Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 02:12 PM EDT

PDB ID	:	3AQM
Title	:	Structure of bacterial protein (form II)
Authors	:	Toh, Y.; Takeshita, D.; Tomita , K.
Deposited on	:	2010-11-09
Resolution	:	3.15 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 (i) 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 (1)) were used in the production of this report:

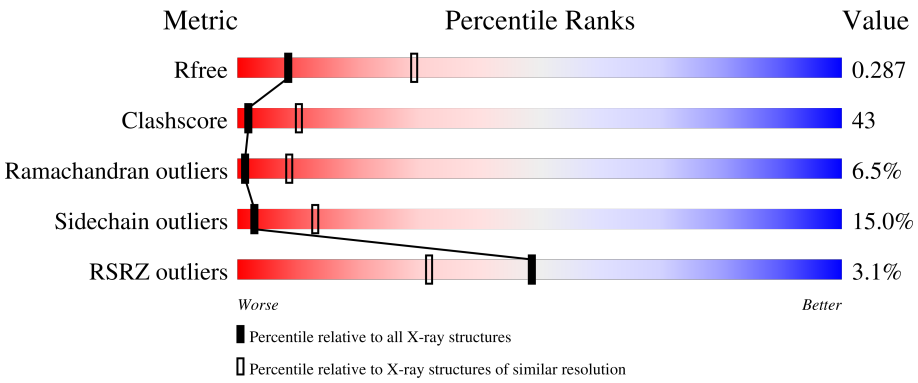
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	415	4% 35% 47% 11% • 7%
1	B	415	2% 35% 44% 14% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6332 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 Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3165	2022	569	560	14	0	0	0
1	B	388	3165	2022	569	560	14	0	0	0

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

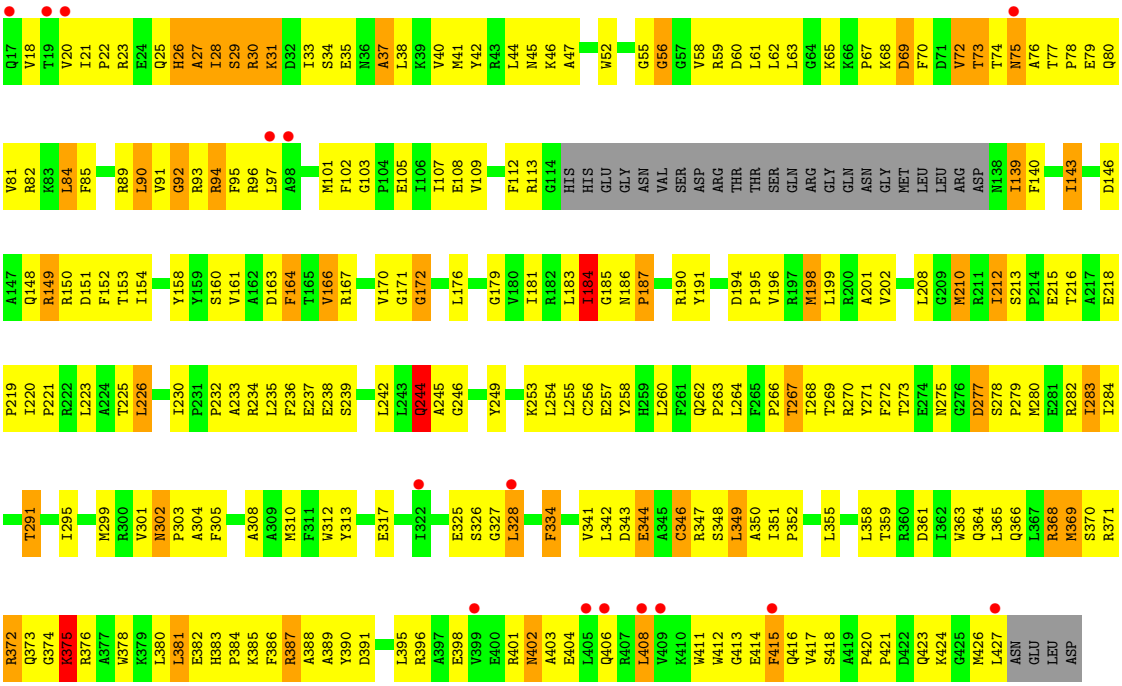
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

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.

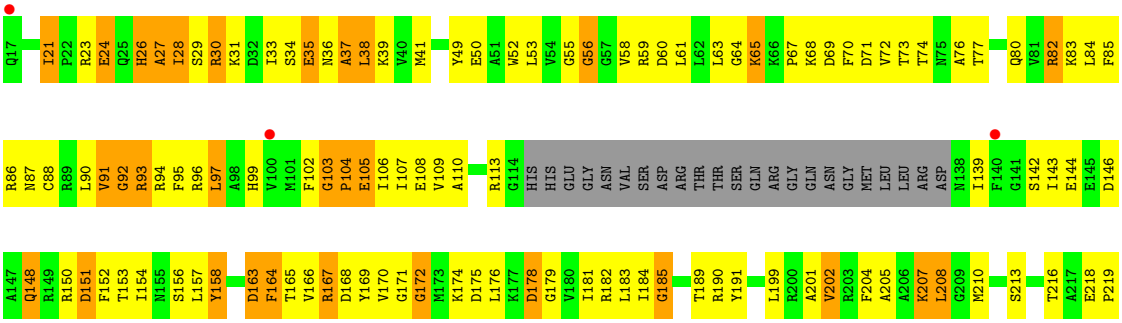
• Molecule 1: Poly(A) polymerase

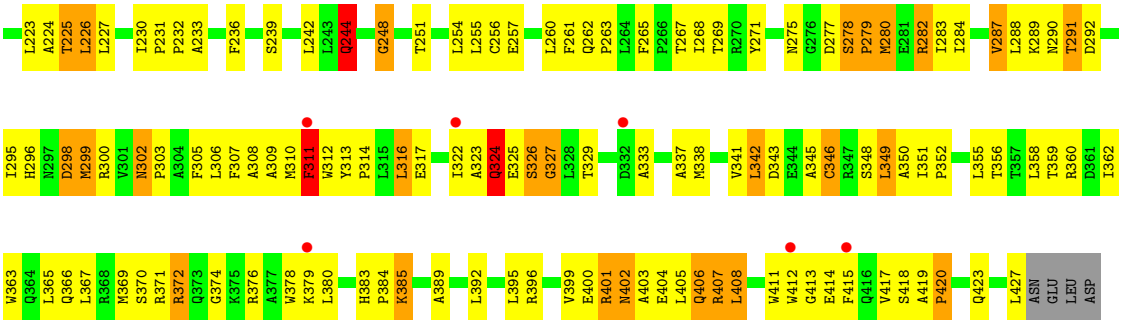
Chain A:



• Molecule 1: Poly(A) polymerase

Chain B:




L223
A224
T225
L226
L227
I230
P231
P232
A233
F236
S239
L242
L243
Q244
G248
T251
L254
L255
C256
E257
L260
F261
Q262
P263
L264
F265
P266
T267
I268
T269
R270
Y271
N275
G276
D277
S278
P279
M280
E281
R282
I283
I284
V287
L288
K289
N290
T291
D292
I295
H296
N297
D298
M299
R300
V301
N302
P303
A304
F305
L306
F307
A308
A309
M310
F311
W312
Y313
P314
L315
L316
E317
I322
A323
Q324
E325
S326
G327
L328
T329
D332
A333
A337
M338
V341
L342
D343
E344
A345
C346
R347
S348
L349
A350
I351
P352
L355
T356
T357
L358
T359
R360
D361
I362
W363
Q364
L365
Q366
L367
R368
M369
S370
R371
R372
Q373
G374
K375
R376
A377
W378
K379
L380
H383
P384
K385
A389
L392
L395
R396
V399
E400
R401
N402
A403
E404
L405
Q406
R407
L408
W411
W412
G413
E414
F415
Q416
V417
S418
A419
P420
Q423
L427
ASN
GLU
LEU
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.25Å 133.25Å 176.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.15 45.52 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.80-3.15) 97.8 (45.52-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.270 , 0.287 0.290 , 0.287	Depositor DCC
R_{free} test set	1364 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	91.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6332	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.40	0/3234	0.71	3/4370 (0.1%)
1	B	0.41	0/3234	0.70	2/4370 (0.0%)
All	All	0.41	0/6468	0.71	5/8740 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	SER	N-CA-C	-7.52	90.69	111.00
1	B	103	GLY	N-CA-C	-5.56	99.19	113.10
1	A	349	LEU	CA-CB-CG	5.40	127.73	115.30
1	B	37	ALA	N-CA-C	-5.31	96.67	111.00
1	A	37	ALA	N-CA-C	-5.26	96.79	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3165	0	3203	286	1
1	B	3165	0	3201	268	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6332	0	6404	549	1

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 43.

