Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:38 PM GMT

PDB ID	:	1Y4U
Title	:	Conformation rearrangement of heat shock protein 90 upon ADP binding
Authors	:	Huai, Q.; Wang, H.; Liu, Y.; Kim, H.; Toft, D.; Ke, H.
Deposited on	:	2004-12-01
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

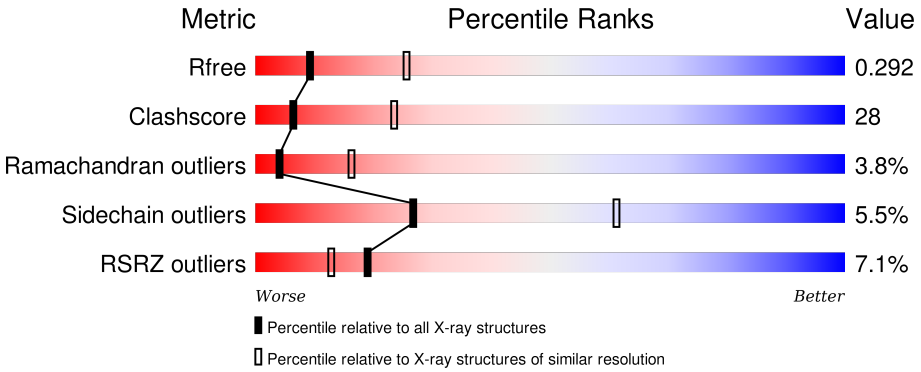
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	559	7% 43% 36% 16%
1	B	559	5% 45% 31% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7536 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.

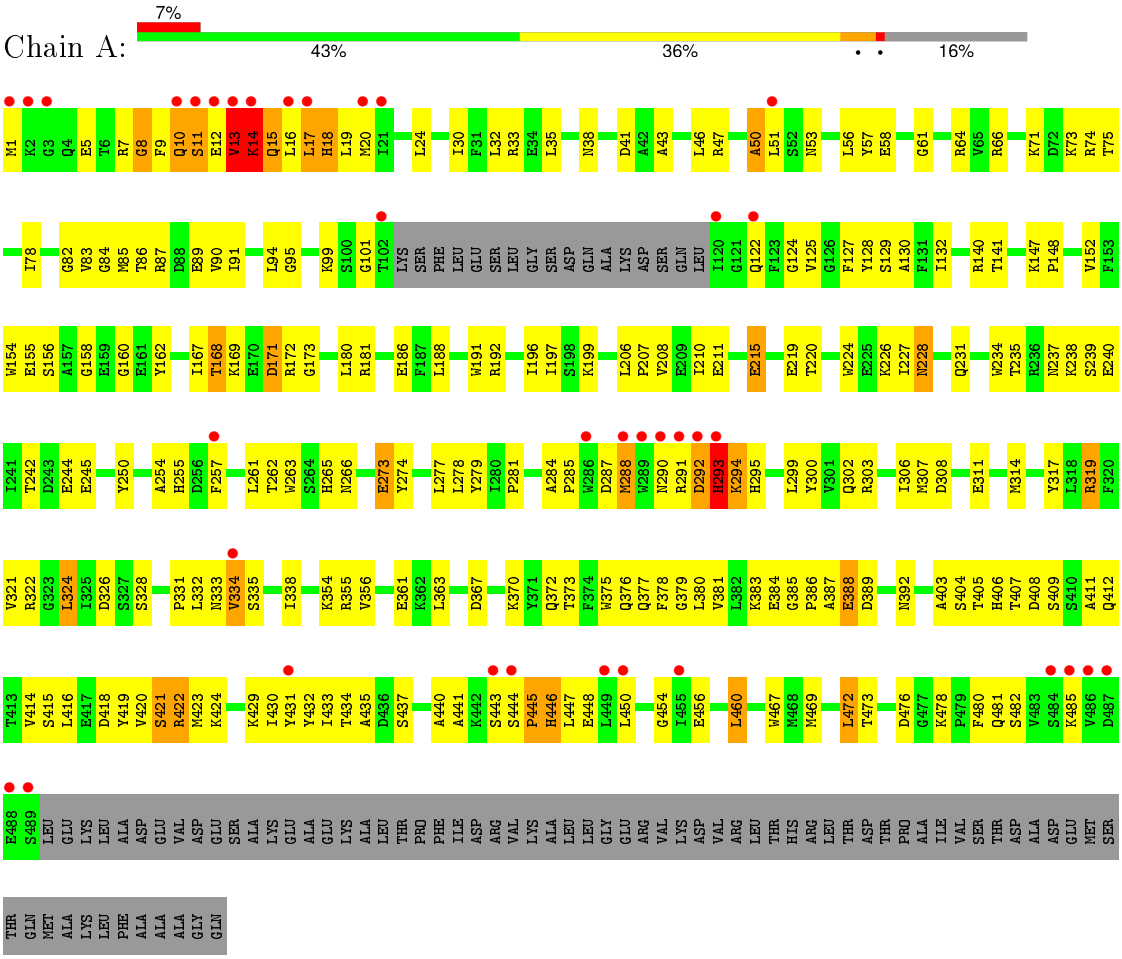
- Molecule 1 is a protein called Chaperone protein htpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3837	2421	660	746	10			
1	B	454	Total	C	N	O	S	0	0	0
			3699	2338	634	718	9			

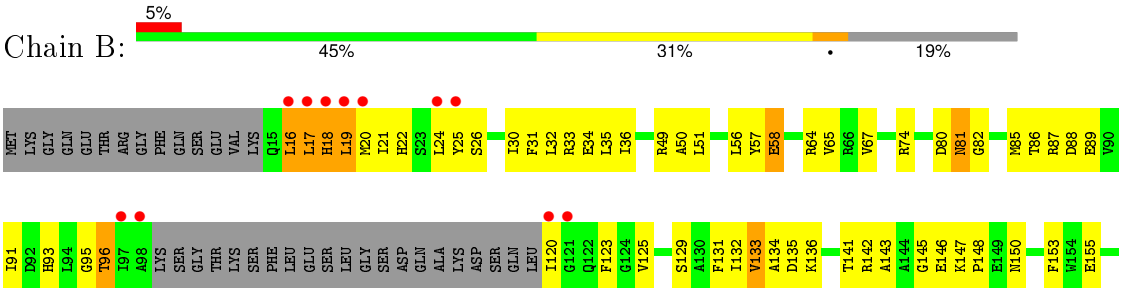
3 Residue-property plots (i)

