



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 AM GMT

PDB ID : 2CG9
Title : CRYSTAL STRUCTURE OF AN HSP90-SBA1 CLOSED CHAPERONE COMPLEX
Authors : Ali, M.M.U.; Roe, S.M.; Prodromou, C.; Pearl, L.H.
Deposited on : 2006-03-01
Resolution : 3.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

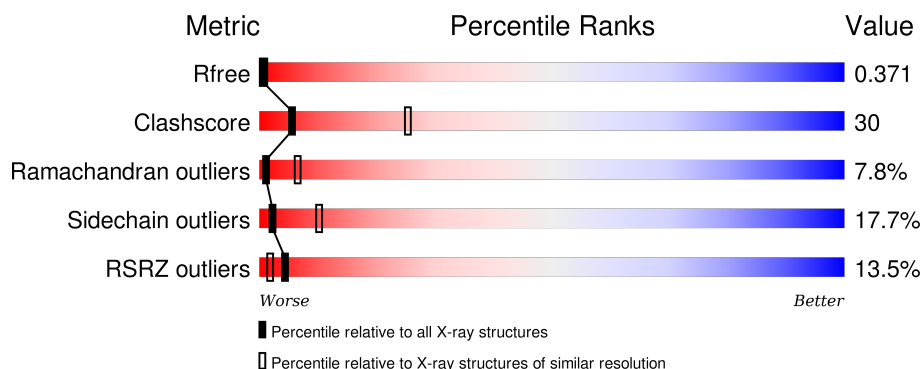
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 $\leq 5\%$. 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	677	
1	B	677	
2	X	134	
2	Y	134	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	B	1678	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11906 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 ATP-DEPENDENT MOLECULAR CHAPERONE HSP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4923	3147	804	963	9			
1	B	618	Total	C	N	O	S	0	0	0
			4997	3195	816	977	9			

- Molecule 2 is a protein called CO-CHAPERONE PROTEIN SBA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	115	Total	C	N	O	S	0	0	0
			962	621	154	185	2			
2	Y	115	Total	C	N	O	S	0	0	0
			962	621	154	185	2			

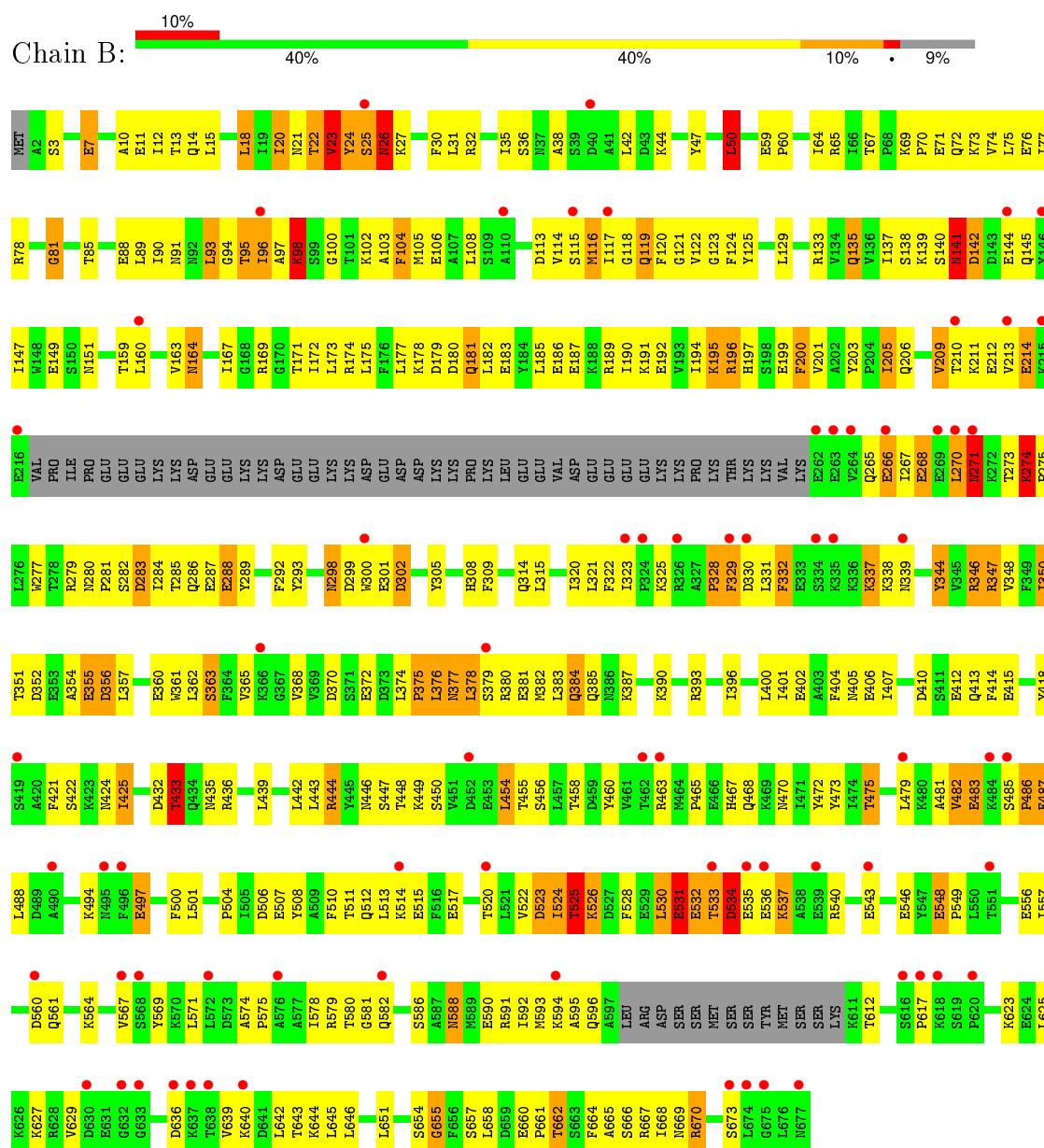
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	127	ALA	GLU	ENGINEERED MUTATION	UNP P28707
Y	127	ALA	GLU	ENGINEERED MUTATION	UNP P28707

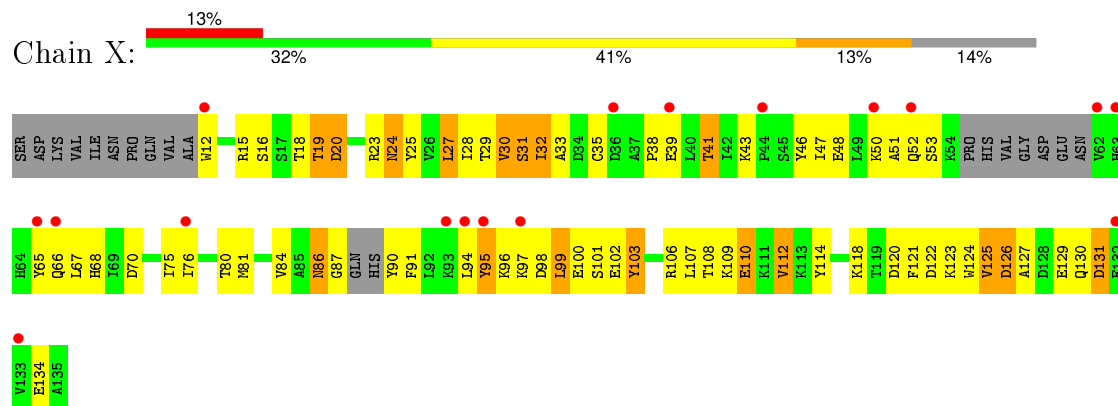
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



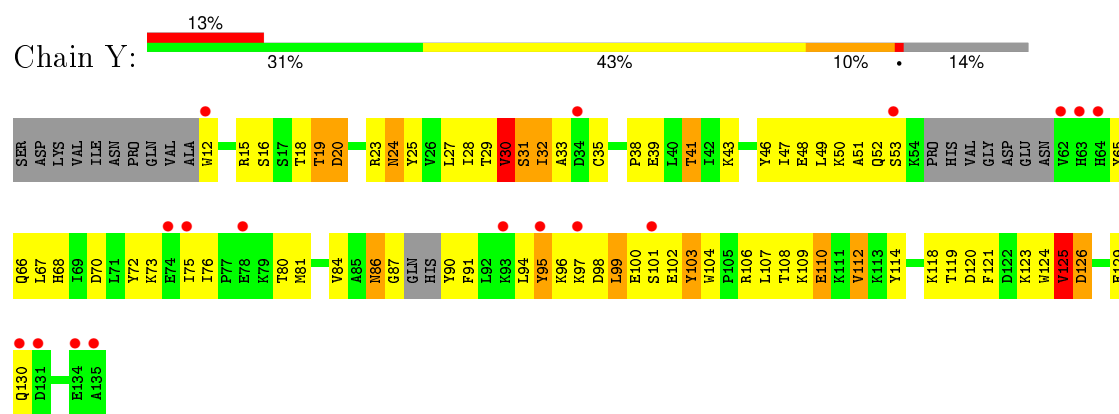
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		



• Molecule 2: CO-CHAPERONE PROTEIN SBA1



• Molecule 2: CO-CHAPERONE PROTEIN SBA1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.73 Å 126.73 Å 279.78 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 3.10 39.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	68.2 (115.47-3.10) 83.9 (39.82-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.48 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.312 , 0.353 0.351 , 0.371	Depositor DCC
R_{free} test set	1249 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 24801 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	11906	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	0.46	0/5004	0.67	2/6743 (0.0%)
1	B	0.46	0/5080	0.67	1/6844 (0.0%)
2	X	0.50	1/986 (0.1%)	0.62	0/1335
2	Y	0.46	0/986	0.62	0/1335
All	All	0.46	1/12056 (0.0%)	0.67	3/16257 (0.0%)

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	5
1	B	0	4
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	134	GLU	CG-CD	5.53	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	LEU	CA-CB-CG	6.01	129.13	115.30
1	B	50	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	24	TYR	N-CA-CB	5.08	119.75	110.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLU	Peptide
1	A	271	ASN	Peptide
1	A	384	GLN	Peptide
1	A	531	GLU	Peptide
1	A	536	GLU	Peptide
1	B	11	GLU	Peptide
1	B	384	GLN	Peptide
1	B	531	GLU	Peptide
1	B	536	GLU	Peptide

