



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2024 – 10:18 PM EST

PDB ID : 2F43  
Title : Rat liver F1-ATPase  
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Deposited on : 2005-11-22  
Resolution : 3.00 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

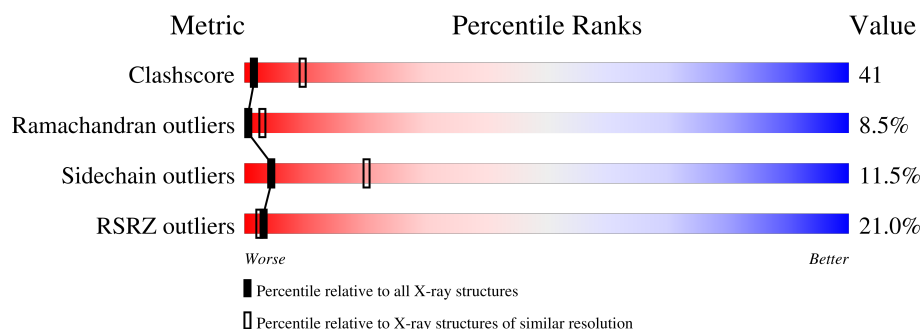
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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  $\geq 3$ , 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	510	
2	B	479	
3	G	273	

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
6	VO4	B	601	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8234 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 synthase alpha chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	13	0
			3659	2301	648	698	12			

- Molecule 2 is a protein called ATP synthase beta chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	471	Total	C	N	O	S	0	20	0
			3556	2253	603	688	12			

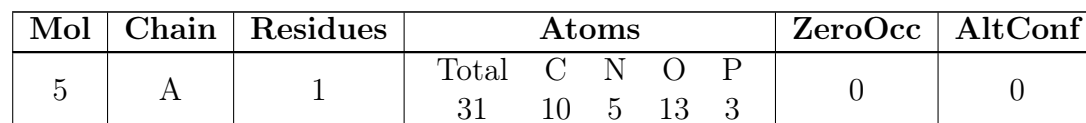
- Molecule 3 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	124	Total	C	N	O	S	0	0	0
			954	592	173	182	7			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	V	0	0
			5	4	1		

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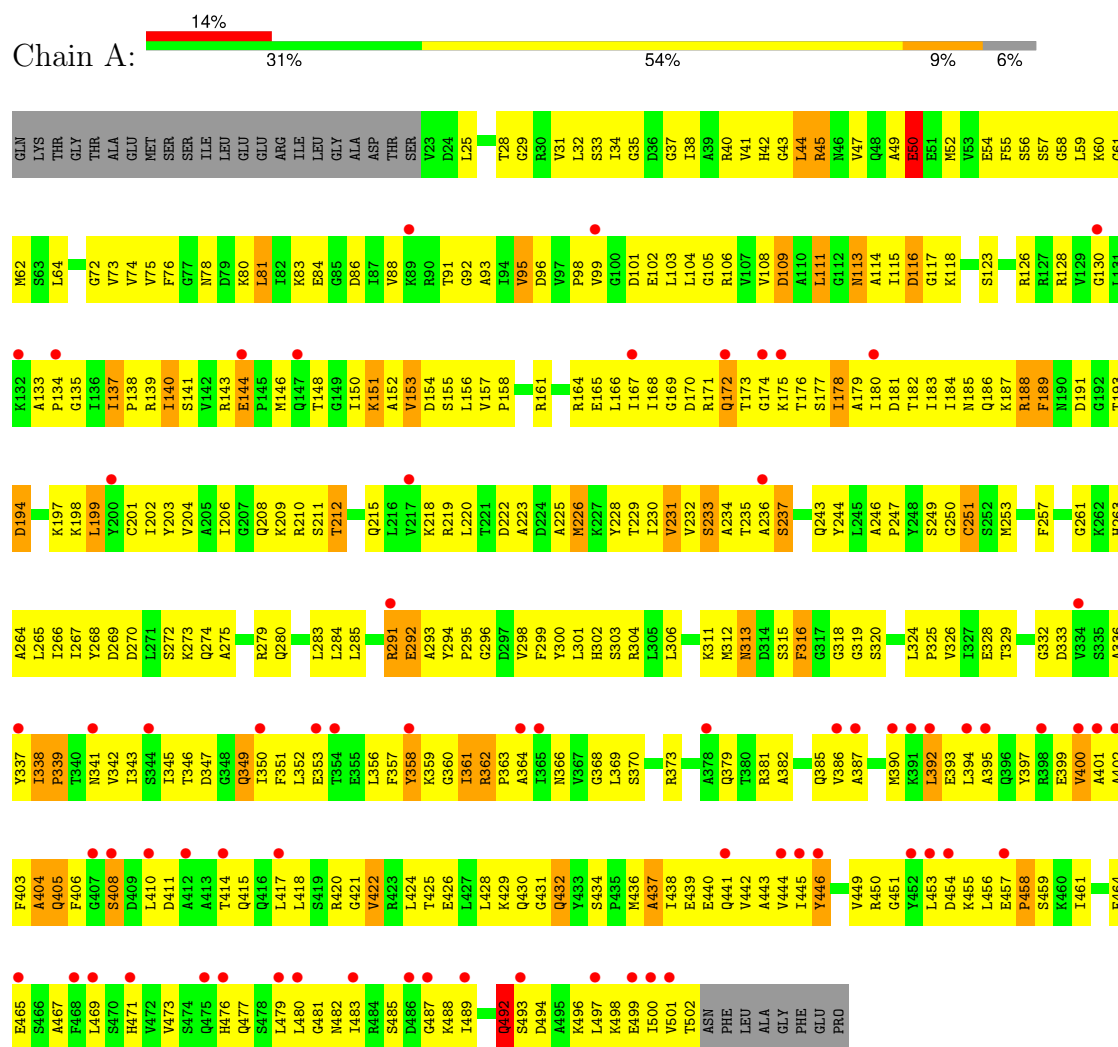


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

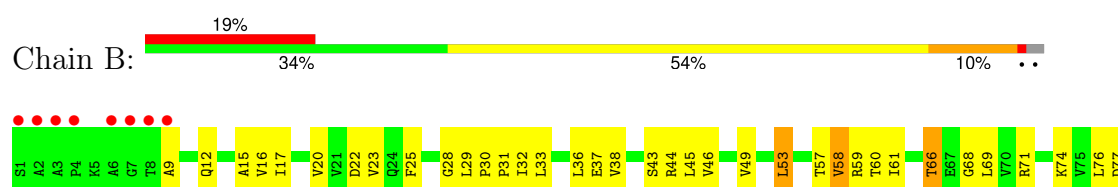
### 3 Residue-property plots

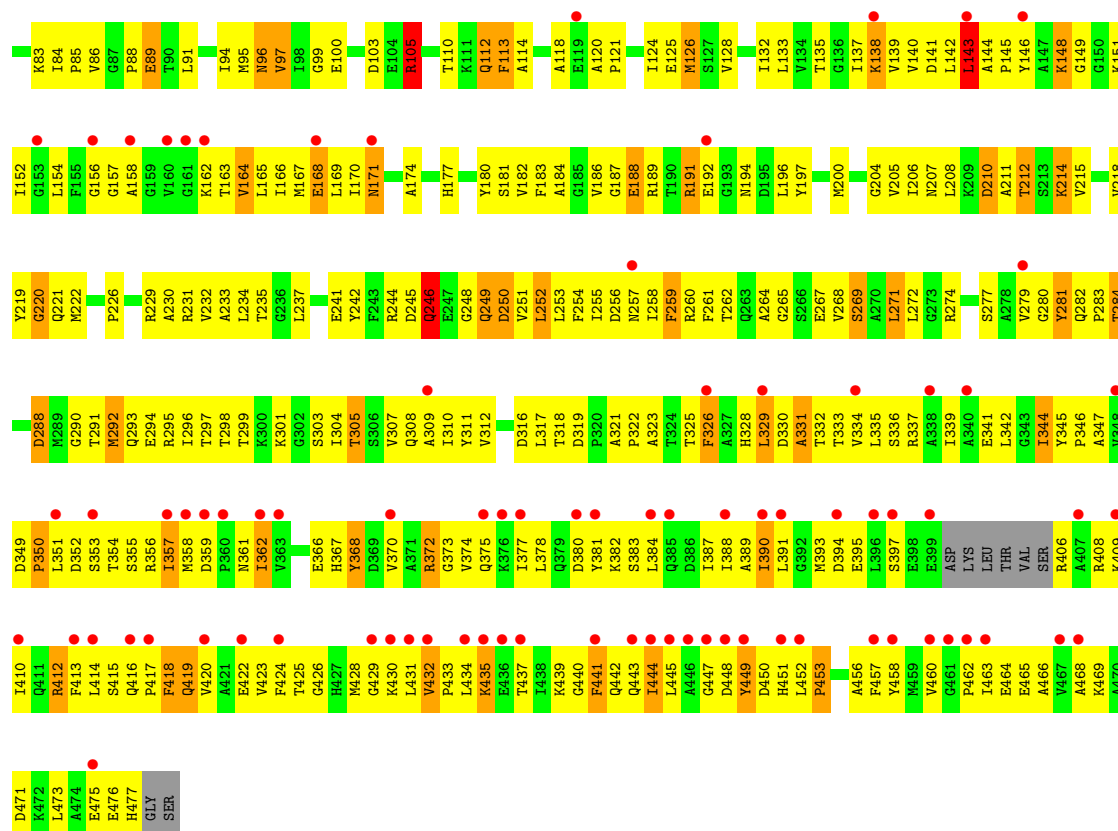
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: ATP synthase alpha chain, mitochondrial

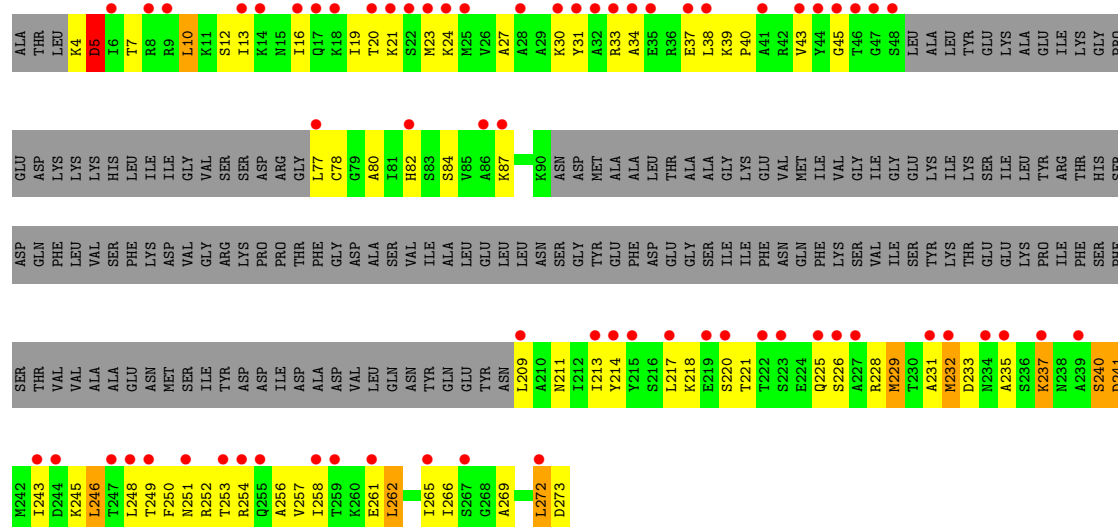


- Molecule 2: ATP synthase beta chain, mitochondrial





● Molecule 3: ATP synthase gamma chain, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.57Å 144.57Å 362.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.97-3.00) 95.8 (19.97-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.306 , 0.320 0.308 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.3	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 86.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.023 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.023 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	8234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, ADP, ATP, MG

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	0.89	0/3708	1.03	2/5003 (0.0%)
2	B	0.90	0/3615	1.01	4/4903 (0.1%)
3	G	0.62	0/958	0.87	1/1276 (0.1%)
All	All	0.87	0/8281	1.01	7/11182 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	246	LEU	CA-CB-CG	8.23	134.23	115.30
1	A	210	ARG	NE-CZ-NH1	-6.19	117.20	120.30
2	B	191	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	61	GLY	N-CA-C	-5.96	98.19	113.10
2	B	244	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	220	GLY	N-CA-C	-5.20	100.09	113.10
2	B	274	ARG	NE-CZ-NH2	-5.20	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3659	0	3761	330	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3556	0	3600	306	0
3	G	954	0	1013	68	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	12	3	0
6	B	5	0	0	2	0
7	B	27	0	12	3	0
All	All	8234	0	8398	689	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 41.

