Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 06:21 PM EDT

PDB ID	:	2DPN
Title	:	Crystal Structure of the glycerol kinase from Thermus thermophilus HB8
Authors	:	Asada, Y.; Sugahara, M.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-05-12
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

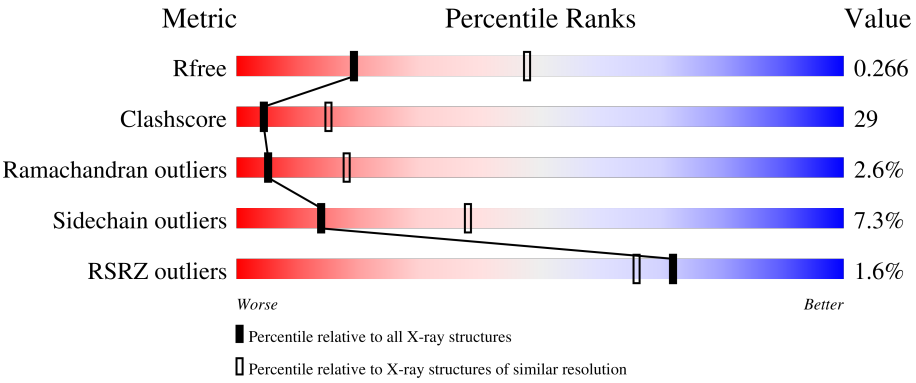
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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% 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	495	65% 31%
1	B	495	3% 46% 46% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7888 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	4	0	0
			3753	2400	664	683	6			
1	B	492	Total	C	N	O	S	4	0	0
			3753	2400	664	683	6			

- Molecule 2 is water.

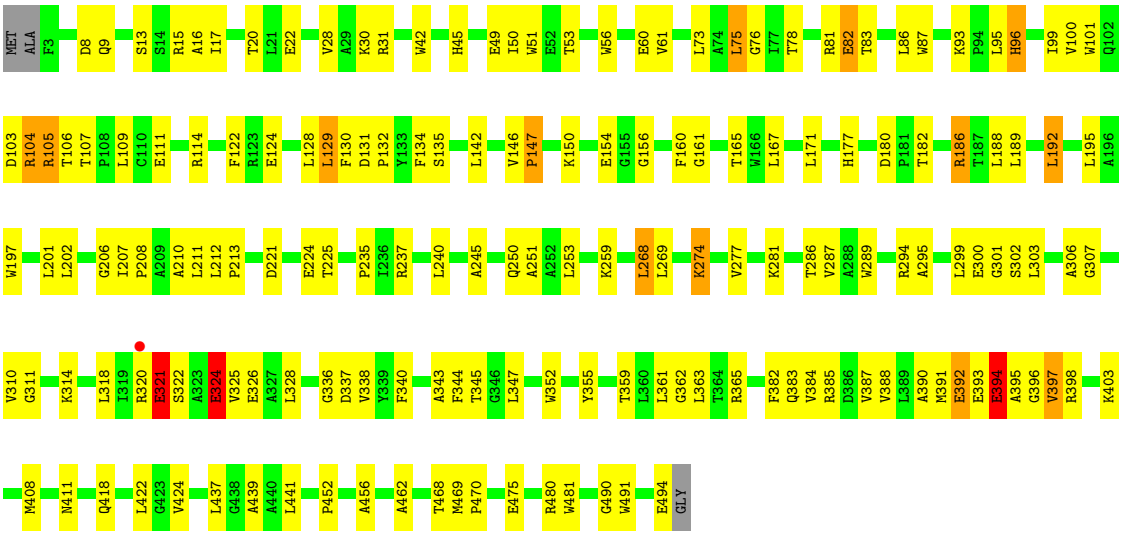
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	243	Total	O	0	0
			243	243		
2	B	139	Total	O	0	0
			139	139		

3 Residue-property plots (i)

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

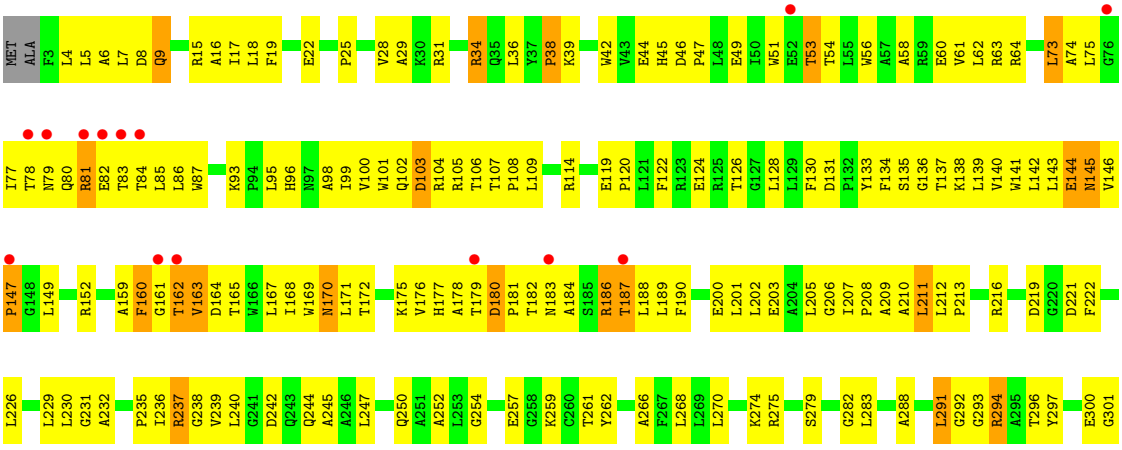
• Molecule 1: Glycerol kinase

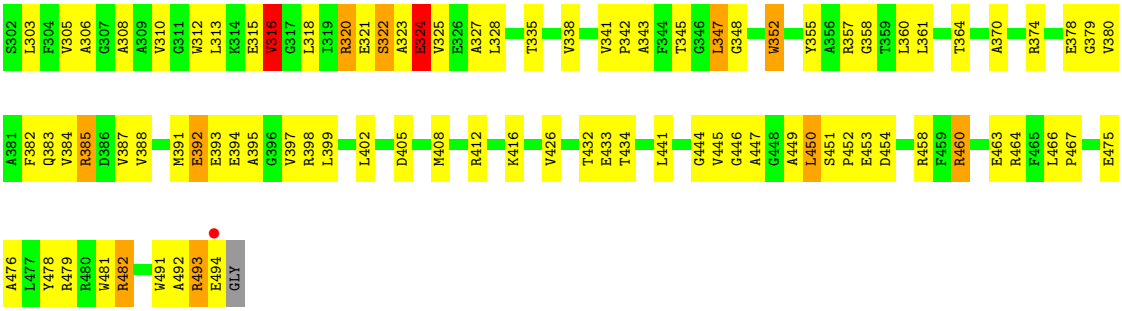
Chain A:



• Molecule 1: Glycerol kinase

Chain B:




S302 L303 F304 V305 A306 G307 A308 A309 V310 G311 W312 L313 K314 E315 V316 G317 L318 I319 R320 E321 S322 A323 E324 V325 E326 A327 L328 T335 V338 V341 P342 A343 F344 T345 G346 L347 G348 W352 Y355 A356 R357 G358 T359 L360 L361 T364 A370 R374 E378 G379 V380
A381 F382 Q383 V384 R385 D386 V387 V388 M391 E392 E393 E394 A395 G396 V397 R398 L399 L402 D405 M408 R412 K416 V426 T432 E433 T434 L441 G444 V445 G446 A447 G448 A449 L450 S451 P452 E453 D454 R458 F459 R460 E463 R464 F465 L466 P467 E475
A476 L477 Y478 R479 R480 W481 R482 W491 A492 R493 E494 GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.99Å 90.51Å 182.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.80 29.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.77-2.80) 99.2 (29.77-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.266 0.213 , 0.266	Depositor DCC
R_{free} test set	1425 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7888	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.46	1/3837 (0.0%)	0.72	0/5221
1	B	0.47	1/3837 (0.0%)	0.72	0/5221
All	All	0.47	2/7674 (0.0%)	0.72	0/10442

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	TRP	NE1-CE2	8.70	1.48	1.37
1	B	352	TRP	NE1-CE2	8.47	1.48	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3753	0	3786	143	0
1	B	3753	0	3786	295	0
2	A	243	0	0	8	0
2	B	139	0	0	9	0
All	All	7888	0	7572	431	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 29.