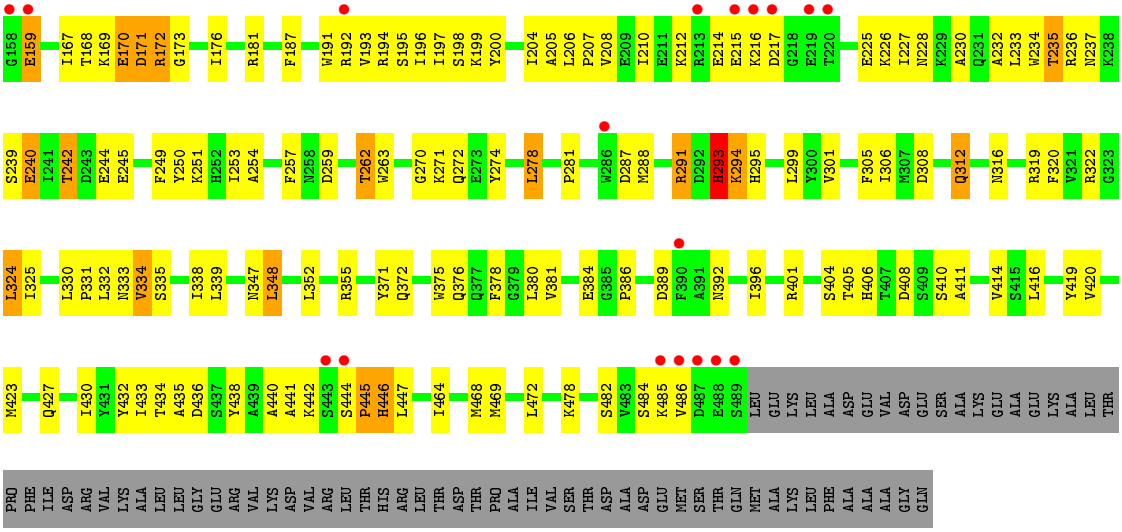
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Chaperone protein htpG



- Molecule 1: Chaperone protein htpG




G158 E159 I167 T168 K169 E170 D171 R172 G173 I176 R181 F187 W191 R192 Y193 R194 S195 I196 I197 S198 K199 Y200 I204 A205 L206 P207 V208 E209 I210 E211 K212 R213 E214 E215 K216 D217 G218 E219 T220 E225 K226 I227 N228 K229 A230 Q231 A232 L233 W234 T235 R236 N237 K238
S239 E240 T241 T242 D243 E244 E245 F249 Y250 K251 H252 I253 A254 F257 N258 D259 T262 W263 G270 K271 Q272 E273 Y274 L278 P281 W286 D287 M288 R291 D292 H293 K294 H295 L299 Y300 V301 F305 I306 M307 D308 Q312 N316 R319 F320 V321 R322 G323
L324 I325 L330 P331 L332 N333 V334 S335 I338 L339 N347 L348 L352 R365 Y371 Q372 W375 Q376 Q377 F378 G379 L380 V381 E384 G385 P386 D389 F390 A391 N392 I396 R401 S404 T405 H406 T407 D408 S409 S410 A411 V414 S415 L416 Y419 V420
M423 Q427 I430 Y431 Y432 I433 T434 A435 D436 S437 Y438 A439 A440 A441 K442 S443 S444 P445 H446 L447 I464 N468 M469 L472 K478 S482 V483 S484 K485 V486 D487 E488 S489 LEU GLU LYS LEU ALA ASP GLU VAL ASP GLU SER ALA LYS GLU ALA GLU LYS ALA LEU THR
PRO PHE ILE ASP ARG VAL LYS ALA LEU LEU GLY GLU ARG VAL LYS ASP VAL ARG LEU THR HIS ARG LEU THR ASP THR PRO ALA ILE VAL SER THR ASP ALA ASP GLU MET SER THR GLN MET ALA LYS LEU PHE ALA ALA ALA GLY GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	158.01Å 158.01Å 117.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 94.04 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 83.5 (94.04-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.82Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.295 0.233 , 0.292	Depositor DCC
R_{free} test set	3001 reflections (9.96%)	DCC
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 32234 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7536	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.73	4/3913 (0.1%)	0.98	9/5277 (0.2%)
1	B	0.47	0/3774	0.72	1/5095 (0.0%)
All	All	0.62	4/7687 (0.1%)	0.86	10/10372 (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	A	0	4
1	B	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	HIS	C-O	29.99	1.80	1.23
1	A	8	GLY	C-N	-16.40	0.96	1.34
1	A	8	GLY	C-O	11.09	1.41	1.23
1	A	10	GLN	C-N	-7.64	1.16	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	GLY	O-C-N	-30.14	74.47	122.70
1	A	293	HIS	O-C-N	-29.82	75.00	122.70
1	A	8	GLY	CA-C-N	18.88	158.73	117.20
1	A	8	GLY	C-N-CA	18.75	168.57	121.70
1	A	8	GLY	CA-C-O	-9.09	104.25	120.60
1	A	13	VAL	N-CA-C	8.84	134.85	111.00
1	A	14	LYS	N-CA-C	8.48	133.91	111.00
1	A	293	HIS	N-CA-C	5.42	125.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	293	HIS	N-CA-C	5.29	125.27	111.00
1	A	13	VAL	CB-CA-C	-5.21	101.49	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ASP	Mainchain
1	A	293	HIS	Mainchain
1	A	8	GLY	Mainchain,Peptide
1	B	371	TYR	Sidechain

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	3837	0	3753	242	0
1	B	3699	0	3612	196	0
All	All	7536	0	7365	411	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 28.