All (689) 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)
3:G:233:ASP:O	3:G:237:LYS:HD3	1.58	1.03
2:B:137:ILE:HG23	2:B:416:GLN:HE22	1.23	1.01
1:A:137:ILE:HD13	1:A:137:ILE:H	1.24	1.00
2:B:271:LEU:HD23	2:B:271:LEU:H	1.31	0.95
3:G:233:ASP:OD2	3:G:237:LYS:NZ	2.04	0.90
2:B:158:ALA:HB2	2:B:311:TYR:HE1	1.37	0.90
2:B:188:GLU:OE2	6:B:601:VO4:O2	1.91	0.87
2:B:310:ILE:HG12	2:B:325:THR:HG21	1.55	0.87
1:A:270:ASP:H	1:A:326:VAL:HB	1.39	0.87
1:A:148:THR:HA	1:A:182:THR:HG23	1.57	0.86
2:B:326:PHE:HA	2:B:329:LEU:HD21	1.58	0.86
2:B:137:ILE:HG23	2:B:416:GLN:NE2	1.89	0.85
2:B:167:MET:HA	2:B:170:ILE:HD12	1.59	0.84
2:B:166:ILE:HA	2:B:169:LEU:HD12	1.58	0.84
1:A:96:ASP:HA	1:A:128:ARG:HA	1.57	0.84
2:B:38:VAL:HG21	2:B:45:LEU:HD23	1.62	0.81
1:A:283:LEU:HD12	2:B:283:PRO:HB3	1.60	0.81
1:A:476:HIS:HB3	1:A:479:LEU:HD13	1.62	0.81
2:B:156:GLY:H	2:B:162:LYS:HE3	1.46	0.81
1:A:386:VAL:HG11	1:A:446:TYR:HB2	1.63	0.81
1:A:59:LEU:HD11	1:A:76:PHE:O	1.82	0.79
1:A:175:LYS:HG2	1:A:352:LEU:HD12	1.63	0.79
3:G:240:SER:O	3:G:243:ILE:N	2.13	0.79
2:B:37:GLU:HB2	2:B:76:LEU:HB3	1.64	0.78
1:A:140:ILE:HG23	1:A:141:SER:H	1.48	0.78
2:B:142:LEU:HG	2:B:367:HIS:NE2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:VAL:HG23	2:B:112:GLN:HE21	1.48	0.77
1:A:137:ILE:H	1:A:137:ILE:CD1	1.97	0.77
2:B:408:ARG:HD2	2:B:412:ARG:HH22	1.49	0.77
2:B:133:LEU:HD13	2:B:148:LYS:HE3	1.66	0.76
2:B:105:ARG:HH21	2:B:208:LEU:HB3	1.50	0.76
1:A:148:THR:HG21	1:A:153:VAL:HG11	1.65	0.76
1:A:397:TYR:HE1	1:A:418:LEU:HA	1.51	0.76
2:B:390[A]:ILE:HD12	3:G:77:LEU:HD21	1.68	0.76
2:B:317:LEU:HD11	2:B:334:VAL:HG11	1.68	0.75
2:B:259:PHE:CE1	2:B:311:TYR:HB3	2.20	0.75
2:B:200:MET:SD	2:B:215:VAL:HG21	2.27	0.75
2:B:299:THR:HG23	2:B:301:LYS:H	1.51	0.74
1:A:49:ALA:O	1:A:50:GLU:HB2	1.85	0.74
1:A:301:LEU:HA	1:A:304:ARG:HH21	1.52	0.74
2:B:368:TYR:O	2:B:372:ARG:HG2	1.88	0.74
1:A:394:LEU:HA	1:A:397:TYR:HB3	1.70	0.74
2:B:66:THR:HG22	2:B:69:LEU:HD12	1.67	0.74
2:B:157:GLY:HA2	2:B:312:VAL:HB	1.69	0.74
2:B:9:ALA:HB1	2:B:77:ASP:HB3	1.70	0.74
3:G:232:MET:SD	3:G:232:MET:N	2.61	0.73
3:G:248:LEU:O	3:G:252:ARG:NH1	2.21	0.73
3:G:250:PHE:O	3:G:254:ARG:N	2.20	0.73
1:A:403[A]:PHE:O	1:A:406[A]:PHE:CD1	2.41	0.73
1:A:184:ILE:HD11	1:A:223:ALA:HB3	1.70	0.73
2:B:158:ALA:HB2	2:B:311:TYR:CE1	2.22	0.73
1:A:444:VAL:HG11	1:A:465:GLU:HG3	1.70	0.72
3:G:249:THR:O	3:G:252:ARG:HB2	1.89	0.72
1:A:98:PRO:HG3	1:A:126:ARG:NE	2.04	0.72
1:A:34:ILE:HD12	1:A:35:GLY:H	1.53	0.72
1:A:137:ILE:HD13	1:A:137:ILE:N	2.04	0.71
2:B:339:ILE:HG23	2:B:344:ILE:HB	1.72	0.71
1:A:148:THR:HB	1:A:150:ILE:HD13	1.72	0.71
1:A:381:ARG:H	1:A:381:ARG:HD2	1.53	0.71
1:A:279:ARG:O	1:A:283:LEU:HG	1.90	0.71
2:B:189:ARG:HB2	2:B:192:GLU:HG2	1.71	0.71
1:A:403[A]:PHE:HA	1:A:406[A]:PHE:HE1	1.54	0.71
2:B:133:LEU:HB2	2:B:148:LYS:HD2	1.70	0.70
1:A:471:HIS:HE1	1:A:500:ILE:HD11	1.55	0.70
1:A:62:MET:SD	1:A:95:VAL:HG21	2.32	0.70
2:B:387[A]:ILE:HG22	2:B:388[A]:ILE:HG13	1.71	0.70
1:A:403[A]:PHE:HA	1:A:406[A]:PHE:CE1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:ARG:O	2:B:409:LYS:HB2	1.92	0.69
2:B:430:LYS:HE3	2:B:460:VAL:HG12	1.74	0.69
1:A:150:ILE:HG23	1:A:430:GLN:HG2	1.74	0.69
1:A:203:TYR:HB3	1:A:231:VAL:HG13	1.73	0.69
2:B:265:GLY:HA2	2:B:268:VAL:HG12	1.75	0.69
2:B:410:ILE:HG13	2:B:444:ILE:HG21	1.74	0.69
1:A:299:PHE:HA	1:A:341:ASN:HD21	1.57	0.68
2:B:339:ILE:HD13	2:B:342:LEU:HD12	1.74	0.68
1:A:209:LYS:HD2	2:B:328:HIS:HA	1.75	0.68
1:A:410[A]:LEU:HD22	1:A:411[A]:ASP:H	1.57	0.68
2:B:96:ASN:HD21	2:B:100:GLU:H	1.41	0.68
3:G:38:LEU:HD13	3:G:218:LYS:HB3	1.76	0.68
2:B:138:LYS:HG3	2:B:414:LEU:HA	1.75	0.68
1:A:158:PRO:HG2	1:A:379:GLN:HB3	1.76	0.68
1:A:209:LYS:HE3	2:B:356:ARG:HH22	1.59	0.68
1:A:32:LEU:HG	1:A:42:HIS:HB2	1.76	0.67
2:B:20:VAL:CG1	2:B:59:ARG:HD2	2.23	0.67
2:B:378:LEU:O	2:B:381[A]:TYR:HB3	1.94	0.67
1:A:108:VAL:HG12	1:A:114:ALA:HA	1.75	0.67
2:B:390[A]:ILE:CD1	3:G:77:LEU:HD21	2.25	0.67
1:A:218:LYS:HD2	2:B:128:VAL:HG11	1.76	0.67
1:A:38:ILE:HG13	1:A:284:LEU:HB3	1.77	0.67
1:A:137:ILE:HG12	1:A:138:PRO:HD3	1.77	0.67
2:B:418:PHE:HA	2:B:430:LYS:H	1.60	0.67
2:B:186:VAL:HG21	2:B:233:ALA:HB2	1.76	0.66
2:B:96:ASN:ND2	2:B:100:GLU:H	1.94	0.66
3:G:27:ALA:HB1	3:G:229:MET:HA	1.77	0.66
3:G:233:ASP:CG	3:G:237:LYS:NZ	2.49	0.66
1:A:488:LYS:HG2	1:A:489:ILE:H	1.60	0.66
2:B:32:ILE:HG22	2:B:33:LEU:HG	1.78	0.66
2:B:257:ASN:H	2:B:309:ALA:HB3	1.61	0.66
1:A:303:SER:HA	1:A:345:ILE:HD13	1.78	0.65
2:B:44:ARG:HH11	2:B:44:ARG:HG2	1.62	0.65
1:A:52:MET:HA	1:A:62:MET:HA	1.79	0.65
2:B:139:VAL:CG2	2:B:414:LEU:HB3	2.27	0.65
2:B:187:GLY:O	2:B:222:MET:HG3	1.96	0.65
2:B:25:PHE:HB2	2:B:29:LEU:HD22	1.79	0.65
1:A:156:LEU:O	1:A:158:PRO:HD3	1.96	0.65
3:G:250:PHE:CE1	3:G:254:ARG:HD2	2.31	0.64
1:A:167:ILE:HG22	1:A:350:ILE:HB	1.79	0.64
2:B:145:PRO:HG2	2:B:357:ILE:HG23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASP:O	1:A:184:ILE:HG22	1.99	0.63
1:A:337:TYR:O	1:A:338:ILE:HB	1.96	0.63
2:B:345:TYR:HA	2:B:346:PRO:C	2.18	0.63
1:A:361:ILE:O	1:A:364:ALA:HB2	1.98	0.63
1:A:458:PRO:HA	1:A:461:ILE:HD11	1.81	0.63
1:A:356:LEU:HD12	1:A:364:ALA:HB1	1.79	0.63
1:A:397:TYR:HA	1:A:400[A]:VAL:CG2	2.28	0.63
2:B:142:LEU:HD11	2:B:441:PHE:HE2	1.63	0.63
1:A:385:GLN:HG2	1:A:489:ILE:HD12	1.81	0.63
2:B:378:LEU:O	2:B:382[A]:LYS:HG2	1.99	0.63
1:A:403[A]:PHE:O	1:A:405[A]:GLN:N	2.32	0.62
2:B:432:VAL:HG11	2:B:435:LYS:HD2	1.81	0.62
1:A:165:GLU:O	1:A:324:LEU:HA	1.98	0.62
1:A:265:LEU:HD11	1:A:324:LEU:HD11	1.80	0.62
3:G:213:ILE:HG13	3:G:213:ILE:O	2.00	0.62
1:A:425:THR:O	1:A:429:LYS:HG3	2.00	0.62
1:A:477:GLN:HA	1:A:477:GLN:HE21	1.65	0.62
1:A:279:ARG:HD2	1:A:293:ALA:HB3	1.81	0.62
2:B:374:VAL:HG23	2:B:445:LEU:HD11	1.81	0.61
1:A:471:HIS:CE1	1:A:500:ILE:HD11	2.34	0.61
2:B:135:THR:OG1	2:B:141:ASP:HB2	2.00	0.61
3:G:250:PHE:CD1	3:G:254:ARG:HD2	2.36	0.61
1:A:106:ARG:CZ	1:A:118:LYS:HB2	2.31	0.61
2:B:346:PRO:HD3	2:B:418:PHE:HE2	1.65	0.61
2:B:118:ALA:HB3	2:B:295:ARG:NH2	2.15	0.60
2:B:253:LEU:HG	2:B:255:ILE:HD11	1.83	0.60
1:A:313:ASN:HD22	1:A:316:PHE:HB2	1.66	0.60
1:A:103:LEU:O	1:A:230:ILE:HG12	2.01	0.60
2:B:408:ARG:HD2	2:B:412:ARG:NH2	2.17	0.60
2:B:441:PHE:HD1	2:B:442:GLN:H	1.48	0.60
2:B:139:VAL:HG22	2:B:414:LEU:HB3	1.82	0.60
1:A:356:LEU:O	1:A:359:LYS:HG3	2.02	0.60
2:B:255:ILE:HD13	2:B:308:GLN:HG2	1.82	0.60
2:B:298:THR:HG23	2:B:303:SER:HB2	1.82	0.60
1:A:106:ARG:O	1:A:231:VAL:HG23	2.02	0.60
1:A:386:VAL:HG23	1:A:387:ALA:H	1.66	0.60
2:B:252:LEU:HG	2:B:305:THR:O	2.02	0.60
2:B:321:ALA:HB3	2:B:322:PRO:HD3	1.83	0.60
2:B:16:VAL:O	2:B:17:ILE:HG13	2.02	0.60
3:G:27:ALA:O	3:G:229:MET:SD	2.60	0.60
1:A:141:SER:HB3	1:A:143:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:PRO:N	2:B:229:ARG:HH21	2.00	0.59
2:B:156:GLY:N	2:B:162:LYS:HE3	2.15	0.59
2:B:36:LEU:O	2:B:46:VAL:HA	2.02	0.59
2:B:319:ASP:HB3	2:B:322:PRO:CD	2.32	0.59
2:B:181:SER:O	2:B:215:VAL:HA	2.03	0.59
2:B:262:THR:HG23	2:B:282:GLN:NE2	2.16	0.59
2:B:180:TYR:HB2	2:B:249:GLN:NE2	2.17	0.59
1:A:393:GLU:O	1:A:397:TYR:HB2	2.03	0.59
2:B:29:LEU:HD13	2:B:30:PRO:HD2	1.84	0.59
2:B:132:ILE:HG13	2:B:133:LEU:N	2.18	0.59
2:B:167:MET:O	2:B:170:ILE:HB	2.03	0.59
3:G:231:ALA:HB3	3:G:232:MET:SD	2.43	0.58
1:A:128:ARG:HG2	1:A:130:GLY:H	1.69	0.58
2:B:138:LYS:CB	2:B:414:LEU:HA	2.34	0.58
2:B:406:ARG:HD2	2:B:444:ILE:O	2.02	0.58
1:A:446:TYR:CE1	1:A:497:LEU:HD13	2.39	0.58
2:B:298:THR:HG22	2:B:299:THR:H	1.68	0.58
1:A:113:ASN:H	1:A:113:ASN:ND2	1.99	0.58
2:B:319:ASP:HB3	2:B:322:PRO:HD3	1.85	0.58
2:B:335:LEU:HB3	2:B:347:ALA:HB3	1.86	0.58
2:B:377:ILE:O	2:B:381[A]:TYR:HB2	2.03	0.58
1:A:424:LEU:HD21	1:A:445:ILE:HD11	1.85	0.58
2:B:133:LEU:HB2	2:B:148:LYS:CD	2.34	0.58
1:A:99:VAL:HG23	1:A:253:MET:HA	1.85	0.57
2:B:186:VAL:HG22	2:B:232:VAL:HG13	1.85	0.57
2:B:200:MET:HB3	2:B:206:ILE:HG13	1.86	0.57
2:B:149:GLY:H	2:B:305:THR:HG23	1.69	0.57
3:G:231:ALA:O	3:G:235:ALA:HB3	2.04	0.57
1:A:212:THR:O	1:A:215:GLN:HB2	2.04	0.57
1:A:294:TYR:HB3	1:A:298:VAL:HG21	1.86	0.57
2:B:242:TYR:HA	2:B:246:GLN:HE22	1.69	0.57
1:A:203:TYR:HB3	1:A:231:VAL:CG1	2.33	0.57
2:B:262:THR:HG23	2:B:282:GLN:HE21	1.69	0.57
3:G:249:THR:HA	3:G:252:ARG:HB2	1.85	0.57
1:A:415:GLN:HA	1:A:418:LEU:HD12	1.86	0.57
2:B:162:LYS:HZ2	2:B:162:LYS:HB2	1.70	0.57
3:G:21:LYS:O	3:G:24:LYS:HB3	2.04	0.57
6:B:601:VO4:O3	7:B:604:ADP:O1B	2.21	0.57
1:A:150:ILE:HD11	1:A:181:ASP:HB2	1.86	0.57
2:B:428:MET:O	2:B:430:LYS:N	2.38	0.57
1:A:184:ILE:HD11	1:A:223:ALA:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:GLN:HA	1:A:477:GLN:NE2	2.20	0.56
2:B:253:LEU:HD12	2:B:254:PHE:N	2.20	0.56
1:A:215:GLN:O	1:A:219:ARG:HB2	2.05	0.56
2:B:85:PRO:HA	2:B:113:PHE:HA	1.88	0.56
1:A:62:MET:CE	1:A:95:VAL:HG21	2.36	0.56
1:A:154:ASP:O	1:A:158:PRO:HG3	2.06	0.56
1:A:211:SER:OG	2:B:126:MET:HG3	2.06	0.56
2:B:465:GLU:HA	2:B:468:ALA:HB3	1.88	0.56
1:A:399:GLU:HG2	1:A:403[A]:PHE:CE1	2.41	0.56
2:B:95:MET:SD	2:B:99:GLY:HA2	2.46	0.56
2:B:269:SER:O	2:B:272:LEU:HB2	2.05	0.56
1:A:249:SER:O	1:A:253:MET:HG2	2.06	0.56
2:B:462:PRO:HB3	2:B:464:GLU:OE1	2.06	0.55
2:B:251:VAL:HG12	2:B:252:LEU:H	1.71	0.55
1:A:37:GLY:O	1:A:38:ILE:HD13	2.06	0.55
1:A:381:ARG:H	1:A:381:ARG:CD	2.19	0.55
3:G:240:SER:O	3:G:241:ASP:C	2.43	0.55
1:A:108:VAL:CG2	1:A:232:VAL:HG12	2.36	0.55
1:A:135:GLY:N	1:A:139:ARG:HH21	2.05	0.55
2:B:154:LEU:HD13	2:B:165:LEU:HD23	1.88	0.55
2:B:449:TYR:CG	2:B:463:ILE:HD11	2.42	0.55
3:G:40:PRO:O	3:G:45:GLY:HA3	2.05	0.55
1:A:188:ARG:HG3	1:A:189:PHE:CD1	2.42	0.55
2:B:126:MET:HE3	2:B:126:MET:HA	1.87	0.55
1:A:115:ILE:C	1:A:117:GLY:H	2.10	0.55
1:A:152:ALA:O	1:A:156:LEU:HB2	2.07	0.55
1:A:410[A]:LEU:CD2	1:A:411[A]:ASP:H	2.18	0.55
1:A:482:ASN:HA	1:A:485:SER:OG	2.07	0.55
2:B:138:LYS:CG	2:B:414:LEU:HA	2.35	0.55
2:B:191:ARG:HH21	2:B:192:GLU:HB3	1.72	0.55
1:A:138:PRO:HA	1:A:316:PHE:HD2	1.72	0.54
1:A:168:ILE:HG12	1:A:329:THR:OG1	2.07	0.54
1:A:338:ILE:HB	1:A:339:PRO:HD3	1.88	0.54
3:G:24:LYS:HB2	3:G:232:MET:HB3	1.88	0.54
1:A:244:TYR:O	1:A:247:PRO:HD2	2.06	0.54
1:A:446:TYR:O	1:A:449:VAL:HG12	2.06	0.54
2:B:140:VAL:HG13	2:B:146:TYR:CZ	2.41	0.54
2:B:346:PRO:HD3	2:B:418:PHE:CE2	2.42	0.54
1:A:106:ARG:NH2	1:A:116:ASP:OD1	2.39	0.54
1:A:151:LYS:HE3	1:A:436:MET:HG3	1.89	0.54
2:B:105:ARG:HE	2:B:208:LEU:HD22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:HG23	1:A:201:CYS:SG	2.47	0.54
1:A:461:ILE:HA	1:A:464:PHE:CD2	2.43	0.54
2:B:375:GLN:HA	2:B:378:LEU:HB2	1.89	0.54
3:G:258:ILE:O	3:G:262:LEU:HB2	2.07	0.54
1:A:144:GLU:O	1:A:144:GLU:HG2	2.08	0.54
1:A:146:MET:HG3	1:A:199:LEU:HD22	1.89	0.54
1:A:183:ILE:HG12	1:A:265:LEU:HD23	1.90	0.54
1:A:483:ILE:O	1:A:487:GLY:HA2	2.08	0.54
2:B:246:GLN:H	2:B:246:GLN:NE2	2.06	0.54
1:A:360:GLY:O	1:A:362:ARG:HG2	2.08	0.54
1:A:385:GLN:OE1	1:A:488:LYS:HG2	2.07	0.54
1:A:399:GLU:O	1:A:403[A]:PHE:CD1	2.61	0.54
2:B:441:PHE:HD1	2:B:442:GLN:N	2.06	0.54
1:A:105:GLY:HA2	1:A:226:MET:O	2.08	0.54
1:A:139:ARG:HA	1:A:311:LYS:O	2.08	0.54
1:A:338:ILE:O	1:A:342:VAL:HG23	2.07	0.54
1:A:31:VAL:HG23	1:A:86:ASP:O	2.07	0.53
1:A:176:THR:O	1:A:180:ILE:HB	2.07	0.53
2:B:138:LYS:HD2	2:B:414:LEU:HD23	1.89	0.53
2:B:476:GLU:O	2:B:477:HIS:HB2	2.08	0.53
1:A:399:GLU:O	1:A:403[A]:PHE:HD1	1.90	0.53
2:B:293:GLN:NE2	2:B:308:GLN:HE22	2.07	0.53
2:B:406:ARG:HD3	2:B:450:ASP:CG	2.28	0.53
1:A:218:LYS:HD3	1:A:219:ARG:N	2.23	0.53
1:A:267:ILE:HD13	1:A:324:LEU:HD13	1.90	0.53
1:A:438:ILE:O	1:A:442:VAL:HG23	2.08	0.53
1:A:417:LEU:O	1:A:420:ARG:HG2	2.08	0.53
3:G:253:THR:HA	3:G:256:ALA:HB3	1.91	0.53
1:A:184:ILE:HD12	1:A:225:ALA:HB2	1.91	0.53
2:B:406:ARG:CZ	2:B:447:GLY:HA2	2.38	0.53
1:A:62:MET:SD	1:A:64:LEU:HD11	2.49	0.53
2:B:257:ASN:HA	2:B:309:ALA:O	2.09	0.53
1:A:91:THR:O	1:A:93:ALA:N	2.42	0.53
1:A:175:LYS:CG	1:A:352:LEU:HD12	2.37	0.53
1:A:180:ILE:HG13	1:A:220:LEU:HD21	1.91	0.53
2:B:255:ILE:HG21	2:B:258:ILE:HB	1.90	0.53
1:A:55:PHE:CE2	1:A:75:VAL:HG22	2.43	0.52
2:B:166:ILE:HG12	2:B:254:PHE:HD2	1.73	0.52
2:B:469:LYS:O	2:B:469:LYS:HD3	2.09	0.52
3:G:30:LYS:HE2	3:G:225:GLN:OE1	2.08	0.52
1:A:174:GLY:O	1:A:178:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HD3	2:B:356:ARG:HH12	1.73	0.52
1:A:313:ASN:HD21	1:A:315:SER:HB2	1.74	0.52
1:A:477:GLN:HE21	1:A:477:GLN:CA	2.21	0.52
2:B:452:LEU:HD22	2:B:466:ALA:HB1	1.90	0.52
3:G:4:LYS:O	3:G:5:ASP:HB3	2.08	0.52
2:B:120:ALA:HB1	2:B:294:GLU:O	2.10	0.52
2:B:212:THR:HG22	2:B:214:LYS:NZ	2.24	0.52
1:A:265:LEU:HD11	1:A:324:LEU:CD1	2.40	0.52
2:B:38:VAL:HG21	2:B:45:LEU:CD2	2.37	0.52
2:B:242:TYR:HA	2:B:246:GLN:NE2	2.25	0.52
2:B:372:ARG:HA	2:B:372:ARG:HE	1.75	0.52
1:A:294:TYR:O	1:A:296:GLY:N	2.34	0.52
1:A:467:ALA:O	1:A:471:HIS:HB2	2.09	0.52
2:B:439:LYS:O	2:B:443:GLN:HG2	2.10	0.52
1:A:431:GLY:CA	5:A:603:ATP:HN62	2.23	0.51
3:G:233:ASP:O	3:G:237:LYS:CD	2.45	0.51
2:B:138:LYS:HB3	2:B:414:LEU:HD23	1.91	0.51
3:G:248:LEU:HG	3:G:252:ARG:HH12	1.75	0.51
1:A:440:GLU:O	1:A:443:ALA:HB3	2.10	0.51
1:A:386:VAL:HG12	1:A:450:ARG:NH2	2.25	0.51
2:B:43:SER:OG	2:B:44:ARG:N	2.42	0.51
2:B:158:ALA:CB	2:B:311:TYR:HE1	2.17	0.51
2:B:434:LEU:O	2:B:437:THR:HG23	2.10	0.51
3:G:249:THR:O	3:G:253:THR:N	2.39	0.51
1:A:362:ARG:HH12	2:B:372:ARG:CD	2.23	0.51
1:A:386:VAL:HG13	1:A:489:ILE:HD11	1.91	0.51
1:A:64:LEU:HD22	1:A:74:VAL:HG11	1.93	0.51
1:A:343:ILE:HD11	1:A:349:GLN:CD	2.31	0.51
2:B:271:LEU:H	2:B:271:LEU:CD2	2.07	0.51
1:A:362:ARG:HH12	2:B:372:ARG:HD2	1.74	0.51
2:B:94:ILE:HB	2:B:103:ASP:HB3	1.93	0.51
1:A:400[A]:VAL:HB	1:A:418:LEU:CD2	2.41	0.51
1:A:441:GLN:O	1:A:445:ILE:HG22	2.11	0.51
2:B:49:VAL:HA	2:B:60:THR:HG22	1.93	0.51
2:B:259:PHE:HZ	2:B:311:TYR:HD2	1.59	0.51
2:B:361:ASN:HB2	2:B:362:ILE:HD13	1.92	0.51
1:A:294:TYR:HB3	1:A:298:VAL:CG2	2.41	0.51
2:B:89:GLU:HB2	2:B:110:THR:HG22	1.92	0.51
2:B:180:TYR:HB2	2:B:249:GLN:HE22	1.75	0.51
2:B:259:PHE:CZ	2:B:311:TYR:HD2	2.29	0.51
2:B:299:THR:HG23	2:B:301:LYS:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TYR:OH	1:A:494:ASP:HA	2.11	0.50
1:A:261:GLY:O	1:A:319:GLY:HA2	2.11	0.50
1:A:479:LEU:HD12	1:A:479:LEU:H	1.76	0.50
2:B:207:ASN:HD21	2:B:210:ASP:H	1.57	0.50
1:A:493:SER:O	1:A:497:LEU:HD12	2.11	0.50
2:B:267:GLU:O	2:B:271:LEU:HD11	2.11	0.50
2:B:406:ARG:HD3	2:B:450:ASP:OD2	2.11	0.50
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.27	0.50
2:B:163:THR:O	2:B:166:ILE:HG22	2.12	0.50
2:B:437:THR:HB	2:B:441:PHE:CE2	2.47	0.50
2:B:207:ASN:HD21	2:B:210:ASP:N	2.10	0.50
1:A:353:GLU:OE1	1:A:366:ASN:HB2	2.11	0.50
2:B:426:GLY:O	2:B:428:MET:HG3	2.12	0.50
3:G:226:SER:O	3:G:229:MET:HB2	2.11	0.50
1:A:397:TYR:CE2	1:A:401[A]:ALA:HB2	2.46	0.50
1:A:483:ILE:HD13	1:A:488:LYS:N	2.27	0.50
2:B:316:ASP:HB3	2:B:318:THR:OG1	2.11	0.50
2:B:383[A]:SER:O	2:B:387[A]:ILE:N	2.43	0.50
1:A:402[A]:ALA:O	1:A:403[A]:PHE:CD1	2.65	0.49
1:A:133:ALA:HB1	1:A:139:ARG:HH22	1.77	0.49
1:A:154:ASP:HB2	1:A:441:GLN:OE1	2.12	0.49
2:B:88:PRO:HA	2:B:91:LEU:HD12	1.94	0.49
2:B:413:PHE:CZ	2:B:444:ILE:HD11	2.47	0.49
3:G:228:ARG:O	3:G:229:MET:C	2.50	0.49
1:A:446:TYR:HA	1:A:449:VAL:HG12	1.94	0.49
2:B:29:LEU:CD1	2:B:58:VAL:HG13	2.42	0.49
2:B:151:LYS:HE2	2:B:296:ILE:HG13	1.94	0.49
2:B:350:PRO:CB	2:B:378:LEU:HD13	2.42	0.49
3:G:23:MET:SD	3:G:228:ARG:HG3	2.52	0.49
1:A:257:PHE:HD2	1:A:264:ALA:HB2	1.77	0.49
1:A:299:PHE:C	1:A:301:LEU:H	2.16	0.49
2:B:350:PRO:HB2	2:B:378:LEU:HD13	1.94	0.49
