.24	0.53
1:E:268:GLN:HE21	1:E:269:TYR:N	2.06	0.53
1:E:277:ARG:HG3	1:E:277:ARG:NH2	2.24	0.53
1:F:321:ILE:HA	1:F:333:THR:O	2.09	0.53
1:H:287:PHE:CZ	1:H:357:HIS:HB2	2.43	0.53
1:B:298:ASP:O	1:B:299:TYR:C	2.45	0.53
1:B:300:LYS:NZ	1:B:300:LYS:CB	2.65	0.53
1:E:321:ILE:HG22	1:F:358:ILE:HG12	1.90	0.53
1:G:288:GLY:HA2	1:G:357:HIS:HD2	1.72	0.53
1:H:287:PHE:CE2	1:H:292:LEU:CD1	2.91	0.53
1:B:299:TYR:HD1	2:B:2047:HOH:O	1.92	0.53
1:H:321:ILE:HG12	2:H:2067:HOH:O	2.07	0.53
1:F:271:VAL:HB	1:F:293:ILE:HD13	1.91	0.53
1:A:348:LYS:HA	2:A:2107:HOH:O	2.07	0.53
1:G:339:LYS:HD3	1:H:331:TRP:CZ3	2.43	0.53
1:E:339:LYS:HD3	2:F:2095:HOH:O	2.08	0.52
1:A:348:LYS:NZ	2:A:2106:HOH:O	2.35	0.52
1:F:348:LYS:HB2	2:F:2068:HOH:O	2.08	0.52
1:F:267:LYS:HD3	1:F:298:ASP:CB	2.36	0.52
1:A:305:ILE:HD13	1:A:353:LEU:HD13	1.91	0.52
1:G:300:LYS:HB3	1:G:301:HIS:CD2	2.45	0.52
1:G:315:PHE:O	1:G:319:SER:OG	2.24	0.52
1:C:284:GLN:HG3	2:C:2032:HOH:O	2.03	0.52
1:F:282:GLN:HE21	1:F:282:GLN:N	2.08	0.52
1:F:289:ASP:CG	1:F:357:HIS:HE1	2.13	0.52
1:E:277:ARG:HG3	1:E:277:ARG:HH21	1.75	0.52
1:D:326:THR:CG2	1:D:331:TRP:HE1	2.23	0.52
1:E:329:GLY:HA2	2:F:2065:HOH:O	2.10	0.52
1:F:318:MET:O	2:F:2048:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:GLN:HE21	1:C:261:GLN:H	1.57	0.51
1:E:344:ASP:OD1	1:E:345:PRO:HD2	2.09	0.51
1:G:306:ALA:C	2:G:2045:HOH:O	2.47	0.51
1:B:305:ILE:HD11	1:B:353:LEU:HD22	1.91	0.51
1:F:264:THR:CG2	1:F:297:THR:HG21	2.31	0.51
1:G:289:ASP:HB2	2:G:2035:HOH:O	2.08	0.51
1:D:281:GLU:O	1:D:283:THR:N	2.43	0.51
1:E:271:VAL:HB	1:E:293:ILE:HA	1.92	0.51
1:H:342:ASP:OD2	1:H:347:PHE:CE1	2.63	0.51
1:A:261:GLN:O	1:B:310:PRO:HA	2.10	0.51
1:D:304:GLN:NE2	2:D:2056:HOH:O	2.39	0.51
1:E:346:GLN:HG3	2:E:2082:HOH:O	2.11	0.51
1:G:316:PHE:HE1	2:H:2054:HOH:O	1.92	0.51
1:D:363:THR:CB	2:D:2112:HOH:O	2.46	0.51
1:E:286:ASN:HD22	1:E:286:ASN:H	1.58	0.51
1:H:352:ILE:O	1:H:355:ASN:HB2	2.09	0.51
1:G:360:ALA:HA	2:G:2083:HOH:O	2.11	0.51
1:H:309:ALA:N	2:H:2054:HOH:O	2.44	0.51
1:G:319:SER:O	1:G:321:ILE:HD12	2.11	0.50
1:B:256:SER:HB3	2:B:2028:HOH:O	2.10	0.50
1:F:361:TYR:O	1:F:361:TYR:HD1	1.92	0.50
2:G:2080:HOH:O	1:H:259:PRO:HB3	2.10	0.50
1:C:351:VAL:HG23	1:D:323:MET:HE1	1.94	0.50
1:B:299:TYR:CE2	1:B:301:HIS:HB2	2.47	0.50
1:G:317:GLY:HA3	1:H:275:PHE:CD1	2.46	0.50
1:A:302:TRP:HB3	1:A:303:PRO:HD3	1.93	0.50
1:F:277:ARG:HH22	1:G:268:GLN:HA	1.75	0.50
1:B:319:SER:HB2	1:B:321:ILE:HD11	1.92	0.50
1:C:267:LYS:O	1:C:267:LYS:HD3	2.12	0.50
1:E:316:PHE:HD1	1:E:321:ILE:HD13	1.76	0.50
1:A:304:GLN:HE21	1:A:350:ASN:HD22	1.58	0.50
1:B:290:GLN:OE1	1:C:294:ARG:CD	2.60	0.50
1:C:326:THR:CG2	1:C:329:GLY:N	2.75	0.50