All (411) 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:293:HIS:C	1:A:293:HIS:O	1.80	1.20
1:A:10:GLN:O	1:A:11:SER:HB2	1.49	1.13
1:B:291:ARG:HD2	1:B:291:ARG:H	1.16	1.04
1:A:242:THR:HG22	1:A:244:GLU:H	1.24	1.01
1:A:293:HIS:O	1:A:294:LYS:N	1.94	0.99
1:B:420:VAL:HA	1:B:423:MET:HE2	1.48	0.95
1:B:86:THR:HB	1:B:89:GLU:HG3	1.49	0.94
1:B:81:ASN:HD22	1:B:81:ASN:H	1.15	0.93
1:A:404:SER:HB3	1:A:414:VAL:HG21	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:HIS:HE1	1:A:485:LYS:HB2	1.33	0.91
1:A:376:GLN:CD	1:B:192:ARG:HH11	1.76	0.88
1:A:376:GLN:HB3	1:B:192:ARG:NH1	1.88	0.88
1:A:295:HIS:HA	1:A:322:ARG:HH12	1.39	0.87
1:B:287:ASP:OD2	1:B:294:LYS:HB3	1.75	0.87
1:B:316:ASN:O	1:B:319:ARG:HG3	1.75	0.87
1:B:125:VAL:O	1:B:129:SER:HB2	1.76	0.86
1:A:242:THR:HB	1:A:245:GLU:HG3	1.58	0.85
1:A:375:TRP:HE1	1:A:412:GLN:HE21	1.20	0.84
1:B:143:ALA:HB3	1:B:146:GLU:HG3	1.60	0.84
1:B:67:VAL:HG11	1:B:197:ILE:HD11	1.59	0.84
1:B:136:LYS:HD2	1:B:155:GLU:OE1	1.78	0.81
1:A:53:ASN:HD22	1:A:56:LEU:HG	1.45	0.81
1:A:376:GLN:HE22	1:B:195:SER:HB3	1.43	0.81
1:A:20:MET:SD	1:B:19:LEU:HD23	2.22	0.80
1:B:242:THR:OG1	1:B:245:GLU:HG3	1.80	0.79
1:B:142:ARG:HB2	1:B:169:LYS:HB3	1.64	0.78
1:A:35:LEU:HD12	1:A:78:ILE:HD12	1.66	0.78
1:B:440:ALA:O	1:B:444:SER:HB3	1.84	0.78
1:B:170:GLU:H	1:B:170:GLU:CD	1.87	0.77
1:A:219:GLU:HG2	1:A:220:THR:H	1.47	0.77
1:B:312:GLN:HG3	1:B:339:LEU:HB3	1.65	0.77
1:B:288:MET:CE	1:B:320:PHE:HB3	2.15	0.76
1:B:291:ARG:CD	1:B:291:ARG:H	1.94	0.76
1:A:411:ALA:HA	1:B:191:TRP:CD1	2.20	0.76
1:A:266:ASN:ND2	1:A:355:ARG:HD3	2.00	0.76
1:A:420:VAL:HA	1:A:423:MET:HE2	1.65	0.76
1:B:446:HIS:HE1	1:B:485:LYS:HG3	1.51	0.75
1:A:219:GLU:HG2	1:A:220:THR:N	2.02	0.75
1:A:443:SER:C	1:A:445:PRO:HD2	2.07	0.75
1:A:335:SER:H	1:A:338:ILE:HD12	1.52	0.74
1:A:376:GLN:HB3	1:B:192:ARG:HH11	1.49	0.74
1:B:420:VAL:HA	1:B:423:MET:CE	2.19	0.73
1:A:129:SER:HA	1:A:132:ILE:HD12	1.71	0.73
1:A:331:PRO:HG2	1:A:334:VAL:HG13	1.70	0.72
1:B:381:VAL:O	1:B:384:GLU:HG2	1.90	0.72
1:A:406:HIS:CD2	1:A:422:ARG:HD2	2.24	0.72
1:A:10:GLN:O	1:A:11:SER:CB	2.26	0.72
1:A:446:HIS:CE1	1:A:485:LYS:HB2	2.22	0.72
1:B:33:ARG:O	1:B:34:GLU:HG2	1.90	0.72
1:B:64:ARG:H	1:B:81:ASN:HD21	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:HB	1:A:227:ILE:HD11	1.72	0.72
1:A:125:VAL:HA	1:B:19:LEU:HD11	1.73	0.71
1:A:30:ILE:HD11	1:A:33:ARG:NH2	2.05	0.71
1:A:122:GLN:HE21	1:A:255:HIS:CE1	2.08	0.71
1:B:446:HIS:CE1	1:B:485:LYS:HG3	2.26	0.71
1:B:81:ASN:HD22	1:B:81:ASN:N	1.87	0.71
1:B:288:MET:HE1	1:B:320:PHE:HB3	1.73	0.70
1:A:10:GLN:HB2	1:A:99:LYS:HD3	1.73	0.70
1:B:64:ARG:HG3	1:B:64:ARG:HH11	1.57	0.70
1:B:170:GLU:HG2	1:B:171:ASP:H	1.57	0.70
1:B:312:GLN:HG3	1:B:339:LEU:CB	2.21	0.69
1:B:21:ILE:HA	1:B:25:TYR:CG	2.27	0.69
1:A:122:GLN:HE21	1:A:255:HIS:HE1	1.38	0.69
1:A:376:GLN:HE22	1:B:195:SER:CB	2.06	0.68
1:A:172:ARG:HG2	1:A:173:GLY:N	2.08	0.68
1:A:376:GLN:CD	1:B:192:ARG:NH1	2.47	0.68
1:A:15:GLN:NE2	1:B:159:GLU:O	2.28	0.67
1:A:376:GLN:OE1	1:B:192:ARG:NH1	2.27	0.67
1:B:445:PRO:HG2	1:B:447:LEU:HD23	1.76	0.67
1:B:446:HIS:CD2	1:B:446:HIS:N	2.62	0.66
1:A:242:THR:HG22	1:A:244:GLU:N	2.05	0.66
1:A:273:GLU:HB3	1:A:328:SER:HB2	1.77	0.66
1:A:180:LEU:HD12	1:A:188:LEU:HD21	1.78	0.66
1:A:375:TRP:HE1	1:A:412:GLN:NE2	1.92	0.65
1:A:24:LEU:HB3	1:A:132:ILE:CD1	2.26	0.65
1:A:335:SER:N	1:A:338:ILE:HD12	2.11	0.65
1:B:423:MET:HE3	1:B:478:LYS:HD2	1.78	0.65
1:B:294:LYS:O	1:B:294:LYS:HG3	1.97	0.65
1:B:372:GLN:O	1:B:376:GLN:HG3	1.96	0.65
1:B:335:SER:HB2	1:B:338:ILE:H	1.61	0.64
1:B:423:MET:CE	1:B:478:LYS:HD2	2.28	0.64
1:A:19:LEU:HD13	1:B:20:MET:HE3	1.79	0.64
1:A:433:ILE:CD1	1:A:445:PRO:HG3	2.26	0.64
1:B:435:ALA:HB3	1:B:441:ALA:HB2	1.79	0.64
1:A:32:LEU:HD23	1:A:196:ILE:HG21	1.80	0.64
1:A:377:GLN:NE2	1:B:192:ARG:NH2	2.47	0.63
1:A:388:GLU:O	1:A:388:GLU:HG3	1.98	0.63
1:A:35:LEU:CD1	1:A:78:ILE:HD12	2.28	0.63
1:A:293:HIS:O	1:A:294:LYS:CA	2.45	0.63
1:A:331:PRO:C	1:A:333:ASN:H	2.01	0.63
1:A:440:ALA:O	1:A:444:SER:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:MET:HG2	1:B:427:GLN:NE2	2.14	0.62
1:A:435:ALA:HB1	1:A:440:ALA:HB3	1.81	0.62
1:B:93:HIS:CE1	1:B:120:ILE:HA	2.35	0.62
1:B:392:ASN:O	1:B:396:ILE:HG13	1.99	0.61
1:A:376:GLN:HG2	1:B:191:TRP:CH2	2.36	0.61
1:A:215:GLU:HA	1:A:220:THR:HA	1.82	0.61
1:B:445:PRO:CG	1:B:447:LEU:HD23	2.30	0.61
1:B:148:PRO:O	1:B:168:THR:HA	2.01	0.61
1:B:93:HIS:HE1	1:B:120:ILE:HG23	1.66	0.61
1:A:191:TRP:CD1	1:B:411:ALA:HA	2.36	0.61
1:A:122:GLN:NE2	1:A:255:HIS:HE1	1.99	0.60
