WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 22, 2023 – 06:06 PM EDT

PDB ID : 1MAB
Title : RAT LIVER F1-ATPASE
Authors : Bianchet, M.A.; Amzel, L.M.
Deposited on : 1998-08-06
Resolution : 2.80 Å(reported)

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

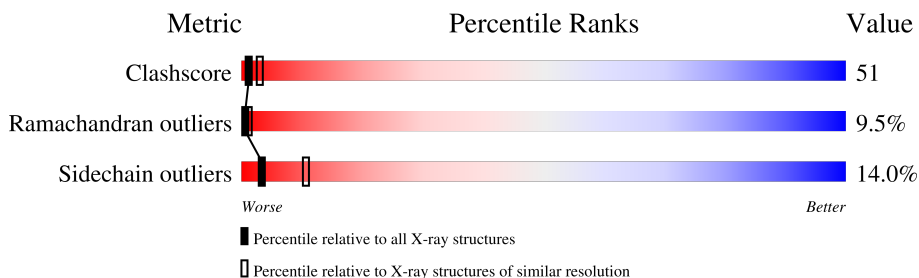|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.80 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	Percentile Ranks	Value
Clashscore		51
Ramachandran outliers		9.5%
Sidechain outliers		14.0%

Worse *Better*

▮ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	510	29% 57% 12% ••
2	B	479	25% 58% 14% •
3	G	270	24% 20% • 54%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 8489 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 PROTEIN (F1-ATPASE ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total 3810	C 2395	N 673	O 730	S 12	0	13	0

- Molecule 2 is a protein called PROTEIN (F1-ATPASE BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	477	Total 3598	C 2279	N 610	O 697	S 12	0	19	0

- Molecule 3 is a protein called PROTEIN (F1-ATPASE GAMMA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	124	Total 956	C 592	N 175	O 182	S 7	0	124	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ARG	LYS	conflict	UNP P35435

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

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
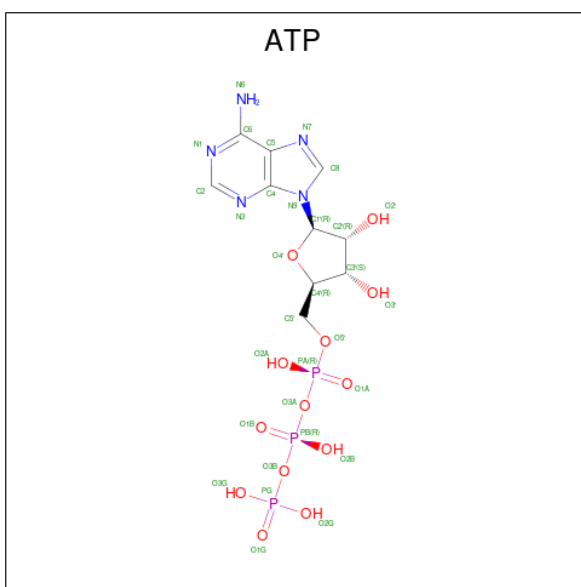
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
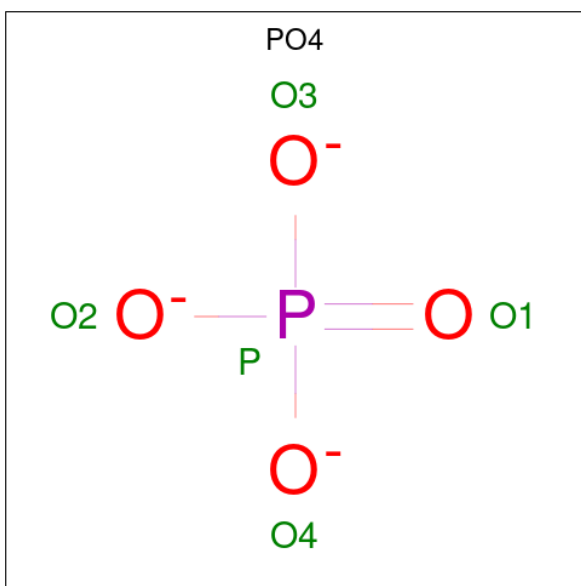
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
6	B	1	5	4	1	0	0

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

ADP

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

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	34	Total	O	0	0
			34	34		
8	B	24	Total	O	0	0
			24	24		
8	G	3	Total	O	0	0
			3	3		

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. 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. 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.
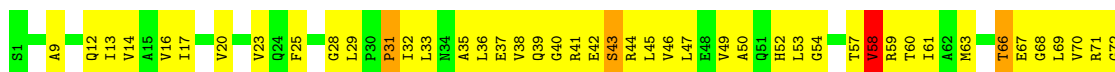
Note EDS was not executed.

• Molecule 1: PROTEIN (F1-ATPASE ALPHA CHAIN)

Chain A:
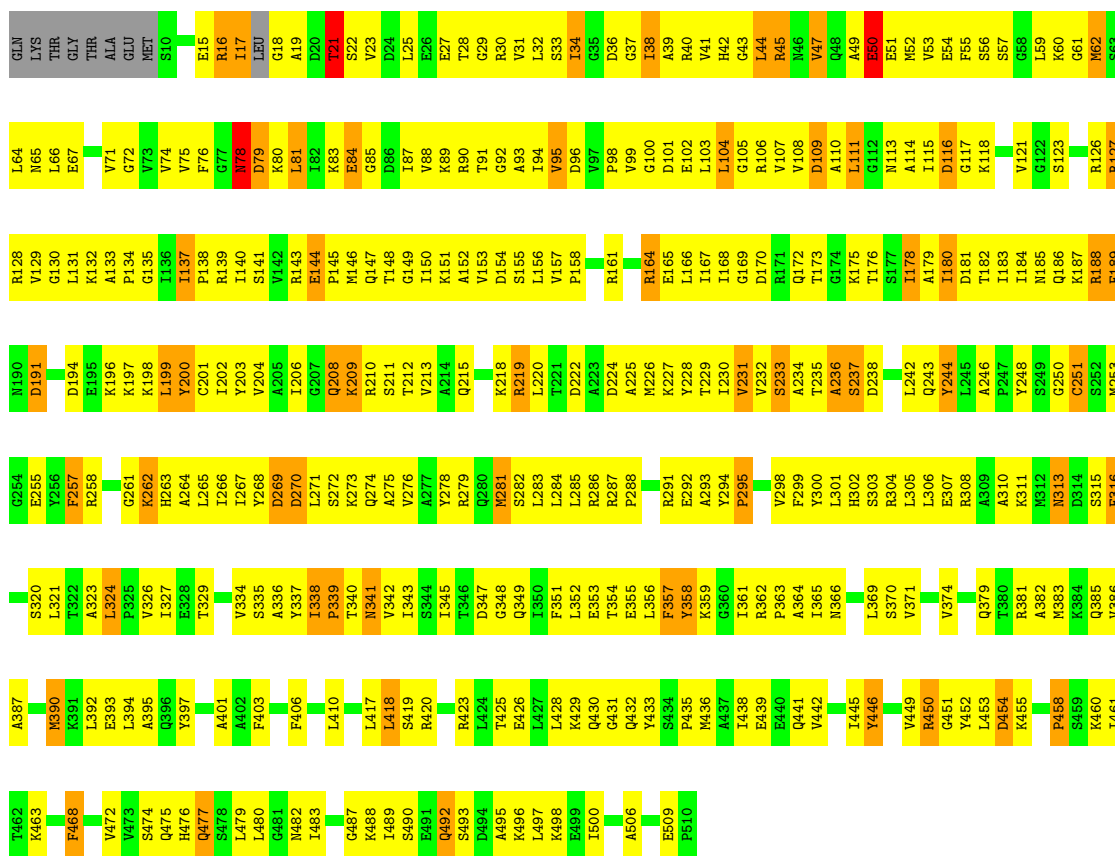
• Molecule 2: PROTEIN (F1-ATPASE BETA CHAIN)

Chain B:
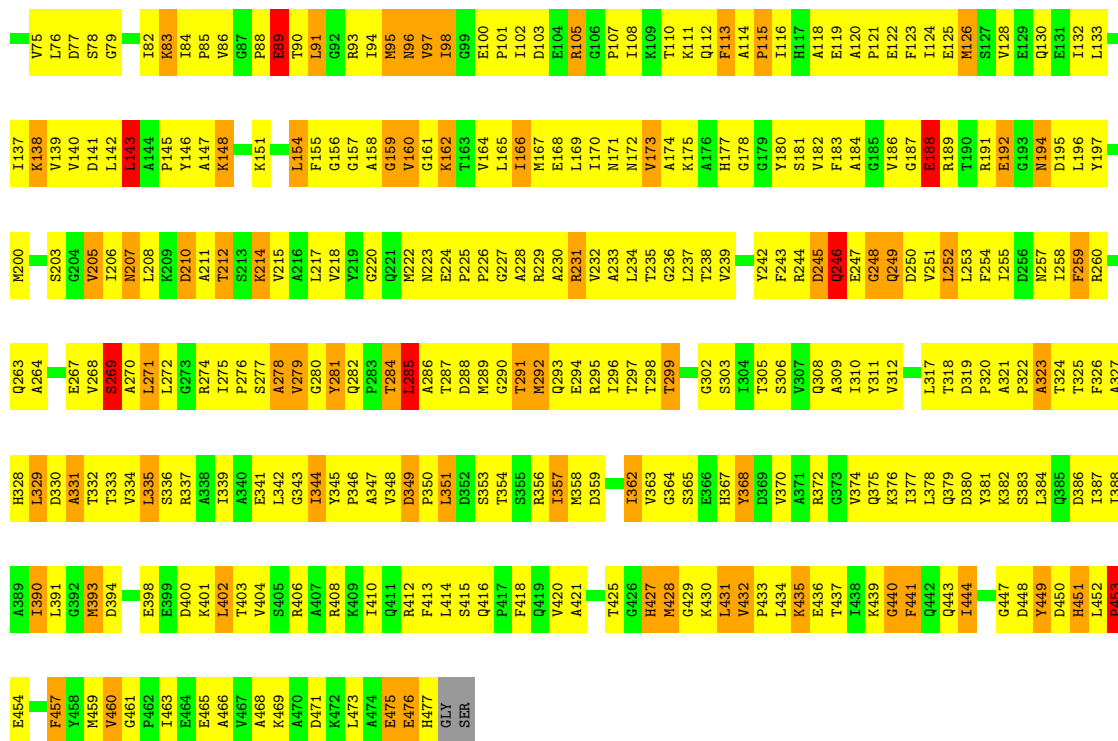
• Molecule 3: PROTEIN (F1-ATPASE GAMMA CHAIN)

Chain G:
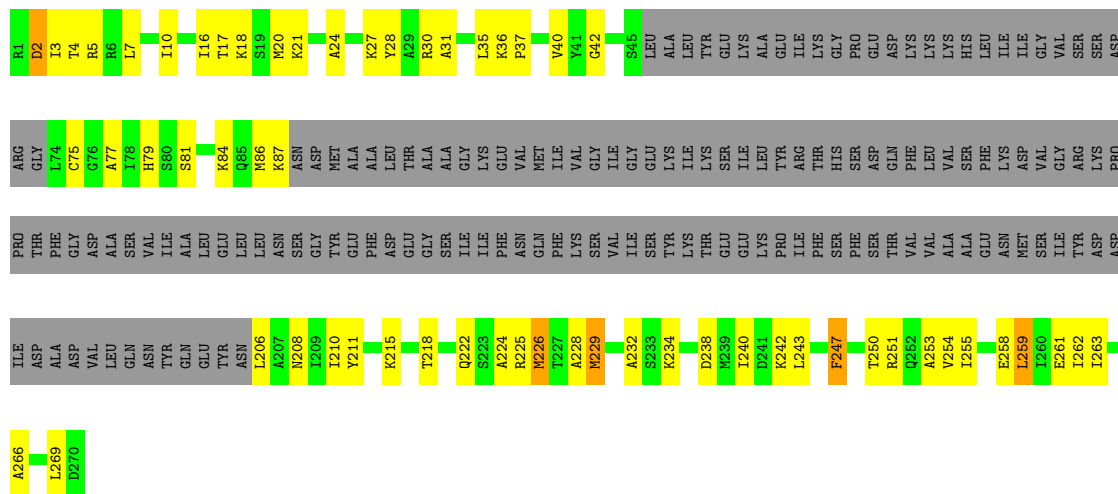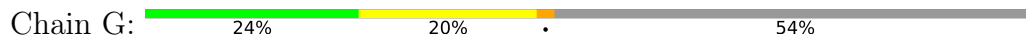
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	143.67Å 143.67Å 361.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	65.0 (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.217 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8489	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ADP, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.47	0/3862	0.78	1/5212 (0.0%)
2	B	0.51	0/3657	0.81	1/4961 (0.0%)
3	G	0.31	0/960	0.53	0/1279
All	All	0.47	0/8479	0.77	2/11452 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	115	PRO	N-CA-CB	5.50	109.90	103.30
1	A	79	ASP	N-CA-C	5.45	125.71	111.00

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	3810	0	3884	406	0
2	B	3598	0	3640	449	0
3	G	956	0	1016	39	0
4	A	1	0	0	0	0
5	A	31	0	12	6	0
6	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	27	0	12	7	0
8	A	34	0	0	12	0
8	B	24	0	0	5	0
8	G	3	0	0	0	0
All	All	8489	0	8564	866	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 51.