All (431) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HG3	1:B:321:GLU:H	1.18	1.07
1:B:47:PRO:HG3	1:B:85:LEU:HD21	1.35	1.06
1:B:186:ARG:HH11	1:B:186:ARG:HB3	1.26	1.00
1:A:86:LEU:HD12	1:A:142:LEU:HD13	1.43	0.98
1:A:17:ILE:HD12	1:A:28:VAL:HG22	1.42	0.96
1:B:397:VAL:HG12	1:B:398:ARG:H	1.30	0.96
1:B:294:ARG:HB3	1:B:294:ARG:HH11	1.33	0.93
1:B:310:VAL:HG11	1:B:325:VAL:HG21	1.48	0.93
1:B:294:ARG:HB3	1:B:294:ARG:NH1	1.83	0.93
1:A:146:VAL:CG1	1:A:147:PRO:HD2	1.98	0.92
1:B:172:THR:HB	1:B:175:LYS:HB2	1.51	0.91
1:B:139:LEU:HD23	1:B:207:ILE:HD13	1.53	0.88
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.57	0.87
1:B:74:ALA:HB1	1:B:237:ARG:HG2	1.56	0.86
1:B:178:ALA:HA	1:B:213:PRO:HB3	1.56	0.86
1:B:202:LEU:HD13	1:B:209:ALA:HB2	1.60	0.84
1:A:224:GLU:OE2	1:A:235:PRO:HA	1.77	0.83
1:A:303:LEU:HD13	1:A:383:GLN:HB3	1.61	0.82
1:B:101:TRP:HA	1:B:138:LYS:HE3	1.61	0.82
1:B:320:ARG:HG3	1:B:321:GLU:N	1.93	0.81
1:B:397:VAL:HG12	1:B:398:ARG:N	1.96	0.79
1:B:200:GLU:O	1:B:203:GLU:HG2	1.84	0.77
1:B:46:ASP:HB3	1:B:49:GLU:HB2	1.66	0.77
1:A:124:GLU:HB3	2:A:518:HOH:O	1.83	0.77
1:B:343:ALA:HB2	1:B:347:LEU:HD13	1.65	0.77
1:B:85:LEU:HD21	1:B:98:ALA:HB2	1.66	0.77
1:B:355:TYR:CE1	1:B:494:GLU:HA	2.20	0.76
1:B:441:LEU:O	1:B:445:VAL:HG23	1.85	0.76
1:B:8:ASP:HA	1:B:78:THR:HG23	1.68	0.76
1:B:146:VAL:CG1	1:B:147:PRO:HD2	2.15	0.76
1:B:47:PRO:HG3	1:B:85:LEU:CD2	2.12	0.76
1:B:312:TRP:O	1:B:316:VAL:HG22	1.86	0.75
1:B:86:LEU:HB3	1:B:95:LEU:HD11	1.66	0.75
1:B:313:LEU:CD2	1:B:318:LEU:HD12	2.17	0.75
1:B:186:ARG:HH11	1:B:186:ARG:CB	1.97	0.74
1:B:114:ARG:HD3	1:B:119:GLU:OE1	1.88	0.74
1:B:133:TYR:O	1:B:138:LYS:HE2	1.88	0.73
1:B:146:VAL:HG13	1:B:147:PRO:HD2	1.70	0.73
1:A:86:LEU:CD1	1:A:142:LEU:HD13	2.17	0.73
1:B:36:LEU:HB2	1:B:44:GLU:HB2	1.70	0.73
1:B:77:ILE:HB	1:B:239:VAL:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:GLN:HG2	1:B:434:THR:HG21	1.70	0.73
1:B:482:ARG:NH2	2:B:539:HOH:O	2.21	0.72
1:A:56:TRP:CZ2	1:A:60:GLU:HG3	2.23	0.72
1:B:202:LEU:HD21	1:B:212:LEU:HD11	1.70	0.72
1:B:79:ASN:ND2	1:B:80:GLN:O	2.23	0.71
1:B:294:ARG:HH11	1:B:294:ARG:CB	2.04	0.71
1:B:114:ARG:NH2	2:B:633:HOH:O	2.22	0.71
1:B:398:ARG:NH2	2:B:589:HOH:O	2.23	0.71
1:B:99:ILE:HG23	1:B:103:ASP:OD2	1.90	0.71
1:B:313:LEU:HD22	1:B:318:LEU:HD12	1.71	0.71
1:A:274:LYS:H	1:A:274:LYS:CE	2.03	0.71
1:B:310:VAL:CG1	1:B:325:VAL:HG21	2.21	0.69
1:A:274:LYS:H	1:A:274:LYS:HE3	1.57	0.69
1:B:294:ARG:HH11	1:B:294:ARG:H	1.40	0.69
1:B:58:ALA:HB1	1:B:230:LEU:HD21	1.74	0.69
1:B:77:ILE:N	1:B:238:GLY:O	2.25	0.68
1:B:4:LEU:O	1:B:18:LEU:HD12	1.94	0.68
1:A:468:THR:HG22	1:A:468:THR:O	1.92	0.68
1:B:168:ILE:HG23	1:B:176:VAL:HG13	1.76	0.68
1:A:274:LYS:H	1:A:274:LYS:CD	2.06	0.68
1:B:320:ARG:CG	1:B:321:GLU:H	2.03	0.68
1:A:392:GLU:O	1:A:394:GLU:N	2.27	0.68
1:A:146:VAL:HG12	1:A:147:PRO:HD2	1.76	0.67
1:B:384:VAL:O	1:B:388:VAL:HG23	1.95	0.67
1:A:182:THR:HG22	1:A:287:VAL:O	1.94	0.67
1:A:195:LEU:HD21	1:A:295:ALA:HB2	1.76	0.66
1:B:51:TRP:CE2	1:B:170:ASN:HB3	2.29	0.66
1:A:359:THR:HG23	1:B:361:LEU:HD23	1.77	0.66
1:B:322:SER:O	1:B:325:VAL:HG23	1.95	0.66
1:B:119:GLU:HB3	1:B:120:PRO:HD3	1.77	0.65
1:B:128:LEU:HD13	1:B:134:PHE:CD2	2.31	0.65
1:B:142:LEU:O	1:B:149:LEU:HD23	1.96	0.65
1:B:141:TRP:O	1:B:145:ASN:HB2	1.95	0.65
1:B:343:ALA:CB	1:B:347:LEU:HD13	2.26	0.65
1:B:236:ILE:C	1:B:237:ARG:HD2	2.16	0.65
1:B:143:LEU:HD23	1:B:207:ILE:HG12	1.79	0.65
1:A:82:GLU:HG2	1:A:101:TRP:CB	2.27	0.64
1:A:390:ALA:O	1:A:394:GLU:HB2	1.97	0.64
1:B:397:VAL:CG1	1:B:398:ARG:H	2.07	0.64
1:B:306:ALA:HB1	1:B:408:MET:CE	2.28	0.63
1:A:311:GLY:O	1:A:314:LYS:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HG	2:A:504:HOH:O	1.98	0.63
1:B:493:ARG:O	1:B:494:GLU:HB2	1.98	0.63
1:A:394:GLU:HA	1:A:394:GLU:OE1	1.97	0.63