1:A:435:ALA:HB3	1:A:441:ALA:HB2	1.82	0.60
1:B:123:PHE:HE2	1:B:176:ILE:HD11	1.66	0.60
1:A:294:LYS:O	1:A:294:LYS:HG2	2.01	0.60
1:A:419:TYR:CE2	1:A:430:ILE:HG23	2.37	0.60
1:A:51:LEU:H	1:A:51:LEU:HD12	1.67	0.60
1:B:272:GLN:NE2	1:B:347:ASN:HB3	2.17	0.59
1:A:86:THR:HG23	1:A:89:GLU:OE1	2.01	0.59
1:A:377:GLN:HE21	1:B:192:ARG:NH2	2.00	0.59
1:B:287:ASP:OD2	1:B:294:LYS:CB	2.49	0.59
1:B:242:THR:HG23	1:B:245:GLU:OE2	2.01	0.59
1:A:299:LEU:HD23	1:A:306:ILE:HG21	1.84	0.59
1:A:306:ILE:HG22	1:A:307:MET:HG2	1.83	0.59
1:B:331:PRO:O	1:B:334:VAL:HG22	2.02	0.59
1:A:242:THR:CG2	1:A:244:GLU:OE1	2.50	0.59
1:B:404:SER:HB3	1:B:414:VAL:HG21	1.84	0.59
1:B:153:PHE:HB2	1:B:167:ILE:HD13	1.85	0.59
1:B:206:LEU:O	1:B:228:ASN:ND2	2.36	0.59
1:A:57:TYR:HD2	1:A:61:GLY:HA2	1.67	0.59
1:A:355:ARG:HH11	1:A:355:ARG:HG3	1.67	0.59
1:A:87:ARG:O	1:A:91:ILE:HG13	2.03	0.59
1:B:416:LEU:O	1:B:420:VAL:HG23	2.03	0.58
1:A:460:LEU:HD23	1:A:460:LEU:N	2.18	0.58
1:A:169:LYS:HG2	1:A:171:ASP:O	2.04	0.58
1:B:433:ILE:HD13	1:B:445:PRO:HG3	1.85	0.58
1:A:226:LYS:HE3	1:A:228:ASN:O	2.03	0.58
1:A:87:ARG:HA	1:A:152:VAL:HG21	1.86	0.58
1:A:387:ALA:HB3	1:A:467:TRP:CH2	2.38	0.58
1:A:290:ASN:HD21	1:A:292:ASP:HB3	1.67	0.58
1:B:33:ARG:HB2	1:B:200:TYR:CG	2.40	0.57
1:A:331:PRO:O	1:A:334:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:SER:N	1:B:445:PRO:CD	2.67	0.57
1:A:290:ASN:ND2	1:A:292:ASP:HB3	2.19	0.57
1:A:376:GLN:NE2	1:B:192:ARG:HD2	2.19	0.57
1:B:207:PRO:HA	1:B:228:ASN:HD22	1.70	0.57
1:A:444:SER:N	1:A:445:PRO:HD2	2.20	0.56
1:A:74:ARG:HH11	1:A:74:ARG:HG2	1.69	0.56
1:B:233:LEU:HD23	1:B:249:PHE:CG	2.40	0.56
1:A:376:GLN:NE2	1:B:195:SER:CB	2.68	0.56
1:A:293:HIS:CD2	1:A:294:LYS:H	2.23	0.56
1:A:266:ASN:HD22	1:A:355:ARG:HD3	1.71	0.56
1:B:194:ARG:NH1	1:B:210:ILE:HD13	2.21	0.56
1:B:212:LYS:HD2	1:B:225:GLU:OE2	2.06	0.56
1:B:86:THR:HG22	1:B:88:ASP:H	1.69	0.56
1:B:21:ILE:HA	1:B:25:TYR:HB2	1.87	0.56
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.71	0.56
1:B:36:ILE:HG22	1:B:204:ILE:CD1	2.36	0.56
1:B:51:LEU:HD21	1:B:332:LEU:HD13	1.88	0.55
1:A:237:ASN:HB2	1:A:240:GLU:HG3	1.89	0.55
1:A:331:PRO:CG	1:A:334:VAL:HG13	2.36	0.55
1:B:244:GLU:CD	1:B:244:GLU:H	2.10	0.55
1:A:86:THR:OG1	1:A:89:GLU:HG3	2.07	0.55
1:A:423:MET:HE1	1:A:478:LYS:HG3	1.88	0.55
1:B:232:ALA:O	1:B:235:THR:HB	2.06	0.55
1:B:281:PRO:HG2	1:B:378:PHE:CZ	2.42	0.55
1:B:205:ALA:HB2	1:B:232:ALA:HA	1.88	0.54
1:B:410:SER:HB3	1:B:438:TYR:CD2	2.42	0.54
1:A:238:LYS:HE2	1:A:265:HIS:O	2.08	0.54
1:A:17:LEU:O	1:A:20:MET:N	2.40	0.54
1:A:262:THR:CG2	1:A:363:LEU:HD13	2.38	0.54
1:B:291:ARG:HD2	1:B:291:ARG:N	2.02	0.54
1:B:419:TYR:CE2	1:B:430:ILE:HG23	2.43	0.54
1:B:324:LEU:C	1:B:324:LEU:HD12	2.28	0.54
1:B:93:HIS:CE1	1:B:120:ILE:HG23	2.43	0.54
1:A:293:HIS:CG	1:A:294:LYS:H	2.25	0.53
1:A:367:ASP:OD2	1:A:370:LYS:HG3	2.08	0.53
1:B:210:ILE:HB	1:B:227:ILE:HD11	1.91	0.53
1:B:81:ASN:ND2	1:B:81:ASN:H	1.96	0.53
1:A:355:ARG:NH1	1:A:355:ARG:HG3	2.22	0.53
1:A:334:VAL:HA	1:A:338:ILE:HD12	1.90	0.53
1:A:90:VAL:HG13	1:A:94:LEU:HD12	1.89	0.53
1:A:257:PHE:HE2	1:B:257:PHE:HE2	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:NH2	1:A:384:GLU:OE2	2.41	0.53
1:A:447:LEU:HD12	1:A:450:LEU:HB2	1.91	0.53
1:A:476:ASP:C	1:A:478:LYS:H	2.13	0.53
1:B:408:ASP:HB2	1:B:442:LYS:HZ1	1.74	0.53
1:B:234:TRP:CE3	1:B:324:LEU:HD21	2.43	0.53
1:A:41:ASP:C	1:A:43:ALA:H	2.11	0.53
1:A:254:ALA:O	1:A:255:HIS:HB2	2.09	0.53
1:B:64:ARG:NH1	1:B:64:ARG:HG3	2.24	0.52
1:A:83:VAL:HG13	1:A:84:GLY:N	2.24	0.52
1:A:125:VAL:HG22	1:B:19:LEU:HD12	1.91	0.52
1:A:1:MET:HG3	1:A:167:ILE:HG22	1.90	0.52
1:B:469:MET:HE1	1:B:472:LEU:HB3	1.91	0.52
1:A:288:MET:CE	1:A:288:MET:HA	2.40	0.52
1:A:53:ASN:ND2	1:A:56:LEU:HG	2.19	0.52
1:A:257:PHE:CE2	1:B:257:PHE:HE2	2.28	0.52
1:B:226:LYS:NZ	1:B:230:ALA:HB3	2.24	0.52
1:B:135:ASP:HB3	1:B:181:ARG:NH1	2.24	0.52
1:A:431:TYR:CD1	1:A:431:TYR:N	2.78	0.52
1:A:13:VAL:O	1:A:17:LEU:HG	2.10	0.52
1:B:33:ARG:O	1:B:33:ARG:HG2	2.09	0.52
1:B:131:PHE:HA	1:B:134:ALA:O	2.10	0.52
1:A:429:LYS:O	1:A:431:TYR:CE1	2.63	0.52
1:A:376:GLN:CB	1:B:192:ARG:HH11	2.20	0.51
1:B:331:PRO:O	1:B:334:VAL:CG2	2.58	0.51
1:A:277:LEU:C	1:A:278:LEU:HD12	2.30	0.51
1:A:431:TYR:HA	1:A:481:GLN:O	2.10	0.51
1:B:85:MET:HB2	1:B:141:THR:HG21	1.92	0.51
1:A:274:TYR:CD1	1:A:274:TYR:C	2.84	0.51
1:A:447:LEU:HD12	1:A:447:LEU:O	2.11	0.51
1:A:235:THR:HG22	1:A:235:THR:O	2.09	0.51
1:B:33:ARG:HB2	1:B:200:TYR:CD2	2.46	0.51
1:A:314:MET:CE	1:A:356:VAL:HG21	2.40	0.51
1:A:19:LEU:HD22	1:B:24:LEU:CD1	2.41	0.50
