Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:59 AM GMT

PDB ID	:	2F43
Title	:	Rat liver F1-ATPase
Authors	:	Chen, C.; Saxena, A.K.; Simcoke, W.N.; Garboczi, D.N.; Pedersen, P.L.; Ko, Y.H.
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

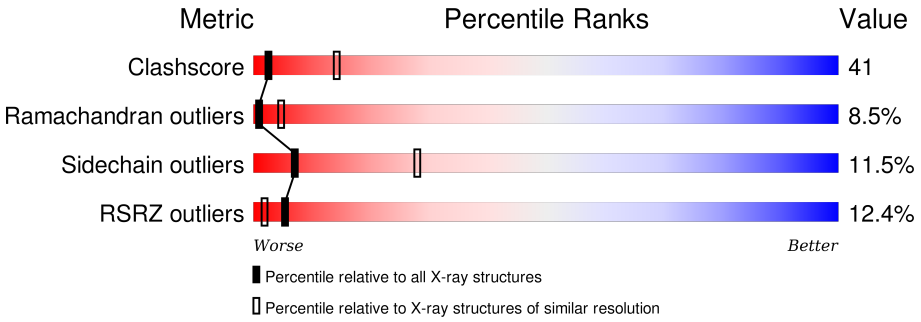
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5% 31% 54% 9% 6%
2	B	479	10% 34% 54% 10%
3	G	273	21% 21% 21% 55%

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
4	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
			Total	C	N	O	S			
1	A	480	3659	2301	648	698	12	0	13	0

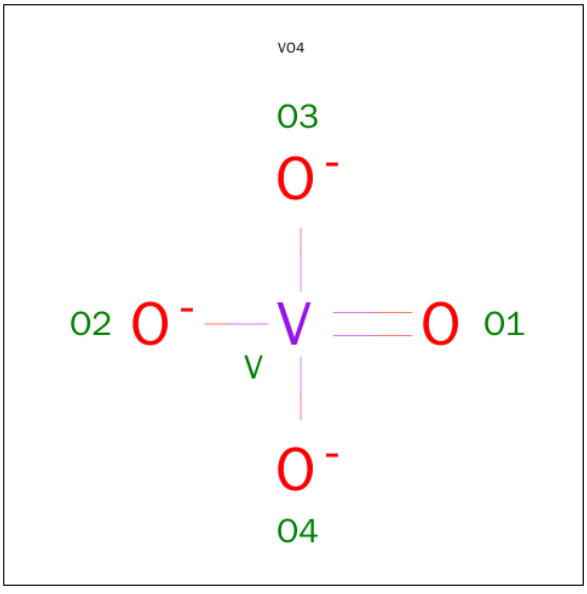
- Molecule 2 is a protein called ATP synthase beta chain, mitochondrial.

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

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

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

- Molecule 4 is VANADATE ION (three-letter code: VO4) (formula: O_4V).

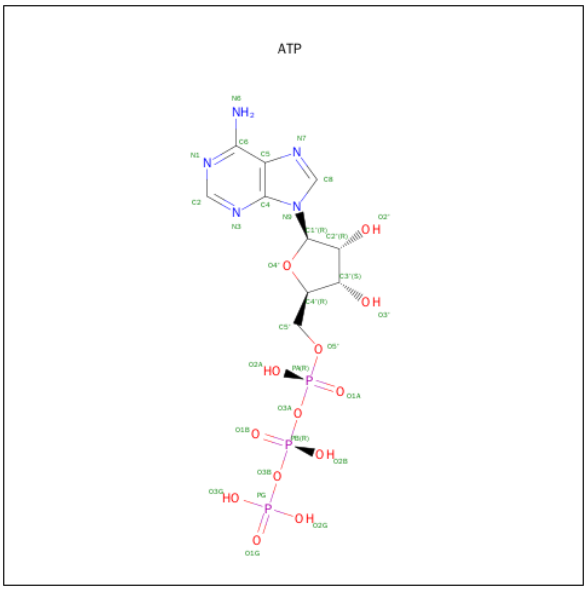


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O V 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

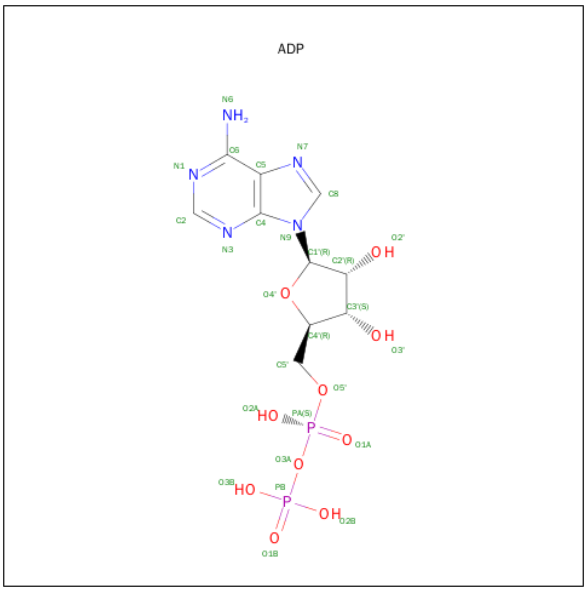
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



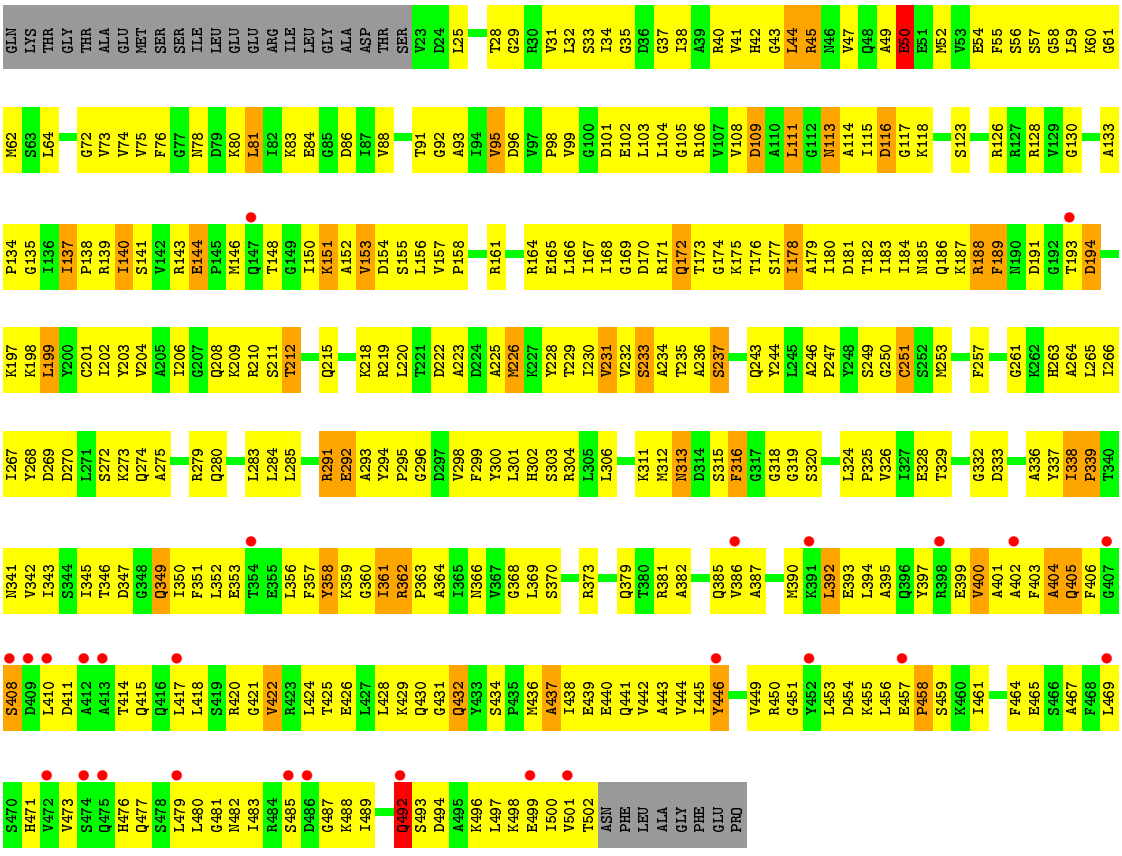
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	27	10	5	10	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