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	4923	0	4960	296	0
1	B	4997	0	5037	316	0
2	X	962	0	936	62	0
2	Y	962	0	936	66	0
3	A	31	0	12	5	0
3	B	31	0	12	13	0
All	All	11906	0	11893	701	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 (701) 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:B:331:LEU:HB3	1:B:332:PHE:HA	1.18	1.17
2:Y:18:THR:HG23	2:Y:120:ASP:HB2	1.18	1.17
1:B:117:ILE:HB	1:B:346:ARG:HD2	1.21	1.13
1:A:475:THR:HG23	1:A:588:ASN:HD21	1.00	1.11
2:X:18:THR:HG23	2:X:120:ASP:HB2	1.16	1.11
1:A:117:ILE:HB	1:A:346:ARG:HD2	1.13	1.11
3:B:1678:ATP:H8	3:B:1678:ATP:H5'2	1.14	1.08
1:B:135:GLN:HB3	1:B:174:ARG:HB2	1.32	1.08
1:A:135:GLN:HB3	1:A:174:ARG:HB2	1.20	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1678:ATP:C8	3:B:1678:ATP:H5'2	1.88	1.07
1:A:385:GLN:HE22	2:X:122:ASP:HA	1.21	1.05
1:B:94:GLY:HA3	1:B:98:LYS:HZ1	1.15	1.04
1:B:331:LEU:CB	1:B:332:PHE:HA	1.88	1.04
1:A:384:GLN:HB3	1:B:23:VAL:CG1	1.89	1.02
1:A:524:ILE:HA	1:A:525:THR:CB	1.86	1.02
2:X:18:THR:CG2	2:X:120:ASP:HB2	1.90	1.01
1:A:524:ILE:HA	1:A:525:THR:HB	1.01	1.01
1:A:94:GLY:HA3	1:A:98:LYS:HZ1	1.24	1.01
2:Y:18:THR:CG2	2:Y:120:ASP:HB2	1.94	0.97
1:A:384:GLN:HE21	1:B:25:SER:HB3	1.29	0.96
1:A:524:ILE:CA	1:A:525:THR:HB	1.93	0.96
1:A:195:LYS:HE2	1:A:268:GLU:OE2	1.65	0.95
1:A:195:LYS:HE2	1:A:268:GLU:CD	1.87	0.95
1:B:525:THR:HG22	1:B:526:LYS:H	1.33	0.94
1:A:475:THR:HG23	1:A:588:ASN:ND2	1.82	0.93
1:B:94:GLY:HA3	1:B:98:LYS:NZ	1.82	0.92
1:B:117:ILE:CB	1:B:346:ARG:HD2	2.00	0.92
1:A:384:GLN:HB3	1:B:23:VAL:HG11	1.49	0.91
1:B:488:LEU:HD21	1:B:579:ARG:HH12	1.36	0.91
1:A:270:LEU:HA	1:A:271:ASN:HB2	1.54	0.89
1:A:117:ILE:CB	1:A:346:ARG:HD2	2.04	0.87
1:A:94:GLY:HA3	1:A:98:LYS:NZ	1.87	0.87
2:X:18:THR:HG23	2:X:120:ASP:CB	2.05	0.86
2:Y:32:ILE:HD13	2:Y:33:ALA:H	1.40	0.86
1:A:18:LEU:HG	1:B:96:ILE:HD12	1.59	0.84
2:Y:106:ARG:NH2	2:Y:109:LYS:HA	1.92	0.84
1:B:285:THR:HG22	1:B:286:GLN:H	1.44	0.82
1:A:284:ILE:HA	1:A:288:GLU:OE1	1.81	0.81
1:A:183:GLU:HA	1:A:186:GLU:OE2	1.81	0.81
1:B:21:ASN:C	1:B:23:VAL:H	1.85	0.81
1:A:275:PRO:HG3	1:A:347:ARG:HH12	1.46	0.80
1:B:24:TYR:HB3	1:B:26:ASN:OD1	1.82	0.80
2:X:97:LYS:HD2	2:X:99:LEU:HD11	1.63	0.80
1:A:270:LEU:HA	1:A:271:ASN:CB	2.12	0.80
2:X:32:ILE:HD13	2:X:33:ALA:H	1.45	0.80
1:B:525:THR:HG22	1:B:526:LYS:N	1.96	0.80
1:B:365:VAL:HG21	1:B:400:LEU:HD21	1.64	0.80
1:B:594:LYS:HZ2	1:B:657:SER:HB2	1.46	0.80
1:B:331:LEU:HB3	1:B:332:PHE:CA	2.08	0.79
2:Y:18:THR:HG23	2:Y:120:ASP:CB	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLU:HA	1:B:186:GLU:OE2	1.82	0.79
1:A:365:VAL:HG21	1:A:400:LEU:HD21	1.63	0.79
1:B:284:ILE:HA	1:B:288:GLU:OE1	1.82	0.78
2:X:106:ARG:NH2	2:X:109:LYS:HA	1.97	0.78
1:A:24:TYR:HB3	1:A:26:ASN:OD1	1.84	0.78
1:B:331:LEU:CB	1:B:332:PHE:CA	2.61	0.78
1:A:18:LEU:HG	1:B:96:ILE:CD1	2.14	0.77
1:B:449:LYS:HD3	1:B:497:GLU:HG2	1.67	0.77
2:Y:97:LYS:HD2	2:Y:99:LEU:HD11	1.68	0.76
1:A:21:ASN:C	1:A:23:VAL:H	1.88	0.76
1:A:486:PRO:HD2	1:B:662:THR:HG21	1.68	0.76
1:A:594:LYS:HZ2	1:A:657:SER:HB2	1.50	0.76
2:X:39:GLU:HB2	2:X:50:LYS:H	1.48	0.75
1:A:275:PRO:HG3	1:A:347:ARG:NH1	2.02	0.75
1:B:588:ASN:O	1:B:591:ARG:HG2	1.86	0.75
1:A:588:ASN:O	1:A:591:ARG:HG2	1.87	0.75
2:Y:106:ARG:HH22	2:Y:109:LYS:HA	1.52	0.74
2:Y:32:ILE:HG13	2:Y:65:TYR:CE1	2.23	0.74
2:X:24:ASN:HD22	2:X:24:ASN:H	1.36	0.74
2:Y:24:ASN:HD22	2:Y:24:ASN:H	1.36	0.74
1:B:525:THR:CG2	1:B:526:LYS:N	2.51	0.74
1:B:473:TYR:O	1:B:523:ASP:HB3	1.89	0.73
2:Y:39:GLU:HB2	2:Y:50:LYS:H	1.54	0.72
1:A:449:LYS:HD3	1:A:497:GLU:HG2	1.70	0.72
1:B:117:ILE:HB	1:B:346:ARG:CD	2.11	0.72
1:A:210:THR:HA	1:A:264:VAL:HA	1.71	0.72
2:X:32:ILE:HG13	2:X:65:TYR:CE1	2.25	0.71
1:B:270:LEU:HA	1:B:271:ASN:HB2	1.69	0.71
2:X:106:ARG:HH22	2:X:109:LYS:HA	1.56	0.71
1:A:18:LEU:O	1:A:22:THR:HB	1.90	0.70
1:A:32:ARG:HD3	1:A:197:HIS:HD2	1.55	0.70
1:A:14:GLN:HB3	1:B:96:ILE:HG22	1.72	0.70
2:X:38:PRO:HB3	2:X:91:PHE:HE2	1.56	0.69
1:A:117:ILE:HB	1:A:346:ARG:CD	2.07	0.69
1:A:285:THR:HG22	1:A:286:GLN:H	1.56	0.69
1:A:195:LYS:CE	1:A:268:GLU:OE2	2.40	0.69
1:A:199:GLU:O	1:A:273:THR:HG23	1.93	0.69
1:B:331:LEU:HB2	1:B:332:PHE:HB3	1.73	0.68
2:X:20:ASP:OD2	2:X:27:LEU:O	2.10	0.68
1:A:25:SER:HB3	1:B:384:GLN:HE21	1.56	0.68
1:B:21:ASN:O	1:B:23:VAL:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:SER:C	1:A:142:ASP:H	1.97	0.68
1:B:119:GLN:O	3:B:1678:ATP:PG	2.52	0.68
1:A:23:VAL:CG1	1:B:384:GLN:HB3	2.24	0.68
3:B:1678:ATP:C5'	3:B:1678:ATP:H8	2.00	0.67
1:A:384:GLN:HG3	1:B:25:SER:H	1.58	0.67
1:A:96:ILE:HG22	1:B:14:GLN:HB3	1.76	0.67
2:X:99:LEU:HB2	2:X:102:GLU:OE1	1.95	0.67
1:B:578:ILE:HD12	1:B:651:LEU:HA	1.76	0.67
1:B:121:GLY:HA2	3:B:1678:ATP:O2A	1.94	0.67
1:B:114:VAL:HB	1:B:346:ARG:NH2	2.08	0.67
1:A:23:VAL:HG13	1:A:24:TYR:H	1.58	0.67
1:A:178:LYS:O	1:A:180:ASP:N	2.26	0.67
1:B:186:GLU:O	1:B:190:ILE:HG13	1.95	0.67
2:Y:24:ASN:HD22	2:Y:24:ASN:N	1.92	0.67
1:B:533:THR:O	1:B:535:GLU:N	2.28	0.67
1:A:37:ASN:OD1	3:A:1678:ATP:O1A	2.13	0.67
1:A:96:ILE:HD12	1:B:18:LEU:HG	1.76	0.67
1:B:594:LYS:NZ	1:B:657:SER:HB2	2.09	0.66
1:A:533:THR:O	1:A:535:GLU:N	2.27	0.66
1:A:21:ASN:O	1:A:23:VAL:N	2.27	0.66
2:Y:70:ASP:O	2:Y:108:THR:HA	1.95	0.66
1:B:567:VAL:HG12	1:B:617:PRO:HG3	1.78	0.66
1:B:18:LEU:O	1:B:22:THR:HB	1.95	0.66
1:A:439:LEU:HA	1:A:442:LEU:HD12	1.78	0.66
1:B:32:ARG:HD3	1:B:197:HIS:HD2	1.61	0.66
1:A:64:ILE:HD11	1:A:205:ILE:HA	1.78	0.66
1:A:23:VAL:HG11	1:B:384:GLN:HB3	1.77	0.66
1:A:65:ARG:HG3	1:A:206:GLN:HB3	1.76	0.66
1:B:344:TYR:O	1:B:370:ASP:HA	1.95	0.66
1:A:96:ILE:CD1	1:B:18:LEU:HG	2.24	0.66
1:A:524:ILE:O	1:A:580:THR:HG23	1.96	0.66
2:Y:99:LEU:HB2	2:Y:102:GLU:OE1	1.95	0.65
1:A:536:GLU:HG2	1:A:536:GLU:O	1.96	0.65
1:A:121:GLY:HA2	3:A:1678:ATP:O3A	1.96	0.65
1:A:271:ASN:H	1:A:272:LYS:C	2.00	0.65
1:B:275:PRO:HG3	1:B:347:ARG:HH12	1.61	0.65
1:A:432:ASP:OD2	1:A:435:ASN:N	2.25	0.65
1:A:384:GLN:HB3	1:B:23:VAL:HG13	1.77	0.65
1:B:65:ARG:HG3	1:B:206:GLN:HB3	1.78	0.65
1:B:275:PRO:HG3	1:B:347:ARG:NH1	2.12	0.65
1:A:32:ARG:HH22	1:A:380:ARG:HB2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:HH21	1:B:206:GLN:HE22	1.45	0.65
1:A:531:GLU:O	1:A:537:LYS:HB2	1.97	0.65
1:A:117:ILE:HD13	1:A:374:LEU:HD22	1.79	0.65
2:Y:38:PRO:HB3	2:Y:91:PHE:HE2	1.62	0.65
1:B:94:GLY:CA	1:B:98:LYS:NZ	2.60	0.64
1:B:439:LEU:HA	1:B:442:LEU:HD12	1.80	0.64
2:Y:15:ARG:HG3	2:Y:65:TYR:CD2	2.32	0.64
1:B:114:VAL:O	1:B:346:ARG:NH1	2.31	0.64
1:B:140:SER:C	1:B:142:ASP:H	1.99	0.64
2:X:24:ASN:HD22	2:X:24:ASN:N	1.94	0.64
1:B:270:LEU:HA	1:B:271:ASN:CB	2.24	0.64
1:B:501:LEU:HD23	1:B:506:ASP:HB3	1.79	0.64
1:A:567:VAL:HG12	1:A:617:PRO:HG3	1.78	0.64
1:B:23:VAL:O	1:B:24:TYR:CG	2.51	0.64
1:B:117:ILE:HD12	1:B:346:ARG:HE	1.63	0.64
1:B:178:LYS:O	1:B:180:ASP:N	2.31	0.63
1:B:195:LYS:HE2	1:B:268:GLU:CD	2.18	0.63
1:B:666:SER:O	1:B:670:ARG:HB2	1.97	0.63
1:A:594:LYS:NZ	1:A:657:SER:HB2	2.13	0.63
2:X:38:PRO:HB3	2:X:91:PHE:CE2	2.33	0.63
1:A:95:THR:HG22	1:A:96:ILE:HG12	1.80	0.63
1:B:114:VAL:O	1:B:346:ARG:CZ	2.47	0.63
2:Y:43:LYS:HB2	2:Y:46:TYR:HB2	1.80	0.62
1:B:24:TYR:O	1:B:26:ASN:N	2.30	0.62
1:A:501:LEU:HD23	1:A:506:ASP:HB3	1.82	0.62
1:A:114:VAL:O	1:A:116:MET:N	2.33	0.62
1:A:388:ILE:HD11	2:X:121:PHE:CD2	2.34	0.62
1:A:578:ILE:HD12	1:A:651:LEU:HA	1.82	0.61
1:A:24:TYR:O	1:A:26:ASN:N	2.30	0.61
2:X:43:LYS:HB2	2:X:46:TYR:HB2	1.81	0.61
1:B:522:VAL:O	1:B:523:ASP:HB2	1.99	0.61
1:B:64:ILE:HD11	1:B:205:ILE:HA	1.80	0.61
1:A:625:LEU:O	1:A:629:VAL:HG23	2.00	0.61
1:B:432:ASP:OD2	1:B:435:ASN:N	2.30	0.61
1:B:328:PRO:HB2	1:B:330:ASP:N	2.15	0.61
1:A:421:PHE:O	1:A:425:ILE:HG22	2.01	0.61
1:A:65:ARG:HH21	1:A:206:GLN:HE22	1.48	0.61
2:X:35:CYS:HA	2:X:53:SER:HA	1.81	0.61