1:A:424:LYS:HD2	1:A:454:GLY:O	2.11	0.50
1:A:469:MET:HE2	1:A:472:LEU:HB3	1.93	0.50
1:B:50:ALA:HB1	1:B:57:TYR:CE1	2.46	0.50
1:A:407:THR:C	1:A:409:SER:H	2.14	0.50
1:A:215:GLU:HA	1:A:219:GLU:O	2.12	0.50
1:A:418:ASP:HB3	1:A:422:ARG:NH2	2.26	0.50
1:A:250:TYR:OH	1:A:281:PRO:HB3	2.11	0.50
1:B:80:ASP:O	1:B:173:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:O	1:B:21:ILE:HG13	2.12	0.50
1:B:20:MET:C	1:B:22:HIS:N	2.64	0.50
1:B:141:THR:HA	1:B:169:LYS:HE3	1.94	0.50
1:A:331:PRO:C	1:A:333:ASN:N	2.65	0.50
1:A:186:GLU:HB2	1:A:192:ARG:HG2	1.94	0.50
1:B:447:LEU:HD12	1:B:447:LEU:O	2.12	0.49
1:A:306:ILE:HG22	1:A:307:MET:N	2.27	0.49
1:A:376:GLN:CB	1:B:192:ARG:NH1	2.70	0.49
1:A:290:ASN:ND2	1:A:292:ASP:O	2.44	0.49
1:A:74:ARG:HG2	1:A:74:ARG:NH1	2.27	0.49
1:B:195:SER:O	1:B:198:SER:HB3	2.11	0.49
1:A:403:ALA:HB2	1:A:412:GLN:HG2	1.93	0.49
1:A:46:LEU:HD21	1:A:172:ARG:NH1	2.27	0.49
1:B:25:TYR:HA	1:B:132:ILE:HD13	1.94	0.49
1:A:469:MET:HE2	1:A:472:LEU:CB	2.42	0.49
1:B:21:ILE:HA	1:B:25:TYR:CB	2.43	0.49
1:B:87:ARG:O	1:B:91:ILE:HG13	2.12	0.49
1:B:125:VAL:O	1:B:129:SER:CB	2.54	0.49
1:B:20:MET:HB3	1:B:25:TYR:CE1	2.48	0.49
1:A:407:THR:O	1:A:409:SER:N	2.46	0.49
1:B:293:HIS:HB2	1:B:295:HIS:ND1	2.27	0.49
1:A:12:GLU:C	1:A:13:VAL:HG23	2.33	0.49
1:B:355:ARG:NH1	1:B:355:ARG:HG2	2.28	0.49
1:A:433:ILE:HG22	1:A:434:THR:N	2.28	0.48
1:B:30:ILE:HD11	1:B:257:PHE:CE1	2.48	0.48
1:A:180:LEU:HD12	1:A:188:LEU:CD2	2.43	0.48
1:A:380:LEU:N	1:A:380:LEU:HD12	2.27	0.48
1:A:17:LEU:O	1:A:18:HIS:C	2.51	0.48
1:B:305:PHE:HZ	1:B:308:ASP:OD1	1.97	0.48
1:A:432:TYR:CZ	1:A:482:SER:HB3	2.49	0.48
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.78	0.48
1:A:404:SER:OG	1:A:405:THR:N	2.47	0.48
1:A:38:ASN:OD1	1:A:122:GLN:OE1	2.32	0.47
1:A:32:LEU:HD23	1:A:196:ILE:CG2	2.42	0.47
1:B:278:LEU:HD12	1:B:278:LEU:N	2.29	0.47
1:A:291:ARG:HH11	1:A:291:ARG:HG2	1.78	0.47
1:A:19:LEU:HD22	1:B:24:LEU:HD11	1.94	0.47
1:B:444:SER:N	1:B:445:PRO:HD2	2.29	0.47
1:B:16:LEU:HG	1:B:17:LEU:N	2.29	0.47
1:A:293:HIS:NE2	1:A:311:GLU:OE2	2.46	0.47
1:B:288:MET:HE3	1:B:320:PHE:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:SER:O	1:A:423:MET:N	2.47	0.47
1:A:262:THR:HG21	1:A:363:LEU:HD13	1.96	0.47
1:A:140:ARG:HH11	1:A:167:ILE:HD12	1.80	0.47
1:A:50:ALA:HB1	1:A:57:TYR:HE1	1.78	0.47
1:A:211:GLU:HB2	1:A:224:TRP:CZ3	2.49	0.47
1:A:57:TYR:CD2	1:A:61:GLY:HA2	2.46	0.47
1:A:210:ILE:CB	1:A:227:ILE:HD11	2.42	0.47
1:B:389:ASP:OD1	1:B:392:ASN:HB2	2.15	0.47
1:A:335:SER:H	1:A:338:ILE:CD1	2.26	0.47
1:B:464:ILE:O	1:B:464:ILE:HG12	2.15	0.47
1:A:87:ARG:CA	1:A:152:VAL:HG21	2.44	0.47
1:B:74:ARG:HG2	1:B:74:ARG:HH11	1.80	0.47
1:B:187:PHE:HA	1:B:193:VAL:HG22	1.96	0.46
1:A:219:GLU:CG	1:A:220:THR:H	2.21	0.46
1:A:429:LYS:HB2	1:A:431:TYR:CZ	2.50	0.46
1:A:210:ILE:CG2	1:A:227:ILE:HD11	2.44	0.46
1:B:147:LYS:HB2	1:B:150:ASN:ND2	2.31	0.46
1:A:433:ILE:CG2	1:A:434:THR:N	2.78	0.46
1:A:433:ILE:HD13	1:A:445:PRO:HG3	1.96	0.46
1:B:187:PHE:HA	1:B:193:VAL:CG2	2.45	0.46
1:B:335:SER:HB2	1:B:338:ILE:HG13	1.98	0.46
1:B:281:PRO:HG2	1:B:378:PHE:HZ	1.81	0.46
1:B:240:GLU:H	1:B:240:GLU:HG2	1.58	0.46
1:B:36:ILE:HG22	1:B:204:ILE:HD12	1.98	0.46
1:A:85:MET:HB2	1:A:141:THR:HG21	1.98	0.46
1:B:404:SER:OG	1:B:405:THR:N	2.49	0.46
1:A:389:ASP:OD1	1:A:392:ASN:ND2	2.49	0.46
1:A:197:ILE:HG23	1:A:208:VAL:HG11	1.98	0.46
1:B:199:LYS:O	1:B:199:LYS:HG2	2.16	0.46
1:B:25:TYR:O	1:B:26:SER:C	2.54	0.45
1:A:206:LEU:O	1:A:228:ASN:OD1	2.34	0.45
1:B:49:ARG:HB3	1:B:56:LEU:CD1	2.46	0.45
1:B:251:LYS:HE3	1:B:259:ASP:OD1	2.16	0.45
1:B:20:MET:HE3	1:B:24:LEU:HD12	1.99	0.45
1:A:86:THR:O	1:A:89:GLU:N	2.49	0.45
1:B:181:ARG:HH11	1:B:181:ARG:HG2	1.81	0.45
1:A:147:LYS:CG	1:A:148:PRO:HD2	2.47	0.45
1:A:331:PRO:HD2	1:A:334:VAL:CG1	2.46	0.45
1:B:272:GLN:HE22	1:B:347:ASN:C	2.20	0.45
1:A:472:LEU:HD22	1:A:480:PHE:CE1	2.52	0.45
1:B:237:ASN:O	1:B:240:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD13	1:B:16:LEU:HA	1.99	0.45
1:A:219:GLU:CG	1:A:220:THR:N	2.75	0.45
1:A:24:LEU:HB3	1:A:132:ILE:HD11	1.99	0.45
1:B:301:VAL:HG23	1:B:306:ILE:HG13	1.98	0.45
1:A:234:TRP:CE3	1:A:324:LEU:HD21	2.52	0.45
1:A:94:LEU:HB3	1:A:154:TRP:CE2	2.52	0.45
1:A:303:ARG:HA	1:A:326:ASP:OD2	2.17	0.45
1:B:253:ILE:HG13	1:B:254:ALA:N	2.31	0.45
1:A:41:ASP:C	1:A:43:ALA:N	2.70	0.44
1:A:14:LYS:O	1:A:15:GLN:C	2.56	0.44
1:B:145:GLY:O	1:B:146:GLU:HG2	2.17	0.44
1:A:331:PRO:O	1:A:333:ASN:N	2.51	0.44
1:A:302:GLN:O	1:A:303:ARG:HB3	2.17	0.44
1:B:331:PRO:HB2	1:B:333:ASN:OD1	2.18	0.44