All (866) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MET:SD	1:A:95:VAL:HG21	1.95	1.07
2:B:37:GLU:HB2	2:B:76:LEU:HB3	1.32	1.05
2:B:38:VAL:HG21	2:B:45:LEU:HD23	1.38	1.05
2:B:133:LEU:HD13	2:B:148:LYS:HE3	1.40	1.04
1:A:151:LYS:HE3	1:A:436:MET:HG3	1.39	1.02
2:B:186:VAL:HG21	2:B:233:ALA:HB2	1.40	1.01
1:A:270:ASP:HB3	1:A:273:LYS:HB2	1.45	0.99
2:B:189:ARG:HB2	2:B:192:GLU:HG2	1.44	0.97
2:B:377:ILE:HG12	2:B:403:THR:HG23	1.49	0.95
1:A:257:PHE:HD2	1:A:264:ALA:HB2	1.33	0.94
1:A:108:VAL:HG12	1:A:114:ALA:HA	1.49	0.94
2:B:154:LEU:HD12	2:B:162:LYS:HA	1.50	0.94
1:A:506:ALA:HA	1:A:509:GLU:HB3	1.49	0.93
1:A:137:ILE:HG12	1:A:138:PRO:HD3	1.47	0.92
2:B:94:ILE:HB	2:B:103:ASP:HB3	1.52	0.90
1:A:150:ILE:HD11	1:A:181:ASP:HB2	1.53	0.90
2:B:243:PHE:HB3	2:B:249:GLN:HE21	1.36	0.90
1:A:32:LEU:HG	1:A:42:HIS:HB2	1.53	0.90
2:B:339:ILE:HD13	2:B:342:LEU:HD12	1.51	0.90
2:B:94:ILE:HG22	2:B:102:ILE:HG13	1.55	0.88
1:A:358:TYR:HE2	2:B:351:LEU:HD12	1.38	0.87
2:B:465:GLU:HA	2:B:468:ALA:HB3	1.54	0.87
1:A:301:LEU:HA	1:A:304:ARG:HH21	1.40	0.85
1:A:203:TYR:HB3	1:A:231:VAL:HG13	1.58	0.84
2:B:105:ARG:HE	2:B:208:LEU:HD22	1.41	0.84
1:A:211:SER:OG	2:B:126:MET:HG3	1.77	0.84
1:A:431:GLY:HA2	5:A:603:ATP:HN62	1.42	0.84
1:A:49:ALA:O	1:A:50:GLU:HB2	1.78	0.83
1:A:158:PRO:HG2	1:A:379:GLN:HB3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ALA:HA	1:A:228:TYR:CE1	2.14	0.82
1:A:271:LEU:HB3	1:A:302:HIS:CE1	2.13	0.82
1:A:140:ILE:HG23	1:A:141:SER:H	1.42	0.82
2:B:88:PRO:HA	2:B:91:LEU:HD12	1.62	0.82
2:B:298:THR:HG22	2:B:299:THR:H	1.43	0.82
1:A:137:ILE:HD13	1:A:137:ILE:H	1.42	0.82
1:A:302:HIS:O	1:A:306:LEU:HD23	1.79	0.81
2:B:289:MET:SD	2:B:293:GLN:NE2	2.53	0.81
1:A:426:GLU:HB2	1:A:461:ILE:HD12	1.63	0.81
1:A:96:ASP:HA	1:A:128:ARG:HA	1.61	0.81
2:B:335:LEU:HB3	2:B:347:ALA:HB3	1.60	0.81
2:B:200:MET:HB3	2:B:206:ILE:HG13	1.64	0.80
1:A:183:ILE:HD11	1:A:267:ILE:HG13	1.62	0.80
1:A:267:ILE:HD13	1:A:324:LEU:HD13	1.60	0.80
1:A:103:LEU:O	1:A:230:ILE:HG12	1.83	0.79
1:A:156:LEU:O	1:A:158:PRO:HD3	1.81	0.79
2:B:184:ALA:HB2	2:B:236:GLY:HA3	1.64	0.79
1:A:141:SER:HB3	1:A:143:ARG:NH2	1.98	0.79
2:B:257:ASN:HA	2:B:309:ALA:O	1.83	0.78
1:A:156:LEU:HD11	1:A:428:LEU:HD21	1.64	0.78
2:B:243:PHE:HB3	2:B:249:GLN:NE2	1.97	0.78
2:B:120:ALA:HB1	2:B:121:PRO:HD2	1.66	0.77
2:B:82:ILE:O	2:B:116:ILE:HG12	1.85	0.77
1:A:152:ALA:O	1:A:156:LEU:HB2	1.85	0.77
1:A:183:ILE:HG23	1:A:201:CYS:SG	2.25	0.77
1:A:52:MET:O	1:A:91:THR:HB	1.86	0.76
1:A:479:LEU:HD23	1:A:497:LEU:HG	1.68	0.76
2:B:155:PHE:HE1	2:B:310:ILE:HB	1.51	0.76
1:A:44:LEU:HD12	1:A:47:VAL:HG23	1.68	0.75
2:B:38:VAL:HG21	2:B:45:LEU:CD2	2.15	0.75
2:B:93:ARG:NH2	2:B:101:PRO:HB3	2.02	0.75
2:B:155:PHE:CE1	2:B:310:ILE:HB	2.22	0.75
1:A:105:GLY:HA2	1:A:226:MET:O	1.87	0.74
2:B:151:LYS:H	2:B:330:ASP:HB3	1.51	0.74
2:B:166:ILE:HG12	2:B:254:PHE:HD2	1.52	0.74
2:B:200:MET:SD	2:B:215:VAL:HG21	2.28	0.74
2:B:86:VAL:HG21	2:B:114:ALA:HB2	1.69	0.73
1:A:133:ALA:HB1	1:A:139:ARG:HH22	1.53	0.73
2:B:63:MET:SD	2:B:227:GLY:O	2.46	0.73
2:B:271:LEU:HD23	2:B:271:LEU:H	1.52	0.73
2:B:259:PHE:CE1	2:B:311:TYR:HB3	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:VAL:O	2:B:272:LEU:HG	1.89	0.73
2:B:335:LEU:HA	2:B:347:ALA:O	1.89	0.73
2:B:339:ILE:HG23	2:B:344:ILE:HB	1.71	0.72
1:A:476:HIS:HB3	1:A:479:LEU:HD13	1.72	0.72
2:B:187:GLY:O	2:B:222:MET:HG3	1.88	0.72
1:A:299:PHE:HA	1:A:341:ASN:HD21	1.54	0.72
1:A:359:LYS:HA	2:B:376:LYS:HB2	1.70	0.72
1:A:386:VAL:HG11	1:A:446:TYR:HB2	1.69	0.72
2:B:253:LEU:HG	2:B:255:ILE:HD11	1.72	0.72
1:A:98:PRO:HA	1:A:126:ARG:HD3	1.71	0.72
1:A:425:THR:O	1:A:429:LYS:HG3	1.90	0.72
1:A:386:VAL:HG12	1:A:450:ARG:NH2	2.05	0.71
2:B:323:ALA:HA	2:B:326:PHE:HD2	1.55	0.71
1:A:303:SER:HA	1:A:345:ILE:HD13	1.72	0.71
1:A:479:LEU:HD12	1:A:479:LEU:H	1.54	0.71
8:A:607:HOH:O	2:B:123:PHE:HB3	1.90	0.71
2:B:137:ILE:HG23	2:B:416:GLN:NE2	2.05	0.71
2:B:326:PHE:HA	2:B:329:LEU:HD21	1.73	0.71
2:B:32:ILE:HG22	2:B:33:LEU:HG	1.73	0.71
2:B:269:SER:OG	2:B:282:GLN:HB3	1.91	0.71
2:B:181:SER:HB3	2:B:215:VAL:HG12	1.73	0.70
1:A:257:PHE:CD2	1:A:264:ALA:HB2	2.23	0.70
2:B:452:LEU:HD22	2:B:466:ALA:HB1	1.72	0.70
1:A:441:GLN:O	1:A:445:ILE:HG22	1.91	0.70
2:B:38:VAL:HB	2:B:45:LEU:HB3	1.73	0.70
2:B:374:VAL:HG13	2:B:410:ILE:HG21	1.74	0.70
2:B:259:PHE:HB3	2:B:310:ILE:HG23	1.73	0.70
1:A:272:SER:O	1:A:275:ALA:HB3	1.92	0.70
1:A:265:LEU:HD11	1:A:324:LEU:HD11	1.73	0.70
2:B:368:TYR:O	2:B:372:ARG:HG2	1.92	0.70
1:A:397:TYR:HE1	1:A:418:LEU:HA	1.56	0.70
2:B:323:ALA:HA	2:B:326:PHE:CD2	2.26	0.69
1:A:40:ARG:HH21	1:A:285:LEU:HD23	1.58	0.69
1:A:351:PHE:O	1:A:365:ILE:HA	1.92	0.69
2:B:9:ALA:HB1	2:B:77:ASP:HB3	1.73	0.69
2:B:310:ILE:HG12	2:B:325:THR:HG21	1.75	0.69
2:B:226:PRO:N	2:B:229:ARG:HH21	1.91	0.68
2:B:439:LYS:O	2:B:443:GLN:HG2	1.92	0.68
2:B:252:LEU:HG	2:B:305:THR:HB	1.76	0.68
2:B:49:VAL:HA	2:B:60:THR:HG22	1.76	0.68
2:B:44:ARG:HH11	2:B:44:ARG:HG2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ALA:HA	2:B:218:VAL:O	1.94	0.68
1:A:279:ARG:O	1:A:283:LEU:HG	1.94	0.67
2:B:255:ILE:HD13	2:B:308:GLN:HG2	1.75	0.67
2:B:292:MET:HE1	2:B:293:GLN:HG2	1.75	0.67
1:A:40:ARG:NH2	1:A:285:LEU:HD23	2.10	0.67
1:A:139:ARG:HG2	1:A:310:ALA:HB1	1.77	0.67
1:A:106:ARG:O	1:A:231:VAL:HG23	1.94	0.67
1:A:151:LYS:CE	1:A:436:MET:HG3	2.22	0.67
2:B:105:ARG:NE	2:B:208:LEU:HD22	2.10	0.67
1:A:358:TYR:CE2	2:B:351:LEU:HD12	2.28	0.66
2:B:317:LEU:HD11	2:B:334:VAL:HG11	1.77	0.66
1:A:59:LEU:HD11	1:A:76:PHE:O	1.96	0.66
1:A:155:SER:HA	1:A:383:MET:SD	2.35	0.66
2:B:335:LEU:HD11	8:B:612:HOH:O	1.95	0.66
2:B:351:LEU:HB3	8:B:628:HOH:O	1.95	0.66
1:A:287:ARG:HG2	8:A:631:HOH:O	1.95	0.66
1:A:182:THR:HG22	1:A:265:LEU:HD21	1.78	0.66
1:A:361:ILE:O	1:A:364:ALA:HB2	1.96	0.66
2:B:378:LEU:O	2:B:381[B]:TYR:HB3	1.96	0.66
1:A:446:TYR:CD2	1:A:489:ILE:HD13	2.30	0.66
2:B:138:LYS:HZ1	2:B:441:PHE:HD2	1.42	0.66
2:B:469:LYS:HE3	2:B:473:LEU:HD13	1.76	0.66
1:A:379:GLN:HB2	1:A:383:MET:HB2	1.77	0.66
2:B:259:PHE:CZ	2:B:311:TYR:HB3	2.31	0.66
1:A:34:ILE:HG23	2:B:52:HIS:HB2	1.77	0.65
1:A:38:ILE:HG13	1:A:284:LEU:HB3	1.78	0.65
2:B:345:TYR:HA	2:B:346:PRO:C	2.16	0.65
1:A:301:LEU:HA	1:A:304:ARG:NH2	2.12	0.65
1:A:141:SER:O	1:A:311:LYS:HG2	1.96	0.65
1:A:203:TYR:HB3	1:A:231:VAL:CG1	2.26	0.65
1:A:167:ILE:HD11	1:A:326:VAL:HG22	1.79	0.65
2:B:121:PRO:HG3	2:B:297:THR:CG2	2.27	0.65
1:A:154:ASP:O	1:A:158:PRO:HG3	1.97	0.65
1:A:175:LYS:HD2	1:A:326:VAL:HG13	1.78	0.65
1:A:246:ALA:HA	8:A:606:HOH:O	1.95	0.65
2:B:84:ILE:HG21	2:B:235:THR:HG22	1.80	0.64
2:B:105:ARG:HH21	2:B:208:LEU:HB3	1.61	0.64
2:B:189:ARG:HD2	2:B:189:ARG:H	1.60	0.64
1:A:110:ALA:HB1	8:A:606:HOH:O	1.96	0.64
3:G:4[A]:THR:HG23	3:G:247[A]:PHE:HE2	1.62	0.64
1:A:32:LEU:CG	1:A:42:HIS:HB2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:VAL:O	2:B:98:ILE:HG12	1.97	0.64
1:A:108:VAL:HG12	1:A:114:ALA:CA	2.26	0.64
2:B:188:GLU:HA	2:B:222:MET:CE	2.28	0.64
2:B:387[B]:ILE:HG22	2:B:388[B]:ILE:HG13	1.80	0.64
1:A:168:ILE:HG12	1:A:329:THR:OG1	1.97	0.64
1:A:215:GLN:O	1:A:219:ARG:HB2	1.98	0.64
1:A:27:GLU:O	1:A:90:ARG:HG3	1.97	0.64
1:A:386:VAL:HG23	1:A:387:ALA:H	1.63	0.64
1:A:442:VAL:O	1:A:446:TYR:HB3	1.98	0.64
2:B:200:MET:HB3	2:B:206:ILE:CG1	2.27	0.64
3:G:37[A]:PRO:O	3:G:42[A]:GLY:HA3	1.97	0.64
1:A:359:LYS:HA	2:B:376:LYS:CB	2.27	0.64
2:B:122:GLU:O	2:B:126:MET:SD	2.56	0.64
2:B:155:PHE:HB2	2:B:334:VAL:HG22	1.80	0.64
2:B:96:ASN:HB3	2:B:102:ILE:CG2	2.28	0.63
2:B:167:MET:SD	2:B:196:LEU:HD13	2.39	0.63
1:A:189:PHE:HD1	1:A:189:PHE:N	1.96	0.63
2:B:32:ILE:O	2:B:33:LEU:HB2	1.99	0.63
2:B:36:LEU:HD23	2:B:77:ASP:HA	1.81	0.63
2:B:61:ILE:HG23	2:B:268:VAL:HG21	1.79	0.63
1:A:189:PHE:N	1:A:189:PHE:CD1	2.67	0.63
2:B:36:LEU:O	2:B:46:VAL:HA	1.98	0.63
2:B:172:ASN:HD21	2:B:431:LEU:HD22	1.63	0.63
1:A:218:LYS:HD3	1:A:219:ARG:N	2.13	0.63
2:B:91:LEU:HD11	2:B:180:TYR:CE2	2.33	0.63
2:B:289:MET:SD	2:B:293:GLN:HG3	2.38	0.63
1:A:16:ARG:HG2	1:A:17:ILE:HG12	1.81	0.63
2:B:378:LEU:O	2:B:382[B]:LYS:HG2	1.98	0.63
2:B:139:VAL:CG2	2:B:414:LEU:HB3	2.29	0.62
2:B:234:LEU:O	2:B:237:LEU:HB3	1.99	0.62
2:B:237:LEU:HD21	2:B:295:ARG:HB3	1.81	0.62
1:A:52:MET:HA	1:A:62:MET:HA	1.81	0.62
2:B:242:TYR:HA	2:B:246:GLN:NE2	2.15	0.62
2:B:259:PHE:CD2	2:B:321:ALA:HB1	2.34	0.62
2:B:402:LEU:O	2:B:406:ARG:HG2	1.99	0.62
2:B:186:VAL:CG2	2:B:233:ALA:HB2	2.24	0.62
2:B:212:THR:HG22	2:B:214:LYS:NZ	2.15	0.62
2:B:440:GLY:HA2	2:B:463:ILE:HG21	1.80	0.62
2:B:251:VAL:HG12	2:B:252:LEU:H	1.65	0.61
1:A:267:ILE:CD1	1:A:324:LEU:HD13	2.31	0.61
2:B:226:PRO:HB3	2:B:267:GLU:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LYS:HD2	2:B:414:LEU:HD23	1.82	0.61
2:B:181:SER:O	2:B:215:VAL:HA	2.00	0.61
2:B:253:LEU:HG	2:B:255:ILE:CD1	2.29	0.61
2:B:475:GLU:O	2:B:476:GLU:HB2	1.99	0.61
1:A:168:ILE:HG23	1:A:351:PHE:HD1	1.64	0.61
2:B:59:ARG:NH1	2:B:272:LEU:HA	2.15	0.61
2:B:86:VAL:HG22	2:B:114:ALA:H	1.66	0.61
2:B:267:GLU:O	2:B:271:LEU:HD21	2.00	0.61
2:B:169:LEU:O	2:B:173:VAL:HB	2.01	0.61
1:A:218:LYS:HD2	2:B:128:VAL:HG11	1.83	0.61
2:B:94:ILE:HG12	2:B:217:LEU:HD12	1.81	0.61
1:A:362:ARG:HD3	5:A:603:ATP:C2	2.35	0.61
2:B:66:THR:HG22	2:B:69:LEU:HD12	1.81	0.61
2:B:85:PRO:O	2:B:90:THR:HG21	2.01	0.61
1:A:164:ARG:HA	1:A:323:ALA:O	2.01	0.61
1:A:337:TYR:O	1:A:338:ILE:HB	1.99	0.61
1:A:366:ASN:ND2	1:A:369:LEU:HD23	2.16	0.61
2:B:36:LEU:HD12	2:B:60:THR:HG21	1.82	0.61
1:A:45:ARG:O	1:A:45:ARG:HD3	2.01	0.60
2:B:244:ARG:O	2:B:248:GLY:HA2	2.01	0.60
1:A:107:VAL:HG13	1:A:231:VAL:HB	1.82	0.60
1:A:144:GLU:O	1:A:144:GLU:HG2	2.01	0.60
2:B:375:GLN:HA	2:B:378:LEU:HB2	1.83	0.60