1:D:260:ARG:NH1	1:D:275:PHE:HA	2.27	0.49
1:F:347:PHE:O	1:F:349:ASP:N	2.45	0.49
1:H:259:PRO:HG3	2:H:2014:HOH:O	2.11	0.49
1:D:316:PHE:CD2	1:D:321:ILE:HD13	2.47	0.49
1:E:302:TRP:NE1	1:E:306:ALA:HB2	2.28	0.49
1:H:266:THR:OG1	1:H:268:GLN:CD	2.51	0.49
1:A:309:ALA:HB1	2:A:2068:HOH:O	2.12	0.49
1:B:355:ASN:O	2:B:2110:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ALA:HB2	2:D:2081:HOH:O	2.11	0.49
1:D:326:THR:HG22	1:D:331:TRP:HE1	1.77	0.49
1:D:318:MET:SD	1:D:338:ILE:CD1	3.00	0.49
1:C:320:ARG:HD2	1:D:284:GLN:O	2.12	0.49
1:F:326:THR:HB	1:F:331:TRP:CE3	2.48	0.49
1:F:264:THR:HG22	1:F:297:THR:CG2	2.34	0.49
2:E:2089:HOH:O	1:F:323:MET:HG2	2.13	0.49
2:F:2016:HOH:O	1:G:277:ARG:CG	2.25	0.49
1:G:315:PHE:HE2	1:G:316:PHE:CE1	2.30	0.49
1:G:332:LEU:HD12	1:H:354:LEU:HD13	1.94	0.49
1:A:294:ARG:NH2	1:A:295:GLN:HE21	2.11	0.49
1:B:275:PHE:HE2	2:B:2022:HOH:O	1.95	0.49
1:C:291:ASP:HB3	1:C:295:GLN:HE22	1.77	0.49
1:C:364:PHE:HB3	2:C:2106:HOH:O	2.12	0.49
1:E:261:GLN:O	1:F:314:ALA:CB	2.61	0.49
1:E:282:GLN:CG	2:E:2035:HOH:O	2.47	0.49
1:F:299:TYR:CE2	1:F:301:HIS:HB2	2.47	0.48
1:G:315:PHE:O	1:G:319:SER:CB	2.61	0.48
1:B:365:PRO:HD2	2:B:2130:HOH:O	2.13	0.48
1:E:362:LYS:CE	1:E:362:LYS:HA	2.41	0.48
1:B:268:GLN:NE2	1:B:268:GLN:H	2.12	0.48
1:A:336:GLY:HA3	1:B:334:TYR:CZ	2.49	0.48
1:G:260:ARG:CD	1:H:339:LYS:HE3	2.40	0.48
1:A:265:ALA:O	1:A:297:THR:HB	2.14	0.48
1:A:355:ASN:O	1:A:357:HIS:N	2.46	0.48
1:E:259:PRO:HD2	1:E:262:LYS:HD2	1.95	0.48
1:G:336:GLY:HA3	1:H:334:TYR:CE1	2.48	0.48
1:F:252:ALA:O	1:F:254:GLU:N	2.45	0.48
1:H:353:LEU:HD23	1:H:354:LEU:CA	2.43	0.48
1:D:251:SER:CA	2:D:2001:HOH:O	2.62	0.48
1:E:332:LEU:HD23	1:F:308:PHE:CB	2.44	0.48
1:F:281:GLU:HG2	1:F:282:GLN:N	2.29	0.48
1:H:329:GLY:O	1:H:331:TRP:CD1	2.67	0.48
1:A:351:VAL:HG22	2:A:2107:HOH:O	2.13	0.47
1:G:278:ARG:HA	1:G:285:GLY:O	2.14	0.47
1:H:353:LEU:CD2	1:H:354:LEU:N	2.77	0.47
1:B:260:ARG:HA	1:B:263:ARG:HD2	1.96	0.47
1:D:314:ALA:HB1	1:D:318:MET:CE	2.45	0.47
1:E:337:ALA:HB1	2:E:2070:HOH:O	2.14	0.47
1:E:361:TYR:CB	1:E:364:PHE:CE2	2.98	0.47
1:F:332:LEU:CD2	1:F:332:LEU:C	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PHE:CE2	2:B:2022:HOH:O	2.55	0.47
1:C:291:ASP:HA	1:C:294:ARG:NE	2.29	0.47
1:C:354:LEU:HD13	1:D:332:LEU:HD13	1.96	0.47
1:E:292:LEU:HD22	1:E:357:HIS:CE1	2.49	0.47
1:G:315:PHE:O	1:G:319:SER:HB2	2.13	0.47
1:H:260:ARG:N	1:H:261:GLN:HE21	2.12	0.47
1:B:270:ASN:HB2	1:B:293:ILE:O	2.14	0.47
1:E:265:ALA:HB3	1:F:313:SER:OG	2.14	0.47
1:G:278:ARG:HD2	1:G:293:ILE:HD11	1.95	0.47
1:D:363:THR:CA	2:D:2112:HOH:O	2.63	0.47
1:E:259:PRO:HD3	1:E:262:LYS:HZ3	1.79	0.47
1:H:361:TYR:OH	1:H:362:LYS:HD2	2.15	0.47