1:A:23:VAL:HG13	1:A:24:TYR:N	2.16	0.61
1:A:666:SER:O	1:A:670:ARG:HB2	2.00	0.61
1:A:350:ILE:HG22	1:A:351:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG23	1:A:125:TYR:CE1	2.36	0.60
1:B:665:ALA:HA	1:B:668:ILE:HD12	1.83	0.60
2:X:99:LEU:HD22	2:X:102:GLU:HB2	1.84	0.60
1:B:151:ASN:O	2:X:86:ASN:HB2	2.01	0.60
1:A:308:HIS:HD2	1:A:309:PHE:N	2.00	0.60
1:B:350:ILE:HG22	1:B:351:THR:N	2.16	0.60
1:A:477:GLU:OE2	1:B:658:LEU:HB2	2.01	0.60
1:A:135:GLN:CB	1:A:174:ARG:HB2	2.13	0.60
1:B:76:GLU:HA	1:B:173:LEU:O	2.00	0.60
2:X:70:ASP:O	2:X:108:THR:HA	2.02	0.60
1:A:114:VAL:O	1:A:346:ARG:CZ	2.50	0.59
2:X:19:THR:HG23	2:X:107:LEU:HD12	1.83	0.59
1:B:97:ALA:O	1:B:98:LYS:HG2	2.01	0.59
1:A:346:ARG:O	1:A:347:ARG:HB2	2.01	0.59
1:B:199:GLU:O	1:B:273:THR:HG23	2.03	0.59
1:B:436:ARG:CZ	1:B:512:GLN:O	2.51	0.59
1:B:625:LEU:O	1:B:629:VAL:HG23	2.02	0.59
1:B:122:VAL:O	1:B:124:PHE:N	2.36	0.59
1:B:100:GLY:N	3:B:1678:ATP:O3'	2.35	0.59
2:Y:38:PRO:HB3	2:Y:91:PHE:CE2	2.37	0.59
1:B:346:ARG:O	1:B:347:ARG:HB2	2.02	0.59
1:A:665:ALA:HA	1:A:668:ILE:HD12	1.82	0.59
1:B:117:ILE:HD12	1:B:346:ARG:NE	2.18	0.59
3:B:1678:ATP:C5'	3:B:1678:ATP:C8	2.78	0.59
1:A:270:LEU:CA	1:A:271:ASN:HB2	2.31	0.59
1:A:122:VAL:O	1:A:124:PHE:N	2.36	0.58
1:B:181:GLN:HA	1:B:181:GLN:NE2	2.18	0.58
1:A:95:THR:HB	1:B:10:ALA:HB2	1.85	0.58
1:A:117:ILE:HD12	1:A:346:ARG:HE	1.69	0.58
1:B:114:VAL:O	1:B:116:MET:N	2.37	0.58
2:Y:15:ARG:NH1	2:Y:32:ILE:H	2.01	0.58
1:A:194:ILE:O	1:A:196:ARG:N	2.34	0.58
1:A:119:GLN:O	3:A:1678:ATP:PG	2.61	0.58
2:Y:35:CYS:HA	2:Y:53:SER:HA	1.86	0.58
2:X:87:GLY:O	2:X:90:TYR:N	2.35	0.58
1:B:163:VAL:O	1:B:164:ASN:HB2	2.04	0.57
1:A:465:PRO:HB2	1:A:467:HIS:CD2	2.39	0.57
1:A:384:GLN:NE2	1:B:25:SER:HB3	2.11	0.57
2:Y:99:LEU:HD22	2:Y:102:GLU:HB2	1.85	0.57
1:B:95:THR:HG23	1:B:125:TYR:CE1	2.38	0.57
2:Y:30:VAL:O	2:Y:31:SER:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:O	1:A:24:TYR:CG	2.58	0.57
1:B:42:LEU:HD23	1:B:81:GLY:N	2.20	0.57
2:X:15:ARG:HG3	2:X:65:TYR:CD2	2.39	0.57
1:A:94:GLY:CA	1:A:98:LYS:NZ	2.65	0.57
2:X:25:TYR:HE1	2:X:27:LEU:HD22	1.70	0.57
1:B:194:ILE:O	1:B:196:ARG:N	2.35	0.57
1:A:436:ARG:CZ	1:A:512:GLN:O	2.52	0.57
1:A:344:TYR:O	1:A:370:ASP:HA	2.05	0.57
1:A:10:ALA:HB2	1:B:95:THR:HB	1.87	0.57
1:A:375:PRO:O	1:A:376:LEU:HB2	2.04	0.56
1:A:285:THR:H	1:A:288:GLU:CD	2.09	0.56
1:B:308:HIS:HD2	1:B:309:PHE:N	2.03	0.56
1:A:591:ARG:O	1:A:595:ALA:HB2	2.04	0.56
1:B:591:ARG:O	1:B:595:ALA:HB2	2.05	0.56
1:B:187:GLU:HG3	1:B:209:VAL:HG11	1.88	0.56
1:A:145:GLN:HE21	1:A:167:ILE:HG12	1.70	0.56
1:B:194:ILE:C	1:B:196:ARG:H	2.09	0.56
1:B:200:PHE:N	1:B:200:PHE:CD2	2.73	0.56
1:B:75:LEU:HB3	1:B:175:LEU:HB2	1.88	0.56
1:A:590:GLU:HA	1:A:593:MET:HG2	1.87	0.56
1:A:210:THR:CG2	1:A:264:VAL:HG22	2.36	0.56
1:B:114:VAL:O	1:B:114:VAL:HG12	2.06	0.56
2:Y:108:THR:HB	2:Y:110:GLU:OE2	2.06	0.56
2:Y:25:TYR:HE1	2:Y:27:LEU:HD22	1.70	0.56
2:Y:76:ILE:HD12	2:Y:96:LYS:HB3	1.87	0.56
2:Y:87:GLY:O	2:Y:90:TYR:N	2.38	0.56
1:A:422:SER:O	1:A:425:ILE:HG23	2.07	0.55
1:B:89:LEU:O	1:B:93:LEU:HD23	2.06	0.55
1:B:658:LEU:HB3	1:B:661:PRO:HB3	1.87	0.55
1:A:341:ILE:HD11	1:A:358:ILE:HB	1.88	0.55
1:B:285:THR:HG22	1:B:286:GLN:N	2.17	0.55
1:A:151:ASN:O	2:Y:86:ASN:HB2	2.06	0.55
1:B:504:PRO:HB3	1:B:592:ILE:HD13	1.87	0.55
1:B:117:ILE:CG1	1:B:346:ARG:HD2	2.35	0.55
2:Y:20:ASP:OD2	2:Y:27:LEU:O	2.24	0.55
1:B:421:PHE:O	1:B:425:ILE:HG22	2.06	0.55
1:B:135:GLN:CB	1:B:174:ARG:HB2	2.22	0.55
2:X:15:ARG:NH1	2:X:32:ILE:H	2.05	0.55
1:A:97:ALA:O	1:A:98:LYS:HG2	2.05	0.55
1:A:89:LEU:O	1:A:93:LEU:HD23	2.07	0.55
1:A:76:GLU:HA	1:A:173:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:PHE:CE2	1:A:114:VAL:HG11	2.42	0.54
2:X:23:ARG:HD3	2:X:24:ASN:HB3	1.89	0.54
1:B:47:TYR:O	1:B:50:LEU:HG	2.08	0.54
1:B:104:PHE:CE2	1:B:114:VAL:HG11	2.41	0.54
1:A:12:ILE:O	1:A:13:THR:C	2.46	0.54
1:B:95:THR:HG22	1:B:96:ILE:HG12	1.90	0.54
1:A:118:GLY:HA2	1:A:380:ARG:HH22	1.73	0.54
1:B:375:PRO:O	1:B:376:LEU:HB2	2.08	0.54
1:A:194:ILE:C	1:A:196:ARG:H	2.10	0.54
1:A:378:LEU:HD13	1:B:24:TYR:HE1	1.73	0.54
1:A:460:TYR:O	1:A:463:ARG:HG2	2.07	0.54
1:B:328:PRO:HB2	1:B:330:ASP:H	1.72	0.54
1:B:460:TYR:O	1:B:463:ARG:HG2	2.08	0.54
1:A:138:SER:HB2	1:A:171:THR:HG23	1.89	0.54
1:B:465:PRO:HB2	1:B:467:HIS:CD2	2.42	0.54
1:A:69:LYS:HD2	1:A:71:GLU:OE1	2.08	0.54
2:X:18:THR:CG2	2:X:120:ASP:CB	2.75	0.54
1:A:186:GLU:O	1:A:190:ILE:HG13	2.08	0.54
1:A:191:LYS:O	1:A:195:LYS:HB2	2.08	0.54
1:A:658:LEU:HB3	1:A:661:PRO:HB3	1.90	0.54
1:A:114:VAL:HG12	1:A:116:MET:O	2.08	0.53
1:A:91:ASN:O	1:A:98:LYS:HG3	2.07	0.53
1:A:96:ILE:HG21	1:B:15:LEU:HA	1.88	0.53
1:B:21:ASN:C	1:B:23:VAL:N	2.55	0.53
2:Y:48:GLU:HA	2:Y:67:LEU:O	2.08	0.53
2:X:131:ASP:N	2:X:131:ASP:OD2	2.41	0.53
1:B:138:SER:HB2	1:B:171:THR:HG23	1.90	0.53
1:B:117:ILE:HD12	1:B:346:ARG:CD	2.39	0.53
1:A:15:LEU:HA	1:B:96:ILE:HG21	1.90	0.53
1:B:590:GLU:HA	1:B:593:MET:HG2	1.91	0.53
1:B:114:VAL:C	1:B:116:MET:H	2.12	0.53
1:B:100:GLY:H	3:B:1678:ATP:C3'	2.21	0.53
1:A:114:VAL:C	1:A:116:MET:N	2.62	0.53
1:B:387:LYS:HA	1:B:390:LYS:HE3	1.90	0.53
1:A:119:GLN:HE22	1:A:374:LEU:HD11	1.74	0.53
1:B:286:GLN:O	1:B:287:GLU:HB2	2.09	0.53
1:A:308:HIS:CD2	1:A:309:PHE:N	2.77	0.52
1:B:332:PHE:HB3	1:B:337:LYS:HD2	1.90	0.52
1:A:64:ILE:O	1:A:206:GLN:HB2	2.09	0.52
1:A:410:ASP:OD2	1:A:413:GLN:HB2	2.10	0.52
2:Y:15:ARG:NH1	2:Y:32:ILE:N	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ASP:OD1	1:A:586:SER:HB2	2.09	0.52
2:X:48:GLU:HA	2:X:67:LEU:O	2.08	0.52
1:B:96:ILE:HA	1:B:120:PHE:O	2.09	0.52
1:A:114:VAL:C	1:A:116:MET:H	2.12	0.52
2:Y:23:ARG:HD3	2:Y:24:ASN:HB3	1.90	0.52
1:A:64:ILE:HD11	1:A:205:ILE:HG23	1.91	0.52
1:B:375:PRO:HB2	1:B:383:LEU:HG	1.91	0.52
1:A:476:GLY:HA2	1:A:591:ARG:HE	1.75	0.52
2:X:30:VAL:O	2:X:31:SER:HB3	2.08	0.52
1:B:200:PHE:CD1	1:B:277:TRP:CH2	2.97	0.52
1:A:668:ILE:HD13	1:B:664:PHE:HZ	1.73	0.52
1:A:390:LYS:O	1:A:393:ARG:HB3	2.10	0.52
1:A:181:GLN:NE2	1:A:181:GLN:HA	2.24	0.52
1:B:69:LYS:HD2	1:B:71:GLU:OE1	2.09	0.52
1:B:308:HIS:O	1:B:309:PHE:HB3	2.10	0.52
1:A:308:HIS:O	1:A:309:PHE:HB3	2.09	0.52
2:Y:24:ASN:H	2:Y:24:ASN:ND2	2.06	0.52
1:B:473:TYR:O	1:B:523:ASP:CB	2.58	0.52
1:B:422:SER:O	1:B:425:ILE:HG23	2.09	0.52
1:A:141:ASN:N	1:A:141:ASN:OD1	2.43	0.52
1:B:284:ILE:HG23	1:B:288:GLU:HB2	1.91	0.51
1:B:510:PHE:HA	1:B:513:LEU:HD12	1.92	0.51
1:B:119:GLN:C	1:B:121:GLY:H	2.14	0.51
1:B:200:PHE:N	1:B:200:PHE:HD2	2.07	0.51
1:B:293:TYR:HB2	1:B:322:PHE:CE1	2.45	0.51
1:B:104:PHE:CZ	1:B:114:VAL:HG11	2.45	0.51
1:A:571:LEU:HD11	1:A:574:ALA:HB3	1.92	0.51
2:X:50:LYS:HG3	2:X:66:GLN:HB3	1.93	0.51
2:Y:38:PRO:HA	2:Y:51:ALA:HB2	1.93	0.51
1:A:65:ARG:HA	1:A:206:GLN:O	2.11	0.51
1:B:59:GLU:OE2	1:B:60:PRO:HD2	2.11	0.51
1:B:274:LYS:HD2	1:B:274:LYS:H	1.76	0.51
1:A:513:LEU:O	1:A:515:GLU:N	2.43	0.51
1:B:410:ASP:OD2	1:B:413:GLN:HB2	2.11	0.51
2:X:24:ASN:H	2:X:24:ASN:ND2	2.07	0.51
1:A:200:PHE:N	1:A:200:PHE:CD2	2.79	0.51
1:A:140:SER:O	1:A:142:ASP:N	2.43	0.51
1:B:639:VAL:HG13	1:B:642:LEU:HD23	1.91	0.51
1:A:444:ARG:HG2	1:A:454:LEU:HB2	1.92	0.51
1:B:32:ARG:HH22	1:B:380:ARG:HB2	1.76	0.50
1:B:569:TYR:C	1:B:571:LEU:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HB3	1:A:175:LEU:HB2	1.92	0.50
1:A:284:ILE:HG23	1:A:288:GLU:HB2	1.92	0.50
1:B:444:ARG:HG2	1:B:454:LEU:HB2	1.92	0.50
1:B:470:ASN:HB2	1:B:472:TYR:HE2	1.76	0.50
1:A:119:GLN:C	1:A:121:GLY:H	2.13	0.50
2:Y:32:ILE:HG13	2:Y:65:TYR:CZ	2.46	0.50
1:B:70:PRO:HA	1:B:185:LEU:HD13	1.93	0.50
1:A:114:VAL:O	1:A:114:VAL:HG12	2.12	0.50
1:B:523:ASP:OD1	1:B:524:ILE:N	2.42	0.50
1:B:64:ILE:O	1:B:206:GLN:HB2	2.11	0.50
1:B:285:THR:H	1:B:288:GLU:CD	2.15	0.50
1:A:517:GLU:OE1	1:A:517:GLU:N	2.45	0.50