3:G:238[A]:ASP:O	3:G:242[A]:LYS:HG2	2.01	0.60
1:A:426:GLU:HA	1:A:429:LYS:HZ2	1.65	0.60
2:B:164:VAL:HG11	7:B:604:ADP:N7	2.16	0.60
2:B:459:MET:O	2:B:460:VAL:HG13	2.00	0.60
1:A:151:LYS:HG2	8:A:609:HOH:O	2.00	0.60
1:A:387:ALA:HA	1:A:390:MET:SD	2.41	0.60
2:B:93:ARG:HH22	2:B:101:PRO:HB3	1.65	0.60
1:A:172:GLN:HG2	2:B:354:THR:HB	1.84	0.60
2:B:410:ILE:HG12	2:B:441:PHE:HE1	1.65	0.60
1:A:446:TYR:CE1	1:A:497:LEU:HD13	2.37	0.60
2:B:406:ARG:HD2	2:B:444:ILE:O	2.01	0.60
1:A:168:ILE:HG23	1:A:351:PHE:CD1	2.37	0.60
2:B:225:PRO:C	2:B:229:ARG:HH21	2.05	0.60
2:B:404:VAL:O	2:B:408:ARG:HG3	2.02	0.59
2:B:413:PHE:HA	2:B:461:GLY:HA2	1.83	0.59
1:A:135:GLY:N	1:A:139:ARG:HH21	1.99	0.59
1:A:279:ARG:HD2	1:A:293:ALA:CB	2.31	0.59
2:B:410:ILE:HG23	2:B:441:PHE:HZ	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG22	1:A:232:VAL:HG12	1.83	0.59
1:A:135:GLY:H	1:A:139:ARG:HE	1.49	0.59
1:A:137:ILE:HD13	1:A:137:ILE:N	2.17	0.59
1:A:176:THR:O	1:A:180:ILE:HB	2.03	0.59
2:B:449:TYR:HB3	2:B:463:ILE:HD11	1.84	0.59
1:A:64:LEU:CD2	1:A:281:MET:SD	2.90	0.59
1:A:426:GLU:HA	1:A:429:LYS:NZ	2.16	0.59
2:B:140:VAL:HG13	2:B:146:TYR:OH	2.01	0.59
2:B:332:THR:HB	2:B:353:SER:HA	1.84	0.59
2:B:342:LEU:HB2	2:B:344:ILE:HG12	1.84	0.59
1:A:386:VAL:HG12	1:A:450:ARG:HH22	1.68	0.59
1:A:431:GLY:CA	5:A:603:ATP:HN62	2.15	0.59
2:B:321:ALA:HB3	2:B:322:PRO:HD3	1.83	0.59
2:B:160:VAL:HA	2:B:345:TYR:OH	2.02	0.59
1:A:49:ALA:O	1:A:50:GLU:CB	2.50	0.58
1:A:78:ASN:H	1:A:78:ASN:ND2	2.01	0.58
1:A:172:GLN:CD	5:A:603:ATP:H4'	2.22	0.58
1:A:243:GLN:O	1:A:274:GLN:HG3	2.03	0.58
1:A:497:LEU:O	1:A:500:ILE:HG22	2.04	0.58
2:B:267:GLU:O	2:B:271:LEU:HD11	2.02	0.58
1:A:99:VAL:HG23	1:A:253:MET:HA	1.85	0.58
2:B:118:ALA:HB3	2:B:295:ARG:NH2	2.19	0.58
2:B:156:GLY:HA3	2:B:160:VAL:HG21	1.85	0.58
2:B:121:PRO:HG3	2:B:297:THR:HG22	1.86	0.58
2:B:133:LEU:HB2	2:B:148:LYS:HD2	1.85	0.58
2:B:252:LEU:HG	2:B:305:THR:O	2.04	0.58
1:A:362:ARG:HH22	2:B:372:ARG:NH1	2.02	0.58
1:A:385:GLN:OE1	1:A:488:LYS:HG2	2.04	0.58
2:B:52:HIS:O	2:B:54:GLY:N	2.36	0.58
2:B:118:ALA:HB3	2:B:295:ARG:HH21	1.68	0.58
2:B:212:THR:HG22	2:B:214:LYS:HZ3	1.69	0.58
2:B:94:ILE:CG2	2:B:102:ILE:HG13	2.33	0.58
2:B:133:LEU:HB2	2:B:148:LYS:CD	2.34	0.58
1:A:57:SER:HB2	1:A:81:LEU:HD22	1.86	0.57
2:B:151:LYS:HB2	2:B:330:ASP:H	1.67	0.57
1:A:472:VAL:HA	1:A:476:HIS:HB2	1.85	0.57
2:B:450:ASP:O	2:B:451:HIS:HB3	2.04	0.57
1:A:101:ASP:O	1:A:104:LEU:HB2	2.04	0.57
1:A:107:VAL:HA	1:A:231:VAL:O	2.02	0.57
1:A:291:ARG:HA	3:G:261[A]:GLU:OE1	2.04	0.57
2:B:23:VAL:O	2:B:57:THR:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:PHE:CE2	2:B:466:ALA:HB2	2.39	0.57
1:A:55:PHE:CE2	1:A:75:VAL:HG22	2.39	0.57
1:A:172:GLN:HB3	2:B:354:THR:HG21	1.86	0.57
1:A:419:SER:O	1:A:423:ARG:HD3	2.04	0.57
2:B:96:ASN:HD22	2:B:96:ASN:C	2.07	0.57
2:B:138:LYS:NZ	2:B:441:PHE:HD2	2.03	0.57
2:B:188:GLU:HA	2:B:222:MET:HE1	1.86	0.57
2:B:231:ARG:O	2:B:234:LEU:HB2	2.05	0.57
1:A:279:ARG:HD2	1:A:293:ALA:HB3	1.85	0.57
2:B:39:GLN:O	2:B:41:ARG:N	2.38	0.57
2:B:94:ILE:HG22	2:B:102:ILE:CG1	2.31	0.57
1:A:99:VAL:HG22	1:A:100:GLY:H	1.70	0.57
2:B:220:GLY:N	2:B:232:VAL:HG21	2.20	0.57
2:B:264:ALA:O	2:B:268:VAL:HG12	2.04	0.57
1:A:78:ASN:HD22	1:A:78:ASN:N	2.03	0.57
1:A:164:ARG:HG2	1:A:306:LEU:HB3	1.86	0.57
1:A:200:TYR:N	1:A:200:TYR:CD1	2.72	0.57
1:A:362:ARG:HH11	5:A:603:ATP:H2	1.51	0.57
2:B:281:TYR:HD1	2:B:281:TYR:H	1.53	0.57
1:A:362:ARG:HH12	2:B:372:ARG:HH11	1.51	0.56
1:A:22:SER:HA	1:A:28:THR:HG21	1.87	0.56
1:A:22:SER:HB3	1:A:87:ILE:HD12	1.87	0.56
1:A:446:TYR:HD2	1:A:489:ILE:HD13	1.69	0.56
1:A:52:MET:SD	1:A:60:LYS:HD2	2.46	0.56
1:A:146:MET:SD	1:A:265:LEU:HD13	2.45	0.56
1:A:166:LEU:O	1:A:349:GLN:HA	2.05	0.56
1:A:62:MET:SD	1:A:95:VAL:CG2	2.84	0.56
1:A:358:TYR:HB2	2:B:375:GLN:HB2	1.87	0.56
1:A:338:ILE:HB	1:A:339:PRO:HD3	1.87	0.56
2:B:118:ALA:H	2:B:295:ARG:NH2	2.04	0.56
2:B:132:ILE:HG13	2:B:133:LEU:N	2.20	0.56
2:B:155:PHE:HB2	2:B:334:VAL:HA	1.87	0.56
2:B:218:VAL:HG11	2:B:235:THR:OG1	2.06	0.56
2:B:311:TYR:O	2:B:322:PRO:HG3	2.04	0.56
2:B:230:ALA:HB2	2:B:264:ALA:HB1	1.87	0.55
1:A:438:ILE:O	1:A:442:VAL:HG23	2.06	0.55
2:B:88:PRO:HA	2:B:91:LEU:CD1	2.35	0.55
1:A:52:MET:HG3	1:A:61:GLY:O	2.07	0.55
1:A:139:ARG:HA	1:A:311:LYS:O	2.06	0.55
1:A:209:LYS:HE3	2:B:356:ARG:NH2	2.20	0.55
1:A:345:ILE:HD12	8:A:605:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:HD13	2:B:75:VAL:HG11	1.89	0.55
2:B:370:VAL:O	2:B:374:VAL:HG23	2.07	0.55
2:B:410:ILE:HG12	2:B:441:PHE:CE1	2.40	0.55
1:A:178:ILE:HG23	1:A:179:ALA:N	2.22	0.55
1:A:299:PHE:HA	1:A:341:ASN:ND2	2.22	0.55
2:B:298:THR:HG22	2:B:299:THR:N	2.15	0.55
3:G:20[A]:MET:SD	3:G:225[A]:ARG:HG3	2.46	0.55
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.88	0.55
1:A:41:VAL:HG12	1:A:42:HIS:O	2.06	0.55
1:A:60:LYS:O	1:A:76:PHE:HB2	2.06	0.55
1:A:165:GLU:O	1:A:324:LEU:HA	2.05	0.55
2:B:154:LEU:HB3	8:B:612:HOH:O	2.05	0.55
2:B:189:ARG:HB2	2:B:192:GLU:CG	2.28	0.55
1:A:32:LEU:O	1:A:84:GLU:HG3	2.06	0.55
1:A:496:LYS:HE2	1:A:496:LYS:HA	1.89	0.55
2:B:85:PRO:HD2	2:B:95:MET:SD	2.47	0.55
1:A:238:ASP:HB3	1:A:242:LEU:HB2	1.88	0.55
1:A:394:LEU:HA	1:A:397:TYR:HB3	1.89	0.55
2:B:207:ASN:HD21	2:B:210:ASP:N	2.05	0.55
1:A:164:ARG:HD3	1:A:164:ARG:N	2.22	0.54
1:A:403[B]:PHE:HA	1:A:406[B]:PHE:CE1	2.42	0.54
2:B:89:GLU:HB3	8:B:622:HOH:O	2.07	0.54
1:A:21:THR:HB	1:A:89:LYS:NZ	2.22	0.54
1:A:148:THR:HG22	1:A:182:THR:HG23	1.89	0.54
2:B:96:ASN:HB3	2:B:102:ILE:HG23	1.89	0.54
1:A:224:ASP:O	1:A:227:LYS:HB3	2.06	0.54
1:A:204:VAL:O	1:A:269:ASP:HB2	2.08	0.54
1:A:313:ASN:HD22	1:A:316:PHE:HB2	1.71	0.54
2:B:410:ILE:HG23	2:B:441:PHE:CZ	2.43	0.54
3:G:250[A]:THR:HA	3:G:253[A]:ALA:HB3	1.90	0.54
1:A:213:VAL:HB	2:B:123:PHE:HE1	1.73	0.54
1:A:52:MET:HG2	1:A:60:LYS:HD2	1.89	0.54
1:A:102:GLU:OE1	1:A:123:SER:HA	2.07	0.54
1:A:166:LEU:HD12	1:A:342:VAL:HG12	1.89	0.54
1:A:248:TYR:CD1	1:A:305:LEU:HD13	2.43	0.54
1:A:269:ASP:O	1:A:270:ASP:HB2	2.08	0.54
2:B:406:ARG:CZ	2:B:447:GLY:HA2	2.37	0.54
2:B:435:LYS:HG2	2:B:436:GLU:HG2	1.90	0.54
1:A:152:ALA:HB2	1:A:428:LEU:O	2.08	0.54
1:A:294:TYR:HB3	1:A:298:VAL:CG2	2.38	0.54
2:B:36:LEU:CD2	2:B:77:ASP:HA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:GLY:O	2:B:368:TYR:HB3	2.07	0.54
1:A:186:GLN:HB2	1:A:228:TYR:CE2	2.43	0.54
1:A:264:ALA:HB3	1:A:321:LEU:CD1	2.38	0.54
2:B:269:SER:HA	2:B:274:ARG:HD2	1.90	0.54
1:A:141:SER:HB3	1:A:143:ARG:HH21	1.71	0.54
2:B:50:ALA:HB2	2:B:61:ILE:CD1	2.38	0.54
3:G:18[A]:LYS:O	3:G:21[A]:LYS:HB3	2.08	0.54
2:B:151:LYS:HD2	2:B:328:HIS:O	2.09	0.53
2:B:377:ILE:O	2:B:381[B]:TYR:HB2	2.07	0.53
2:B:84:ILE:C	2:B:113:PHE:HB3	2.29	0.53
2:B:140:VAL:HG13	2:B:146:TYR:CZ	2.42	0.53
2:B:259:PHE:CE2	2:B:321:ALA:HB1	2.42	0.53
3:G:228[A]:ALA:O	3:G:232[A]:ALA:HB3	2.08	0.53
2:B:237:LEU:HD21	2:B:295:ARG:CB	2.38	0.53
1:A:64:LEU:HD11	8:A:633:HOH:O	2.09	0.53
1:A:115:ILE:HG13	1:A:116:ASP:N	2.24	0.53
1:A:336:ALA:O	1:A:339:PRO:HD2	2.09	0.53
1:A:348:GLY:HA2	1:A:371:VAL:O	2.07	0.53
1:A:393:GLU:O	1:A:397:TYR:HB2	2.08	0.53
1:A:44:LEU:O	1:A:47:VAL:HB	2.09	0.53
1:A:148:THR:O	1:A:185:ASN:HB2	2.09	0.53
2:B:50:ALA:HB2	2:B:61:ILE:HD11	1.91	0.53
2:B:89:GLU:HB2	2:B:110:THR:HG22	1.90	0.53
2:B:230:ALA:HB3	2:B:231:ARG:HD3	1.91	0.53
2:B:277:SER:O	2:B:280:GLY:N	2.38	0.53
1:A:52:MET:CG	1:A:60:LYS:HD2	2.39	0.53
2:B:113:PHE:CD1	2:B:113:PHE:N	2.76	0.53
2:B:378:LEU:HD23	2:B:381[B]:TYR:CD2	2.44	0.53
1:A:279:ARG:CD	1:A:293:ALA:HB3	2.39	0.53
2:B:66:THR:HG22	2:B:69:LEU:CD1	2.39	0.53
2:B:94:ILE:HG12	2:B:217:LEU:HB2	1.90	0.53
2:B:443:GLN:HB3	2:B:448:ASP:O	2.09	0.53
1:A:235:THR:O	1:A:237:SER:N	2.41	0.53
1:A:172:GLN:HG3	1:A:172:GLN:O	2.09	0.52
2:B:119:GLU:HA	2:B:119:GLU:OE1	2.09	0.52
3:G:247[A]:PHE:CE1	3:G:251[A]:ARG:HD2	2.43	0.52
1:A:179:ALA:HB1	1:A:267:ILE:HD12	1.90	0.52
1:A:383:MET:HB3	1:A:387:ALA:HB3	1.90	0.52
2:B:394[B]:ASP:O	2:B:401:LYS:HE2	2.09	0.52
1:A:450:ARG:HB3	1:A:452:TYR:CE2	2.44	0.52
2:B:84:ILE:O	2:B:113:PHE:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:GLY:HA2	7:B:604:ADP:O3A	2.09	0.52
2:B:182:VAL:HG21	2:B:239:VAL:HG12	1.90	0.52
3:G:229[A]:MET:SD	3:G:229[A]:MET:N	2.82	0.52
1:A:78:ASN:H	1:A:78:ASN:HD22	1.57	0.52
2:B:94:ILE:CB	2:B:103:ASP:HB3	2.33	0.52
2:B:242:TYR:HA	2:B:246:GLN:HE22	1.74	0.52
2:B:83:LYS:HB3	2:B:115:PRO:HA	1.91	0.52
1:A:31:VAL:HG12	1:A:84:GLU:HA	1.91	0.52
1:A:47:VAL:HG11	1:A:71:VAL:HG11	1.91	0.52
1:A:278:TYR:CD2	1:A:301:LEU:HD22	2.45	0.52
2:B:96:ASN:HB3	2:B:102:ILE:HG21	1.91	0.52
2:B:457:PHE:CZ	2:B:463:ILE:HA	2.44	0.52
2:B:86:VAL:HG22	2:B:114:ALA:N	2.25	0.52
2:B:165:LEU:O	2:B:165:LEU:HD12	2.10	0.52
3:G:75[A]:CYS:SG	3:G:224[A]:ALA:HB1	2.49	0.52
1:A:140:ILE:HB	1:A:313:ASN:HB2	1.90	0.51
3:G:218[A]:THR:O	3:G:222[A]:GLN:HG2	2.10	0.51
1:A:403[B]:PHE:HA	1:A:406[B]:PHE:CZ	2.45	0.51
1:A:282:SER:O	1:A:285:LEU:N	2.43	0.51
2:B:156:GLY:HA3	2:B:160:VAL:CG2	2.41	0.51
2:B:285:LEU:HD11	2:B:320:PRO:O	2.10	0.51
1:A:131:LEU:HD12	1:A:132:LYS:H	1.75	0.51
1:A:173:THR:HG21	1:A:352:LEU:C	2.31	0.51
2:B:271:LEU:HD23	2:B:271:LEU:N	2.25	0.51
1:A:34:ILE:CG2	2:B:52:HIS:HB2	2.41	0.51
1:A:116:ASP:O	1:A:118:LYS:N	2.44	0.51
1:A:343:ILE:HD11	1:A:349:GLN:NE2	2.26	0.51
2:B:330:ASP:HB2	2:B:356:ARG:HH21	1.76	0.51
2:B:32:ILE:HA	2:B:49:VAL:HG12	1.92	0.51
1:A:300:TYR:O	1:A:304:ARG:HB3	2.11	0.51
2:B:357:ILE:HG13	2:B:357:ILE:O	2.09	0.51
2:B:457:PHE:CE2	2:B:463:ILE:HA	2.46	0.51
1:A:84:GLU:HB2	2:B:52:HIS:HB3	1.93	0.51
1:A:116:ASP:OD2	1:A:118:LYS:HD2	2.11	0.51
1:A:156:LEU:C	1:A:158:PRO:HD3	2.30	0.51
1:A:436:MET:HB2	8:A:609:HOH:O	2.10	0.51
2:B:431:LEU:O	2:B:432:VAL:HB	2.11	0.51