1:H:354:LEU:O	1:H:358:ILE:HG13	2.14	0.47
1:F:294:ARG:HD3	2:G:2034:HOH:O	2.15	0.47
1:G:321:ILE:HA	1:G:333:THR:O	2.15	0.47
1:A:297:THR:HG23	1:A:297:THR:O	2.15	0.47
1:B:253:ALA:HB3	2:B:2001:HOH:O	2.15	0.47
1:B:347:PHE:O	1:B:351:VAL:HG23	2.14	0.47
1:C:350:ASN:O	1:C:354:LEU:HG	2.14	0.47
1:E:334:TYR:HE1	1:F:338:ILE:HG13	1.79	0.47
1:H:314:ALA:O	1:H:318:MET:HG3	2.14	0.47
1:E:358:ILE:CD1	1:F:321:ILE:HG22	2.45	0.47
1:E:364:PHE:HA	1:E:365:PRO:HD3	1.64	0.47
1:B:294:ARG:HA	2:B:2045:HOH:O	2.15	0.47
1:H:282:GLN:HG2	1:H:283:THR:N	2.29	0.47
1:B:254:GLU:OE1	1:B:255:ALA:N	2.46	0.46
1:D:251:SER:HA	2:D:2001:HOH:O	2.14	0.46
1:E:265:ALA:O	1:E:266:THR:CG2	2.64	0.46
1:G:301:HIS:CD2	1:G:301:HIS:N	2.83	0.46
1:B:278:ARG:HD3	1:B:293:ILE:HD11	1.97	0.46
1:E:355:ASN:O	1:E:358:ILE:N	2.28	0.46
1:C:326:THR:HG22	1:C:329:GLY:H	1.80	0.46
1:H:321:ILE:CG2	1:H:332:LEU:HD11	2.43	0.46
1:E:260:ARG:CZ	1:F:318:MET:HB3	2.45	0.46
1:G:340:LEU:CB	1:G:347:PHE:CE1	2.89	0.46
2:A:2013:HOH:O	1:B:318:MET:HA	2.16	0.46
1:C:318:MET:HG2	1:D:260:ARG:NH1	2.31	0.46
1:D:307:GLN:NE2	2:D:2059:HOH:O	2.44	0.46
1:E:309:ALA:HB3	2:E:2049:HOH:O	2.15	0.46
1:D:290:GLN:HB3	1:D:290:GLN:HE21	1.56	0.46
1:F:272:THR:N	1:F:293:ILE:CD1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:GLY:HA2	1:E:292:LEU:HD23	1.97	0.46
1:G:263:ARG:NH1	2:G:2011:HOH:O	2.49	0.46
1:B:295:GLN:HB3	1:B:299:TYR:N	2.31	0.46
1:C:260:ARG:HA	1:C:263:ARG:CD	2.46	0.46
1:C:281:GLU:N	1:C:281:GLU:OE2	2.42	0.46
1:E:319:SER:HB3	1:E:335:HIS:O	2.16	0.46
1:C:309:ALA:HA	1:C:310:PRO:HD2	1.78	0.46
1:F:326:THR:OG1	1:F:327:PRO:HD2	2.16	0.46
1:E:321:ILE:HG13	2:E:2059:HOH:O	2.16	0.45
1:E:338:ILE:N	2:E:2070:HOH:O	2.49	0.45
1:E:296:GLY:O	1:E:299:TYR:HB3	2.17	0.45
1:A:309:ALA:O	1:B:262:LYS:HE2	2.16	0.45
1:B:286:ASN:HD22	1:B:286:ASN:H	1.65	0.45
1:G:325:VAL:N	2:G:2056:HOH:O	2.49	0.45
1:G:325:VAL:HG22	1:G:330:THR:HG23	1.97	0.45
1:H:282:GLN:CD	1:H:282:GLN:H	2.18	0.45
1:A:352:ILE:HD12	1:A:352:ILE:C	2.37	0.45
1:D:346:GLN:NE2	2:D:2094:HOH:O	2.48	0.45
1:C:300:LYS:HD3	1:C:300:LYS:O	2.15	0.45
1:F:352:ILE:HG21	2:F:2077:HOH:O	2.16	0.45
1:G:303:PRO:HA	1:G:306:ALA:HB3	1.97	0.45
1:H:355:ASN:HA	1:H:358:ILE:CD1	2.47	0.45
1:H:261:GLN:HG2	1:H:262:LYS:N	2.31	0.45
1:B:300:LYS:HZ2	1:B:300:LYS:HB3	1.79	0.45
1:E:260:ARG:HH22	1:F:318:MET:CB	2.30	0.45
1:H:266:THR:OG1	1:H:268:GLN:OE1	2.35	0.45
1:F:274:ALA:HB1	1:F:275:PHE:CE2	2.52	0.45
1:F:325:VAL:HG13	1:F:330:THR:OG1	2.15	0.45
1:H:271:VAL:HG13	1:H:275:PHE:HD1	1.82	0.45
1:C:360:ALA:C	1:C:362:LYS:N	2.71	0.45
1:D:268:GLN:H	1:D:268:GLN:NE2	2.15	0.45
1:G:270:ASN:HB3	1:G:273:GLN:HG3	1.98	0.45
1:A:290:GLN:HG3	2:A:2055:HOH:O	2.17	0.44