1:A:166:LEU:HD12	1:A:342:VAL:HG12	1.95	0.49
1:A:291:ARG:O	1:A:294:TYR:HB2	2.13	0.49
2:B:408:ARG:O	2:B:412:ARG:HG2	2.12	0.49
2:B:378:LEU:HA	2:B:381[A]:TYR:HB3	1.94	0.49
2:B:381[A]:TYR:HA	2:B:384[A]:LEU:CD2	2.42	0.49
1:A:280:GLN:OE1	2:B:284:THR:HA	2.13	0.49
1:A:397:TYR:CZ	1:A:421:GLY:HA3	2.47	0.49
1:A:445:ILE:HG23	1:A:446:TYR:N	2.27	0.49
2:B:44:ARG:HG2	2:B:44:ARG:NH1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:TYR:HD1	2:B:281:TYR:H	1.61	0.49
2:B:358:MET:HE3	2:B:368:TYR:HB2	1.94	0.49
2:B:362:ILE:HD13	2:B:362:ILE:N	2.27	0.49
1:A:386:VAL:O	1:A:449:VAL:HG21	2.12	0.49
2:B:96:ASN:HD22	2:B:96:ASN:C	2.16	0.49
2:B:174:ALA:O	2:B:177:HIS:HB3	2.12	0.49
3:G:82:HIS:H	3:G:82:HIS:CD2	2.30	0.49
1:A:417:LEU:HA	1:A:420:ARG:NE	2.27	0.49
1:A:186:GLN:O	1:A:189:PHE:HB2	2.13	0.48
1:A:138:PRO:HA	1:A:316:PHE:CD2	2.48	0.48
1:A:178:ILE:HG23	1:A:179:ALA:N	2.28	0.48
2:B:15:ALA:HB3	2:B:22:ASP:HB2	1.95	0.48
2:B:138:LYS:HB3	2:B:414:LEU:HA	1.94	0.48
2:B:373:GLY:O	2:B:377:ILE:HG22	2.13	0.48
1:A:137:ILE:CG1	1:A:138:PRO:HD3	2.43	0.48
1:A:410[A]:LEU:HD22	1:A:411[A]:ASP:N	2.26	0.48
2:B:196:LEU:HD23	2:B:219:TYR:OH	2.12	0.48
3:G:78:CYS:SG	3:G:78:CYS:O	2.71	0.48
3:G:233:ASP:CG	3:G:237:LYS:HZ2	2.17	0.48
1:A:403[A]:PHE:O	1:A:404[A]:ALA:C	2.51	0.48
1:A:422:VAL:O	1:A:425:THR:HB	2.14	0.48
1:A:59:LEU:HD12	1:A:60:LYS:H	1.78	0.48
2:B:226:PRO:HB3	2:B:267:GLU:OE1	2.14	0.48
1:A:102:GLU:OE1	1:A:123:SER:HA	2.14	0.48
2:B:251:VAL:HG12	2:B:252:LEU:N	2.28	0.48
1:A:392:LEU:HA	1:A:395:ALA:HB2	1.96	0.48
2:B:113:PHE:CD1	2:B:113:PHE:N	2.81	0.48
2:B:268:VAL:O	2:B:272:LEU:HG	2.14	0.48
3:G:23:MET:HB3	3:G:232:MET:HG2	1.96	0.48
1:A:386:VAL:HG23	1:A:387:ALA:N	2.29	0.47
2:B:253:LEU:HG	2:B:255:ILE:CD1	2.42	0.47
3:G:250:PHE:HE1	3:G:254:ARG:HH11	1.60	0.47
1:A:98:PRO:HA	1:A:126:ARG:HD3	1.95	0.47
1:A:385:GLN:CG	1:A:489:ILE:HD12	2.43	0.47
2:B:319:ASP:C	2:B:321:ALA:H	2.17	0.47
1:A:57:SER:CB	1:A:81:LEU:HB2	2.44	0.47
2:B:234:LEU:O	2:B:237:LEU:HB3	2.14	0.47
2:B:259:PHE:CD1	2:B:259:PHE:C	2.87	0.47
2:B:370:VAL:O	2:B:374:VAL:HG23	2.13	0.47
3:G:241:ASP:O	3:G:245:LYS:N	2.48	0.47
1:A:492:GLN:HE21	1:A:492:GLN:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:VAL:HG22	2:B:410:ILE:HD13	1.97	0.47
3:G:251:ASN:HA	3:G:254:ARG:HB3	1.97	0.47
1:A:223:ALA:C	1:A:225:ALA:H	2.18	0.47
1:A:356:LEU:HB2	1:A:364:ALA:HB1	1.96	0.47
2:B:38:VAL:HG11	2:B:69:LEU:HD21	1.96	0.47
2:B:212:THR:HG22	2:B:214:LYS:HZ1	1.79	0.47
2:B:296:ILE:HD13	2:B:308:GLN:OE1	2.13	0.47
1:A:81:LEU:HD12	1:A:81:LEU:H	1.79	0.47
1:A:173:THR:HG22	1:A:352:LEU:HB3	1.96	0.47
2:B:237:LEU:HD23	2:B:241:GLU:HG3	1.97	0.47
2:B:378:LEU:HD23	2:B:381[A]:TYR:HD2	1.80	0.47
3:G:249:THR:HA	3:G:252:ARG:HH11	1.79	0.47
1:A:34:ILE:HD12	1:A:35:GLY:N	2.27	0.47
1:A:171:ARG:HH12	2:B:354:THR:HG21	1.79	0.47
1:A:177:SER:O	1:A:180:ILE:HG22	2.15	0.47
1:A:359:LYS:HB2	1:A:361:ILE:HG12	1.97	0.47
1:A:498:LYS:HA	1:A:501:VAL:HG22	1.96	0.47
2:B:258:ILE:O	2:B:258:ILE:HG13	2.14	0.47
2:B:268:VAL:O	2:B:271:LEU:HG	2.14	0.47
2:B:335:LEU:HA	2:B:347:ALA:O	2.15	0.47
1:A:313:ASN:ND2	1:A:316:PHE:HB2	2.29	0.47
2:B:194:ASN:O	2:B:197:TYR:HB3	2.15	0.47
1:A:56:SER:C	1:A:58:GLY:H	2.18	0.47
1:A:263:HIS:HB3	1:A:320:SER:OG	2.15	0.47
1:A:358:TYR:HE2	2:B:351:LEU:HD12	1.80	0.47
1:A:397:TYR:CE1	1:A:418:LEU:HA	2.41	0.47
1:A:410[A]:LEU:CD2	1:A:411[A]:ASP:N	2.78	0.47
2:B:220:GLY:N	2:B:232:VAL:HG21	2.29	0.47
2:B:389[A]:ALA:HA	2:B:395[A]:GLU:HG3	1.97	0.47
1:A:33:SER:OG	1:A:40:ARG:HB2	2.15	0.47
2:B:139:VAL:HG23	2:B:414:LEU:HB3	1.97	0.47
2:B:145:PRO:HD3	2:B:358:MET:HG3	1.97	0.47
3:G:249:THR:CA	3:G:252:ARG:HB2	2.45	0.47
1:A:45:ARG:O	1:A:45:ARG:HD3	2.14	0.46
1:A:152:ALA:HB2	1:A:428:LEU:O	2.16	0.46
1:A:299:PHE:HA	1:A:341:ASN:ND2	2.27	0.46
2:B:20:VAL:HG11	2:B:59:ARG:HD2	1.94	0.46
2:B:186:VAL:HG13	2:B:232:VAL:CG1	2.45	0.46
2:B:298:THR:HG22	2:B:299:THR:N	2.31	0.46
1:A:135:GLY:O	1:A:138:PRO:HD2	2.15	0.46
1:A:299:PHE:C	1:A:301:LEU:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:VAL:HG23	2:B:45:LEU:O	2.16	0.46
2:B:469:LYS:HE3	2:B:473:LEU:HD13	1.96	0.46
3:G:250:PHE:O	3:G:254:ARG:HB2	2.16	0.46
2:B:432:VAL:CG1	2:B:435:LYS:HD2	2.44	0.46
1:A:209:LYS:CD	2:B:356:ARG:HH12	2.29	0.46
2:B:86:VAL:HG23	2:B:112:GLN:NE2	2.24	0.46
1:A:204:VAL:HA	1:A:232:VAL:HG23	1.98	0.46
1:A:399:GLU:O	1:A:402[A]:ALA:HB3	2.15	0.46
1:A:404[A]:ALA:C	1:A:406[A]:PHE:H	2.18	0.46
2:B:137:ILE:HA	2:B:416:GLN:OE1	2.16	0.46
2:B:269:SER:OG	2:B:282:GLN:HB3	2.16	0.46
3:G:19:ILE:N	3:G:19:ILE:HD12	2.30	0.46
1:A:188:ARG:HG3	1:A:189:PHE:HD1	1.78	0.46
1:A:390:MET:SD	1:A:449:VAL:HB	2.56	0.46
3:G:217:LEU:O	3:G:221:THR:N	2.45	0.46
1:A:336:ALA:C	1:A:339:PRO:HD2	2.36	0.46
3:G:261:GLU:O	3:G:265:ILE:HG13	2.16	0.46
1:A:164:ARG:HD3	1:A:164:ARG:N	2.30	0.45
1:A:178:ILE:HG23	1:A:179:ALA:H	1.81	0.45
1:A:202:ILE:O	1:A:266:ILE:HA	2.16	0.45
1:A:312:MET:HB2	1:A:319:GLY:O	2.15	0.45
1:A:386:VAL:HG12	1:A:450:ARG:HH21	1.80	0.45
2:B:258:ILE:O	2:B:261:PHE:HB3	2.16	0.45
2:B:157:GLY:O	2:B:158:ALA:HB3	2.16	0.45
2:B:362:ILE:HD13	2:B:362:ILE:H	1.82	0.45
1:A:156:LEU:HG	1:A:428:LEU:HD11	1.97	0.45
1:A:343:ILE:HD11	1:A:349:GLN:NE2	2.31	0.45
1:A:426:GLU:HB2	1:A:461:ILE:HD12	1.97	0.45
2:B:196:LEU:HD11	2:B:200:MET:HE2	1.99	0.45
2:B:357:ILE:HG13	2:B:357:ILE:O	2.17	0.45
1:A:138:PRO:O	1:A:313:ASN:HB3	2.16	0.45
1:A:170:ASP:CG	1:A:329:THR:HB	2.37	0.45
1:A:302:HIS:O	1:A:306:LEU:HD23	2.16	0.45
3:G:231:ALA:C	3:G:232:MET:SD	2.94	0.45
1:A:78:ASN:N	1:A:78:ASN:ND2	2.65	0.45
1:A:336:ALA:O	1:A:339:PRO:HD2	2.16	0.45
2:B:144:ALA:HB2	2:B:353:SER:O	2.15	0.45
3:G:84:SER:HA	3:G:87:LYS:HE2	1.99	0.45
1:A:25:LEU:HA	1:A:28:THR:O	2.15	0.45
1:A:225:ALA:HA	1:A:228:TYR:CE1	2.52	0.45
2:B:121:PRO:HG3	2:B:297:THR:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:SER:O	2:B:280:GLY:N	2.47	0.45
1:A:41:VAL:HG12	1:A:42:HIS:O	2.17	0.45
3:G:24:LYS:HE2	3:G:233:ASP:HB2	1.97	0.45
1:A:431:GLY:HA2	5:A:603:ATP:HN62	1.81	0.45
1:A:453:LEU:O	1:A:456:LEU:HG	2.16	0.45
2:B:235:THR:C	2:B:237:LEU:H	2.20	0.45
2:B:378:LEU:C	2:B:381[A]:TYR:HB3	2.36	0.45
1:A:81:LEU:HD12	1:A:81:LEU:N	2.31	0.45
1:A:153:VAL:O	1:A:157:VAL:N	2.49	0.45
1:A:300:TYR:O	1:A:304:ARG:HB3	2.16	0.45
1:A:469:LEU:O	1:A:473:VAL:HG22	2.17	0.45
2:B:86:VAL:O	2:B:112:GLN:NE2	2.50	0.45
2:B:284:THR:HB	2:B:288:ASP:OD1	2.16	0.45
1:A:211:SER:O	1:A:215:GLN:HG2	2.17	0.44
1:A:382:ALA:O	1:A:386:VAL:HG22	2.17	0.44
2:B:162:LYS:HE2	2:B:311:TYR:HA	1.98	0.44
2:B:250:ASP:HA	2:B:303:SER:O	2.16	0.44
2:B:267:GLU:O	2:B:271:LEU:HD21	2.17	0.44
2:B:469:LYS:HD3	2:B:469:LYS:C	2.37	0.44
1:A:219:ARG:HA	1:A:222:ASP:OD2	2.18	0.44
1:A:453:LEU:H	1:A:453:LEU:HD12	1.82	0.44
2:B:187:GLY:O	2:B:221:GLN:HB3	2.17	0.44
2:B:298:THR:HG23	2:B:303:SER:CB	2.45	0.44
2:B:335:LEU:HD23	2:B:347:ALA:H	1.81	0.44
2:B:416:GLN:HE21	2:B:418:PHE:HD2	1.64	0.44
1:A:199:LEU:HD21	1:A:265:LEU:HB2	2.00	0.44
1:A:209:LYS:HB2	1:A:212:THR:OG1	2.18	0.44
2:B:152:ILE:HB	2:B:307:VAL:HA	2.00	0.44
1:A:158:PRO:HG2	1:A:379:GLN:OE1	2.17	0.44
1:A:417:LEU:C	1:A:420:ARG:HG2	2.37	0.44
2:B:32:ILE:HA	2:B:49:VAL:HG12	2.00	0.44
2:B:332:THR:HB	2:B:354:THR:H	1.83	0.44
3:G:20:THR:O	3:G:232:MET:HG3	2.18	0.44
1:A:25:LEU:HB3	1:A:43:GLY:HA2	1.99	0.44
1:A:234:ALA:HB1	1:A:243:GLN:HA	2.00	0.44
1:A:235:THR:O	1:A:237:SER:N	2.51	0.44
1:A:246:ALA:O	1:A:249:SER:HB2	2.18	0.44
1:A:38:ILE:HG23	1:A:285:LEU:HD23	2.00	0.44
1:A:104:LEU:HD22	1:A:230:ILE:HD11	1.98	0.44
1:A:146:MET:SD	1:A:265:LEU:HD13	2.57	0.44
1:A:312:MET:O	1:A:318:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LEU:HD13	1:A:424:LEU:C	2.38	0.44
2:B:258:ILE:HD11	2:B:292:MET:SD	2.57	0.44
2:B:419:GLN:HE21	2:B:419:GLN:HB2	1.59	0.44
3:G:4:LYS:O	3:G:5:ASP:CB	2.66	0.44
3:G:10:LEU:HD23	3:G:13:ILE:HD12	1.99	0.44
1:A:140:ILE:HG23	1:A:141:SER:N	2.25	0.44
1:A:206:ILE:HD11	1:A:247:PRO:HG3	1.99	0.44
1:A:422:VAL:HG12	1:A:458:PRO:HG2	1.99	0.44
2:B:16:VAL:C	2:B:17:ILE:HG13	2.38	0.44
2:B:137:ILE:O	2:B:141:ASP:HB3	2.18	0.44
2:B:336:SER:O	2:B:339:ILE:HB	2.18	0.44
1:A:501:VAL:HG23	1:A:502:THR:N	2.32	0.44
2:B:319:ASP:HB3	2:B:322:PRO:HD2	2.00	0.44
2:B:412:ARG:HD2	2:B:458:TYR:HD1	1.82	0.44
3:G:257:VAL:O	3:G:261:GLU:HG2	2.18	0.44
1:A:111:LEU:HB3	1:A:113:ASN:HD21	1.82	0.44
1:A:188:ARG:CZ	1:A:437:ALA:HB2	2.48	0.44
1:A:257:PHE:CD2	1:A:264:ALA:HB2	2.53	0.44
1:A:338:ILE:CB	1:A:339:PRO:HD3	2.48	0.44
1:A:436:MET:O	1:A:437:ALA:O	2.36	0.44
2:B:66:THR:HG22	2:B:69:LEU:CD1	2.44	0.44
2:B:259:PHE:CD2	2:B:321:ALA:HB1	2.53	0.44
1:A:62:MET:HG3	1:A:64:LEU:HD13	2.00	0.43
1:A:74:VAL:HG13	1:A:74:VAL:O	2.17	0.43
1:A:150:ILE:HB	1:A:153:VAL:HB	1.99	0.43
2:B:259:PHE:HB3	2:B:310:ILE:HG23	1.98	0.43
1:A:479:LEU:HD23	1:A:497:LEU:HG	1.99	0.43
2:B:256:ASP:O	2:B:257:ASN:HB2	2.18	0.43
2:B:268:VAL:HA	2:B:271:LEU:HG	2.00	0.43
1:A:64:LEU:HD22	1:A:74:VAL:CG1	2.48	0.43
1:A:153:VAL:HG12	1:A:154:ASP:N	2.33	0.43
1:A:189:PHE:CD1	1:A:189:PHE:N	2.86	0.43
1:A:135:GLY:H	1:A:139:ARG:HE	1.66	0.43
1:A:204:VAL:HA	1:A:232:VAL:CG2	2.49	0.43
1:A:272:SER:O	1:A:275:ALA:HB3	2.18	0.43
2:B:76:LEU:HG	2:B:77:ASP:N	2.32	0.43
2:B:149:GLY:HA2	2:B:304:ILE:O	2.18	0.43
2:B:158:ALA:O	2:B:337:ARG:NH2	2.52	0.43
1:A:194:ASP:HB3	1:A:197:LYS:HB3	2.00	0.43
2:B:23:VAL:O	2:B:57:THR:HG23	2.19	0.43
2:B:255:ILE:N	2:B:255:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:ASP:O	2:B:331:ALA:HB2	2.19	0.43
1:A:267:ILE:CD1	1:A:324:LEU:HD13	2.48	0.43
1:A:270:ASP:HB3	1:A:273:LYS:HB2	2.00	0.43
2:B:456:ALA:O	2:B:469:LYS:HD2	2.19	0.43
3:G:24:LYS:O	3:G:27:ALA:HB3	2.18	0.43
1:A:101:ASP:O	1:A:104:LEU:HB2	2.19	0.43
1:A:363:PRO:O	1:A:364:ALA:HB3	2.19	0.43
1:A:493:SER:HA	1:A:496:LYS:HB2	2.00	0.43
2:B:151:LYS:NZ	2:B:293:GLN:O	2.41	0.43
1:A:29:GLY:HA3	1:A:42:HIS:O	2.19	0.43
1:A:292:GLU:C	1:A:294:TYR:H	2.23	0.43
1:A:299:PHE:CD2	1:A:303:SER:OG	2.71	0.43
1:A:390:MET:CE	1:A:449:VAL:HB	2.48	0.43
1:A:404[A]:ALA:O	1:A:406[A]:PHE:N	2.52	0.43
1:A:480:LEU:HD12	1:A:481:GLY:N	2.34	0.43
2:B:32:ILE:O	2:B:33:LEU:HB2	2.19	0.43
2:B:142:LEU:HG	2:B:367:HIS:CD2	2.54	0.43
2:B:374:VAL:O	2:B:378:LEU:HD12	2.18	0.43
1:A:172:GLN:HA	1:A:172:GLN:OE1	2.18	0.42
1:A:397:TYR:HA	1:A:400[A]:VAL:HG22	2.00	0.42
2:B:148:LYS:HA	2:B:305:THR:HG23	2.00	0.42
2:B:162:LYS:HB3	7:B:604:ADP:O2B	2.19	0.42
2:B:182:VAL:HG12	2:B:183:PHE:N	2.34	0.42
1:A:148:THR:O	1:A:185:ASN:HB2	2.19	0.42
3:G:257:VAL:HG12	3:G:261:GLU:CD	2.39	0.42
1:A:44:LEU:HD12	1:A:47:VAL:HB	2.01	0.42
1:A:381:ARG:HD2	1:A:381:ARG:N	2.26	0.42
1:A:458:PRO:O	1:A:461:ILE:HG13	2.18	0.42
2:B:188:GLU:HA	2:B:222:MET:CE	2.50	0.42
2:B:230:ALA:HB2	2:B:264:ALA:HB1	2.00	0.42
2:B:412:ARG:HD2	2:B:458:TYR:CD1	2.54	0.42
2:B:378:LEU:HD23	2:B:381[A]:TYR:CD2	2.54	0.42
3:G:24:LYS:HA	3:G:232:MET:CB	2.50	0.42
3:G:249:THR:C	3:G:252:ARG:H	2.23	0.42
1:A:171:ARG:HH12	2:B:354:THR:CG2	2.32	0.42
1:A:368:GLY:C	1:A:369:LEU:HD22	2.40	0.42
2:B:61:ILE:HG23	2:B:268:VAL:HG21	2.01	0.42
2:B:293:GLN:CD	2:B:308:GLN:HE22	2.22	0.42
3:G:217:LEU:HA	3:G:220:SER:HB2	2.01	0.42
1:A:25:LEU:HD22	1:A:43:GLY:HA3	2.01	0.42
1:A:189:PHE:HD1	1:A:189:PHE:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:THR:HG22	1:A:230:ILE:N	2.35	0.42
1:A:338:ILE:HD13	1:A:338:ILE:HA	1.97	0.42
2:B:53:LEU:HD12	2:B:57:THR:HG22	2.00	0.42
2:B:140:VAL:HG13	2:B:146:TYR:OH	2.20	0.42
2:B:165:LEU:HG	2:B:169:LEU:HD11	2.02	0.42
2:B:189:ARG:HD2	2:B:189:ARG:H	1.85	0.42
2:B:441:PHE:CD1	2:B:442:GLN:N	2.85	0.42
1:A:50:GLU:O	1:A:95:VAL:HG23	2.20	0.42
1:A:98:PRO:HG3	1:A:126:ARG:CZ	2.50	0.42
1:A:113:ASN:ND2	1:A:113:ASN:N	2.66	0.42
1:A:411[A]:ASP:O	1:A:414:THR:HG22	2.19	0.42
2:B:164:VAL:HG11	7:B:604:ADP:N7	2.35	0.42
2:B:345:TYR:HD2	2:B:346:PRO:HA	1.85	0.42
2:B:418:PHE:HA	2:B:430:LYS:N	2.31	0.42
3:G:249:THR:O	3:G:252:ARG:CB	2.63	0.42
3:G:257:VAL:HG12	3:G:261:GLU:OE2	2.20	0.42
1:A:165:GLU:OE2	1:A:350:ILE:HD11	2.20	0.42
1:A:445:ILE:CG2	1:A:446:TYR:N	2.82	0.42
2:B:410:ILE:HD11	2:B:445:LEU:HG	2.02	0.42
1:A:38:ILE:CG2	1:A:285:LEU:HD23	2.49	0.42
1:A:165:GLU:O	1:A:325:PRO:HD2	2.20	0.42
1:A:169:GLY:HA2	1:A:352:LEU:O	2.20	0.42
1:A:146:MET:HA	1:A:161:ARG:HH21	1.84	0.41
1:A:209:LYS:HE3	2:B:356:ARG:NH2	2.32	0.41
1:A:251:CYS:SG	1:A:268:TYR:OH	2.77	0.41
2:B:149:GLY:N	2:B:305:THR:HG23	2.33	0.41
2:B:187:GLY:O	2:B:188:GLU:O	2.38	0.41
2:B:253:LEU:HD12	2:B:254:PHE:H	1.85	0.41
1:A:403[A]:PHE:O	1:A:406[A]:PHE:HD1	1.97	0.41
3:G:249:THR:C	3:G:252:ARG:HB2	2.40	0.41
1:A:324:LEU:HD12	1:A:324:LEU:N	2.36	0.41
1:A:349:GLN:OE1	1:A:370:SER:HA	2.20	0.41
1:A:397:TYR:CE2	1:A:421:GLY:HA3	2.55	0.41
1:A:431:GLY:HA2	5:A:603:ATP:N6	2.35	0.41
3:G:272:LEU:HB3	3:G:273:ASP:H	1.75	0.41
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.91	0.41
2:B:255:ILE:HG12	2:B:258:ILE:HD13	2.01	0.41
1:A:52:MET:O	1:A:91:THR:HB	2.20	0.41
2:B:344:ILE:HG23	2:B:415:SER:OG	2.20	0.41
3:G:39:LYS:HD2	3:G:39:LYS:HA	1.72	0.41
1:A:140:ILE:HB	1:A:313:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLY:O	1:A:253:MET:HB2	2.21	0.41
2:B:168:GLU:O	2:B:171:ASN:HB3	2.21	0.41
2:B:447:GLY:O	2:B:450:ASP:HB3	2.21	0.41
1:A:349:GLN:CD	1:A:370:SER:HA	2.41	0.41
1:A:351:PHE:CZ	1:A:353:GLU:HG2	2.55	0.41
2:B:366:GLU:O	2:B:370:VAL:HG22	2.20	0.41
2:B:382[A]:LYS:HE2	2:B:382[A]:LYS:HA	2.02	0.41
1:A:73:VAL:HG12	1:A:74:VAL:N	2.36	0.41
1:A:329:THR:HG22	1:A:332:GLY:H	1.85	0.41
1:A:397:TYR:HA	1:A:400[A]:VAL:HG23	2.03	0.41
2:B:143:LEU:O	2:B:145:PRO:HD3	2.21	0.41
2:B:156:GLY:HA3	2:B:162:LYS:NZ	2.36	0.41
2:B:332:THR:O	2:B:333:THR:HG23	2.21	0.41
1:A:135:GLY:C	1:A:138:PRO:HD2	2.41	0.41
1:A:300:TYR:O	1:A:304:ARG:NE	2.54	0.41
1:A:441:GLN:HE21	1:A:441:GLN:HB2	1.64	0.41
2:B:230:ALA:C	2:B:231:ARG:HD3	2.40	0.41
3:G:245:LYS:HA	3:G:245:LYS:HD2	1.90	0.41
1:A:54:GLU:O	1:A:88:VAL:HA	2.21	0.41
1:A:109:ASP:O	1:A:233:SER:N	2.54	0.41
2:B:184:ALA:HA	2:B:218:VAL:O	2.21	0.41
3:G:12:SER:O	3:G:16:ILE:HG13	2.21	0.41
1:A:198:LYS:O	1:A:199:LEU:HB2	2.21	0.40
2:B:30:PRO:HG2	2:B:58:VAL:HG11	2.02	0.40
2:B:86:VAL:HG21	2:B:114:ALA:HB2	2.03	0.40
2:B:417:PRO:HD2	2:B:430:LYS:HG3	2.02	0.40
3:G:37:GLU:O	3:G:40:PRO:HD2	2.20	0.40
1:A:349:GLN:O	1:A:370:SER:HB2	2.20	0.40
2:B:186:VAL:HG12	2:B:260:ARG:HB2	2.03	0.40
2:B:259:PHE:HD2	2:B:321:ALA:HB1	1.87	0.40
2:B:282:GLN:C	2:B:284:THR:H	2.25	0.40
1:A:148:THR:O	1:A:182:THR:HA	2.21	0.40
2:B:84:ILE:C	2:B:113:PHE:HB3	2.41	0.40
1:A:155:SER:OG	1:A:156:LEU:N	2.54	0.40
1:A:279:ARG:HD2	1:A:293:ALA:CB	2.51	0.40
1:A:333:ASP:OD2	1:A:336:ALA:HB2	2.20	0.40
2:B:138:LYS:HD2	2:B:414:LEU:CD2	2.51	0.40
2:B:145:PRO:CD	2:B:358:MET:HG3	2.50	0.40
2:B:339:ILE:HG21	2:B:347:ALA:HA	2.02	0.40
1:A:246:ALA:HB3	1:A:247:PRO:HD3	2.04	0.40
1:A:299:PHE:O	1:A:303:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LYS:N	2:B:74:LYS:HD2	2.36	0.40
2:B:96:ASN:ND2	2:B:100:GLU:N	2.67	0.40
2:B:299:THR:C	2:B:301:LYS:H	2.24	0.40
2:B:355:SER:OG	2:B:357:ILE:HG22	2.22	0.40
2:B:422:GLU:C	2:B:424:PHE:H	2.24	0.40
3:G:209:LEU:O	3:G:213:ILE:HG22	2.22	0.40
3:G:266:ILE:HA	3:G:269:ALA:HB3	2.03	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	478/510 (94%)	354 (74%)	85 (18%)	39 (8%)	1	3
2	B	467/479 (98%)	316 (68%)	104 (22%)	47 (10%)	0	2
3	G	118/273 (43%)	92 (78%)	22 (19%)	4 (3%)	3	17
All	All	1063/1262 (84%)	762 (72%)	211 (20%)	90 (8%)	0	3