2:B:120:ALA:HB1	2:B:294:GLU:O	2.11	0.51
2:B:142:LEU:HD23	2:B:143:LEU:N	2.26	0.51
2:B:186:VAL:HG13	2:B:232:VAL:HG13	1.92	0.51
3:G:255[A]:ILE:O	3:G:259[A]:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:VAL:HG23	1:A:387:ALA:N	2.26	0.51
3:G:24[A]:ALA:HB1	3:G:226[A]:MET:HA	1.93	0.51
3:G:35[A]:LEU:HD13	3:G:215[A]:LYS:HB3	1.93	0.51
1:A:234:ALA:HB1	1:A:243:GLN:HA	1.93	0.50
2:B:44:ARG:HG2	2:B:44:ARG:NH1	2.24	0.50
2:B:287:THR:O	2:B:291:THR:N	2.44	0.50
1:A:108:VAL:CG2	1:A:232:VAL:HG12	2.41	0.50
1:A:189:PHE:HB3	1:A:197:LYS:O	2.11	0.50
2:B:161:GLY:O	7:B:604:ADP:PB	2.70	0.50
2:B:398[B]:GLU:HA	2:B:401:LYS:CB	2.40	0.50
1:A:480:LEU:O	1:A:483:ILE:HB	2.12	0.50
2:B:96:ASN:C	2:B:96:ASN:ND2	2.65	0.50
2:B:184:ALA:O	2:B:255:ILE:HA	2.11	0.50
2:B:186:VAL:HG13	2:B:232:VAL:CG1	2.41	0.50
1:A:300:TYR:O	1:A:304:ARG:NE	2.45	0.50
2:B:288:ASP:C	2:B:290:GLY:N	2.65	0.50
2:B:290:GLY:O	2:B:292:MET:N	2.45	0.50
2:B:427:HIS:HE1	2:B:459:MET:SD	2.34	0.50
3:G:24[A]:ALA:O	3:G:226[A]:MET:SD	2.69	0.50
1:A:452:TYR:HE1	8:A:610:HOH:O	1.94	0.50
2:B:137:ILE:HG23	2:B:416:GLN:HE22	1.74	0.50
2:B:336:SER:O	2:B:339:ILE:HB	2.11	0.50
3:G:75[A]:CYS:SG	3:G:75[A]:CYS:O	2.69	0.50
1:A:53:VAL:N	1:A:61:GLY:O	2.44	0.50
1:A:474:SER:O	1:A:475:GLN:HG3	2.12	0.50
2:B:91:LEU:HD21	2:B:180:TYR:CD2	2.46	0.49
2:B:139:VAL:HG23	2:B:414:LEU:HB3	1.93	0.49
1:A:204:VAL:HG13	1:A:232:VAL:CG2	2.41	0.49
1:A:370:SER:O	1:A:371:VAL:HG13	2.13	0.49
2:B:449:TYR:CB	2:B:463:ILE:HD11	2.42	0.49
1:A:482:ASN:OD1	1:A:490:SER:HB2	2.12	0.49
2:B:231:ARG:N	2:B:231:ARG:CD	2.74	0.49
3:G:20[A]:MET:HB3	3:G:229[A]:MET:HG2	1.95	0.49
1:A:31:VAL:HB	1:A:85:GLY:H	1.77	0.49
1:A:198:LYS:O	1:A:199:LEU:HB2	2.13	0.49
2:B:257:ASN:HB3	2:B:260:ARG:HG2	1.94	0.49
1:A:156:LEU:CD2	1:A:390:MET:HB3	2.42	0.49
2:B:377:ILE:HD11	2:B:403:THR:HA	1.94	0.49
1:A:29:GLY:HA3	1:A:42:HIS:O	2.13	0.49
1:A:153:VAL:O	1:A:157:VAL:N	2.45	0.49
1:A:313:ASN:ND2	1:A:316:PHE:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:PHE:CD1	2:B:259:PHE:C	2.84	0.49
2:B:332:THR:HB	2:B:354:THR:N	2.28	0.49
2:B:381[B]:TYR:CD1	2:B:403:THR:HG22	2.47	0.49
1:A:57:SER:CB	1:A:81:LEU:HB2	2.42	0.49
1:A:181:ASP:O	1:A:184:ILE:HG22	2.13	0.49
1:A:91:THR:O	1:A:93:ALA:N	2.46	0.49
1:A:153:VAL:HG13	1:A:157:VAL:HG23	1.95	0.49
1:A:180:ILE:O	1:A:184:ILE:HB	2.13	0.49
2:B:41:ARG:HG3	2:B:42:GLU:H	1.78	0.49
2:B:166:ILE:HG12	2:B:254:PHE:CD2	2.40	0.49
2:B:284:THR:O	2:B:286:ALA:N	2.45	0.49
2:B:330:ASP:O	2:B:331:ALA:HB2	2.12	0.49
1:A:139:ARG:NH1	1:A:310:ALA:HB2	2.28	0.48
1:A:175:LYS:HG2	1:A:352:LEU:HD12	1.95	0.48
2:B:374:VAL:O	2:B:377:ILE:HG22	2.12	0.48
1:A:28:THR:HG21	1:A:89:LYS:HZ3	1.77	0.48
1:A:167:ILE:O	1:A:167:ILE:HG13	2.13	0.48
1:A:203:TYR:O	1:A:231:VAL:HA	2.13	0.48
2:B:13:ILE:HD13	2:B:69:LEU:HD13	1.95	0.48
2:B:97:VAL:HG21	2:B:228:ALA:HB1	1.96	0.48
2:B:191:ARG:HH21	2:B:192:GLU:HB3	1.78	0.48
1:A:204:VAL:HG13	1:A:232:VAL:HG23	1.95	0.48
1:A:472:VAL:O	1:A:476:HIS:N	2.44	0.48
2:B:381[B]:TYR:OH	2:B:408:ARG:HG2	2.13	0.48
1:A:128:ARG:HG2	1:A:130:GLY:H	1.77	0.48
2:B:469:LYS:CE	2:B:473:LEU:HD13	2.43	0.48
2:B:476:GLU:O	2:B:477:HIS:HB2	2.13	0.48
3:G:250[A]:THR:O	3:G:250[A]:THR:HG22	2.13	0.48
1:A:219:ARG:HA	1:A:222:ASP:OD2	2.13	0.48
1:A:362:ARG:HD3	5:A:603:ATP:H2	1.78	0.48
1:A:158:PRO:CG	1:A:379:GLN:HB3	2.38	0.48
1:A:225:ALA:HA	1:A:228:TYR:HE1	1.74	0.48
1:A:28:THR:HG21	1:A:89:LYS:NZ	2.29	0.48
2:B:188:GLU:HA	2:B:222:MET:HE3	1.95	0.48
2:B:312:VAL:HG12	2:B:312:VAL:O	2.13	0.48
1:A:37:GLY:O	1:A:38:ILE:HD13	2.14	0.48
2:B:255:ILE:HG21	2:B:258:ILE:HD13	1.96	0.48
2:B:277:SER:OG	2:B:278:ALA:N	2.46	0.48
1:A:135:GLY:N	1:A:139:ARG:HE	2.11	0.48
2:B:36:LEU:HB2	2:B:47:LEU:O	2.14	0.48
2:B:298:THR:HG23	2:B:303:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:79[A]:HIS:CD2	3:G:79[A]:HIS:H	2.30	0.48
1:A:99:VAL:HG22	1:A:100:GLY:N	2.29	0.47
1:A:127:ARG:HG2	1:A:127:ARG:HH11	1.79	0.47
1:A:495:ALA:O	1:A:498:LYS:HB3	2.13	0.47
2:B:142:LEU:HG	2:B:367:HIS:NE2	2.29	0.47
2:B:167:MET:SD	2:B:196:LEU:CD1	3.02	0.47
1:A:211:SER:O	1:A:215:GLN:HG2	2.14	0.47
1:A:397:TYR:CE1	1:A:418:LEU:HA	2.43	0.47
2:B:332:THR:O	2:B:333:THR:HG23	2.13	0.47
1:A:25:LEU:HA	1:A:28:THR:O	2.14	0.47
1:A:446:TYR:CE2	1:A:489:ILE:HG21	2.50	0.47
1:A:262:LYS:C	1:A:263:HIS:HD1	2.17	0.47
1:A:356:LEU:HD12	1:A:364:ALA:HB1	1.96	0.47
1:A:150:ILE:HD11	1:A:181:ASP:CB	2.37	0.47
1:A:172:GLN:CG	2:B:354:THR:HB	2.45	0.47
1:A:356:LEU:O	1:A:359:LYS:HG3	2.14	0.47
2:B:139:VAL:HG13	2:B:143:LEU:HG	1.96	0.47
1:A:140:ILE:HG13	1:A:143:ARG:HH22	1.79	0.47
1:A:149:GLY:HA3	1:A:435:PRO:HB2	1.97	0.47
1:A:349:GLN:CD	1:A:370:SER:HA	2.35	0.47
2:B:39:GLN:C	2:B:41:ARG:H	2.17	0.47
2:B:143:LEU:O	2:B:145:PRO:HD3	2.14	0.47
2:B:164:VAL:HG23	7:B:604:ADP:O2A	2.15	0.47
2:B:165:LEU:HA	2:B:168:GLU:HB3	1.96	0.47
2:B:187:GLY:O	2:B:188:GLU:O	2.33	0.47
2:B:319:ASP:C	2:B:321:ALA:H	2.18	0.47
1:A:99:VAL:HG11	1:A:127:ARG:HB2	1.97	0.47
2:B:164:VAL:HG21	7:B:604:ADP:C8	2.50	0.47
2:B:384[B]:LEU:HD22	2:B:400:ASP:HB3	1.96	0.47
1:A:36:ASP:O	1:A:38:ILE:HG12	2.15	0.47
1:A:137:ILE:H	1:A:137:ILE:CD1	2.16	0.47
2:B:344:ILE:HG23	2:B:415:SER:OG	2.15	0.47
2:B:381[B]:TYR:HA	2:B:384[B]:LEU:CD2	2.44	0.47
2:B:374:VAL:HG22	2:B:410:ILE:HD13	1.97	0.47
2:B:469:LYS:HE2	2:B:473:LEU:HD22	1.96	0.47
2:B:350:PRO:CB	2:B:378:LEU:HD13	2.45	0.46
1:A:164:ARG:HD3	1:A:164:ARG:H	1.79	0.46
1:A:178:ILE:HG23	1:A:179:ALA:H	1.81	0.46
2:B:378:LEU:HD23	2:B:381[B]:TYR:HD2	1.78	0.46
1:A:363:PRO:O	1:A:364:ALA:HB3	2.15	0.46
2:B:84:ILE:HG21	2:B:235:THR:CG2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:2[A]:ASP:HA	3:G:5[A]:ARG:HH12	1.80	0.46
1:A:45:ARG:HD3	1:A:45:ARG:C	2.36	0.46
1:A:382:ALA:O	1:A:386:VAL:HG22	2.16	0.46
1:A:397:TYR:CE2	1:A:401[B]:ALA:HB2	2.50	0.46
2:B:137:ILE:O	2:B:141:ASP:N	2.49	0.46
1:A:31:VAL:HG13	1:A:33:SER:O	2.15	0.46
1:A:66:LEU:HB3	8:A:618:HOH:O	2.16	0.46
2:B:154:LEU:HA	2:B:333:THR:OG1	2.16	0.46
2:B:186:VAL:CG1	2:B:260:ARG:HB2	2.46	0.46
2:B:237:LEU:CD2	2:B:295:ARG:HD3	2.44	0.46
2:B:349:ASP:OD1	2:B:350:PRO:HD2	2.16	0.46
2:B:428:MET:HB3	2:B:430:LYS:HE2	1.97	0.46
2:B:160:VAL:O	2:B:345:TYR:CE2	2.69	0.46
2:B:257:ASN:H	2:B:309:ALA:HB3	1.80	0.46
2:B:323:ALA:O	2:B:325:THR:N	2.49	0.46
2:B:78:SER:OG	2:B:79:GLY:N	2.49	0.46
2:B:145:PRO:C	2:B:146:TYR:HD1	2.19	0.46
2:B:151:LYS:NZ	2:B:293:GLN:O	2.47	0.46
2:B:251:VAL:HG12	2:B:252:LEU:O	2.16	0.46
2:B:330:ASP:HB2	2:B:356:ARG:NH2	2.31	0.46
1:A:54:GLU:HB3	1:A:89:LYS:HB2	1.97	0.46
1:A:184:ILE:HD12	1:A:225:ALA:HB2	1.98	0.46
1:A:208:GLN:O	1:A:235:THR:HG22	2.15	0.46
2:B:44:ARG:NH1	2:B:44:ARG:CG	2.79	0.46
2:B:398[B]:GLU:HA	2:B:401:LYS:HB2	1.97	0.46
1:A:150:ILE:CG2	1:A:153:VAL:HG23	2.46	0.45
2:B:222:MET:C	2:B:224:GLU:H	2.18	0.45
2:B:298:THR:O	2:B:299:THR:HB	2.16	0.45
1:A:104:LEU:HD22	1:A:230:ILE:HD11	1.97	0.45
1:A:219:ARG:NH1	1:A:433:TYR:CE2	2.83	0.45
2:B:145:PRO:HG3	2:B:363:VAL:HG11	1.97	0.45
2:B:155:PHE:O	2:B:335:LEU:N	2.49	0.45
2:B:194:ASN:O	2:B:197:TYR:HB3	2.16	0.45
1:A:453:LEU:H	1:A:453:LEU:HD12	1.81	0.45
2:B:383[B]:SER:O	2:B:387[B]:ILE:N	2.49	0.45
1:A:477:GLN:HA	1:A:477:GLN:HE21	1.81	0.45
2:B:96:ASN:HB3	2:B:102:ILE:HD13	1.97	0.45
2:B:278:ALA:O	2:B:279:VAL:HB	2.15	0.45
2:B:374:VAL:HG12	2:B:378:LEU:HD12	1.98	0.45
3:G:3[A]:ILE:HG23	3:G:243[A]:LEU:HD12	1.98	0.45
1:A:55:PHE:CE2	1:A:75:VAL:CG2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TYR:O	1:A:449:VAL:HG12	2.17	0.45
1:A:144:GLU:O	1:A:161:ARG:HB2	2.17	0.45
1:A:175:LYS:CG	1:A:352:LEU:HD12	2.47	0.45
2:B:96:ASN:ND2	2:B:100:GLU:H	2.15	0.45
2:B:400:ASP:O	2:B:403:THR:HB	2.17	0.45
1:A:166:LEU:HD23	1:A:167:ILE:N	2.32	0.45
2:B:36:LEU:HD13	2:B:75:VAL:CG1	2.46	0.45
3:G:258[A]:GLU:O	3:G:262[A]:ILE:HG13	2.16	0.45
1:A:71:VAL:HG12	1:A:71:VAL:O	2.16	0.45
1:A:106:ARG:CZ	1:A:118:LYS:HB2	2.47	0.45
1:A:183:ILE:HD11	1:A:267:ILE:CG1	2.40	0.45
1:A:326:VAL:O	1:A:327:ILE:HD13	2.16	0.45
2:B:180:TYR:CD2	2:B:249:GLN:NE2	2.80	0.45
1:A:147:GLN:OE1	1:A:438:ILE:HB	2.16	0.45
2:B:171:ASN:HA	2:B:175:LYS:HE3	1.98	0.45
1:A:157:VAL:HG23	1:A:157:VAL:O	2.17	0.45
1:A:270:ASP:CB	1:A:273:LYS:HB2	2.32	0.45
1:A:106:ARG:NH2	1:A:118:LYS:HB2	2.32	0.44
1:A:250:GLY:HA2	1:A:253:MET:CG	2.47	0.44
2:B:16:VAL:HG21	2:B:69:LEU:HB3	1.99	0.44
2:B:38:VAL:HG12	2:B:39:GLN:O	2.17	0.44
2:B:128:VAL:O	2:B:130:GLN:HG3	2.18	0.44
2:B:386[B]:ASP:O	2:B:390[B]:ILE:HA	2.17	0.44
3:G:254[A]:VAL:O	3:G:258[A]:GLU:HG2	2.17	0.44
1:A:209:LYS:NZ	1:A:209:LYS:HB2	2.33	0.44
1:A:306:LEU:CD2	1:A:306:LEU:H	2.30	0.44
1:A:359:LYS:HG2	2:B:376:LYS:HA	1.98	0.44
1:A:460:LYS:O	1:A:463:LYS:HB2	2.18	0.44
2:B:94:ILE:CG1	2:B:217:LEU:HD12	2.47	0.44
2:B:365:SER:HA	2:B:368:TYR:CD1	2.52	0.44
2:B:94:ILE:HG12	2:B:217:LEU:CB	2.47	0.44
2:B:244:ARG:HE	2:B:245:ASP:CG	2.20	0.44
2:B:296:ILE:O	2:B:296:ILE:HG13	2.17	0.44
1:A:51:GLU:HG3	1:A:51:GLU:O	2.17	0.44
1:A:169:GLY:HA2	1:A:352:LEU:O	2.16	0.44
2:B:20:VAL:CG1	2:B:59:ARG:HD2	2.48	0.44
2:B:57:THR:HG22	2:B:58:VAL:O	2.18	0.44
2:B:251:VAL:HG12	2:B:252:LEU:N	2.32	0.44
1:A:65:ASN:HB3	1:A:67:GLU:OE2	2.16	0.44
1:A:298:VAL:HG11	1:A:337:TYR:HE1	1.83	0.44
1:A:306:LEU:H	1:A:306:LEU:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:TYR:O	2:B:147:ALA:HB2	2.18	0.44
2:B:336:SER:HB3	2:B:339:ILE:CG1	2.47	0.44
1:A:106:ARG:HD3	1:A:121:VAL:HG21	2.00	0.44
1:A:140:ILE:HG23	1:A:141:SER:N	2.20	0.44
1:A:169:GLY:N	1:A:175:LYS:HD3	2.33	0.44
1:A:189:PHE:CD2	1:A:197:LYS:O	2.70	0.44
2:B:133:LEU:CD1	2:B:148:LYS:HE3	2.29	0.44
1:A:62:MET:HG3	1:A:64:LEU:HD13	2.00	0.44
1:A:188:ARG:HG3	1:A:189:PHE:CD1	2.53	0.44
