



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:45 PM UTC

PDB ID : 2CG9 / pdb_00002cg9
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

<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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

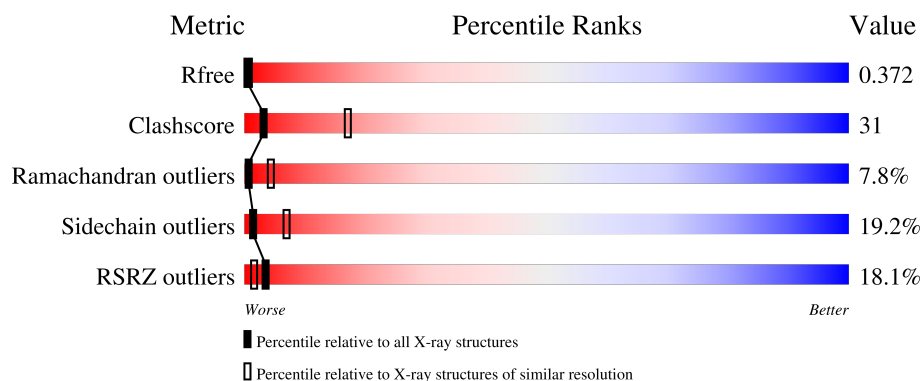
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	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 criteria:

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:

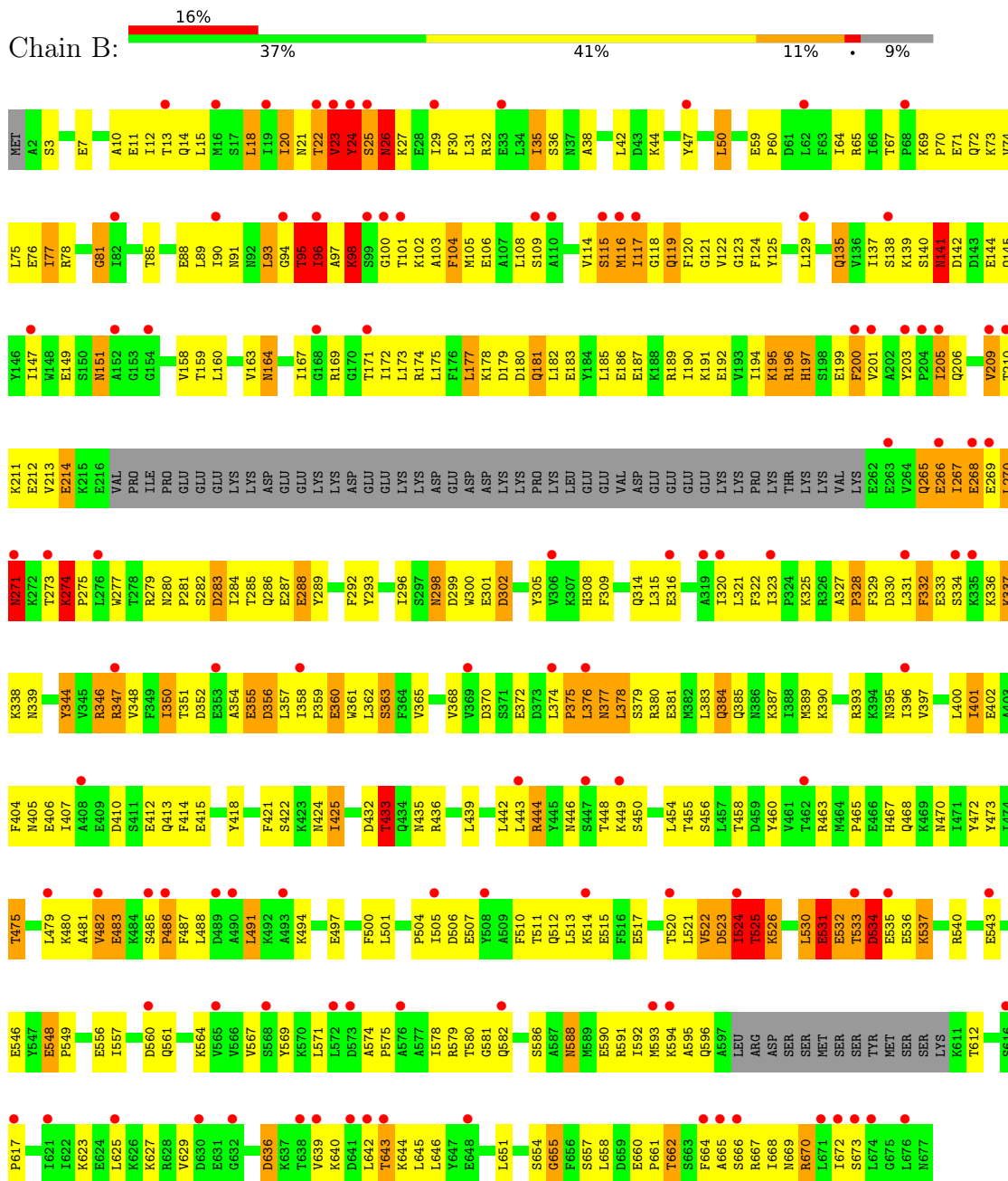
Chain	Residue	Modelled	Actual	Comment	Reference
X	127	ALA	GLU	engineered mutation	UNP P28707
Y	127	ALA	GLU	engineered mutation	UNP P28707

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

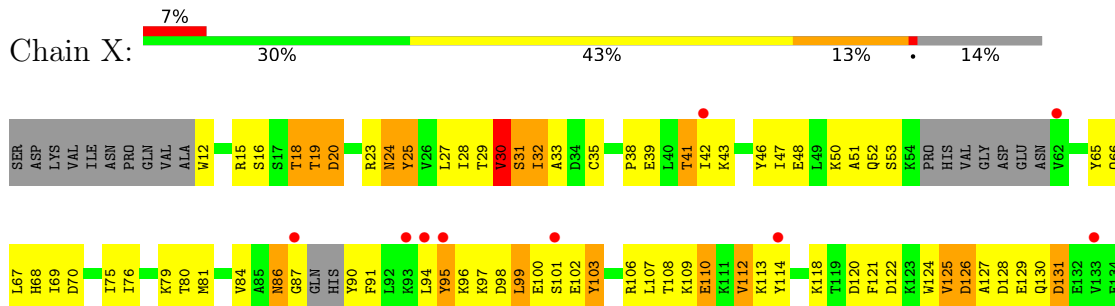


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 1: ATP-DEPENDENT MOLECULAR CHAPERONE HSP82

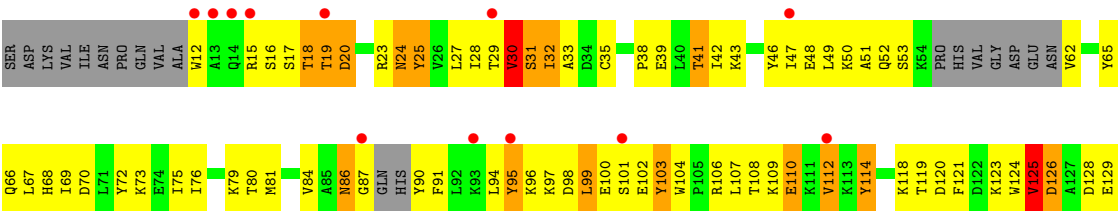


- Molecule 2: CO-CHAPERONE PROTEIN SBA1





● 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	126.73Å 126.73Å 279.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.47 – 3.10 115.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	68.2 (115.47-3.10) 83.8 (115.44-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.312 , 0.353 0.353 , 0.372	Depositor DCC
R_{free} test set	1250 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.58	1/5004 (0.0%)	0.97	13/6743 (0.2%)
1	B	0.58	0/5080	0.98	14/6844 (0.2%)
2	X	0.57	0/986	0.88	3/1335 (0.2%)
2	Y	0.55	0/986	0.89	6/1335 (0.4%)
All	All	0.57	1/12056 (0.0%)	0.96	36/16257 (0.2%)

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)
1	A	285	THR	CA-CB	5.85	1.61	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	LYS	CA-C-N	8.72	130.74	119.84
1	B	274	LYS	C-N-CA	8.72	130.74	119.84
1	A	274	LYS	CA-C-N	7.67	129.43	119.84
1	A	274	LYS	C-N-CA	7.67	129.43	119.84
1	B	269	GLU	N-CA-C	-7.17	102.97	112.72
1	A	672	ILE	N-CA-C	-7.16	106.03	112.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	17	SER	N-CA-C	7.07	117.60	108.34
1	B	95	THR	N-CA-C	6.82	119.85	110.24
1	B	672	ILE	N-CA-C	-6.73	106.44	112.90
1	A	380	ARG	N-CA-C	6.71	118.76	110.91
1	A	269	GLU	N-CA-C	-6.53	103.84	112.72
2	X	18	THR	N-CA-C	6.52	118.28	107.20
2	Y	18	THR	N-CA-C	6.45	118.17	107.20
1	B	327	ALA	CA-C-N	6.39	127.82	119.84
1	B	327	ALA	C-N-CA	6.39	127.82	119.84
1	B	491	LEU	N-CA-C	-6.29	106.24	114.04
1	A	491	LEU	N-CA-C	-6.20	106.35	114.04
1	A	358	ILE	N-CA-C	6.07	114.65	107.73
1	A	95	THR	N-CA-C	6.07	118.80	110.24
1	A	531	GLU	CA-C-N	5.90	129.21	120.95
1	A	531	GLU	C-N-CA	5.90	129.21	120.95
1	B	358	ILE	N-CA-C	5.74	114.28	107.73
2	X	113	LYS	N-CA-C	-5.69	104.75	112.26
1	A	274	LYS	N-CA-C	5.65	122.29	109.81
1	A	537	LYS	N-CA-C	5.61	122.74	110.80
1	A	24	TYR	N-CA-CB	5.48	119.75	110.49
2	Y	25	TYR	N-CA-C	5.39	117.00	108.96
2	X	25	TYR	N-CA-C	5.33	116.90	108.96
1	B	24	TYR	N-CA-C	-5.27	99.58	110.80
2	Y	114	TYR	CA-C-N	5.25	124.88	119.05
2	Y	114	TYR	C-N-CA	5.25	124.88	119.05
1	B	274	LYS	N-CA-C	5.22	121.34	109.81
1	B	24	TYR	N-CA-CB	5.15	119.20	110.49
2	Y	18	THR	CB-CA-C	-5.09	105.12	111.43
1	B	265	GLN	N-CA-C	5.08	115.84	107.20
1	B	378	LEU	N-CA-C	-5.01	103.43	110.50

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	318	0
1	B	4997	0	5037	331	0
2	X	962	0	936	63	0
2	Y	962	0	936	67	0
3	A	31	0	12	7	0
3	B	31	0	12	13	0
All	All	11906	0	11893	740	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 31.

