



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:27 pm BST

PDB ID : 3LQR
Title : Structure of CED-4:CED-3 complex
Authors : Qi, S.; Pang, Y.; Shi, Y.; Yan, N.
Deposited on : 2010-02-09
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

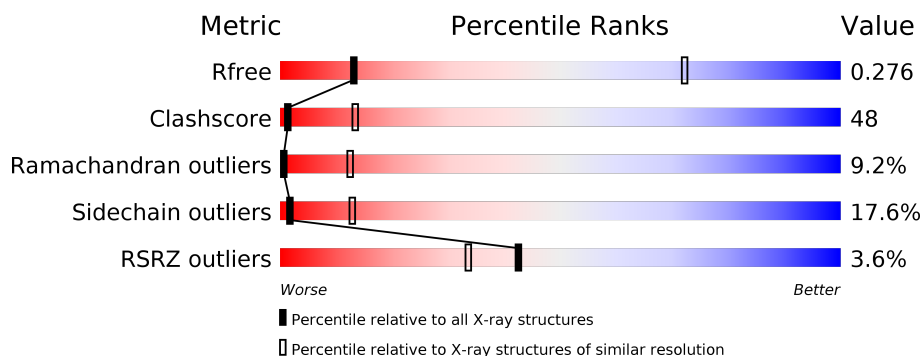
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	549	<div> <div>2%</div> <div> <div></div> <div>26%</div> <div>49%</div> <div>15%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	549	<div> <div>5%</div> <div> <div></div> <div>25%</div> <div>50%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>

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	A	602	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8124 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.

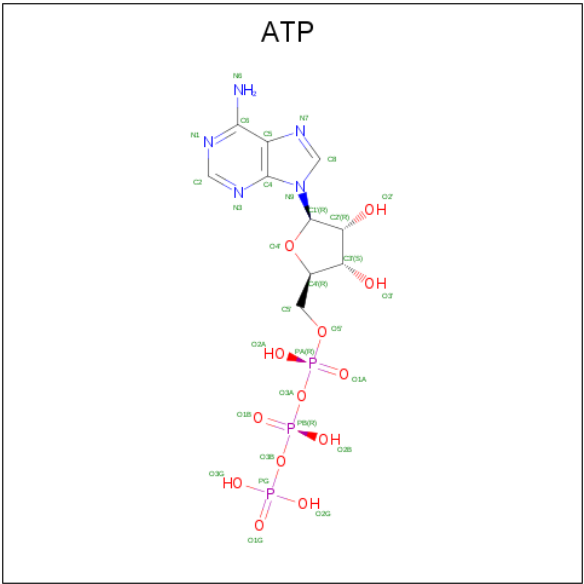
- Molecule 1 is a protein called Cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4039	2575	676	759	29			
1	B	501	Total	C	N	O	S	0	0	0
			4021	2565	673	754	29			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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

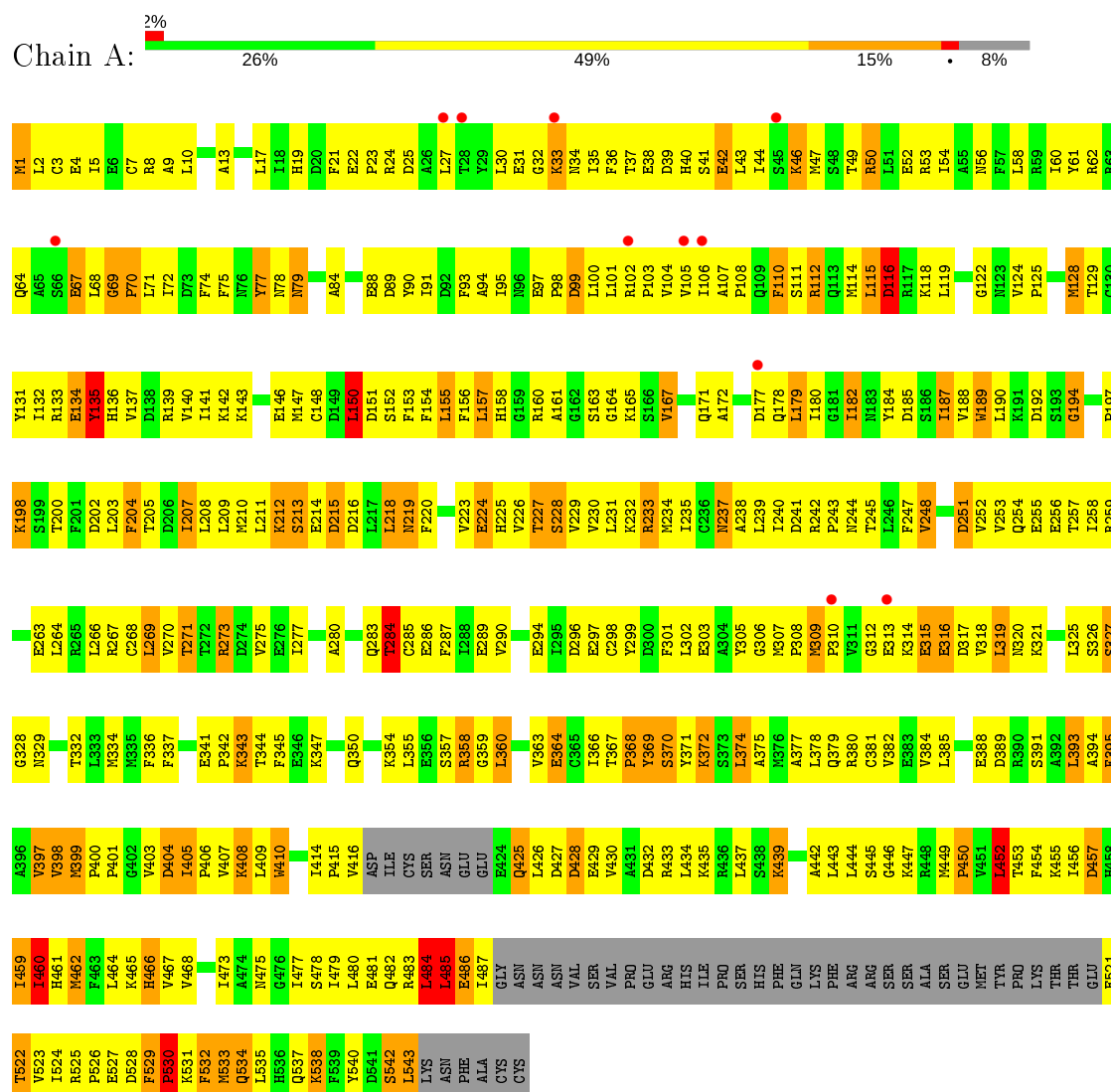


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

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

• Molecule 1: Cell death protein 4



• Molecule 1: Cell death protein 4



V523	I460	V397	R265	T200	E134	E87	M1
I524	H461	V398	L266	F201	I135	L68	L2
R525	M462	M399	R267	D202	H136	G69	C3
P526	F463	P400	C268	L203	V137	F70	E4
E527	L464	P401	L269	F204	D138	L71	I5
D528	K465	G402	K334	T205	R139	I72	E6
F529	H466	V403	K335	D206	V140	H73	C7
P530	V467	D404	F336	L207	I141	F74	R8
K531	V468	I405	R273	L208	K142	F75	A9
F532	I473	P406	D274	L209	K143	H76	L10
M533	A474	V407	V275	D210	I146	Y77	A13
Q534	N475	K408	E276	L211	M147	H78	L17
L535	G476	L409	L277	K212	C148	H79	L17
H536	I477	W410	S278	S213	D149	H82	F21
Q537	I478	I414	N279	E214	L150	L83	E22
F539	S478	P415	S282	D215	D151	A84	P23
Y540	I479	V416	D216	L217	S152		P24
D541	L480	ASP	T284	L218	F153	L87	R24
S542	Q482	ILE	C285	N219	F154	E88	D25
LYS	R483	CYS	E286	V223	L155	D89	A26
ASN	L484	SER	F287	E224	F156	Y90	L27
PHE	L485	ASN	L288	H225	L157	I91	T28
ALA	E496	GLU	E289	H226	H158	D92	Y29
CYS	L497	GLU	V290	V226	G159	F93	L30
	GLY	GLU		T227	R160	A94	E31
	ASN	GLN	L293	S228	A161	I95	G32
	ASN	L426	E294	V229	G162	I96	K33
	VAL	D427	D296	V230	S163	P97	N34
	SER	D428	E297	L231	G164	P98	I35
	VAL	E429	C365	K232	K165	D99	F36
	VAL	V430	T366	R233	S166	L100	T37
	PRO	A431	T367	T234	V167	L101	E38
	GLU	R432	D300	L235	S170	R102	D39
	HIS	L434	F301	C236	P103	P103	H40
	ILE	K435	S370	N237	Q171	Y104	S41
	PRO	R436	V371	A238	A172	V105	E42
	SER	L437	K372	L239	I106	I106	L43
	PHE	S438	S373	I240	A107	P108	I44
	GLN	K439	L374	D241	Q109	K46	S45
	LYS	A442	A377	P243	F110	M47	K46
	PHE	L443	L378	T244	S111	R112	T49
	ARG	L444	Q379	T245	R112	Q113	S48
	ARG	S445	R380	L246	I182	L114	R50
	SER	G446	C381	F247	H183	L115	L51
	SER	K447	V382	V248	Y184	E52	E52
	ALA	R448	E383		D185	D116	R53
	SER	M449	V384	D251	S186	R117	N56
	GLU	P450	L385	V252	I187	L121	F57
	MET	V451	E388	V253	V188	G122	L58
	TYR	L452	D389	Q254	W189		R59
	PRO	T453	R390	E255		Q127	I60
	LYS	F454	S391	T257	D192	M128	Y61
	THR	K455	L392	T258	S193	T129	R62
	THR	I456	L393	R259	G194	G130	R63
	GLU	D457	F395	E263	P197	Y131	Q64
		H458	S327	L264	K198	I132	A65
		I459	G328		S199	R133	S66

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.33Å 181.33Å 202.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 3.90 39.78 – 3.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.78-3.90) 96.6 (39.78-3.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.255 , 0.283 0.254 , 0.276	Depositor DCC
R_{free} test set	689 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	143.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 183.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å ²)	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: MG, 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	0.43	0/4113	0.66	0/5558
1	B	0.43	0/4095	0.65	0/5534
All	All	0.43	0/8208	0.66	0/11092

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4039	0	4066	405	0
1	B	4021	0	4052	401	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	10	0
3	B	31	0	12	4	0
All	All	8124	0	8142	786	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 48.