1:B:145:GLN:HE21	1:B:167:ILE:HG12	1.76	0.50
1:A:104:PHE:HB2	1:A:116:MET:HE1	1.93	0.50
1:A:378:LEU:HD13	1:B:24:TYR:CE1	2.47	0.50
1:A:32:ARG:HD3	1:A:197:HIS:CD2	2.43	0.50
2:X:15:ARG:NH1	2:X:32:ILE:N	2.59	0.50
1:A:21:ASN:C	1:A:23:VAL:N	2.58	0.50
1:A:23:VAL:CG1	1:A:24:TYR:N	2.74	0.50
1:A:37:ASN:HB3	3:A:1678:ATP:N7	2.27	0.49
2:Y:121:PHE:HA	2:Y:124:TRP:HB3	1.94	0.49
1:B:299:ASP:OD1	1:B:300:TRP:N	2.45	0.49
1:A:201:VAL:HG23	1:A:203:TYR:O	2.12	0.49
2:X:76:ILE:HD12	2:X:96:LYS:HB3	1.93	0.49
1:A:96:ILE:HA	1:A:120:PHE:O	2.12	0.49
1:A:285:THR:HG22	1:A:286:GLN:N	2.27	0.49
2:Y:24:ASN:ND2	2:Y:24:ASN:N	2.60	0.49
1:B:517:GLU:N	1:B:517:GLU:OE1	2.45	0.49
1:A:286:GLN:O	1:A:287:GLU:HB2	2.12	0.49
2:Y:50:LYS:HG3	2:Y:66:GLN:HB3	1.93	0.49
1:B:140:SER:O	1:B:142:ASP:N	2.44	0.49
1:B:396:ILE:O	1:B:400:LEU:HB2	2.13	0.49
1:B:74:VAL:HA	1:B:175:LEU:O	2.12	0.49
1:A:387:LYS:HA	1:A:390:LYS:HE3	1.94	0.49
1:A:569:TYR:C	1:A:571:LEU:H	2.14	0.49
2:X:28:ILE:HD12	2:X:95:TYR:HE1	1.77	0.49
1:A:340:ASN:O	1:A:342:LYS:HG3	2.12	0.49
1:B:283:ASP:C	1:B:284:ILE:HG13	2.32	0.49
1:A:293:TYR:HB2	1:A:322:PHE:CE1	2.46	0.49
1:A:10:ALA:CB	1:B:95:THR:HB	2.42	0.49
1:A:308:HIS:HD2	1:A:309:PHE:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLN:NE2	1:B:470:ASN:O	2.43	0.49
1:A:35:ILE:O	1:A:38:ALA:N	2.45	0.49
2:Y:18:THR:CG2	2:Y:120:ASP:CB	2.78	0.49
1:B:374:LEU:O	1:B:376:LEU:N	2.45	0.49
1:B:460:TYR:CE1	1:B:497:GLU:HB3	2.48	0.49
1:B:308:HIS:HD2	1:B:309:PHE:H	1.61	0.49
1:B:94:GLY:CA	1:B:98:LYS:HZ1	2.05	0.48
1:B:191:LYS:O	1:B:195:LYS:HB2	2.13	0.48
1:B:410:ASP:OD1	1:B:413:GLN:N	2.45	0.48
1:A:283:ASP:C	1:A:284:ILE:HG13	2.33	0.48
1:A:210:THR:HG23	1:A:264:VAL:HG13	1.95	0.48
1:B:140:SER:C	1:B:142:ASP:N	2.67	0.48
2:X:38:PRO:HA	2:X:51:ALA:HB2	1.95	0.48
1:B:481:ALA:O	1:B:482:VAL:HB	2.13	0.48
2:Y:18:THR:HG22	2:Y:18:THR:O	2.13	0.48
2:Y:15:ARG:HE	2:Y:31:SER:H	1.62	0.48
1:A:187:GLU:HG3	1:A:209:VAL:HG11	1.94	0.48
1:A:481:ALA:O	1:A:482:VAL:HB	2.13	0.48
1:B:104:PHE:HB2	1:B:116:MET:HE1	1.94	0.48
1:A:95:THR:HB	1:B:10:ALA:CB	2.43	0.48
1:B:475:THR:HB	1:B:501:LEU:HB2	1.95	0.48
1:B:351:THR:OG1	1:B:352:ASP:N	2.47	0.48
1:A:299:ASP:OD1	1:A:300:TRP:N	2.47	0.48
1:A:114:VAL:HB	1:A:346:ARG:NH2	2.29	0.48
1:A:513:LEU:C	1:A:515:GLU:H	2.15	0.48
1:A:64:ILE:CD1	1:A:205:ILE:HA	2.44	0.48
1:B:390:LYS:O	1:B:393:ARG:HB3	2.13	0.48
1:A:74:VAL:HA	1:A:175:LEU:O	2.12	0.48
1:A:639:VAL:HG13	1:A:642:LEU:HD23	1.95	0.48
1:A:47:TYR:O	1:A:50:LEU:HG	2.14	0.48
1:A:402:GLU:HA	1:A:405:ASN:HB2	1.95	0.48
1:B:212:GLU:HG2	1:B:214:GLU:H	1.79	0.48
3:B:1678:ATP:O2A	3:B:1678:ATP:O2B	2.31	0.48
1:A:32:ARG:HH22	1:A:380:ARG:CB	2.25	0.48
1:A:385:GLN:NE2	2:X:122:ASP:HA	2.06	0.48
1:B:308:HIS:CD2	1:B:309:PHE:N	2.81	0.48
1:A:483:GLU:HA	1:A:500:PHE:CE2	2.49	0.48
1:B:35:ILE:O	1:B:38:ALA:N	2.47	0.48
1:A:644:LYS:HD3	1:A:667:ARG:HH21	1.79	0.47
2:Y:28:ILE:HD12	2:Y:95:TYR:HE1	1.78	0.47
1:A:279:ARG:HG3	1:A:284:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:30:VAL:HG23	2:X:91:PHE:O	2.14	0.47
1:A:140:SER:C	1:A:142:ASP:N	2.65	0.47
1:B:30:PHE:CG	1:B:31:LEU:N	2.82	0.47
2:X:108:THR:HB	2:X:110:GLU:OE2	2.13	0.47
1:B:163:VAL:O	1:B:164:ASN:CB	2.61	0.47
1:B:571:LEU:HD11	1:B:574:ALA:HB3	1.95	0.47
1:A:163:VAL:O	1:A:164:ASN:HB2	2.14	0.47
3:B:1678:ATP:O3A	3:B:1678:ATP:O1G	2.31	0.47
1:B:64:ILE:HD11	1:B:205:ILE:HG23	1.95	0.47
1:B:141:ASN:N	1:B:141:ASN:OD1	2.44	0.47
1:B:91:ASN:O	1:B:98:LYS:HG3	2.14	0.47
2:X:32:ILE:HG13	2:X:65:TYR:CZ	2.50	0.47
1:B:531:GLU:O	1:B:537:LYS:HB2	2.14	0.47
1:B:27:LYS:HB2	1:B:129:LEU:HD13	1.96	0.47
1:B:644:LYS:HD3	1:B:667:ARG:HH21	1.79	0.47
1:A:207:LEU:O	1:A:207:LEU:HG	2.15	0.47
1:A:64:ILE:HD11	1:A:205:ILE:CG2	2.45	0.47
1:B:378:LEU:O	1:B:380:ARG:N	2.48	0.47
1:B:65:ARG:HA	1:B:206:GLN:O	2.15	0.47
1:A:289:TYR:O	1:A:292:PHE:HB3	2.15	0.47
1:B:201:VAL:HG23	1:B:203:TYR:O	2.15	0.47
3:A:1678:ATP:O1G	3:A:1678:ATP:O1B	2.33	0.47
1:B:344:TYR:CD2	1:B:344:TYR:N	2.83	0.47
1:B:73:LYS:HD3	1:B:182:LEU:HD21	1.97	0.47
1:B:199:GLU:HB3	1:B:200:PHE:HD2	1.80	0.47
1:A:510:PHE:HA	1:A:513:LEU:HD12	1.96	0.47
1:A:70:PRO:HA	1:A:185:LEU:HD13	1.95	0.47
1:B:483:GLU:HA	1:B:500:PHE:CE2	2.50	0.47
1:A:375:PRO:HB2	1:A:383:LEU:HG	1.96	0.47
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.77	0.47
1:A:95:THR:CB	1:B:10:ALA:HB2	2.44	0.47
1:B:114:VAL:C	1:B:116:MET:N	2.66	0.46
1:A:351:THR:OG1	1:A:352:ASP:N	2.48	0.46
1:A:85:THR:HG23	1:A:88:GLU:H	1.80	0.46
2:X:47:ILE:O	2:X:68:HIS:HA	2.15	0.46
1:A:340:ASN:O	1:A:342:LYS:N	2.48	0.46
1:A:475:THR:HB	1:A:501:LEU:HB2	1.96	0.46
1:A:104:PHE:CZ	1:A:114:VAL:HG11	2.51	0.46
2:X:38:PRO:CB	2:X:91:PHE:HE2	2.27	0.46
1:A:25:SER:H	1:B:384:GLN:HG3	1.80	0.46
1:B:513:LEU:O	1:B:515:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ILE:HG13	1:B:129:LEU:HD23	1.96	0.46
2:Y:47:ILE:O	2:Y:68:HIS:HA	2.15	0.46
1:B:443:LEU:O	1:B:456:SER:HA	2.15	0.46
1:B:23:VAL:HG13	1:B:24:TYR:N	2.31	0.46
1:A:463:ARG:HH11	1:A:497:GLU:HG3	1.80	0.46
1:A:410:ASP:OD1	1:A:413:GLN:N	2.48	0.46
1:B:534:ASP:OD1	1:B:537:LYS:HG2	2.15	0.46
2:Y:18:THR:HB	2:Y:29:THR:H	1.81	0.46
1:B:346:ARG:HG2	1:B:372:GLU:HA	1.97	0.46
1:A:210:THR:HG23	1:A:264:VAL:HG22	1.97	0.46
1:A:534:ASP:OD1	1:A:537:LYS:HG2	2.15	0.46
1:A:468:GLN:NE2	1:A:470:ASN:O	2.45	0.46
1:A:10:ALA:HB2	1:B:95:THR:CB	2.46	0.46
1:B:279:ARG:HG3	1:B:284:ILE:HD11	1.97	0.46
1:A:178:LYS:C	1:A:180:ASP:H	2.19	0.46
1:B:180:ASP:C	1:B:182:LEU:H	2.19	0.46
1:A:30:PHE:CG	1:A:31:LEU:N	2.84	0.46
2:X:121:PHE:HA	2:X:124:TRP:HB3	1.96	0.46
1:A:344:TYR:N	1:A:344:TYR:CD2	2.84	0.46
2:X:41:THR:HB	2:X:48:GLU:HB3	1.98	0.46
1:B:44:LYS:NZ	1:B:103:ALA:HB1	2.30	0.46
1:A:470:ASN:HB2	1:A:472:TYR:HE2	1.81	0.46
1:A:564:LYS:HG3	1:A:612:THR:HG23	1.98	0.46
1:A:114:VAL:O	1:A:115:SER:C	2.55	0.45
1:B:178:LYS:C	1:B:180:ASP:H	2.20	0.45
1:B:212:GLU:CD	1:B:214:GLU:HB3	2.36	0.45
1:B:331:LEU:HB2	1:B:332:PHE:CB	2.41	0.45
1:A:200:PHE:N	1:A:200:PHE:HD2	2.14	0.45
1:B:213:VAL:O	1:B:213:VAL:HG12	2.15	0.45
1:B:302:ASP:O	1:B:325:LYS:HE3	2.15	0.45
2:Y:99:LEU:HB2	2:Y:100:GLU:H	1.66	0.45
1:A:460:TYR:CE1	1:A:497:GLU:HB3	2.51	0.45
1:B:280:ASN:HA	1:B:281:PRO:HD2	1.75	0.45
1:A:507:GLU:CD	1:A:589:MET:HA	2.36	0.45
1:B:12:ILE:O	1:B:13:THR:C	2.54	0.45
1:B:119:GLN:O	3:B:1678:ATP:O2G	2.35	0.45
1:A:73:LYS:HD3	1:A:182:LEU:HD21	1.97	0.45
1:B:64:ILE:CD1	1:B:205:ILE:HA	2.46	0.45
1:A:401:ILE:HA	1:A:404:PHE:CD2	2.50	0.45
1:A:623:LYS:O	1:A:627:LYS:HG2	2.17	0.45
1:A:354:ALA:O	1:A:356:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ILE:HD12	1:A:643:THR:HG21	1.97	0.45
1:B:362:LEU:O	1:B:363:SER:C	2.55	0.45
1:A:200:PHE:CD1	1:A:277:TRP:CH2	3.05	0.45
1:B:331:LEU:HD13	1:B:337:LYS:HE3	1.98	0.45
2:X:15:ARG:HE	2:X:31:SER:H	1.63	0.45
1:B:513:LEU:C	1:B:515:GLU:H	2.19	0.45
1:B:119:GLN:O	1:B:120:PHE:HB2	2.17	0.45
1:A:383:LEU:HD21	1:A:389:MET:HE2	1.99	0.45
2:Y:30:VAL:CG2	2:Y:91:PHE:HB3	2.47	0.45
1:B:463:ARG:HH11	1:B:497:GLU:HG3	1.81	0.45
1:B:623:LYS:O	1:B:627:LYS:HG2	2.17	0.45
1:B:446:ASN:HA	1:B:446:ASN:HD22	1.67	0.45
1:B:402:GLU:HA	1:B:405:ASN:HB2	1.99	0.45
1:A:374:LEU:O	1:A:376:LEU:N	2.50	0.44
1:A:524:ILE:O	1:A:580:THR:CG2	2.64	0.44
1:A:195:LYS:HE3	1:A:270:LEU:O	2.16	0.44
2:Y:32:ILE:CD1	2:Y:33:ALA:H	2.20	0.44
2:X:23:ARG:HB2	2:X:130:GLN:HE22	1.81	0.44
1:A:16:MET:O	1:A:19:ILE:N	2.50	0.44
1:B:104:PHE:CE2	1:B:114:VAL:CG1	3.01	0.44
2:X:18:THR:O	2:X:18:THR:HG22	2.17	0.44
1:B:526:LYS:HZ2	1:B:581:GLY:HA2	1.82	0.44
2:Y:15:ARG:HH11	2:Y:32:ILE:H	1.64	0.44
1:A:284:ILE:CG2	1:A:288:GLU:HB2	2.48	0.44
1:A:350:ILE:HG22	1:A:351:THR:H	1.79	0.44
1:A:8:PHE:CB	1:B:12:ILE:HG21	2.47	0.44
1:A:44:LYS:HD2	1:A:44:LYS:HA	1.90	0.44
1:B:557:ILE:HD12	1:B:643:THR:HG21	1.98	0.44