1:B:302:TRP:HB3	1:B:303:PRO:HD3	2.00	0.44
1:H:274:ALA:HB1	1:H:275:PHE:CD2	2.52	0.44
1:B:300:LYS:HZ2	1:B:300:LYS:CB	2.28	0.44
1:D:316:PHE:HD2	1:D:321:ILE:HD13	1.81	0.44
1:D:348:LYS:HZ2	1:D:348:LYS:HG2	1.65	0.44
1:E:289:ASP:HB2	1:E:357:HIS:ND1	2.33	0.44
1:E:334:TYR:CE1	1:F:338:ILE:HG13	2.53	0.44
1:E:346:GLN:N	2:E:2082:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:LEU:O	1:E:342:ASP:N	2.51	0.44
1:A:326:THR:HB	1:A:327:PRO:HD2	1.98	0.44
1:D:278:ARG:HD2	1:D:293:ILE:HD12	2.00	0.44
1:E:354:LEU:O	1:E:358:ILE:HG12	2.17	0.44
2:G:2077:HOH:O	1:H:323:MET:HG2	2.18	0.44
1:H:353:LEU:O	1:H:354:LEU:C	2.55	0.44
1:B:363:THR:O	1:B:363:THR:HG22	2.17	0.44
1:A:332:LEU:C	1:A:332:LEU:CD2	2.86	0.44
1:E:329:GLY:CA	2:F:2065:HOH:O	2.65	0.44
1:F:326:THR:CG2	1:F:331:TRP:CH2	2.90	0.44
1:G:348:LYS:O	1:G:351:VAL:HG12	2.17	0.44
1:H:287:PHE:CE2	1:H:292:LEU:HD13	2.53	0.44
1:C:347:PHE:CD2	1:C:348:LYS:HD3	2.52	0.44
1:F:347:PHE:O	1:F:348:LYS:C	2.56	0.44
1:G:299:TYR:HB3	1:G:302:TRP:HB2	2.00	0.44
1:H:348:LYS:HG3	1:H:348:LYS:H	1.61	0.44
1:A:301:HIS:HB3	1:A:353:LEU:HD11	2.00	0.43
1:E:338:ILE:HD12	1:E:339:LYS:H	1.81	0.43
1:F:253:ALA:O	1:F:268:GLN:NE2	2.44	0.43
1:G:288:GLY:HA2	1:G:357:HIS:CD2	2.53	0.43
1:A:278:ARG:HD2	1:A:293:ILE:HD11	1.99	0.43
1:A:353:LEU:O	1:A:357:HIS:HD2	2.01	0.43
1:B:291:ASP:HB3	2:B:2047:HOH:O	2.17	0.43
1:C:297:THR:HG22	1:C:302:TRP:CE2	2.53	0.43
1:C:326:THR:HG21	1:C:331:TRP:NE1	2.33	0.43
1:E:302:TRP:CE2	1:E:306:ALA:HB2	2.53	0.43
1:E:312:ALA:HA	1:F:309:ALA:CB	2.48	0.43
1:G:287:PHE:HE1	1:G:292:LEU:HD11	1.83	0.43
1:H:351:VAL:HG12	1:H:355:ASN:ND2	2.34	0.43
1:A:356:LYS:HD3	2:A:2113:HOH:O	2.18	0.43
1:H:353:LEU:HD23	1:H:354:LEU:HA	2.01	0.43
1:H:354:LEU:HG	1:H:354:LEU:H	1.52	0.43
1:H:361:TYR:CZ	1:H:362:LYS:HG3	2.52	0.43
1:A:261:GLN:HE21	1:A:261:GLN:N	2.11	0.43
1:B:300:LYS:HD2	1:B:301:HIS:CE1	2.54	0.43
1:B:275:PHE:CZ	2:B:2022:HOH:O	2.72	0.43
1:C:262:LYS:HA	1:C:262:LYS:HD2	1.74	0.43
1:E:342:ASP:HA	1:E:347:PHE:CG	2.54	0.43
1:G:309:ALA:C	2:G:2044:HOH:O	2.56	0.43
1:G:309:ALA:N	2:G:2045:HOH:O	1.97	0.43
1:B:268:GLN:CD	1:B:268:GLN:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:GLN:CA	1:F:282:GLN:HE21	2.32	0.43
1:E:260:ARG:NH2	1:F:318:MET:HB3	2.34	0.43
1:B:261:GLN:HB3	2:B:2017:HOH:O	2.18	0.43
1:C:326:THR:HG23	1:C:329:GLY:H	1.83	0.43
1:C:257:LYS:O	1:E:345:PRO:HG3	2.19	0.43
1:G:299:TYR:OH	1:G:357:HIS:HE1	2.01	0.43
1:G:358:ILE:HD13	1:G:358:ILE:C	2.38	0.43
1:E:345:PRO:C	2:E:2082:HOH:O	2.57	0.43
1:F:326:THR:CG2	1:F:328:SER:H	2.32	0.43
1:A:281:GLU:H	1:A:284:GLN:HE21	1.65	0.43
1:B:305:ILE:CD1	1:B:353:LEU:HD13	2.49	0.43