All (786) 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:110:PHE:HA	1:B:113:GLN:HB2	1.34	1.08
1:B:4:GLU:O	1:B:8:ARG:HB2	1.59	1.01
1:B:484:LEU:HD11	1:B:533:MET:HG2	1.44	1.00
1:A:484:LEU:HD11	1:A:533:MET:HG2	1.45	0.99
1:A:534:GLN:HA	1:A:534:GLN:HE21	1.25	0.98
1:A:4:GLU:O	1:A:8:ARG:HB2	1.63	0.96
1:B:534:GLN:HE21	1:B:534:GLN:HA	1.27	0.96
1:B:468:VAL:HG23	1:B:473:ILE:HD11	1.48	0.96
1:A:342:PRO:HB3	1:B:448:ARG:HH11	1.31	0.94
1:A:468:VAL:HG23	1:A:473:ILE:HD11	1.50	0.94
1:B:114:MET:SD	1:B:177:ASP:HA	2.07	0.93
1:A:164:GLY:HA2	3:A:602:ATP:O1A	1.72	0.89
1:B:540:TYR:O	1:B:543:LEU:HD23	1.72	0.89
1:B:101:LEU:HD11	1:B:106:ILE:HD12	1.53	0.88
1:A:540:TYR:O	1:A:543:LEU:HD23	1.74	0.86
1:A:128:MET:HE2	1:A:129:THR:H	1.42	0.84
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.43	0.84
1:A:78:ASN:OD1	1:B:37:THR:HG21	1.77	0.84
1:A:299:TYR:HA	1:A:302:LEU:HD12	1.61	0.82
1:A:47:MET:HB2	1:A:53:ARG:HG3	1.62	0.82
1:B:299:TYR:HA	1:B:302:LEU:HD12	1.60	0.81
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.63	0.81
1:B:47:MET:HB2	1:B:53:ARG:HG3	1.62	0.81
1:A:93:PHE:HB2	1:A:101:LEU:HD13	1.61	0.81
1:A:160:ARG:HB3	1:A:163:SER:HB3	1.61	0.80
1:A:189:TRP:HE3	1:A:248:VAL:HG21	1.46	0.80
1:A:524:ILE:HD12	1:A:525:ARG:H	1.46	0.79
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.64	0.79
1:B:443:LEU:O	1:B:460:ILE:HD12	1.83	0.79
1:A:44:ILE:O	1:A:53:ARG:HG2	1.83	0.79
1:A:305:TYR:O	1:A:307:MET:HG2	1.83	0.79
1:B:197:PRO:HD2	1:B:198:LYS:HG2	1.65	0.79
1:A:165:LYS:HZ2	1:A:273:ARG:HD3	1.49	0.78
1:B:524:ILE:HD12	1:B:525:ARG:H	1.48	0.78
1:A:197:PRO:HD2	1:A:198:LYS:HG2	1.66	0.77
1:A:247:PHE:CE1	1:A:266:LEU:HD13	2.19	0.77
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.67	0.77
1:B:527:GLU:HA	1:B:530:PRO:HG3	1.65	0.77
1:A:443:LEU:O	1:A:460:ILE:HD12	1.85	0.77
1:B:189:TRP:HE3	1:B:248:VAL:HG21	1.48	0.77
1:A:399:MET:SD	1:A:400:PRO:HD2	2.25	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:HB3	1:B:163:SER:HB3	1.65	0.77
1:A:233:ARG:HH11	1:A:233:ARG:HG3	1.49	0.77
1:B:305:TYR:O	1:B:307:MET:HG2	1.85	0.77
1:A:527:GLU:HA	1:A:530:PRO:HG3	1.65	0.77
1:B:264:LEU:HB3	1:B:266:LEU:HD21	1.66	0.76
1:A:156:PHE:HB2	1:A:287:PHE:HD2	1.50	0.76
1:A:408:LYS:HE2	1:A:427:ASP:HB2	1.68	0.75
1:A:313:GLU:O	1:A:316:GLU:HG3	1.86	0.75
1:A:112:ARG:NH1	1:A:115:LEU:HD12	2.01	0.75
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.68	0.75
1:B:247:PHE:CE1	1:B:266:LEU:HD13	2.21	0.75
1:A:264:LEU:HB3	1:A:266:LEU:HD21	1.68	0.74
1:B:399:MET:SD	1:B:400:PRO:HD2	2.26	0.74
1:B:313:GLU:O	1:B:316:GLU:HG3	1.88	0.74
1:B:542:SER:C	1:B:543:LEU:HD22	2.07	0.73
1:B:233:ARG:CG	1:B:233:ARG:HH11	2.01	0.73
1:A:189:TRP:CE3	1:A:248:VAL:HG21	2.24	0.73
1:A:208:LEU:HD23	1:A:235:ILE:HG12	1.71	0.73
1:B:331:ALA:HA	3:B:602:ATP:O2'	1.89	0.73
1:A:88:GLU:O	1:A:91:ILE:HG22	1.89	0.73
1:B:133:ARG:O	1:B:137:VAL:HG23	1.88	0.73
1:A:122:GLY:HA3	1:A:187:ILE:HG23	1.70	0.72
1:B:408:LYS:HE2	1:B:427:ASP:HB2	1.71	0.72
1:A:347:LYS:HD3	1:A:347:LYS:O	1.90	0.72
1:B:241:ASP:C	1:B:243:PRO:HD3	2.10	0.72
1:B:128:MET:HE2	1:B:129:THR:H	1.54	0.72
1:B:208:LEU:HD23	1:B:235:ILE:HG12	1.71	0.72
1:A:167:VAL:HG21	3:A:602:ATP:N7	2.05	0.72
1:B:44:ILE:O	1:B:53:ARG:HG2	1.90	0.72
1:B:216:ASP:HB3	1:B:219:ASN:HB3	1.72	0.71
1:A:452:LEU:H	1:A:452:LEU:HD23	1.55	0.71
1:B:156:PHE:HB2	1:B:287:PHE:HD2	1.56	0.71
1:A:216:ASP:HB3	1:A:219:ASN:HB3	1.73	0.71
1:B:7:CYS:SG	1:B:62:ARG:HD3	2.30	0.71
1:A:524:ILE:HD12	1:A:525:ARG:N	2.06	0.71
1:B:182:ILE:N	1:B:182:ILE:HD12	2.06	0.71
1:B:5:ILE:HD13	1:B:94:ALA:HB1	1.71	0.71
1:A:167:VAL:HG21	3:A:602:ATP:C8	2.25	0.71
1:A:374:LEU:CD1	1:A:378:LEU:HG	2.21	0.71
1:B:122:GLY:HA3	1:B:187:ILE:HG23	1.71	0.71
1:A:133:ARG:O	1:A:137:VAL:HG23	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.31	0.70
1:B:524:ILE:HD12	1:B:525:ARG:N	2.06	0.70
1:B:347:LYS:HD3	1:B:347:LYS:O	1.90	0.70
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.05	0.70
1:B:88:GLU:O	1:B:91:ILE:HG22	1.91	0.70
1:A:480:LEU:HD23	1:A:481:GLU:OE2	1.91	0.70
1:A:542:SER:C	1:A:543:LEU:HD22	2.12	0.70
1:B:534:GLN:HE21	1:B:534:GLN:CA	2.04	0.70
1:B:189:TRP:CE3	1:B:248:VAL:HG21	2.27	0.70
1:A:342:PRO:HB3	1:B:448:ARG:NH1	2.04	0.69
1:A:294:GLU:HB2	1:A:297:GLU:OE1	1.93	0.69
1:B:326:SER:O	1:B:328:GLY:N	2.25	0.69
1:B:374:LEU:CD1	1:B:378:LEU:HG	2.23	0.69
1:A:482:GLN:O	1:A:485:LEU:HD11	1.93	0.69
1:A:534:GLN:HA	1:A:534:GLN:NE2	2.06	0.69
1:B:42:GLU:O	1:B:46:LYS:HG3	1.93	0.69
1:A:301:PHE:HE1	1:A:305:TYR:HE1	1.41	0.69
1:A:326:SER:O	1:A:328:GLY:N	2.26	0.69
1:A:165:LYS:NZ	1:A:273:ARG:HD3	2.07	0.69
1:B:301:PHE:HE1	1:B:305:TYR:HE1	1.41	0.68
1:B:294:GLU:HB2	1:B:297:GLU:OE1	1.93	0.68
1:B:480:LEU:HD23	1:B:481:GLU:OE2	1.93	0.68
1:B:406:PRO:HA	1:B:453:THR:HG22	1.74	0.68
1:B:110:PHE:CA	1:B:113:GLN:HB2	2.18	0.68
1:A:165:LYS:HG3	3:A:602:ATP:O2B	1.94	0.68
1:B:482:GLN:O	1:B:485:LEU:HD11	1.94	0.68
1:A:156:PHE:HB2	1:A:287:PHE:CD2	2.29	0.68
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.74	0.68
1:B:165:LYS:NZ	1:B:273:ARG:HD3	2.09	0.68
1:B:443:LEU:HB2	1:B:444:LEU:HD12	1.76	0.68
1:A:141:ILE:HG23	1:A:179:LEU:HD21	1.76	0.67
1:A:406:PRO:HA	1:A:453:THR:HG22	1.76	0.67
1:B:447:LYS:NZ	1:B:450:PRO:HD2	2.08	0.67
1:B:128:MET:HA	1:B:128:MET:HE3	1.75	0.67
1:A:443:LEU:HB2	1:A:444:LEU:HD12	1.76	0.67
1:A:98:PRO:O	1:A:99:ASP:HB2	1.95	0.67
1:B:35:ILE:O	1:B:35:ILE:HG22	1.95	0.67
1:B:452:LEU:H	1:B:452:LEU:HD23	1.60	0.67
1:B:415:PRO:O	1:B:416:VAL:HG23	1.94	0.66
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.76	0.66
1:A:182:ILE:N	1:A:182:ILE:HD12	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:HD22	1:B:204:PHE:CE1	2.30	0.66
1:A:255:GLU:CB	1:A:277:ILE:HG22	2.25	0.66
1:A:5:ILE:HD13	1:A:94:ALA:HB1	1.76	0.66
1:A:241:ASP:C	1:A:243:PRO:HD3	2.16	0.66
1:B:91:ILE:O	1:B:95:ILE:HG12	1.95	0.66
1:B:255:GLU:CB	1:B:277:ILE:HG22	2.26	0.65
1:A:447:LYS:NZ	1:A:450:PRO:HD2	2.11	0.65
1:A:394:ALA:O	1:A:397:VAL:HG23	1.96	0.65
1:B:312:GLY:H	1:B:315:GLU:CD	1.99	0.65
1:A:72:ILE:HG23	1:A:84:ALA:HB1	1.79	0.65
1:B:203:LEU:HD22	1:B:204:PHE:CD1	2.31	0.65
1:B:165:LYS:HG3	3:B:602:ATP:O2B	1.97	0.65
1:B:259:ARG:O	1:B:263:GLU:HG3	1.97	0.65
1:B:319:LEU:HD23	1:B:320:ASN:N	2.12	0.65
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.77	0.65
1:B:318:VAL:HG12	1:B:318:VAL:O	1.96	0.65
1:A:218:LEU:HG	1:A:219:ASN:H	1.61	0.65
1:A:318:VAL:O	1:A:318:VAL:HG12	1.96	0.65
1:B:371:TYR:CD1	1:B:377:ALA:HB2	2.33	0.64
1:A:158:HIS:O	1:A:290:VAL:HG23	1.98	0.64
1:B:72:ILE:HG23	1:B:84:ALA:HB1	1.80	0.64
1:A:483:ARG:O	1:A:485:LEU:HD12	1.98	0.64
1:A:203:LEU:HD22	1:A:204:PHE:CE1	2.33	0.64
1:B:468:VAL:CG2	1:B:473:ILE:HD11	2.25	0.64
1:B:156:PHE:HB2	1:B:287:PHE:CD2	2.33	0.63
1:A:384:VAL:HG23	1:A:385:LEU:HD23	1.80	0.63
1:A:37:THR:OG1	1:A:40:HIS:HD2	1.81	0.63
1:A:91:ILE:O	1:A:95:ILE:HG12	1.98	0.63
1:B:114:MET:HG2	1:B:180:ILE:HB	1.81	0.63
1:B:39:ASP:O	1:B:43:LEU:HB2	1.98	0.63
1:A:312:GLY:H	1:A:315:GLU:CD	2.01	0.63
1:B:108:PRO:O	1:B:109:GLN:HB2	1.98	0.63
1:B:49:THR:HG22	1:B:50:ARG:N	2.14	0.63
1:A:40:HIS:ND1	1:A:60:ILE:HD13	2.14	0.63
1:A:415:PRO:O	1:A:416:VAL:HG23	1.99	0.63
1:B:141:ILE:HG23	1:B:179:LEU:HD21	1.81	0.63
1:B:218:LEU:HG	1:B:219:ASN:H	1.63	0.63
1:B:447:LYS:CE	1:B:450:PRO:HD2	2.29	0.63
1:B:534:GLN:HA	1:B:534:GLN:NE2	2.08	0.63
1:A:42:GLU:O	1:A:46:LYS:HG3	1.97	0.62
1:B:527:GLU:CA	1:B:530:PRO:HG3	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:VAL:HG13	1:B:172:ALA:HB2	1.81	0.62
1:B:298:CYS:O	1:B:302:LEU:HG	2.00	0.62
1:B:40:HIS:ND1	1:B:60:ILE:HD13	2.13	0.62
1:B:77:TYR:O	1:B:77:TYR:CD1	2.53	0.62
1:A:477:ILE:O	1:A:480:LEU:HB3	1.99	0.62
1:B:447:LYS:HE3	1:B:450:PRO:HD2	1.80	0.62
1:A:366:ILE:H	1:A:366:ILE:HD12	1.64	0.62
1:A:259:ARG:O	1:A:263:GLU:HG3	2.00	0.62
1:A:443:LEU:HB2	1:A:444:LEU:CD1	2.30	0.62
1:A:329:ASN:HB2	1:A:459:ILE:HD13	1.81	0.62
1:A:371:TYR:CD1	1:A:377:ALA:HB2	2.35	0.62
1:B:485:LEU:HD12	1:B:486:GLU:HG3	1.81	0.62
1:B:405:ILE:HG12	1:B:410:TRP:CZ3	2.35	0.62
1:A:410:TRP:CZ3	1:A:454:PHE:HB2	2.35	0.61
1:A:203:LEU:HD22	1:A:204:PHE:CD1	2.35	0.61
1:A:298:CYS:O	1:A:302:LEU:HG	2.01	0.61
1:A:468:VAL:CG2	1:A:473:ILE:HD11	2.27	0.61
1:B:255:GLU:CA	1:B:277:ILE:HG22	2.30	0.61
1:A:447:LYS:HE3	1:A:450:PRO:HD2	1.82	0.61
1:A:527:GLU:CA	1:A:530:PRO:HG3	2.29	0.61
1:B:22:GLU:HB3	1:B:25:ASP:OD2	2.00	0.61
1:B:264:LEU:HB3	1:B:266:LEU:CD2	2.30	0.61
1:B:165:LYS:HZ2	1:B:273:ARG:HD3	1.65	0.61
1:B:158:HIS:O	1:B:290:VAL:HG23	2.00	0.61
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.82	0.61
1:A:22:GLU:HB2	1:B:63:ARG:NH1	2.16	0.61
1:A:255:GLU:CA	1:A:277:ILE:HG22	2.30	0.61
1:A:350:GLN:NE2	1:B:428:ASP:HB3	2.15	0.61
1:B:241:ASP:O	1:B:243:PRO:HD3	2.01	0.61
1:A:35:ILE:HG22	1:A:35:ILE:O	2.01	0.60
1:B:182:ILE:H	1:B:182:ILE:HD12	1.63	0.60
1:B:483:ARG:O	1:B:485:LEU:N	2.34	0.60
1:B:404:ASP:OD1	1:B:447:LYS:HD3	2.01	0.60
1:B:443:LEU:HB2	1:B:444:LEU:CD1	2.31	0.60
1:B:394:ALA:O	1:B:397:VAL:HG23	2.01	0.60
1:A:194:GLY:O	1:A:254:GLN:HG3	2.01	0.60
1:A:483:ARG:O	1:A:485:LEU:N	2.34	0.60
1:A:79:ASN:ND2	1:B:36:PHE:H	1.99	0.60
1:A:33:LYS:HD3	1:A:70:PRO:HB3	1.84	0.60
1:A:39:ASP:O	1:A:43:LEU:HB2	2.02	0.60
1:A:77:TYR:CD1	1:A:77:TYR:O	2.54	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:HG21	1:B:256:GLU:HB3	1.84	0.60
1:B:37:THR:OG1	1:B:40:HIS:HD2	1.85	0.60
1:A:319:LEU:HD23	1:A:320:ASN:N	2.17	0.59
1:A:310:PRO:CB	1:A:316:GLU:HB3	2.33	0.59
1:A:443:LEU:HB3	1:A:460:ILE:HD11	1.83	0.59
1:A:447:LYS:CE	1:A:450:PRO:HD2	2.32	0.59
1:B:255:GLU:HA	1:B:277:ILE:HG22	1.84	0.59
1:A:264:LEU:HB3	1:A:266:LEU:CD2	2.31	0.59
1:A:37:THR:OG1	1:A:40:HIS:CD2	2.55	0.59
1:B:301:PHE:HE1	1:B:305:TYR:CE1	2.20	0.59
1:B:384:VAL:HG23	1:B:385:LEU:HD23	1.85	0.59
1:B:167:VAL:O	1:B:171:GLN:HG3	2.02	0.59
1:B:122:GLY:HA2	1:B:187:ILE:O	2.03	0.59
1:A:105:VAL:O	1:A:105:VAL:HG12	2.02	0.59
1:A:475:ASN:O	1:A:479:ILE:HG13	2.03	0.59
1:B:310:PRO:CB	1:B:316:GLU:HB3	2.33	0.59
1:B:483:ARG:O	1:B:485:LEU:HD12	2.02	0.59
1:A:49:THR:HB	1:A:52:GLU:OE1	2.03	0.59
1:B:342:PRO:O	1:B:343:LYS:CB	2.51	0.59
1:B:410:TRP:CZ3	1:B:454:PHE:HB2	2.38	0.59
1:B:484:LEU:HD11	1:B:533:MET:CG	2.26	0.59
1:B:480:LEU:HD22	1:B:540:TYR:HE2	1.68	0.59
1:B:49:THR:HG22	1:B:50:ARG:H	1.67	0.58
1:A:251:ASP:HA	1:A:271:THR:O	2.03	0.58
1:A:401:PRO:HA	1:A:456:ILE:HG23	1.85	0.58
1:B:443:LEU:HB3	1:B:460:ILE:HD11	1.84	0.58
1:A:301:PHE:HE1	1:A:305:TYR:CE1	2.21	0.58
1:A:426:LEU:HB3	1:A:428:ASP:OD2	2.03	0.58
1:A:49:THR:HG22	1:A:50:ARG:N	2.18	0.58
1:B:477:ILE:O	1:B:480:LEU:HB3	2.03	0.58
1:A:178:GLN:O	1:A:182:ILE:HB	2.02	0.58
1:B:101:LEU:HD21	1:B:106:ILE:HD11	1.85	0.58
1:B:177:ASP:O	1:B:182:ILE:HD13	2.04	0.58
1:A:177:ASP:O	1:A:182:ILE:HD13	2.04	0.58
1:B:136:HIS:O	1:B:140:VAL:HG23	2.04	0.58
1:B:24:ARG:HA	1:B:27:LEU:HD12	1.85	0.58
1:B:533:MET:HE3	1:B:533:MET:O	2.04	0.58
1:B:135:TYR:CE1	1:B:139:ARG:HD2	2.39	0.57
1:B:233:ARG:CG	1:B:233:ARG:NH1	2.65	0.57
1:B:426:LEU:HB3	1:B:428:ASP:OD2	2.04	0.57
1:B:10:LEU:HD22	1:B:58:LEU:HD21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:PRO:HA	1:B:456:ILE:HG23	1.86	0.57
1:A:414:ILE:HG21	1:A:430:VAL:HG22	1.86	0.57
1:B:178:GLN:O	1:B:182:ILE:HB	2.04	0.57
1:B:366:ILE:H	1:B:366:ILE:HD12	1.70	0.57
1:A:241:ASP:O	1:A:243:PRO:HD3	2.04	0.57
1:A:410:TRP:CH2	1:A:454:PHE:HB2	2.40	0.57
1:A:47:MET:HE2	1:A:52:GLU:HB3	1.86	0.57
1:A:69:GLY:H	1:A:70:PRO:HD2	1.70	0.57
1:A:342:PRO:O	1:A:343:LYS:CB	2.52	0.57
1:A:366:ILE:N	1:A:366:ILE:HD12	2.19	0.57
1:B:248:VAL:CG1	1:B:269:LEU:HD12	2.35	0.57
1:B:251:ASP:HA	1:B:271:THR:O	2.04	0.57
1:A:135:TYR:CE1	1:A:139:ARG:HD2	2.40	0.57
1:B:153:PHE:CE2	1:B:267:ARG:HG2	2.40	0.57
1:A:327:SER:HB2	1:A:459:ILE:CG1	2.35	0.56
1:A:485:LEU:HD12	1:A:486:GLU:HG3	1.86	0.56
1:A:9:ALA:HB2	1:A:90:TYR:CD2	2.40	0.56
1:A:119:LEU:HB3	1:B:265:ARG:HH12	1.70	0.56
1:A:405:ILE:HG12	1:A:410:TRP:CZ3	2.40	0.56
1:A:192:ASP:OD2	1:A:252:VAL:HG22	2.05	0.56
1:A:24:ARG:NE	1:A:53:ARG:HH11	2.03	0.56
1:B:32:GLY:C	1:B:34:ASN:H	2.09	0.56
1:A:255:GLU:HA	1:A:277:ILE:HG22	1.87	0.56
1:B:114:MET:O	1:B:114:MET:HE3	2.05	0.56
1:B:327:SER:HB2	1:B:459:ILE:CG1	2.36	0.56
1:A:182:ILE:H	1:A:182:ILE:HD12	1.68	0.56
1:A:67:GLU:HG2	1:A:68:LEU:N	2.21	0.56
1:A:314:LYS:HA	1:A:317:ASP:HB2	1.88	0.56
1:A:400:PRO:HB2	1:A:403:VAL:HB	1.88	0.56
1:A:404:ASP:OD1	1:A:447:LYS:HD3	2.05	0.56
1:B:9:ALA:HB2	1:B:90:TYR:CD2	2.40	0.56
1:A:315:GLU:HB2	1:A:345:PHE:CE2	2.41	0.56
1:B:117:ARG:O	1:B:121:LEU:HG	2.05	0.56
1:B:369:TYR:HD1	1:B:370:SER:H	1.53	0.56
1:B:33:LYS:HD3	1:B:70:PRO:HB3	1.88	0.56
1:A:32:GLY:C	1:A:34:ASN:H	2.10	0.56
1:A:136:HIS:O	1:A:140:VAL:HG23	2.06	0.55
1:B:525:ARG:HD3	1:B:535:LEU:HD13	1.88	0.55
1:B:153:PHE:HE2	1:B:267:ARG:HG2	1.71	0.55
1:B:37:THR:O	1:B:40:HIS:HB2	2.06	0.55
1:B:72:ILE:HG21	1:B:88:GLU:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:HIS:HB3	1:B:1:MET:HB2	1.88	0.55
1:A:158:HIS:HB2	1:A:275:VAL:HG22	1.88	0.55
1:A:72:ILE:HG21	1:A:88:GLU:HG2	1.88	0.55
1:B:47:MET:HB2	1:B:53:ARG:CG	2.34	0.55
1:A:167:VAL:O	1:A:171:GLN:HG3	2.06	0.55
1:A:354:LYS:O	1:A:358:ARG:HB2	2.06	0.55
1:B:315:GLU:HB2	1:B:345:PHE:CE2	2.42	0.55
1:B:37:THR:OG1	1:B:40:HIS:CD2	2.58	0.55
1:B:46:LYS:HE3	1:B:46:LYS:O	2.06	0.55
1:A:137:VAL:HG13	1:A:172:ALA:HB2	1.89	0.55
1:A:141:ILE:HG23	1:A:179:LEU:CD2	2.37	0.55
1:B:109:GLN:C	1:B:111:SER:H	2.09	0.55
1:B:314:LYS:HA	1:B:317:ASP:HB2	1.89	0.55
1:B:49:THR:HB	1:B:52:GLU:OE1	2.07	0.55
1:A:223:VAL:O	1:A:226:VAL:HG23	2.06	0.55
1:A:37:THR:O	1:A:40:HIS:HB2	2.07	0.55
1:B:342:PRO:HD2	1:B:347:LYS:HG3	1.89	0.55
1:A:460:ILE:HG23	1:A:460:ILE:O	2.06	0.55
1:A:525:ARG:HD3	1:A:535:LEU:HD13	1.89	0.55
1:A:79:ASN:HD21	1:B:34:ASN:C	2.11	0.55
1:A:112:ARG:HD3	1:A:112:ARG:O	2.07	0.54
1:B:475:ASN:O	1:B:479:ILE:HG13	2.06	0.54
1:A:207:ILE:HG22	1:A:208:LEU:N	2.22	0.54
1:B:223:VAL:O	1:B:226:VAL:HG23	2.07	0.54
1:B:329:ASN:HB2	1:B:459:ILE:HD13	1.89	0.54
1:B:393:LEU:HD23	1:B:437:LEU:HD22	1.90	0.54
1:A:122:GLY:HA2	1:A:187:ILE:O	2.08	0.54
1:A:52:GLU:O	1:A:56:ASN:HB2	2.07	0.54
1:B:366:ILE:N	1:B:366:ILE:HD12	2.23	0.54
1:B:410:TRP:CH2	1:B:454:PHE:HB2	2.42	0.54
1:A:327:SER:O	1:A:459:ILE:HD11	2.08	0.54
1:A:153:PHE:CE2	1:A:267:ARG:HG2	2.43	0.54
1:A:303:GLU:HG3	1:A:309:MET:HE1	1.89	0.54
1:B:468:VAL:HG23	1:B:473:ILE:CD1	2.32	0.54
1:B:67:GLU:HG2	1:B:68:LEU:N	2.23	0.54
1:A:22:GLU:HB3	1:A:25:ASP:OD2	2.07	0.54
1:A:47:MET:HB2	1:A:53:ARG:CG	2.36	0.54
1:B:327:SER:HB2	1:B:459:ILE:HG13	1.90	0.54
1:A:115:LEU:CD2	1:A:180:ILE:HB	2.39	0.53
1:B:459:ILE:C	1:B:461:HIS:H	2.11	0.53
1:B:167:VAL:HG21	3:B:602:ATP:N3	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:GLU:O	1:A:530:PRO:HD3	2.09	0.53
1:B:534:GLN:NE2	1:B:537:GLN:HB2	2.23	0.53
1:B:24:ARG:NE	1:B:53:ARG:HH11	2.06	0.53
1:A:188:VAL:HB	1:A:247:PHE:CD2	2.44	0.53
1:B:47:MET:HE2	1:B:52:GLU:HB3	1.91	0.53
1:A:480:LEU:HD22	1:A:540:TYR:HE2	1.72	0.53
1:A:533:MET:C	1:A:533:MET:HE2	2.28	0.53
1:B:228:SER:O	1:B:232:LYS:HG3	2.09	0.53
1:B:342:PRO:CD	1:B:347:LYS:HG3	2.38	0.53
1:B:429:GLU:HA	1:B:432:ASP:OD2	2.09	0.53
1:A:24:ARG:HA	1:A:27:LEU:HD12	1.90	0.53
1:B:189:TRP:HB2	1:B:248:VAL:HG23	1.91	0.53
1:B:391:SER:OG	1:B:415:PRO:HG2	2.09	0.53
1:B:4:GLU:O	1:B:8:ARG:CB	2.47	0.53
1:A:369:TYR:HD1	1:A:370:SER:H	1.55	0.53
1:A:534:GLN:HE21	1:A:534:GLN:CA	2.04	0.53
1:B:178:GLN:HA	1:B:182:ILE:HD13	1.91	0.53
1:B:194:GLY:O	1:B:254:GLN:HG3	2.09	0.53
1:B:69:GLY:H	1:B:70:PRO:HD2	1.72	0.53
1:A:153:PHE:HE2	1:A:267:ARG:HG2	1.74	0.52
1:A:468:VAL:HG23	1:A:473:ILE:CD1	2.33	0.52
1:B:256:GLU:HA	1:B:259:ARG:HG3	1.90	0.52
1:A:131:TYR:CD2	1:A:301:PHE:HA	2.44	0.52
1:A:449:MET:HA	1:A:450:PRO:C	2.30	0.52
1:A:534:GLN:NE2	1:A:537:GLN:HB2	2.23	0.52
1:B:478:SER:O	1:B:482:GLN:HG2	2.08	0.52
1:B:538:LYS:C	1:B:538:LYS:HD3	2.30	0.52
1:A:13:ALA:O	1:A:17:LEU:HD12	2.08	0.52
1:A:205:THR:HA	1:A:231:LEU:HD11	1.91	0.52
1:A:538:LYS:HD3	1:A:538:LYS:C	2.30	0.52
1:B:27:LEU:HD22	1:B:41:SER:HA	1.91	0.52
1:B:30:LEU:HD22	1:B:35:ILE:HB	1.90	0.52
1:B:52:GLU:O	1:B:56:ASN:HB2	2.08	0.52
1:B:10:LEU:HD13	1:B:58:LEU:CD2	2.40	0.52
1:A:178:GLN:HA	1:A:182:ILE:HD13	1.92	0.52
1:B:141:ILE:HG23	1:B:179:LEU:CD2	2.39	0.52
1:B:207:ILE:HG22	1:B:208:LEU:N	2.24	0.52
1:A:364:GLU:HG3	1:A:372:LYS:HB3	1.92	0.52
1:A:27:LEU:HD22	1:A:41:SER:HA	1.92	0.52
1:A:342:PRO:CD	1:A:347:LYS:HG3	2.40	0.52
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PRO:HB3	1:A:316:GLU:HB3	1.92	0.52
1:A:429:GLU:HA	1:A:432:ASP:OD2	2.09	0.52
1:B:400:PRO:HB2	1:B:403:VAL:HB	1.92	0.52
1:A:533:MET:O	1:A:533:MET:HE3	2.10	0.52
1:A:165:LYS:NZ	3:A:602:ATP:O1G	2.43	0.52
1:A:407:VAL:HG23	1:A:452:LEU:O	2.10	0.51
1:A:46:LYS:O	1:A:46:LYS:HE3	2.10	0.51
1:B:310:PRO:HB3	1:B:316:GLU:HB3	1.92	0.51
1:B:101:LEU:HD11	1:B:106:ILE:CD1	2.34	0.51
1:B:354:LYS:O	1:B:358:ARG:HB2	2.11	0.51
1:B:460:ILE:O	1:B:460:ILE:HG23	2.11	0.51
1:B:533:MET:C	1:B:533:MET:HE2	2.30	0.51
1:B:128:MET:CE	1:B:128:MET:HA	2.41	0.51
1:B:213:SER:C	1:B:215:ASP:N	2.64	0.51
1:A:256:GLU:HA	1:A:259:ARG:HG3	1.92	0.51
1:A:207:ILE:CG2	1:A:208:LEU:N	2.74	0.51
1:A:478:SER:O	1:A:482:GLN:HG2	2.10	0.51
1:B:35:ILE:CG2	1:B:35:ILE:O	2.58	0.51
1:B:426:LEU:HB3	1:B:428:ASP:OD1	2.11	0.51
1:A:93:PHE:O	1:A:101:LEU:HB2	2.11	0.51
1:A:391:SER:OG	1:A:415:PRO:HG2	2.10	0.51
1:A:459:ILE:C	1:A:461:HIS:H	2.14	0.51
1:B:360:LEU:HD23	1:B:374:LEU:HB3	1.93	0.51
1:A:128:MET:CE	1:A:128:MET:HA	2.41	0.51
1:A:132:ILE:HG13	1:A:171:GLN:NE2	2.25	0.51