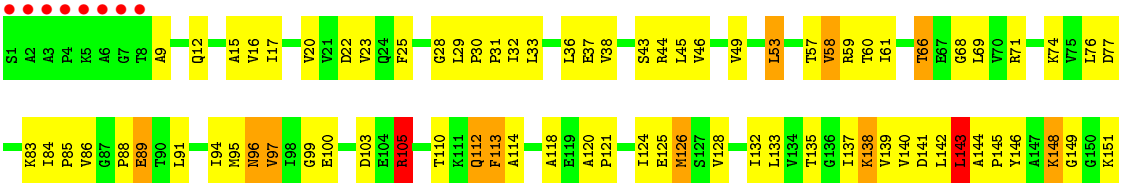
- Molecule 1: ATP synthase alpha chain, mitochondrial

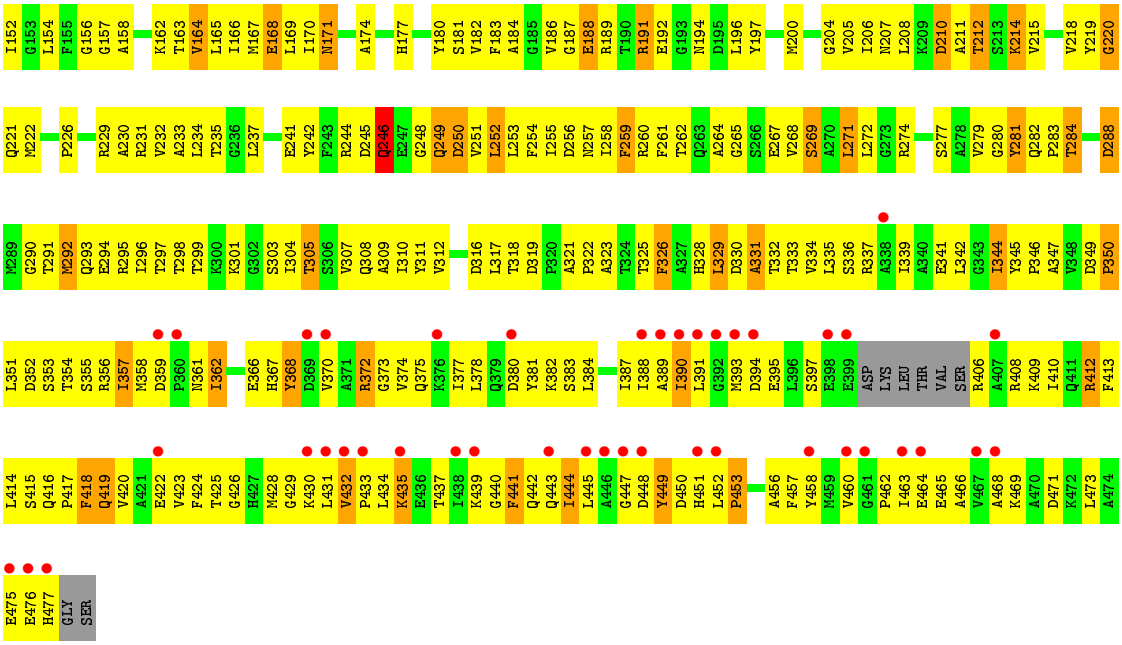
Chain A:



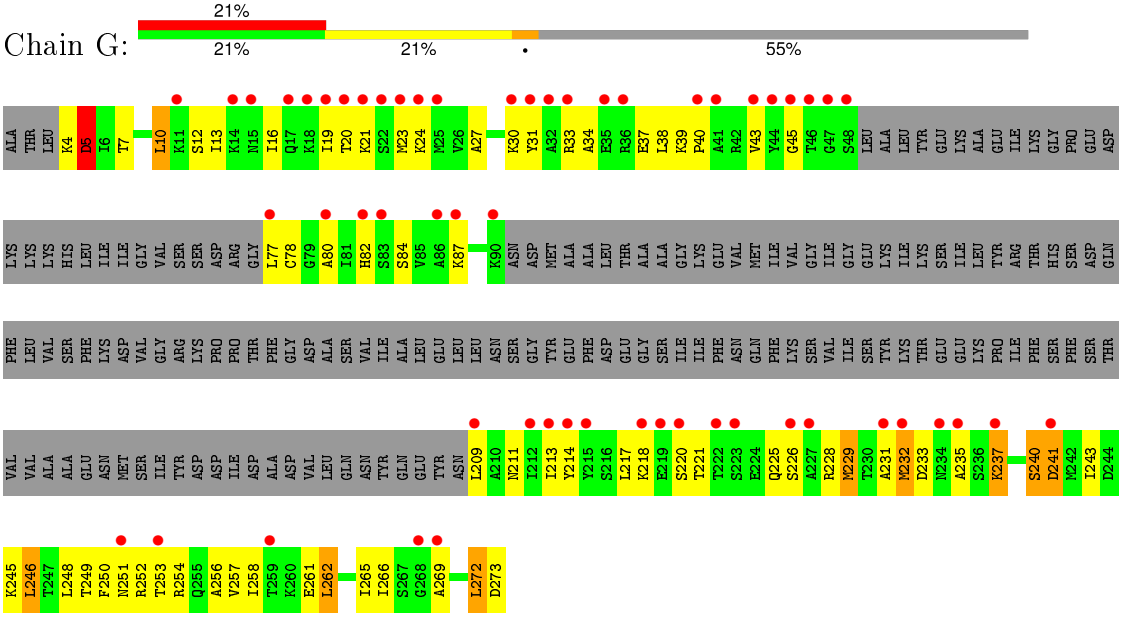
- Molecule 2: ATP synthase beta chain, mitochondrial

Chain B:





• Molecule 3: ATP synthase gamma chain, mitochondrial



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	144.57Å 144.57Å 362.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.00 19.82 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.97-3.00) 96.0 (19.82-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.49 (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.	DCC
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 91.1	EDS
Estimated twinning fraction	0.016 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.021 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 0.022 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 29849 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8234	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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(^{o})	Ideal(^{o})
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