1:A:383:LYS:O	1:A:386:PRO:HD2	2.18	0.44
1:B:270:GLY:O	1:B:271:LYS:C	2.55	0.44
1:A:140:ARG:NH1	1:A:167:ILE:HD12	2.32	0.44
1:A:196:ILE:O	1:A:199:LYS:HB3	2.17	0.44
1:A:314:MET:HE2	1:A:321:VAL:HB	2.00	0.44
1:A:71:LYS:HA	1:A:188:LEU:HD13	1.98	0.44
1:B:226:LYS:HE3	1:B:228:ASN:O	2.17	0.44
1:A:317:TYR:CD1	1:A:385:GLY:HA3	2.53	0.44
1:B:294:LYS:HG3	1:B:322:ARG:NH2	2.33	0.44
1:A:415:SER:HB3	1:A:418:ASP:CG	2.37	0.44
1:B:301:VAL:CG1	1:B:332:LEU:HD23	2.48	0.44
1:B:133:VAL:HG11	1:B:187:PHE:CE1	2.53	0.44
1:A:373:THR:O	1:A:376:GLN:HB2	2.18	0.43
1:A:443:SER:C	1:A:445:PRO:CD	2.81	0.43
1:B:445:PRO:HB2	1:B:446:HIS:H	1.61	0.43
1:A:331:PRO:CD	1:A:334:VAL:HG13	2.48	0.43
1:A:122:GLN:C	1:A:124:GLY:H	2.20	0.43
1:A:423:MET:O	1:A:424:LYS:C	2.56	0.43
1:A:122:GLN:C	1:A:124:GLY:N	2.71	0.43
1:A:7:ARG:NH1	1:A:91:ILE:HD13	2.34	0.43
1:B:226:LYS:HZ1	1:B:230:ALA:HB3	1.83	0.43
1:A:444:SER:N	1:A:445:PRO:CD	2.81	0.43
1:B:214:GLU:HB3	1:B:216:LYS:HE3	1.99	0.43
1:B:438:TYR:CZ	1:B:442:LYS:HD2	2.54	0.43
1:A:319:ARG:NH2	1:A:381:VAL:HG13	2.34	0.43
1:B:274:TYR:CD1	1:B:274:TYR:C	2.92	0.43
1:B:31:PHE:CG	1:B:32:LEU:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HB3	1:A:224:TRP:CZ3	2.54	0.43
1:B:432:TYR:O	1:B:482:SER:HA	2.19	0.43
1:A:12:GLU:O	1:A:13:VAL:HG23	2.17	0.43
1:A:415:SER:HB3	1:A:418:ASP:OD1	2.19	0.43
1:A:273:GLU:HB3	1:A:328:SER:CB	2.48	0.43
1:B:194:ARG:HH21	1:B:225:GLU:CD	2.22	0.43
1:B:18:HIS:O	1:B:20:MET:N	2.52	0.43
1:A:432:TYR:C	1:A:432:TYR:CD1	2.92	0.43
1:B:49:ARG:HH11	1:B:49:ARG:HG2	1.84	0.43
1:B:375:TRP:CE2	1:B:401:ARG:HB2	2.54	0.43
1:A:324:LEU:C	1:A:324:LEU:HD12	2.39	0.42
1:B:469:MET:CE	1:B:472:LEU:HD23	2.49	0.42
1:A:263:TRP:HB3	1:A:279:TYR:CD2	2.53	0.42
1:B:330:LEU:HD23	1:B:331:PRO:HD2	1.99	0.42
1:B:325:ILE:HD12	1:B:352:LEU:HD11	2.00	0.42
1:B:348:LEU:O	1:B:352:LEU:HG	2.18	0.42
1:A:47:ARG:O	1:A:50:ALA:HB3	2.19	0.42
1:A:372:GLN:O	1:A:376:GLN:HG3	2.20	0.42
1:A:125:VAL:HG23	1:B:18:HIS:NE2	2.34	0.42
1:A:12:GLU:O	1:A:13:VAL:CG2	2.67	0.42
1:B:226:LYS:O	1:B:226:LYS:HG3	2.18	0.42
1:B:194:ARG:NH2	1:B:225:GLU:CD	2.72	0.42
1:A:314:MET:HE1	1:A:356:VAL:HG21	2.00	0.42
1:B:262:THR:HG22	1:B:263:TRP:H	1.84	0.42
1:A:370:LYS:O	1:A:373:THR:HB	2.19	0.42
1:A:95:GLY:HA2	1:A:162:TYR:CE2	2.54	0.42
1:A:127:PHE:O	1:A:130:ALA:HB3	2.19	0.42
1:A:73:LYS:HB2	1:A:75:THR:HG23	2.01	0.42
1:B:420:VAL:HG13	1:B:423:MET:CE	2.49	0.42
1:A:472:LEU:HD22	1:A:480:PHE:HE1	1.85	0.42
1:A:261:LEU:HD12	1:A:281:PRO:O	2.20	0.42
1:B:20:MET:O	1:B:22:HIS:N	2.53	0.42
1:A:331:PRO:HD2	1:A:334:VAL:HG13	2.01	0.42
1:A:273:GLU:CB	1:A:328:SER:HB2	2.48	0.42
1:A:234:TRP:HA	1:A:265:HIS:CE1	2.55	0.42
1:B:406:HIS:ND1	1:B:406:HIS:O	2.53	0.42
1:B:170:GLU:CG	1:B:171:ASP:H	2.29	0.41
1:A:406:HIS:HD2	1:A:422:ARG:HD2	1.81	0.41
1:A:30:ILE:O	1:A:33:ARG:N	2.53	0.41
1:B:35:LEU:HD22	1:B:176:ILE:CD1	2.50	0.41
1:B:386:PRO:HG2	1:B:468:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD12	1:A:207:PRO:HD2	2.02	0.41
1:A:375:TRP:CZ3	1:A:379:GLY:HA2	2.55	0.41
1:A:13:VAL:HG12	1:A:14:LYS:N	2.32	0.41
1:A:416:LEU:HD23	1:A:416:LEU:HA	1.82	0.41
1:B:406:HIS:CG	1:B:406:HIS:O	2.72	0.41
1:B:65:VAL:HG13	1:B:208:VAL:HA	2.03	0.41
1:B:322:ARG:HA	1:B:322:ARG:HD3	1.64	0.41
1:A:406:HIS:HB2	1:A:456:GLU:OE1	2.21	0.41
1:A:419:TYR:CD2	1:A:430:ILE:HG23	2.55	0.41
1:B:250:TYR:OH	1:B:281:PRO:HB3	2.21	0.41
1:A:319:ARG:CZ	1:A:381:VAL:HG13	2.51	0.41
1:A:168:THR:O	1:A:168:THR:CG2	2.67	0.41
1:A:86:THR:O	1:A:87:ARG:C	2.59	0.41
1:B:74:ARG:NH1	1:B:74:ARG:HG2	2.36	0.41
1:A:378:PHE:O	1:A:379:GLY:C	2.58	0.41
1:A:14:LYS:HB3	1:A:15:GLN:H	1.54	0.41
1:A:17:LEU:O	1:A:19:LEU:N	2.53	0.41
1:A:418:ASP:O	1:A:421:SER:HB2	2.20	0.41
1:B:469:MET:HE1	1:B:472:LEU:HD23	2.03	0.41
1:A:288:MET:HA	1:A:288:MET:HE3	2.03	0.41
1:A:156:SER:C	1:A:158:GLY:H	2.24	0.41
1:A:155:GLU:O	1:A:156:SER:HB2	2.21	0.41
1:A:300:TYR:CE1	1:A:324:LEU:HD22	2.56	0.41
1:A:181:ARG:NH1	1:A:181:ARG:HG2	2.36	0.40
1:B:196:ILE:O	1:B:197:ILE:C	2.57	0.40
1:B:446:HIS:H	1:B:446:HIS:CD2	2.39	0.40
1:A:333:ASN:O	1:A:334:VAL:O	2.40	0.40
1:A:51:LEU:HD12	1:A:51:LEU:N	2.34	0.40
1:B:82:GLY:O	1:B:172:ARG:HD2	2.22	0.40
1:A:354:LYS:HB2	1:A:354:LYS:HE3	1.84	0.40
1:B:95:GLY:O	1:B:96:THR:C	2.60	0.40
1:B:312:GLN:HG3	1:B:339:LEU:HB2	2.00	0.40
1:A:284:ALA:HA	1:A:285:PRO:HD3	1.94	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	468/559 (84%)	386 (82%)	60 (13%)	22 (5%)	3 11
1	B	450/559 (80%)	397 (88%)	40 (9%)	13 (3%)	6 23
All	All	918/1118 (82%)	783 (85%)	100 (11%)	35 (4%)	4 16