1:B:305:TYR:OH	1:B:406:GLU:OE1	2.31	0.44
1:B:507:GLU:O	1:B:511:THR:HG23	2.17	0.44
1:B:117:ILE:HG23	1:B:119:GLN:OE1	2.16	0.44
1:B:119:GLN:C	1:B:121:GLY:N	2.69	0.44
1:A:180:ASP:C	1:A:182:LEU:H	2.20	0.44
2:Y:19:THR:HG23	2:Y:107:LEU:HD12	1.99	0.44
1:A:274:LYS:HD2	1:A:274:LYS:H	1.83	0.44
1:A:101:THR:O	1:A:104:PHE:N	2.29	0.44
2:X:99:LEU:HB2	2:X:100:GLU:H	1.67	0.44
1:B:387:LYS:HA	1:B:390:LYS:CE	2.47	0.44
1:A:651:LEU:O	1:A:656:PHE:HB2	2.18	0.44
1:A:507:GLU:O	1:A:511:THR:HG23	2.18	0.44
1:B:32:ARG:HD3	1:B:197:HIS:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD23	1:A:81:GLY:N	2.33	0.44
2:Y:18:THR:HA	2:Y:118:LYS:O	2.18	0.44
1:A:119:GLN:O	1:A:120:PHE:HB2	2.18	0.44
1:A:199:GLU:HB3	1:A:200:PHE:HD2	1.82	0.44
1:A:435:ASN:O	1:A:436:ARG:C	2.57	0.44
1:A:378:LEU:O	1:A:380:ARG:N	2.51	0.44
1:B:59:GLU:H	1:B:169:ARG:HH12	1.66	0.44
1:A:127:LEU:C	1:A:127:LEU:HD12	2.38	0.44
1:B:7:GLU:H	1:B:7:GLU:CD	2.22	0.44
1:B:323:ILE:HD12	1:B:407:ILE:CD1	2.48	0.44
1:B:119:GLN:O	3:B:1678:ATP:O3B	2.36	0.43
1:B:31:LEU:HD12	1:B:31:LEU:HA	1.85	0.43
2:Y:125:VAL:O	2:Y:126:ASP:O	2.36	0.43
1:B:414:PHE:O	1:B:418:TYR:N	2.49	0.43
1:A:119:GLN:C	1:A:121:GLY:N	2.72	0.43
1:B:64:ILE:HD11	1:B:205:ILE:CG2	2.48	0.43
2:Y:41:THR:HB	2:Y:48:GLU:HB3	2.00	0.43
1:A:35:ILE:HG22	1:A:36:SER:N	2.33	0.43
1:A:85:THR:HG22	1:A:88:GLU:CG	2.48	0.43
1:A:507:GLU:OE2	1:A:589:MET:HA	2.19	0.43
1:B:485:SER:C	1:B:487:PHE:H	2.21	0.43
2:X:126:ASP:O	2:X:127:ALA:HB3	2.19	0.43
1:A:20:ILE:HG13	1:A:129:LEU:HD23	1.99	0.43
1:B:85:THR:HG22	1:B:88:GLU:CG	2.47	0.43
1:B:401:ILE:HA	1:B:404:PHE:CD2	2.53	0.43
1:B:22:THR:HG23	1:B:24:TYR:CZ	2.53	0.43
1:B:117:ILE:HD13	1:B:374:LEU:HD22	2.01	0.43
1:A:513:LEU:C	1:A:515:GLU:N	2.71	0.43
2:X:112:VAL:HA	2:X:114:TYR:HD2	1.84	0.43
2:Y:112:VAL:HA	2:Y:114:TYR:HD2	1.83	0.43
1:B:77:ILE:HG22	1:B:77:ILE:O	2.18	0.43
1:B:177:LEU:H	1:B:177:LEU:HD22	1.84	0.43
1:A:31:LEU:O	1:A:32:ARG:C	2.57	0.43
1:B:564:LYS:HG3	1:B:612:THR:HG23	2.01	0.43
2:Y:103:TYR:CD2	2:Y:103:TYR:N	2.84	0.43
1:B:375:PRO:CB	1:B:383:LEU:HG	2.48	0.43
1:A:75:LEU:HD23	1:A:175:LEU:HD12	2.00	0.43
1:A:137:ILE:HB	1:A:172:ILE:HG22	1.99	0.43
1:B:137:ILE:HB	1:B:172:ILE:CG2	2.48	0.43
1:B:289:TYR:O	1:B:292:PHE:HB3	2.19	0.43
1:B:320:ILE:O	1:B:321:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ILE:CG2	1:B:288:GLU:HB2	2.49	0.43
2:Y:43:LYS:CB	2:Y:46:TYR:HB2	2.48	0.43
1:B:314:GLN:HG2	2:Y:119:THR:CG2	2.49	0.43
1:A:77:ILE:HG22	1:A:77:ILE:O	2.18	0.43
2:Y:23:ARG:HB2	2:Y:130:GLN:HE22	1.83	0.43
1:A:485:SER:C	1:A:487:PHE:H	2.22	0.43
1:A:97:ALA:O	1:A:98:LYS:O	2.36	0.43
1:A:137:ILE:HB	1:A:172:ILE:CG2	2.48	0.43
1:B:346:ARG:CZ	1:B:372:GLU:OE2	2.67	0.42
2:X:18:THR:HA	2:X:118:LYS:O	2.18	0.42
1:A:104:PHE:CE2	1:A:114:VAL:CG1	3.01	0.42
2:X:24:ASN:N	2:X:24:ASN:ND2	2.61	0.42
1:B:350:ILE:HG22	1:B:351:THR:H	1.82	0.42
1:A:290:ASN:HB2	1:A:303:PRO:HD2	2.01	0.42
1:B:100:GLY:H	3:B:1678:ATP:H3'	1.84	0.42
1:A:591:ARG:HA	1:A:594:LYS:NZ	2.34	0.42
2:X:19:THR:HG22	2:X:20:ASP:H	1.84	0.42
1:A:59:GLU:OE2	1:A:60:PRO:HD2	2.18	0.42
1:B:285:THR:CG2	1:B:286:GLN:H	2.24	0.42
2:Y:24:ASN:O	2:Y:96:LYS:HG3	2.19	0.42
1:B:137:ILE:HG12	1:B:147:ILE:HG13	2.01	0.42
1:A:7:GLU:CD	1:A:7:GLU:H	2.22	0.42
2:X:18:THR:HB	2:X:29:THR:H	1.85	0.42
1:A:380:ARG:O	1:A:381:GLU:HB2	2.19	0.42
2:Y:30:VAL:HG23	2:Y:91:PHE:O	2.18	0.42
1:B:137:ILE:HB	1:B:172:ILE:HG22	2.01	0.42
1:B:354:ALA:O	1:B:356:ASP:N	2.52	0.42
1:B:543:GLU:O	1:B:546:GLU:HB2	2.19	0.42
1:B:118:GLY:HA2	1:B:380:ARG:HH22	1.84	0.42
1:A:308:HIS:CD2	1:A:309:PHE:H	2.37	0.42
1:B:75:LEU:HD23	1:B:175:LEU:HD12	2.00	0.42
1:B:421:PHE:O	1:B:422:SER:C	2.58	0.42
1:A:487:PHE:CZ	1:A:524:ILE:HD13	2.55	0.42
1:B:42:LEU:HA	1:B:81:GLY:HA2	2.02	0.42
1:A:548:GLU:N	1:A:549:PRO:HD2	2.34	0.42
1:B:525:THR:CG2	1:B:582:GLN:HG3	2.50	0.42
2:Y:97:LYS:HD3	2:Y:104:TRP:NE1	2.34	0.42
1:B:548:GLU:N	1:B:549:PRO:HD2	2.35	0.42
1:B:525:THR:HG23	1:B:582:GLN:HG3	2.01	0.42
1:B:85:THR:HG23	1:B:88:GLU:H	1.85	0.42
1:B:31:LEU:O	1:B:32:ARG:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:20:ASP:CG	2:X:27:LEU:O	2.58	0.42
1:A:432:ASP:OD2	1:A:433:THR:N	2.53	0.42
1:A:616:SER:HA	1:A:617:PRO:HD3	1.90	0.42
1:B:265:GLN:O	1:B:267:ILE:HG23	2.20	0.42
1:A:209:VAL:CG2	1:A:267:ILE:HG12	2.49	0.42
1:A:507:GLU:OE1	1:A:589:MET:HA	2.20	0.42
1:A:320:ILE:O	1:A:321:LEU:HD23	2.20	0.42
1:B:412:GLU:OE1	1:B:415:GLU:HB2	2.20	0.42
1:B:525:THR:HG23	1:B:582:GLN:HA	2.02	0.41
2:Y:15:ARG:HH11	2:Y:32:ILE:N	2.17	0.41
2:X:24:ASN:O	2:X:96:LYS:HG3	2.20	0.41
1:B:195:LYS:HD3	1:B:199:GLU:OE2	2.20	0.41
1:A:482:VAL:HG13	1:A:500:PHE:CD2	2.55	0.41
1:B:139:LYS:HB2	1:B:145:GLN:HG3	2.02	0.41
1:B:627:LYS:H	1:B:627:LYS:HG2	1.63	0.41
1:B:560:ASP:O	1:B:561:GLN:HG3	2.20	0.41
1:A:615:ILE:HG23	1:A:622:ILE:HG12	2.03	0.41
1:A:369:VAL:HG12	1:A:370:ASP:N	2.35	0.41
1:B:654:SER:O	1:B:655:GLY:C	2.59	0.41
1:A:302:ASP:O	1:A:325:LYS:HE3	2.20	0.41
1:A:96:ILE:HG13	1:B:15:LEU:HD13	2.02	0.41
1:B:277:TRP:HA	1:B:308:HIS:CE1	2.55	0.41
2:Y:72:TYR:CD2	2:Y:73:LYS:HG3	2.54	0.41
1:B:374:LEU:C	1:B:376:LEU:N	2.74	0.41
1:A:590:GLU:O	1:A:594:LYS:HB3	2.21	0.41
1:B:328:PRO:HB2	1:B:329:PHE:CA	2.50	0.41
1:A:387:LYS:HA	1:A:390:LYS:CE	2.51	0.41
1:B:78:ARG:CA	1:B:172:ILE:HD12	2.50	0.41
1:B:432:ASP:CG	1:B:433:THR:N	2.74	0.41
2:Y:19:THR:HG22	2:Y:20:ASP:H	1.86	0.41
1:A:543:GLU:O	1:A:546:GLU:HB2	2.20	0.41
2:X:103:TYR:N	2:X:103:TYR:CD2	2.87	0.41
1:B:522:VAL:O	1:B:523:ASP:CB	2.67	0.41
1:B:314:GLN:NE2	2:Y:124:TRP:HD1	2.18	0.41
1:B:44:LYS:HA	1:B:44:LYS:HD2	1.86	0.41
1:A:560:ASP:O	1:A:561:GLN:HG3	2.19	0.41
2:Y:15:ARG:HB3	2:Y:30:VAL:HG12	2.02	0.41
1:A:550:LEU:HD13	1:A:629:VAL:CG2	2.51	0.41
2:Y:25:TYR:CE1	2:Y:27:LEU:HD22	2.54	0.41
1:A:44:LYS:NZ	1:A:103:ALA:HB1	2.36	0.41
1:A:17:SER:HA	1:A:20:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TRP:O	1:A:424:ASN:HB3	2.21	0.41
1:A:135:GLN:HB2	1:A:176:PHE:HE2	1.86	0.41
1:B:433:THR:HA	1:B:436:ARG:HD3	2.03	0.41
1:B:470:ASN:HB2	1:B:472:TYR:CE2	2.56	0.41
1:B:331:LEU:HB2	1:B:332:PHE:CA	2.45	0.41
1:B:135:GLN:HE22	1:B:149:GLU:CD	2.24	0.41
2:X:15:ARG:HH11	2:X:32:ILE:H	1.67	0.41
1:B:35:ILE:O	1:B:36:SER:C	2.57	0.41
1:A:290:ASN:OD1	1:A:291:ALA:N	2.53	0.41
1:B:361:TRP:O	1:B:424:ASN:HB3	2.21	0.41
2:X:15:ARG:HH11	2:X:32:ILE:N	2.19	0.40
1:B:460:TYR:OH	1:B:497:GLU:O	2.30	0.40
2:Y:49:LEU:O	2:Y:66:GLN:HA	2.21	0.40
1:A:664:PHE:HZ	1:B:668:ILE:HD13	1.86	0.40
1:A:122:VAL:CG2	1:A:123:GLY:N	2.85	0.40
1:B:645:LEU:HD13	1:B:667:ARG:HB2	2.02	0.40
1:A:654:SER:O	1:A:655:GLY:C	2.59	0.40
1:B:189:ARG:HD2	1:B:192:GLU:OE1	2.21	0.40
1:B:114:VAL:HG12	1:B:116:MET:O	2.21	0.40
1:A:384:GLN:CB	1:B:23:VAL:HG13	2.47	0.40
1:A:432:ASP:CG	1:A:433:THR:N	2.74	0.40
1:B:432:ASP:OD2	1:B:433:THR:N	2.52	0.40
1:B:314:GLN:HG2	2:Y:119:THR:HG21	2.03	0.40
1:B:645:LEU:HD13	1:B:667:ARG:CB	2.51	0.40
1:B:485:SER:HA	1:B:486:PRO:HD2	1.95	0.40
1:B:190:ILE:HG13	1:B:190:ILE:H	1.70	0.40
1:B:151:ASN:O	2:X:86:ASN:CB	2.68	0.40
1:A:211:LYS:HB3	1:A:212:GLU:H	1.74	0.40
1:A:18:LEU:HD21	1:B:120:PHE:HA	2.03	0.40
1:B:267:ILE:HB	1:B:268:GLU:H	1.72	0.40
1:A:341:ILE:HG13	1:A:341:ILE:H	1.49	0.40
1:A:159:THR:HG23	1:B:3:SER:HA	2.04	0.40
1:A:315:LEU:HD12	1:A:317:PHE:HD2	1.87	0.40
1:A:14:GLN:HG3	1:B:97:ALA:HA	2.04	0.40
1:A:668:ILE:HD13	1:B:664:PHE:CZ	2.56	0.40
1:B:35:ILE:HG22	1:B:36:SER:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	601/677 (89%)	447 (74%)	107 (18%)	47 (8%)	1	6
1	B	612/677 (90%)	447 (73%)	117 (19%)	48 (8%)	1	6
2	X	109/134 (81%)	83 (76%)	18 (16%)	8 (7%)	1	7
2	Y	109/134 (81%)	82 (75%)	19 (17%)	8 (7%)	1	7
All	All	1431/1622 (88%)	1059 (74%)	261 (18%)	111 (8%)	1	6