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	80	LYS
1	A	92	GLY
1	A	109	ASP
1	A	134	PRO
1	A	187	LYS
1	A	208	GLN
1	A	236	ALA
1	A	295	PRO
1	A	338	ILE

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Mol	Chain	Res	Type
1	A	357	PHE
1	A	404[A]	ALA
1	A	408[A]	SER
1	A	437	ALA
1	A	454	ASP
1	A	455	LYS
1	A	458	PRO
1	A	459	SER
2	B	53	LEU
2	B	71	ARG
2	B	97	VAL
2	B	138	LYS
2	B	188	GLU
2	B	210	ASP
2	B	211	ALA
2	B	279	VAL
2	B	281	TYR
2	B	323	ALA
2	B	331	ALA
2	B	418	PHE
2	B	429	GLY
2	B	435	LYS
2	B	453	PRO
3	G	5	ASP
3	G	80	ALA
1	A	84	GLU
1	A	95	VAL
1	A	153	VAL
1	A	194	ASP
1	A	451	GLY
2	B	205	VAL
2	B	245	ASP
2	B	246	GLN
2	B	248	GLY
2	B	269	SER
2	B	288	ASP
2	B	423	VAL
2	B	440	GLY
2	B	451	HIS
1	A	44	LEU
1	A	116	ASP
1	A	151	LYS