All (740) 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
3:B:1678:ATP:H5'2	3:B:1678:ATP:C8	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLY:HA3	1:A:98:LYS:HZ1	1.24	1.01
1:A:524:ILE:HA	1:A:525:THR:HB	1.01	1.01
2:X:18:THR:CG2	2:X:120:ASP:HB2	1.90	1.01
1:A:195:LYS:HE2	1:A:268:GLU:CD	1.87	0.99
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: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:94:GLY:HA3	1:A:98:LYS:NZ	1.87	0.87
1:A:117:ILE:CB	1:A:346:ARG:HD2	2.04	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:B:21:ASN:C	1:B:23:VAL:H	1.85	0.85
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:A:21:ASN:C	1:A:23:VAL:H	1.88	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:365:VAL:HG21	1:B:400:LEU:HD21	1.64	0.80
1:B:594:LYS:HZ2	1:B:657:SER:HB2	1.46	0.79
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
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:525:THR:HG22	1:B:526:LYS:N	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:CB	1:B:332:PHE:CA	2.61	0.78
1:A:119:GLN:O	3:A:1678:ATP:O3B	2.02	0.77
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: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
1:A:99:SER:OG	3:A:1678:ATP:O2B	2.02	0.75
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:H	2:X:24:ASN:HD22	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
1:A:140:SER:C	1:A:142:ASP:H	1.97	0.72
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:A:210:THR:HA	1:A:264:VAL:HA	1.71	0.72
1:B:117:ILE:HB	1:B:346:ARG:CD	2.11	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:B:140:SER:C	1:B:142:ASP:H	1.99	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:A:271:ASN:H	1:A:272:LYS:C	2.00	0.68
1:B:195:LYS:HE2	1:B:268:GLU:CD	2.18	0.68
1:B:21:ASN:O	1:B:23:VAL:N	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:CG1	1:B:384:GLN:HB3	2.24	0.68
1:B:119:GLN:O	3:B:1678:ATP:PG	2.52	0.68
3:B:1678:ATP:H8	3:B:1678:ATP:C5'	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:A:23:VAL:HG13	1:A:24:TYR:H	1.58	0.67
1:B:114:VAL:HB	1:B:346:ARG:NH2	2.08	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:A:533:THR:O	1:A:535:GLU:N	2.27	0.66
1:B:594:LYS:NZ	1:B:657:SER:HB2	2.09	0.66
1:A:21:ASN:O	1:A:23:VAL:N	2.27	0.66
1:B:567:VAL:HG12	1:B:617:PRO:HG3	1.78	0.66
2:Y:70:ASP:O	2:Y:108:THR:HA	1.95	0.66
1:A:439:LEU:HA	1:A:442:LEU:HD12	1.78	0.66
1:B:18:LEU:O	1:B:22:THR:HB	1.95	0.66
1:A:64:ILE:HD11	1:A:205:ILE:HA	1.78	0.66
1:B:32:ARG:HD3	1:B:197:HIS:HD2	1.61	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:O	1:A:536:GLU:HG2	1.96	0.65
1:A:121:GLY:HA2	3:A:1678:ATP:O3A	1.96	0.65
1:A:432:ASP:OD2	1:A:435:ASN:N	2.25	0.65
1:B:275:PRO:HG3	1:B:347:ARG:HH12	1.61	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
1:A:531:GLU:O	1:A:537:LYS:HB2	1.97	0.65
1:B:65:ARG:HH21	1:B:206:GLN:HE22	1.45	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:X:24:ASN:HD22	2:X:24:ASN:N	1.94	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: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: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:501:LEU:HD23	1:A:506:ASP:HB3	1.82	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:A:21:ASN:C	1:A:23:VAL:N	2.58	0.61
1:A:625:LEU:O	1:A:629:VAL:HG23	2.00	0.61
1:B:64:ILE:HD11	1:B:205:ILE:HA	1.80	0.61
1:B:522:VAL:O	1:B:523:ASP:HB2	1.99	0.61
1:B:328:PRO:HB2	1:B:330:ASP:N	2.15	0.61
1:B:432:ASP:OD2	1:B:435:ASN:N	2.30	0.61
1:A:285:THR:H	1:A:288:GLU:CD	2.09	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:350:ILE:HG22	1:A:351:THR:N	2.15	0.61
1:A:666:SER:O	1:A:670:ARG:HB2	2.00	0.61
1:B:194:ILE:C	1:B:196:ARG:H	2.09	0.61
1:A:95:THR:HG23	1:A:125:TYR:CE1	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:477:GLU:OE2	1:B:658:LEU:HB2	2.01	0.60
1:B:350:ILE:HG22	1:B:351:THR:N	2.16	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:A:346:ARG:O	1:A:347:ARG:HB2	2.01	0.59
1:B:97:ALA:O	1:B:98:LYS:HG2	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:A:12:ILE:O	1:A:13:THR:C	2.46	0.59
1:A:665:ALA:HA	1:A:668:ILE:HD12	1.82	0.59
1:B:346:ARG:O	1:B:347:ARG:HB2	2.02	0.59
1:B:117:ILE:HD12	1:B:346:ARG:NE	2.18	0.59
1:A:194:ILE:C	1:A:196:ARG:H	2.10	0.59
1:A:270:LEU:CA	1:A:271:ASN:HB2	2.31	0.59
3:B:1678:ATP:C8	3:B:1678:ATP:C5'	2.78	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:X:87:GLY:O	2:X:90:TYR:N	2.35	0.58
2:Y:35:CYS:HA	2:Y:53:SER:HA	1.86	0.58
1:A:114:VAL:C	1:A:116:MET:H	2.12	0.58
1:A:465:PRO:HB2	1:A:467:HIS:CD2	2.39	0.57
1:B:163:VAL:O	1:B:164:ASN:HB2	2.04	0.57
1:A:384:GLN:NE2	1:B:25:SER:HB3	2.11	0.57
1:B:21:ASN:C	1:B:23:VAL:N	2.55	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:99:LEU:HD22	2:Y:102:GLU:HB2	1.85	0.57
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
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
1:B:114:VAL:C	1:B:116:MET:H	2.12	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
1:B:194:ILE:O	1:B:196:ARG:N	2.35	0.57
2:X:25:TYR:HE1	2:X:27:LEU:HD22	1.70	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:B:308:HIS:HD2	1:B:309:PHE:N	2.03	0.56
1:A:145:GLN:HE21	1:A:167:ILE:HG12	1.70	0.56
1:A:591:ARG:O	1:A:595:ALA:HB2	2.04	0.56
1:B:187:GLU:HG3	1:B:209:VAL:HG11	1.88	0.56
1:B:591:ARG:O	1:B:595:ALA:HB2	2.05	0.56
1:B:75:LEU:HB3	1:B:175:LEU:HB2	1.88	0.56
1:B:119:GLN:C	1:B:121:GLY:H	2.14	0.56
1:B:200:PHE:CD2	1:B:200:PHE:N	2.73	0.56
1:B:569:TYR:C	1:B:571:LEU:H	2.13	0.56
1:A:210:THR:CG2	1:A:264:VAL:HG22	2.36	0.56
1:A:590:GLU:HA	1:A:593:MET:HG2	1.87	0.56
1:B:114:VAL:O	1:B:114:VAL:HG12	2.06	0.56
2:Y:25:TYR:HE1	2:Y:27:LEU:HD22	1.70	0.56
2:Y:108:THR:HB	2:Y:110:GLU:OE2	2.06	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:A:341:ILE:HD11	1:A:358:ILE:HB	1.88	0.55
1:B:658:LEU:HB3	1:B:661:PRO:HB3	1.87	0.55
1:A:151:ASN:O	2:Y:86:ASN:HB2	2.06	0.55
1:B:104:PHE:HB2	1:B:116:MET:HE1	1.89	0.55
1:B:285:THR:HG22	1:B:286:GLN:N	2.17	0.55
1:B:285:THR:H	1:B:288:GLU:CD	2.15	0.55
1:B:504:PRO:HB3	1:B:592:ILE:HD13	1.87	0.55
1:A:119:GLN:C	1:A:121:GLY:H	2.13	0.55
1:B:117:ILE:CG1	1:B:346:ARG:HD2	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:LEU:O	1:A:93:LEU:HD23	2.07	0.55
1:A:97:ALA:O	1:A:98:LYS:HG2	2.05	0.55
1:A:76:GLU:HA	1:A:173:LEU:O	2.07	0.54
1:A:104:PHE:CE2	1:A:114:VAL:HG11	2.42	0.54
1:A:114:VAL:C	1:A:116:MET:N	2.62	0.54
1:B:47:TYR:O	1:B:50:LEU:HG	2.08	0.54
2:X:23:ARG:HD3	2:X:24:ASN:HB3	1.89	0.54
1:B:104:PHE:CE2	1:B:114:VAL:HG11	2.41	0.54
1:A:118:GLY:HA2	1:A:380:ARG:HH22	1.73	0.54
1:B:95:THR:HG22	1:B:96:ILE:HG12	1.90	0.54
1:B:375:PRO:O	1:B:376:LEU:HB2	2.08	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:A:69:LYS:HD2	1:A:71:GLU:OE1	2.08	0.54
1:A:104:PHE:HB2	1:A:116:MET:HE1	1.90	0.54
1:A:138:SER:HB2	1:A:171:THR:HG23	1.89	0.54
1:A:569:TYR:C	1:A:571:LEU:H	2.14	0.54
1:B:460:TYR:O	1:B:463:ARG:HG2	2.08	0.54
1:B:465:PRO:HB2	1:B:467:HIS:CD2	2.42	0.54
1:A:186:GLU:O	1:A:190:ILE:HG13	2.08	0.54
1:B:283:ASP:C	1:B:284:ILE:HG13	2.32	0.54
2:X:18:THR:CG2	2:X:120:ASP:CB	2.75	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:91:ASN:O	1:A:98:LYS:HG3	2.07	0.53
1:A:114:VAL:HG12	1:A:116:MET:O	2.08	0.53
1:A:96:ILE:HG21	1:B:15:LEU:HA	1.88	0.53
1:A:283:ASP:C	1:A:284:ILE:HG13	2.33	0.53
2:Y:48:GLU:HA	2:Y:67:LEU:O	2.08	0.53
2:X:131:ASP:OD2	2:X:131:ASP:N	2.41	0.53
1:B:138:SER:HB2	1:B:171:THR:HG23	1.90	0.53
1:A:15:LEU:HA	1:B:96:ILE:HG21	1.90	0.53
1:B:117:ILE:HD12	1:B:346:ARG:CD	2.39	0.53
1:B:590:GLU:HA	1:B:593:MET:HG2	1.91	0.53
1:B:100:GLY:H	3:B:1678:ATP:C3'	2.21	0.53
1:B:387:LYS:HA	1:B:390:LYS:HE3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:HE22	1:A:374:LEU:HD11	1.74	0.53
1:A:513:LEU:C	1:A:515:GLU:H	2.15	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: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
1:B:332:PHE:HB3	1:B:337:LYS:HD2	1.90	0.52
1:A:523:ASP:OD1	1:A:586:SER:HB2	2.09	0.52
1:B:140:SER:C	1:B:142:ASP:N	2.67	0.52
2:X:48:GLU:HA	2:X:67:LEU:O	2.08	0.52
2:Y:15:ARG:NH1	2:Y:32:ILE:N	2.57	0.52
1:A:64:ILE:HD11	1:A:205:ILE:HG23	1.91	0.52
1:B:96:ILE:HA	1:B:120:PHE:O	2.09	0.52