All (549) 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:183:LEU:HD23	1:B:184:ILE:H	1.07	1.20
1:A:95:PHE:CD1	1:A:96:ARG:HG3	1.78	1.18
1:A:149:ARG:HH11	1:A:149:ARG:HB3	1.22	1.04
1:A:372:ARG:NH1	1:A:372:ARG:HA	1.71	1.03
1:B:233:ALA:HA	1:B:350:ALA:HB3	1.43	0.98
1:A:95:PHE:CE1	1:A:96:ARG:HG3	2.00	0.96
1:B:170:VAL:HG12	1:B:171:GLY:H	1.28	0.95
1:A:378:TRP:HB3	1:B:299:MET:SD	2.07	0.94
1:A:212:ILE:H	1:A:212:ILE:HD12	1.30	0.94
1:A:375:LYS:H	1:A:375:LYS:HD2	1.32	0.94
1:B:372:ARG:HE	1:B:407:ARG:HH21	0.98	0.94
1:A:184:ILE:HG22	1:A:190:ARG:NH1	1.84	0.92
1:A:37:ALA:O	1:A:40:VAL:HG12	1.69	0.92
1:A:77:THR:H	1:A:80:GLN:HE21	0.97	0.92
1:B:374:GLY:HA3	1:B:427:LEU:HD22	1.51	0.92
1:A:372:ARG:HA	1:A:372:ARG:HH11	1.33	0.90
1:B:372:ARG:HE	1:B:407:ARG:NH2	1.69	0.90
1:A:95:PHE:CE1	1:A:96:ARG:CG	2.55	0.89
1:A:113:ARG:HG2	1:A:146:ASP:OD1	1.73	0.88
1:B:28:ILE:HG13	1:B:29:SER:H	1.37	0.88
1:B:183:LEU:HD23	1:B:184:ILE:N	1.88	0.88
1:A:196:VAL:HG21	1:A:234:ARG:NH2	1.87	0.88
1:A:271:TYR:HE1	1:A:317:GLU:HG2	1.39	0.87
1:B:244:GLN:HE22	1:B:303:PRO:HA	1.39	0.86
1:B:28:ILE:HB	1:B:30:ARG:HD2	1.57	0.85
1:A:242:LEU:HD13	1:A:255:LEU:HD11	1.57	0.85
1:B:55:GLY:O	1:B:58:VAL:HG12	1.76	0.84
1:A:184:ILE:HG22	1:A:190:ARG:HH12	1.43	0.84
1:B:103:GLY:O	1:B:105:GLU:N	2.10	0.84
1:B:184:ILE:HG22	1:B:185:GLY:N	1.92	0.84
1:A:302:ASN:HD21	1:A:385:LYS:NZ	1.75	0.84
1:B:183:LEU:HB2	1:B:216:THR:HG23	1.59	0.84
1:A:262:GLN:HB3	1:A:263:PRO:HD3	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLU:HB3	1:A:219:PRO:HD3	1.61	0.83
1:B:352:PRO:HG2	1:B:355:LEU:HD23	1.61	0.83
1:A:149:ARG:HB3	1:A:149:ARG:NH1	1.94	0.82
1:A:195:PRO:HB2	1:A:230:ILE:HD11	1.58	0.82
1:A:95:PHE:HE1	1:A:96:ARG:HE	1.24	0.82
1:A:196:VAL:HG21	1:A:234:ARG:HH22	1.44	0.82
1:B:30:ARG:CZ	1:B:33:ILE:HD11	2.10	0.82
1:A:184:ILE:CG2	1:A:185:GLY:N	2.44	0.81
1:A:291:THR:O	1:A:295:ILE:HG12	1.81	0.80
1:B:154:ILE:HG22	1:B:176:LEU:HB2	1.64	0.80
1:A:183:LEU:HD23	1:A:184:ILE:N	1.97	0.79
1:A:77:THR:N	1:A:80:GLN:HE21	1.79	0.79
1:A:191:TYR:CE1	1:A:198:MET:HG3	2.18	0.78
1:A:184:ILE:HG22	1:A:185:GLY:H	1.48	0.78
1:A:244:GLN:O	1:A:246:GLY:N	2.13	0.78
1:A:78:PRO:O	1:A:82:ARG:HG3	1.85	0.77
1:A:35:GLU:OE1	1:A:105:GLU:HG3	1.84	0.76
1:A:235:LEU:HD22	1:A:264:LEU:HD21	1.67	0.76
1:B:308:ALA:HB2	1:B:359:THR:HG23	1.67	0.76
1:B:93:ARG:O	1:B:94:ARG:HB2	1.84	0.76
1:A:77:THR:H	1:A:80:GLN:NE2	1.80	0.75
1:A:28:ILE:HG23	1:A:30:ARG:HG2	1.68	0.75
1:B:34:SER:O	1:B:35:GLU:O	2.04	0.75
1:B:372:ARG:NE	1:B:407:ARG:HH21	1.81	0.75
1:A:223:LEU:O	1:A:226:LEU:HB2	1.86	0.75
1:A:75:ASN:H	1:A:75:ASN:HD22	1.35	0.74
1:A:153:THR:HG22	1:A:170:VAL:CG1	2.18	0.74
1:B:183:LEU:CD2	1:B:184:ILE:H	1.95	0.74
1:A:232:PRO:HB2	1:A:350:ALA:HB2	1.68	0.74
1:B:170:VAL:HG12	1:B:171:GLY:N	2.03	0.73
1:B:218:GLU:HB3	1:B:219:PRO:HD3	1.69	0.73
1:B:324:GLN:O	1:B:324:GLN:HG2	1.89	0.73
1:A:374:GLY:HA2	1:A:427:LEU:HD22	1.71	0.73
1:A:153:THR:HG22	1:A:170:VAL:HG12	1.72	0.72
1:B:34:SER:O	1:B:35:GLU:C	2.27	0.72
1:A:21:ILE:HG23	1:A:166:VAL:HG13	1.72	0.72
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.55	0.72
1:B:248:GLY:O	1:B:288:LEU:HD13	1.90	0.72
1:A:244:GLN:HE22	1:A:303:PRO:HA	1.52	0.72
1:A:218:GLU:O	1:A:221:PRO:HD2	1.90	0.71
1:B:303:PRO:HG2	1:B:355:LEU:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PRO:CG	1:B:355:LEU:HD23	2.21	0.71
1:A:101:MET:O	1:A:102:PHE:HD1	1.73	0.70
1:A:308:ALA:HB2	1:A:359:THR:HG23	1.73	0.70
1:A:170:VAL:HG12	1:A:171:GLY:N	2.05	0.70
1:A:302:ASN:HD21	1:A:385:LYS:HZ1	1.39	0.70
1:B:96:ARG:O	1:B:97:LEU:O	2.08	0.70
1:B:307:PHE:CD2	1:B:351:ILE:HD11	2.27	0.70
1:B:278:SER:HB2	1:B:279:PRO:CD	2.22	0.70
1:A:238:GLU:O	1:A:242:LEU:HG	1.92	0.69
1:B:97:LEU:HD11	1:B:108:GLU:HG2	1.73	0.69
1:A:223:LEU:HD23	1:A:226:LEU:HD12	1.75	0.69
1:B:95:PHE:O	1:B:96:ARG:HB3	1.93	0.69
1:B:202:VAL:HG12	1:B:254:LEU:HB3	1.75	0.69
1:B:28:ILE:HB	1:B:30:ARG:CD	2.23	0.68
1:B:36:ASN:HD22	1:B:39:LYS:HG3	1.59	0.68
1:B:287:VAL:HG23	1:B:395:LEU:CD1	2.24	0.67
1:B:144:GLU:HA	1:B:169:TYR:CD1	2.30	0.67
1:A:299:MET:SD	1:B:378:TRP:HB3	2.34	0.67
1:A:302:ASN:ND2	1:A:385:LYS:NZ	2.42	0.67
1:A:52:TRP:CZ3	1:A:160:SER:HB2	2.29	0.67
1:A:82:ARG:NH1	1:A:82:ARG:HB2	2.09	0.67
1:B:233:ALA:CA	1:B:350:ALA:HB3	2.24	0.67
1:A:150:ARG:HH21	1:A:150:ARG:HG3	1.60	0.66
1:B:60:ASP:HA	1:B:63:LEU:HD12	1.77	0.66
1:B:232:PRO:HB2	1:B:350:ALA:HB2	1.77	0.66
1:B:402:ASN:ND2	1:B:404:GLU:H	1.93	0.66
1:A:26:HIS:O	1:A:26:HIS:CD2	2.48	0.66
1:B:244:GLN:HE21	1:B:303:PRO:HB3	1.61	0.66
1:A:371:ARG:O	1:A:373:GLN:N	2.29	0.66
1:A:184:ILE:HG22	1:A:185:GLY:N	2.09	0.65
1:B:150:ARG:O	1:B:184:ILE:HG13	1.96	0.65
1:A:183:LEU:HD23	1:A:184:ILE:H	1.59	0.65
1:B:244:GLN:NE2	1:B:303:PRO:HA	2.10	0.65
1:B:278:SER:HB2	1:B:279:PRO:HD2	1.77	0.65
1:A:269:THR:HA	1:A:272:PHE:CE2	2.32	0.65
1:A:220:ILE:HB	1:A:221:PRO:HD3	1.79	0.65
1:B:271:TYR:HB2	1:B:280:MET:HE1	1.79	0.65
1:B:280:MET:CE	1:B:314:PRO:HG3	2.27	0.64
1:A:22:PRO:HG2	1:A:25:GLN:HE21	1.61	0.64
1:A:34:SER:HB3	1:A:38:LEU:HD21	1.77	0.64
1:A:402:ASN:ND2	1:A:404:GLU:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PHE:HE1	1:B:345:ALA:CB	2.10	0.64
1:A:198:MET:HG2	1:A:220:ILE:HG23	1.79	0.64
1:B:223:LEU:O	1:B:226:LEU:HB2	1.96	0.64
1:B:380:LEU:HD22	1:B:412:TRP:CH2	2.32	0.64
1:B:257:GLU:O	1:B:257:GLU:HG2	1.95	0.64
1:B:30:ARG:NE	1:B:33:ILE:HD11	2.12	0.64
1:A:325:GLU:O	1:A:325:GLU:HG2	1.97	0.63
1:A:402:ASN:HD22	1:A:403:ALA:N	1.96	0.63
1:B:385:LYS:HA	1:B:385:LYS:NZ	2.14	0.63
1:B:280:MET:HE2	1:B:314:PRO:HG3	1.80	0.63
1:A:40:VAL:HG23	1:A:85:PHE:CE2	2.33	0.63
1:A:26:HIS:O	1:A:28:ILE:N	2.32	0.62
1:A:31:LYS:HE3	1:A:38:LEU:CD1	2.30	0.62
1:A:75:ASN:H	1:A:75:ASN:ND2	1.96	0.62
1:A:40:VAL:HG23	1:A:85:PHE:HE2	1.62	0.62
1:A:170:VAL:HG12	1:A:171:GLY:H	1.63	0.62
1:A:79:GLU:HA	1:A:82:ARG:CZ	2.29	0.62
1:B:183:LEU:HB2	1:B:216:THR:CG2	2.29	0.62
1:B:184:ILE:CG2	1:B:185:GLY:N	2.63	0.62
1:B:278:SER:O	1:B:282:ARG:HD2	1.99	0.62
1:B:199:LEU:HD22	1:B:242:LEU:HD11	1.80	0.62