2:B:214:LYS:HD3	2:B:214:LYS:N	2.33	0.44
1:A:27:GLU:OE1	1:A:90:ARG:NH1	2.51	0.44
1:A:219:ARG:HH11	1:A:433:TYR:HE2	1.66	0.44
2:B:33:LEU:HA	2:B:33:LEU:HD23	1.60	0.44
2:B:230:ALA:CB	2:B:231:ARG:HD3	2.47	0.44
2:B:246:GLN:H	2:B:246:GLN:HE21	1.66	0.44
2:B:269:SER:O	2:B:272:LEU:N	2.43	0.44
1:A:170:ASP:HA	1:A:329:THR:O	2.18	0.44
1:A:261:GLY:O	1:A:263:HIS:CE1	2.70	0.44
1:A:313:ASN:ND2	1:A:316:PHE:N	2.66	0.44
1:A:458:PRO:HB3	1:A:461:ILE:HD11	1.99	0.44
2:B:89:GLU:H	2:B:89:GLU:HG2	1.57	0.44
2:B:157:GLY:C	2:B:311:TYR:HE1	2.21	0.44
2:B:200:MET:SD	2:B:205:VAL:HG11	2.58	0.44
2:B:259:PHE:HD2	2:B:321:ALA:HB1	1.78	0.44
2:B:367:HIS:C	2:B:367:HIS:CD2	2.91	0.44
1:A:29:GLY:N	1:A:44:LEU:HD22	2.32	0.43
1:A:29:GLY:O	1:A:88:VAL:N	2.51	0.43
1:A:99:VAL:CG2	1:A:253:MET:HA	2.46	0.43
1:A:209:LYS:HE3	2:B:356:ARG:HH22	1.83	0.43
2:B:83:LYS:NZ	2:B:113:PHE:O	2.51	0.43
1:A:483:ILE:O	1:A:487:GLY:HA2	2.18	0.43
2:B:70:VAL:O	2:B:72:GLY:N	2.51	0.43
2:B:86:VAL:HG21	2:B:114:ALA:CB	2.41	0.43
3:G:206[A]:LEU:O	3:G:210[A]:ILE:HG22	2.17	0.43
1:A:248:TYR:OH	1:A:301:LEU:HD12	2.18	0.43
2:B:98:ILE:HG22	2:B:98:ILE:O	2.17	0.43
2:B:154:LEU:HD12	2:B:162:LYS:CA	2.34	0.43
3:G:16[A]:ILE:HD12	3:G:16[A]:ILE:N	2.33	0.43
3:G:228[A]:ALA:HB3	3:G:229[A]:MET:SD	2.58	0.43
1:A:155:SER:N	1:A:441:GLN:OE1	2.51	0.43
2:B:177:HIS:CE1	2:B:178:GLY:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:HIS:CD2	2:B:178:GLY:O	2.72	0.43
2:B:393[B]:MET:SD	2:B:404:VAL:HG11	2.58	0.43
1:A:79:ASP:O	1:A:81:LEU:N	2.51	0.43
1:A:94:ILE:HG22	1:A:95:VAL:N	2.33	0.43
1:A:200:TYR:N	1:A:200:TYR:HD1	2.15	0.43
1:A:426:GLU:CD	1:A:429:LYS:HZ1	2.22	0.43
2:B:42:GLU:O	2:B:43:SER:HB2	2.19	0.43
2:B:130:GLN:HB3	2:B:357:ILE:HD13	2.01	0.43
2:B:222:MET:O	2:B:224:GLU:N	2.52	0.43
2:B:326:PHE:C	2:B:328:HIS:H	2.21	0.43
1:A:59:LEU:HD21	1:A:76:PHE:O	2.18	0.43
1:A:286:ARG:HA	2:B:275:ILE:HD12	2.00	0.43
1:A:355:GLU:HG2	2:B:379:GLN:NE2	2.33	0.43
1:A:429:LYS:NZ	1:A:429:LYS:HB2	2.34	0.43
2:B:90:THR:HG22	2:B:108:ILE:CG2	2.49	0.43
2:B:118:ALA:N	2:B:295:ARG:NH2	2.66	0.43
2:B:296:ILE:HD12	2:B:306:SER:OG	2.19	0.43
1:A:22:SER:HB3	1:A:87:ILE:CD1	2.48	0.43
1:A:180:ILE:HD12	1:A:180:ILE:HA	1.80	0.43
1:A:196:LYS:HB3	1:A:196:LYS:NZ	2.32	0.43
1:A:386:VAL:HG13	1:A:489:ILE:HD11	2.01	0.43
1:A:500:ILE:HD12	1:A:500:ILE:HA	1.84	0.43
2:B:139:VAL:HG11	2:B:348:VAL:CG1	2.49	0.43
2:B:168:GLU:N	2:B:420:VAL:HG21	2.33	0.43
2:B:326:PHE:O	2:B:328:HIS:N	2.51	0.43
2:B:406:ARG:O	2:B:410:ILE:HG13	2.19	0.43
1:A:109:ASP:O	1:A:233:SER:N	2.51	0.43
1:A:168:ILE:HD13	1:A:334:VAL:HG12	2.01	0.43
1:A:200:TYR:O	1:A:264:ALA:HA	2.18	0.43
1:A:263:HIS:HB3	1:A:320:SER:OG	2.18	0.43
2:B:88:PRO:C	2:B:90:THR:H	2.21	0.43
1:A:87:ILE:HA	1:A:87:ILE:HD13	1.81	0.43
1:A:255:GLU:HG2	1:A:258:ARG:NH1	2.34	0.43
2:B:203:SER:HA	8:B:620:HOH:O	2.19	0.43
2:B:319:ASP:OD1	2:B:320:PRO:HD2	2.19	0.43
2:B:333:THR:HA	2:B:353:SER:OG	2.19	0.43
1:A:186:GLN:HB2	1:A:228:TYR:HE2	1.83	0.43
1:A:229:THR:HG22	1:A:230:ILE:N	2.34	0.43
2:B:35:ALA:HB2	2:B:82:ILE:N	2.34	0.43
2:B:161:GLY:O	2:B:162:LYS:HB2	2.18	0.43
2:B:268:VAL:HA	2:B:271:LEU:HG	2.01	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:CB	2.67	0.43
2:B:428:MET:O	2:B:430:LYS:N	2.52	0.43
1:A:228:TYR:CD2	1:A:228:TYR:O	2.72	0.42
2:B:188:GLU:HG3	6:B:601:PO4:O3	2.18	0.42
2:B:200:MET:HB3	2:B:206:ILE:CD1	2.49	0.42
1:A:173:THR:HG22	1:A:352:LEU:HB3	2.01	0.42
1:A:276:VAL:HG12	2:B:286:ALA:HB2	2.01	0.42
1:A:294:TYR:HB3	1:A:298:VAL:HG22	2.01	0.42
2:B:220:GLY:HA3	2:B:232:VAL:HB	2.01	0.42
3:G:17[A]:THR:HG22	3:G:229[A]:MET:HA	2.00	0.42
1:A:127:ARG:HG2	1:A:127:ARG:NH1	2.35	0.42
1:A:313:ASN:HD21	1:A:315:SER:HB2	1.84	0.42
2:B:118:ALA:N	2:B:295:ARG:HH22	2.18	0.42
2:B:253:LEU:CG	2:B:255:ILE:HD11	2.47	0.42
2:B:292:MET:CE	2:B:293:GLN:HG2	2.46	0.42
2:B:358:MET:O	2:B:358:MET:HG2	2.19	0.42
2:B:465:GLU:O	2:B:469:LYS:N	2.52	0.42
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.74	0.42
1:A:306:LEU:C	1:A:308:ARG:H	2.23	0.42
2:B:142:LEU:HG	2:B:367:HIS:CD2	2.54	0.42
2:B:452:LEU:HA	2:B:453:PRO:HD3	1.92	0.42
3:G:86[A]:MET:O	3:G:87[A]:LYS:HG3	2.19	0.42
1:A:468:PHE:O	1:A:472:VAL:HG23	2.19	0.42
2:B:259:PHE:CE1	2:B:263:GLN:OE1	2.72	0.42
1:A:251:CYS:SG	1:A:268:TYR:OH	2.69	0.42
1:A:351:PHE:CZ	1:A:353:GLU:HG2	2.54	0.42
1:A:479:LEU:H	1:A:479:LEU:CD1	2.28	0.42
2:B:111:LYS:HB2	2:B:112:GLN:OE1	2.20	0.42
2:B:182:VAL:HG12	2:B:183:PHE:N	2.34	0.42
1:A:202:ILE:HD11	1:A:257:PHE:HE2	1.85	0.42
1:A:381:ARG:H	1:A:381:ARG:HD2	1.85	0.42
2:B:164:VAL:HG21	7:B:604:ADP:N7	2.34	0.42
2:B:285:LEU:O	2:B:285:LEU:HG	2.19	0.42
2:B:350:PRO:HB2	2:B:378:LEU:HD13	2.02	0.42
2:B:428:MET:CB	2:B:430:LYS:HE2	2.49	0.42
1:A:490:SER:HB3	1:A:493:SER:HB2	2.00	0.42
2:B:158:ALA:H	2:B:337:ARG:NH2	2.18	0.42
2:B:234:LEU:O	2:B:238:THR:N	2.49	0.42
2:B:244:ARG:HG3	2:B:302:GLY:HA3	2.01	0.42
3:G:81[A]:SER:HA	3:G:84[A]:LYS:HE2	2.00	0.42
1:A:202:ILE:O	1:A:266:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HE3	2:B:356:ARG:CZ	2.50	0.42
1:A:286:ARG:HA	2:B:275:ILE:CD1	2.50	0.42
2:B:29:LEU:HD12	2:B:58:VAL:HG13	2.01	0.42
2:B:258:ILE:HD11	2:B:292:MET:SD	2.60	0.42
2:B:433:PRO:O	2:B:435:LYS:N	2.53	0.42
1:A:140:ILE:HG12	1:A:143:ARG:HH12	1.84	0.42
1:A:164:ARG:HB3	1:A:306:LEU:HD12	2.01	0.42
1:A:173:THR:CG2	1:A:352:LEU:HB3	2.50	0.42
2:B:138:LYS:HD2	2:B:414:LEU:CD2	2.48	0.42
3:G:10[A]:ILE:HG21	3:G:240[A]:ILE:HG13	2.01	0.42
3:G:27[A]:LYS:HE2	3:G:222[A]:GLN:OE1	2.20	0.42
3:G:36[A]:LYS:HD2	3:G:36[A]:LYS:HA	1.82	0.42
1:A:16:ARG:O	1:A:18:GLY:N	2.52	0.41
1:A:129:VAL:O	1:A:308:ARG:NH1	2.53	0.41
1:A:150:ILE:HG21	1:A:153:VAL:HG23	2.01	0.41
1:A:496:LYS:HE2	1:A:496:LYS:CA	2.49	0.41
2:B:16:VAL:O	2:B:17:ILE:HG13	2.20	0.41
2:B:97:VAL:C	2:B:98:ILE:HG12	2.40	0.41
2:B:230:ALA:HB2	2:B:264:ALA:CB	2.49	0.41
1:A:306:LEU:O	1:A:308:ARG:N	2.54	0.41
2:B:25:PHE:HE2	2:B:77:ASP:HB2	1.84	0.41
2:B:86:VAL:O	2:B:112:GLN:NE2	2.53	0.41
2:B:401:LYS:HB2	2:B:401:LYS:HE3	1.79	0.41
1:A:44:LEU:HD21	1:A:88:VAL:HB	2.02	0.41
1:A:244:TYR:O	1:A:274:GLN:NE2	2.54	0.41
1:A:338:ILE:CB	1:A:339:PRO:HD3	2.49	0.41
2:B:378:LEU:C	2:B:381[B]:TYR:HB3	2.40	0.41
2:B:421:ALA:HB2	7:B:604:ADP:C6	2.54	0.41
1:A:423:ARG:HG2	1:A:454:ASP:O	2.21	0.41
1:A:74:VAL:HG13	1:A:74:VAL:O	2.20	0.41
1:A:282:SER:OG	1:A:287:ARG:HB2	2.20	0.41
2:B:255:ILE:N	2:B:255:ILE:HD12	2.36	0.41
3:G:7[A]:LEU:HD23	3:G:10[A]:ILE:HD12	2.02	0.41
1:A:185:ASN:OD1	1:A:188:ARG:NH2	2.53	0.41
1:A:270:ASP:H	1:A:326:VAL:HB	1.84	0.41
2:B:180:TYR:HB3	2:B:181:SER:H	1.71	0.41
2:B:381[B]:TYR:HB2	2:B:403:THR:HG21	2.02	0.41
2:B:398[B]:GLU:HA	2:B:401:LYS:HB3	2.01	0.41
1:A:42:HIS:CG	1:A:43:GLY:N	2.89	0.41
2:B:244:ARG:HG2	2:B:245:ASP:N	2.32	0.41
1:A:84:GLU:CD	2:B:54:GLY:HA2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HG23	1:A:430:GLN:HG2	2.02	0.41
1:A:294:TYR:HA	1:A:295:PRO:HD3	1.63	0.41
1:A:351:PHE:HD2	1:A:366:ASN:HB3	1.86	0.41
1:A:381:ARG:H	1:A:381:ARG:CD	2.33	0.41
1:A:492:GLN:O	1:A:496:LYS:HG2	2.21	0.41
2:B:84:ILE:HD11	2:B:238:THR:HB	2.02	0.41
2:B:126:MET:HE1	2:B:297:THR:HG21	2.03	0.41
2:B:139:VAL:HG22	2:B:414:LEU:HD22	2.03	0.41
2:B:151:LYS:O	2:B:330:ASP:N	2.53	0.41
2:B:365:SER:O	2:B:368:TYR:HD1	2.04	0.41
1:A:64:LEU:HD21	8:A:633:HOH:O	2.19	0.41
1:A:96:ASP:CA	1:A:128:ARG:HA	2.41	0.41
1:A:156:LEU:HG	1:A:428:LEU:HD11	2.02	0.41
1:A:168:ILE:O	1:A:352:LEU:N	2.51	0.41
1:A:294:TYR:HB3	1:A:298:VAL:HG21	2.02	0.41
1:A:358:TYR:CB	2:B:375:GLN:HB2	2.49	0.41
2:B:177:HIS:NE2	2:B:178:GLY:O	2.54	0.41
2:B:186:VAL:O	2:B:260:ARG:HG3	2.20	0.41
2:B:237:LEU:HD21	2:B:295:ARG:HD3	2.03	0.41
2:B:332:THR:O	2:B:353:SER:HB3	2.20	0.41
2:B:416:GLN:NE2	2:B:431:LEU:HD23	2.36	0.41
3:G:24[A]:ALA:HB1	3:G:226[A]:MET:HG3	2.02	0.41
3:G:259[A]:LEU:HA	3:G:259[A]:LEU:HD22	1.85	0.41
8:A:607:HOH:O	2:B:124:ILE:HG13	2.20	0.41
2:B:63:MET:HG3	2:B:82:ILE:HD11	2.03	0.41
2:B:90:THR:HG22	2:B:108:ILE:HG21	2.03	0.41
2:B:126:MET:HA	2:B:126:MET:CE	2.50	0.41
1:A:28:THR:C	1:A:44:LEU:HD22	2.42	0.40
1:A:251:CYS:SG	1:A:308:ARG:NE	2.95	0.40
2:B:43:SER:OG	2:B:44:ARG:N	2.52	0.40
2:B:164:VAL:HG13	2:B:420:VAL:CG1	2.50	0.40
2:B:235:THR:C	2:B:237:LEU:N	2.75	0.40
2:B:332:THR:HB	2:B:354:THR:H	1.87	0.40
1:A:165:GLU:O	1:A:324:LEU:HB3	2.21	0.40
1:A:189:PHE:CE2	1:A:197:LYS:HE2	2.56	0.40
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.88	0.40
1:A:354:THR:HG23	1:A:355:GLU:N	2.36	0.40
2:B:86:VAL:HG11	2:B:114:ALA:HB3	2.03	0.40
2:B:126:MET:SD	2:B:126:MET:N	2.94	0.40
2:B:139:VAL:HA	2:B:143:LEU:HB2	2.03	0.40
2:B:247:GLU:O	2:B:249:GLN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:PRO:HB3	2:B:378:LEU:HD13	2.04	0.40
1:A:81:LEU:HD12	1:A:81:LEU:H	1.86	0.40
1:A:99:VAL:CG1	1:A:127:ARG:HB2	2.51	0.40
2:B:343:GLY:O	2:B:345:TYR:HD1	2.04	0.40
2:B:362:ILE:HD13	2:B:362:ILE:N	2.36	0.40
3:G:250[A]:THR:O	3:G:254[A]:VAL:HG23	2.21	0.40
3:G:263[A]:ILE:HA	3:G:266[A]:ALA:HB3	2.04	0.40
1:A:149:GLY:HA3	1:A:435:PRO:CB	2.51	0.40
1:A:188:ARG:HG3	1:A:189:PHE:CE1	2.56	0.40
1:A:236:ALA:HB3	2:B:294:GLU:HG3	2.02	0.40
1:A:335:SER:O	1:A:340:THR:HG23	2.21	0.40
2:B:189:ARG:O	2:B:192:GLU:HG3	2.21	0.40
2:B:250:ASP:HA	2:B:303:SER:O	2.21	0.40
2:B:469:LYS:HD3	2:B:469:LYS:O	2.22	0.40
1:A:349:GLN:NE2	1:A:370:SER:HA	2.37	0.40
1:A:417:LEU:O	1:A:420:ARG:HG2	2.22	0.40
3:G:10[A]:ILE:H	3:G:10[A]:ILE:HG13	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/510 (98%)	357 (72%)	101 (20%)	41 (8%)	1	2
2	B	475/479 (99%)	307 (65%)	109 (23%)	59 (12%)	0	1
3	G	118/270 (44%)	96 (81%)	18 (15%)	4 (3%)	3	13
All	All	1092/1259 (87%)	760 (70%)	228 (21%)	104 (10%)	0	1

