Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:38 AM GMT

PDB ID	:	3MH4
Title	:	HtrA proteases are activated by a conserved mechanism that can be triggered by distinct molecular cues
Authors	:	Krojer, T.; Sawa, J.; Huber, R.; Clausen, T.
Deposited on	:	2010-04-07
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

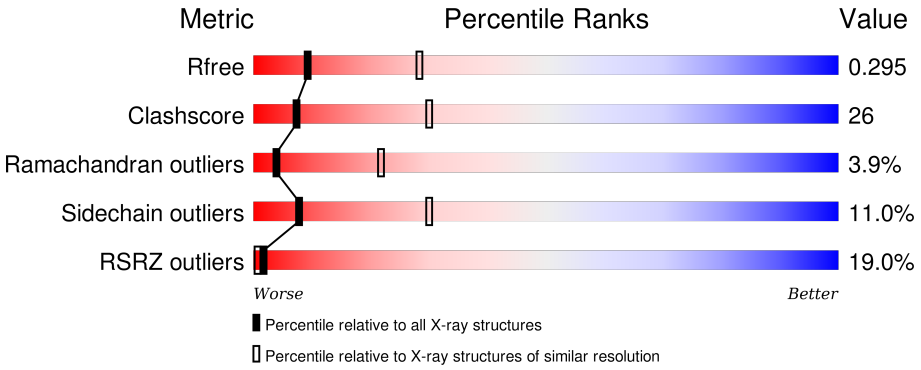
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	456	14% 36% 25% 5% • 34%
1	B	456	15% 47% 31% 5% • 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5007 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 Protease do.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2194	1367	390	425	12			
1	B	383	Total	C	N	O	S	0	0	0
			2813	1752	499	549	13			

There are 18 discrepancies between the modelled and reference sequences:

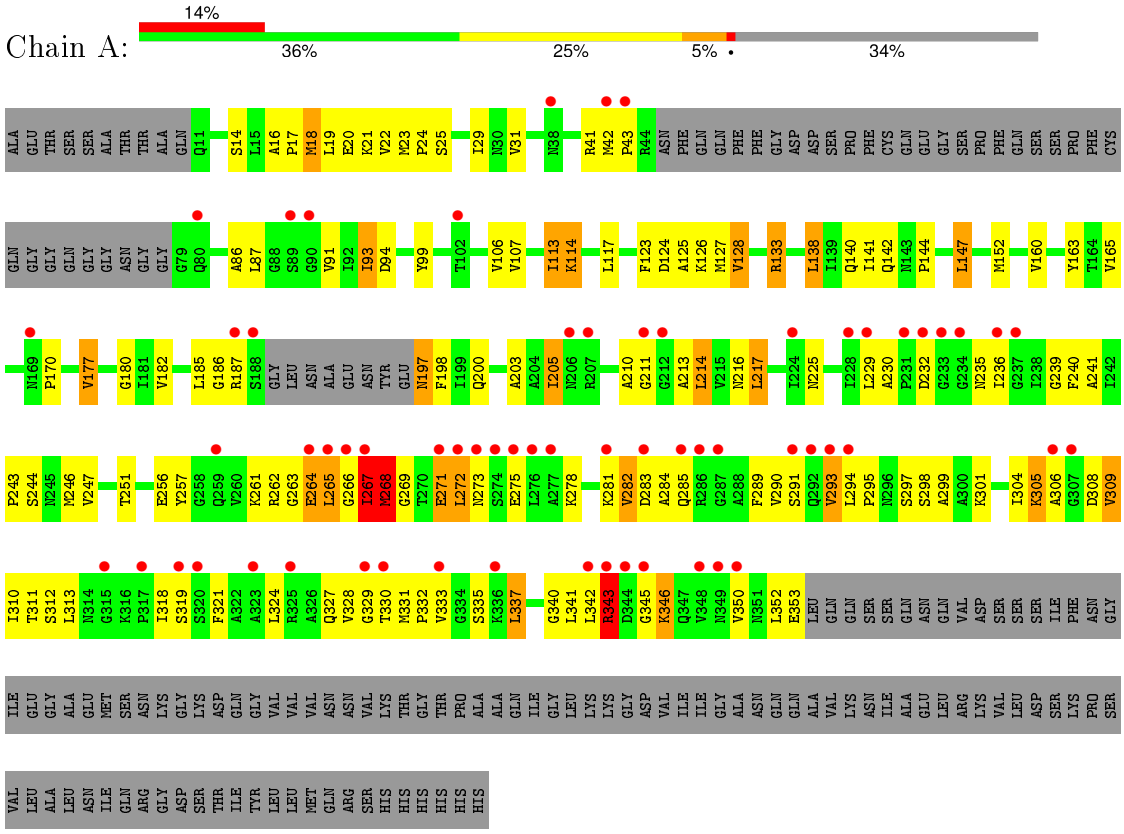
Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	SER	ENGINEERED	UNP P0C0V0
A	449	ARG	-	EXPRESSION TAG	UNP P0C0V0
A	450	SER	-	EXPRESSION TAG	UNP P0C0V0
A	451	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	452	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	453	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
A	456	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	210	ALA	SER	ENGINEERED	UNP P0C0V0
B	449	ARG	-	EXPRESSION TAG	UNP P0C0V0
B	450	SER	-	EXPRESSION TAG	UNP P0C0V0
B	451	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	452	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	453	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	454	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	455	HIS	-	EXPRESSION TAG	UNP P0C0V0
B	456	HIS	-	EXPRESSION TAG	UNP P0C0V0