1:A:191:TYR:CD1	1:A:198:MET:HG3	2.34	0.62
1:A:196:VAL:CG2	1:A:234:ARG:HH22	2.11	0.61
1:A:82:ARG:CB	1:A:82:ARG:HH11	2.12	0.61
1:B:170:VAL:HG11	1:B:184:ILE:CD1	2.30	0.61
1:B:271:TYR:HE1	1:B:317:GLU:HG2	1.66	0.61
1:A:271:TYR:CE1	1:A:317:GLU:HG2	2.30	0.61
1:B:97:LEU:CD1	1:B:108:GLU:HG2	2.29	0.61
1:B:56:GLY:HA2	1:B:59:ARG:HH12	1.65	0.61
1:B:346:CYS:HA	1:B:349:LEU:O	2.00	0.61
1:A:196:VAL:CG2	1:A:234:ARG:NH2	2.60	0.61
1:B:213:SER:HB3	1:B:216:THR:OG1	2.01	0.61
1:B:72:VAL:HG23	1:B:109:VAL:HG22	1.81	0.61
1:A:34:SER:CB	1:A:38:LEU:HD21	2.31	0.61
1:A:279:PRO:HA	1:A:282:ARG:HD3	1.82	0.61
1:A:368:ARG:NH1	1:A:380:LEU:HD11	2.15	0.61
1:B:179:GLY:CA	1:B:210:MET:HG2	2.30	0.61
1:B:37:ALA:CB	1:B:107:ILE:HG12	2.31	0.60
1:B:82:ARG:HG3	1:B:82:ARG:HH11	1.65	0.60
1:A:271:TYR:HB2	1:A:280:MET:CE	2.30	0.60
1:A:402:ASN:HD22	1:A:402:ASN:C	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PRO:HG3	1:B:70:PHE:CZ	2.37	0.60
1:A:75:ASN:HB3	1:A:112:PHE:CE1	2.36	0.60
1:B:34:SER:HB2	1:B:38:LEU:HD21	1.83	0.60
1:B:50:GLU:HG3	1:B:52:TRP:NE1	2.15	0.60
1:B:158:TYR:O	1:B:166:VAL:HA	2.01	0.60
1:B:204:PHE:O	1:B:208:LEU:HD12	2.02	0.60
1:B:262:GLN:HB3	1:B:263:PRO:HD3	1.84	0.60
1:A:223:LEU:CD2	1:A:226:LEU:HD12	2.31	0.60
1:A:344:GLU:O	1:A:347:ARG:HB2	2.02	0.60
1:B:268:ILE:HD11	1:B:310:MET:HB3	1.82	0.60
1:B:337:ALA:O	1:B:341:VAL:HG23	2.01	0.60
1:A:75:ASN:HB3	1:A:112:PHE:CD1	2.38	0.59
1:B:30:ARG:H	1:B:30:ARG:HD3	1.68	0.59
1:B:365:LEU:HD12	1:B:389:ALA:HB2	1.84	0.59
1:A:418:SER:C	1:A:423:GLN:HE21	2.06	0.58
1:A:199:LEU:O	1:A:202:VAL:HG12	2.02	0.58
1:B:28:ILE:HG13	1:B:29:SER:N	2.15	0.58
1:A:187:PRO:O	1:A:191:TYR:HD2	1.86	0.58
1:B:184:ILE:HG22	1:B:185:GLY:H	1.68	0.58
1:B:190:ARG:HG3	1:B:190:ARG:HH11	1.67	0.58
1:A:26:HIS:O	1:A:27:ALA:C	2.41	0.58
1:A:77:THR:C	1:A:79:GLU:H	2.05	0.58
1:B:154:ILE:HD13	1:B:210:MET:HE2	1.85	0.58
1:A:257:GLU:HG2	1:A:257:GLU:O	2.03	0.57
1:B:224:ALA:O	1:B:227:LEU:HG	2.04	0.57
1:B:407:ARG:HG2	1:B:407:ARG:HH11	1.69	0.57
1:A:35:GLU:O	1:A:37:ALA:N	2.35	0.57
1:B:143:ILE:HG23	1:B:169:TYR:HE1	1.69	0.57
1:B:154:ILE:HD13	1:B:210:MET:CE	2.34	0.57
1:B:202:VAL:CG1	1:B:254:LEU:HB3	2.33	0.57
1:A:184:ILE:HG23	1:A:185:GLY:N	2.18	0.57
1:A:150:ARG:HG3	1:A:150:ARG:NH2	2.17	0.57
1:B:59:ARG:NE	1:B:208:LEU:HD21	2.19	0.57
1:B:271:TYR:CE1	1:B:317:GLU:HG2	2.40	0.57
1:A:33:ILE:O	1:A:33:ILE:HG22	2.05	0.57
1:B:27:ALA:O	1:B:28:ILE:C	2.43	0.57
1:A:20:VAL:HG23	1:A:167:ARG:NE	2.19	0.57
1:A:95:PHE:CE1	1:A:96:ARG:HG2	2.38	0.57
1:B:50:GLU:HG3	1:B:52:TRP:HE1	1.70	0.57
1:B:163:ASP:O	1:B:165:THR:HG23	2.05	0.57
1:B:287:VAL:HG21	1:B:309:ALA:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:C	1:A:79:GLU:N	2.56	0.57
1:A:271:TYR:HB2	1:A:280:MET:HE1	1.86	0.57
1:A:179:GLY:O	1:A:210:MET:HB2	2.05	0.56
1:A:235:LEU:HD22	1:A:264:LEU:CD2	2.36	0.56
1:B:41:MET:HE1	1:B:53:LEU:HD13	1.86	0.56
1:A:79:GLU:HA	1:A:82:ARG:NH2	2.20	0.56
1:A:181:ILE:CD1	1:A:210:MET:HG3	2.35	0.56
1:A:190:ARG:NH1	1:A:190:ARG:HG3	2.16	0.56
1:A:220:ILE:CG2	1:A:260:LEU:HD11	2.35	0.56
1:B:358:LEU:O	1:B:362:ILE:HG13	2.05	0.56
1:B:342:LEU:O	1:B:346:CYS:HB2	2.06	0.56
1:A:212:ILE:H	1:A:212:ILE:CD1	2.03	0.56
1:B:68:LYS:HE3	1:B:207:LYS:NZ	2.20	0.56
1:A:20:VAL:HG23	1:A:167:ARG:CD	2.36	0.56
1:A:368:ARG:CZ	1:A:380:LEU:HD11	2.36	0.56
1:A:299:MET:SD	1:B:378:TRP:HE3	2.28	0.56
1:A:299:MET:SD	1:B:378:TRP:CE3	2.98	0.56
1:B:179:GLY:HA2	1:B:210:MET:HG2	1.88	0.56
1:B:323:ALA:O	1:B:327:GLY:HA2	2.05	0.56
1:B:406:GLN:O	1:B:406:GLN:HG2	2.06	0.56
1:A:74:THR:HG23	1:A:76:ALA:H	1.69	0.56
1:B:26:HIS:NE2	1:B:29:SER:HB3	2.21	0.56
1:B:59:ARG:HE	1:B:208:LEU:HD21	1.71	0.56
1:B:302:ASN:OD1	1:B:385:LYS:HE3	2.06	0.56
1:B:312:TRP:CE2	1:B:316:LEU:HD22	2.41	0.55
1:B:174:LYS:HE3	1:B:178:ASP:OD2	2.07	0.55
1:A:52:TRP:O	1:A:72:VAL:HA	2.05	0.55
1:A:68:LYS:O	1:A:69:ASP:HB2	2.05	0.55
1:B:56:GLY:HA2	1:B:59:ARG:NH1	2.22	0.55
1:B:244:GLN:NE2	1:B:303:PRO:HB3	2.21	0.55
1:B:303:PRO:HG2	1:B:355:LEU:CD1	2.37	0.55
1:B:41:MET:CE	1:B:53:LEU:HD13	2.37	0.55
1:B:374:GLY:CA	1:B:427:LEU:HD22	2.30	0.55
1:A:82:ARG:HB2	1:A:82:ARG:HH11	1.71	0.55
1:A:365:LEU:HD12	1:A:389:ALA:HB2	1.88	0.55
1:A:52:TRP:CE3	1:A:160:SER:HB2	2.40	0.55
1:A:76:ALA:HB3	1:A:81:VAL:HG22	1.89	0.55
1:A:181:ILE:HD11	1:A:210:MET:HG3	1.88	0.55
1:A:77:THR:HB	1:A:80:GLN:HG3	1.89	0.55
1:B:50:GLU:CG	1:B:52:TRP:HE1	2.20	0.55
1:B:418:SER:O	1:B:423:GLN:NE2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:THR:HG23	1:B:76:ALA:H	1.72	0.54
1:A:143:ILE:HD11	1:A:158:TYR:CD2	2.42	0.54
1:A:418:SER:O	1:A:423:GLN:NE2	2.40	0.54
1:A:358:LEU:HD12	1:A:358:LEU:H	1.73	0.54
1:B:405:LEU:C	1:B:407:ARG:H	2.09	0.54
1:B:153:THR:HG21	1:B:175:ASP:OD2	2.07	0.54
1:A:277:ASP:O	1:A:282:ARG:HD2	2.07	0.54
1:B:34:SER:CB	1:B:38:LEU:HD21	2.38	0.54
1:A:244:GLN:NE2	1:A:303:PRO:HA	2.21	0.54
1:B:342:LEU:HD21	1:B:363:TRP:HZ3	1.72	0.54
1:A:280:MET:HA	1:A:313:TYR:CD2	2.42	0.54
1:A:342:LEU:O	1:A:346:CYS:HB2	2.07	0.54
1:B:405:LEU:C	1:B:407:ARG:N	2.59	0.54
1:B:311:PHE:HE1	1:B:345:ALA:HB2	1.72	0.53
1:B:53:LEU:HD12	1:B:71:ASP:O	2.09	0.53
1:A:18:VAL:HG13	1:A:18:VAL:O	2.09	0.53
1:A:414:GLU:HB3	1:A:426:MET:HE1	1.89	0.53
1:B:151:ASP:HB3	1:B:152:PHE:CD2	2.44	0.53
1:A:262:GLN:CB	1:A:263:PRO:HD3	2.37	0.53
1:B:152:PHE:CZ	1:B:201:ALA:HA	2.44	0.53
1:B:183:LEU:HD12	1:B:191:TYR:CE1	2.44	0.53
1:A:72:VAL:HG22	1:A:109:VAL:HG22	1.90	0.53
1:A:216:THR:HG22	1:A:216:THR:O	2.06	0.53
1:B:278:SER:O	1:B:282:ARG:HG3	2.09	0.52
1:A:28:ILE:HG23	1:A:28:ILE:O	2.10	0.52
1:A:326:SER:O	1:A:328:LEU:N	2.42	0.52
1:B:82:ARG:HG3	1:B:82:ARG:NH1	2.24	0.52
1:B:385:LYS:HA	1:B:385:LYS:HZ3	1.74	0.52
1:A:60:ASP:HA	1:A:63:LEU:HD12	1.91	0.52
1:B:68:LYS:HE3	1:B:207:LYS:HZ2	1.74	0.52
1:B:73:THR:HA	1:B:110:ALA:O	2.09	0.52
1:A:196:VAL:HG21	1:A:234:ARG:CZ	2.39	0.52
1:A:270:ARG:HD2	1:A:271:TYR:CE2	2.43	0.52
1:B:170:VAL:HG11	1:B:184:ILE:HD11	1.91	0.52
1:A:402:ASN:ND2	1:A:404:GLU:N	2.58	0.52
1:B:183:LEU:CD2	1:B:184:ILE:N	2.65	0.52