1:A:49:THR:HG22	1:A:50:ARG:H	1.76	0.51
1:B:207:ILE:O	1:B:211:LEU:HG	2.11	0.51
1:A:10:LEU:HD22	1:A:58:LEU:HD21	1.93	0.51
1:A:69:GLY:H	1:A:70:PRO:CD	2.23	0.51
1:B:142:LYS:HE2	1:B:146:GLU:OE2	2.11	0.51
1:B:182:ILE:H	1:B:182:ILE:CD1	2.24	0.51
1:B:449:MET:HA	1:B:450:PRO:C	2.31	0.50
1:B:240:ILE:HG13	1:B:241:ASP:OD1	2.11	0.50
1:B:334:MET:HA	1:B:337:PHE:HD1	1.77	0.50
1:A:218:LEU:HG	1:A:219:ASN:N	2.26	0.50
1:A:368:PRO:HG3	1:B:279:ASN:O	2.11	0.50
1:B:35:ILE:O	1:B:36:PHE:CD2	2.65	0.50
1:B:527:GLU:O	1:B:530:PRO:HD3	2.12	0.50
1:A:248:VAL:CG1	1:A:269:LEU:HD12	2.42	0.50
1:A:532:PHE:HD1	1:A:532:PHE:O	1.95	0.50
1:B:40:HIS:O	1:B:43:LEU:HB3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:O	1:B:116:ASP:C	2.49	0.50
1:B:182:ILE:N	1:B:182:ILE:CD1	2.74	0.50
1:A:4:GLU:OE2	1:A:267:ARG:NH2	2.44	0.50
1:B:364:GLU:HG3	1:B:372:LYS:HB3	1.94	0.50
1:A:327:SER:CB	1:A:457:ASP:HB3	2.42	0.50
1:A:434:LEU:HB3	1:A:454:PHE:CZ	2.47	0.50
1:A:79:ASN:ND2	1:B:34:ASN:C	2.65	0.50
1:B:207:ILE:CG2	1:B:208:LEU:N	2.74	0.49
1:B:401:PRO:HA	1:B:456:ILE:O	2.12	0.49
1:B:187:ILE:HD11	1:B:248:VAL:CG2	2.42	0.49
1:A:1:MET:HE3	1:A:240:ILE:HG22	1.94	0.49
1:A:40:HIS:O	1:A:43:LEU:HB3	2.12	0.49
1:A:529:PHE:N	1:A:530:PRO:HD3	2.27	0.49
1:A:44:ILE:HD11	1:A:60:ILE:HD12	1.93	0.49
1:B:158:HIS:HB2	1:B:275:VAL:HG22	1.94	0.49
1:B:321:LYS:O	1:B:325:LEU:HG	2.12	0.49
1:A:342:PRO:HD2	1:A:347:LYS:HG3	1.94	0.49
1:A:35:ILE:O	1:A:36:PHE:CD2	2.66	0.49
1:A:388:GLU:HB2	1:A:433:ARG:HH21	1.77	0.49
1:B:483:ARG:N	1:B:483:ARG:HD2	2.28	0.49
1:B:532:PHE:HD1	1:B:532:PHE:O	1.95	0.49
1:A:273:ARG:CZ	1:A:380:ARG:HH21	2.24	0.49
1:B:31:GLU:OE1	1:B:38:GLU:HG2	2.12	0.49
1:A:350:GLN:CD	1:B:428:ASP:HB3	2.33	0.49
1:A:380:ARG:C	1:A:382:VAL:H	2.15	0.49
1:B:529:PHE:N	1:B:530:PRO:HD3	2.27	0.49
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.95	0.49
1:A:401:PRO:HA	1:A:456:ILE:O	2.13	0.49
1:B:197:PRO:HD2	1:B:198:LYS:HE2	1.95	0.49
1:B:407:VAL:HG23	1:B:452:LEU:O	2.12	0.49
1:B:414:ILE:HG21	1:B:430:VAL:HG22	1.94	0.49
1:A:128:MET:HE2	1:A:129:THR:N	2.21	0.49
1:A:233:ARG:NH1	1:A:233:ARG:CG	2.69	0.49
1:B:188:VAL:HB	1:B:247:PHE:CD2	2.47	0.49
1:B:69:GLY:H	1:B:70:PRO:CD	2.25	0.49
1:A:360:LEU:HD23	1:A:374:LEU:HB3	1.95	0.49
1:A:484:LEU:HD11	1:A:533:MET:CG	2.29	0.49
1:A:10:LEU:HD13	1:A:58:LEU:CD2	2.42	0.49
1:A:155:LEU:HD23	1:A:286:GLU:O	2.12	0.49
1:B:132:ILE:HG13	1:B:171:GLN:NE2	2.28	0.49
1:B:218:LEU:HG	1:B:219:ASN:N	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ILE:HG12	1:B:410:TRP:CE3	2.48	0.48
1:B:533:MET:CE	1:B:533:MET:O	2.60	0.48
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.13	0.48
1:A:4:GLU:OE2	1:A:244:ASN:ND2	2.46	0.48
1:A:393:LEU:CD1	1:A:464:LEU:HD21	2.43	0.48
1:B:115:LEU:CD2	1:B:116:ASP:H	2.26	0.48
1:B:257:THR:HG22	1:B:258:ILE:HD12	1.93	0.48
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.41	0.48
1:A:150:LEU:HD11	1:A:284:THR:HG21	1.95	0.48
1:A:426:LEU:HB3	1:A:428:ASP:OD1	2.12	0.48
1:B:388:GLU:HB2	1:B:433:ARG:HH21	1.77	0.48
1:A:230:VAL:HG12	1:A:234:MET:HE3	1.96	0.48
1:B:342:PRO:HD2	1:B:347:LYS:CG	2.42	0.48
1:B:13:ALA:O	1:B:17:LEU:HD12	2.14	0.48
1:A:321:LYS:O	1:A:325:LEU:HG	2.13	0.48
1:A:484:LEU:C	1:A:485:LEU:HG	2.34	0.48
1:A:528:ASP:HB2	1:A:529:PHE:CE2	2.48	0.48
1:B:225:HIS:CD2	1:B:225:HIS:O	2.66	0.48
1:B:327:SER:CB	1:B:457:ASP:HB3	2.43	0.48
1:B:273:ARG:CZ	1:B:380:ARG:HH21	2.26	0.48
1:B:528:ASP:HB2	1:B:529:PHE:CE2	2.49	0.48
1:A:104:VAL:HG12	1:A:105:VAL:HG23	1.95	0.48
1:A:164:GLY:HA2	3:A:602:ATP:PA	2.52	0.48
1:A:395:PHE:O	1:A:398:VAL:HG22	2.14	0.48
1:A:533:MET:CE	1:A:533:MET:O	2.61	0.48
1:B:264:LEU:O	1:B:266:LEU:HD23	2.13	0.48
1:B:398:VAL:HG23	1:B:398:VAL:O	2.14	0.48
1:A:167:VAL:HG23	3:A:602:ATP:O1A	2.13	0.48
1:B:205:THR:HA	1:B:231:LEU:HD11	1.95	0.48
1:B:242:ARG:HB3	1:B:245:THR:OG1	2.14	0.48
1:A:533:MET:H	1:A:533:MET:HG3	1.43	0.48
1:A:69:GLY:C	1:A:71:LEU:H	2.18	0.48
1:A:128:MET:HE3	1:A:128:MET:HA	1.95	0.47
1:A:205:THR:O	1:A:209:LEU:HG	2.14	0.47
1:A:213:SER:C	1:A:215:ASP:N	2.66	0.47
1:B:204:PHE:CD1	1:B:204:PHE:N	2.82	0.47
1:A:182:ILE:N	1:A:182:ILE:CD1	2.78	0.47
1:A:483:ARG:HD2	1:A:483:ARG:H	1.80	0.47
1:A:225:HIS:CD2	1:A:225:HIS:O	2.67	0.47
1:A:483:ARG:HD2	1:A:483:ARG:N	2.29	0.47
1:A:242:ARG:HB3	1:A:245:THR:OG1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:CE	1:A:427:ASP:HB2	2.41	0.47
1:B:101:LEU:HD21	1:B:106:ILE:CD1	2.44	0.47
1:B:327:SER:O	1:B:459:ILE:HD11	2.14	0.47
1:B:426:LEU:HB3	1:B:428:ASP:CG	2.34	0.47
1:A:187:ILE:HD11	1:A:248:VAL:CG2	2.44	0.47
1:B:131:TYR:CD2	1:B:301:PHE:HA	2.49	0.47
1:B:203:LEU:C	1:B:203:LEU:HD23	2.35	0.47
1:B:307:MET:HG3	1:B:337:PHE:CD2	2.49	0.47
1:B:434:LEU:HB3	1:B:454:PHE:CZ	2.50	0.47
1:A:143:LYS:O	1:A:147:MET:HG3	2.14	0.47
1:A:426:LEU:HB3	1:A:428:ASP:CG	2.34	0.47
1:B:89:ASP:O	1:B:93:PHE:HD2	1.98	0.47
1:A:397:VAL:O	1:A:399:MET:N	2.48	0.47
1:A:455:LYS:HG2	1:A:456:ILE:N	2.30	0.47
1:A:167:VAL:CG2	3:A:602:ATP:O1A	2.63	0.47
1:A:334:MET:HA	1:A:337:PHE:HD1	1.80	0.47
1:A:434:LEU:HB3	1:A:454:PHE:CE2	2.49	0.47
1:A:479:ILE:HG23	1:A:483:ARG:NH2	2.30	0.47
1:A:204:PHE:O	1:A:231:LEU:HD21	2.14	0.47
1:A:380:ARG:C	1:A:382:VAL:N	2.67	0.47
1:A:35:ILE:CG2	1:A:35:ILE:O	2.61	0.46
1:A:156:PHE:CD1	1:A:287:PHE:CE2	3.03	0.46
1:A:158:HIS:CE1	1:A:289:GLU:HA	2.50	0.46
1:B:69:GLY:C	1:B:71:LEU:H	2.19	0.46
1:B:397:VAL:O	1:B:399:MET:N	2.48	0.46
1:B:84:ALA:O	1:B:88:GLU:HG2	2.15	0.46
1:A:240:ILE:HG13	1:A:241:ASP:OD1	2.16	0.46
1:A:255:GLU:HB3	1:A:277:ILE:HG22	1.96	0.46
1:A:342:PRO:HD2	1:A:347:LYS:CG	2.46	0.46
1:B:479:ILE:HG23	1:B:483:ARG:NH2	2.30	0.46
1:A:188:VAL:HB	1:A:247:PHE:HD2	1.80	0.46
1:A:227:THR:HB	1:A:229:VAL:HG22	1.96	0.46
1:A:374:LEU:HD11	1:A:378:LEU:HG	1.98	0.46
1:A:405:ILE:HG12	1:A:410:TRP:CE3	2.51	0.46
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.67	0.46
1:B:143:LYS:O	1:B:147:MET:HG3	2.14	0.46
1:B:212:LYS:HA	1:B:212:LYS:HD3	1.49	0.46
1:A:160:ARG:HB3	1:A:163:SER:CB	2.40	0.46
1:A:31:GLU:OE1	1:A:38:GLU:HG2	2.15	0.46
1:A:79:ASN:OD1	1:B:34:ASN:O	2.33	0.46
1:A:98:PRO:O	1:A:99:ASP:CB	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD22	1:B:270:VAL:H	1.80	0.46
1:A:182:ILE:H	1:A:182:ILE:CD1	2.28	0.46
1:A:307:MET:HG3	1:A:337:PHE:CD2	2.51	0.46
1:B:192:ASP:OD2	1:B:252:VAL:HG22	2.15	0.46
1:A:107:ALA:N	1:A:108:PRO:CD	2.79	0.46
1:B:233:ARG:O	1:B:233:ARG:HD2	2.16	0.46
1:B:367:THR:C	1:B:369:TYR:H	2.19	0.46
1:A:93:PHE:CB	1:A:101:LEU:HD13	2.37	0.46
1:A:100:LEU:HG	1:A:104:VAL:HG21	1.97	0.46
1:A:207:ILE:O	1:A:211:LEU:HG	2.16	0.46
1:A:212:LYS:HD3	1:A:212:LYS:HA	1.51	0.46
1:A:23:PRO:HG2	1:A:53:ARG:HB3	1.98	0.46
1:A:50:ARG:O	1:A:54:ILE:HG13	2.16	0.46
1:A:164:GLY:CA	3:A:602:ATP:O1A	2.55	0.46
1:B:213:SER:C	1:B:215:ASP:H	2.19	0.46
1:A:128:MET:HE1	1:B:282:SER:HB2	1.96	0.46
1:A:307:MET:HG3	1:A:337:PHE:HD2	1.80	0.45
1:B:187:ILE:HD13	1:B:188:VAL:N	2.31	0.45
1:B:202:ASP:O	1:B:205:THR:HB	2.16	0.45
1:A:118:LYS:HD3	1:A:180:ILE:HG22	1.97	0.45
1:A:224:GLU:OE2	1:A:225:HIS:HB2	2.17	0.45
1:B:197:PRO:HD2	1:B:198:LYS:CG	2.42	0.45
1:B:247:PHE:HB2	1:B:268:CYS:HB3	1.97	0.45
1:B:466:HIS:ND1	1:B:466:HIS:N	2.63	0.45
1:B:483:ARG:H	1:B:483:ARG:HD2	1.81	0.45
1:B:484:LEU:C	1:B:485:LEU:HG	2.36	0.45
1:A:190:LEU:CD1	1:A:207:ILE:HG13	2.47	0.45
1:A:30:LEU:HD22	1:A:35:ILE:HB	1.98	0.45
1:A:393:LEU:HD23	1:A:437:LEU:HD22	1.98	0.45
1:A:89:ASP:O	1:A:93:PHE:HD2	2.00	0.45
1:B:216:ASP:HB3	1:B:219:ASN:CB	2.44	0.45
1:B:374:LEU:HD11	1:B:378:LEU:HG	1.99	0.45
1:A:204:PHE:N	1:A:204:PHE:CD1	2.85	0.45
1:B:150:LEU:HD11	1:B:284:THR:HG21	1.99	0.45
1:A:122:GLY:O	1:A:189:TRP:HB3	2.17	0.45
1:A:216:ASP:HB3	1:A:219:ASN:CB	2.44	0.45
1:B:112:ARG:O	1:B:117:ARG:HG2	2.17	0.45
1:A:115:LEU:O	1:A:118:LYS:N	2.49	0.45
1:A:79:ASN:HD22	1:B:36:PHE:H	1.62	0.45
1:B:533:MET:H	1:B:533:MET:HG3	1.43	0.45
1:B:164:GLY:HA2	3:B:602:ATP:O1A	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:VAL:HG23	1:A:398:VAL:O	2.16	0.45
1:A:61:TYR:HE2	1:A:68:LEU:HD23	1.82	0.45
1:B:204:PHE:O	1:B:231:LEU:HD21	2.17	0.45
1:B:385:LEU:HD23	1:B:385:LEU:N	2.32	0.45
1:B:434:LEU:HB3	1:B:454:PHE:CE2	2.52	0.45
1:A:7:CYS:HB2	1:A:243:PRO:HG2	1.98	0.45
1:B:102:ARG:O	1:B:104:VAL:HG23	2.17	0.45
1:B:197:PRO:HG2	1:B:198:LYS:HE2	1.99	0.45
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.98	0.45
1:A:197:PRO:HG2	1:A:198:LYS:HE2	1.98	0.44
1:A:202:ASP:O	1:A:205:THR:HB	2.17	0.44
1:A:354:LYS:HA	1:A:354:LYS:HD3	1.72	0.44
1:A:487:ILE:HG13	1:A:487:ILE:H	1.50	0.44
1:A:535:LEU:O	1:A:535:LEU:HD23	2.17	0.44
1:B:101:LEU:HD22	1:B:106:ILE:HG13	1.99	0.44
1:B:325:LEU:C	1:B:327:SER:H	2.21	0.44
1:B:334:MET:HA	1:B:337:PHE:CD1	2.52	0.44
1:B:393:LEU:CD1	1:B:464:LEU:HD21	2.47	0.44
1:A:367:THR:C	1:A:369:TYR:H	2.21	0.44
1:A:203:LEU:HD23	1:A:203:LEU:C	2.38	0.44
1:A:307:MET:HA	1:A:308:PRO:HD3	1.60	0.44
1:B:227:THR:HB	1:B:229:VAL:HG22	1.98	0.44
1:A:414:ILE:HA	1:A:415:PRO:HD3	1.78	0.44
1:A:456:ILE:HD13	1:A:461:HIS:HD2	1.83	0.44
1:B:109:GLN:C	1:B:111:SER:N	2.71	0.44
1:B:115:LEU:HD23	1:B:116:ASP:H	1.81	0.44
1:B:21:PHE:HZ	1:B:57:PHE:CD2	2.35	0.44
1:A:115:LEU:O	1:A:116:ASP:C	2.55	0.44
1:A:23:PRO:HG2	1:A:53:ARG:CB	2.48	0.44
1:A:50:ARG:HE	1:A:50:ARG:HB3	1.50	0.44
1:B:158:HIS:CE1	1:B:289:GLU:HA	2.51	0.44
1:B:307:MET:HG3	1:B:337:PHE:HD2	1.80	0.44
1:B:72:ILE:HG21	1:B:88:GLU:CG	2.47	0.44
1:A:216:ASP:HA	1:A:218:LEU:HG	1.99	0.44
1:A:72:ILE:CG2	1:A:84:ALA:HB1	2.47	0.44
1:B:204:PHE:HD1	1:B:204:PHE:H	1.66	0.44
1:B:205:THR:O	1:B:209:LEU:HG	2.17	0.44
1:B:380:ARG:C	1:B:382:VAL:H	2.21	0.44
1:A:385:LEU:HD23	1:A:385:LEU:N	2.33	0.44
1:B:229:VAL:HG23	1:B:230:VAL:N	2.33	0.44
1:B:542:SER:O	1:B:543:LEU:HD22	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:THR:HG22	1:A:258:ILE:HD12	2.00	0.44
1:B:155:LEU:HD23	1:B:286:GLU:O	2.17	0.44
1:B:408:LYS:CE	1:B:427:ASP:HB2	2.45	0.44
1:A:542:SER:O	1:A:543:LEU:HD22	2.17	0.44
1:A:75:PHE:CB	1:A:84:ALA:HB2	2.43	0.44
1:B:395:PHE:O	1:B:398:VAL:HG22	2.18	0.44
1:A:111:SER:HB3	1:A:114:MET:HB2	1.99	0.43
1:A:264:LEU:O	1:A:266:LEU:HD23	2.18	0.43
1:B:189:TRP:HB2	1:B:248:VAL:CG2	2.48	0.43
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.85	0.43
1:B:163:SER:O	1:B:330:PRO:HG2	2.17	0.43
1:B:455:LYS:HG2	1:B:456:ILE:N	2.33	0.43
1:B:525:ARG:HH11	1:B:535:LEU:HD13	1.83	0.43
1:B:68:LEU:HD21	1:B:71:LEU:HB3	1.98	0.43
1:A:210:MET:HB3	1:A:210:MET:HE3	1.91	0.43
1:A:357:SER:O	1:A:358:ARG:HG3	2.18	0.43
1:B:332:THR:HA	1:B:335:MET:SD	2.58	0.43
1:B:49:THR:CG2	1:B:50:ARG:N	2.80	0.43
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.84	0.43
1:A:22:GLU:HA	1:A:23:PRO:HD3	1.83	0.43
1:A:25:ASP:HB3	1:A:78:ASN:HD21	1.82	0.43
1:A:334:MET:HE3	1:A:334:MET:HA	2.00	0.43
1:A:466:HIS:ND1	1:A:466:HIS:N	2.65	0.43
1:A:84:ALA:O	1:A:88:GLU:HG2	2.18	0.43
1:A:128:MET:SD	1:B:282:SER:HB2	2.58	0.43
1:A:214:GLU:O	1:A:216:ASP:N	2.51	0.43
1:A:156:PHE:HD1	1:A:287:PHE:CE2	2.37	0.43
1:A:522:THR:O	1:A:523:VAL:HG23	2.18	0.43
1:A:72:ILE:HG21	1:A:88:GLU:CG	2.46	0.43
1:B:310:PRO:HA	1:B:345:PHE:HZ	1.83	0.43
1:B:354:LYS:HA	1:B:354:LYS:HD3	1.74	0.43
1:B:35:ILE:CD1	1:B:70:PRO:HG2	2.48	0.43
1:A:148:CYS:HA	1:A:184:TYR:CZ	2.53	0.43
1:A:457:ASP:O	1:A:460:ILE:HG22	2.18	0.43
1:A:79:ASN:ND2	1:B:36:PHE:N	2.66	0.43
1:B:23:PRO:HG2	1:B:53:ARG:HB3	2.00	0.43
1:A:197:PRO:HD2	1:A:198:LYS:CG	2.43	0.43
1:A:1:MET:CE	1:A:240:ILE:HG22	2.48	0.43
1:A:161:ALA:HB2	1:A:273:ARG:HD2	2.00	0.43
1:B:148:CYS:HA	1:B:184:TYR:CZ	2.54	0.43
1:B:465:LYS:HD3	1:B:466:HIS:HE1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ARG:CD	1:B:483:ARG:H	2.30	0.43
1:B:525:ARG:HA	1:B:526:PRO:HD3	1.68	0.43
1:A:2:LEU:O	1:A:3:CYS:HB3	2.19	0.43
1:B:380:ARG:C	1:B:382:VAL:N	2.72	0.43
1:B:451:VAL:O	1:B:453:THR:HG23	2.18	0.43
1:B:487:ILE:HG22	1:B:487:ILE:O	2.18	0.43
1:A:233:ARG:HD2	1:A:233:ARG:O	2.19	0.43
1:B:142:LYS:O	1:B:146:GLU:HG3	2.19	0.43
1:B:188:VAL:HB	1:B:247:PHE:HD2	1.84	0.43
1:A:128:MET:CE	1:B:282:SER:HB2	2.48	0.43
1:B:303:GLU:HG3	1:B:309:MET:HE1	2.00	0.43
1:B:318:VAL:O	1:B:318:VAL:CG1	2.66	0.43
1:A:325:LEU:C	1:A:327:SER:H	2.21	0.43
1:A:326:SER:O	1:A:327:SER:C	2.57	0.43
1:A:318:VAL:O	1:A:318:VAL:CG1	2.66	0.42
1:A:435:LYS:NZ	1:A:446:GLY:HA3	2.34	0.42
1:B:102:ARG:O	1:B:104:VAL:N	2.52	0.42
1:B:351:LEU:N	1:B:351:LEU:HD23	2.33	0.42
1:B:522:THR:O	1:B:523:VAL:HG23	2.19	0.42
1:B:535:LEU:O	1:B:535:LEU:HD23	2.19	0.42
1:B:72:ILE:C	1:B:74:PHE:H	2.22	0.42
1:A:158:HIS:CE1	1:A:289:GLU:HB2	2.54	0.42
1:A:259:ARG:HG2	1:A:280:ALA:HB1	2.01	0.42
1:A:7:CYS:CB	1:A:243:PRO:HG2	2.49	0.42
1:B:114:MET:C	1:B:114:MET:CE	2.87	0.42
1:B:39:ASP:O	1:B:43:LEU:CB	2.66	0.42
1:A:112:ARG:HH12	1:A:115:LEU:HD12	1.82	0.42
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.82	0.42
1:B:61:TYR:HE2	1:B:68:LEU:HD23	1.83	0.42
1:A:378:LEU:O	1:A:379:GLN:C	2.56	0.42
3:A:602:ATP:O1B	3:A:602:ATP:O2G	2.37	0.42
1:B:310:PRO:HA	1:B:345:PHE:CZ	2.55	0.42
1:B:406:PRO:CA	1:B:453:THR:HG22	2.47	0.42
1:A:122:GLY:CA	1:A:187:ILE:O	2.67	0.42
1:A:479:ILE:HG23	1:A:483:ARG:HH22	1.84	0.42
1:B:134:GLU:O	1:B:135:TYR:C	2.57	0.42
1:B:29:TYR:CE2	1:B:33:LYS:HD2	2.54	0.42
1:A:247:PHE:HB2	1:A:268:CYS:HB3	2.02	0.42
1:B:357:SER:O	1:B:358:ARG:HG3	2.18	0.42
1:A:334:MET:HA	1:A:337:PHE:CD1	2.55	0.42
1:A:366:ILE:HG22	1:A:366:ILE:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:O	1:A:439:LYS:N	2.47	0.42
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.69	0.42
1:B:44:ILE:HD11	1:B:60:ILE:HD12	2.01	0.42
1:A:406:PRO:CA	1:A:453:THR:HG22	2.45	0.42
1:A:483:ARG:CD	1:A:483:ARG:H	2.32	0.42
1:A:97:GLU:OE1	1:A:100:LEU:HD23	2.19	0.42
1:A:310:PRO:HA	1:A:345:PHE:HZ	1.84	0.42
1:A:404:ASP:O	1:A:524:ILE:HD13	2.19	0.42
1:B:101:LEU:CD2	1:B:106:ILE:HG13	2.50	0.42
1:B:141:ILE:HD13	1:B:176:SER:HB3	2.02	0.42
1:B:307:MET:HA	1:B:308:PRO:HD3	1.61	0.42
1:B:327:SER:N	1:B:459:ILE:HG12	2.34	0.42
1:A:527:GLU:OE1	1:A:527:GLU:N	2.51	0.41
1:A:530:PRO:O	1:A:532:PHE:N	2.53	0.41
1:A:72:ILE:C	1:A:74:PHE:H	2.22	0.41
1:B:30:LEU:HB3	1:B:36:PHE:CD2	2.55	0.41
1:B:72:ILE:CG2	1:B:84:ALA:HB1	2.48	0.41
1:A:374:LEU:O	1:A:375:ALA:C	2.58	0.41
1:A:79:ASN:HD22	1:B:36:PHE:N	2.19	0.41
1:B:158:HIS:CE1	1:B:289:GLU:HB2	2.55	0.41
1:B:122:GLY:O	1:B:189:TRP:HB3	2.20	0.41
1:B:161:ALA:HB2	1:B:273:ARG:HD2	2.02	0.41
1:B:342:PRO:O	1:B:343:LYS:HB2	2.21	0.41
1:B:458:HIS:O	1:B:461:HIS:HB3	2.21	0.41
1:B:49:THR:CG2	1:B:50:ARG:H	2.32	0.41
1:A:269:LEU:HD22	1:A:270:VAL:H	1.85	0.41
1:A:343:LYS:O	1:A:343:LYS:HG2	2.21	0.41
1:A:525:ARG:HH11	1:A:535:LEU:HD13	1.86	0.41
1:A:71:LEU:HD11	1:A:75:PHE:HE1	1.85	0.41
1:B:113:GLN:OE1	1:B:113:GLN:HA	2.19	0.41
1:A:189:TRP:HB2	1:A:248:VAL:HG23	2.03	0.41
1:B:2:LEU:O	1:B:3:CYS:HB3	2.20	0.41
1:A:134:GLU:O	1:A:135:TYR:C	2.57	0.41
1:A:219:ASN:O	1:A:220:PHE:C	2.59	0.41
1:A:154:PHE:CE1	1:A:283:GLN:NE2	2.89	0.41
1:A:487:ILE:HG22	1:A:487:ILE:O	2.21	0.41
1:A:527:GLU:CD	1:A:527:GLU:N	2.74	0.41
1:A:237:ASN:O	1:A:239:LEU:N	2.53	0.41
1:A:79:ASN:HD21	1:B:34:ASN:HA	1.85	0.41
1:A:99:ASP:C	1:A:101:LEU:H	2.22	0.41
1:B:23:PRO:HG2	1:B:53:ARG:CB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:MET:HE3	1:B:334:MET:HA	2.01	0.41
1:A:102:ARG:HB2	1:A:103:PRO:HD3	2.02	0.41
1:A:204:PHE:H	1:A:204:PHE:HD1	1.69	0.41
1:A:283:GLN:O	1:A:285:CYS:N	2.54	0.41
1:A:23:PRO:CG	1:A:53:ARG:O	2.69	0.41
1:B:127:GLN:HA	1:B:170:SER:OG	2.21	0.41
1:B:122:GLY:CA	1:B:187:ILE:O	2.67	0.41
1:B:326:SER:O	1:B:327:SER:C	2.59	0.41
1:B:393:LEU:HD12	1:B:464:LEU:HD21	2.03	0.41
1:A:213:SER:C	1:A:215:ASP:H	2.23	0.41
1:A:310:PRO:HA	1:A:345:PHE:CZ	2.56	0.41
1:B:25:ASP:HB3	1:B:78:ASN:HD21	1.86	0.41
1:B:479:ILE:HG23	1:B:483:ARG:HH22	1.86	0.41
1:A:228:SER:O	1:A:232:LYS:HG3	2.21	0.41
1:B:189:TRP:C	1:B:189:TRP:CD1	2.95	0.41
1:B:541:ASP:O	1:B:543:LEU:N	2.48	0.41
1:A:110:PHE:C	1:A:110:PHE:CD2	2.94	0.41
1:A:35:ILE:CD1	1:A:70:PRO:HG2	2.51	0.41
1:B:216:ASP:HA	1:B:218:LEU:HG	2.02	0.41
1:B:224:GLU:OE2	1:B:225:HIS:HB2	2.20	0.41
1:B:330:PRO:O	1:B:333:LEU:HB2	2.21	0.41
1:B:374:LEU:HD12	1:B:378:LEU:CD1	2.50	0.41
1:B:527:GLU:N	1:B:527:GLU:OE1	2.54	0.41
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.95	0.40
1:A:342:PRO:O	1:A:343:LYS:HB2	2.21	0.40
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.78	0.40
1:A:119:LEU:CB	1:B:265:ARG:HH12	2.32	0.40
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.81	0.40
1:A:1:MET:HE2	1:A:240:ILE:HB	2.03	0.40
1:A:374:LEU:HD12	1:A:378:LEU:CD1	2.51	0.40
1:A:68:LEU:HD21	1:A:71:LEU:HB3	2.04	0.40
1:B:106:ILE:O	1:B:106:ILE:CG2	2.69	0.40
1:B:154:PHE:CE1	1:B:283:GLN:NE2	2.89	0.40
1:B:69:GLY:N	1:B:70:PRO:CD	2.85	0.40
1:A:157:LEU:HA	1:A:157:LEU:HD23	1.75	0.40
1:A:528:ASP:C	1:A:530:PRO:HD3	2.42	0.40
1:B:365:CYS:SG	1:B:366:ILE:N	2.92	0.40
1:B:444:LEU:HD12	1:B:444:LEU:N	2.36	0.40
1:B:477:ILE:HD11	1:B:543:LEU:HG	2.03	0.40
1:B:527:GLU:CD	1:B:527:GLU:N	2.75	0.40
1:B:201:PHE:CD2	1:B:201:PHE:C	2.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:VAL:HG13	1:B:269:LEU:HD12	2.03	0.40
1:B:23:PRO:CG	1:B:53:ARG:O	2.69	0.40
1:A:359:GLY:HA2	1:A:462:MET:HB3	2.03	0.40
1:B:179:LEU:HA	1:B:179:LEU:HD12	1.87	0.40
1:B:283:GLN:O	1:B:285:CYS:N	2.53	0.40
1:B:435:LYS:HZ2	1:B:446:GLY:HA3	1.87	0.40
1:B:47:MET:CB	1:B:53:ARG:HG3	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/549 (90%)	364 (73%)	87 (18%)	46 (9%)	0	12
1	B	495/549 (90%)	359 (72%)	91 (18%)	45 (9%)	1	12
All	All	992/1098 (90%)	723 (73%)	178 (18%)	91 (9%)	1	12