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Mol	Chain	Res	Type
1	A	193	THR
1	A	346	THR
1	A	405[A]	GLN
2	B	68	GLY
2	B	124	ILE
2	B	143	LEU
2	B	291	THR
2	B	344	ILE
2	B	391[A]	LEU
2	B	394[A]	ASP
2	B	397[A]	SER
2	B	433	PRO
3	G	34	ALA
1	A	72	GLY
1	A	172	GLN
1	A	188	ARG
1	A	199	LEU
1	A	432	GLN
2	B	105	ARG
2	B	326	PHE
2	B	431	LEU
2	B	432	VAL
3	G	43	VAL
1	A	492	GLN
2	B	171	ASN
2	B	204	GLY
2	B	393[A]	MET
2	B	420	VAL
1	A	361	ILE
1	A	373	ARG
2	B	357	ILE
2	B	390[A]	ILE
1	A	140	ILE
2	B	28	GLY
2	B	444	ILE
2	B	290	GLY
1	A	422	VAL
2	B	350	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	392/416 (94%)	354 (90%)	38 (10%)	6	27
2	B	377/384 (98%)	330 (88%)	47 (12%)	3	17
3	G	103/230 (45%)	88 (85%)	15 (15%)	2	12
All	All	872/1030 (85%)	772 (88%)	100 (12%)	4	20