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	24	TYR
1	A	25	SER
1	A	98	LYS
1	A	164	ASN
1	A	179	ASP
1	A	355	GLU
1	A	363	SER
1	A	376	LEU
1	A	379	SER
1	A	433	THR
1	A	482	VAL
1	A	530	LEU
1	A	534	ASP
1	A	537	LYS
1	B	23	VAL
1	B	24	TYR
1	B	25	SER
1	B	98	LYS
1	B	115	SER
1	B	164	ASN
1	B	179	ASP

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Mol	Chain	Res	Type
1	B	355	GLU
1	B	363	SER
1	B	376	LEU
1	B	379	SER
1	B	433	THR
1	B	482	VAL
1	B	523	ASP
1	B	525	THR
1	B	530	LEU
1	B	534	ASP
2	X	20	ASP
2	X	126	ASP
2	Y	20	ASP
2	Y	126	ASP
1	A	22	THR
1	A	90	ILE
1	A	115	SER
1	A	123	GLY
1	A	141	ASN
1	A	266	GLU
1	A	271	ASN
1	A	381	GLU
1	A	483	GLU
1	A	514	LYS
1	A	525	THR
1	B	22	THR
1	B	123	GLY
1	B	141	ASN
1	B	195	LYS
1	B	266	GLU
1	B	271	ASN
1	B	298	ASN
1	B	339	ASN
1	B	483	GLU
1	B	514	LYS
1	B	655	GLY
2	X	30	VAL
2	X	86	ASN
2	X	129	GLU
2	Y	30	VAL
2	Y	86	ASN
2	Y	129	GLU