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	343	LYS
1	A	398	VAL
1	A	452	LEU
1	A	484	LEU
1	A	485	LEU
1	A	486	GLU
1	B	109	GLN
1	B	116	ASP
1	B	327	SER
1	B	343	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	398	VAL
1	B	452	LEU
1	B	484	LEU
1	B	485	LEU
1	B	486	GLU
1	A	99	ASP
1	A	115	LEU
1	A	116	ASP
1	A	134	GLU
1	A	215	ASP
1	A	238	ALA
1	A	284	THR
1	A	306	GLY
1	A	442	ALA
1	A	460	ILE
1	A	465	LYS
1	B	104	VAL
1	B	115	LEU
1	B	134	GLU
1	B	215	ASP
1	B	238	ALA
1	B	284	THR
1	B	306	GLY
1	B	442	ALA
1	B	460	ILE
1	B	465	LYS
1	A	21	PHE
1	A	106	ILE
1	A	135	TYR
1	A	237	ASN
1	A	251	ASP
1	A	372	LYS
1	A	425	GLN
1	A	439	LYS
1	A	445	SER
1	A	522	THR
1	A	531	LYS
1	B	21	PHE
1	B	103	PRO
1	B	135	TYR
1	B	237	ASN
1	B	251	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	439	LYS
1	B	445	SER
1	B	531	LYS
1	A	33	LYS
1	A	150	LEU
1	A	152	SER
1	A	182	ILE
1	A	364	GLU
1	A	542	SER
1	B	33	LYS
1	B	152	SER
1	B	182	ILE
1	B	364	GLU
1	B	372	LYS
1	B	522	THR
1	B	542	SER
1	A	70	PRO
1	A	212	LYS
1	A	358	ARG
1	A	530	PRO
1	B	70	PRO
1	B	150	LEU
1	B	212	LYS
1	B	530	PRO
1	A	69	GLY
1	A	213	SER
1	A	368	PRO
1	B	69	GLY
1	B	358	ARG
1	B	368	PRO
1	B	102	ARG
1	A	194	GLY
1	A	467	VAL
1	B	397	VAL
1	B	467	VAL
1	A	397	VAL
1	A	450	PRO
1	B	450	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/501 (91%)	379 (83%)	79 (17%)	2	14
1	B	456/501 (91%)	374 (82%)	82 (18%)	1	12
All	All	914/1002 (91%)	753 (82%)	161 (18%)	2	13

