



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:11 AM UTC

PDB ID : 1Y4U / pdb_00001y4u
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

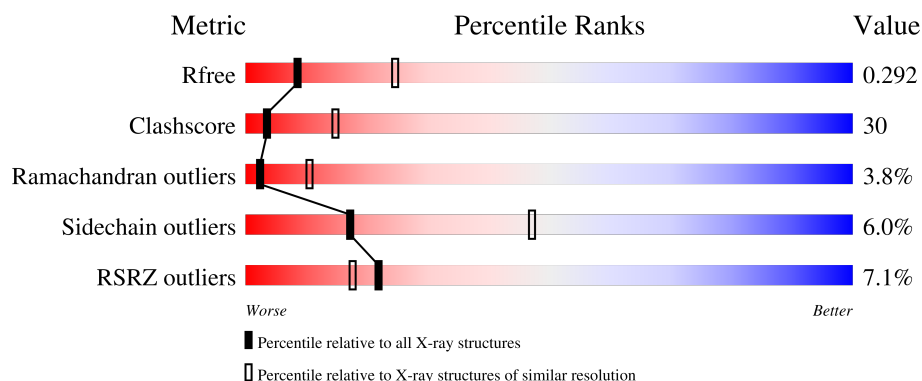
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	7% 41% 37% 6% 16%
1	B	559	5% 44% 31% 6% 19%

2 Entry composition

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.

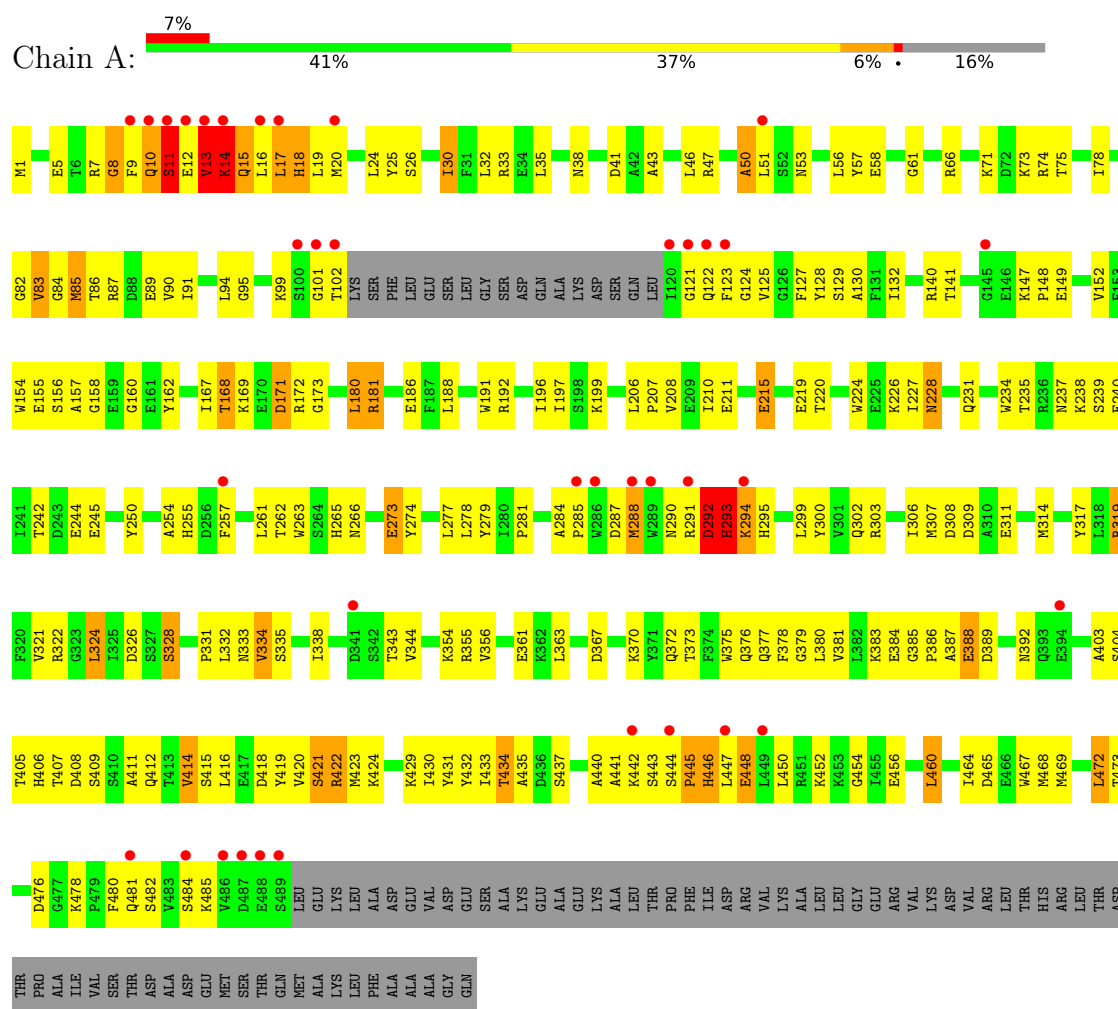
- Molecule 1 is a protein called Chaperone protein htpG.