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	17	ILE
1	A	44	LEU
1	A	50	GLU
1	A	78	ASN
1	A	80	LYS
1	A	84	GLU
1	A	92	GLY
1	A	95	VAL
1	A	109	ASP
1	A	111	LEU
1	A	117	GLY
1	A	134	PRO
1	A	208	GLN
1	A	236	ALA
1	A	295	PRO
1	A	338	ILE
1	A	357	PHE
1	A	451	GLY
1	A	458	PRO
2	B	53	LEU
2	B	97	VAL
2	B	138	LYS
2	B	143	LEU
2	B	188	GLU
2	B	210	ASP
2	B	211	ALA
2	B	245	ASP
2	B	248	GLY
2	B	269	SER
2	B	279	VAL
2	B	281	TYR
2	B	291	THR
2	B	327	ALA
2	B	331	ALA
2	B	344	ILE
2	B	418	PHE
2	B	451	HIS
2	B	453	PRO
3	G	2[A]	ASP
3	G	77[A]	ALA
1	A	19	ALA
1	A	72	GLY

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Mol	Chain	Res	Type
1	A	116	ASP
1	A	191	ASP
1	A	194	ASP
1	A	454	ASP
2	B	40	GLY
2	B	43	SER
2	B	71	ARG
2	B	162	LYS
2	B	174	ALA
2	B	205	VAL
2	B	285	LEU
2	B	393[B]	MET
2	B	431	LEU
2	B	434	LEU
1	A	16	ARG
1	A	21	THR
1	A	34	ILE
1	A	395	ALA
1	A	455	LYS
2	B	67	GLU
2	B	89	GLU
2	B	223	ASN
2	B	246	GLN
2	B	276	PRO
2	B	278	ALA
2	B	323	ALA
2	B	324	THR
2	B	391[B]	LEU
2	B	428	MET
2	B	476	GLU
3	G	31[A]	ALA
3	G	40[A]	VAL
1	A	145	PRO
1	A	307	GLU
2	B	98	ILE
2	B	160	VAL
2	B	270	ALA
2	B	351	LEU
2	B	432	VAL
2	B	435	LYS
2	B	444	ILE
2	B	454	GLU