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Mol	Chain	Res	Type
1	A	40	ASP
1	A	195	LYS
1	A	298	ASN
1	A	360	GLU
1	A	533	THR
1	A	655	GLY
1	B	328	PRO
1	B	368	VAL
1	B	532	GLU
1	B	533	THR
2	Y	31	SER
1	A	181	GLN
1	A	377	ASN
1	B	81	GLY
1	B	90	ILE
1	B	360	GLU
1	B	375	PRO
1	B	377	ASN
1	B	381	GLU
1	B	524	ILE
1	B	531	GLU
2	X	31	SER
1	A	13	THR
1	A	26	ASN
1	A	286	GLN
1	A	328	PRO
1	A	341	ILE
1	A	375	PRO
1	B	181	GLN
1	B	274	LYS
1	B	385	GLN
1	A	350	ILE
1	A	486	PRO
1	B	26	ASN
1	B	350	ILE
1	B	486	PRO
1	A	365	VAL
2	X	125	VAL
1	A	96	ILE
1	A	368	VAL
2	X	75	ILE
2	Y	75	ILE

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Mol	Chain	Res	Type
2	Y	125	VAL
1	A	575	PRO
1	B	96	ILE
1	B	575	PRO
1	A	451	VAL

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	546/615 (89%)	454 (83%)	92 (17%)	2	11
1	B	554/615 (90%)	457 (82%)	97 (18%)	2	10
2	X	106/124 (86%)	84 (79%)	22 (21%)	1	6
2	Y	106/124 (86%)	85 (80%)	21 (20%)	1	7
All	All	1312/1478 (89%)	1080 (82%)	232 (18%)	2	10

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	20	ILE
1	A	23	VAL
1	A	26	ASN
1	A	35	ILE
1	A	50	LEU
1	A	72	GLN
1	A	93	LEU
1	A	95	THR
1	A	98	LYS
1	A	102	LYS
1	A	104	PHE
1	A	105	MET
1	A	106	GLU
1	A	108	LEU
1	A	113	ASP

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Mol	Chain	Res	Type
1	A	116	MET
1	A	119	GLN
1	A	133	ARG
1	A	135	GLN
1	A	141	ASN
1	A	142	ASP
1	A	144	GLU
1	A	159	THR
1	A	160	LEU
1	A	179	ASP
1	A	196	ARG
1	A	197	HIS
1	A	200	PHE
1	A	205	ILE
1	A	209	VAL
1	A	210	THR
1	A	266	GLU
1	A	268	GLU
1	A	270	LEU
1	A	271	ASN
1	A	274	LYS
1	A	282	SER
1	A	283	ASP
1	A	288	GLU
1	A	298	ASN
1	A	301	GLU
1	A	302	ASP
1	A	315	LEU
1	A	329	PHE
1	A	341	ILE
1	A	346	ARG
1	A	347	ARG
1	A	348	VAL
1	A	355	GLU
1	A	356	ASP
1	A	377	ASN
1	A	378	LEU
1	A	382	MET
1	A	425	ILE
1	A	433	THR
1	A	444	ARG
1	A	448	THR

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Mol	Chain	Res	Type
1	A	450	SER
1	A	454	LEU
1	A	455	THR
1	A	458	THR
1	A	475	THR
1	A	479	LEU
1	A	485	SER
1	A	487	PHE
1	A	494	LYS
1	A	497	GLU
1	A	508	TYR
1	A	520	THR
1	A	522	VAL
1	A	523	ASP
1	A	524	ILE
1	A	528	PHE
1	A	532	GLU
1	A	534	ASP
1	A	537	LYS
1	A	540	ARG
1	A	548	GLU
1	A	556	GLU
1	A	580	THR
1	A	586	SER
1	A	588	ASN
1	A	596	GLN
1	A	636	ASP
1	A	640	LYS
1	A	646	LEU
1	A	660	GLU
1	A	662	THR
1	A	669	ASN
1	A	670	ARG
1	A	673	SER
1	B	7	GLU
1	B	18	LEU
1	B	20	ILE
1	B	23	VAL
1	B	26	ASN
1	B	50	LEU
1	B	67	THR
1	B	72	GLN

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Mol	Chain	Res	Type
1	B	93	LEU
1	B	95	THR
1	B	98	LYS
1	B	102	LYS
1	B	104	PHE
1	B	105	MET
1	B	106	GLU
1	B	108	LEU
1	B	113	ASP
1	B	116	MET
1	B	119	GLN
1	B	133	ARG
1	B	135	GLN
1	B	141	ASN
1	B	142	ASP
1	B	144	GLU
1	B	159	THR
1	B	160	LEU
1	B	196	ARG
1	B	200	PHE
1	B	205	ILE
1	B	209	VAL
1	B	210	THR
1	B	211	LYS
1	B	214	GLU
1	B	266	GLU
1	B	268	GLU
1	B	270	LEU
1	B	271	ASN
1	B	274	LYS
1	B	282	SER
1	B	283	ASP
1	B	288	GLU
1	B	298	ASN
1	B	301	GLU
1	B	302	ASP
1	B	315	LEU
1	B	329	PHE
1	B	332	PHE
1	B	337	LYS
1	B	338	LYS
1	B	344	TYR

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Mol	Chain	Res	Type
1	B	346	ARG
1	B	347	ARG
1	B	348	VAL
1	B	355	GLU
1	B	356	ASP
1	B	357	LEU
1	B	377	ASN
1	B	378	LEU
1	B	382	MET
1	B	425	ILE
1	B	433	THR
1	B	444	ARG
1	B	447	SER
1	B	448	THR
1	B	450	SER
1	B	454	LEU
1	B	455	THR
1	B	458	THR
1	B	475	THR
1	B	479	LEU
1	B	487	PHE
1	B	494	LYS
1	B	497	GLU
1	B	508	TYR
1	B	520	THR
1	B	525	THR
1	B	526	LYS
1	B	528	PHE
1	B	530	LEU
1	B	532	GLU
1	B	534	ASP
1	B	537	LYS
1	B	540	ARG
1	B	548	GLU
1	B	556	GLU
1	B	580	THR
1	B	586	SER
1	B	588	ASN
1	B	596	GLN
1	B	636	ASP
1	B	640	LYS
1	B	646	LEU