1:B:158:TYR:O	1:B:166:VAL:HG23	2.10	0.52
1:A:249:TYR:CE1	1:A:253:LYS:HE3	2.44	0.52
1:B:150:ARG:HD3	1:B:156:SER:OG	2.10	0.52
1:A:76:ALA:HB3	1:A:81:VAL:CG2	2.39	0.52
1:A:202:VAL:CG2	1:A:254:LEU:HB3	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HD23	1:A:415:PHE:CE2	2.45	0.52
1:B:322:ILE:HG22	1:B:333:ALA:HB1	1.91	0.52
1:B:383:HIS:ND1	1:B:384:PRO:HD2	2.24	0.52
1:A:387:ARG:HG2	1:A:387:ARG:HH11	1.75	0.51
1:B:185:GLY:H	1:B:190:ARG:NH1	2.08	0.51
1:B:302:ASN:O	1:B:305:PHE:HB3	2.10	0.51
1:A:45:ASN:C	1:A:47:ALA:H	2.13	0.51
1:B:77:THR:HG23	1:B:80:GLN:NE2	2.24	0.51
1:A:369:MET:O	1:A:408:LEU:HD12	2.10	0.51
1:B:72:VAL:CG2	1:B:109:VAL:HG22	2.41	0.51
1:A:361:ASP:O	1:A:365:LEU:HG	2.11	0.51
1:A:383:HIS:ND1	1:A:384:PRO:HD2	2.25	0.51
1:B:170:VAL:CG1	1:B:171:GLY:H	2.13	0.51
1:B:419:ALA:HB1	1:B:420:PRO:HD2	1.91	0.51
1:A:97:LEU:HD21	1:A:108:GLU:OE1	2.11	0.51
1:A:390:TYR:HE2	1:B:417:VAL:O	1.93	0.51
1:A:158:TYR:O	1:A:166:VAL:HA	2.11	0.51
1:A:183:LEU:HB2	1:A:216:THR:HG23	1.93	0.51
1:A:284:ILE:HG23	1:A:310:MET:HG2	1.92	0.51
1:B:183:LEU:CD1	1:B:191:TYR:CE1	2.94	0.51
1:B:190:ARG:HG3	1:B:190:ARG:NH1	2.25	0.51
1:A:283:ILE:HG22	1:A:284:ILE:N	2.26	0.51
1:A:55:GLY:O	1:A:56:GLY:C	2.49	0.50
1:A:181:ILE:HD11	1:A:210:MET:CG	2.41	0.50
1:B:82:ARG:HH22	1:B:86:ARG:NH2	2.09	0.50
1:B:365:LEU:O	1:B:369:MET:HG3	2.11	0.50
1:A:312:TRP:CE2	1:A:396:ARG:HD2	2.46	0.50
1:A:164:PHE:N	1:A:164:PHE:CD1	2.79	0.50
1:B:244:GLN:NE2	1:B:303:PRO:CA	2.74	0.50
1:A:61:LEU:HD23	1:A:67:PRO:HD3	1.91	0.50
1:A:75:ASN:HD22	1:A:75:ASN:N	1.98	0.50
1:A:233:ALA:HA	1:A:350:ALA:HB3	1.94	0.50
1:B:289:LYS:O	1:B:292:ASP:HB2	2.10	0.50
1:A:387:ARG:HG2	1:A:387:ARG:NH1	2.26	0.50
1:A:59:ARG:HE	1:A:208:LEU:HD21	1.77	0.49
1:B:55:GLY:O	1:B:58:VAL:CG1	2.56	0.49
1:A:38:LEU:O	1:A:42:TYR:CD1	2.65	0.49
1:A:40:VAL:HG11	1:A:107:ILE:HG21	1.93	0.49
1:A:301:VAL:HG22	1:A:302:ASN:N	2.27	0.49
1:A:170:VAL:CG1	1:A:171:GLY:N	2.74	0.49
1:B:61:LEU:CD2	1:B:67:PRO:HD3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLY:HA2	1:B:210:MET:HE3	1.94	0.49
1:A:213:SER:HB3	1:A:216:THR:HB	1.95	0.49
1:A:372:ARG:HA	1:A:372:ARG:CZ	2.38	0.49
1:B:312:TRP:NE1	1:B:396:ARG:HD2	2.28	0.49
1:B:24:GLU:OE1	1:B:24:GLU:N	2.46	0.49
1:A:380:LEU:C	1:A:382:GLU:N	2.65	0.49
1:B:150:ARG:HH21	1:B:150:ARG:HG3	1.77	0.49
1:A:63:LEU:HD21	1:A:176:LEU:HD11	1.94	0.49
1:A:77:THR:CB	1:A:80:GLN:HG3	2.43	0.48
1:B:28:ILE:HD12	1:B:30:ARG:HH21	1.78	0.48
1:B:148:GLN:O	1:B:184:ILE:HG21	2.13	0.48
1:B:325:GLU:C	1:B:327:GLY:N	2.66	0.48
1:A:35:GLU:HG2	1:A:105:GLU:OE1	2.12	0.48
1:B:152:PHE:CD1	1:B:181:ILE:HG22	2.48	0.48
1:A:402:ASN:ND2	1:A:402:ASN:C	2.66	0.48
1:B:30:ARG:CD	1:B:33:ILE:HD11	2.44	0.48
1:B:244:GLN:HE22	1:B:303:PRO:CA	2.20	0.48
1:B:367:LEU:O	1:B:370:SER:HB3	2.14	0.48
1:A:302:ASN:ND2	1:A:385:LYS:HZ1	2.08	0.48
1:B:90:LEU:C	1:B:92:GLY:H	2.17	0.48
1:B:280:MET:HE2	1:B:314:PRO:CG	2.43	0.48
1:B:287:VAL:HG21	1:B:309:ALA:HB1	1.94	0.48
1:B:374:GLY:C	1:B:376:ARG:H	2.17	0.48
1:A:72:VAL:CG2	1:A:109:VAL:HG22	2.43	0.47
1:A:75:ASN:ND2	1:A:75:ASN:N	2.60	0.47
1:B:56:GLY:O	1:B:59:ARG:HB3	2.14	0.47
1:A:38:LEU:HB3	1:A:42:TYR:CE1	2.48	0.47
1:B:34:SER:O	1:B:38:LEU:HD23	2.14	0.47
1:B:157:LEU:HD21	1:B:172:GLY:HA3	1.95	0.47
1:A:90:LEU:CD2	1:A:90:LEU:H	2.27	0.47
1:A:35:GLU:HB2	1:A:70:PHE:CE1	2.50	0.47
1:A:160:SER:HB3	1:A:163:ASP:OD1	2.14	0.47
1:A:61:LEU:CD2	1:A:67:PRO:HD3	2.44	0.47
1:A:103:GLY:C	1:A:105:GLU:H	2.18	0.47
1:A:191:TYR:HD1	1:A:198:MET:HE2	1.79	0.47
1:A:373:GLN:HG2	1:A:376:ARG:HG3	1.95	0.47
1:B:82:ARG:HH22	1:B:86:ARG:HH21	1.61	0.47
1:B:227:LEU:O	1:B:230:ILE:HB	2.14	0.47
1:B:376:ARG:O	1:B:379:LYS:HB3	2.14	0.47
1:A:154:ILE:HG22	1:A:176:LEU:HB2	1.97	0.47
1:A:303:PRO:HD2	1:A:304:ALA:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:VAL:HG23	1:B:400:GLU:N	2.29	0.47
1:B:271:TYR:HB2	1:B:280:MET:CE	2.44	0.47
1:B:26:HIS:HD2	1:B:27:ALA:O	1.97	0.47
1:A:22:PRO:HG2	1:A:25:GLN:NE2	2.29	0.46
1:B:90:LEU:HA	1:B:99:HIS:O	2.15	0.46
1:B:153:THR:HG22	1:B:170:VAL:HG12	1.97	0.46
1:B:311:PHE:H	1:B:311:PHE:HD2	1.63	0.46
1:A:374:GLY:CA	1:A:427:LEU:HD22	2.42	0.46
1:B:261:PHE:CE2	1:B:265:PHE:HB2	2.50	0.46
1:B:356:THR:O	1:B:360:ARG:HG2	2.15	0.46
1:A:273:THR:HG23	1:A:278:SER:HB2	1.97	0.46
1:B:26:HIS:O	1:B:26:HIS:CD2	2.68	0.46
1:A:95:PHE:CE1	1:A:96:ARG:NE	2.80	0.46
1:A:370:SER:HA	1:A:408:LEU:CD1	2.46	0.46
1:B:392:LEU:HD12	1:B:392:LEU:O	2.16	0.46
1:B:358:LEU:HB3	1:B:385:LYS:HD2	1.98	0.46
1:A:235:LEU:O	1:A:239:SER:HB3	2.15	0.46
1:A:20:VAL:O	1:A:20:VAL:HG13	2.16	0.46
1:A:171:GLY:O	1:A:172:GLY:C	2.54	0.46
1:A:236:PHE:O	1:A:237:GLU:C	2.53	0.46
1:A:270:ARG:HD2	1:A:271:TYR:HE2	1.81	0.46
1:A:271:TYR:HB2	1:A:280:MET:HE3	1.97	0.46
1:A:304:ALA:HB2	1:A:355:LEU:HD12	1.98	0.46
1:B:30:ARG:NH2	1:B:33:ILE:HD11	2.30	0.46
1:A:37:ALA:O	1:A:40:VAL:CG1	2.53	0.45
1:B:278:SER:CB	1:B:279:PRO:CD	2.93	0.45
1:A:152:PHE:CZ	1:A:201:ALA:HA	2.52	0.45
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.76	0.45
1:A:283:ILE:CG2	1:A:284:ILE:N	2.80	0.45
1:B:23:ARG:HB3	1:B:164:PHE:O	2.17	0.45
1:B:97:LEU:HD11	1:B:108:GLU:CG	2.45	0.45
1:B:208:LEU:HD12	1:B:208:LEU:H	1.81	0.45
1:A:411:TRP:C	1:A:413:GLY:N	2.70	0.45
1:B:28:ILE:O	1:B:29:SER:C	2.54	0.45
1:B:325:GLU:HG2	1:B:326:SER:N	2.31	0.45
1:B:402:ASN:ND2	1:B:402:ASN:C	2.69	0.45
1:A:21:ILE:HG13	1:A:25:GLN:HG3	1.99	0.45
1:A:170:VAL:CG1	1:A:171:GLY:H	2.30	0.45
1:A:219:PRO:O	1:A:223:LEU:HD12	2.17	0.45
1:A:220:ILE:HG23	1:A:260:LEU:HD11	1.99	0.45
1:B:244:GLN:NE2	1:B:303:PRO:CB	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASP:OD2	1:B:182:ARG:NH1	2.49	0.45
1:A:47:ALA:CB	1:A:84:LEU:HD21	2.47	0.45
1:A:77:THR:HB	1:A:80:GLN:H	1.82	0.45
1:A:385:LYS:HA	1:A:385:LYS:HD3	1.59	0.45
1:B:67:PRO:CG	1:B:70:PHE:CZ	3.00	0.45
1:A:268:ILE:O	1:A:269:THR:C	2.56	0.45
1:B:91:VAL:O	1:B:92:GLY:O	2.34	0.45
1:A:151:ASP:HB3	1:A:152:PHE:CD2	2.53	0.44
1:B:36:ASN:O	1:B:102:PHE:CE1	2.71	0.44