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	42	GLU
1	A	46	LYS
1	A	50	ARG
1	A	64	GLN
1	A	67	GLU
1	A	77	TYR
1	A	79	ASN
1	A	110	PHE
1	A	112	ARG
1	A	116	ASP
1	A	128	MET
1	A	135	TYR
1	A	150	LEU
1	A	151	ASP
1	A	155	LEU
1	A	157	LEU
1	A	167	VAL
1	A	179	LEU
1	A	185	ASP
1	A	187	ILE
1	A	189	TRP
1	A	198	LYS
1	A	204	PHE
1	A	207	ILE
1	A	218	LEU
1	A	219	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	224	GLU
1	A	227	THR
1	A	228	SER
1	A	233	ARG
1	A	248	VAL
1	A	253	VAL
1	A	269	LEU
1	A	271	THR
1	A	273	ARG
1	A	284	THR
1	A	296	ASP
1	A	309	MET
1	A	315	GLU
1	A	316	GLU
1	A	319	LEU
1	A	332	THR
1	A	336	PHE
1	A	344	THR
1	A	355	LEU
1	A	360	LEU
1	A	363	VAL
1	A	369	TYR
1	A	370	SER
1	A	374	LEU
1	A	381	CYS
1	A	389	ASP
1	A	393	LEU
1	A	395	PHE
1	A	399	MET
1	A	404	ASP
1	A	405	ILE
1	A	408	LYS
1	A	409	LEU
1	A	410	TRP
1	A	425	GLN
1	A	428	ASP
1	A	452	LEU
1	A	457	ASP
1	A	459	ILE
1	A	460	ILE
1	A	462	MET
1	A	466	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	484	LEU
1	A	485	LEU
1	A	521	GLU
1	A	529	PHE
1	A	530	PRO
1	A	532	PHE
1	A	533	MET
1	A	534	GLN
1	A	538	LYS
1	A	543	LEU
1	B	1	MET
1	B	42	GLU
1	B	46	LYS
1	B	50	ARG
1	B	64	GLN
1	B	67	GLU
1	B	77	TYR
1	B	79	ASN
1	B	99	ASP
1	B	109	GLN
1	B	112	ARG
1	B	114	MET
1	B	115	LEU
1	B	116	ASP
1	B	121	LEU
1	B	128	MET
1	B	135	TYR
1	B	150	LEU
1	B	151	ASP
1	B	155	LEU
1	B	157	LEU
1	B	167	VAL
1	B	179	LEU
1	B	185	ASP
1	B	187	ILE
1	B	189	TRP
1	B	198	LYS
1	B	204	PHE
1	B	207	ILE
1	B	218	LEU
1	B	219	ASN
1	B	224	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	227	THR
1	B	228	SER
1	B	233	ARG
1	B	248	VAL
1	B	253	VAL
1	B	257	THR
1	B	269	LEU
1	B	271	THR
1	B	273	ARG
1	B	284	THR
1	B	296	ASP
1	B	309	MET
1	B	315	GLU
1	B	316	GLU
1	B	319	LEU
1	B	332	THR
1	B	336	PHE
1	B	344	THR
1	B	355	LEU
1	B	360	LEU
1	B	363	VAL
1	B	369	TYR
1	B	370	SER
1	B	374	LEU
1	B	381	CYS
1	B	389	ASP
1	B	393	LEU
1	B	395	PHE
1	B	399	MET
1	B	404	ASP
1	B	405	ILE
1	B	408	LYS
1	B	409	LEU
1	B	410	TRP
1	B	428	ASP
1	B	452	LEU
1	B	457	ASP
1	B	459	ILE
1	B	460	ILE
1	B	462	MET
1	B	466	HIS
1	B	484	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	485	LEU
1	B	521	GLU
1	B	529	PHE
1	B	532	PHE
1	B	533	MET
1	B	534	GLN
1	B	538	LYS
1	B	543	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	40	HIS
1	A	64	GLN
1	A	79	ASN
1	A	123	ASN
1	A	158	HIS
1	A	171	GLN
1	A	219	ASN
1	A	225	HIS
1	A	283	GLN
1	A	461	HIS
1	A	471	GLN
1	A	475	ASN
1	A	534	GLN
1	B	34	ASN
1	B	40	HIS
1	B	64	GLN
1	B	123	ASN
1	B	158	HIS
1	B	171	GLN
1	B	219	ASN
1	B	225	HIS
1	B	244	ASN
1	B	461	HIS
1	B	471	GLN
1	B	475	ASN
1	B	534	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	B	602	2	26,33,33	1.11	3 (11%)	31,52,52	1.67	7 (22%)
3	ATP	A	602	2	26,33,33	1.08	3 (11%)	31,52,52	1.79	9 (29%)