1:B:327:PRO:HD2	2:B:2075:HOH:O	2.18	0.43
1:C:326:THR:HG22	1:C:329:GLY:N	2.34	0.43
1:C:360:ALA:C	1:C:362:LYS:H	2.22	0.43
1:D:282:GLN:HG2	2:D:2039:HOH:O	2.18	0.43
1:D:361:TYR:HA	1:D:364:PHE:CD2	2.54	0.43
1:E:334:TYR:HD1	2:E:2068:HOH:O	2.01	0.43
1:E:346:GLN:O	1:E:347:PHE:C	2.57	0.43
1:H:329:GLY:O	1:H:331:TRP:HD1	2.01	0.43
1:B:281:GLU:HG3	2:B:2039:HOH:O	2.19	0.42
1:G:330:THR:C	1:G:331:TRP:CD1	2.91	0.42
1:H:359:ASP:HA	1:H:361:TYR:HE2	1.83	0.42
1:D:354:LEU:O	1:D:358:ILE:HG13	2.18	0.42
1:G:286:ASN:OD1	1:H:320:ARG:HA	2.19	0.42
1:B:259:PRO:O	1:B:260:ARG:C	2.58	0.42
1:B:295:GLN:CD	2:B:2047:HOH:O	2.58	0.42
1:A:264:THR:HA	1:B:313:SER:HB3	2.01	0.42
1:E:266:THR:OG1	1:E:268:GLN:HG3	2.19	0.42
1:H:261:GLN:H	1:H:261:GLN:HE21	1.67	0.42
1:H:268:GLN:HG3	1:H:268:GLN:H	1.42	0.42
1:D:346:GLN:HA	2:D:2090:HOH:O	2.19	0.42
1:E:286:ASN:O	1:E:358:ILE:O	2.38	0.42
1:E:292:LEU:HD13	1:E:299:TYR:CG	2.54	0.42
1:E:328:SER:HB2	2:E:2066:HOH:O	2.19	0.42
1:H:295:GLN:O	1:H:296:GLY:C	2.57	0.42
1:E:358:ILE:HA	1:E:358:ILE:HD13	1.98	0.42
1:G:331:TRP:CZ3	2:H:2001:HOH:O	2.71	0.42
1:B:289:ASP:OD2	1:B:289:ASP:C	2.58	0.42
1:F:343:LYS:O	2:F:2066:HOH:O	2.21	0.42
1:E:310:PRO:HA	1:F:261:GLN:O	2.20	0.42
1:H:361:TYR:OH	1:H:362:LYS:NZ	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:NZ	2:A:2025:HOH:O	2.41	0.42
1:D:346:GLN:CD	2:D:2094:HOH:O	2.57	0.42
1:E:321:ILE:HD12	1:F:287:PHE:CB	2.50	0.42
1:F:320:ARG:CG	1:F:335:HIS:HD2	2.32	0.42
1:H:359:ASP:HA	1:H:361:TYR:CE2	2.55	0.42
1:B:305:ILE:HD13	1:B:353:LEU:HD13	2.00	0.42
1:C:314:ALA:HA	1:D:275:PHE:CZ	2.54	0.42
1:D:289:ASP:C	1:D:289:ASP:OD1	2.57	0.42
1:F:295:GLN:HE21	1:F:295:GLN:HB2	1.52	0.42
1:H:341:ASP:HB2	2:H:2081:HOH:O	2.19	0.42
1:G:292:LEU:O	1:G:292:LEU:HD23	2.19	0.42
1:H:272:THR:CG2	1:H:273:GLN:N	2.83	0.42
1:H:361:TYR:HA	1:H:364:PHE:CE2	2.54	0.42
1:B:328:SER:OG	2:B:2077:HOH:O	2.21	0.41
1:E:346:GLN:NE2	2:E:2081:HOH:O	2.52	0.41
1:G:289:ASP:O	1:G:293:ILE:HG12	2.20	0.41
1:G:331:TRP:HB3	1:H:337:ALA:CB	2.36	0.41
1:E:283:THR:CG2	2:E:2039:HOH:O	2.60	0.41
1:A:282:GLN:NE2	2:A:2046:HOH:O	2.53	0.41
1:F:271:VAL:CB	1:F:293:ILE:HG12	2.48	0.41
1:B:300:LYS:HB2	2:B:2050:HOH:O	2.19	0.41
1:A:331:TRP:CZ3	1:B:339:LYS:HB2	2.56	0.41
1:C:273:GLN:NE2	2:C:2028:HOH:O	2.53	0.41
1:E:361:TYR:CD2	1:E:361:TYR:C	2.94	0.41
1:H:350:ASN:O	1:H:354:LEU:HG	2.19	0.41
1:B:364:PHE:N	1:B:365:PRO:CD	2.83	0.41
2:E:2089:HOH:O	1:F:323:MET:HE2	2.21	0.41
1:G:287:PHE:CG	1:H:321:ILE:HD12	2.56	0.41
1:G:338:ILE:HG22	1:H:332:LEU:CB	2.36	0.41
1:A:358:ILE:O	1:A:359:ASP:HB2	2.21	0.41
1:E:282:GLN:NE2	2:E:2033:HOH:O	2.53	0.41
1:F:325:VAL:HA	1:F:330:THR:HA	2.02	0.41