1:B:280:MET:O	1:B:284:ILE:HG13	2.17	0.44
1:A:112:PHE:O	1:A:140:PHE:HB3	2.18	0.44
1:A:380:LEU:O	1:A:382:GLU:N	2.50	0.44
1:B:144:GLU:HA	1:B:169:TYR:CE1	2.53	0.44
1:A:20:VAL:HG23	1:A:167:ARG:HD3	1.99	0.44
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.87	0.44
1:B:37:ALA:HB2	1:B:107:ILE:HG12	1.99	0.44
1:B:164:PHE:CD1	1:B:164:PHE:N	2.85	0.44
1:B:311:PHE:CD2	1:B:311:PHE:N	2.86	0.44
1:A:42:TYR:HB3	1:A:46:LYS:NZ	2.32	0.44
1:A:91:VAL:O	1:A:92:GLY:O	2.35	0.44
1:A:218:GLU:HB3	1:A:219:PRO:CD	2.40	0.44
1:A:143:ILE:HD11	1:A:158:TYR:CG	2.52	0.44
1:A:148:GLN:O	1:A:184:ILE:HG21	2.18	0.44
1:A:283:ILE:HG13	1:A:313:TYR:HE2	1.83	0.44
1:B:338:MET:O	1:B:342:LEU:HD22	2.18	0.44
1:B:152:PHE:CD2	1:B:152:PHE:N	2.86	0.44
1:B:158:TYR:CD1	1:B:158:TYR:N	2.86	0.44
1:A:179:GLY:C	1:A:210:MET:HB2	2.39	0.43
1:B:168:ASP:OD1	1:B:170:VAL:O	2.35	0.43
1:A:101:MET:C	1:A:102:PHE:HD1	2.21	0.43
1:B:202:VAL:O	1:B:205:ALA:HB3	2.19	0.43
1:A:42:TYR:HB3	1:A:46:LYS:HZ3	1.82	0.43
1:A:52:TRP:HB2	1:A:73:THR:HG23	2.00	0.43
1:B:153:THR:HG22	1:B:170:VAL:CG1	2.48	0.43
1:A:77:THR:O	1:A:81:VAL:HG23	2.18	0.43
1:A:387:ARG:NH2	1:A:416:GLN:HE22	2.16	0.43
1:A:421:PRO:O	1:A:424:LYS:HB2	2.18	0.43
1:B:83:LYS:C	1:B:85:PHE:H	2.22	0.43
1:B:93:ARG:HG2	1:B:94:ARG:H	1.83	0.43
1:A:202:VAL:HG11	1:A:255:LEU:CD2	2.48	0.43
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:HG3	1:B:97:LEU:H	1.84	0.43
1:B:290:ASN:C	1:B:292:ASP:N	2.72	0.43
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.82	0.43
1:A:194:ASP:OD2	1:A:196:VAL:HG23	2.18	0.43
1:B:72:VAL:HG23	1:B:109:VAL:HA	2.01	0.43
1:B:227:LEU:HD11	1:B:260:LEU:HD22	2.01	0.43
1:B:311:PHE:CE1	1:B:345:ALA:HB1	2.54	0.43
1:B:411:TRP:O	1:B:414:GLU:N	2.51	0.43
1:B:26:HIS:CD2	1:B:26:HIS:C	2.91	0.43
1:B:34:SER:C	1:B:35:GLU:O	2.56	0.43
1:B:150:ARG:O	1:B:184:ILE:CG1	2.66	0.43
1:B:184:ILE:HB	1:B:190:ARG:HH12	1.83	0.43
1:A:93:ARG:O	1:A:94:ARG:O	2.37	0.43
1:A:266:PRO:O	1:A:268:ILE:N	2.52	0.43
1:B:251:THR:O	1:B:255:LEU:HG	2.18	0.43
1:B:167:ARG:HG2	1:B:167:ARG:NH1	2.33	0.42
1:B:280:MET:HE3	1:B:314:PRO:HG3	2.01	0.42
1:A:191:TYR:HE1	1:A:198:MET:HG3	1.78	0.42
1:A:387:ARG:HH22	1:A:416:GLN:HE22	1.65	0.42
1:B:53:LEU:O	1:B:58:VAL:HG21	2.19	0.42
1:A:358:LEU:O	1:A:359:THR:C	2.58	0.42
1:A:415:PHE:O	1:A:415:PHE:CG	2.72	0.42
1:A:358:LEU:HD23	1:A:385:LYS:CE	2.49	0.42
1:A:388:ALA:O	1:A:389:ALA:C	2.58	0.42
1:A:413:GLY:O	1:A:417:VAL:HG22	2.20	0.42
1:A:30:ARG:HD2	1:A:33:ILE:HD11	2.01	0.42
1:A:41:MET:O	1:A:44:LEU:HB2	2.19	0.42
1:B:33:ILE:HG22	1:B:33:ILE:O	2.19	0.42
1:B:102:PHE:HB2	1:B:105:GLU:O	2.19	0.42
1:B:311:PHE:HE1	1:B:345:ALA:HB1	1.80	0.42
1:A:95:PHE:O	1:A:96:ARG:HB2	2.20	0.42
1:A:267:THR:HG21	1:A:341:VAL:HG13	2.00	0.42
1:A:334:PHE:C	1:A:334:PHE:CD2	2.93	0.42
1:A:363:TRP:O	1:A:366:GLN:HB2	2.20	0.42
1:A:374:GLY:C	1:A:376:ARG:H	2.22	0.42
1:A:408:LEU:O	1:A:412:TRP:HD1	2.03	0.42
1:B:287:VAL:HG11	1:B:306:LEU:HD12	2.02	0.42
1:B:312:TRP:CE2	1:B:396:ARG:HD2	2.54	0.42
1:B:407:ARG:HG2	1:B:407:ARG:NH1	2.34	0.42
1:B:291:THR:O	1:B:295:ILE:HG12	2.19	0.42
1:A:76:ALA:O	1:A:77:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:THR:OG1	1:A:275:ASN:HB3	2.20	0.42
1:B:415:PHE:O	1:B:415:PHE:CG	2.72	0.42
1:A:374:GLY:O	1:A:376:ARG:N	2.52	0.42
1:A:402:ASN:HD21	1:A:404:GLU:HB3	1.84	0.42
1:B:199:LEU:O	1:B:202:VAL:HG23	2.20	0.42
1:B:362:ILE:O	1:B:366:GLN:HG2	2.19	0.42
1:B:372:ARG:HB2	1:B:372:ARG:HH11	1.85	0.42
1:B:418:SER:O	1:B:423:GLN:HG3	2.20	0.42
1:B:288:LEU:O	1:B:289:LYS:C	2.59	0.42
1:A:26:HIS:O	1:A:26:HIS:HD2	2.02	0.41
1:A:82:ARG:NH1	1:A:82:ARG:CB	2.74	0.41
1:A:152:PHE:CE1	1:A:201:ALA:HA	2.55	0.41
1:B:30:ARG:HD3	1:B:33:ILE:HD11	2.01	0.41
1:B:402:ASN:HD22	1:B:403:ALA:N	2.17	0.41
1:A:355:LEU:N	1:A:355:LEU:HD22	2.36	0.41
1:A:414:GLU:HB3	1:A:426:MET:CE	2.50	0.41
1:B:218:GLU:CB	1:B:219:PRO:HD3	2.43	0.41
1:B:303:PRO:CG	1:B:355:LEU:HD11	2.47	0.41
1:B:370:SER:HA	1:B:408:LEU:HD11	2.02	0.41
1:A:28:ILE:O	1:A:30:ARG:HG2	2.20	0.41
1:B:96:ARG:CG	1:B:97:LEU:N	2.83	0.41
1:B:113:ARG:HD3	1:B:146:ASP:OD1	2.20	0.41
1:B:236:PHE:CE2	1:B:351:ILE:HG12	2.56	0.41
1:A:158:TYR:CD1	1:A:158:TYR:N	2.89	0.41
1:A:58:VAL:O	1:A:62:LEU:HD12	2.21	0.41
1:A:302:ASN:HB3	1:A:305:PHE:HB2	2.02	0.41
1:B:358:LEU:N	1:B:358:LEU:HD12	2.35	0.41
1:A:97:LEU:HD22	1:A:108:GLU:HG2	2.03	0.41
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.93	0.41
1:A:212:ILE:HD13	1:A:258:TYR:OH	2.19	0.41
1:A:358:LEU:H	1:A:358:LEU:CD1	2.33	0.41
1:B:411:TRP:C	1:B:413:GLY:N	2.74	0.41
1:A:351:ILE:HA	1:A:352:PRO:HD3	1.92	0.41
1:B:279:PRO:CD	1:B:280:MET:H	2.34	0.41
1:B:400:GLU:C	1:B:402:ASN:H	2.24	0.41
1:A:23:ARG:HA	1:A:26:HIS:CE1	2.56	0.41
1:A:26:HIS:CD2	1:A:26:HIS:C	2.94	0.41
1:A:42:TYR:O	1:A:46:LYS:HG3	2.20	0.41
1:A:234:ARG:C	1:A:236:PHE:N	2.72	0.41
1:A:273:THR:C	1:A:275:ASN:N	2.71	0.41
1:A:395:LEU:O	1:A:398:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:HB	1:B:166:VAL:HG12	2.02	0.41
1:B:313:TYR:N	1:B:314:PRO:CD	2.84	0.41
1:B:352:PRO:HG3	1:B:355:LEU:HD23	2.03	0.41
1:B:411:TRP:O	1:B:413:GLY:N	2.54	0.41
1:A:139:ILE:HG22	1:A:140:PHE:N	2.36	0.41
1:A:385:LYS:O	1:A:386:PHE:C	2.59	0.41
1:B:49:TYR:CE1	1:B:80:GLN:OE1	2.74	0.41
1:B:231:PRO:HA	1:B:232:PRO:HD3	1.89	0.41
1:B:158:TYR:N	1:B:158:TYR:HD1	2.19	0.40
1:A:186:ASN:O	1:A:187:PRO:C	2.58	0.40
1:B:311:PHE:C	1:B:314:PRO:HD2	2.42	0.40
1:A:90:LEU:H	1:A:90:LEU:HD23	1.85	0.40
1:A:184:ILE:CG2	1:A:190:ARG:HH12	2.21	0.40
1:A:391:ASP:O	1:A:395:LEU:HD13	2.21	0.40
1:B:49:TYR:CD1	1:B:76:ALA:HB2	2.55	0.40
1:B:61:LEU:HD21	1:B:67:PRO:HD3	2.03	0.40
1:B:170:VAL:CG1	1:B:171:GLY:N	2.75	0.40
1:A:152:PHE:CD2	1:A:152:PHE:N	2.88	0.40
1:B:59:ARG:HD2	1:B:154:ILE:HD12	2.04	0.40
1:B:85:PHE:C	1:B:87:ASN:N	2.74	0.40
1:A:20:VAL:HG23	1:A:167:ARG:HE	1.84	0.40
1:A:262:GLN:NE2	1:A:269:THR:HG21	2.36	0.40
1:B:55:GLY:N	1:B:58:VAL:HG11	2.36	0.40
1:B:64:GLY:O	1:B:65:LYS:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH1	1:A:361:ASP:OD1[2_545]	1.75	0.45