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	305	0
3	G	954	0	1013	68	0
4	B	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	31	0	12	3	0
7	B	27	0	12	3	0
All	All	8234	0	8398	688	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 (688) 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:H	1:A:137:ILE:HD13	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: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
2:B:326:PHE:HA	2:B:329:LEU:HD21	1.58	0.86
1:A:148:THR:HA	1:A:182:THR:HG23	1.57	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
3:G:240:SER:O	3:G:243:ILE:N	2.13	0.79
1:A:175:LYS:HG2	1:A:352:LEU:HD12	1.63	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
2:B:86:VAL:HG23	2:B:112:GLN:HE21	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:CD1	1:A:137:ILE:H	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
2:B:157:GLY:HA2	2:B:312:VAL:HB	1.69	0.74
2:B:66:THR:HG22	2:B:69:LEU:HD12	1.67	0.74
1:A:394:LEU:HA	1:A:397:TYR:HB3	1.70	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
2:B:158:ALA:HB2	2:B:311:TYR:CE1	2.22	0.73
1:A:184:ILE:HD11	1:A:223:ALA:HB3	1.70	0.73
3:G:249:THR:O	3:G:252:ARG:HB2	1.89	0.72
1:A:444:VAL:HG11	1:A:465:GLU:HG3	1.70	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:N	1:A:137:ILE:HD13	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:HD2	1:A:381:ARG:H	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
2:B:406:ARG:O	2:B:409:LYS:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LYS:HE3	2:B:460:VAL:HG12	1.74	0.69
2:B:265:GLY:HA2	2:B:268:VAL:HG12	1.75	0.69
1:A:150:ILE:HG23	1:A:430:GLN:HG2	1.74	0.69
2:B:410:ILE:HG13	2:B:444:ILE:HG21	1.74	0.69
1:A:203:TYR:HB3	1:A:231:VAL:HG13	1.73	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
2:B:418:PHE:HA	2:B:430:LYS:H	1.60	0.67
1:A:137:ILE:HG12	1:A:138:PRO:HD3	1.77	0.67
1:A:38:ILE:HG13	1:A:284:LEU:HB3	1.77	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:233:ASP:CG	3:G:237:LYS:NZ	2.49	0.66
3:G:27:ALA:HB1	3:G:229:MET:HA	1.77	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:HG2	2:B:44:ARG:HH11	1.62	0.65
2:B:187:GLY:O	2:B:222:MET:HG3	1.96	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: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
2:B:145:PRO:HG2	2:B:357:ILE:HG23	1.78	0.64
1:A:167:ILE:HG22	1:A:350:ILE:HB	1.79	0.64
1:A:181:ASP:O	1:A:184:ILE:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:TYR:HA	2:B:346:PRO:C	2.18	0.63
1:A:337:TYR:O	1:A:338:ILE:HB	1.96	0.63
1:A:458:PRO:HA	1:A:461:ILE:HD11	1.81	0.63
1:A:361:ILE:O	1:A:364:ALA:HB2	1.98	0.63
1:A:397:TYR:HA	1:A:400[A]:VAL:CG2	2.28	0.63
1:A:356:LEU:HD12	1:A:364:ALA:HB1	1.79	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:HE21	1:A:477:GLN:HA	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
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:471:HIS:CE1	1:A:500:ILE:HD11	2.34	0.61
2:B:346:PRO:HD3	2:B:418:PHE:HE2	1.65	0.61
1:A:106:ARG:CZ	1:A:118:LYS:HB2	2.31	0.61
2:B:253:LEU:HG	2:B:255:ILE:HD11	1.83	0.60
2:B:118:ALA:HB3	2:B:295:ARG:NH2	2.15	0.60
1:A:313:ASN:HD22	1:A:316:PHE:HB2	1.66	0.60
2:B:408:ARG:HD2	2:B:412:ARG:NH2	2.17	0.60
1:A:103:LEU:O	1:A:230:ILE:HG12	2.01	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
2:B:321:ALA:HB3	2:B:322:PRO:HD3	1.83	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
1:A:106:ARG:O	1:A:231:VAL:HG23	2.02	0.60
3:G:27:ALA:O	3:G:229:MET:SD	2.60	0.60
2:B:16:VAL:O	2:B:17:ILE:HG13	2.02	0.60
1:A:141:SER:HB3	1:A:143:ARG:NH2	2.17	0.59
2:B:226:PRO:N	2:B:229:ARG:HH21	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:GLY:N	2:B:162:LYS:HE3	2.15	0.59
2:B:319:ASP:HB3	2:B:322:PRO:CD	2.32	0.59
2:B:36:LEU:O	2:B:46:VAL:HA	2.02	0.59
2:B:262:THR:HG23	2:B:282:GLN:NE2	2.16	0.59
2:B:181:SER:O	2:B:215:VAL:HA	2.03	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:167:MET:O	2:B:170:ILE:HB	2.03	0.59
2:B:132:ILE:HG13	2:B:133:LEU:N	2.18	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:406:ARG:HD2	2:B:444:ILE:O	2.02	0.58
2:B:138:LYS:CB	2:B:414:LEU:HA	2.34	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
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:113:ASN:H	1:A:113:ASN:ND2	1.99	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
2:B:200:MET:HB3	2:B:206:ILE:HG13	1.86	0.57
2:B:186:VAL:HG22	2:B:232:VAL:HG13	1.85	0.57
1:A:99:VAL:HG23	1:A:253:MET:HA	1.85	0.57
3:G:231:ALA:O	3:G:235:ALA:HB3	2.04	0.57
2:B:149:GLY:H	2:B:305:THR:HG23	1.69	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
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:203:TYR:HB3	1:A:231:VAL:CG1	2.33	0.57