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			

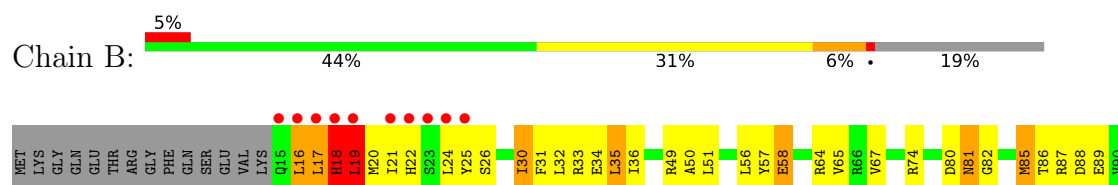
3 Residue-property plots

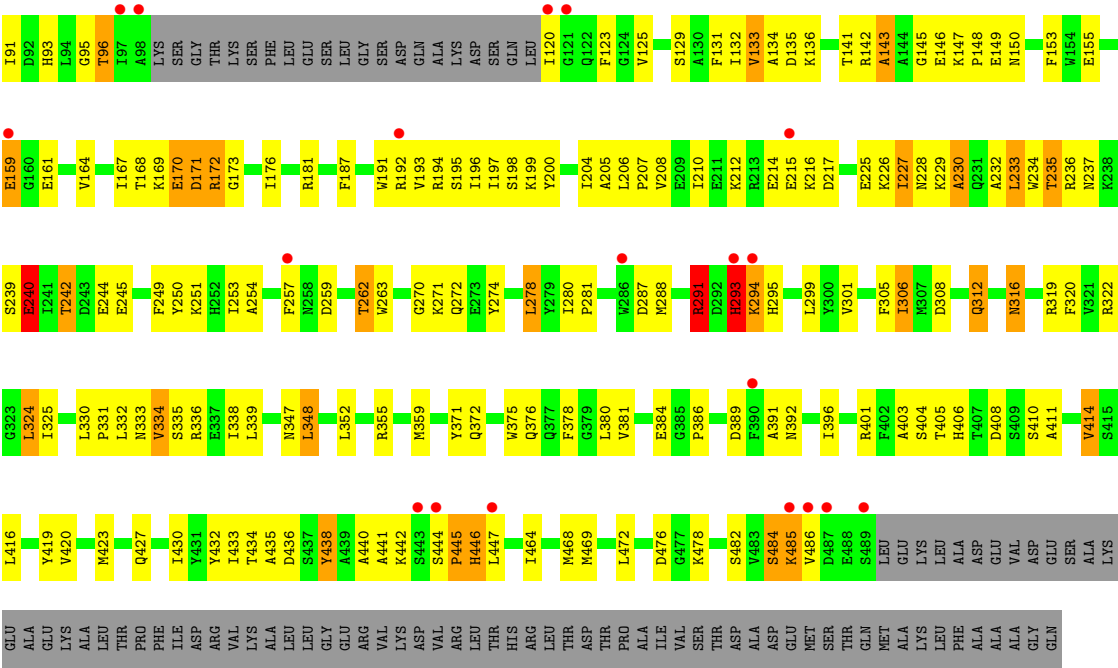
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Chaperone protein htpG