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	B	602	2	-	7/18/38/38	0/3/3/3
3	ATP	A	602	2	-	7/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ATP	C5-C4	3.03	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ATP	C5-C4	2.85	1.48	1.40
3	B	602	ATP	O4'-C1'	2.46	1.44	1.41
3	A	602	ATP	O4'-C1'	2.41	1.44	1.41
3	B	602	ATP	C2-N3	2.34	1.35	1.32
3	A	602	ATP	C2-N3	2.19	1.35	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ATP	PB-O3B-PG	-5.32	114.57	132.83
3	B	602	ATP	PA-O3A-PB	-3.74	119.99	132.83
3	B	602	ATP	C1'-N9-C4	3.40	132.62	126.64
3	A	602	ATP	N3-C2-N1	-3.26	123.58	128.68
3	B	602	ATP	N3-C2-N1	-2.98	124.02	128.68
3	B	602	ATP	PB-O3B-PG	-2.87	122.98	132.83
3	A	602	ATP	C4-C5-N7	-2.59	106.70	109.40
3	A	602	ATP	PA-O3A-PB	-2.46	124.39	132.83
3	A	602	ATP	C3'-C2'-C1'	2.45	104.67	100.98
3	B	602	ATP	O3G-PG-O3B	-2.43	96.48	104.64
3	A	602	ATP	O4'-C1'-C2'	-2.43	103.37	106.93
3	A	602	ATP	O3G-PG-O2G	2.40	116.81	107.64
3	B	602	ATP	C4-C5-N7	-2.10	107.21	109.40
3	A	602	ATP	O5'-C5'-C4'	-2.10	101.78	108.99
3	B	602	ATP	N6-C6-N1	2.03	122.79	118.57
3	A	602	ATP	O5'-PA-O1A	-2.02	101.16	109.07