3:G:21:LYS:O	3:G:24:LYS:HB3	2.04	0.57
2:B:162:LYS:HB2	2:B:162:LYS:HZ2	1.70	0.57
1:A:415:GLN:HA	1:A:418:LEU:HD12	1.86	0.57
4:B:601:VO4:O3	7:B:604:ADP:O1B	2.21	0.57
2:B:428:MET:O	2:B:430:LYS:N	2.38	0.57
1:A:150:ILE:HD11	1:A:181:ASP:HB2	1.86	0.57
1:A:184:ILE:HD11	1:A:223:ALA:CB	2.35	0.56
1:A:477:GLN:NE2	1:A:477:GLN:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:ASP:O	1:A:158:PRO:HG3	2.06	0.56
1:A:62:MET:CE	1:A:95:VAL:HG21	2.36	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
2:B:269:SER:O	2:B:272:LEU:HB2	2.05	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
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
3:G:240:SER:O	3:G:241:ASP:C	2.43	0.55
1:A:381:ARG:CD	1:A:381:ARG:H	2.19	0.55
1:A:37:GLY:O	1:A:38:ILE:HD13	2.06	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
1:A:108:VAL:CG2	1:A:232:VAL:HG12	2.36	0.55
3:G:40:PRO:O	3:G:45:GLY:HA3	2.05	0.55
2:B:449:TYR:CG	2:B:463:ILE:HD11	2.42	0.55
2:B:126:MET:HA	2:B:126:MET:HE3	1.87	0.55
1:A:188:ARG:HG3	1:A:189:PHE:CD1	2.42	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
2:B:191:ARG:HH21	2:B:192:GLU:HB3	1.72	0.55
1:A:410[A]:LEU:CD2	1:A:411[A]:ASP:H	2.18	0.55
2:B:138:LYS:CG	2:B:414:LEU:HA	2.35	0.55
1:A:482:ASN:HA	1:A:485:SER:OG	2.07	0.55
3:G:24:LYS:HB2	3:G:232:MET:HB3	1.88	0.54
1:A:138:PRO:HA	1:A:316:PHE:HD2	1.72	0.54
1:A:338:ILE:HB	1:A:339:PRO:HD3	1.88	0.54
1:A:168:ILE:HG12	1:A:329:THR:OG1	2.07	0.54
2:B:346:PRO:HD3	2:B:418:PHE:CE2	2.42	0.54
1:A:446:TYR:O	1:A:449:VAL:HG12	2.06	0.54
1:A:244:TYR:O	1:A:247:PRO:HD2	2.06	0.54
2:B:140:VAL:HG13	2:B:146:TYR:CZ	2.41	0.54
1:A:106:ARG:NH2	1:A:116:ASP:OD1	2.39	0.54
2:B:105:ARG:HE	2:B:208:LEU:HD22	1.73	0.54
1:A:151:LYS:HE3	1:A:436:MET:HG3	1.89	0.54
2:B:375:GLN:HA	2:B:378:LEU:HB2	1.89	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
3:G:258:ILE:O	3:G:262:LEU:HB2	2.07	0.54
1:A:483:ILE:O	1:A:487:GLY:HA2	2.08	0.54
1:A:183:ILE:HG12	1:A:265:LEU:HD23	1.90	0.54
1:A:146:MET:HG3	1:A:199:LEU:HD22	1.89	0.54
2:B:246:GLN:NE2	2:B:246:GLN:H	2.06	0.54
1:A:144:GLU:O	1:A:144:GLU:HG2	2.08	0.54
1:A:385:GLN:OE1	1:A:488:LYS:HG2	2.07	0.54
2:B:441:PHE:HD1	2:B:442:GLN:N	2.06	0.54
1:A:360:GLY:O	1:A:362:ARG:HG2	2.08	0.54
1:A:399:GLU:O	1:A:403[A]:PHE:CD1	2.61	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:105:GLY:HA2	1:A:226:MET:O	2.08	0.54
2:B:138:LYS:HD2	2:B:414:LEU:HD23	1.89	0.53
1:A:31:VAL:HG23	1:A:86:ASP:O	2.07	0.53
2:B:476:GLU:O	2:B:477:HIS:HB2	2.08	0.53
1:A:176:THR:O	1:A:180:ILE:HB	2.07	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
3:G:253:THR:HA	3:G:256:ALA:HB3	1.91	0.53
1:A:417:LEU:O	1:A:420:ARG:HG2	2.08	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:175:LYS:CG	1:A:352:LEU:HD12	2.37	0.53
1:A:91:THR:O	1:A:93:ALA:N	2.42	0.53
2:B:255:ILE:HG21	2:B:258:ILE:HB	1.90	0.53
1:A:180:ILE:HG13	1:A:220:LEU:HD21	1.91	0.53
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
1:A:55:PHE:CE2	1:A:75:VAL:HG22	2.43	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
1:A:313:ASN:HD21	1:A:315:SER:HB2	1.74	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:477:GLN:CA	1:A:477:GLN:HE21	2.21	0.52
3:G:4:LYS:O	3:G:5:ASP:HB3	2.08	0.52
2:B:452:LEU:HD22	2:B:466:ALA:HB1	1.90	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
2:B:38:VAL:HG21	2:B:45:LEU:CD2	2.37	0.52
2:B:372:ARG:HE	2:B:372:ARG:HA	1.75	0.52
1:A:265:LEU:HD11	1:A:324:LEU:CD1	2.40	0.52
2:B:242:TYR:HA	2:B:246:GLN:NE2	2.25	0.52
1:A:467:ALA:O	1:A:471:HIS:HB2	2.09	0.52
1:A:294:TYR:O	1:A:296:GLY:N	2.34	0.52
2:B:439:LYS:O	2:B:443:GLN:HG2	2.10	0.52
3:G:233:ASP:O	3:G:237:LYS:CD	2.45	0.51
1:A:431:GLY:CA	6:A:603:ATP:HN62	2.23	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
2:B:158:ALA:CB	2:B:311:TYR:HE1	2.17	0.51
1:A:386:VAL:HG12	1:A:450:ARG:NH2	2.25	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
2:B:43:SER:OG	2:B:44:ARG:N	2.42	0.51
1:A:386:VAL:HG13	1:A:489:ILE:HD11	1.91	0.51
1:A:362:ARG:HH12	2:B:372:ARG:CD	2.23	0.51
2:B:271:LEU:CD2	2:B:271:LEU:H	2.07	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
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
2:B:259:PHE:HZ	2:B:311:TYR:HD2	1.59	0.51
1:A:441:GLN:O	1:A:445:ILE:HG22	2.11	0.51
1:A:400[A]:VAL:HB	1:A:418:LEU:CD2	2.41	0.51
2:B:49:VAL:HA	2:B:60:THR:HG22	1.93	0.51
2:B:361:ASN:HB2	2:B:362:ILE:HD13	1.92	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
2:B:180:TYR:HB2	2:B:249:GLN:HE22	1.75	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
1:A:446:TYR:OH	1:A:494:ASP:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:GLY:O	1:A:319:GLY:HA2	2.11	0.50