4 Data and refinement statistics

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 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 90.1 (50.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	3219 reflections (9.99%)	wwPDB-VP
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 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	7/3913 (0.2%)	1.47	24/5277 (0.5%)
1	B	0.57	0/3774	1.05	22/5095 (0.4%)
All	All	0.84	7/7687 (0.1%)	1.28	46/10372 (0.4%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	HIS	C-O	44.72	1.80	1.24
1	A	8	GLY	C-N	-26.69	0.96	1.33
1	A	8	GLY	C-O	12.92	1.41	1.23
1	A	10	GLN	C-N	-12.30	1.16	1.33
1	A	13	VAL	CA-C	8.44	1.63	1.52
1	A	14	LYS	N-CA	5.87	1.53	1.46
1	A	11	SER	N-CA	5.65	1.53	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	GLY	O-C-N	-53.79	74.47	123.42
1	A	293	HIS	O-C-N	-35.79	75.00	122.59
1	A	8	GLY	CA-C-N	24.62	168.57	121.54
1	A	8	GLY	C-N-CA	24.62	168.57	121.54
1	A	8	GLY	CA-C-O	-17.00	104.25	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	VAL	N-CA-C	12.27	134.85	109.34
1	A	14	LYS	N-CA-C	10.85	133.91	110.80
1	B	336	ARG	N-CA-C	-9.89	100.50	111.28
1	A	25	TYR	N-CA-C	-8.60	102.17	114.12
1	B	438	TYR	N-CA-C	-7.42	103.13	111.07
1	A	83	VAL	N-CA-C	7.31	117.40	110.53
1	B	230	ALA	N-CA-C	7.27	121.27	111.24
1	A	293	HIS	N-CA-C	6.97	125.64	110.80
1	B	403	ALA	N-CA-C	-6.90	101.24	110.55
1	A	180	LEU	N-CA-C	6.82	120.19	109.96
1	B	293	HIS	N-CA-C	6.79	125.27	110.80
1	A	442	LYS	N-CA-C	6.20	117.73	110.97
1	A	157	ALA	N-CA-C	-6.12	105.86	113.15
1	B	484	SER	N-CA-C	6.06	123.70	110.80
1	A	13	VAL	CB-CA-C	-5.97	101.49	111.29
1	A	11	SER	N-CA-C	5.90	123.36	110.80
1	A	414	VAL	N-CA-C	5.80	117.10	108.23
1	B	391	ALA	N-CA-C	-5.79	104.93	112.23
1	B	35	LEU	N-CA-C	-5.78	104.98	111.28
1	B	240	GLU	N-CA-C	5.73	119.26	112.72
1	A	30	ILE	N-CA-C	5.69	116.42	110.62
1	B	18	HIS	N-CA-C	5.55	122.63	110.80
1	B	143	ALA	N-CA-C	5.55	117.23	110.41
1	A	8	GLY	N-CA-C	5.49	119.63	111.18
1	A	181	ARG	N-CA-C	-5.46	103.28	110.43
1	B	306	ILE	CB-CA-C	-5.45	107.08	111.71
1	B	485	LYS	N-CA-C	5.44	118.47	110.59
1	A	328	SER	N-CA-C	-5.40	106.70	113.72
1	A	484	SER	N-CA-C	5.37	117.65	110.35
1	B	229	LYS	N-CA-C	-5.36	106.00	112.54
1	B	227	ILE	CA-C-N	5.36	128.47	120.87
1	B	227	ILE	C-N-CA	5.36	128.47	120.87
1	B	233	LEU	N-CA-C	5.25	117.41	111.11
1	A	292	ASP	N-CA-C	-5.25	104.15	110.44
1	B	161	GLU	N-CA-C	5.22	117.25	108.73
1	B	30	ILE	N-CA-C	5.21	115.83	110.36
1	A	26	SER	N-CA-C	-5.21	106.19	112.54
1	B	85	MET	N-CA-C	5.19	117.31	109.41
1	B	291	ARG	N-CA-C	-5.15	105.84	111.82
1	B	414	VAL	N-CA-C	5.14	115.98	108.58
1	A	85	MET	N-CA-C	5.04	117.47	109.50