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	ATP	C5'-O5'-PA-O1A
3	B	602	ATP	C5'-O5'-PA-O2A
3	B	602	ATP	C3'-C4'-C5'-O5'
3	A	602	ATP	C5'-O5'-PA-O2A
3	A	602	ATP	C5'-O5'-PA-O3A
3	A	602	ATP	O4'-C4'-C5'-O5'
3	A	602	ATP	C3'-C4'-C5'-O5'
3	B	602	ATP	O4'-C4'-C5'-O5'
3	B	602	ATP	PA-O3A-PB-O1B
3	A	602	ATP	PA-O3A-PB-O1B
3	A	602	ATP	C5'-O5'-PA-O1A
3	B	602	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

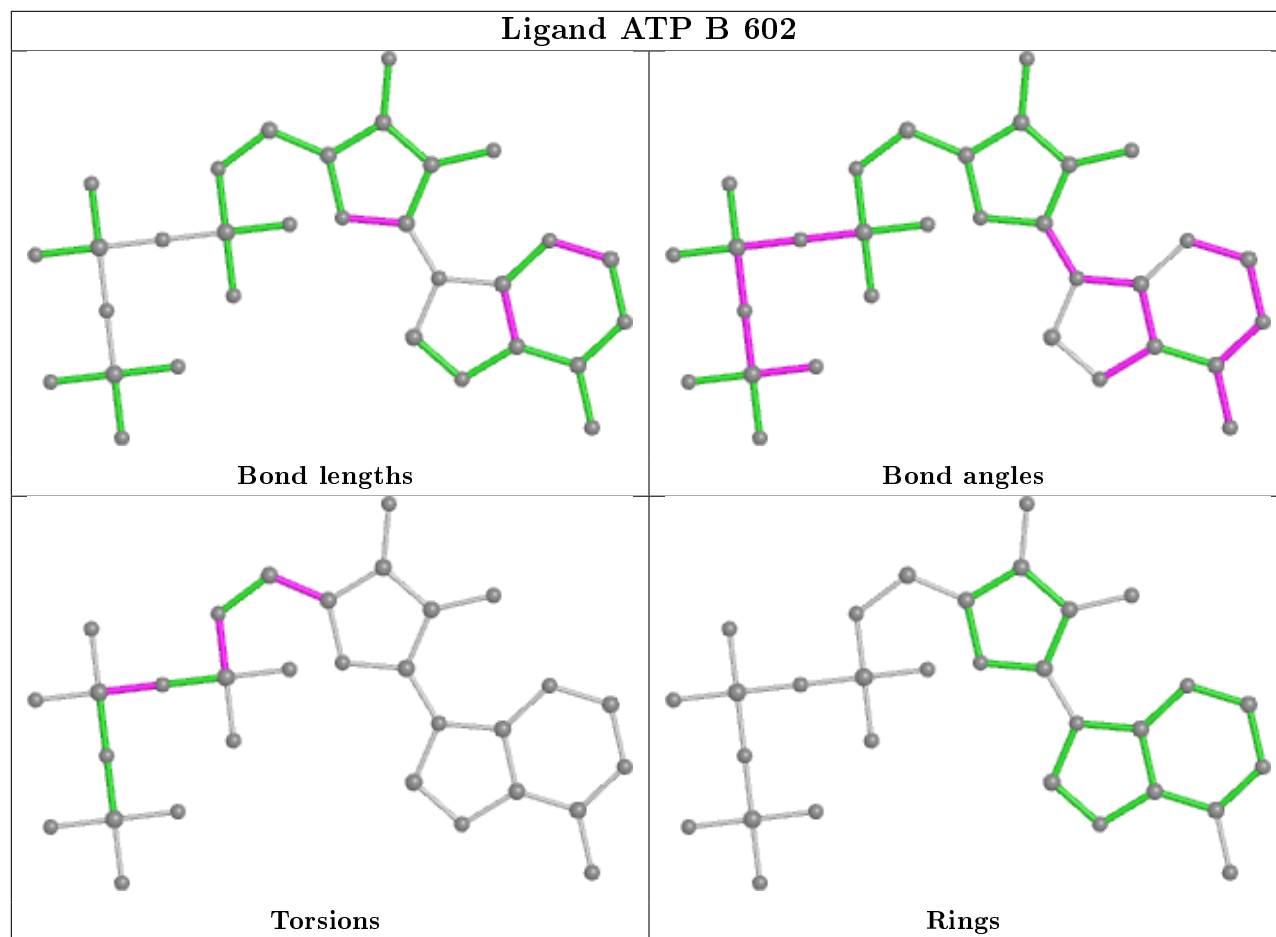
Mol	Chain	Res	Type	Atoms
3	B	602	ATP	PA-O3A-PB-O2B
3	A	602	ATP	PA-O3A-PB-O2B