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	50	GLU
1	A	81	LEU
1	A	83	LYS
1	A	111	LEU
1	A	113	ASN
1	A	137	ILE
1	A	144	GLU
1	A	178	ILE
1	A	189	PHE
1	A	191	ASP
1	A	212	THR
1	A	226	MET
1	A	231	VAL
1	A	233	SER
1	A	237	SER
1	A	251	CYS
1	A	269	ASP
1	A	291	ARG
1	A	292	GLU
1	A	313	ASN
1	A	316	PHE
1	A	328	GLU
1	A	339	PRO
1	A	347	ASP
1	A	349	GLN

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Mol	Chain	Res	Type
1	A	358	TYR
1	A	362	ARG
1	A	392	LEU
1	A	400[A]	VAL
1	A	408[A]	SER
1	A	432	GLN
1	A	434	SER
1	A	439	GLU
1	A	446	TYR
1	A	457	GLU
1	A	492	GLN
1	A	499	GLU
2	B	12	GLN
2	B	31	PRO
2	B	58	VAL
2	B	66	THR
2	B	83	LYS
2	B	89	GLU
2	B	96	ASN
2	B	97	VAL
2	B	105	ARG
2	B	112	GLN
2	B	113	PHE
2	B	125	GLU
2	B	126	MET
2	B	143	LEU
2	B	148	LYS
2	B	164	VAL
2	B	168	GLU
2	B	212	THR
2	B	214	LYS
2	B	246	GLN
2	B	249	GLN
2	B	250	ASP
2	B	252	LEU
2	B	259	PHE
2	B	271	LEU
2	B	284	THR
2	B	292	MET
2	B	305	THR
2	B	329	LEU
2	B	341	GLU

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Mol	Chain	Res	Type
2	B	349	ASP
2	B	352	ASP
2	B	359	ASP
2	B	362	ILE
2	B	368	TYR
2	B	372	ARG
2	B	380[A]	ASP
2	B	412	ARG
2	B	419	GLN
2	B	425	THR
2	B	441	PHE
2	B	448	ASP
2	B	449	TYR
2	B	453	PRO
2	B	457	PHE
2	B	471	ASP
2	B	475	GLU
3	G	5	ASP
3	G	7	THR
3	G	10	LEU
3	G	31	TYR
3	G	33	ARG
3	G	211	ASN
3	G	214	TYR
3	G	229	MET
3	G	232	MET
3	G	237	LYS
3	G	240	SER
3	G	241	ASP
3	G	246	LEU
3	G	262	LEU
3	G	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	113	ASN
1	A	190	ASN
1	A	208	GLN
1	A	215	GLN
1	A	260	ASN

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	471	HIS
1	A	477	GLN
1	A	492	GLN
2	B	12	GLN
2	B	24	GLN
2	B	39	GLN
2	B	96	ASN
2	B	112	GLN
2	B	130	GLN
2	B	207	ASN
2	B	246	GLN
2	B	249	GLN
2	B	308	GLN
2	B	419	GLN
3	G	88	GLN
3	G	255	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
6	VO4	B	601	7,4	1,4,4	0.16	0	-		
5	ATP	A	603	4	28,33,33	2.61	8 (28%)	34,52,52	2.92	14 (41%)
7	ADP	B	604	6,4	24,29,29	1.73	6 (25%)	29,45,45	1.81	7 (24%)