1:B:17:ILE:HD12	1:B:28:VAL:HG22	1.80	0.63
1:B:51:TRP:CH2	1:B:171:LEU:CD2	2.81	0.63
1:B:165:THR:OG1	1:B:179:THR:HB	1.98	0.63
1:B:254:GLY:O	1:B:257:GLU:HB2	1.99	0.62
1:A:422:LEU:O	1:A:424:VAL:HG23	1.99	0.62
1:A:310:VAL:CG1	1:A:325:VAL:HG21	2.29	0.62
1:B:47:PRO:CG	1:B:85:LEU:HD21	2.20	0.62
1:B:450:LEU:HD23	1:B:450:LEU:H	1.65	0.62
1:B:492:ALA:O	1:B:494:GLU:N	2.33	0.62
1:B:237:ARG:HD2	1:B:237:ARG:N	2.14	0.62
1:B:444:GLY:HA3	1:B:450:LEU:HD21	1.81	0.62
1:A:344:PHE:HB3	1:B:364:THR:HA	1.82	0.62
1:B:310:VAL:HG11	1:B:325:VAL:CG2	2.25	0.62
1:B:445:VAL:HA	1:B:450:LEU:O	2.00	0.62
1:A:324:GLU:O	1:A:328:LEU:HB2	2.00	0.62
1:B:310:VAL:CG1	1:B:325:VAL:CG2	2.77	0.62
1:A:300:GLU:HG2	1:A:301:GLY:N	2.14	0.61
1:B:104:ARG:HD2	1:B:345:THR:HB	1.82	0.61
1:A:128:LEU:HD22	1:A:134:PHE:CE2	2.35	0.61
1:B:45:HIS:O	1:B:47:PRO:HD3	2.00	0.61
1:B:82:GLU:OE2	1:B:186:ARG:NH1	2.34	0.61
1:B:86:LEU:CD1	1:B:149:LEU:HD21	2.31	0.61
1:A:82:GLU:O	1:A:135:SER:HB3	2.01	0.61
1:A:310:VAL:HG11	1:A:325:VAL:HG21	1.82	0.61
1:B:104:ARG:HD2	1:B:345:THR:O	2.00	0.61
1:B:31:ARG:HD2	1:B:53:THR:HG22	1.83	0.60
1:A:150:LYS:HE3	1:A:154:GLU:OE1	2.01	0.60
1:B:279:SER:HB2	1:B:394:GLU:HG2	1.83	0.60
1:A:281:LYS:HD2	1:A:394:GLU:CG	2.32	0.60
1:B:458:ARG:HD2	2:B:517:HOH:O	2.01	0.60
1:A:221:ASP:OD1	1:A:237:ARG:NH1	2.35	0.59
1:B:61:VAL:HG23	1:B:62:LEU:H	1.67	0.59
1:B:8:ASP:HA	1:B:78:THR:O	2.02	0.59
1:B:47:PRO:CG	1:B:85:LEU:CD2	2.80	0.59
1:B:84:THR:HG23	1:B:160:PHE:CE1	2.37	0.59
1:B:122:PHE:CE1	1:B:201:LEU:HG	2.38	0.59
1:A:82:GLU:HG2	1:A:101:TRP:HB3	1.83	0.58
1:B:328:LEU:HB3	1:B:370:ALA:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HD3	1:B:433:GLU:OE2	2.03	0.58
1:A:307:GLY:N	1:A:408:MET:HE1	2.17	0.58
1:B:122:PHE:CZ	1:B:201:LEU:HG	2.38	0.58
1:B:321:GLU:HG3	1:B:322:SER:N	2.17	0.58
1:A:314:LYS:HD3	1:A:314:LYS:C	2.24	0.58
1:B:167:LEU:O	1:B:171:LEU:HG	2.04	0.58
1:A:177:HIS:NE2	1:A:213:PRO:HB3	2.19	0.57
1:B:392:GLU:OE2	1:B:399:LEU:N	2.36	0.57
1:A:8:ASP:HA	1:A:78:THR:CG2	2.34	0.57
1:B:81:ARG:NH2	1:B:300:GLU:OE1	2.37	0.57
1:B:180:ASP:OD1	1:B:183:ASN:HB2	2.05	0.57
1:B:178:ALA:HA	1:B:213:PRO:CB	2.32	0.57
1:B:283:LEU:HD13	1:B:391:MET:HG2	1.86	0.57
1:B:450:LEU:HD23	1:B:450:LEU:N	2.18	0.57
1:B:244:GLN:HB3	1:B:288:ALA:O	2.05	0.57
1:B:64:ARG:HD3	2:B:519:HOH:O	2.04	0.56
1:A:338:VAL:HG22	1:A:362:GLY:O	2.05	0.56
1:B:160:PHE:CD1	1:B:161:GLY:N	2.73	0.56
1:B:355:TYR:CD1	1:B:494:GLU:HA	2.40	0.56
1:B:168:ILE:CG2	1:B:176:VAL:HG13	2.35	0.56
1:A:16:ALA:O	1:A:17:ILE:HD13	2.05	0.56
1:A:75:LEU:HD23	1:A:76:GLY:N	2.20	0.56
1:A:146:VAL:HG12	1:A:147:PRO:CD	2.35	0.56
1:B:16:ALA:O	1:B:17:ILE:HD13	2.05	0.56
1:A:78:THR:HB	1:A:439:ALA:HB2	1.88	0.56
1:B:321:GLU:HG3	1:B:322:SER:H	1.70	0.56
1:B:348:GLY:O	1:B:352:TRP:N	2.34	0.55
1:B:475:GLU:O	1:B:479:ARG:HG3	2.07	0.55
1:B:7:LEU:HD23	1:B:7:LEU:N	2.21	0.55
1:B:143:LEU:O	1:B:144:GLU:HG3	2.07	0.55
1:B:160:PHE:CG	1:B:161:GLY:N	2.74	0.55
1:B:343:ALA:HB2	1:B:347:LEU:CD1	2.34	0.55
1:B:301:GLY:HA3	1:B:387:VAL:HG11	1.87	0.55
1:B:451:SER:O	1:B:454:ASP:HB2	2.06	0.55
1:A:8:ASP:HA	1:A:78:THR:HG23	1.89	0.55
1:B:86:LEU:HD13	1:B:149:LEU:HD21	1.88	0.55
1:B:211:LEU:N	1:B:211:LEU:HD23	2.22	0.54
1:B:51:TRP:CH2	1:B:171:LEU:HD21	2.43	0.54
1:B:84:THR:HG23	1:B:160:PHE:HE1	1.73	0.54
1:A:274:LYS:HD2	1:A:274:LYS:N	2.23	0.54
1:A:306:ALA:C	1:A:408:MET:HE1	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:O	1:A:422:LEU:HB2	2.07	0.54
1:B:140:VAL:HG21	1:B:205:LEU:HD22	1.89	0.54
1:A:82:GLU:HG2	1:A:101:TRP:HB2	1.90	0.54
1:A:167:LEU:O	1:A:171:LEU:HG	2.07	0.54
1:A:274:LYS:H	1:A:274:LYS:HD2	1.72	0.54
1:A:385:ARG:NH2	1:A:475:GLU:OE2	2.41	0.54
1:A:17:ILE:HD12	1:A:28:VAL:CG2	2.28	0.53
1:B:51:TRP:CH2	1:B:171:LEU:HD23	2.42	0.53
1:A:394:GLU:C	1:A:396:GLY:H	2.11	0.53