2:B:267:GLU:O	2:B:271:LEU:HD11	2.11	0.50
1:A:493:SER:O	1:A:497:LEU:HD12	2.11	0.50
2:B:406:ARG:HD3	2:B:450:ASP:OD2	2.11	0.50
2:B:163:THR:O	2:B:166:ILE:HG22	2.12	0.50
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.27	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
2:B:426:GLY:O	2:B:428:MET:HG3	2.12	0.50
1:A:353:GLU:OE1	1:A:366:ASN:HB2	2.11	0.50
3:G:226:SER:O	3:G:229:MET:HB2	2.11	0.50
1:A:483:ILE:HD13	1:A:488:LYS:N	2.27	0.50
1:A:397:TYR:CE2	1:A:401[A]:ALA:HB2	2.46	0.50
2:B:383[A]:SER:O	2:B:387[A]:ILE:N	2.43	0.50
2:B:316:ASP:HB3	2:B:318:THR:OG1	2.11	0.50
1:A:402[A]:ALA:O	1:A:403[A]:PHE:CD1	2.65	0.49
3:G:228:ARG:O	3:G:229:MET:C	2.50	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:413:PHE:CZ	2:B:444:ILE:HD11	2.47	0.49
2:B:88:PRO:HA	2:B:91:LEU:HD12	1.94	0.49
3:G:23:MET:SD	3:G:228:ARG:HG3	2.52	0.49
1:A:446:TYR:HA	1:A:449:VAL:HG12	1.94	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
2:B:29:LEU:CD1	2:B:58:VAL:HG13	2.42	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:257:PHE:HD2	1:A:264:ALA:HB2	1.77	0.49
2:B:408:ARG:O	2:B:412:ARG:HG2	2.12	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: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:445:ILE:HG23	1:A:446:TYR:N	2.27	0.49
1:A:397:TYR:CZ	1:A:421:GLY:HA3	2.47	0.49
2:B:358:MET:HE3	2:B:368:TYR:HB2	1.94	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:362:ILE:N	2:B:362:ILE:HD13	2.27	0.49
2:B:281:TYR:HD1	2:B:281:TYR:H	1.61	0.49
1:A:386:VAL:O	1:A:449:VAL:HG21	2.12	0.49
2:B:96:ASN:C	2:B:96:ASN:HD22	2.16	0.49
2:B:174:ALA:O	2:B:177:HIS:HB3	2.12	0.49
3:G:82:HIS:CD2	3:G:82:HIS:H	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
2:B:373:GLY:O	2:B:377:ILE:HG22	2.13	0.48
2:B:138:LYS:HB3	2:B:414:LEU:HA	1.94	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
3:G:233:ASP:CG	3:G:237:LYS:HZ2	2.17	0.48
1:A:137:ILE:CG1	1:A:138:PRO:HD3	2.43	0.48
2:B:196:LEU:HD23	2:B:219:TYR:OH	2.12	0.48
1:A:410[A]:LEU:HD22	1:A:411[A]:ASP:N	2.26	0.48
3:G:78:CYS:SG	3:G:78:CYS:O	2.71	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
2:B:251:VAL:HG12	2:B:252:LEU:N	2.28	0.48
1:A:102:GLU:OE1	1:A:123:SER:HA	2.14	0.48
3:G:23:MET:HB3	3:G:232:MET:HG2	1.96	0.48
2:B:268:VAL:O	2:B:272:LEU:HG	2.14	0.48
2:B:113:PHE:N	2:B:113:PHE:CD1	2.81	0.48
1:A:392:LEU:HA	1:A:395:ALA:HB2	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
2:B:319:ASP:C	2:B:321:ALA:H	2.17	0.47
1:A:385:GLN:CG	1:A:489:ILE:HD12	2.43	0.47
1:A:98:PRO:HA	1:A:126:ARG:HD3	1.95	0.47
2:B:259:PHE:CD1	2:B:259:PHE:C	2.87	0.47
3:G:241:ASP:O	3:G:245:LYS:N	2.48	0.47
2:B:370:VAL:O	2:B:374:VAL:HG23	2.13	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
3:G:251:ASN:HA	3:G:254:ARG:HB3	1.97	0.47
2:B:374:VAL:HG22	2:B:410:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLN:HA	1:A:492:GLN:HE21	1.79	0.47
1:A:223:ALA:C	1:A:225:ALA:H	2.18	0.47
2:B:296:ILE:HD13	2:B:308:GLN:OE1	2.13	0.47
2:B:38:VAL:HG11	2:B:69:LEU:HD21	1.96	0.47
1:A:356:LEU:HB2	1:A:364:ALA:HB1	1.96	0.47
2:B:212:THR:HG22	2:B:214:LYS:HZ1	1.79	0.47
1:A:173:THR:HG22	1:A:352:LEU:HB3	1.96	0.47
3:G:249:THR:HA	3:G:252:ARG:HH11	1.79	0.47
2:B:378:LEU:HD23	2:B:381[A]:TYR:HD2	1.80	0.47
1:A:81:LEU:HD12	1:A:81:LEU:H	1.79	0.47
2:B:237:LEU:HD23	2:B:241:GLU:HG3	1.97	0.47
2:B:268:VAL:O	2:B:271:LEU:HG	2.14	0.47
2:B:258:ILE:O	2:B:258:ILE:HG13	2.14	0.47
1:A:34:ILE:HD12	1:A:35:GLY:N	2.27	0.47
2:B:335:LEU:HA	2:B:347:ALA:O	2.15	0.47
1:A:359:LYS:HB2	1:A:361:ILE:HG12	1.97	0.47
1:A:177:SER:O	1:A:180:ILE:HG22	2.15	0.47
1:A:171:ARG:HH12	2:B:354:THR:HG21	1.79	0.47
1:A:498:LYS:HA	1:A:501:VAL:HG22	1.96	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: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
1:A:358:TYR:HE2	2:B:351:LEU:HD12	1.80	0.47
2:B:389[A]:ALA:HA	2:B:395[A]:GLU:HG3	1.97	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
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
2:B:139:VAL:HG23	2:B:414:LEU:HB3	1.97	0.47
1:A:33:SER:OG	1:A:40:ARG:HB2	2.15	0.47
1:A:152:ALA:HB2	1:A:428:LEU:O	2.16	0.46
2:B:298:THR:HG22	2:B:299:THR:N	2.31	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
1:A:45:ARG:O	1:A:45:ARG:HD3	2.14	0.46
1:A:135:GLY:O	1:A:138:PRO:HD2	2.15	0.46
2:B:38:VAL:HG23	2:B:45:LEU:O	2.16	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)
3:G:250:PHE:O	3:G:254:ARG:HB2	2.16	0.46
2:B:469:LYS:HE3	2:B:473:LEU:HD13	1.96	0.46
2:B:432:VAL:CG1	2:B:435:LYS:HD2	2.44	0.46
2:B:86:VAL:HG23	2:B:112:GLN:NE2	2.24	0.46
1:A:209:LYS:CD	2:B:356:ARG:HH12	2.29	0.46