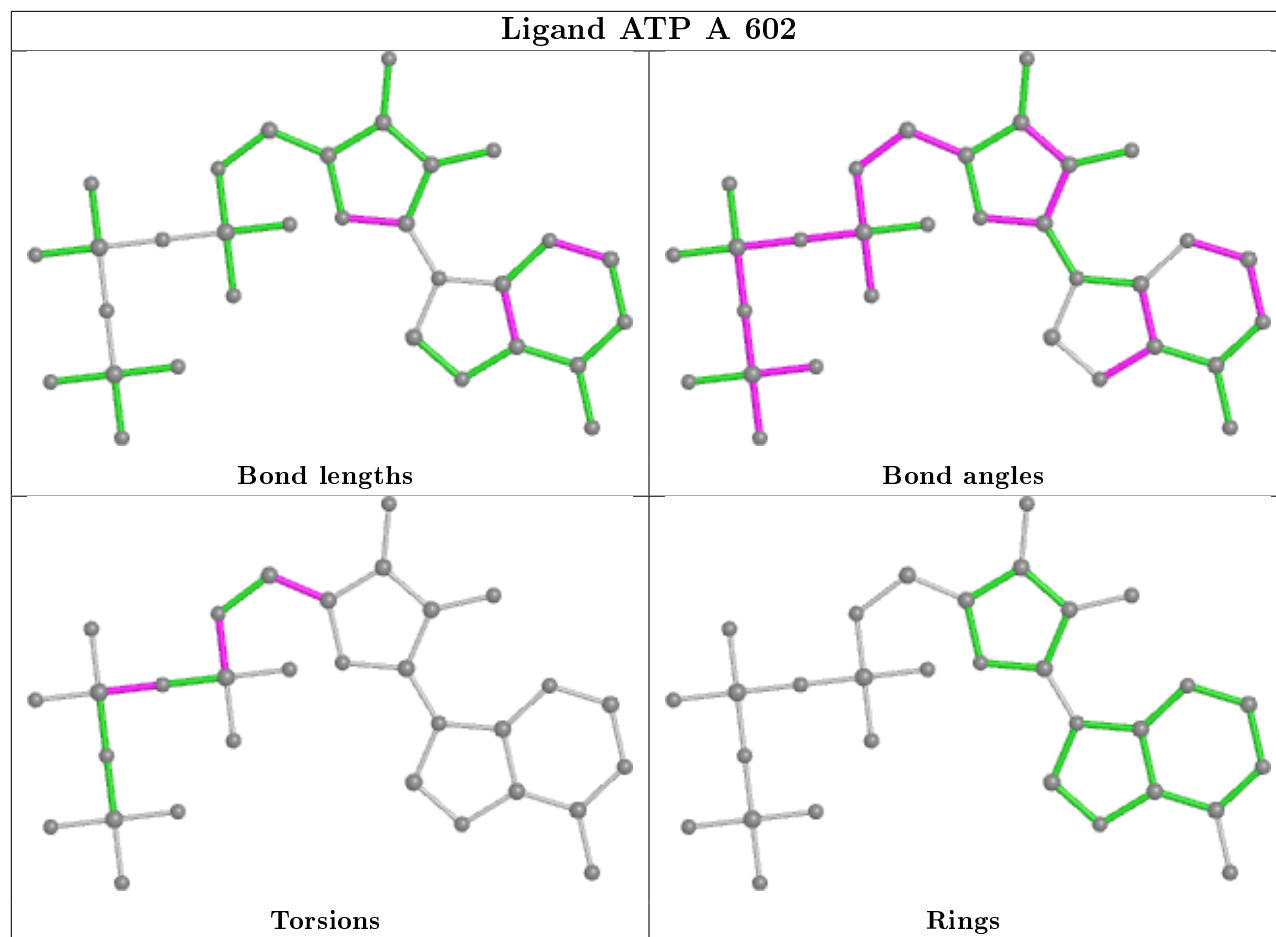
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	ATP	4	0
3	A	602	ATP	10	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	503/549 (91%)	-0.05	11 (2%) 62 51	120, 188, 268, 332	0
1	B	501/549 (91%)	0.04	25 (4%) 28 24	121, 188, 270, 362	0
All	All	1004/1098 (91%)	-0.01	36 (3%) 42 33	120, 188, 269, 362	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	4.9
1	B	100	LEU	4.6
1	B	56	ASN	4.1
1	A	177	ASP	3.9
1	A	66	SER	3.8
1	B	51	LEU	3.6
1	B	105	VAL	3.6
1	B	94	ALA	3.4
1	B	308	PRO	3.1
1	B	521	GLU	3.0
1	B	92	ASP	3.0
1	B	61	TYR	2.8
1	B	90	TYR	2.8
1	B	36	PHE	2.7
1	B	65	ALA	2.7
1	B	96	ASN	2.7
1	B	95	ILE	2.7
1	B	72	ILE	2.5
1	B	6	GLU	2.5
1	A	102	ARG	2.5
1	B	97	GLU	2.5
1	B	87	LEU	2.4
1	A	310	PRO	2.4
1	B	91	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	313	GLU	2.3
1	B	64	GLN	2.3
1	A	28	THR	2.3
1	A	33	LYS	2.2
1	B	68	LEU	2.2
1	A	106	ILE	2.2
1	B	60	ILE	2.2
1	B	284	THR	2.1
1	A	27	LEU	2.1
1	A	45	SER	2.1
1	B	52	GLU	2.0
1	B	82	HIS	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](#)

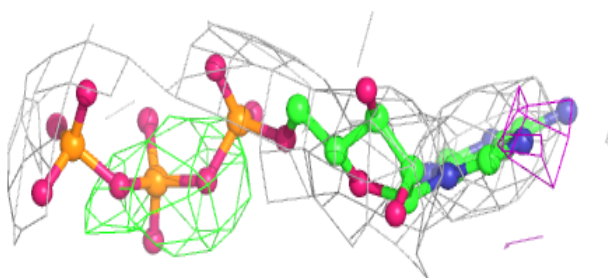
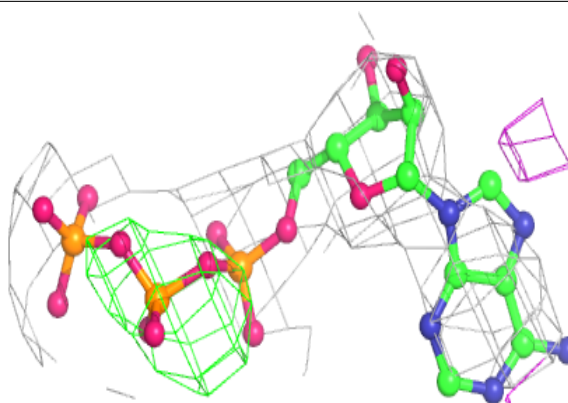
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	602	31/31	0.95	0.29	95,155,196,334	0
3	ATP	A	602	31/31	0.96	0.26	109,150,189,351	0
2	MG	A	601	1/1	0.97	0.27	120,120,120,120	0
2	MG	B	601	1/1	0.98	0.22	104,104,104,104	0

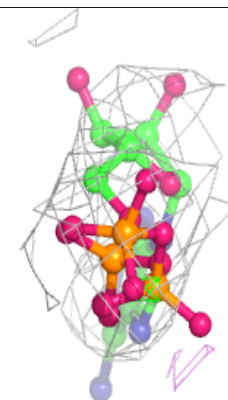
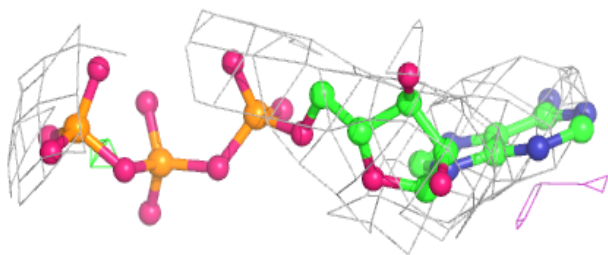
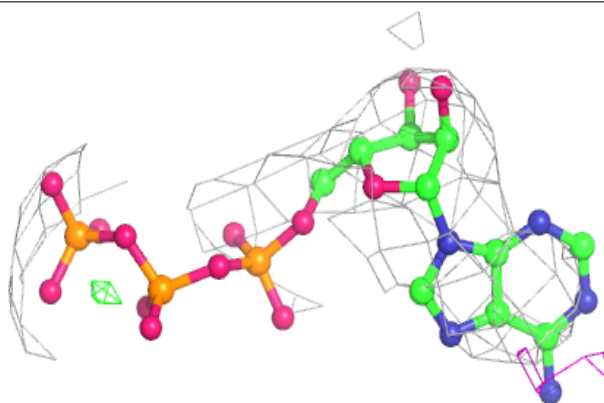
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP A 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.