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Mol	Chain	Res	Type
1	B	660	GLU
1	B	662	THR
1	B	669	ASN
1	B	670	ARG
1	B	673	SER
2	X	12	TRP
2	X	16	SER
2	X	19	THR
2	X	24	ASN
2	X	27	LEU
2	X	32	ILE
2	X	41	THR
2	X	52	GLN
2	X	80	THR
2	X	81	MET
2	X	84	VAL
2	X	94	LEU
2	X	95	TYR
2	X	98	ASP
2	X	99	LEU
2	X	101	SER
2	X	103	TYR
2	X	110	GLU
2	X	112	VAL
2	X	123	LYS
2	X	125	VAL
2	X	131	ASP
2	Y	12	TRP
2	Y	16	SER
2	Y	19	THR
2	Y	24	ASN
2	Y	30	VAL
2	Y	32	ILE
2	Y	41	THR
2	Y	52	GLN
2	Y	80	THR
2	Y	81	MET
2	Y	84	VAL
2	Y	94	LEU
2	Y	95	TYR
2	Y	98	ASP
2	Y	99	LEU

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Mol	Chain	Res	Type
2	Y	101	SER
2	Y	103	TYR
2	Y	110	GLU
2	Y	112	VAL
2	Y	123	LYS
2	Y	125	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	135	GLN
1	A	181	GLN
1	A	197	HIS
1	A	271	ASN
1	A	308	HIS
1	A	314	GLN
1	A	340	ASN
1	A	384	GLN
1	A	385	GLN
1	A	446	ASN
1	A	467	HIS
1	A	561	GLN
1	A	588	ASN
1	B	72	GLN
1	B	135	GLN
1	B	181	GLN
1	B	197	HIS
1	B	308	HIS
1	B	339	ASN
1	B	384	GLN
1	B	446	ASN
1	B	467	HIS
1	B	561	GLN
1	B	588	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	1678	1	24,33,33	1.12	2 (8%)	31,52,52	2.21	6 (19%)
3	ATP	B	1678	-	24,33,33	0.98	1 (4%)	31,52,52	2.27	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	1678	1	-	0/18/38/38	0/3/3/3
3	ATP	B	1678	-	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1678	ATP	O4'-C1'	2.01	1.43	1.41
3	B	1678	ATP	C5-C4	2.93	1.47	1.40
3	A	1678	ATP	C5-C4	3.63	1.48	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1678	ATP	N3-C2-N1	-6.79	123.69	128.89
3	A	1678	ATP	N3-C2-N1	-6.66	123.80	128.89
3	A	1678	ATP	PA-O3A-PB	-6.45	114.63	132.73
3	B	1678	ATP	PA-O3A-PB	-6.03	115.80	132.73
3	B	1678	ATP	PB-O3B-PG	-5.49	114.27	132.67
3	A	1678	ATP	PB-O3B-PG	-5.26	115.04	132.67
3	A	1678	ATP	C4-C5-N7	-2.65	107.04	109.48
3	A	1678	ATP	O3A-PA-O5'	-2.06	97.48	102.94
3	B	1678	ATP	O3G-PG-O2G	2.00	115.00	107.38
3	B	1678	ATP	N6-C6-N1	2.14	123.79	119.20
3	A	1678	ATP	O2G-PG-O1G	2.15	117.52	110.58
3	B	1678	ATP	O2G-PG-O1G	2.18	117.61	110.58
3	B	1678	ATP	O2B-PB-O3A	2.39	115.93	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1678	ATP	5	0
3	B	1678	ATP	13	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	609/677 (89%)	1.04	92 (15%) 3 1	63, 72, 74, 79	0
1	B	618/677 (91%)	0.86	71 (11%) 6 2	66, 72, 75, 88	0
2	X	115/134 (85%)	0.82	17 (14%) 3 1	69, 71, 74, 82	0
2	Y	115/134 (85%)	0.94	17 (14%) 3 1	69, 71, 74, 83	0
All	All	1457/1622 (89%)	0.94	197 (13%) 4 2	63, 72, 74, 88	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	ALA	9.0
1	A	25	SER	7.3
1	B	673	SER	7.0
1	A	532	GLU	6.8
1	A	549	PRO	6.7
1	A	597	ALA	6.2
1	A	638	THR	6.0
1	A	533	THR	5.6
1	A	535	GLU	5.6
1	A	531	GLU	5.5
1	B	271	ASN	5.3
1	A	674	LEU	4.8
1	A	567	VAL	4.8
1	A	529	GLU	4.7
1	A	58	THR	4.7
2	Y	135	ALA	4.7
2	X	62	VAL	4.6
1	A	547	TYR	4.4
1	A	550	LEU	4.4
2	Y	62	VAL	4.3
1	A	110	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	263	GLU	4.3
1	A	585	TRP	4.0
1	A	572	LEU	4.0
1	A	641	ASP	4.0
1	B	535	GLU	4.0
1	A	530	LEU	4.0
1	A	215	LYS	3.9
1	B	568	SER	3.9
1	A	553	ALA	3.9
1	B	560	ASP	3.9
1	A	568	SER	3.9
1	B	334	SER	3.9
1	A	637	LYS	3.8
1	A	624	GLU	3.8
1	A	536	GLU	3.8
1	A	573	ASP	3.7
1	A	170	GLY	3.7
1	A	635	GLN	3.7
1	B	616	SER	3.7
1	A	546	GLU	3.6
1	B	115	SER	3.6
1	A	563	GLU	3.6
1	A	673	SER	3.6
1	A	169	ARG	3.6
1	A	586	SER	3.6
1	A	379	SER	3.5
1	B	462	THR	3.4
2	Y	12	TRP	3.4
2	Y	134	GLU	3.4
1	B	637	LYS	3.4
1	A	560	ASP	3.3
1	A	596	GLN	3.3
1	B	330	ASP	3.3
1	A	328	PRO	3.3
1	A	146	TYR	3.3
1	B	216	GLU	3.2
1	B	632	GLY	3.2
1	A	620	PRO	3.2
1	A	539	GLU	3.2
1	B	617	PRO	3.2
1	B	269	GLU	3.2
2	X	132	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	300	TRP	3.2
1	A	485	SER	3.2
1	A	496	PHE	3.1
1	B	543	GLU	3.1
1	B	638	THR	3.1
1	A	564	LYS	3.1
1	B	452	ASP	3.1
1	A	263	GLU	3.1
1	A	554	LEU	3.1
1	A	326	ARG	3.1
1	B	533	THR	3.0
1	B	490	ALA	3.0
1	A	271	ASN	3.0
1	B	630	ASP	3.0
1	A	642	LEU	3.0
1	A	534	ASP	3.0
1	A	138	SER	3.0
1	B	326	ARG	2.9
1	B	262	GLU	2.9
1	B	572	LEU	2.9
2	Y	95	TYR	2.9
1	A	484	LYS	2.9
1	B	636	ASP	2.9
2	X	50	LYS	2.9
1	B	379	SER	2.9
1	B	576	ALA	2.8
1	A	618	LYS	2.8
2	X	12	TRP	2.8
1	B	551	THR	2.8
1	B	495	ASN	2.8
1	B	640	LYS	2.8
1	A	542	LYS	2.8
2	X	97	LYS	2.8
2	X	63	HIS	2.8
1	A	630	ASP	2.8
1	A	270	LEU	2.7
2	Y	34	ASP	2.7
2	X	95	TYR	2.7
1	B	567	VAL	2.7
1	A	541	GLU	2.7
1	A	633	GLY	2.7
2	X	36	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLN	2.7
1	B	520	THR	2.7
1	A	581	GLY	2.6
2	Y	64	HIS	2.6
1	B	213	VAL	2.6
1	A	583	PHE	2.6
1	A	449	LYS	2.6
1	A	467	HIS	2.6
1	B	514	LYS	2.6
1	A	579	ARG	2.6
2	Y	130	GLN	2.6
1	B	210	THR	2.6
1	B	25	SER	2.6
2	X	94	LEU	2.5
1	A	566	VAL	2.5
1	B	335	LYS	2.5
1	A	515	GLU	2.5
1	B	266	GLU	2.5
1	B	144	GLU	2.5
1	B	675	GLY	2.5
1	B	339	ASN	2.5
1	A	631	GLU	2.5
1	B	110	ALA	2.5
1	A	300	TRP	2.5
1	B	633	GLY	2.5
1	B	485	SER	2.4
1	A	211	LYS	2.4
1	A	640	LYS	2.4
1	B	618	LYS	2.4
1	B	323	ILE	2.4
2	X	65	TYR	2.4
2	Y	93	LYS	2.4
1	A	528	PHE	2.4
2	Y	97	LYS	2.4
1	B	270	LEU	2.4
1	B	324	PRO	2.4
1	A	623	LYS	2.3
1	A	466	GLU	2.3
2	Y	53	SER	2.3
1	A	117	ILE	2.3
1	B	215	LYS	2.3
1	A	21	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	632	GLY	2.3
1	B	484	LYS	2.3
1	A	210	THR	2.3
1	B	674	LEU	2.3
1	A	551	THR	2.3
1	A	629	VAL	2.3
1	B	329	PHE	2.2
1	A	527	ASP	2.2
1	A	495	ASN	2.2
1	A	213	VAL	2.2
1	A	486	PRO	2.2
2	X	39	GLU	2.2
1	A	639	VAL	2.2
2	Y	131	ASP	2.2
1	A	621	ILE	2.2
1	A	582	GLN	2.2
1	B	536	GLU	2.2
2	X	76	ILE	2.2
1	B	419	SER	2.2
1	B	479	LEU	2.2
1	A	285	THR	2.1
2	Y	63	HIS	2.1
2	X	52	GLN	2.1
2	Y	74	GLU	2.1
1	B	677	ASN	2.1
1	B	96	ILE	2.1
2	Y	75	ILE	2.1
1	A	574	ALA	2.1
1	B	620	PRO	2.1
1	B	594	LYS	2.1
1	A	565	VAL	2.1
2	Y	78	GLU	2.1
2	X	66	GLN	2.1
2	X	44	PRO	2.1
2	Y	101	SER	2.1
1	B	582	GLN	2.1
1	B	117	ILE	2.1
1	B	146	TYR	2.1
1	B	40	ASP	2.1
1	B	539	GLU	2.1
1	B	264	VAL	2.1
2	X	133	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	468	GLN	2.1
1	B	160	LEU	2.1
1	B	496	PHE	2.0
1	B	366	LYS	2.0
1	A	264	VAL	2.0
1	A	562	VAL	2.0
2	X	93	LYS	2.0
1	B	463	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ATP	A	1678	31/31	0.94	0.19	-2.15	21,30,32,33	0
3	ATP	B	1678	31/31	0.94	0.20	-2.44	18,29,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.