1:E:305:ILE:HG12	1:E:354:LEU:CD2	2.51	0.41
1:F:326:THR:HG23	1:F:328:SER:H	1.85	0.41
1:G:299:TYR:OH	1:G:357:HIS:CE1	2.74	0.41
1:G:306:ALA:O	2:G:2045:HOH:O	2.21	0.41
1:H:344:ASP:OD1	1:H:346:GLN:CB	2.69	0.41
1:E:337:ALA:C	2:E:2070:HOH:O	2.58	0.41
1:G:278:ARG:HG2	1:G:278:ARG:H	1.66	0.41
1:A:354:LEU:O	1:A:358:ILE:HG13	2.21	0.41
1:D:345:PRO:O	2:D:2089:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:LYS:HG2	1:E:262:LYS:CD	2.51	0.41
1:E:293:ILE:HB	1:E:294:ARG:HD2	2.03	0.41
1:F:358:ILE:O	1:F:359:ASP:HB2	2.21	0.41
1:H:278:ARG:NH2	1:H:285:GLY:HA3	2.35	0.41
1:A:332:LEU:HB2	1:B:340:LEU:HD21	2.01	0.41
1:C:278:ARG:HD3	1:C:287:PHE:O	2.21	0.41
1:E:290:GLN:O	1:E:291:ASP:C	2.60	0.41
1:C:361:TYR:CD1	1:C:361:TYR:C	2.94	0.40
1:E:281:GLU:HB3	1:E:283:THR:HG22	2.03	0.40
1:F:350:ASN:O	1:F:351:VAL:C	2.60	0.40
1:B:319:SER:HB2	1:B:321:ILE:CD1	2.50	0.40
1:C:348:LYS:O	1:C:352:ILE:HG12	2.21	0.40
1:D:262:LYS:NZ	2:D:2021:HOH:O	2.49	0.40
1:C:261:GLN:CB	1:D:338:ILE:HD12	2.42	0.40
1:E:334:TYR:CE2	1:F:319:SER:OG	2.74	0.40
1:H:316:PHE:HA	1:H:321:ILE:HD11	2.03	0.40
1:E:288:GLY:HA2	1:E:357:HIS:HB3	2.04	0.40
1:E:270:ASN:HD22	1:E:294:ARG:HA	1.86	0.40
1:E:316:PHE:HD1	1:E:321:ILE:CD1	2.34	0.40
1:G:293:ILE:HD12	2:G:2025:HOH:O	2.21	0.40
1:C:291:ASP:HB3	1:C:295:GLN:NE2	2.36	0.40
1:E:259:PRO:HD2	1:E:262:LYS:CD	2.52	0.40
1:E:260:ARG:HH22	1:F:318:MET:HB3	1.87	0.40
1:E:330:THR:N	2:E:2067:HOH:O	2.55	0.40
1:H:309:ALA:CB	2:H:2054:HOH:O	2.69	0.40
1:H:315:PHE:CZ	1:H:334:TYR:CG	3.09	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ASP:O	1:H:352:ILE:CG2[4_455]	1.93	0.27
2:B:2069:HOH:O	2:D:2097:HOH:O[4_455]	2.06	0.14

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	113/128 (88%)	98 (87%)	12 (11%)	3 (3%)	5 7
1	B	111/128 (87%)	99 (89%)	9 (8%)	3 (3%)	5 7
1	C	111/128 (87%)	105 (95%)	4 (4%)	2 (2%)	8 14
1	D	113/128 (88%)	104 (92%)	5 (4%)	4 (4%)	3 4
1	E	108/128 (84%)	82 (76%)	17 (16%)	9 (8%)	1 1
1	F	110/128 (86%)	84 (76%)	17 (16%)	9 (8%)	1 1
1	G	107/128 (84%)	83 (78%)	18 (17%)	6 (6%)	2 1
1	H	108/128 (84%)	87 (81%)	14 (13%)	7 (6%)	1 1
All	All	881/1024 (86%)	742 (84%)	96 (11%)	43 (5%)	2 2

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	ASP
1	E	260	ARG
1	E	355	ASN
1	E	356	LYS
1	E	358	ILE
1	F	326	THR
1	F	347	PHE
1	F	348	LYS
1	F	361	TYR
1	G	260	ARG
1	H	326	THR
1	H	356	LYS
1	H	363	THR
1	A	252	ALA
1	B	255	ALA
1	B	299	TYR
1	B	358	ILE
1	C	254	GLU
1	C	361	TYR
1	D	282	GLN
1	E	289	ASP
1	E	348	LYS
1	F	253	ALA

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Mol	Chain	Res	Type
1	G	356	LYS
1	H	270	ASN
1	D	252	ALA
1	D	359	ASP
1	F	307	GLN
1	G	281	GLU
1	H	290	GLN
1	E	293	ILE
1	F	270	ASN