1:B:135:SER:HA	1:B:138:LYS:HD2	1.90	0.53
1:B:168:ILE:HG22	1:B:176:VAL:O	2.08	0.53
1:B:313:LEU:HD22	1:B:318:LEU:CD1	2.36	0.53
1:B:82:GLU:HB2	1:B:101:TRP:HB3	1.89	0.53
1:B:387:VAL:O	1:B:391:MET:HG3	2.09	0.53
1:B:83:THR:HG23	1:B:100:VAL:HA	1.90	0.53
1:B:237:ARG:HG3	1:B:447:ALA:HB2	1.91	0.53
1:B:283:LEU:CD1	1:B:391:MET:HG2	2.38	0.53
1:B:74:ALA:CB	1:B:237:ARG:HG2	2.35	0.53
1:B:460:ARG:HG3	2:B:577:HOH:O	2.09	0.53
1:A:17:ILE:CD1	1:A:28:VAL:HG22	2.27	0.52
1:B:324:GLU:OE1	1:B:327:ALA:HB3	2.09	0.52
1:B:453:GLU:CD	1:B:453:GLU:H	2.11	0.52
1:A:20:THR:OG1	1:A:22:GLU:HG2	2.09	0.52
1:B:244:GLN:HG3	1:B:288:ALA:HA	1.91	0.52
1:B:335:THR:HG22	1:B:374:ARG:HB3	1.89	0.52
1:B:164:ASP:O	1:B:168:ILE:HD13	2.09	0.52
1:B:187:THR:HG23	1:B:189:LEU:H	1.73	0.52
1:B:305:VAL:HG13	1:B:308:ALA:HB3	1.91	0.52
1:B:119:GLU:HA	1:B:130:PHE:CE2	2.45	0.52
1:B:159:ALA:HB1	1:B:177:HIS:NE2	2.25	0.52
1:A:78:THR:HA	1:A:240:LEU:O	2.09	0.52
1:A:336:GLY:O	1:A:337:ASP:HB3	2.08	0.52
1:B:453:GLU:CD	1:B:453:GLU:N	2.63	0.52
1:A:177:HIS:CD2	1:A:213:PRO:HB3	2.45	0.52
1:B:8:ASP:HA	1:B:78:THR:CG2	2.39	0.52
1:B:313:LEU:HD23	1:B:318:LEU:HD12	1.92	0.52
1:A:397:VAL:HG12	1:A:398:ARG:H	1.74	0.52
1:A:480:ARG:HD3	1:B:493:ARG:HD3	1.92	0.52
1:B:109:LEU:HD12	1:B:109:LEU:H	1.74	0.52
1:A:15:ARG:HG2	1:A:30:LYS:HB2	1.92	0.52
1:B:6:ALA:C	1:B:7:LEU:HD23	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ALA:HB1	1:B:408:MET:HE2	1.90	0.52
1:B:186:ARG:NH2	1:B:300:GLU:OE2	2.43	0.51
1:B:343:ALA:O	1:B:357:ARG:HA	2.10	0.51
1:B:452:PRO:HG2	1:B:453:GLU:OE1	2.10	0.51
1:B:139:LEU:CD2	1:B:207:ILE:HD13	2.34	0.51
1:B:262:TYR:CB	1:B:408:MET:HB2	2.40	0.51
1:B:186:ARG:HH11	1:B:186:ARG:CG	2.23	0.51
1:B:211:LEU:HD23	1:B:211:LEU:H	1.75	0.51
1:A:15:ARG:HH11	1:A:30:LYS:HD2	1.76	0.51
1:B:382:PHE:HB3	1:B:481:TRP:CE2	2.45	0.51
1:A:274:LYS:CD	1:A:274:LYS:N	2.73	0.51
1:B:216:ARG:HB2	1:B:222:PHE:CZ	2.45	0.51
1:B:45:HIS:O	1:B:98:ALA:HB3	2.10	0.51
1:B:51:TRP:NE1	1:B:170:ASN:HB3	2.26	0.50
1:B:310:VAL:HG13	1:B:325:VAL:HG22	1.92	0.50
1:A:186:ARG:HH21	1:A:300:GLU:CD	2.15	0.50
1:A:394:GLU:O	1:A:396:GLY:N	2.45	0.50
1:B:380:VAL:HG11	1:B:408:MET:HE1	1.93	0.50
1:B:412:ARG:NH2	1:B:463:GLU:OE1	2.45	0.50
1:A:122:PHE:CE1	1:A:201:LEU:HD22	2.47	0.50
1:A:124:GLU:HG3	2:A:549:HOH:O	2.11	0.50
1:B:42:TRP:HA	1:B:103:ASP:OD1	2.12	0.50
1:B:262:TYR:HB2	1:B:408:MET:HB2	1.94	0.50
1:B:275:ARG:HG2	1:B:275:ARG:HH11	1.77	0.50
1:A:56:TRP:CH2	1:A:60:GLU:HG3	2.46	0.49
1:A:302:SER:C	1:A:303:LEU:HD23	2.31	0.49
1:A:104:ARG:HD2	1:A:345:THR:HB	1.95	0.49
1:A:382:PHE:HB3	1:A:481:TRP:CE2	2.46	0.49
1:B:172:THR:CB	1:B:175:LYS:HB2	2.33	0.49
1:A:111:GLU:OE2	1:A:355:TYR:OH	2.29	0.49
1:B:172:THR:O	1:B:175:LYS:HG3	2.11	0.49
1:B:380:VAL:HG11	1:B:408:MET:CE	2.42	0.49
1:A:491:TRP:CZ3	1:B:361:LEU:HD13	2.48	0.49
1:B:126:THR:HG21	1:B:188:LEU:O	2.12	0.49
1:B:188:LEU:O	1:B:201:LEU:HD23	2.12	0.49
1:B:320:ARG:CZ	1:B:320:ARG:HB2	2.42	0.49
1:B:146:VAL:HG12	1:B:147:PRO:HD2	1.95	0.49
1:B:172:THR:HG21	1:B:176:VAL:HG12	1.94	0.49
1:B:323:ALA:C	1:B:325:VAL:H	2.16	0.49
1:A:129:LEU:HD12	1:A:130:PHE:O	2.12	0.49
1:A:268:LEU:HD12	1:A:384:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:HB2	1:B:138:LYS:NZ	2.28	0.49
1:A:300:GLU:HG2	1:A:301:GLY:H	1.76	0.49
1:A:384:VAL:O	1:A:388:VAL:HG23	2.12	0.49
1:A:240:LEU:HD23	1:A:245:ALA:HA	1.95	0.48
1:B:393:GLU:O	1:B:395:ALA:N	2.46	0.48
1:B:324:GLU:OE1	1:B:328:LEU:HG	2.13	0.48
1:B:476:ALA:HA	1:B:479:ARG:NH1	2.29	0.48
1:A:363:LEU:HB2	1:B:358:GLY:HA3	1.94	0.48
1:A:104:ARG:NH2	1:A:131:ASP:OD1	2.47	0.48
1:B:165:THR:OG1	1:B:178:ALA:O	2.30	0.48
1:B:379:GLY:O	1:B:383:GLN:HG3	2.14	0.48
1:A:156:GLY:HA2	1:A:210:ALA:HB1	1.96	0.48
1:A:197:TRP:CZ2	1:A:212:LEU:HD22	2.49	0.48
1:A:268:LEU:C	1:A:269:LEU:HD12	2.34	0.48