1:B:114:VAL:C	1:B:116:MET:N	2.66	0.52
2:Y:23:ARG:HD3	2:Y:24:ASN:HB3	1.90	0.52
1:A:476:GLY:HA2	1:A:591:ARG:HE	1.75	0.52
1:A:668:ILE:HD13	1:B:664:PHE:HZ	1.73	0.52
1:B:200:PHE:CD1	1:B:277:TRP:CH2	2.97	0.52
1:B:375:PRO:HB2	1:B:383:LEU:HG	1.91	0.52
2:X:30:VAL:O	2:X:31:SER:HB3	2.08	0.52
1:A:140:SER:C	1:A:142:ASP:N	2.65	0.52
1:A:181:GLN:HA	1:A:181:GLN:NE2	2.24	0.52
1:A:383:LEU:HD21	1:A:389:MET:HE2	1.91	0.52
1:A:390:LYS:O	1:A:393:ARG:HB3	2.10	0.52
1:B:69:LYS:HD2	1:B:71:GLU:OE1	2.09	0.52
1:A:308:HIS:O	1:A:309:PHE:HB3	2.09	0.52
1:B:308:HIS:O	1:B:309:PHE:HB3	2.10	0.52
1:A:141:ASN:OD1	1:A:141:ASN:N	2.43	0.52
1:B:422:SER:O	1:B:425:ILE:HG23	2.09	0.52
1:B:473:TYR:O	1:B:523:ASP:CB	2.58	0.52
2:Y:24:ASN:H	2:Y:24:ASN:ND2	2.06	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: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
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:H	1:B:274:LYS:HD2	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:38:PRO:HA	2:Y:51:ALA:HB2	1.93	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
1:A:140:SER:O	1:A:142:ASP:N	2.43	0.51
1:A:178:LYS:C	1:A:180:ASP:H	2.19	0.51
1:A:200:PHE:N	1:A:200:PHE:CD2	2.79	0.51
1:A:444:ARG:HG2	1:A:454:LEU:HB2	1.92	0.51
1:B:639:VAL:HG13	1:B:642:LEU:HD23	1.91	0.51
2:X:24:ASN:H	2:X:24:ASN:ND2	2.07	0.51
1:A:75:LEU:HB3	1:A:175:LEU:HB2	1.92	0.50
1:B:32:ARG:HH22	1:B:380:ARG:HB2	1.76	0.50
1:B:180:ASP:C	1:B:182:LEU:H	2.19	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:114:VAL:O	1:A:115:SER:C	2.55	0.50
1:B:70:PRO:HA	1:B:185:LEU:HD13	1.93	0.50
2:Y:32:ILE:HG13	2:Y:65:TYR:CZ	2.46	0.50
1:A:114:VAL:O	1:A:114:VAL:HG12	2.12	0.50
1:B:64:ILE:O	1:B:206:GLN:HB2	2.11	0.50
1:B:178:LYS:C	1:B:180:ASP:H	2.20	0.50
1:B:212:GLU:CD	1:B:214:GLU:HB3	2.36	0.50
1:B:523:ASP:OD1	1:B:524:ILE:N	2.42	0.50
1:A:507:GLU:CD	1:A:589:MET:HA	2.36	0.50
1:A:517:GLU:N	1:A:517:GLU:OE1	2.45	0.50
1:B:12:ILE:O	1:B:13:THR:C	2.54	0.50
1:B:145:GLN:HE21	1:B:167:ILE:HG12	1.76	0.50
1:A:378:LEU:HD13	1:B:24:TYR:CE1	2.47	0.50
1:A:23:VAL:CG1	1:A:24:TYR:N	2.74	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:37:ASN:HB3	3:A:1678:ATP:N7	2.27	0.49
1:B:299:ASP:OD1	1:B:300:TRP:N	2.45	0.49
1:B:362:LEU:O	1:B:363:SER:C	2.55	0.49
2:Y:121:PHE:HA	2:Y:124:TRP:HB3	1.94	0.49
1:A:201:VAL:HG23	1:A:203:TYR:O	2.12	0.49
1:B:513:LEU:C	1:B:515:GLU:H	2.19	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
1:B:119:GLN:C	1:B:121:GLY:N	2.69	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:GLU:N	1:B:517:GLU:OE1	2.45	0.49
2:Y:24:ASN:N	2:Y:24:ASN:ND2	2.60	0.49
1:A:286:GLN:O	1:A:287:GLU:HB2	2.12	0.49
1:B:140:SER:O	1:B:142:ASP:N	2.44	0.49
2:Y:50:LYS:HG3	2:Y:66:GLN:HB3	1.93	0.49
1:A:340:ASN:O	1:A:342:LYS:HG3	2.12	0.49
1:A:387:LYS:HA	1:A:390:LYS:HE3	1.94	0.49
1:B:74:VAL:HA	1:B:175:LEU:O	2.12	0.49
1:B:396:ILE:O	1:B:400:LEU:HB2	2.13	0.49
2:X:28:ILE:HD12	2:X:95:TYR:HE1	1.77	0.49
1:A:180:ASP:C	1:A:182:LEU:H	2.20	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:35:ILE:O	1:A:38:ALA:N	2.45	0.49
1:A:308:HIS:HD2	1:A:309:PHE:H	1.60	0.49
1:B:468:GLN:NE2	1:B:470:ASN:O	2.43	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
2:Y:18:THR:CG2	2:Y:120:ASP:CB	2.78	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:210:THR:HG23	1:A:264:VAL:HG13	1.95	0.48
1:A:435:ASN:O	1:A:436:ARG:C	2.57	0.48
1:B:7:GLU:CD	1:B:7:GLU:H	2.22	0.48
1:B:481:ALA:O	1:B:482:VAL:HB	2.13	0.48
2:X:38:PRO:HA	2:X:51:ALA:HB2	1.95	0.48
1:A:187:GLU:HG3	1:A:209:VAL:HG11	1.94	0.48
1:B:305:TYR:OH	1:B:406:GLU:OE1	2.31	0.48
2:Y:15:ARG:HE	2:Y:31:SER:H	1.62	0.48
2:Y:18:THR:HG22	2:Y:18:THR:O	2.13	0.48
1:A:95:THR:HB	1:B:10:ALA:CB	2.43	0.48
1:A:127:LEU:C	1:A:127:LEU:HD12	2.38	0.48
1:A:299:ASP:OD1	1:A:300:TRP:N	2.47	0.48
1:B:351:THR:OG1	1:B:352:ASP:N	2.47	0.48
1:B:475:THR:HB	1:B:501:LEU:HB2	1.95	0.48
1:A:114:VAL:HB	1:A:346:ARG:NH2	2.29	0.48
1:A:47:TYR:O	1:A:50:LEU:HG	2.14	0.48
1:A:64:ILE:CD1	1:A:205:ILE:HA	2.44	0.48
1:A:74:VAL:HA	1:A:175:LEU:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:HA	1:A:405:ASN:HB2	1.95	0.48
1:A:639:VAL:HG13	1:A:642:LEU:HD23	1.95	0.48
1:B:212:GLU:HG2	1:B:214:GLU:H	1.79	0.48
1:B:390:LYS:O	1:B:393:ARG:HB3	2.13	0.48
1:A:31:LEU:O	1:A:32:ARG:C	2.57	0.48
1:A:485:SER:C	1:A:487:PHE:H	2.22	0.48
1:A:513:LEU:C	1:A:515:GLU:N	2.71	0.48
1:B:485:SER:C	1:B:487:PHE:H	2.21	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: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:B:308:HIS:CD2	1:B:309:PHE:N	2.81	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
1:A:481:ALA:O	1:A:482:VAL:HB	2.13	0.47
1:A:163:VAL:O	1:A:164:ASN:HB2	2.14	0.47
1:B:30:PHE:CG	1:B:31:LEU:N	2.82	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
2:X:30:VAL:HG23	2:X:91:PHE:O	2.14	0.47
2:X:108:THR:HB	2:X:110:GLU:OE2	2.13	0.47
1:A:119:GLN:C	1:A:121:GLY:N	2.72	0.47
1:B:64:ILE:HD11	1:B:205:ILE:HG23	1.95	0.47
1:B:141:ASN:OD1	1:B:141:ASN:N	2.44	0.47
1:B:526:LYS:HZ2	1:B:581:GLY:HA2	1.78	0.47
3:B:1678:ATP:O1G	3:B:1678:ATP:O3A	2.31	0.47
1:B:27:LYS:HB2	1:B:129:LEU:HD13	1.96	0.47
1:B:91:ASN:O	1:B:98:LYS:HG3	2.14	0.47
1:B:531:GLU:O	1:B:537:LYS:HB2	2.14	0.47
1:B:644:LYS:HD3	1:B:667:ARG:HH21	1.79	0.47
2:X:32:ILE:HG13	2:X:65:TYR:CZ	2.50	0.47
1:A:7:GLU:CD	1:A:7:GLU:H	2.22	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:421:PHE:O	1:B:422:SER:C	2.58	0.47
1:A:289:TYR:O	1:A:292:PHE:HB3	2.15	0.47
1:B:65:ARG:HA	1:B:206:GLN:O	2.15	0.47
1:B:201:VAL:HG23	1:B:203:TYR:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HA	1:A:185:LEU:HD13	1.95	0.47
1:A:510:PHE:HA	1:A:513:LEU:HD12	1.96	0.47
3:A:1678:ATP:O1G	3:A:1678:ATP:O1B	2.33	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:B:344:TYR:N	1:B:344:TYR:CD2	2.83	0.47
1:B:483:GLU:HA	1:B:500:PHE:CE2	2.50	0.47
1:A:95:THR:CB	1:B:10:ALA:HB2	2.44	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:85:THR:HG23	1:A:88:GLU:H	1.80	0.46
1:A:351:THR:OG1	1:A:352:ASP:N	2.48	0.46
1:B:31:LEU:O	1:B:32:ARG:C	2.58	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
2:X:20:ASP:CG	2:X:27:LEU:O	2.58	0.46
1:A:25:SER:H	1:B:384:GLN:HG3	1.80	0.46
1:A:104:PHE:CZ	1:A:114:VAL:HG11	2.51	0.46
1:A:475:THR:HB	1:A:501:LEU:HB2	1.96	0.46
1:B:20:ILE:HG13	1:B:129:LEU:HD23	1.96	0.46
1:B:443:LEU:O	1:B:456:SER:HA	2.15	0.46
1:B:513:LEU:O	1:B:515:GLU:N	2.48	0.46
2:X:38:PRO:CB	2:X:91:PHE:HE2	2.27	0.46
2:Y:47:ILE:O	2:Y:68:HIS:HA	2.15	0.46
1:B:23:VAL:HG13	1:B:24:TYR:N	2.31	0.46
1:A:410:ASP:OD1	1:A:413:GLN:N	2.48	0.46
1:A:463:ARG:HH11	1:A:497:GLU:HG3	1.80	0.46
1:B:534:ASP:OD1	1:B:537:LYS:HG2	2.15	0.46
1:B:654:SER:O	1:B:655:GLY:C	2.59	0.46
1:A:210:THR:HG23	1:A:264:VAL:HG22	1.97	0.46
1:A:468:GLN:NE2	1:A:470:ASN:O	2.45	0.46
1:A:534:ASP:OD1	1:A:537:LYS:HG2	2.15	0.46
1:B:346:ARG:HG2	1:B:372:GLU:HA	1.97	0.46
1:B:432:ASP:CG	1:B:433:THR:N	2.74	0.46
2:Y:18:THR:HB	2:Y:29:THR:H	1.81	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:B:374:LEU:C	1:B:376:LEU:N	2.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:NZ	1:B:103:ALA:HB1	2.30	0.46
2:X:41:THR:HB	2:X:48:GLU:HB3	1.98	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:B:47:TYR:OH	1:B:109:SER:OG	2.29	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
1:B:331:LEU:HB2	1:B:332:PHE:CB	2.41	0.45
1:A:383:LEU:CD2	1:A:389:MET:HE2	2.46	0.45
1:A:460:TYR:CE1	1:A:497:GLU:HB3	2.51	0.45
1:A:654:SER:O	1:A:655:GLY:C	2.59	0.45
1:B:35:ILE:O	1:B:36:SER:C	2.57	0.45
1:B:280:ASN:HA	1:B:281:PRO:HD2	1.75	0.45
2:Y:99:LEU:HB2	2:Y:100:GLU:H	1.66	0.45
1:B:135:GLN:HE22	1:B:149:GLU:CD	2.24	0.45
1:A:73:LYS:HD3	1:A:182:LEU:HD21	1.97	0.45
1:B:119:GLN:O	3:B:1678:ATP:O2G	2.35	0.45
1:A:401:ILE:HA	1:A:404:PHE:CD2	2.50	0.45
1:A:432:ASP:CG	1:A:433:THR:N	2.74	0.45
1:A:623:LYS:O	1:A:627:LYS:HG2	2.17	0.45
1:B:64:ILE:CD1	1:B:205:ILE:HA	2.46	0.45
1:A:354:ALA:O	1:A:356:ASP:N	2.50	0.45
1:A:557:ILE:HD12	1:A:643:THR:HG21	1.97	0.45
1:A:200:PHE:CD1	1:A:277:TRP:CH2	3.05	0.45
1:A:487:PHE:CD1	1:A:487:PHE:C	2.95	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:119:GLN:O	1:B:120:PHE:HB2	2.17	0.45
1:B:194:ILE:C	1:B:196:ARG:N	2.74	0.45