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 ⓘ

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	3754	262	0
1	B	3699	0	3612	207	0
All	All	7536	0	7366	441	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (441) 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:O	1:A:293:HIS:C	1.80	1.25
1:A:10:GLN:O	1:A:11:SER:HB2	1.49	1.13
1:B:291:ARG:H	1:B:291:ARG:HD2	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:423:MET:HE1	1:B:478:LYS:HD2	1.47	0.97
1:A:314:MET:HE1	1:A:356:VAL:HG21	1.47	0.96
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:B:420:VAL:HA	1:B:423:MET:HE2	1.50	0.93
1:A:376:GLN:CD	1:B:192:ARG:HH11	1.76	0.93
1:B:468:MET:HE3	1:B:469:MET:HE3	1.52	0.92
1:A:404:SER:HB3	1:A:414:VAL:HG21	1.50	0.91
1:A:446:HIS:HE1	1:A:485:LYS:HB2	1.33	0.91
1:B:288:MET:HE1	1:B:320:PHE:HB3	1.52	0.90
1:A:376:GLN:HB3	1:B:192:ARG:NH1	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:GLU:CD	1:B:170:GLU:H	1.87	0.82
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:A:443:SER:C	1:A:445:PRO:HD2	2.07	0.80
1:A:420:VAL:HA	1:A:423:MET:HE2	1.64	0.79
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: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:H	1:B:291:ARG:CD	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:B:20:MET:HE3	1:B:24:LEU:HD12	1.67	0.76
1:A:219:GLU:HG2	1:A:220:THR:N	2.02	0.75
1:B:446:HIS:HE1	1:B:485:LYS:HG3	1.51	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:469:MET:HE1	1:B:472:LEU:HD23	1.70	0.73
1:A:129:SER:HA	1:A:132:ILE:HD12	1.71	0.73
1:B:420:VAL:HA	1:B:423:MET:CE	2.19	0.73
1:A:331:PRO:HG2	1:A:334:VAL:HG13	1.70	0.72
1:A:376:GLN:CD	1:B:192:ARG:NH1	2.47	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:A:210:ILE:HB	1:A:227:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:H	1:B:81:ASN:HD21	1.37	0.72
1:A:30:ILE:HD11	1:A:33:ARG:NH2	2.05	0.71
1:A:125:VAL:HA	1:B:19:LEU:HD11	1.73	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: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:288:MET:HE3	1:A:288:MET:HA	1.76	0.68
1:A:331:PRO:C	1:A:333:ASN:H	2.01	0.67
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:N	1:B:446:HIS:CD2	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: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: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:HG3	1:A:388:GLU:O	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:314:MET:HE2	1:A:321:VAL:HB	1.81	0.62
1:A:440:ALA:O	1:A:444:SER:HB3	1.99	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ASN:O	1:B:396:ILE:HG13	1.99	0.61
1:A:215:GLU:HA	1:A:220:THR:HA	1.82	0.61
1:A:376:GLN:HG2	1:B:191:TRP:CH2	2.36	0.61
1:B:148:PRO:O	1:B:168:THR:HA	2.01	0.61
1:B:445:PRO:CG	1:B:447:LEU:HD23	2.30	0.61
1:A:191:TRP:CD1	1:B:411:ALA:HA	2.36	0.61
1:B:93:HIS:HE1	1:B:120:ILE:HG23	1.66	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:244:GLU:CD	1:B:244:GLU:H	2.10	0.60
1:A:86:THR:HG23	1:A:89:GLU:OE1	2.01	0.59
1:B:272:GLN:NE2	1:B:347:ASN:HB3	2.17	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:A:377:GLN:HE21	1:B:192:ARG:NH2	2.00	0.59
1:B:242:THR:HG23	1:B:245:GLU:OE2	2.01	0.59
1:B:287:ASP:OD2	1:B:294:LYS:CB	2.49	0.59
1:B:331:PRO:O	1:B:334:VAL:HG22	2.02	0.59
1:B:469:MET:HE2	1:B:469:MET:HA	1.84	0.59
1:A:242:THR:CG2	1:A:244:GLU:OE1	2.50	0.59
1:B:153:PHE:HB2	1:B:167:ILE:HD13	1.85	0.59
1:B:404:SER:HB3	1:B:414:VAL:HG21	1.84	0.59
1:A:57:TYR:HD2	1:A:61:GLY:HA2	1.67	0.59
1:B:206:LEU:O	1:B:228:ASN:ND2	2.36	0.59
1:B:423:MET:CE	1:B:478:LYS:HD2	2.28	0.59
1:A:355:ARG:HG3	1:A:355:ARG:HH11	1.67	0.59
1:A:468:MET:HE3	1:A:469:MET:HE3	1.85	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:169:LYS:HG2	1:A:171:ASP:O	2.04	0.58