1	F	327	PRO
1	F	358	ILE
1	G	256	SER
1	G	280	PRO
1	D	311	SER
1	E	261	GLN
1	E	341	ASP
1	G	261	GLN
1	H	307	GLN
1	H	353	LEU
1	A	326	THR

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	93/106 (88%)	84 (90%)	9 (10%)	8 16
1	B	93/106 (88%)	81 (87%)	12 (13%)	4 8
1	C	92/106 (87%)	84 (91%)	8 (9%)	10 20
1	D	93/106 (88%)	82 (88%)	11 (12%)	5 10
1	E	91/106 (86%)	75 (82%)	16 (18%)	2 3
1	F	90/106 (85%)	78 (87%)	12 (13%)	4 7
1	G	90/106 (85%)	77 (86%)	13 (14%)	3 6
1	H	89/106 (84%)	69 (78%)	20 (22%)	1 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	731/848 (86%)	630 (86%)	101 (14%)	3 6

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	264	THR
1	A	278	ARG
1	A	281	GLU
1	A	297	THR
1	A	323	MET
1	A	328	SER
1	A	353	LEU
1	A	354	LEU
1	B	254	GLU
1	B	264	THR
1	B	277	ARG
1	B	278	ARG
1	B	282	GLN
1	B	286	ASN
1	B	300	LYS
1	B	324	GLU
1	B	348	LYS
1	B	353	LEU
1	B	356	LYS
1	B	359	ASP
1	C	261	GLN
1	C	278	ARG
1	C	281	GLU
1	C	300	LYS
1	C	320	ARG
1	C	328	SER
1	C	346	GLN
1	C	348	LYS
1	D	258	LYS
1	D	260	ARG
1	D	264	THR
1	D	278	ARG
1	D	286	ASN
1	D	291	ASP
1	D	300	LYS
1	D	324	GLU

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Mol	Chain	Res	Type
1	D	339	LYS
1	D	342	ASP
1	D	353	LEU
1	E	258	LYS
1	E	262	LYS
1	E	267	LYS
1	E	268	GLN
1	E	270	ASN
1	E	272	THR
1	E	286	ASN
1	E	289	ASP
1	E	290	GLN
1	E	292	LEU
1	E	307	GLN
1	E	319	SER
1	E	326	THR
1	E	338	ILE
1	E	362	LYS
1	E	364	PHE
1	F	260	ARG
1	F	262	LYS
1	F	264	THR
1	F	272	THR
1	F	278	ARG
1	F	282	GLN
1	F	293	ILE
1	F	295	GLN
1	F	326	THR
1	F	332	LEU
1	F	335	HIS
1	F	356	LYS
1	G	257	LYS
1	G	277	ARG
1	G	278	ARG
1	G	282	GLN
1	G	301	HIS
1	G	320	ARG
1	G	323	MET
1	G	333	THR
1	G	339	LYS
1	G	349	ASP
1	G	353	LEU

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Mol	Chain	Res	Type
1	G	356	LYS
1	G	358	ILE
1	H	258	LYS
1	H	260	ARG
1	H	261	GLN
1	H	268	GLN
1	H	270	ASN
1	H	278	ARG
1	H	281	GLU
1	H	282	GLN
1	H	284	GLN
1	H	289	ASP
1	H	307	GLN
1	H	320	ARG
1	H	323	MET
1	H	325	VAL
1	H	330	THR
1	H	339	LYS
1	H	340	LEU
1	H	348	LYS
1	H	358	ILE
1	H	363	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	284	GLN
1	A	301	HIS
1	A	350	ASN
1	A	355	ASN
1	B	268	GLN
1	B	284	GLN
1	B	286	ASN
1	B	307	GLN
1	B	350	ASN
1	B	355	ASN
1	C	261	GLN
1	C	304	GLN
1	C	335	HIS
1	C	350	ASN
1	C	355	ASN

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Mol	Chain	Res	Type
1	D	268	GLN
1	D	282	GLN
1	D	286	ASN
1	D	290	GLN
1	D	295	GLN
1	D	301	HIS
1	D	307	GLN
1	D	357	HIS
1	E	268	GLN
1	E	286	ASN
1	E	301	HIS
1	E	346	GLN
1	F	282	GLN
1	F	284	GLN
1	F	295	GLN
1	G	295	GLN
1	G	335	HIS
1	G	357	HIS
1	H	261	GLN
1	H	270	ASN
1	H	284	GLN
1	H	290	GLN
1	H	295	GLN