1:B:402:GLU:HA	1:B:405:ASN:HB2	1.99	0.45
1:B:446:ASN:HD22	1:B:446:ASN:HA	1.67	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
2:Y:30:VAL:CG2	2:Y:91:PHE:HB3	2.47	0.45
1:A:16:MET:O	1:A:19:ILE:N	2.50	0.44
1:A:195:LYS:HE3	1:A:270:LEU:O	2.16	0.44
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:526:LYS:HZ2	1:A:581:GLY:HA2	1.82	0.44
1:B:513:LEU:C	1:B:515:GLU:N	2.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:23:ARG:HB2	2:X:130:GLN:HE22	1.81	0.44
2:Y:32:ILE:CD1	2:Y:33:ALA:H	2.20	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: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:B:104:PHE:CE2	1:B:114:VAL:CG1	3.01	0.44
1:B:507:GLU:O	1:B:511:THR:HG23	2.17	0.44
1:B:557:ILE:HD12	1:B:643:THR:HG21	1.98	0.44
2:X:18:THR:O	2:X:18:THR:HG22	2.17	0.44
2:Y:15:ARG:HH11	2:Y:32:ILE:H	1.64	0.44
1:A:274:LYS:H	1:A:274:LYS:HD2	1.83	0.44
1:A:362:LEU:O	1:A:363:SER:C	2.60	0.44
1:B:117:ILE:HG23	1:B:119:GLN:OE1	2.16	0.44
2:Y:19:THR:HG23	2:Y:107:LEU:HD12	1.99	0.44
1:A:101:THR:O	1:A:104:PHE:N	2.29	0.44
1:B:29:ILE:O	1:B:30:PHE:C	2.59	0.44
1:B:387:LYS:HA	1:B:390:LYS:CE	2.47	0.44
2:X:99:LEU:HB2	2:X:100:GLU:H	1.67	0.44
1:A:194:ILE:C	1:A:196:ARG:N	2.75	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:A:42:LEU:HD23	1:A:81:GLY:N	2.33	0.44
1:B:32:ARG:HD3	1:B:197:HIS:CD2	2.48	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
2:Y:18:THR:HA	2:Y:118:LYS:O	2.18	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:B:323:ILE:HD12	1:B:407:ILE:CD1	2.48	0.44
1:B:31:LEU:HD12	1:B:31:LEU:HA	1.85	0.43
1:B:119:GLN:O	3:B:1678:ATP:O3B	2.36	0.43
1:B:414:PHE:O	1:B:418:TYR:N	2.49	0.43
2:Y:125:VAL:O	2:Y:126:ASP:O	2.36	0.43
1:A:20:ILE:HG13	1:A:129:LEU:HD23	1.99	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:104:PHE:CB	1:A:116:MET:HE1	2.48	0.43
1:A:507:GLU:OE2	1:A:589:MET:HA	2.19	0.43
1:B:64:ILE:HD11	1:B:205:ILE:CG2	2.48	0.43
1:B:85:THR:HG22	1:B:88:GLU:CG	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ILE:HA	1:B:404:PHE:CD2	2.53	0.43
2:X:126:ASP:O	2:X:127:ALA:HB3	2.19	0.43
2:Y:41:THR:HB	2:Y:48:GLU:HB3	2.00	0.43
1:A:432:ASP:CG	1:A:433:THR:H	2.26	0.43
1:B:22:THR:HG23	1:B:24:TYR:CZ	2.53	0.43
1:B:435:ASN:O	1:B:436:ARG:C	2.61	0.43
1:B:77:ILE:O	1:B:77:ILE:HG22	2.18	0.43
1:B:114:VAL:O	1:B:115:SER:C	2.61	0.43
1:B:117:ILE:HD13	1:B:374:LEU:HD22	2.01	0.43
1:B:177:LEU:H	1:B:177:LEU:HD22	1.84	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:A:297:SER:O	1:A:298:ASN:C	2.61	0.43
1:A:636:ASP:CG	1:A:639:VAL:HB	2.44	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: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:A:395:ASN:C	1:A:397:VAL:N	2.76	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
1:B:375:PRO:CB	1:B:383:LEU:HG	2.48	0.43
1:A:24:TYR:C	1:A:26:ASN:N	2.77	0.43
1:A:77:ILE:O	1:A:77:ILE:HG22	2.18	0.43
1:B:284:ILE:CG2	1:B:288:GLU:HB2	2.49	0.43
1:B:314:GLN:HG2	2:Y:119:THR:CG2	2.49	0.43
2:Y:43:LYS:CB	2:Y:46:TYR:HB2	2.48	0.43
2:Y:23:ARG:HB2	2:Y:130:GLN:HE22	1.83	0.43
1:A:29:ILE:O	1:A:30:PHE:C	2.61	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:A:421:PHE:O	1:A:422:SER:C	2.60	0.43
2:Y:126:ASP:C	2:Y:128:ASP:H	2.27	0.43
1:A:104:PHE:CE2	1:A:114:VAL:CG1	3.01	0.42
1:A:207:LEU:O	1:A:207:LEU:HG	2.15	0.42
1:A:290:ASN:HB2	1:A:303:PRO:HD2	2.01	0.42
1:A:374:LEU:C	1:A:376:LEU:N	2.77	0.42
1:B:346:ARG:CZ	1:B:372:GLU:OE2	2.67	0.42
1:B:350:ILE:HG22	1:B:351:THR:H	1.82	0.42
1:B:432:ASP:CG	1:B:433:THR:H	2.25	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:18:THR:HA	2:X:118:LYS:O	2.18	0.42
1:A:59:GLU:OE2	1:A:60:PRO:HD2	2.18	0.42
1:A:591:ARG:HA	1:A:594:LYS:NZ	2.34	0.42
1:B:100:GLY:H	3:B:1678:ATP:H3'	1.84	0.42
1:B:334:SER:C	1:B:336:LYS:H	2.27	0.42
2:X:19:THR:HG22	2:X:20:ASP:H	1.84	0.42
1:B:137:ILE:HG12	1:B:147:ILE:HG13	2.01	0.42
1:B:285:THR:CG2	1:B:286:GLN:H	2.24	0.42
1:B:487:PHE:CD1	1:B:487:PHE:C	2.97	0.42
2:Y:24:ASN:O	2:Y:96:LYS:HG3	2.19	0.42
1:A:380:ARG:O	1:A:381:GLU:HB2	2.19	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
2:X:18:THR:HB	2:X:29:THR:H	1.85	0.42
2:Y:30:VAL:HG23	2:Y:91:PHE:O	2.18	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:118:GLY:HA2	1:B:380:ARG:HH22	1.84	0.42
1:A:487:PHE:CZ	1:A:524:ILE:HD13	2.55	0.42
1:A:548:GLU:N	1:A:549:PRO:HD2	2.34	0.42
1:B:42:LEU:HA	1:B:81:GLY:HA2	2.02	0.42
1:B:525:THR:CG2	1:B:582:GLN:HG3	2.50	0.42
1:B:548:GLU:N	1:B:549:PRO:HD2	2.35	0.42
2:Y:97:LYS:HD3	2:Y:104:TRP:NE1	2.34	0.42
1:B:85:THR:HG23	1:B:88:GLU:H	1.85	0.42
1:B:525:THR:HG23	1:B:582:GLN:HG3	2.01	0.42
1:A:209:VAL:CG2	1:A:267:ILE:HG12	2.49	0.42
1:A:320:ILE:O	1:A:321:LEU:HD23	2.20	0.42
1:A:432:ASP:OD2	1:A:433:THR:N	2.53	0.42
1:A:507:GLU:OE1	1:A:589:MET:HA	2.20	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:B:412:GLU:OE1	1:B:415:GLU:HB2	2.20	0.42
1:A:482:VAL:HG13	1:A:500:PHE:CD2	2.55	0.41
1:B:195:LYS:HD3	1:B:199:GLU:OE2	2.20	0.41
1:B:525:THR:HG23	1:B:582:GLN:HA	2.02	0.41
2:X:24:ASN:O	2:X:96:LYS:HG3	2.20	0.41
2:Y:15:ARG:HH11	2:Y:32:ILE:N	2.17	0.41
1:A:135:GLN:HE22	1:A:149:GLU:CD	2.28	0.41
1:A:615:ILE:HG23	1:A:622:ILE:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:O	1:B:102:LYS:C	2.63	0.41
1:B:139:LYS:HB2	1:B:145:GLN:HG3	2.02	0.41
1:B:560:ASP:O	1:B:561:GLN:HG3	2.20	0.41
1:B:627:LYS:HG2	1:B:627:LYS:H	1.63	0.41
1:A:101:THR:O	1:A:102:LYS:C	2.62	0.41
1:A:302:ASP:O	1:A:325:LYS:HE3	2.20	0.41
1:A:369:VAL:HG12	1:A:370:ASP:N	2.35	0.41
1:B:24:TYR:C	1:B:26:ASN:N	2.77	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
1:B:636:ASP:CG	1:B:639:VAL:HB	2.45	0.41
2:Y:72:TYR:CD2	2:Y:73:LYS:HG3	2.54	0.41
1:A:387:LYS:HA	1:A:390:LYS:CE	2.51	0.41
1:A:590:GLU:O	1:A:594:LYS:HB3	2.21	0.41
1:B:78:ARG:CA	1:B:172:ILE:HD12	2.50	0.41
1:B:328:PRO:HB2	1:B:329:PHE:CA	2.50	0.41
1:B:361:TRP:CD1	1:B:361:TRP:H	2.38	0.41
1:A:543:GLU:O	1:A:546:GLU:HB2	2.20	0.41
2:X:103:TYR:CD2	2:X:103:TYR:N	2.87	0.41
2:Y:19:THR:HG22	2:Y:20:ASP:H	1.86	0.41
1:A:560:ASP:O	1:A:561:GLN:HG3	2.19	0.41
1:B:44:LYS:HA	1:B:44:LYS:HD2	1.86	0.41
1:B:314:GLN:NE2	2:Y:124:TRP:HD1	2.18	0.41
1:B:522:VAL:O	1:B:523:ASP:CB	2.67	0.41
1:A:16:MET:C	1:A:18:LEU:N	2.79	0.41
1:A:17:SER:HA	1:A:20:ILE:HG23	2.02	0.41
1:A:44:LYS:NZ	1:A:103:ALA:HB1	2.36	0.41
1:A:361:TRP:O	1:A:424:ASN:HB3	2.21	0.41
1:A:550:LEU:HD13	1:A:629:VAL:CG2	2.51	0.41
2:X:126:ASP:C	2:X:128:ASP:H	2.28	0.41
2:Y:15:ARG:HB3	2:Y:30:VAL:HG12	2.02	0.41
2:Y:25:TYR:CE1	2:Y:27:LEU:HD22	2.54	0.41
1:A:135:GLN:HB2	1:A:176:PHE:HE2	1.86	0.41
1:B:359:PRO:O	1:B:360:GLU:C	2.64	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
2:X:15:ARG:HE	2:X:31:SER:C	2.28	0.41
1:A:290:ASN:OD1	1:A:291:ALA:N	2.53	0.41
1:B:331:LEU:HB2	1:B:332:PHE:CA	2.45	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:H	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:CG2	1:A:123:GLY:N	2.85	0.40
1:A:664:PHE:HZ	1:B:668:ILE:HD13	1.86	0.40
1:B:189:ARG:HD2	1:B:192:GLU:OE1	2.21	0.40
1:B:460:TYR:OH	1:B:497:GLU:O	2.30	0.40
1:B:645:LEU:HD13	1:B:667:ARG:HB2	2.02	0.40
2:X:15:ARG:HH11	2:X:32:ILE:N	2.19	0.40
2:Y:49:LEU:O	2:Y:66:GLN:HA	2.21	0.40
1:A:384:GLN:CB	1:B:23:VAL:HG13	2.47	0.40
1:B:114:VAL:HG12	1:B:116:MET:O	2.21	0.40
1:B:314:GLN:HG2	2:Y:119:THR:HG21	2.03	0.40
1:B:395:ASN:C	1:B:397:VAL:N	2.77	0.40
1:B:432:ASP:OD2	1:B:433:THR:N	2.52	0.40
1:B:485:SER:HA	1:B:486:PRO:HD2	1.95	0.40
1:B:645:LEU:HD13	1:B:667:ARG:CB	2.51	0.40
1:A:211:LYS:HB3	1:A:212:GLU:H	1.74	0.40
1:B:151:ASN:O	2:X:86:ASN:CB	2.68	0.40
1:B:190:ILE:HG13	1:B:190:ILE:H	1.70	0.40
1:A:18:LEU:HD21	1:B:120:PHE:HA	2.03	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:341:ILE:H	1:A:341:ILE:HG13	1.49	0.40
1:A:382:MET:O	1:A:383:LEU:C	2.65	0.40
1:A:393:ARG:O	1:A:394:LYS:C	2.63	0.40
1:B:267:ILE:HB	1:B:268:GLU:H	1.72	0.40
1:A:14:GLN:HG3	1:B:97:ALA:HA	2.04	0.40
1:A:35:ILE:O	1:A:36:SER:C	2.65	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	4
1	B	612/677 (90%)	447 (73%)	117 (19%)	48 (8%)	1	4
2	X	109/134 (81%)	83 (76%)	18 (16%)	8 (7%)	1	5
2	Y	109/134 (81%)	82 (75%)	19 (17%)	8 (7%)	1	5
All	All	1431/1622 (88%)	1059 (74%)	261 (18%)	111 (8%)	1	4