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
5	ATP	A	603	4	-	6/18/38/38	0/3/3/3
7	ADP	B	604	6,4	-	5/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	ATP	C4-N3	7.47	1.45	1.35
5	A	603	ATP	C2-N3	6.21	1.41	1.32
5	A	603	ATP	C2-N1	6.11	1.44	1.33
7	B	604	ADP	C2-N1	3.86	1.40	1.33
5	A	603	ATP	O4'-C4'	-3.52	1.37	1.45
7	B	604	ADP	O4'-C1'	3.50	1.45	1.40
5	A	603	ATP	O4'-C1'	2.63	1.44	1.40
7	B	604	ADP	PB-O2B	-2.47	1.45	1.54
7	B	604	ADP	C2-N3	2.43	1.35	1.32
5	A	603	ATP	C5'-C4'	2.42	1.58	1.51
5	A	603	ATP	C6-N1	2.27	1.45	1.36
7	B	604	ADP	C1'-N9	2.27	1.55	1.49
5	A	603	ATP	O5'-C5'	-2.25	1.36	1.44
7	B	604	ADP	C4-N3	2.12	1.38	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	ATP	O4'-C1'-N9	-10.57	94.73	108.75
5	A	603	ATP	N3-C2-N1	-7.96	117.87	128.67
5	A	603	ATP	C4'-O4'-C1'	5.49	114.95	109.92
5	A	603	ATP	C5-C6-N6	3.92	126.29	120.31
7	B	604	ADP	O4'-C1'-N9	3.85	113.84	108.75
7	B	604	ADP	N3-C2-N1	-3.62	123.76	128.67
7	B	604	ADP	C5-C6-N6	3.54	125.70	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	604	ADP	C4'-O4'-C1'	3.16	112.82	109.92
5	A	603	ATP	C4-C5-N7	-2.71	106.47	109.34
7	B	604	ADP	O2A-PA-O3A	2.66	114.46	107.27
5	A	603	ATP	O5'-C5'-C4'	2.61	117.89	108.99
7	B	604	ADP	C5-C6-N1	-2.60	114.04	120.23
5	A	603	ATP	O2'-C2'-C3'	2.57	120.05	111.82
5	A	603	ATP	O2B-PB-O3A	2.51	114.07	107.27
5	A	603	ATP	O2A-PA-O3A	2.42	113.81	107.27
5	A	603	ATP	N6-C6-N1	-2.40	113.20	118.33
5	A	603	ATP	O3A-PA-O1A	-2.35	103.62	110.70
5	A	603	ATP	O2G-PG-O3B	2.30	112.35	104.64
5	A	603	ATP	O4'-C4'-C5'	-2.13	102.50	109.33
5	A	603	ATP	O3'-C3'-C4'	-2.10	105.05	111.08
7	B	604	ADP	O3A-PA-O1A	-2.09	104.41	110.70

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	603	ATP	C5'-O5'-PA-O3A
5	A	603	ATP	C4'-C5'-O5'-PA
7	B	604	ADP	PA-O3A-PB-O3B
5	A	603	ATP	O4'-C4'-C5'-O5'
5	A	603	ATP	C3'-C4'-C5'-O5'
5	A	603	ATP	PA-O3A-PB-O1B
5	A	603	ATP	PA-O3A-PB-O2B
7	B	604	ADP	PA-O3A-PB-O1B
7	B	604	ADP	PA-O3A-PB-O2B
7	B	604	ADP	PB-O3A-PA-O1A
7	B	604	ADP	PB-O3A-PA-O2A

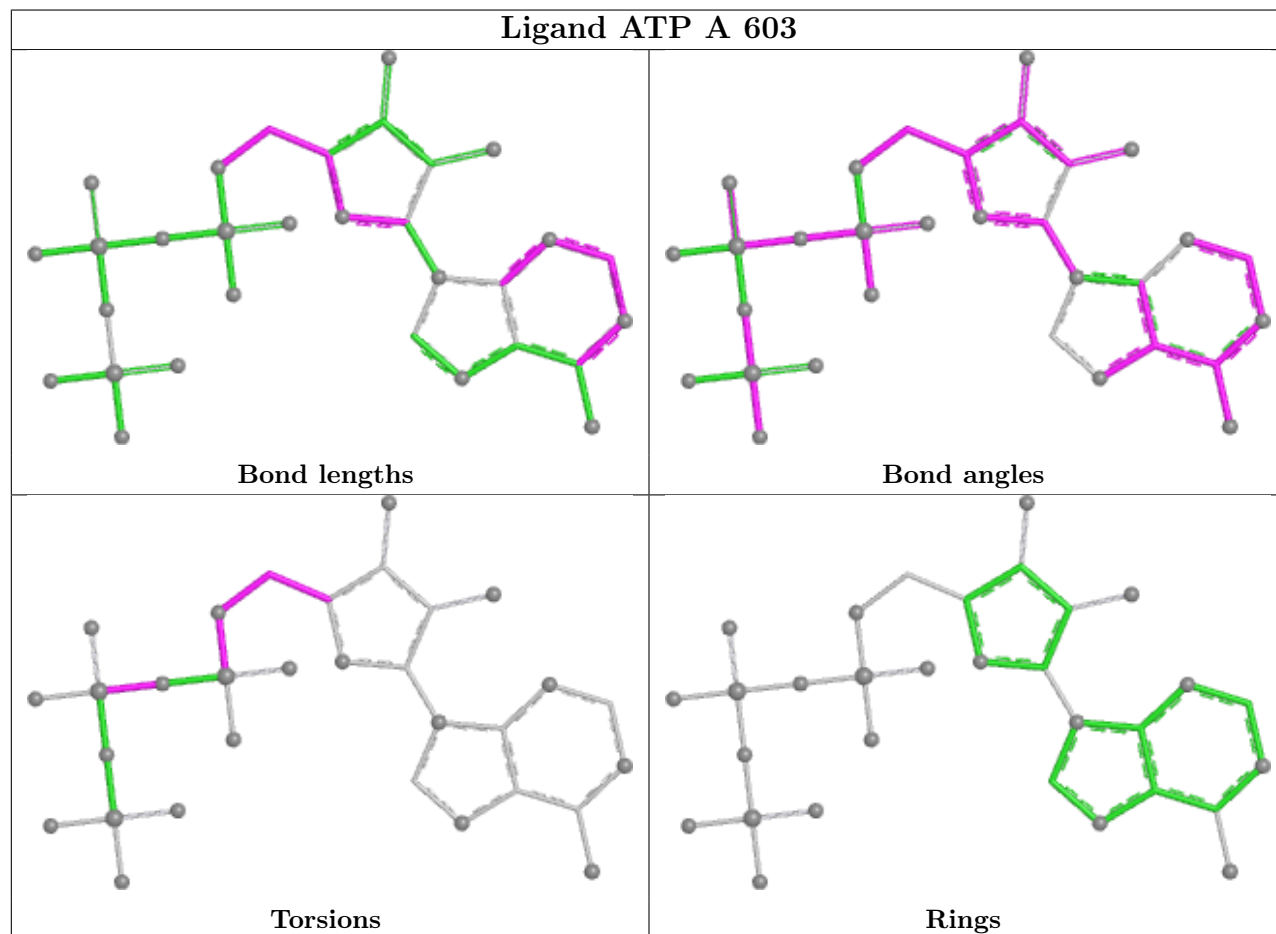
There are no ring outliers.