1:B:103:ASP:HB2	1:B:138:LYS:HZ1	1.79	0.48
1:B:270:LEU:HD22	1:B:391:MET:HE3	1.96	0.48
1:B:149:LEU:O	1:B:149:LEU:HG	2.14	0.48
1:B:182:THR:OG1	1:B:240:LEU:HD12	2.14	0.48
1:A:171:LEU:O	1:A:225:THR:HA	2.14	0.48
1:B:22:GLU:O	1:B:458:ARG:HD3	2.13	0.48
1:B:39:LYS:O	1:B:42:TRP:HB2	2.14	0.48
1:B:44:GLU:HA	1:B:98:ALA:O	2.14	0.48
1:B:61:VAL:HG23	1:B:62:LEU:N	2.28	0.47
1:A:106:THR:OG1	1:A:132:PRO:HA	2.14	0.47
1:A:384:VAL:O	1:A:387:VAL:HG22	2.14	0.47
1:B:426:VAL:O	1:B:464:ARG:HA	2.14	0.47
1:B:385:ARG:HG2	1:B:478:TYR:CE1	2.48	0.47
1:A:268:LEU:HD13	1:A:387:VAL:CG2	2.44	0.47
1:B:178:ALA:CA	1:B:213:PRO:HB3	2.36	0.47
1:B:203:GLU:HB2	2:B:514:HOH:O	2.14	0.47
1:A:95:LEU:O	1:A:96:HIS:HB2	2.14	0.47
1:B:19:PHE:HA	1:B:25:PRO:HA	1.95	0.47
1:B:51:TRP:CE3	1:B:54:THR:HB	2.50	0.47
1:B:162:THR:O	1:B:164:ASP:N	2.48	0.47
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.69	0.47
1:A:103:ASP:C	1:A:104:ARG:HG2	2.35	0.47
1:B:186:ARG:HH21	1:B:300:GLU:CD	2.17	0.47
1:B:268:LEU:HD11	1:B:388:VAL:HG22	1.95	0.47
1:A:83:THR:HG23	1:A:100:VAL:HA	1.96	0.47
1:B:38:PRO:HG3	1:B:44:GLU:OE1	2.15	0.47
1:B:184:ALA:O	1:B:187:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:NH1	1:B:221:ASP:O	2.44	0.47
1:B:294:ARG:HH11	1:B:294:ARG:N	2.10	0.47
1:A:146:VAL:CG1	1:A:147:PRO:CD	2.80	0.47
1:B:95:LEU:HD22	1:B:149:LEU:HD13	1.97	0.46
1:B:124:GLU:N	1:B:124:GLU:OE2	2.48	0.46
1:B:131:ASP:C	1:B:133:TYR:H	2.18	0.46
1:B:140:VAL:HG23	1:B:207:ILE:HD11	1.97	0.46
1:A:281:LYS:HD2	1:A:394:GLU:CD	2.36	0.46
1:A:398:ARG:HH11	1:A:398:ARG:HG3	1.81	0.46
1:B:100:VAL:HG12	1:B:101:TRP:N	2.31	0.46
1:B:80:GLN:NE2	1:B:163:VAL:HG21	2.30	0.46
1:A:326:GLU:OE2	2:A:594:HOH:O	2.20	0.46
1:B:103:ASP:OD1	1:B:105:ARG:HD2	2.15	0.46
1:B:323:ALA:C	1:B:325:VAL:N	2.69	0.46
1:A:345:THR:HA	2:A:531:HOH:O	2.14	0.46
1:B:86:LEU:O	1:B:95:LEU:HG	2.15	0.46
1:B:235:PRO:HB3	1:B:237:ARG:NH1	2.31	0.46
1:A:268:LEU:HD22	1:A:391:MET:SD	2.56	0.46
1:A:318:LEU:HG	1:B:318:LEU:HD21	1.98	0.46
1:B:294:ARG:NH1	1:B:294:ARG:H	2.12	0.46
1:B:397:VAL:HG13	2:B:507:HOH:O	2.15	0.46
1:B:432:THR:O	1:B:434:THR:N	2.48	0.46
1:B:449:ALA:HB3	1:B:450:LEU:HD23	1.98	0.46
1:B:231:GLY:O	1:B:232:ALA:HB2	2.16	0.46
1:A:49:GLU:O	1:A:53:THR:HG23	2.15	0.46
1:B:95:LEU:O	1:B:96:HIS:HB2	2.16	0.46
1:B:219:ASP:O	1:B:446:GLY:HA3	2.16	0.46
1:A:268:LEU:O	1:A:269:LEU:HD12	2.16	0.45
1:A:437:LEU:O	1:A:441:LEU:HG	2.16	0.45
1:A:122:PHE:CD1	1:A:201:LEU:HD22	2.51	0.45
1:A:303:LEU:HD13	1:A:383:GLN:CB	2.40	0.45
1:B:85:LEU:HD23	1:B:98:ALA:HA	1.98	0.45
1:B:451:SER:HB2	1:B:452:PRO:HD2	1.97	0.45
1:B:51:TRP:HH2	1:B:171:LEU:CD2	2.27	0.45
1:B:164:ASP:CG	1:B:165:THR:N	2.70	0.45
1:B:181:PRO:HD3	1:B:216:ARG:O	2.16	0.45
1:A:302:SER:O	1:A:303:LEU:HD23	2.17	0.45
1:B:5:LEU:HB3	1:B:75:LEU:HD12	1.98	0.45
1:B:36:LEU:O	1:B:38:PRO:HD3	2.15	0.45
1:B:179:THR:HG22	1:B:213:PRO:HB2	1.99	0.45
1:B:135:SER:O	1:B:138:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:MET:HA	1:A:470:PRO:HD3	1.90	0.45
1:A:277:VAL:O	1:A:299:LEU:HD21	2.16	0.45
1:A:73:LEU:HD21	2:A:638:HOH:O	2.16	0.45
1:B:186:ARG:HB3	1:B:186:ARG:NH1	2.09	0.45
1:A:365:ARG:HG3	1:A:365:ARG:HH11	1.82	0.45
1:A:22:GLU:N	1:A:22:GLU:OE1	2.50	0.44
1:A:107:THR:O	1:A:111:GLU:HG3	2.17	0.44
1:B:274:LYS:O	1:B:297:TYR:CD2	2.70	0.44
1:A:321:GLU:OE1	1:A:321:GLU:HA	2.17	0.44
1:B:310:VAL:HG13	1:B:325:VAL:CG2	2.47	0.44
1:B:160:PHE:H	1:B:211:LEU:HB2	1.82	0.44
1:B:247:LEU:CD1	1:B:252:ALA:HB3	2.48	0.44
1:A:192:LEU:HD12	1:A:192:LEU:N	2.32	0.44
1:A:250:GLN:O	1:A:251:ALA:HB3	2.17	0.44
1:A:253:LEU:HD12	1:A:456:ALA:HB2	2.00	0.44
1:B:163:VAL:HG12	1:B:163:VAL:O	2.18	0.44
1:B:128:LEU:HD13	1:B:134:PHE:CE2	2.52	0.44
1:B:294:ARG:NH1	1:B:294:ARG:CB	2.68	0.44
1:A:250:GLN:HB3	1:A:403:LYS:HE3	1.99	0.43
1:B:85:LEU:CD2	1:B:98:ALA:HB2	2.42	0.43