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	447 (82%)	99 (18%)	2	8
1	B	554/615 (90%)	450 (81%)	104 (19%)	1	7
2	X	106/124 (86%)	82 (77%)	24 (23%)	1	4
2	Y	106/124 (86%)	81 (76%)	25 (24%)	1	3
All	All	1312/1478 (89%)	1060 (81%)	252 (19%)	1	7

All (252) 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	35	ILE
1	A	50	LEU
1	A	67	THR
1	A	72	GLN
1	A	77	ILE
1	A	93	LEU
1	A	95	THR
1	A	96	ILE
1	A	98	LYS
1	A	104	PHE
1	A	105	MET
1	A	106	GLU
1	A	108	LEU
1	A	113	ASP
1	A	116	MET
1	A	117	ILE
1	A	119	GLN
1	A	122	VAL
1	A	135	GLN
1	A	141	ASN
1	A	144	GLU
1	A	151	ASN
1	A	158	VAL
1	A	159	THR
1	A	160	LEU
1	A	172	ILE
1	A	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	267	ILE
1	A	268	GLU
1	A	270	LEU
1	A	271	ASN
1	A	274	LYS
1	A	278	THR
1	A	282	SER
1	A	288	GLU
1	A	298	ASN
1	A	301	GLU
1	A	302	ASP
1	A	315	LEU
1	A	341	ILE
1	A	344	TYR
1	A	346	ARG
1	A	347	ARG
1	A	348	VAL
1	A	355	GLU
1	A	356	ASP
1	A	357	LEU
1	A	377	ASN
1	A	389	MET
1	A	401	ILE
1	A	425	ILE
1	A	433	THR
1	A	444	ARG
1	A	448	THR
1	A	450	SER
1	A	455	THR
1	A	458	THR
1	A	475	THR
1	A	479	LEU
1	A	480	LYS
1	A	485	SER
1	A	491	LEU
1	A	494	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	503	ASP
1	A	505	ILE
1	A	520	THR
1	A	521	LEU
1	A	522	VAL
1	A	523	ASP
1	A	524	ILE
1	A	526	LYS
1	A	530	LEU
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	643	THR
1	A	646	LEU
1	A	660	GLU
1	A	662	THR
1	A	669	ASN
1	A	670	ARG
1	B	18	LEU
1	B	20	ILE
1	B	23	VAL
1	B	26	ASN
1	B	35	ILE
1	B	50	LEU
1	B	67	THR
1	B	72	GLN
1	B	77	ILE
1	B	93	LEU
1	B	95	THR
1	B	96	ILE
1	B	98	LYS
1	B	104	PHE
1	B	105	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	106	GLU
1	B	108	LEU
1	B	116	MET
1	B	117	ILE
1	B	119	GLN
1	B	135	GLN
1	B	141	ASN
1	B	144	GLU
1	B	151	ASN
1	B	158	VAL
1	B	159	THR
1	B	160	LEU
1	B	177	LEU
1	B	196	ARG
1	B	197	HIS
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	267	ILE
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	296	ILE
1	B	298	ASN
1	B	301	GLU
1	B	302	ASP
1	B	315	LEU
1	B	316	GLU
1	B	332	PHE
1	B	333	GLU
1	B	337	LYS
1	B	338	LYS
1	B	344	TYR
1	B	346	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	389	MET
1	B	401	ILE
1	B	425	ILE
1	B	433	THR
1	B	444	ARG
1	B	448	THR
1	B	450	SER
1	B	455	THR
1	B	458	THR
1	B	475	THR
1	B	479	LEU
1	B	480	LYS
1	B	491	LEU
1	B	494	LYS
1	B	505	ILE
1	B	520	THR
1	B	521	LEU
1	B	522	VAL
1	B	524	ILE
1	B	525	THR
1	B	526	LYS
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	643	THR
1	B	646	LEU