1	H	307	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	115/128 (89%)	0.17	6 (5%)	27	29	3, 16, 43, 55	0
1	B	113/128 (88%)	0.16	9 (7%)	12	12	3, 20, 38, 67	0
1	C	113/128 (88%)	0.14	2 (1%)	68	71	2, 22, 44, 46	0
1	D	115/128 (89%)	0.17	4 (3%)	44	47	3, 15, 41, 52	0
1	E	110/128 (85%)	1.30	26 (23%)	0	0	18, 38, 58, 64	0
1	F	112/128 (87%)	1.24	22 (19%)	1	1	23, 43, 57, 59	0
1	G	109/128 (85%)	1.18	19 (17%)	1	1	15, 41, 54, 58	0
1	H	110/128 (85%)	1.17	24 (21%)	0	0	20, 38, 54, 65	0
All	All	897/1024 (87%)	0.68	112 (12%)	3	3	2, 31, 53, 67	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	329	GLY	7.6
1	D	255	ALA	6.5
1	F	253	ALA	6.0
1	F	326	THR	6.0
1	G	269	TYR	6.0
1	B	365	PRO	5.7
1	G	358	ILE	5.2
1	F	327	PRO	5.1
1	E	280	PRO	5.0
1	E	331	TRP	4.6
1	H	328	SER	4.2
1	E	337	ALA	4.0
1	G	346	GLN	3.7
1	H	281	GLU	3.6
1	A	251	SER	3.6
1	E	325	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	358	ILE	3.5
1	F	264	THR	3.5
1	F	306	ALA	3.4
1	H	264	THR	3.3
1	G	359	ASP	3.3
1	B	364	PHE	3.3
1	G	350	ASN	3.2
1	A	326	THR	3.2
1	E	358	ILE	3.1
1	A	327	PRO	3.1
1	H	354	LEU	3.1
1	E	347	PHE	3.1
1	B	363	THR	3.1
1	E	327	PRO	3.1
1	H	345	PRO	3.1
1	D	325	VAL	3.0
1	G	325	VAL	3.0
1	H	342	ASP	2.9
1	G	351	VAL	2.9
1	H	353	LEU	2.9
1	F	361	TYR	2.9
1	F	347	PHE	2.8
1	G	297	THR	2.8
1	F	265	ALA	2.8
1	F	283	THR	2.8
1	A	328	SER	2.8
1	H	365	PRO	2.8
1	B	254	GLU	2.7
1	G	298	ASP	2.7
1	H	346	GLN	2.7
1	B	328	SER	2.6
1	E	321	ILE	2.6
1	G	285	GLY	2.6
1	E	314	ALA	2.6
1	G	338	ILE	2.6
1	E	293	ILE	2.6
1	D	252	ALA	2.5
1	E	271	VAL	2.5
1	H	343	LYS	2.5
1	A	252	ALA	2.5
1	E	315	PHE	2.5
1	F	342	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	343	LYS	2.4
1	D	254	GLU	2.4
1	F	328	SER	2.4
1	C	327	PRO	2.4
1	H	347	PHE	2.4
1	G	336	GLY	2.4
1	H	267	LYS	2.3
1	B	345	PRO	2.3
1	F	273	GLN	2.3
1	A	253	ALA	2.3
1	H	280	PRO	2.3
1	E	282	GLN	2.3
1	H	324	GLU	2.3
1	G	255	ALA	2.3
1	F	276	GLY	2.3
1	E	359	ASP	2.3
1	B	253	ALA	2.3
1	H	298	ASP	2.3
1	B	315	PHE	2.3
1	E	319	SER	2.3
1	F	274	ALA	2.3
1	G	361	TYR	2.3
1	F	309	ALA	2.3
1	H	348	LYS	2.3
1	F	252	ALA	2.3
1	F	354	LEU	2.3
1	G	259	PRO	2.2
1	F	329	GLY	2.2
1	G	274	ALA	2.2
1	E	363	THR	2.2
1	H	331	TRP	2.2
1	B	327	PRO	2.2
1	E	357	HIS	2.2
1	E	287	PHE	2.2
1	H	308	PHE	2.2
1	E	288	GLY	2.1
1	H	355	ASN	2.1
1	F	360	ALA	2.1
1	H	327	PRO	2.1
1	H	356	LYS	2.1
1	E	292	LEU	2.1
1	G	266	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	364	PHE	2.1
1	E	334	TYR	2.1
1	F	305	ILE	2.1
1	E	361	TYR	2.1
1	E	267	LYS	2.1
1	E	345	PRO	2.1
1	H	352	ILE	2.1
1	G	275	PHE	2.1
1	F	331	TRP	2.0
1	G	271	VAL	2.0
1	F	275	PHE	2.0
1	C	365	PRO	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.