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	LYS
1	A	15	GLN
1	A	17	LEU
1	A	293	HIS
1	A	294	LYS
1	A	334	VAL
1	A	422	ARG
1	B	17	LEU
1	B	18	HIS
1	B	159	GLU
1	B	217	ASP
1	B	293	HIS
1	B	294	LYS
1	B	484	SER
1	A	9	PHE
1	A	13	VAL
1	A	58	GLU
1	A	101	GLY
1	A	287	ASP
1	A	408	ASP
1	A	421	SER
1	A	448	GLU
1	B	19	LEU
1	B	58	GLU

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Mol	Chain	Res	Type
1	B	215	GLU
1	B	486	VAL
1	A	160	GLY
1	B	96	THR
1	B	445	PRO
1	A	82	GLY
1	A	332	LEU
1	A	18	HIS
1	A	50	ALA
1	A	445	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	416/488 (85%)	395 (95%)	21 (5%)	30 65
1	B	401/488 (82%)	377 (94%)	24 (6%)	24 57
All	All	817/976 (84%)	772 (94%)	45 (6%)	27 61

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	64	ARG
1	A	128	TYR
1	A	168	THR
1	A	171	ASP
1	A	215	GLU
1	A	228	ASN
1	A	231	GLN
1	A	239	SER
1	A	273	GLU
1	A	288	MET
1	A	308	ASP
1	A	319	ARG