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	384/415 (92%)	291 (76%)	72 (19%)	21 (6%)	2 12
1	B	384/415 (92%)	298 (78%)	57 (15%)	29 (8%)	1 6
All	All	768/830 (92%)	589 (77%)	129 (17%)	50 (6%)	1 8

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	92	GLY
1	A	245	ALA
1	A	372	ARG
1	A	375	LYS
1	B	28	ILE
1	B	35	GLU
1	B	65	LYS
1	B	92	GLY
1	B	104	PRO
1	B	105	GLU
1	B	278	SER
1	B	298	ASP
1	A	27	ALA
1	A	56	GLY
1	A	65	LYS
1	A	69	ASP
1	A	94	ARG
1	A	139	ILE
1	A	172	GLY
1	A	267	THR
1	A	327	GLY
1	A	401	ARG
1	B	27	ALA
1	B	56	GLY
1	B	97	LEU
1	B	151	ASP
1	B	172	GLY
1	B	311	PHE
1	B	327	GLY
1	A	31	LYS
1	A	369	MET
1	B	225	THR
1	B	244	GLN

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Mol	Chain	Res	Type
1	B	299	MET
1	A	244	GLN
1	B	88	CYS
1	B	185	GLY
1	B	207	LYS
1	B	401	ARG
1	B	91	VAL
1	B	93	ARG
1	B	324	GLN
1	A	184	ILE
1	A	415	PHE
1	B	31	LYS
1	B	84	LEU
1	B	248	GLY
1	B	279	PRO
1	A	187	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	334/358 (93%)	291 (87%)	43 (13%)	4 18
1	B	334/358 (93%)	277 (83%)	57 (17%)	2 9
All	All	668/716 (93%)	568 (85%)	100 (15%)	3 13