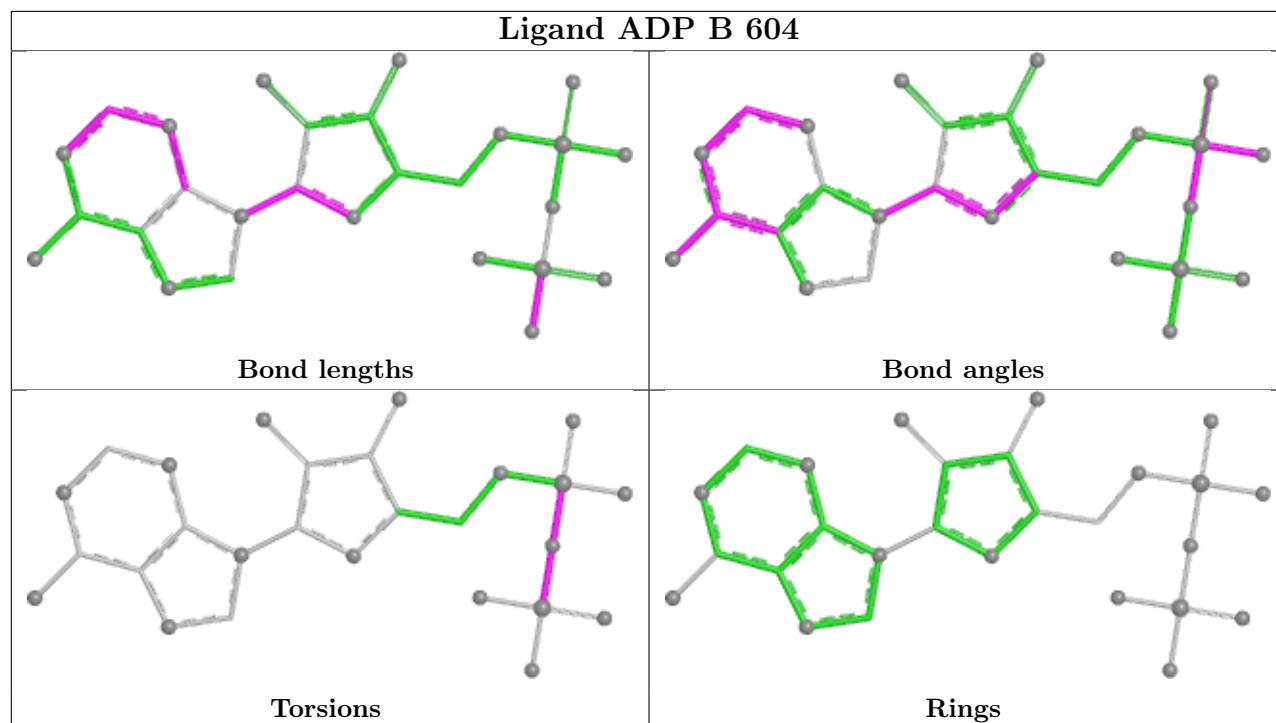
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	VO4	2	0
5	A	603	ATP	3	0
7	B	604	ADP	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	480/510 (94%)	0.99	69 (14%) 7 4	23, 68, 122, 134	13 (2%)
2	B	471/479 (98%)	0.99	90 (19%) 4 3	13, 62, 116, 136	21 (4%)
3	G	124/273 (45%)	2.31	67 (54%) 0 0	4, 14, 19, 20	124 (100%)
All	All	1075/1262 (85%)	1.15	226 (21%) 3 2	4, 60, 117, 136	158 (14%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	77	LEU	10.4
3	G	32	ALA	7.4
2	B	463	ILE	6.7
3	G	22	SER	6.3
1	A	489	ILE	6.1
3	G	223	SER	6.0
1	A	407[A]	GLY	6.0
1	A	501	VAL	6.0
3	G	253	THR	5.7
3	G	265	ILE	5.5
3	G	234	ASN	5.4
2	B	407	ALA	5.3
2	B	431	LEU	5.1
3	G	259	THR	5.1
3	G	235	ALA	5.0
1	A	391	LYS	5.0
2	B	417	PRO	4.8
3	G	21	LYS	4.5
1	A	497	LEU	4.5
2	B	460	VAL	4.5
1	A	147	GLN	4.5
3	G	20	THR	4.4
3	G	14	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	370	VAL	4.4
2	B	457	PHE	4.3
2	B	390[A]	ILE	4.3
3	G	17	GLN	4.3
2	B	162	LYS	4.3
3	G	25	MET	4.2
2	B	2	ALA	4.2
1	A	354	THR	4.2
3	G	48	SER	4.2
3	G	209	LEU	4.2
3	G	251	ASN	4.1
2	B	413	PHE	4.0
2	B	362	ILE	4.0
2	B	8	THR	3.9
1	A	401[A]	ALA	3.9
3	G	227	ALA	3.8
3	G	46	THR	3.8
1	A	172	GLN	3.8
2	B	452	LEU	3.6
3	G	23	MET	3.6
2	B	329	LEU	3.6
2	B	381[A]	TYR	3.6
1	A	469	LEU	3.6
2	B	334	VAL	3.6
2	B	399[A]	GLU	3.6
3	G	255	GLN	3.5
2	B	4	PRO	3.5
2	B	391[A]	LEU	3.5
1	A	445	ILE	3.5
2	B	376	LYS	3.5
1	A	465	GLU	3.5
3	G	219	GLU	3.5
3	G	87	LYS	3.5
2	B	359	ASP	3.5
3	G	45	GLY	3.5
3	G	231	ALA	3.4
2	B	7	GLY	3.4
1	A	394	LEU	3.3
2	B	462	PRO	3.3
2	B	451	HIS	3.3
2	B	380[A]	ASP	3.3
1	A	167	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	441	GLN	3.3
2	B	397[A]	SER	3.3
3	G	47	GLY	3.3
2	B	396[A]	LEU	3.3
3	G	44	TYR	3.3
1	A	365	ILE	3.2
3	G	28	ALA	3.2
1	A	499	GLU	3.2
2	B	410	ILE	3.2
3	G	261	GLU	3.1
2	B	416	GLN	3.1
1	A	99	VAL	3.1
1	A	358	TYR	3.1
2	B	384[A]	LEU	3.1
1	A	390	MET	3.1
3	G	9	ARG	3.1
2	B	461	GLY	3.1
2	B	168	GLU	3.1
3	G	232	MET	3.1
1	A	410[A]	LEU	3.1
3	G	220	SER	3.0
3	G	215	TYR	3.0
2	B	394[A]	ASP	3.0
1	A	479	LEU	3.0
1	A	500	ILE	3.0
3	G	31	TYR	3.0
3	G	226	SER	3.0
1	A	402[A]	ALA	3.0
3	G	243	ILE	3.0
3	G	18	LYS	2.9
3	G	33	ARG	2.9
1	A	144	GLU	2.9
1	A	180	ILE	2.8
3	G	41	ALA	2.8
1	A	475	GLN	2.8
2	B	429	GLY	2.8
2	B	357	ILE	2.8
2	B	377	ILE	2.8
2	B	458	TYR	2.8
2	B	437	THR	2.8
1	A	134	PRO	2.8
2	B	3	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	G	248	LEU	2.8
3	G	222	THR	2.8
2	B	375	GLN	2.8
3	G	6	ILE	2.8
1	A	417	LEU	2.8
3	G	35	GLU	2.8
1	A	217	VAL	2.8
3	G	249	THR	2.7
1	A	291	ARG	2.7
2	B	385[A]	GLN	2.7
3	G	214	TYR	2.7
2	B	432	VAL	2.7
3	G	239	ALA	2.7
2	B	449	TYR	2.7
2	B	430	LYS	2.7
2	B	309	ALA	2.7
2	B	446	ALA	2.6
1	A	400[A]	VAL	2.6
2	B	467	VAL	2.6
2	B	409	LYS	2.6
2	B	448	ASP	2.6
2	B	6	ALA	2.6
1	A	392	LEU	2.6
2	B	358	MET	2.5
2	B	363	VAL	2.5
2	B	435	LYS	2.5
1	A	337	TYR	2.5
3	G	254	ARG	2.5
2	B	9	ALA	2.5
2	B	171	ASN	2.5
2	B	445	LEU	2.5
2	B	146	TYR	2.5
2	B	119	GLU	2.5
1	A	132	LYS	2.5
1	A	452	TYR	2.5
1	A	334	VAL	2.5
2	B	279	VAL	2.5
2	B	351	LEU	2.4
1	A	476	HIS	2.4
3	G	86	ALA	2.4
1	A	486	ASP	2.4
1	A	175	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	156	GLY	2.4
2	B	444	ILE	2.4
3	G	258	ILE	2.4
2	B	447	GLY	2.4
2	B	158	ALA	2.4
2	B	340	ALA	2.4
2	B	388[A]	ILE	2.4
1	A	236	ALA	2.4
1	A	387	ALA	2.4
1	A	344	SER	2.3
2	B	1	SER	2.3
2	B	348	VAL	2.3
3	G	244	ASP	2.3
3	G	30	LYS	2.3
3	G	213	ILE	2.3
1	A	408[A]	SER	2.3
1	A	493	SER	2.3
3	G	267	SER	2.3
1	A	457	GLU	2.3
1	A	364	ALA	2.3
1	A	386	VAL	2.3
2	B	353	SER	2.3
3	G	217	LEU	2.3
1	A	200	TYR	2.3
1	A	487	GLY	2.3
1	A	446	TYR	2.2
1	A	174	GLY	2.2
3	G	272	LEU	2.2
1	A	483	ILE	2.2
3	G	16	ILE	2.2
1	A	480	LEU	2.2
2	B	338	ALA	2.2
1	A	414	THR	2.2
2	B	160	VAL	2.2
1	A	453	LEU	2.2
3	G	34	ALA	2.2
2	B	257	ASN	2.2
1	A	350	ILE	2.2
3	G	37	GLU	2.2
3	G	82	HIS	2.2
2	B	360	PRO	2.2
3	G	43	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	153	GLY	2.1
1	A	398	ARG	2.1
1	A	468	PHE	2.1
2	B	441	PHE	2.1
3	G	237	LYS	2.1
2	B	192	GLU	2.1
2	B	475	GLU	2.1
1	A	412[A]	ALA	2.1
2	B	468	ALA	2.1
3	G	225	GLN	2.1
1	A	130	GLY	2.1
2	B	161	GLY	2.1
3	G	13	ILE	2.1
2	B	420	VAL	2.1
1	A	395	ALA	2.1
1	A	341	ASN	2.1
1	A	444	VAL	2.1
1	A	378	ALA	2.1
2	B	443	GLN	2.1
2	B	434	LEU	2.1
3	G	38	LEU	2.1
2	B	436	GLU	2.1
2	B	326	PHE	2.0
2	B	424	PHE	2.0
2	B	143	LEU	2.0
2	B	414	LEU	2.0
2	B	138	LYS	2.0
2	B	422	GLU	2.0
3	G	8	ARG	2.0
3	G	247	THR	2.0
1	A	454	ASP	2.0
1	A	89	LYS	2.0
1	A	471	HIS	2.0
3	G	24	LYS	2.0
1	A	353	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

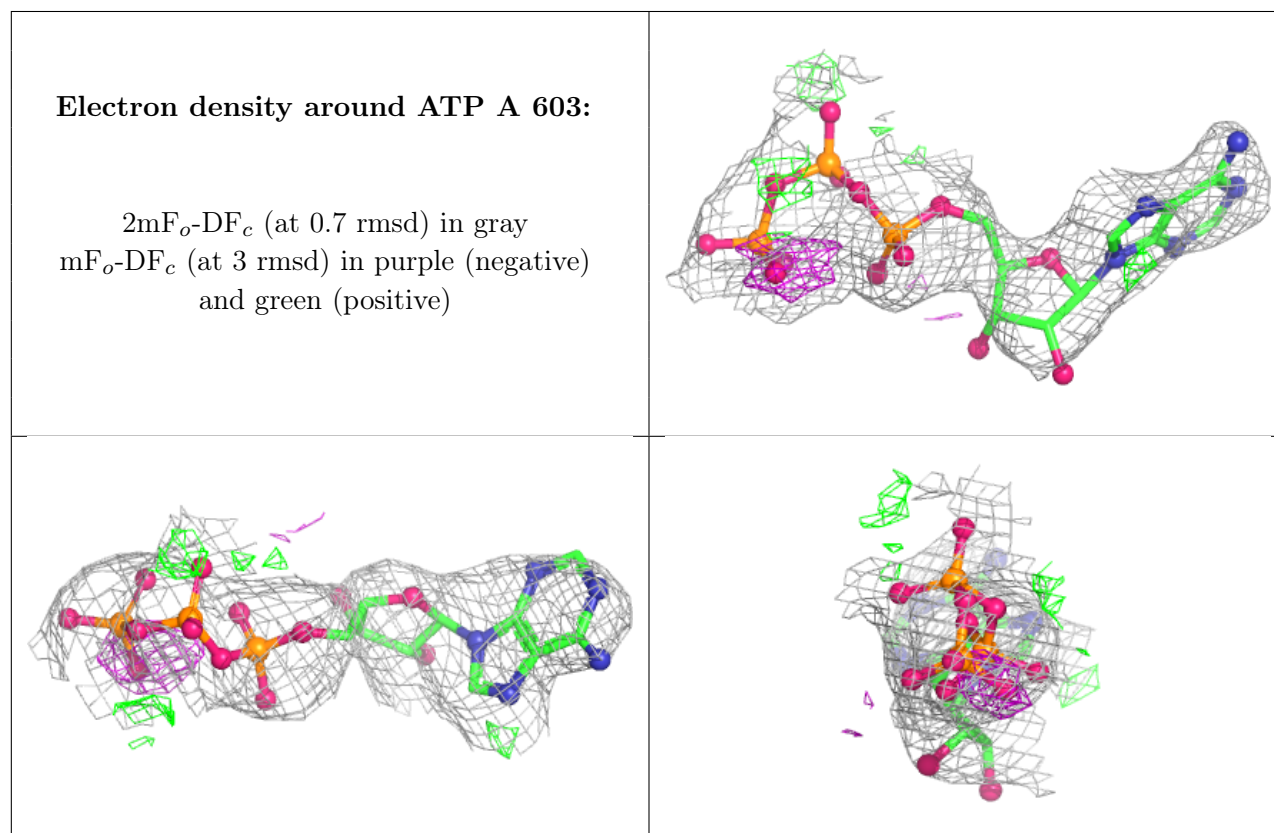
There are no monosaccharides in this entry.

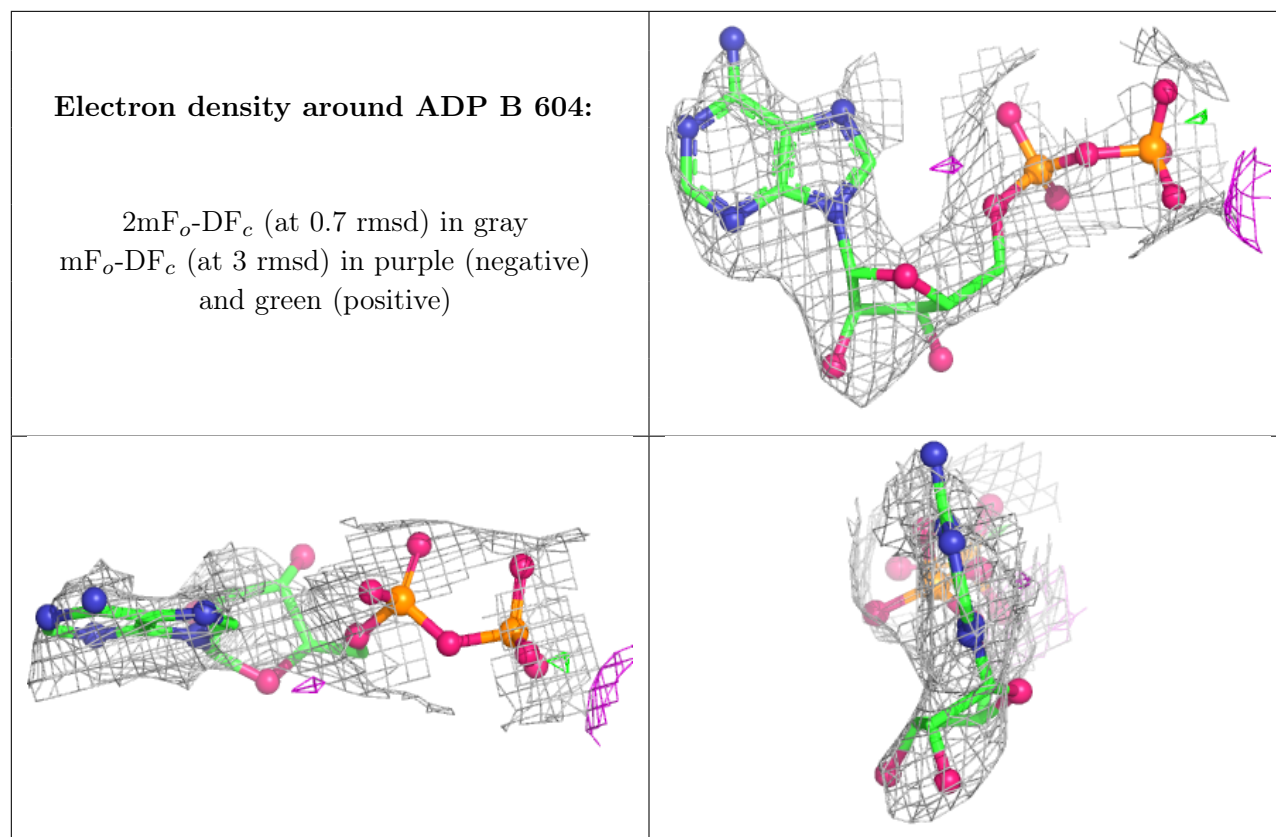
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	MG	A	602	1/1	0.60	0.28	55,55,55,55	0
5	ATP	A	603	31/31	0.77	0.14	57,68,73,74	0
7	ADP	B	604	27/27	0.79	0.18	97,100,102,102	0
4	MG	B	605	1/1	0.82	0.15	40,40,40,40	0
6	VO4	B	601	5/5	0.90	0.34	43,44,45,48	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.