1:A:204:VAL:HA	1:A:232:VAL:HG23	1.98	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
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
3:G:19:ILE:N	3:G:19:ILE:HD12	2.30	0.46
1:A:390:MET:SD	1:A:449:VAL:HB	2.56	0.46
1:A:188:ARG:HG3	1:A:189:PHE:HD1	1.78	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:386:VAL:HG12	1:A:450:ARG:HH21	1.80	0.45
1:A:178:ILE:HG23	1:A:179:ALA:H	1.81	0.45
1:A:312:MET:HB2	1:A:319:GLY:O	2.15	0.45
1:A:164:ARG:N	1:A:164:ARG:HD3	2.30	0.45
1:A:202:ILE:O	1:A:266:ILE:HA	2.16	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:H	2:B:362:ILE:HD13	1.82	0.45
1:A:156:LEU:HG	1:A:428:LEU:HD11	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:426:GLU:HB2	1:A:461:ILE:HD12	1.97	0.45
1:A:343:ILE:HD11	1:A:349:GLN:NE2	2.31	0.45
3:G:231:ALA:C	3:G:232:MET:SD	2.94	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
1:A:336:ALA:O	1:A:339:PRO:HD2	2.16	0.45
3:G:84:SER:HA	3:G:87:LYS:HE2	1.99	0.45
1:A:78:ASN:N	1:A:78:ASN:ND2	2.65	0.45
2:B:144:ALA:HB2	2:B:353:SER:O	2.15	0.45
1:A:225:ALA:HA	1:A:228:TYR:CE1	2.52	0.45
2:B:277:SER:O	2:B:280:GLY:N	2.47	0.45
2:B:121:PRO:HG3	2:B:297:THR:CG2	2.47	0.45
1:A:25:LEU:HA	1:A:28:THR:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:24:LYS:HE2	3:G:233:ASP:HB2	1.97	0.45
1:A:41:VAL:HG12	1:A:42:HIS:O	2.17	0.45
2:B:378:LEU:C	2:B:381[A]:TYR:HB3	2.36	0.45
1:A:431:GLY:HA2	6:A:603:ATP:HN62	1.81	0.45
2:B:235:THR:C	2:B:237:LEU:H	2.20	0.45
1:A:453:LEU:O	1:A:456:LEU:HG	2.16	0.45
2:B:284:THR:HB	2:B:288:ASP:OD1	2.16	0.45
1:A:153:VAL:O	1:A:157:VAL:N	2.49	0.45
2:B:86:VAL:O	2:B:112:GLN:NE2	2.50	0.45
1:A:300:TYR:O	1:A:304:ARG:HB3	2.16	0.45
1:A:81:LEU:HD12	1:A:81:LEU:N	2.31	0.45
1:A:469:LEU:O	1:A:473:VAL:HG22	2.17	0.45
2:B:267:GLU:O	2:B:271:LEU:HD21	2.17	0.44
2:B:162:LYS:HE2	2:B:311:TYR:HA	1.98	0.44
1:A:382:ALA:O	1:A:386:VAL:HG22	2.17	0.44
2:B:250:ASP:HA	2:B:303:SER:O	2.16	0.44
1:A:211:SER:O	1:A:215:GLN:HG2	2.17	0.44
2:B:469:LYS:C	2:B:469:LYS:HD3	2.37	0.44
2:B:416:GLN:HE21	2:B:418:PHE:HD2	1.64	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
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
1:A:209:LYS:HB2	1:A:212:THR:OG1	2.18	0.44
1:A:199:LEU:HD21	1:A:265:LEU:HB2	2.00	0.44
2:B:152:ILE:HB	2:B:307:VAL:HA	2.00	0.44
3:G:20:THR:O	3:G:232:MET:HG3	2.18	0.44
1:A:158:PRO:HG2	1:A:379:GLN:OE1	2.17	0.44
2:B:32:ILE:HA	2:B:49:VAL:HG12	2.00	0.44
1:A:417:LEU:C	1:A:420:ARG:HG2	2.37	0.44
2:B:332:THR:HB	2:B:354:THR:H	1.83	0.44
1:A:246:ALA:O	1:A:249:SER:HB2	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: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
1:A:38:ILE:HG23	1:A:285:LEU:HD23	2.00	0.44
1:A:146:MET:SD	1:A:265:LEU:HD13	2.57	0.44
1:A:104:LEU:HD22	1:A:230:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:LYS:O	3:G:5:ASP:CB	2.66	0.44
1:A:312:MET:O	1:A:318:GLY:HA2	2.17	0.44
2:B:419:GLN:HB2	2:B:419:GLN:HE21	1.59	0.44
3:G:10:LEU:HD23	3:G:13:ILE:HD12	1.99	0.44
2:B:137:ILE:O	2:B:141:ASP:HB3	2.18	0.44
1:A:140:ILE:HG23	1:A:141:SER:N	2.25	0.44
2:B:336:SER:O	2:B:339:ILE:HB	2.18	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
1:A:206:ILE:HD11	1:A:247:PRO:HG3	1.99	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
1:A:501:VAL:HG23	1:A:502:THR:N	2.32	0.44
3:G:257:VAL:O	3:G:261:GLU:HG2	2.18	0.44
2:B:259:PHE:CD2	2:B:321:ALA:HB1	2.53	0.44
2:B:66:THR:HG22	2:B:69:LEU:CD1	2.44	0.44
1:A:338:ILE:CB	1:A:339:PRO:HD3	2.48	0.44
1:A:111:LEU:HB3	1:A:113:ASN:HD21	1.82	0.44
1:A:436:MET:O	1:A:437:ALA:O	2.36	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
2:B:259:PHE:HB3	2:B:310:ILE:HG23	1.98	0.43
1:A:150:ILE:HB	1:A:153:VAL:HB	1.99	0.43
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
2:B:268:VAL:HA	2:B:271:LEU:HG	2.00	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
1:A:153:VAL:HG12	1:A:154:ASP:N	2.33	0.43
1:A:64:LEU:HD22	1:A:74:VAL:CG1	2.48	0.43
1:A:189:PHE:N	1:A:189:PHE:CD1	2.86	0.43
1:A:135:GLY:H	1:A:139:ARG:HE	1.66	0.43
2:B:76:LEU:HG	2:B:77:ASP:N	2.32	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:158:ALA:O	2:B:337:ARG:NH2	2.52	0.43
2:B:149:GLY:HA2	2:B:304:ILE:O	2.18	0.43
2:B:255:ILE:HD12	2:B:255:ILE:N	2.33	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:330:ASP:O	2:B:331:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASP:HB3	1:A:273:LYS:HB2	2.00	0.43
1:A:267:ILE:CD1	1:A:324:LEU:HD13	2.48	0.43
3:G:24:LYS:O	3:G:27:ALA:HB3	2.18	0.43
2:B:456:ALA:O	2:B:469:LYS:HD2	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:363:PRO:O	1:A:364:ALA:HB3	2.19	0.43
1:A:101:ASP:O	1:A:104:LEU:HB2	2.19	0.43
1:A:390:MET:CE	1:A:449:VAL:HB	2.48	0.43