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

Mol	Chain	Res	Type
1	A	26	HIS
1	A	29	SER
1	A	30	ARG
1	A	72	VAL
1	A	73	THR
1	A	75	ASN
1	A	84	LEU

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Mol	Chain	Res	Type
1	A	89	ARG
1	A	90	LEU
1	A	143	ILE
1	A	149	ARG
1	A	161	VAL
1	A	164	PHE
1	A	166	VAL
1	A	184	ILE
1	A	198	MET
1	A	210	MET
1	A	212	ILE
1	A	215	GLU
1	A	225	THR
1	A	226	LEU
1	A	244	GLN
1	A	256	CYS
1	A	277	ASP
1	A	283	ILE
1	A	291	THR
1	A	302	ASN
1	A	328	LEU
1	A	334	PHE
1	A	343	ASP
1	A	344	GLU
1	A	346	CYS
1	A	348	SER
1	A	349	LEU
1	A	364	GLN
1	A	368	ARG
1	A	375	LYS
1	A	381	LEU
1	A	387	ARG
1	A	402	ASN
1	A	406	GLN
1	A	408	LEU
1	A	420	PRO
1	B	21	ILE
1	B	24	GLU
1	B	26	HIS
1	B	30	ARG
1	B	38	LEU
1	B	69	ASP

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Mol	Chain	Res	Type
1	B	82	ARG
1	B	104	PRO
1	B	106	ILE
1	B	139	ILE
1	B	142	SER
1	B	148	GLN
1	B	158	TYR
1	B	163	ASP
1	B	164	PHE
1	B	167	ARG
1	B	178	ASP
1	B	189	THR
1	B	202	VAL
1	B	208	LEU
1	B	225	THR
1	B	226	LEU
1	B	239	SER
1	B	244	GLN
1	B	256	CYS
1	B	267	THR
1	B	269	THR
1	B	275	ASN
1	B	277	ASP
1	B	280	MET
1	B	282	ARG
1	B	283	ILE
1	B	287	VAL
1	B	291	THR
1	B	296	HIS
1	B	298	ASP
1	B	300	ARG
1	B	302	ASN
1	B	311	PHE
1	B	316	LEU
1	B	324	GLN
1	B	326	SER
1	B	329	THR
1	B	342	LEU
1	B	343	ASP
1	B	346	CYS
1	B	348	SER
1	B	349	LEU

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Mol	Chain	Res	Type
1	B	371	ARG
1	B	372	ARG
1	B	385	LYS
1	B	401	ARG
1	B	402	ASN
1	B	406	GLN
1	B	407	ARG
1	B	408	LEU
1	B	420	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	HIS
1	A	36	ASN
1	A	45	ASN
1	A	75	ASN
1	A	80	GLN
1	A	87	ASN
1	A	138	ASN
1	A	155	ASN
1	A	244	GLN
1	A	262	GLN
1	A	275	ASN
1	A	286	GLN
1	A	290	ASN
1	A	302	ASN
1	A	364	GLN
1	A	402	ASN
1	A	406	GLN
1	A	416	GLN
1	A	423	GLN
1	B	26	HIS
1	B	36	ASN
1	B	45	ASN
1	B	87	ASN
1	B	138	ASN
1	B	155	ASN
1	B	186	ASN
1	B	244	GLN
1	B	275	ASN

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Mol	Chain	Res	Type
1	B	290	ASN
1	B	364	GLN
1	B	373	GLN
1	B	402	ASN
1	B	406	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	388/415 (93%)	0.33	15 (3%)	39	24	71, 101, 141, 169	0
1	B	388/415 (93%)	0.28	9 (2%)	60	46	66, 104, 145, 166	0
All	All	776/830 (93%)	0.30	24 (3%)	49	32	66, 103, 143, 169	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	GLN	3.9
1	B	100	VAL	3.3
1	A	328	LEU	2.7
1	A	409	VAL	2.7
1	A	405	LEU	2.7
1	A	98	ALA	2.7
1	B	140	PHE	2.5
1	B	311	PHE	2.5
1	B	379	LYS	2.5
1	A	399	VAL	2.5
1	B	17	GLN	2.4
1	B	322	ILE	2.4
1	A	75	ASN	2.4
1	A	427	LEU	2.4
1	A	20	VAL	2.4
1	A	406	GLN	2.3
1	B	332	ASP	2.3
1	A	97	LEU	2.3
1	A	408	LEU	2.3
1	B	415	PHE	2.2
1	A	19	THR	2.2
1	A	415	PHE	2.1
1	A	322	ILE	2.1
1	B	412	TRP	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	501	1/1	0.84	0.18	37,37,37,37	0
2	MG	A	501	1/1	0.88	0.23	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.