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Mol	Chain	Res	Type
1	A	324	LEU
1	A	361	GLU
1	A	388	GLU
1	A	437	SER
1	A	446	HIS
1	A	460	LEU
1	A	472	LEU
1	A	473	THR
1	B	16	LEU
1	B	58	GLU
1	B	81	ASN
1	B	133	VAL
1	B	170	GLU
1	B	171	ASP
1	B	172	ARG
1	B	235	THR
1	B	236	ARG
1	B	239	SER
1	B	240	GLU
1	B	242	THR
1	B	262	THR
1	B	278	LEU
1	B	291	ARG
1	B	299	LEU
1	B	312	GLN
1	B	324	LEU
1	B	334	VAL
1	B	348	LEU
1	B	380	LEU
1	B	434	THR
1	B	436	ASP
1	B	446	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	53	ASN
1	A	122	GLN
1	A	203	HIS
1	A	228	ASN
1	A	255	HIS

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Mol	Chain	Res	Type
1	A	266	ASN
1	A	290	ASN
1	A	347	ASN
1	A	376	GLN
1	A	412	GLN
1	B	81	ASN
1	B	93	HIS
1	B	150	ASN
1	B	203	HIS
1	B	228	ASN
1	B	231	GLN
1	B	255	HIS
1	B	266	ASN
1	B	272	GLN
1	B	283	GLN
1	B	446	HIS

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	472/559 (84%)	0.49	37 (7%)	16	10	34, 66, 101, 101	0
1	B	454/559 (81%)	0.43	29 (6%)	23	16	19, 46, 99, 101	0
All	All	926/1118 (82%)	0.46	66 (7%)	19	13	19, 57, 101, 101	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	12.3
1	A	488	GLU	9.8
1	B	487	ASP	9.7
1	A	489	SER	8.8
1	A	12	GLU	8.7
1	B	486	VAL	8.6
1	A	11	SER	7.1
1	B	18	HIS	7.1
1	B	98	ALA	6.7
1	A	289	TRP	6.6
1	A	10	GLN	6.5
1	B	25	TYR	6.0
1	B	17	LEU	5.9
1	A	487	ASP	5.5
1	B	120	ILE	5.3
1	B	97	ILE	4.9
1	B	485	LYS	4.7
1	B	19	LEU	4.5
1	A	17	LEU	4.4
1	B	489	SER	4.3
1	B	215	GLU	4.1
1	B	488	GLU	4.0
1	A	122	GLN	3.9
1	A	486	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	291	ARG	3.5
1	A	20	MET	3.4
1	A	484	SER	3.4
1	A	444	SER	3.1
1	B	443	SER	3.1
1	B	216	LYS	3.0
1	A	120	ILE	3.0
1	B	286	TRP	2.9
1	B	159	GLU	2.9
1	B	220	THR	2.9
1	A	51	LEU	2.9
1	B	24	LEU	2.8
1	A	14	LYS	2.8
1	A	3	GLY	2.8
1	B	20	MET	2.8
1	A	292	ASP	2.8
1	B	213	ARG	2.7
1	A	1	MET	2.7
1	B	16	LEU	2.7
1	A	449	LEU	2.7
1	A	431	TYR	2.6
1	B	217	ASP	2.6
1	B	192	ARG	2.6
1	A	485	LYS	2.6
1	B	121	GLY	2.5
1	A	2	LYS	2.5
1	A	286	TRP	2.5
1	A	443	SER	2.4
1	A	102	THR	2.4
1	A	450	LEU	2.4
1	A	455	ILE	2.3
1	B	219	GLU	2.3
1	A	257	PHE	2.3
1	A	334	VAL	2.3
1	A	290	ASN	2.2
1	B	390	PHE	2.2
1	A	16	LEU	2.2
1	A	288	MET	2.2
1	B	444	SER	2.1
1	A	21	ILE	2.1
1	B	158	GLY	2.1
1	A	293	HIS	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.