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Mol	Chain	Res	Type
1	A	38	ILE
1	A	199	LEU
1	A	210	ARG
1	A	262	LYS
1	A	270	ASP
2	B	31	PRO
2	B	440	GLY
1	A	187	LYS
1	A	288	PRO
2	B	390[B]	ILE
1	A	23	VAL
2	B	28	GLY
2	B	68	GLY
2	B	429	GLY
2	B	58	VAL
2	B	107	PRO
2	B	357	ILE
2	B	159	GLY
2	B	173	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/416 (97%)	348 (86%)	56 (14%)	3	11
2	B	381/384 (99%)	323 (85%)	58 (15%)	3	8
3	G	103/228 (45%)	93 (90%)	10 (10%)	8	24
All	All	888/1028 (86%)	764 (86%)	124 (14%)	3	11

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	30	ARG
1	A	45	ARG

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Mol	Chain	Res	Type
1	A	47	VAL
1	A	50	GLU
1	A	56	SER
1	A	62	MET
1	A	78	ASN
1	A	81	LEU
1	A	83	LYS
1	A	104	LEU
1	A	111	LEU
1	A	113	ASN
1	A	127	ARG
1	A	137	ILE
1	A	144	GLU
1	A	164	ARG
1	A	178	ILE
1	A	180	ILE
1	A	188	ARG
1	A	189	PHE
1	A	191	ASP
1	A	200	TYR
1	A	206	ILE
1	A	209	LYS
1	A	212	THR
1	A	219	ARG
1	A	231	VAL
1	A	233	SER
1	A	237	SER
1	A	244	TYR
1	A	251	CYS
1	A	257	PHE
1	A	269	ASP
1	A	281	MET
1	A	292	GLU
1	A	313	ASN
1	A	316	PHE
1	A	324	LEU
1	A	339	PRO
1	A	341	ASN
1	A	347	ASP
1	A	357	PHE
1	A	358	TYR
1	A	374	VAL