2:B:142:LEU:HG	2:B:367:HIS:CD2	2.54	0.43
1:A:299:PHE:CD2	1:A:303:SER:OG	2.71	0.43
1:A:404[A]:ALA:O	1:A:406[A]:PHE:N	2.52	0.43
2:B:374:VAL:O	2:B:378:LEU:HD12	2.18	0.43
1:A:29:GLY:HA3	1:A:42:HIS:O	2.19	0.43
2:B:32:ILE:O	2:B:33:LEU:HB2	2.19	0.43
1:A:292:GLU:C	1:A:294:TYR:H	2.23	0.43
1:A:480:LEU:HD12	1:A:481:GLY:N	2.34	0.43
2:B:162:LYS:HB3	7:B:604:ADP:O2B	2.19	0.42
2:B:148:LYS:HA	2:B:305:THR:HG23	2.00	0.42
1:A:397:TYR:HA	1:A:400[A]:VAL:HG22	2.00	0.42
2:B:182:VAL:HG12	2:B:183:PHE:N	2.34	0.42
1:A:172:GLN:HA	1:A:172:GLN:OE1	2.18	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
2:B:188:GLU:HA	2:B:222:MET:CE	2.50	0.42
2:B:412:ARG:HD2	2:B:458:TYR:CD1	2.54	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
1:A:44:LEU:HD12	1:A:47:VAL:HB	2.01	0.42
2:B:230:ALA:HB2	2:B:264:ALA:HB1	2.00	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
2:B:378:LEU:HD23	2:B:381[A]:TYR:CD2	2.54	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
1:A:171:ARG:HH12	2:B:354:THR:CG2	2.32	0.42
3:G:217:LEU:HA	3:G:220:SER:HB2	2.01	0.42
1:A:368:GLY:C	1:A:369:LEU:HD22	2.40	0.42
2:B:165:LEU:HG	2:B:169:LEU:HD11	2.02	0.42
2:B:441:PHE:CD1	2:B:442:GLN:N	2.85	0.42
2:B:189:ARG:HD2	2:B:189:ARG:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:HD13	1:A:338:ILE:HA	1.97	0.42
1:A:229:THR:HG22	1:A:230:ILE:N	2.35	0.42
1:A:189:PHE:N	1:A:189:PHE:HD1	2.18	0.42
2:B:140:VAL:HG13	2:B:146:TYR:OH	2.20	0.42
1:A:25:LEU:HD22	1:A:43:GLY:HA3	2.01	0.42
2:B:53:LEU:HD12	2:B:57:THR:HG22	2.00	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
2:B:164:VAL:HG11	7:B:604:ADP:N7	2.35	0.42
1:A:50:GLU:O	1:A:95:VAL:HG23	2.20	0.42
3:G:249:THR:O	3:G:252:ARG:CB	2.63	0.42
1:A:98:PRO:HG3	1:A:126:ARG:CZ	2.50	0.42
1:A:411[A]:ASP:O	1:A:414:THR:HG22	2.19	0.42
1:A:113:ASN:ND2	1:A:113:ASN:N	2.66	0.42
3:G:257:VAL:HG12	3:G:261:GLU:OE2	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:165:GLU:OE2	1:A:350:ILE:HD11	2.20	0.42
1:A:169:GLY:HA2	1:A:352:LEU:O	2.20	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
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
2:B:149:GLY:N	2:B:305:THR:HG23	2.33	0.41
1:A:209:LYS:HE3	2:B:356:ARG:NH2	2.32	0.41
1:A:146:MET:HA	1:A:161:ARG:HH21	1.84	0.41
1:A:251:CYS:SG	1:A:268:TYR:OH	2.77	0.41
3:G:249:THR:C	3:G:252:ARG:HB2	2.40	0.41
1:A:403[A]:PHE:O	1:A:406[A]:PHE:HD1	1.97	0.41
1:A:397:TYR:CE2	1:A:421:GLY:HA3	2.55	0.41
1:A:324:LEU:N	1:A:324:LEU:HD12	2.36	0.41
1:A:431:GLY:HA2	6:A:603:ATP:N6	2.35	0.41
1:A:349:GLN:OE1	1:A:370:SER:HA	2.20	0.41
3:G:272:LEU:HB3	3:G:273:ASP:H	1.75	0.41
2:B:255:ILE:HG12	2:B:258:ILE:HD13	2.01	0.41
1:A:199:LEU:HA	1:A:199:LEU:HD12	1.91	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:HA	3:G:39:LYS:HD2	1.72	0.41
1:A:140:ILE:HB	1:A:313:ASN:HB2	2.02	0.41
2:B:447:GLY:O	2:B:450:ASP:HB3	2.21	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: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: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:156:GLY:HA3	2:B:162:LYS:NZ	2.36	0.41
1:A:397:TYR:HA	1:A:400[A]:VAL:HG23	2.03	0.41
1:A:73:VAL:HG12	1:A:74:VAL:N	2.36	0.41
2:B:143:LEU:O	2:B:145:PRO:HD3	2.21	0.41
1:A:329:THR:HG22	1:A:332:GLY:H	1.85	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:441:GLN:HB2	1:A:441:GLN:HE21	1.64	0.41
3:G:245:LYS:HD2	3:G:245:LYS:HA	1.90	0.41
1:A:300:TYR:O	1:A:304:ARG:NE	2.54	0.41
2:B:230:ALA:C	2:B:231:ARG:HD3	2.40	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
2:B:417:PRO:HD2	2:B:430:LYS:HG3	2.02	0.40
2:B:86:VAL:HG21	2:B:114:ALA:HB2	2.03	0.40
2:B:30:PRO:HG2	2:B:58:VAL:HG11	2.02	0.40
1:A:198:LYS:O	1:A:199:LEU:HB2	2.21	0.40
3:G:37:GLU:O	3:G:40:PRO:HD2	2.20	0.40
2:B:282:GLN:C	2:B:284:THR:H	2.25	0.40
2:B:259:PHE:HD2	2:B:321:ALA:HB1	1.87	0.40
2:B:186:VAL:HG12	2:B:260:ARG:HB2	2.03	0.40
1:A:349:GLN:O	1:A:370:SER:HB2	2.20	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
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
2:B:138:LYS:HD2	2:B:414:LEU:CD2	2.51	0.40
1:A:333:ASP:OD2	1:A:336:ALA:HB2	2.20	0.40
2:B:299:THR:C	2:B:301:LYS:H	2.24	0.40
1:A:299:PHE:O	1:A:303:SER:N	2.54	0.40
2:B:355:SER:OG	2:B:357:ILE:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ASN:ND2	2:B:100:GLU:N	2.67	0.40
3:G:209:LEU:O	3:G:213:ILE:HG22	2.22	0.40
1:A:246:ALA:HB3	1:A:247:PRO:HD3	2.04	0.40
2:B:74:LYS:N	2:B:74:LYS:HD2	2.36	0.40
2:B:422:GLU:C	2:B:424:PHE:H	2.24	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 5
2	B	467/479 (98%)	316 (68%)	104 (22%)	47 (10%)	1 3
3	G	118/273 (43%)	92 (78%)	22 (19%)	4 (3%)	5 25
All	All	1063/1262 (84%)	762 (72%)	211 (20%)	90 (8%)	1 5