1:A:460:LEU:HD23	1:A:460:LEU:N	2.18	0.58
1:B:324:LEU:C	1:B:324:LEU:HD12	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:290:ASN:ND2	1:A:292:ASP:HB3	2.19	0.57
1:A:476:ASP:C	1:A:478:LYS:H	2.13	0.57
1:B:444:SER:N	1:B:445:PRO:CD	2.67	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: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:277:LEU:C	1:A:278:LEU:HD12	2.30	0.56
1:A:376:GLN:NE2	1:B:195:SER:CB	2.68	0.56
1:A:444:SER:N	1:A:445:PRO:HD2	2.20	0.56
1:A:41:ASP:C	1:A:43:ALA:H	2.11	0.56
1:A:266:ASN:HD22	1:A:355:ARG:HD3	1.71	0.56
1:A:293:HIS:CD2	1:A:294:LYS:H	2.23	0.56
1:A:274:TYR:CD1	1:A:274:TYR:C	2.84	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:21:ILE:HA	1:B:25:TYR:HB2	1.87	0.56
1:B:86:THR:HG22	1:B:88:ASP:H	1.69	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:A:237:ASN:HB2	1:A:240:GLU:HG3	1.89	0.55
1:B:51:LEU:HD21	1:B:332:LEU:HD13	1.88	0.55
1:A:331:PRO:CG	1:A:334:VAL:HG13	2.36	0.55
1:A:86:THR:OG1	1:A:89:GLU:HG3	2.07	0.55
1:A:407:THR:C	1:A:409:SER:H	2.14	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:20:MET:C	1:B:22:HIS:N	2.64	0.54
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: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:A:12:GLU:C	1:A:13:VAL:HG23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:MET:HE2	1:A:469:MET:HA	1.90	0.53
1:B:210:ILE:HB	1:B:227:ILE:HD11	1.91	0.53
1:A:334:VAL:HA	1:A:338:ILE:HD12	1.90	0.53
1:A:355:ARG:HG3	1:A:355:ARG:NH1	2.22	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
1:A:469:MET:HE1	1:A:472:LEU:CD1	2.38	0.53
1:A:17:LEU:O	1:A:18:HIS:C	2.51	0.53
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:443:SER:C	1:A:445:PRO:CD	2.81	0.53
1:B:234:TRP:CE3	1:B:324:LEU:HD21	2.43	0.53
1:A:254:ALA:O	1:A:255:HIS:HB2	2.09	0.53
1:A:83:VAL:HG13	1:A:84:GLY:N	2.24	0.52
1:B:64:ARG:HG3	1:B:64:ARG:NH1	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: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:A:431:TYR:N	1:A:431:TYR:CD1	2.78	0.52
1:A:469:MET:HE1	1:A:472:LEU:HD13	1.91	0.52
1:B:135:ASP:HB3	1:B:181:ARG:NH1	2.24	0.52
1:B:226:LYS:NZ	1:B:230:ALA:HB3	2.24	0.52
1:A:13:VAL:O	1:A:17:LEU:HG	2.10	0.52
1:A:314:MET:HE2	1:A:321:VAL:CB	2.39	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:423:MET:HE1	1:A:478:LYS:HG3	1.91	0.52
1:A:429:LYS:O	1:A:431:TYR:CE1	2.63	0.52
1:A:19:LEU:HD13	1:B:20:MET:HE1	1.91	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: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:235:THR:HG22	1:A:235:THR:O	2.09	0.51
1:A:447:LEU:HD12	1:A:447:LEU:O	2.11	0.51
1:B:33:ARG:HB2	1:B:200:TYR:CD2	2.46	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:331:PRO:C	1:A:333:ASN:N	2.65	0.50
1:A:288:MET:HA	1:A:288:MET:CE	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:O	1:B:26:SER:C	2.54	0.50
1:B:50:ALA:HB1	1:B:57:TYR:CE1	2.46	0.50
1:A:215:GLU:HA	1:A:219:GLU:O	2.12	0.50
1:A:16:LEU:HB3	1:A:20:MET:HE3	1.94	0.50
1:A:250:TYR:OH	1:A:281:PRO:HB3	2.11	0.50
1:A:418:ASP:HB3	1:A:422:ARG:NH2	2.26	0.50
1:B:80:ASP:O	1:B:173:GLY:HA3	2.11	0.50
1:B:17:LEU:O	1:B:21:ILE:HG13	2.12	0.50
1:B:141:THR:HA	1:B:169:LYS:HE3	1.94	0.50
1:A:186:GLU:HB2	1:A:192:ARG:HG2	1.94	0.50
1:A:306:ILE:HG22	1:A:307:MET:N	2.27	0.49
1:A:415:SER:HB3	1:A:418:ASP:CG	2.37	0.49
1:B:447:LEU:HD12	1:B:447:LEU:O	2.12	0.49
1:A:74:ARG:HG2	1:A:74:ARG:NH1	2.27	0.49
1:A:290:ASN:ND2	1:A:292:ASP:O	2.44	0.49
1:A:376:GLN:CB	1:B:192:ARG:NH1	2.70	0.49
1:B:272:GLN:HE22	1:B:347:ASN:C	2.20	0.49
1:A:46:LEU:HD21	1:A:172:ARG:NH1	2.27	0.49
1:A:403:ALA:HB2	1:A:412:GLN:HG2	1.93	0.49
1:B:195:SER:O	1:B:198:SER:HB3	2.11	0.49
1:A:41:ASP:C	1:A:43:ALA:N	2.70	0.49
1:B:25:TYR:HA	1:B:132:ILE:HD13	1.94	0.49