Continued on next page...

Continued from previous page...

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	30	VAL
2	X	32	ILE
2	X	41	THR
2	X	42	ILE
2	X	52	GLN
2	X	69	ILE
2	X	79	LYS
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	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	42	ILE
2	Y	52	GLN
2	Y	62	VAL
2	Y	69	ILE
2	Y	79	LYS
2	Y	80	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	81	MET
2	Y	84	VAL
2	Y	94	LEU
2	Y	95	TYR
2	Y	98	ASP
2	Y	99	LEU
2	Y	101	SER
2	Y	103	TYR
2	Y	110	GLU
2	Y	112	VAL
2	Y	123	LYS
2	Y	125	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	119	GLN
1	A	135	GLN
1	A	145	GLN
1	A	181	GLN
1	A	197	HIS
1	A	206	GLN
1	A	271	ASN
1	A	308	HIS
1	A	340	ASN
1	A	384	GLN
1	A	385	GLN
1	A	413	GLN
1	A	446	ASN
1	A	467	HIS
1	A	561	GLN
1	A	588	ASN
1	B	72	GLN
1	B	92	ASN
1	B	119	GLN
1	B	135	GLN
1	B	145	GLN
1	B	181	GLN
1	B	197	HIS
1	B	308	HIS
1	B	384	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	446	ASN
1	B	467	HIS
1	B	561	GLN
1	B	588	ASN
2	X	66	GLN
2	Y	66	GLN

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](#)

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	-	32,33,33	1.41	4 (12%)	48,52,52	1.75	8 (16%)
3	ATP	B	1678	-	32,33,33	1.34	3 (9%)	48,52,52	1.87	12 (25%)

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	-	-	3/22/38/38	0/3/3/3
3	ATP	B	1678	-	-	9/22/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1678	ATP	C5-C4	5.38	1.48	1.39
3	B	1678	ATP	C5-C4	4.50	1.47	1.39
3	B	1678	ATP	C5-N7	-3.19	1.33	1.39
3	A	1678	ATP	C5-C6	2.90	1.49	1.41
3	A	1678	ATP	C8-N7	2.42	1.36	1.31
3	B	1678	ATP	C4-N9	-2.33	1.32	1.37
3	A	1678	ATP	C5-N7	-2.24	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1678	ATP	C5-C4-N3	-6.01	118.44	126.72
3	B	1678	ATP	C5-C4-N3	-5.39	119.29	126.72
3	B	1678	ATP	N3-C4-N9	4.72	135.19	127.17
3	A	1678	ATP	N3-C4-N9	4.65	135.08	127.17
3	B	1678	ATP	O3A-PB-O1B	-3.80	99.27	110.70
3	A	1678	ATP	C2-N3-C4	3.74	120.95	111.83
3	B	1678	ATP	C2-N3-C4	3.23	119.73	111.83
3	B	1678	ATP	N3-C2-N1	-3.23	123.69	128.58
3	B	1678	ATP	O2B-PB-O3A	3.20	115.93	107.27
3	A	1678	ATP	N3-C2-N1	-3.16	123.80	128.58
3	A	1678	ATP	C4-C5-N7	-3.10	107.04	110.58
3	B	1678	ATP	C3'-C2'-C1'	2.61	106.39	101.46
3	A	1678	ATP	C3'-C2'-C1'	2.53	106.24	101.46
3	B	1678	ATP	N6-C6-N1	2.43	123.79	118.38
3	B	1678	ATP	O2B-PB-O1B	2.33	123.27	112.44
3	B	1678	ATP	C4-C5-N7	-2.22	108.04	110.58
3	B	1678	ATP	C2-N1-C6	2.17	122.30	118.73
3	A	1678	ATP	O2B-PB-O1B	2.11	122.27	112.44
3	A	1678	ATP	O3A-PA-O1A	-2.10	104.40	110.70
3	B	1678	ATP	C4-N9-C8	2.03	107.87	105.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

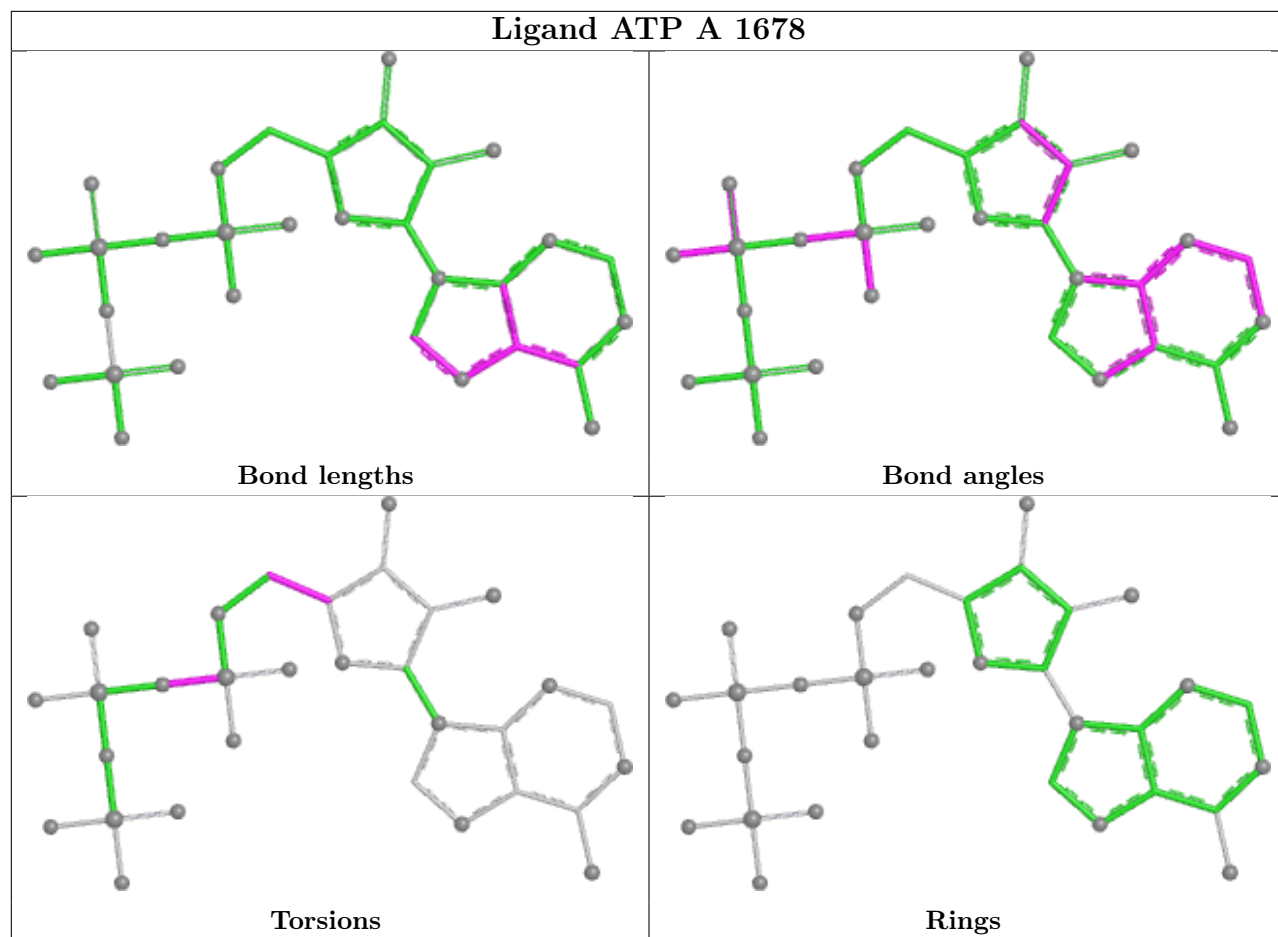
Mol	Chain	Res	Type	Atoms
3	A	1678	ATP	PB-O3A-PA-O5'
3	A	1678	ATP	O4'-C4'-C5'-O5'
3	A	1678	ATP	C3'-C4'-C5'-O5'
3	B	1678	ATP	C3'-C4'-C5'-O5'
3	B	1678	ATP	O4'-C4'-C5'-O5'
3	B	1678	ATP	C4'-C5'-O5'-PA
3	B	1678	ATP	PB-O3B-PG-O1G
3	B	1678	ATP	PA-O3A-PB-O1B
3	B	1678	ATP	PA-O3A-PB-O2B
3	B	1678	ATP	PB-O3A-PA-O1A
3	B	1678	ATP	PB-O3B-PG-O2G
3	B	1678	ATP	PB-O3A-PA-O2A