1:B:101:TRP:CZ3	1:B:102:GLN:HG2	2.53	0.43
1:B:143:LEU:HD21	1:B:208:PRO:HD2	2.00	0.43
1:B:203:GLU:O	1:B:206:GLY:N	2.44	0.43
1:A:268:LEU:CD1	1:A:384:VAL:HG13	2.49	0.43
1:B:58:ALA:CB	1:B:230:LEU:HD21	2.47	0.43
1:B:77:ILE:CB	1:B:239:VAL:HG22	2.44	0.43
1:A:82:GLU:OE2	1:A:186:ARG:HB3	2.19	0.43
1:B:235:PRO:HB3	1:B:237:ARG:HH11	1.83	0.43
1:B:34:ARG:HB3	2:B:524:HOH:O	2.17	0.43
1:B:77:ILE:HB	1:B:239:VAL:HA	2.00	0.43
1:B:86:LEU:HD21	1:B:211:LEU:HD12	2.00	0.43
1:B:107:THR:N	1:B:108:PRO:HD2	2.33	0.43
1:B:402:LEU:O	1:B:426:VAL:HA	2.19	0.43
1:A:13:SER:HB2	1:A:31:ARG:O	2.18	0.43
1:B:126:THR:HG22	1:B:190:PHE:O	2.18	0.43
1:B:382:PHE:HB3	1:B:481:TRP:CD2	2.54	0.43
1:A:343:ALA:HB2	1:A:347:LEU:CD2	2.49	0.43
1:A:468:THR:O	1:A:468:THR:CG2	2.63	0.43
1:B:279:SER:HA	1:B:394:GLU:OE2	2.19	0.43
1:B:323:ALA:O	1:B:325:VAL:N	2.52	0.43
1:A:452:PRO:HG3	2:A:654:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ARG:HG2	1:B:82:GLU:OE2	2.19	0.42
1:B:219:ASP:HB2	1:B:446:GLY:CA	2.49	0.42
1:A:253:LEU:HD23	1:A:289:TRP:CZ2	2.54	0.42
1:B:275:ARG:HG2	1:B:275:ARG:NH1	2.33	0.42
1:A:310:VAL:HG13	1:A:325:VAL:HG21	2.00	0.42
1:A:87:TRP:HH2	1:A:165:THR:HG22	1.84	0.42
1:A:114:ARG:NH2	2:A:503:HOH:O	2.45	0.42
1:A:207:ILE:HA	1:A:208:PRO:HD3	1.88	0.42
1:A:397:VAL:HG12	1:A:398:ARG:N	2.34	0.42
1:B:81:ARG:HB3	1:B:82:GLU:OE2	2.19	0.42
1:B:291:LEU:O	1:B:293:GLY:N	2.53	0.42
1:B:398:ARG:HG3	1:B:398:ARG:HH11	1.85	0.42
1:B:106:THR:HB	1:B:137:THR:HB	2.01	0.42
1:B:165:THR:HG21	1:B:213:PRO:HG3	2.00	0.42
1:A:160:PHE:CG	1:A:161:GLY:N	2.86	0.42
1:A:361:LEU:HD13	1:B:491:TRP:CZ3	2.55	0.42
1:B:208:PRO:C	1:B:210:ALA:H	2.23	0.42
1:A:192:LEU:HD12	1:A:192:LEU:H	1.85	0.42
1:B:51:TRP:CE3	1:B:51:TRP:HA	2.55	0.42
1:B:105:ARG:NH2	1:B:141:TRP:CH2	2.85	0.42
1:B:186:ARG:NH1	1:B:186:ARG:CG	2.82	0.42
1:B:240:LEU:HD23	1:B:245:ALA:HA	2.01	0.42
1:B:282:GLY:O	1:B:352:TRP:NE1	2.41	0.42
1:A:17:ILE:CD1	1:A:28:VAL:HG13	2.49	0.41
1:B:9:GLN:O	1:B:80:GLN:N	2.53	0.41
1:B:75:LEU:N	1:B:235:PRO:O	2.53	0.41
1:B:360:LEU:HD23	1:B:360:LEU:HA	1.88	0.41
1:A:150:LYS:NZ	1:A:206:GLY:O	2.53	0.41
1:A:388:VAL:O	1:A:392:GLU:HB2	2.19	0.41
1:B:81:ARG:CB	1:B:81:ARG:HH11	2.33	0.41
1:B:338:VAL:HA	1:B:361:LEU:O	2.20	0.41
1:A:111:GLU:CD	1:A:355:TYR:HH	2.23	0.41
1:B:29:ALA:CB	1:B:60:GLU:HB3	2.51	0.41
1:B:78:THR:OG1	1:B:242:ASP:HA	2.19	0.41
1:B:87:TRP:HB2	1:B:93:LYS:O	2.21	0.41
1:B:135:SER:HA	1:B:138:LYS:HB2	2.02	0.41
1:B:261:THR:HA	1:B:405:ASP:O	2.20	0.41
1:B:452:PRO:HG2	1:B:453:GLU:CD	2.40	0.41
1:B:31:ARG:NH2	1:B:56:TRP:CZ2	2.88	0.41
1:A:355:TYR:CE1	1:A:494:GLU:HA	2.56	0.41
1:B:73:LEU:C	1:B:73:LEU:CD2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:HIS:HB3	1:A:50:ILE:HD11	2.01	0.41
1:B:341:VAL:O	1:B:358:GLY:HA2	2.21	0.41
1:B:374:ARG:O	1:B:378:GLU:HG3	2.21	0.41
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.86	0.41
1:A:394:GLU:C	1:A:396:GLY:N	2.75	0.40
1:B:226:LEU:HB2	1:B:229:LEU:HG	2.04	0.40
1:A:83:THR:HA	1:A:99:ILE:O	2.21	0.40
1:B:78:THR:HA	1:B:240:LEU:O	2.21	0.40
1:B:136:GLY:HA3	1:B:188:LEU:HB2	2.02	0.40
1:B:143:LEU:O	1:B:143:LEU:HG	2.22	0.40
1:B:466:LEU:HA	1:B:467:PRO:HD3	1.85	0.40
1:A:42:TRP:CE2	1:A:105:ARG:HB3	2.56	0.40
1:A:51:TRP:CH2	1:A:171:LEU:HD23	2.55	0.40
1:A:189:LEU:HB3	1:A:202:LEU:CD2	2.51	0.40
1:B:60:GLU:OE1	1:B:64:ARG:NE	2.54	0.40
1:A:51:TRP:HH2	1:A:171:LEU:HD23	1.86	0.40
1:B:45:HIS:HB2	1:B:98:ALA:HB3	2.02	0.40
1:B:54:THR:HG21	1:B:167:LEU:HD22	2.03	0.40
1:A:320:ARG:O	1:A:321:GLU:HB2	2.19	0.40
1:B:266:ALA:HB3	1:B:303:LEU:HB2	2.03	0.40
1:B:452:PRO:HG2	1:B:453:GLU:OE2	2.21	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	490/495 (99%)	452 (92%)	26 (5%)	12 (2%)	6 20
1	B	490/495 (99%)	424 (86%)	53 (11%)	13 (3%)	5 17
All	All	980/990 (99%)	876 (89%)	79 (8%)	25 (3%)	5 18