1:A:14:LYS:O	1:A:15:GLN:C	2.56	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:A:407:THR:O	1:A:409:SER:N	2.46	0.49
1:B:20:MET:HB3	1:B:25:TYR:CE1	2.48	0.49
1:B:270:GLY:O	1:B:271:LYS:C	2.55	0.49
1:B:293:HIS:HB2	1:B:295:HIS:ND1	2.27	0.49
1:B:355:ARG:HG2	1:B:355:ARG:NH1	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:HD12	1:A:380:LEU:N	2.27	0.48
1:A:423:MET:O	1:A:424:LYS:C	2.56	0.48
1:B:305:PHE:HZ	1:B:308:ASP:OD1	1.97	0.48
1:A:122:GLN:C	1:A:124:GLY:H	2.20	0.48
1:A:432:TYR:CZ	1:A:482:SER:HB3	2.49	0.48
1:A:181:ARG:HG2	1:A:181:ARG:HH11	1.78	0.48
1:A:404:SER:OG	1:A:405:THR:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:TYR:CD1	1:B:274:TYR:C	2.92	0.48
1:A:32:LEU:HD23	1:A:196:ILE:CG2	2.42	0.47
1:A:38:ASN:OD1	1:A:122:GLN:OE1	2.32	0.47
1:A:122:GLN:C	1:A:124:GLY:N	2.71	0.47
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.78	0.47
1:B:278:LEU:N	1:B:278:LEU:HD12	2.29	0.47
1:A:19:LEU:HD22	1:B:24:LEU:HD11	1.94	0.47
1:B:194:ARG:HH21	1:B:225:GLU:CD	2.22	0.47
1:B:444:SER:N	1:B:445:PRO:HD2	2.29	0.47
1:A:432:TYR:CD1	1:A:432:TYR:C	2.92	0.47
1:B:16:LEU:HG	1:B:17:LEU:N	2.29	0.47
1:A:140:ARG:HH11	1:A:167:ILE:HD12	1.80	0.47
1:A:262:THR:HG21	1:A:363:LEU:HD13	1.96	0.47
1:A:293:HIS:NE2	1:A:311:GLU:OE2	2.46	0.47
1:A:324:LEU:HD12	1:A:324:LEU:C	2.39	0.47
1:A:421:SER:O	1:A:423:MET:N	2.47	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:20:MET:HE2	1:B:20:MET:HG3	1.97	0.47
1:A:210:ILE:CB	1:A:227:ILE:HD11	2.42	0.47
1:B:194:ARG:NH2	1:B:225:GLU:CD	2.72	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:HG12	1:B:464:ILE:O	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:B:85:MET:HE1	1:B:123:PHE: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:240:GLU:H	1:B:240:GLU:HG2	1.58	0.46
1:B:281:PRO:HG2	1:B:378:PHE:HZ	1.81	0.46
1:A:85:MET:HB2	1:A:141:THR:HG21	1.98	0.46
1:B:36:ILE:HG22	1:B:204:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:O	1:A:87:ARG:C	2.59	0.46
1:A:197:ILE:HG23	1:A:208:VAL:HG11	1.98	0.46
1:A:389:ASP:OD1	1:A:392:ASN:ND2	2.49	0.46
1:B:199:LYS:O	1:B:199:LYS:HG2	2.16	0.46
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:A:156:SER:C	1:A:158:GLY:H	2.24	0.45
1:B:251:LYS:HE3	1:B:259:ASP:OD1	2.16	0.45
1:A:86:THR:O	1:A:89:GLU:N	2.49	0.45
1:B:181:ARG:HG2	1:B:181:ARG:HH11	1.81	0.45
1:B:196:ILE:O	1:B:197:ILE:C	2.57	0.45
1:A:147:LYS:CG	1:A:148:PRO:HD2	2.47	0.45
1:B:408:ASP:HB2	1:B:442:LYS:HZ3	1.80	0.45
1:B:81:ASN:H	1:B:81:ASN:ND2	1.96	0.45
1:B:95:GLY:O	1:B:96:THR:C	2.60	0.45
1:A:331:PRO:HD2	1:A:334:VAL:CG1	2.46	0.45
1:A:472:LEU:HD22	1:A:480:PHE:CE1	2.52	0.45
1:B:20:MET:C	1:B:22:HIS:H	2.24	0.45
1:B:237:ASN:O	1:B:240:GLU:HG2	2.16	0.45
1:A:16:LEU:HD13	1:B:16:LEU:HA	1.99	0.45
1:A:24:LEU:HB3	1:A:132:ILE:HD11	1.99	0.45
1:A:219:GLU:CG	1:A:220:THR:N	2.75	0.45
1:B:301:VAL:HG23	1:B:306:ILE:HG13	1.98	0.45
1:A:94:LEU:HB3	1:A:154:TRP:CE2	2.52	0.45
1:A:234:TRP:CE3	1:A:324:LEU:HD21	2.52	0.45
1:A:303:ARG:HA	1:A:326:ASP:OD2	2.17	0.45
1:A:464:ILE:O	1:A:465:ASP:C	2.60	0.45
1:B:253:ILE:HG13	1:B:254:ALA:N	2.31	0.45
1:B:288:MET:HE1	1:B:378:PHE:CD2	2.52	0.44
1:B:404:SER:OG	1:B:405:THR:N	2.49	0.44
1:A:302:GLN:O	1:A:303:ARG:HB3	2.17	0.44
1:A:331:PRO:O	1:A:333:ASN:N	2.51	0.44
1:B:145:GLY:O	1:B:146:GLU:HG2	2.17	0.44
1:A:383:LYS:O	1:A:386:PRO:HD2	2.18	0.44
1:B:331:PRO:HB2	1:B:333:ASN:OD1	2.18	0.44
1:A:121:GLY:C	1:A:123:PHE:N	2.76	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:378:PHE:O	1:A:379:GLY:C	2.58	0.44
1:B:226:LYS:HZ2	1:B:230:ALA:HB3	1.82	0.44
1:A:71:LYS:HA	1:A:188:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TYR:CD1	1:A:385:GLY:HA3	2.53	0.44
1:B:226:LYS:HE3	1:B:228:ASN:O	2.17	0.44
1:B:133:VAL:HG11	1:B:187:PHE:CE1	2.53	0.44
1:B:294:LYS:HG3	1:B:322:ARG:NH2	2.33	0.44