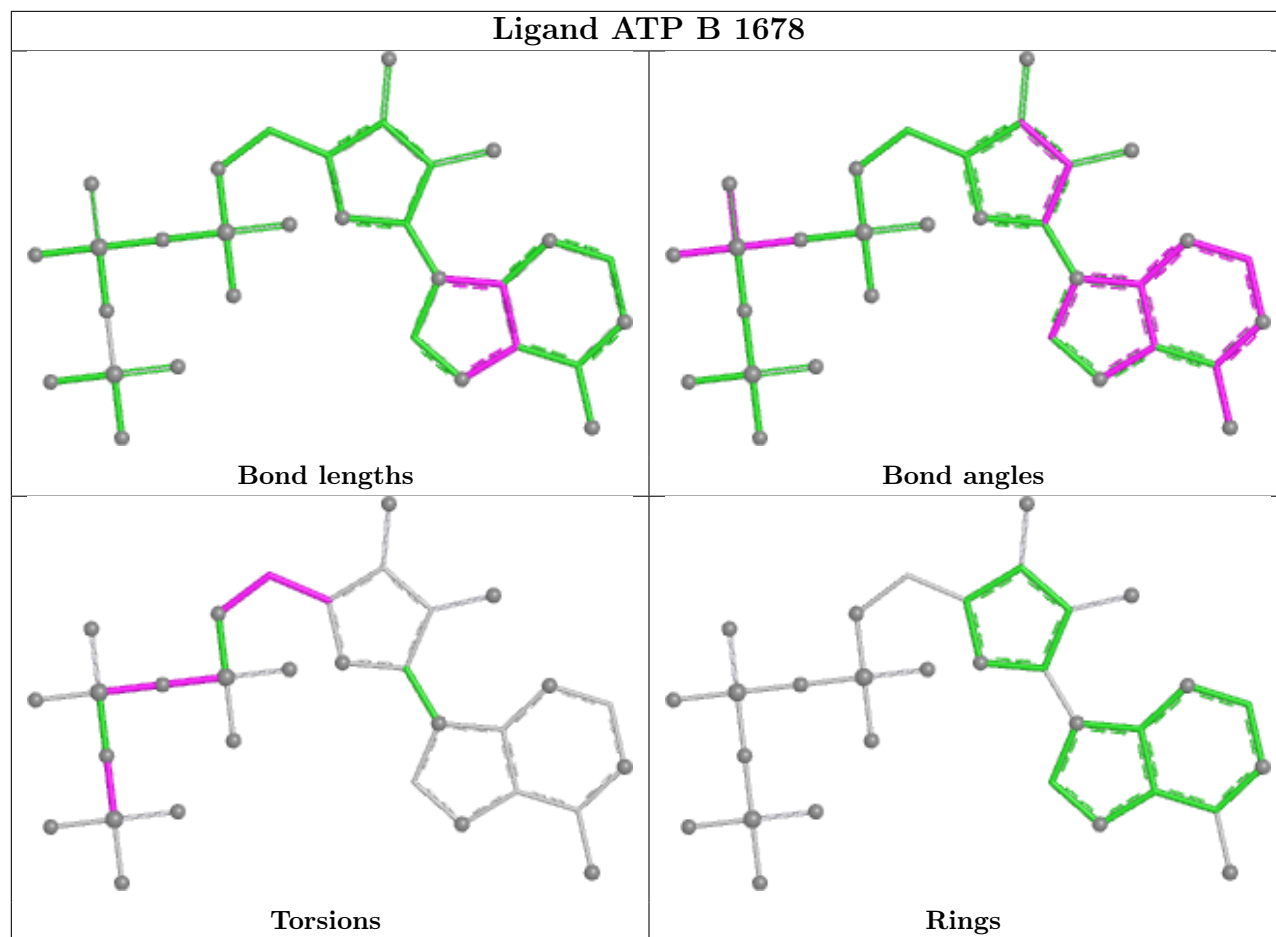
There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1678	ATP	7	0
3	B	1678	ATP	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	1.37	132 (21%) 2 1	63, 72, 74, 78	0
1	B	618/677 (91%)	1.24	109 (17%) 4 2	66, 72, 75, 88	0
2	X	115/134 (85%)	0.89	10 (8%) 16 9	69, 71, 74, 82	0
2	Y	115/134 (85%)	1.13	12 (10%) 11 6	69, 71, 74, 83	0
All	All	1457/1622 (89%)	1.26	263 (18%) 3 1	63, 72, 74, 88	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	SER	7.6
1	B	96	ILE	7.0
1	A	550	LEU	6.4
1	A	538	ALA	6.0
1	A	549	PRO	5.2
1	A	532	GLU	5.2
1	A	659	ASP	5.2
1	A	642	LEU	5.2
1	A	96	ILE	5.1
1	B	263	GLU	5.0
1	B	673	SER	4.8
1	A	553	ALA	4.8
1	A	531	GLU	4.8
1	A	567	VAL	4.8
1	B	271	ASN	4.6
1	A	597	ALA	4.4
1	A	638	THR	4.4
1	A	568	SER	4.3
1	A	379	SER	4.3
1	A	170	GLY	4.1
1	A	547	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	110	ALA	4.1
1	A	100	GLY	4.0
2	Y	87	GLY	4.0
1	A	271	ASN	4.0
1	A	620	PRO	4.0
1	B	543	GLU	3.9
1	A	572	LEU	3.7
1	B	524	ILE	3.6
1	B	535	GLU	3.6
1	B	117	ILE	3.6
1	B	672	ILE	3.6
1	B	29	ILE	3.5
1	A	117	ILE	3.5
1	A	110	ALA	3.5
1	A	641	ASP	3.5
1	A	575	PRO	3.5
1	B	116	MET	3.5
1	A	374	LEU	3.4
1	A	632	GLY	3.4
1	B	572	LEU	3.4
1	B	205	ILE	3.4
1	B	621	ILE	3.4
1	B	115	SER	3.4
1	A	639	VAL	3.3
1	B	479	LEU	3.3
1	A	535	GLU	3.3
2	Y	14	GLN	3.3
1	A	383	LEU	3.3
1	B	320	ILE	3.3
1	A	588	ASN	3.2
1	A	650	ALA	3.2
1	B	100	GLY	3.2
1	A	554	LEU	3.2
1	A	586	SER	3.2
2	X	87	GLY	3.2
1	A	529	GLU	3.2
1	B	664	PHE	3.2
1	B	13	THR	3.2
1	A	566	VAL	3.1
1	A	621	ILE	3.1
1	B	129	LEU	3.1
1	A	574	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	285	THR	3.1
1	B	374	LEU	3.1
1	A	478	SER	3.1
2	Y	93	LYS	3.1
1	A	624	GLU	3.1
1	A	585	TRP	3.0
1	B	376	LEU	3.0
1	B	616	SER	3.0
1	A	276	LEU	3.0
1	A	24	TYR	3.0
1	B	210	THR	3.0
1	A	657	SER	3.0
1	B	101	THR	2.9
1	A	205	ILE	2.9
1	A	201	VAL	2.9
1	B	203	TYR	2.9
2	Y	19	THR	2.9
1	B	82	ILE	2.9
1	A	637	LYS	2.9
1	B	594	LYS	2.9
2	X	133	VAL	2.9
1	B	25	SER	2.8
2	X	101	SER	2.8
1	A	169	ARG	2.8
1	B	485	SER	2.8
1	B	665	ALA	2.8
1	A	581	GLY	2.8
1	A	270	LEU	2.8
2	Y	95	TYR	2.8
1	A	562	VAL	2.8
1	B	138	SER	2.8
1	A	375	PRO	2.7
1	A	263	GLU	2.7
1	A	477	GLU	2.7
1	A	524	ILE	2.7
1	B	24	TYR	2.7
1	B	576	ALA	2.7
1	B	200	PHE	2.7
1	B	209	VAL	2.7
1	B	674	LEU	2.7
1	B	648	GLU	2.7
1	A	629	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	625	LEU	2.7
1	A	674	LEU	2.7
2	X	94	LEU	2.7
1	A	273	THR	2.6
1	A	533	THR	2.6
1	B	273	THR	2.6
1	B	642	LEU	2.6
2	Y	13	ALA	2.6
1	B	568	SER	2.6
1	B	268	GLU	2.6
1	B	490	ALA	2.6
1	A	596	GLN	2.6
1	B	154	GLY	2.6
1	B	676	LEU	2.6
1	A	622	ILE	2.5
1	B	593	MET	2.5
1	B	266	GLU	2.5
1	B	316	GLU	2.5
1	A	350	ILE	2.5
1	B	323	ILE	2.5
1	A	617	PRO	2.5
1	A	571	LEU	2.5
1	B	514	LYS	2.5
1	A	345	VAL	2.5
1	B	565	VAL	2.5
1	A	635	GLN	2.5
1	A	343	LEU	2.5
1	B	493	ALA	2.5
1	B	19	ILE	2.5
2	X	42	ILE	2.5
1	A	525	THR	2.5
2	X	93	LYS	2.5
1	B	152	ALA	2.4
1	A	592	ILE	2.4
1	A	591	ARG	2.4
1	A	23	VAL	2.4
1	B	168	GLY	2.4
1	A	11	GLU	2.4
1	A	93	LEU	2.4
1	A	115	SER	2.4
1	A	485	SER	2.4
2	Y	29	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	489	ASP	2.4
1	A	146	TYR	2.4
1	A	19	ILE	2.4
1	B	353	GLU	2.4
1	B	369	VAL	2.4
1	B	643	THR	2.4
1	A	578	ILE	2.4
2	Y	47	ILE	2.4
1	B	62	LEU	2.4
1	A	262	GLU	2.4
1	A	490	ALA	2.3
1	A	579	ARG	2.3
1	A	558	LEU	2.3
1	B	269	GLU	2.3
1	A	475	THR	2.3
1	A	557	ILE	2.3
1	B	347	ARG	2.3
1	B	520	THR	2.3
1	A	577	ALA	2.3
1	A	630	ASP	2.3
1	B	671	LEU	2.3
1	A	486	PRO	2.3
1	B	617	PRO	2.3
1	B	462	THR	2.3
1	A	479	LEU	2.3
1	A	163	VAL	2.3
1	B	147	ILE	2.3
1	A	319	ALA	2.3
1	B	171	THR	2.3
1	B	533	THR	2.3
2	Y	101	SER	2.3
1	B	560	ASP	2.3
1	A	536	GLU	2.3
1	A	541	GLU	2.3
1	B	639	VAL	2.3
1	A	401	ILE	2.3
1	A	527	ASP	2.3
1	A	573	ASP	2.3
1	B	630	ASP	2.3
1	A	118	GLY	2.2
1	B	16	MET	2.2
1	A	304	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	SER	2.2
1	B	99	SER	2.2
2	X	114	TYR	2.2
1	A	565	VAL	2.2
1	A	20	ILE	2.2
1	A	58	THR	2.2
1	A	95	THR	2.2
1	A	101	THR	2.2
1	A	570	LYS	2.2
1	B	335	LYS	2.2
1	B	94	GLY	2.2
1	B	276	LEU	2.2
2	Y	12	TRP	2.2
1	A	278	THR	2.2
1	A	344	TYR	2.2
1	B	23	VAL	2.2
1	B	482	VAL	2.2
1	A	126	SER	2.2
1	A	150	SER	2.2
1	A	615	ILE	2.2
1	B	443	LEU	2.2
1	A	514	LYS	2.2
1	B	573	ASP	2.2
1	A	551	THR	2.2
1	B	306	VAL	2.2
2	X	95	TYR	2.2
1	B	334	SER	2.2
1	B	447	SER	2.2
1	A	168	GLY	2.2
1	B	68	PRO	2.2
2	Y	112	VAL	2.1
1	B	508	TYR	2.1
1	A	39	SER	2.1
1	A	590	GLU	2.1
1	B	632	GLY	2.1
1	B	641	ASP	2.1
1	A	320	ILE	2.1
1	B	204	PRO	2.1
1	A	474	ILE	2.1
1	B	625	LEU	2.1
1	B	582	GLN	2.1
1	A	266	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	109	SER	2.1
1	B	201	VAL	2.1
1	A	82	ILE	2.1
1	A	129	LEU	2.1
1	A	315	LEU	2.1
1	A	652	LEU	2.1
1	B	90	ILE	2.1
1	B	22	THR	2.1
2	Y	15	ARG	2.1
1	A	661	PRO	2.1
1	B	33	GLU	2.1
1	B	666	SER	2.1
2	X	62	VAL	2.1
1	A	480	LYS	2.1
1	A	378	LEU	2.1
1	B	396	ILE	2.1
1	A	580	THR	2.1
1	B	486	PRO	2.1
1	A	136	VAL	2.0
1	A	673	SER	2.0
1	A	47	TYR	2.0
1	A	202	ALA	2.0
1	B	47	TYR	2.0
1	B	319	ALA	2.0
1	A	563	GLU	2.0
1	B	449	LYS	2.0
1	B	505	ILE	2.0
1	B	408	ALA	2.0
1	B	638	THR	2.0
2	X	135	ALA	2.0
1	B	331	LEU	2.0
1	B	358	ILE	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](#)