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	393	GLU
1	A	397	VAL
1	B	493	ARG
1	A	96	HIS
1	A	395	ALA
1	B	170	ASN
1	A	392	GLU
1	B	34	ARG
1	B	38	PRO
1	B	147	PRO
1	B	169	TRP
1	A	321	GLU
1	A	324	GLU
1	A	462	ALA
1	B	315	GLU
1	B	144	GLU
1	B	163	VAL
1	B	316	VAL
1	B	324	GLU
1	A	322	SER
1	A	394	GLU
1	B	292	GLY
1	A	490	GLY
1	B	342	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	371/372 (100%)	347 (94%)	24 (6%)	17 44
1	B	371/372 (100%)	341 (92%)	30 (8%)	11 33
All	All	742/744 (100%)	688 (93%)	54 (7%)	14 38

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	61	VAL
1	A	75	LEU
1	A	81	ARG
1	A	82	GLU
1	A	93	LYS
1	A	104	ARG
1	A	105	ARG
1	A	129	LEU
1	A	180	ASP
1	A	186	ARG
1	A	188	LEU
1	A	192	LEU
1	A	211	LEU
1	A	259	LYS
1	A	268	LEU
1	A	274	LYS
1	A	286	THR
1	A	294	ARG
1	A	321	GLU
1	A	324	GLU
1	A	340	PHE
1	A	394	GLU
1	A	411	ASN
1	B	9	GLN
1	B	53	THR
1	B	63	ARG
1	B	73	LEU
1	B	81	ARG
1	B	103	ASP
1	B	145	ASN
1	B	152	ARG
1	B	160	PHE
1	B	162	THR
1	B	180	ASP
1	B	186	ARG
1	B	187	THR
1	B	211	LEU
1	B	237	ARG
1	B	259	LYS
1	B	291	LEU
1	B	294	ARG
1	B	296	THR

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Mol	Chain	Res	Type
1	B	316	VAL
1	B	320	ARG
1	B	322	SER
1	B	324	GLU
1	B	347	LEU
1	B	385	ARG
1	B	392	GLU
1	B	416	LYS
1	B	450	LEU
1	B	460	ARG
1	B	482	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	411	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	492/495 (99%)	-0.56	1 (0%) 95 94	13, 29, 49, 77	1 (0%)
1	B	492/495 (99%)	-0.01	15 (3%) 50 40	16, 57, 82, 88	1 (0%)
All	All	984/990 (99%)	-0.28	16 (1%) 72 66	13, 35, 78, 88	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	THR	3.1
1	B	76	GLY	2.7
1	B	81	ARG	2.7
1	B	147	PRO	2.6
1	B	161	GLY	2.6
1	B	179	THR	2.5
1	B	494	GLU	2.3
1	B	183	ASN	2.3
1	B	187	THR	2.2
1	B	84	THR	2.2
1	B	82	GLU	2.2
1	B	52	GLU	2.2
1	B	162	THR	2.1
1	A	320	ARG	2.1
1	B	78	THR	2.1
1	B	79	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.