1:B:301:VAL:CG1	1:B:332:LEU:HD23	2.48	0.44
1:A:373:THR:O	1:A:376:GLN:HB2	2.18	0.43
1:B:85:MET:HE1	1:B:123:PHE:CE1	2.53	0.43
1:A:331:PRO:CD	1:A:334:VAL:HG13	2.48	0.43
1:B:445:PRO:HB2	1:B:446:HIS:H	1.61	0.43
1:A:7:ARG:NH1	1:A:91:ILE:HD13	2.34	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:31:PHE:CG	1:B:32:LEU:N	2.86	0.43
1:A:66:ARG:HB3	1:A:224:TRP:CZ3	2.54	0.43
1:B:319:ARG:HH21	1:B:384:GLU:CD	2.25	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:273:GLU:HB3	1:A:328:SER:CB	2.48	0.43
1:A:383:LYS:C	1:A:386:PRO:HD2	2.44	0.43
1:A:415:SER:HB3	1:A:418:ASP:OD1	2.19	0.43
1:B:18:HIS:O	1:B:20:MET:N	2.52	0.43
1:B:49:ARG:HG2	1:B:49:ARG:HH11	1.84	0.43
1:B:375:TRP:CE2	1:B:401:ARG:HB2	2.54	0.43
1:A:263:TRP:HB3	1:A:279:TYR:CD2	2.53	0.42
1:B:170:GLU:CD	1:B:170:GLU:N	2.63	0.42
1:B:325:ILE:HD12	1:B:352:LEU:HD11	2.00	0.42
1:B:330:LEU:HD23	1:B:331:PRO:HD2	1.99	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:407:THR:C	1:A:409:SER:N	2.77	0.42
1:A:12:GLU:O	1:A:13:VAL:CG2	2.67	0.42
1:A:125:VAL:HG23	1:B:18:HIS:NE2	2.34	0.42
1:A:372:GLN:O	1:A:376:GLN:HG3	2.20	0.42
1:B:226:LYS:O	1:B:226:LYS:HG3	2.18	0.42
1:B:262:THR:HG22	1:B:263:TRP:H	1.84	0.42
1:A:95:GLY:HA2	1:A:162:TYR:CE2	2.54	0.42
1:A:370:LYS:O	1:A:373:THR:HB	2.19	0.42
1:A:73:LYS:HB2	1:A:75:THR:HG23	2.01	0.42
1:A:121:GLY:C	1:A:123:PHE:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:O	1:A:130:ALA:HB3	2.19	0.42
1:A:261:LEU:HD12	1:A:281:PRO:O	2.20	0.42
1:A:472:LEU:HD22	1:A:480:PHE:HE1	1.85	0.42
1:A:476:ASP:C	1:A:478:LYS:N	2.77	0.42
1:B:420:VAL:HG13	1:B:423:MET:CE	2.49	0.42
1:A:234:TRP:HA	1:A:265:HIS:CE1	2.55	0.42
1:A:273:GLU:CB	1:A:328:SER:HB2	2.48	0.42
1:A:331:PRO:HD2	1:A:334:VAL:HG13	2.01	0.42
1:B:20:MET:O	1:B:22:HIS:N	2.53	0.42
1:B:406:HIS:ND1	1:B:406:HIS:O	2.53	0.42
1:A:30:ILE:O	1:A:33:ARG:N	2.53	0.41
1:A:308:ASP:O	1:A:309:ASP:C	2.62	0.41
1:A:406:HIS:HD2	1:A:422:ARG:HD2	1.81	0.41
1:A:447:LEU:O	1:A:448:GLU:C	2.61	0.41
1:B:35:LEU:HD22	1:B:176:ILE:CD1	2.50	0.41
1:B:170:GLU:CG	1:B:171:ASP:H	2.29	0.41
1:B:386:PRO:HG2	1:B:468:MET:HG3	2.01	0.41
1:A:206:LEU:HD12	1:A:207:PRO:HD2	2.02	0.41
1:A:333:ASN:O	1:A:334:VAL:C	2.62	0.41
1:A:13:VAL:HG12	1:A:14:LYS:N	2.32	0.41
1:A:15:GLN:O	1:A:16:LEU:C	2.63	0.41
1:A:375:TRP:CZ3	1:A:379:GLY:HA2	2.55	0.41
1:A:452:LYS:C	1:A:454:GLY:N	2.77	0.41
1:A:383:LYS:NZ	1:A:465:ASP:OD1	2.49	0.41
1:A:416:LEU:HD23	1:A:416:LEU:HA	1.82	0.41
1:B:33:ARG:C	1:B:34:GLU:HG2	2.45	0.41
1:B:65:VAL:HG13	1:B:208:VAL:HA	2.03	0.41
1:B:147:LYS:C	1:B:149:GLU:N	2.78	0.41
1:B:406:HIS:O	1:B:406:HIS:CG	2.72	0.41
1:A:168:THR:O	1:A:168:THR:CG2	2.67	0.41
1:A:319:ARG:CZ	1:A:381:VAL:HG13	2.51	0.41
1:A:343:THR:O	1:A:344:VAL:C	2.63	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:B:322:ARG:HD3	1:B:322:ARG:HA	1.64	0.41
1:A:452:LYS:C	1:A:454:GLY:H	2.29	0.41
1:B:476:ASP:O	1:B:476:ASP:CG	2.64	0.41
1:B:74:ARG:HG2	1:B:74:ARG:NH1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:C	1:A:149:GLU:H	2.29	0.41
1:A:155:GLU:O	1:A:156:SER:HB2	2.21	0.41
1:A:418:ASP:O	1:A:421:SER:HB2	2.20	0.41
1:B:147:LYS:C	1:B:149:GLU:H	2.29	0.41
1:A:300:TYR:CE1	1:A:324:LEU:HD22	2.56	0.41
1:A:181:ARG:HG2	1:A:181:ARG:NH1	2.36	0.40
1:A:51:LEU:HD12	1:A:51:LEU:N	2.34	0.40
1:A:333:ASN:O	1:A:334:VAL:O	2.40	0.40
1:B:82:GLY:O	1:B:172:ARG:HD2	2.22	0.40
1:B:280:ILE:CD1	1:B:359:MET:HE3	2.52	0.40
1:B:446:HIS:CD2	1:B:446:HIS:H	2.39	0.40
1:A:147:LYS:C	1:A:149:GLU:N	2.79	0.40
1:A:354:LYS:HB2	1:A:354:LYS:HE3	1.84	0.40
1:A:284:ALA:HA	1:A:285:PRO:HD3	1.94	0.40
1:B:312:GLN:HG3	1:B:339:LEU:HB2	2.00	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%)	2	7
1	B	450/559 (80%)	397 (88%)	40 (9%)	13 (3%)	3	15
All	All	918/1118 (82%)	783 (85%)	100 (11%)	35 (4%)	2	10