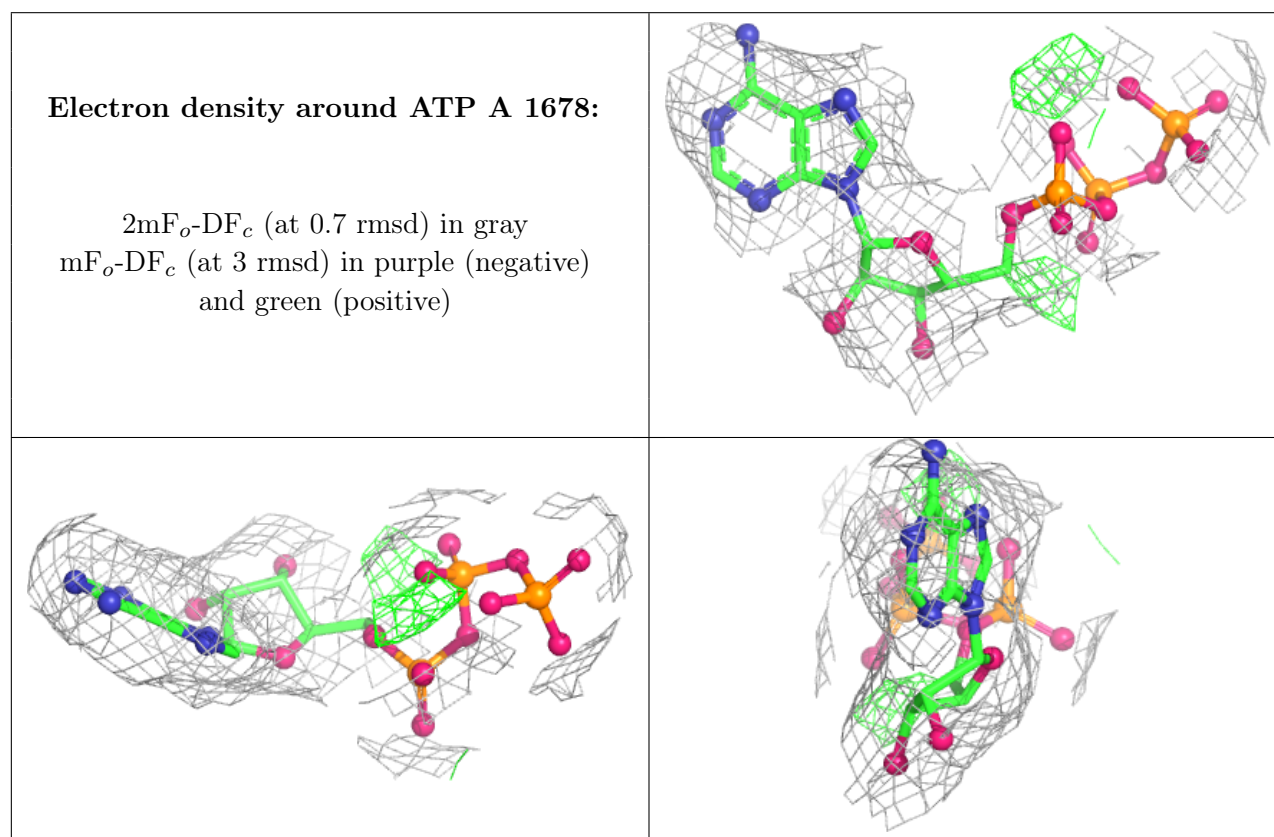
There are no oligosaccharides in this entry.

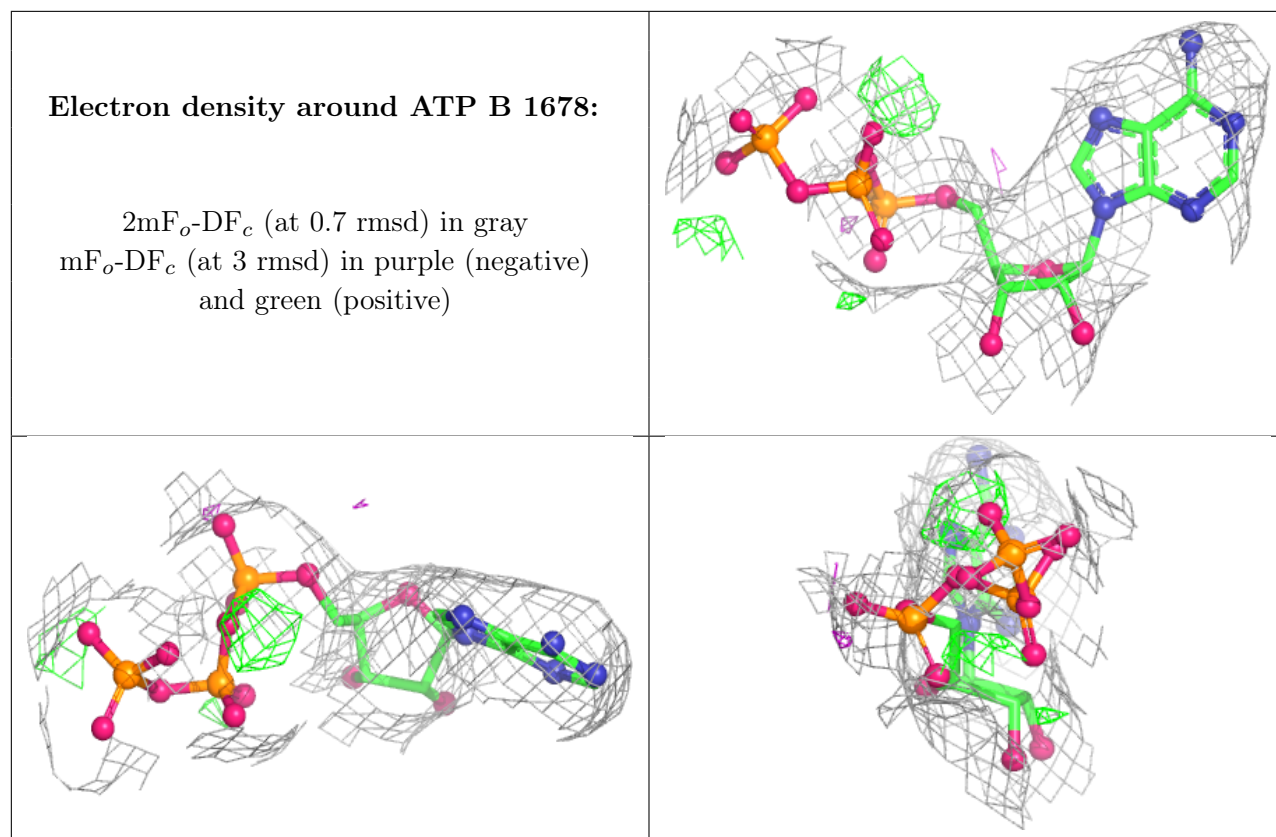
6.4 Ligands ⓘ

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. 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	B-factors(Å ²)	Q<0.9
3	ATP	A	1678	31/31	0.95	0.08	21,30,32,33	0
3	ATP	B	1678	31/31	0.96	0.08	18,29,31,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.