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Mol	Chain	Res	Type
1	A	390	MET
1	A	392	LEU
1	A	410[B]	LEU
1	A	418	LEU
1	A	432	GLN
1	A	439	GLU
1	A	446	TYR
1	A	450	ARG
1	A	468	PHE
1	A	477	GLN
1	A	492	GLN
2	B	12	GLN
2	B	14	VAL
2	B	31	PRO
2	B	58	VAL
2	B	66	THR
2	B	83	LYS
2	B	89	GLU
2	B	91	LEU
2	B	95	MET
2	B	96	ASN
2	B	105	ARG
2	B	113	PHE
2	B	125	GLU
2	B	126	MET
2	B	143	LEU
2	B	148	LYS
2	B	154	LEU
2	B	166	ILE
2	B	170	ILE
2	B	188	GLU
2	B	192	GLU
2	B	194	ASN
2	B	195	ASP
2	B	207	ASN
2	B	212	THR
2	B	214	LYS
2	B	231	ARG
2	B	246	GLN
2	B	249	GLN
2	B	252	LEU
2	B	259	PHE

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Mol	Chain	Res	Type
2	B	269	SER
2	B	271	LEU
2	B	284	THR
2	B	285	LEU
2	B	292	MET
2	B	299	THR
2	B	318	THR
2	B	329	LEU
2	B	335	LEU
2	B	341	GLU
2	B	349	ASP
2	B	359	ASP
2	B	362	ILE
2	B	368	TYR
2	B	380[B]	ASP
2	B	402	LEU
2	B	412	ARG
2	B	425	THR
2	B	427	HIS
2	B	437	THR
2	B	441	PHE
2	B	449	TYR
2	B	453	PRO
2	B	457	PHE
2	B	460	VAL
2	B	471	ASP
2	B	475	GLU
3	G	28[A]	TYR
3	G	30[A]	ARG
3	G	208[A]	ASN
3	G	211[A]	TYR
3	G	226[A]	MET
3	G	229[A]	MET
3	G	234[A]	LYS
3	G	247[A]	PHE
3	G	259[A]	LEU
3	G	269[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	208	GLN
1	A	366	ASN
1	A	477	GLN
1	A	492	GLN
2	B	24	GLN
2	B	73	GLN
2	B	96	ASN
2	B	207	ASN
2	B	246	GLN
2	B	249	GLN
2	B	263	GLN
2	B	416	GLN
2	B	427	HIS
2	B	442	GLN
3	G	85[A]	GLN
3	G	252[A]	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is 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
7	ADP	B	604	-	24,29,29	1.10	2 (8%)	29,45,45	1.62	6 (20%)
5	ATP	A	603	4	26,33,33	1.14	3 (11%)	31,52,52	1.70	6 (19%)
6	PO4	B	601	-	4,4,4	1.95	3 (75%)	6,6,6	0.41	0

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	603	ATP	PG-O3G	-2.64	1.44	1.54
5	A	603	ATP	C2-N3	2.63	1.36	1.32
7	B	604	ADP	C2'-C1'	-2.42	1.50	1.53
6	B	601	PO4	P-O3	-2.32	1.47	1.54
7	B	604	ADP	C2-N3	2.15	1.35	1.32
6	B	601	PO4	P-O4	-2.05	1.48	1.54
6	B	601	PO4	P-O2	-2.05	1.48	1.54
5	A	603	ATP	C2'-C1'	-2.01	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	603	ATP	C1'-N9-C4	5.64	136.54	126.64
7	B	604	ADP	O3'-C3'-C2'	4.27	125.64	111.82
5	A	603	ATP	O5'-C5'-C4'	3.84	122.21	108.99
7	B	604	ADP	O2'-C2'-C3'	3.42	122.87	111.82
7	B	604	ADP	C5-C6-N6	3.28	125.33	120.35
7	B	604	ADP	O2B-PB-O1B	3.06	122.65	110.68
5	A	603	ATP	PB-O3B-PG	2.33	140.83	132.83
5	A	603	ATP	O3'-C3'-C4'	2.31	117.73	111.05
5	A	603	ATP	C4-C5-N7	2.24	111.74	109.40
7	B	604	ADP	O4'-C4'-C3'	-2.23	100.69	105.11
7	B	604	ADP	N3-C2-N1	-2.05	125.48	128.68
5	A	603	ATP	O2'-C2'-C3'	2.01	118.32	111.82

There are no chirality outliers.
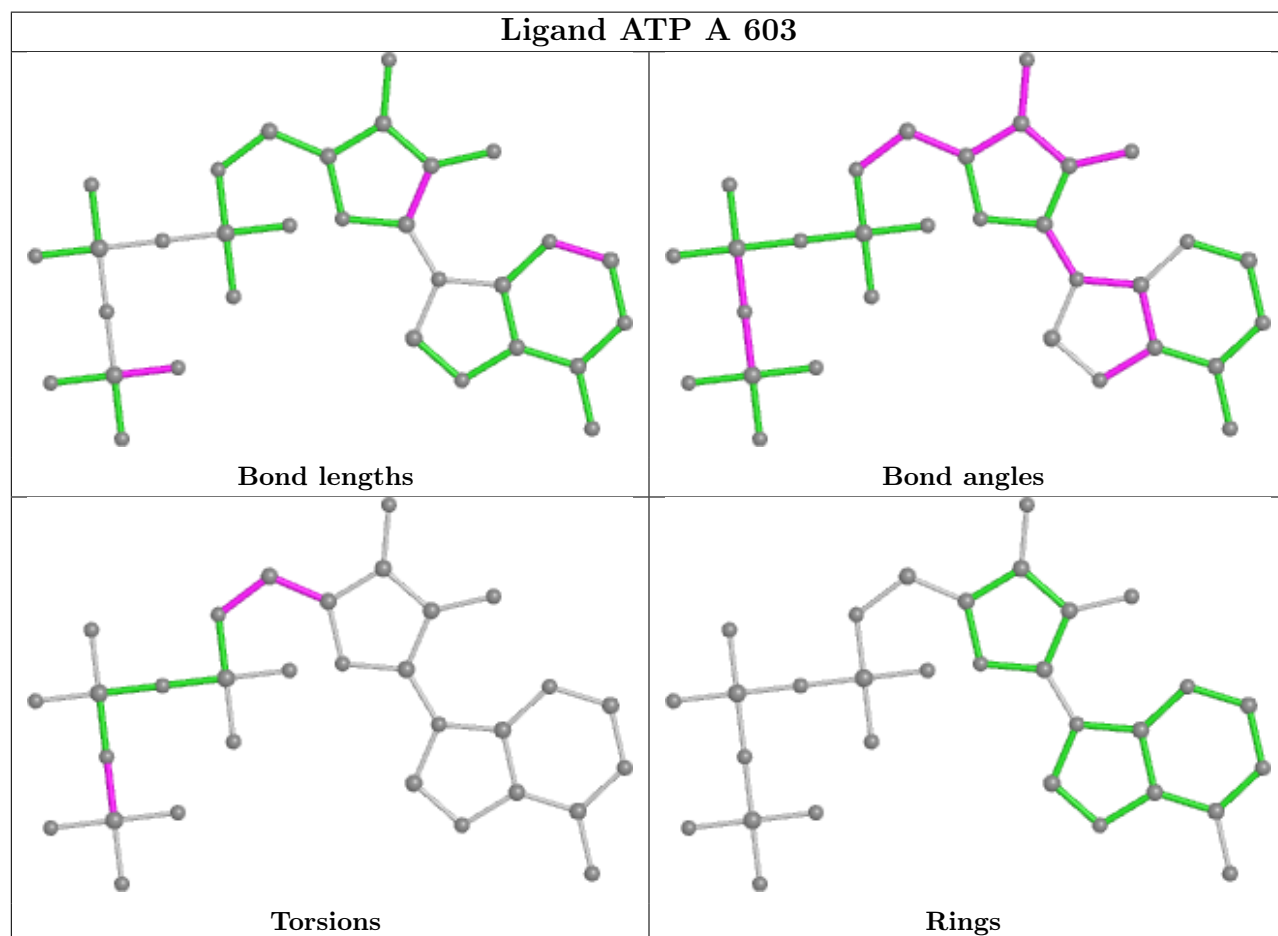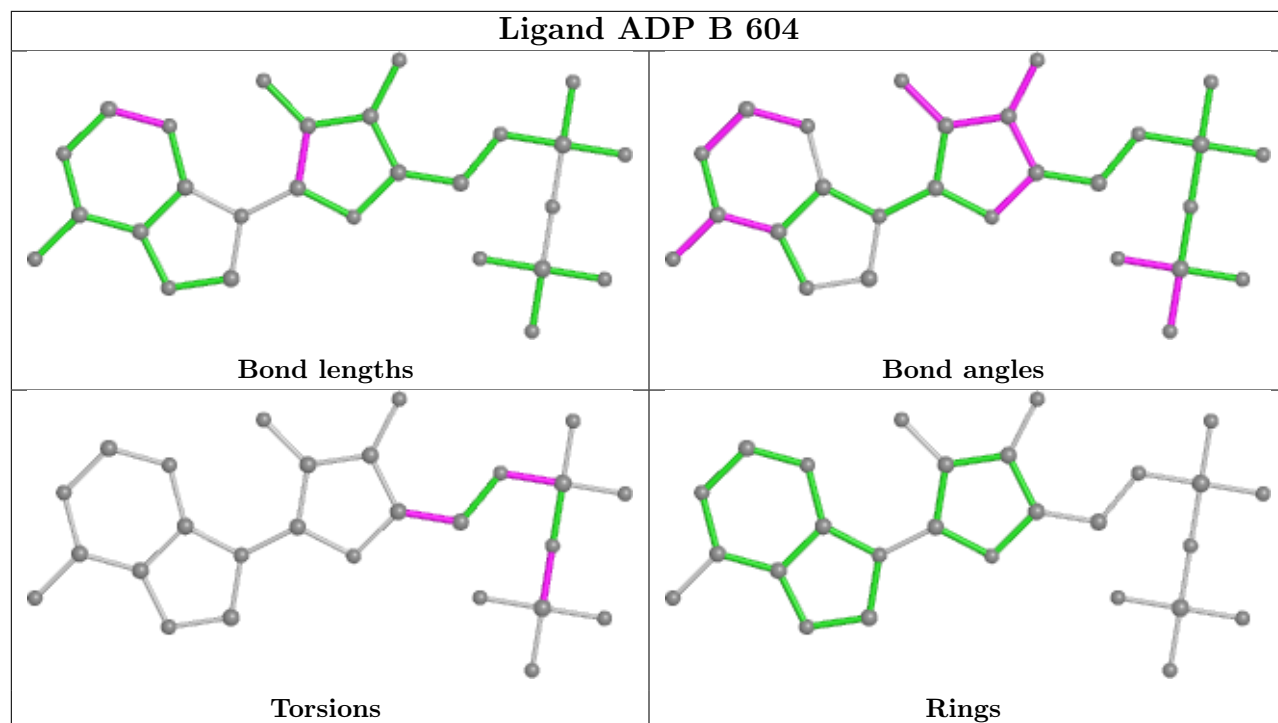
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	603	ATP	PB-O3B-PG-O2G
7	B	604	ADP	PA-O3A-PB-O2B
7	B	604	ADP	C5'-O5'-PA-O2A
7	B	604	ADP	O4'-C4'-C5'-O5'
7	B	604	ADP	C3'-C4'-C5'-O5'
5	A	603	ATP	C3'-C4'-C5'-O5'
5	A	603	ATP	O4'-C4'-C5'-O5'
5	A	603	ATP	C4'-C5'-O5'-PA
7	B	604	ADP	PA-O3A-PB-O1B
7	B	604	ADP	C5'-O5'-PA-O3A
7	B	604	ADP	C5'-O5'-PA-O1A
5	A	603	ATP	PB-O3B-PG-O1G

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	604	ADP	7	0
5	A	603	ATP	6	0
6	B	601	PO4	1	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 then 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.

Ligand ADP B 604

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 603

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.