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	14	LYS
1	A	15	GLN

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	394 (95%)	22 (5%)	20	52
1	B	401/488 (82%)	374 (93%)	27 (7%)	15	43
All	All	817/976 (84%)	768 (94%)	49 (6%)	17	47

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	14	LYS
1	A	102	THR
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	319	ARG
1	A	324	LEU
1	A	361	GLU
1	A	388	GLU
1	A	434	THR
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	19	LEU
1	B	58	GLU
1	B	81	ASN
1	B	133	VAL
1	B	164	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

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Mol	Chain	Res	Type
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	316	ASN
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	10	GLN
1	A	15	GLN
1	A	53	ASN
1	A	122	GLN
1	A	203	HIS
1	A	228	ASN
1	A	255	HIS
1	A	266	ASN
1	A	272	GLN
1	A	290	ASN
1	A	316	ASN
1	A	376	GLN
1	A	412	GLN
1	B	81	ASN
1	B	93	HIS
1	B	122	GLN
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

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Mol	Chain	Res	Type
1	B	312	GLN
1	B	347	ASN
1	B	427	GLN
1	B	446	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	10:GLN	C	11:SER	N	1.16
1	A	8:GLY	C	9:PHE	N	0.96

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, 95th 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%)	0.47	37 (7%)	19 16	34, 66, 101, 101	0
1	B	454/559 (81%)	0.09	29 (6%)	25 20	19, 46, 99, 101	0
All	All	926/1118 (82%)	0.28	66 (7%)	22 17	19, 57, 101, 101	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	8.6
1	B	487	ASP	6.1
1	A	486	VAL	5.8
1	B	486	VAL	5.7
1	B	25	TYR	5.5
1	B	120	ILE	4.6
1	A	122	GLN	4.5
1	B	16	LEU	4.3
1	A	17	LEU	4.2
1	A	120	ILE	4.2
1	A	488	GLU	4.1
1	B	24	LEU	4.1
1	B	444	SER	4.0
1	A	286	TRP	4.0
1	B	18	HIS	4.0
1	A	487	ASP	3.9
1	A	257	PHE	3.9
1	B	286	TRP	3.8
1	B	17	LEU	3.8
1	A	102	THR	3.8
1	A	12	GLU	3.8
1	A	289	TRP	3.7
1	A	20	MET	3.6
1	B	98	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	10	GLN	3.5
1	B	257	PHE	3.5
1	B	97	ILE	3.5
1	A	447	LEU	3.4
1	A	11	SER	3.4
1	B	19	LEU	3.3
1	A	123	PHE	3.3
1	B	390	PHE	3.3
1	B	21	ILE	3.3
1	B	121	GLY	3.3
1	A	489	SER	3.3
1	A	51	LEU	3.2
1	B	192	ARG	3.2
1	B	22	HIS	3.2
1	A	14	LYS	3.2
1	A	294	LYS	3.1
1	B	15	GLN	3.1
1	A	449	LEU	3.1
1	A	9	PHE	3.1
1	B	443	SER	3.0
1	A	121	GLY	3.0
1	B	23	SER	2.9
1	A	16	LEU	2.8
1	B	485	LYS	2.8
1	A	285	PRO	2.8
1	A	484	SER	2.7
1	B	293	HIS	2.6
1	B	447	LEU	2.6
1	A	444	SER	2.6
1	A	291	ARG	2.5
1	A	145	GLY	2.5
1	B	159	GLU	2.4
1	B	294	LYS	2.4
1	B	215	GLU	2.4
1	A	288	MET	2.4
1	A	481	GLN	2.2
1	A	100	SER	2.2
1	A	101	GLY	2.2
1	B	489	SER	2.1
1	A	341	ASP	2.0
1	A	394	GLU	2.0
1	A	442	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 oligosaccharides 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.