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
1	A	357	PHE

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Mol	Chain	Res	Type
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
1	A	193	THR

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Mol	Chain	Res	Type
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 (i)

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%)	10 37
2	B	377/384 (98%)	330 (88%)	47 (12%)	6 24
3	G	103/230 (45%)	88 (85%)	15 (15%)	4 18
All	All	872/1030 (85%)	772 (88%)	100 (12%)	7 28

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
1	A	358	TYR
1	A	362	ARG
1	A	392	LEU
1	A	400[A]	VAL

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Mol	Chain	Res	Type
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
2	B	349	ASP
2	B	352	ASP
2	B	359	ASP
2	B	362	ILE

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Mol	Chain	Res	Type
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

Some 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
1	A	341	ASN
1	A	471	HIS
1	A	477	GLN
1	A	492	GLN

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Mol	Chain	Res	Type
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

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 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	ATP	A	603	5	24,33,33	2.60	8 (33%)	31,52,52	3.48	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	VO4	B	601	2,5,7	1,4,4	0.07	0	0,6,6	0.00	-
7	ADP	B	604	5,4	22,29,29	1.64	4 (18%)	27,45,45	2.05	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	A	603	5	-	0/18/38/38	0/3/3/3
4	VO4	B	601	2,5,7	-	0/0/0/0	0/0/0/0
7	ADP	B	604	5,4	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	ATP	O4'-C4'	-3.40	1.37	1.45
7	B	604	ADP	PB-O2B	-2.53	1.45	1.54
6	A	603	ATP	O5'-C5'	-2.13	1.36	1.44
7	B	604	ADP	C2-N3	2.07	1.35	1.32
6	A	603	ATP	C5'-C4'	2.22	1.58	1.51
6	A	603	ATP	O4'-C1'	2.48	1.44	1.41
6	A	603	ATP	C5-C4	2.61	1.46	1.40
7	B	604	ADP	O4'-C1'	3.39	1.45	1.41
7	B	604	ADP	C2-N1	3.63	1.40	1.33
6	A	603	ATP	C2-N3	5.39	1.41	1.32
6	A	603	ATP	C2-N1	5.73	1.44	1.33
6	A	603	ATP	C4-N3	6.83	1.45	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	603	ATP	N3-C2-N1	-14.39	117.87	128.89
7	B	604	ADP	N3-C2-N1	-6.71	123.76	128.89
6	A	603	ATP	O4'-C1'-N9	-6.38	94.73	108.10
7	B	604	ADP	C2'-C1'-N9	-3.76	108.55	114.29
6	A	603	ATP	C4-C5-N7	-3.27	106.47	109.48
6	A	603	ATP	N6-C6-N1	-2.79	113.20	119.20
6	A	603	ATP	PB-O3B-PG	-2.66	123.74	132.67
6	A	603	ATP	O3'-C3'-C4'	-2.00	105.05	111.05
6	A	603	ATP	C2-N1-C6	2.04	122.42	118.77
7	B	604	ADP	O2A-PA-O3A	2.06	114.46	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	603	ATP	O5'-C5'-C4'	2.38	117.89	109.12
6	A	603	ATP	O2'-C2'-C3'	2.53	120.05	111.83
7	B	604	ADP	O4'-C1'-N9	2.74	113.84	108.10
7	B	604	ADP	C2-N1-C6	2.82	123.81	118.77
7	B	604	ADP	C4'-O4'-C1'	2.82	112.82	109.72
6	A	603	ATP	C4'-O4'-C1'	4.76	114.95	109.72
6	A	603	ATP	C2'-C1'-N9	5.81	123.17	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	ATP	3	0
4	B	601	VO4	1	0
7	B	604	ADP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	480/510 (94%)	0.13	27 (5%) 28 11	23, 68, 124, 141	13 (2%)
2	B	471/479 (98%)	0.27	50 (10%) 8 3	13, 62, 116, 136	21 (4%)
3	G	124/273 (45%)	2.32	56 (45%) 0 0	11, 42, 58, 60	124 (100%)
All	All	1075/1262 (85%)	0.44	133 (12%) 5 2	11, 60, 120, 141	158 (14%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	48	SER	12.2
3	G	32	ALA	10.1
3	G	209	LEU	10.0
3	G	223	SER	7.3
3	G	47	GLY	7.3
3	G	20	THR	7.1
3	G	43	VAL	6.8
3	G	41	ALA	5.5
3	G	31	TYR	5.4
3	G	86	ALA	5.3
2	B	431	LEU	5.3
3	G	46	THR	5.2
3	G	22	SER	5.1
1	A	475	GLN	5.1
3	G	253	THR	5.1
3	G	44	TYR	4.9
3	G	30	LYS	4.8
2	B	432	VAL	4.7
3	G	35	GLU	4.7
2	B	475	GLU	4.6
2	B	7	GLY	4.6
3	G	40	PRO	4.5
1	A	486	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	391[A]	LEU	4.4
2	B	5	LYS	4.4
2	B	476	GLU	4.3
3	G	268	GLY	4.3
2	B	8	THR	4.2
1	A	452	TYR	4.2
2	B	451	HIS	4.2
2	B	399[A]	GLU	4.1
1	A	407[A]	GLY	4.1
3	G	234	ASN	4.1
2	B	477	HIS	4.1
2	B	398[A]	GLU	4.0
2	B	6	ALA	4.0
3	G	25	MET	4.0
2	B	4	PRO	4.0
2	B	370	VAL	3.8
3	G	17	GLN	3.8
2	B	1	SER	3.8
2	B	443	GLN	3.8
2	B	439	LYS	3.8
3	G	33	ARG	3.7
2	B	376	LYS	3.7
3	G	227	ALA	3.7
3	G	36	ARG	3.7
2	B	448	ASP	3.7
2	B	338	ALA	3.6
3	G	18	LYS	3.6
2	B	467	VAL	3.6
2	B	2	ALA	3.6
2	B	3	ALA	3.5
1	A	413	ALA	3.5
3	G	213	ILE	3.5
3	G	24	LYS	3.4
3	G	23	MET	3.4
2	B	463	ILE	3.4
3	G	226	SER	3.3
2	B	452	LEU	3.3
3	G	215	TYR	3.3
1	A	402[A]	ALA	3.3
1	A	417	LEU	3.3
2	B	407	ALA	3.2
3	G	259	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	235	ALA	3.1
2	B	435	LYS	3.1
2	B	447	GLY	3.1
2	B	445	LEU	3.1
2	B	460	VAL	3.1
3	G	21	LYS	3.1
1	A	193	THR	2.9
3	G	219	GLU	2.9
3	G	231	ALA	2.9
2	B	392[A]	GLY	2.9
3	G	212	ILE	2.9
3	G	220	SER	2.9
2	B	446	ALA	2.9
3	G	87	LYS	2.9
3	G	251	ASN	2.8
3	G	77	LEU	2.8
1	A	474	SER	2.8
3	G	241	ASP	2.8
3	G	80	ALA	2.8
3	G	19	ILE	2.8
1	A	409[A]	ASP	2.7
3	G	232	MET	2.7
2	B	390[A]	ILE	2.7
1	A	408[A]	SER	2.7
3	G	222	THR	2.6
2	B	461	GLY	2.6
1	A	391	LYS	2.6
1	A	501	VAL	2.6
2	B	438	ILE	2.6
2	B	422	GLU	2.6
2	B	388[A]	ILE	2.6
2	B	380[A]	ASP	2.5
2	B	433	PRO	2.5
2	B	369	ASP	2.5
1	A	410[A]	LEU	2.5
3	G	269	ALA	2.4
2	B	360	PRO	2.4
2	B	389[A]	ALA	2.4
3	G	214	TYR	2.4
2	B	394[A]	ASP	2.3
1	A	469	LEU	2.3
2	B	468	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	398	ARG	2.3
3	G	14	LYS	2.3
3	G	15	ASN	2.3
2	B	458	TYR	2.3
3	G	11	LYS	2.2
1	A	499	GLU	2.2
2	B	359	ASP	2.2
1	A	492	GLN	2.2
1	A	479	LEU	2.2
3	G	82	HIS	2.1
3	G	45	GLY	2.1
2	B	430	LYS	2.1
3	G	83	SER	2.1
1	A	446	TYR	2.1
2	B	393[A]	MET	2.1
2	B	464	GLU	2.1
1	A	412[A]	ALA	2.1
3	G	218	LYS	2.1
1	A	457	GLU	2.1
3	G	90	LYS	2.1
1	A	354	THR	2.1
3	G	237	LYS	2.1
1	A	386	VAL	2.1
1	A	147	GLN	2.0
1	A	472	VAL	2.0
1	A	485	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	VO4	B	601	5/5	0.87	0.44	2.57	43,44,45,48	0
7	ADP	B	604	27/27	0.82	0.29	-0.07	97,100,102,102	0
5	MG	B	605	1/1	0.87	0.24	-0.50	40,40,40,40	0
6	ATP	A	603	31/31	0.88	0.21	-0.51	57,68,73,74	0
5	MG	A	602	1/1	0.84	0.42	-	55,55,55,55	0

6.5 Other polymers

There are no such residues in this entry.