3 Residue-property plots (i)

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

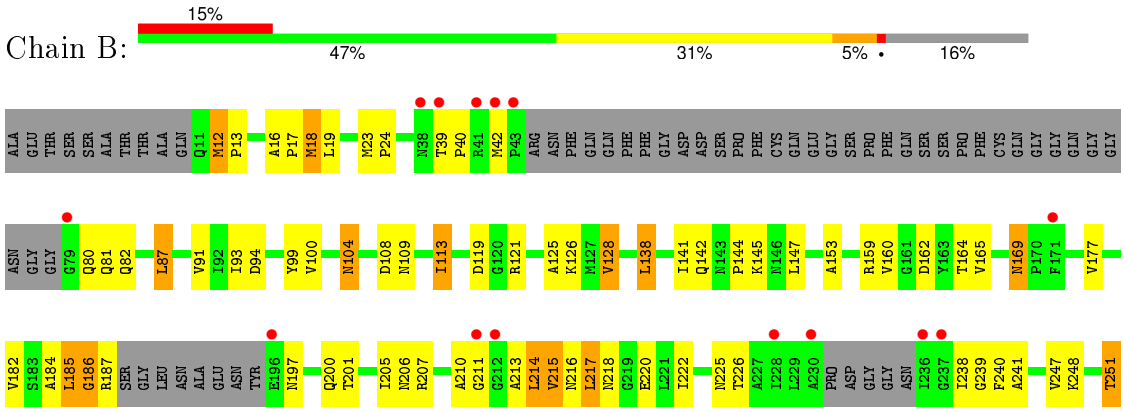
- Molecule 1: Protease do

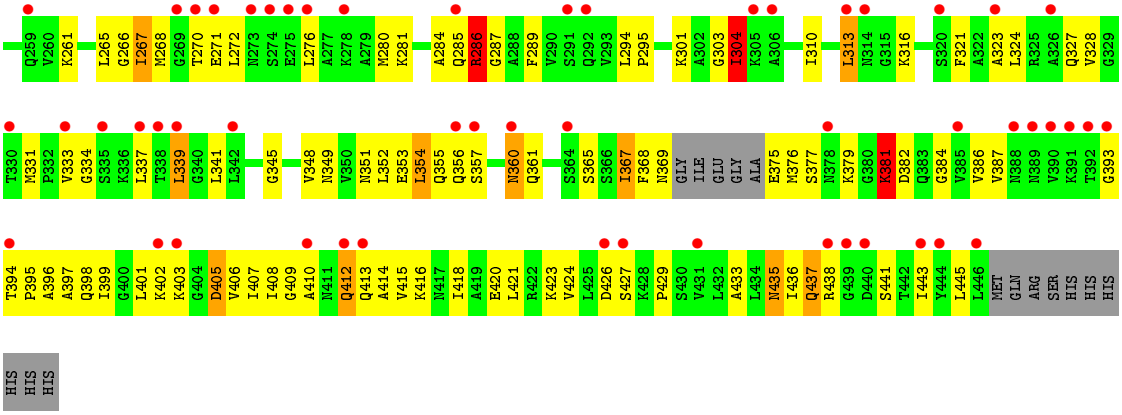
Chain A:



- Molecule 1: Protease do

Chain B:




Q259 V260 K261 L265 G266 I267 M268 G269 T270 E271 L272 N273 S274 E275 L276 A277 K278 A279 M280 K281 A284 Q285 R286 G287 A288 F289 V290 S291 Q292 V293 L294 P295 K301 A302 G303 A304 K305 A306 I310 L313 N314 G315 K316 S320 F321 A322 A323 L324 R325 A326 Q327 V328 G329
T330 M331 P332 V333 G334 S335 K336 L337 T338 L339 G340 L341 L342 G345 V348 N349 V350 N351 L352 E353 L354 Q355 Q356 S357 N360 Q361 S364 S365 S366 I367 F368 N369 GLY ILE GLU GLY ALA E375 M376 S377 N378 K379 G380 K381 D382 Q383 G384 V385 V386 V387 N388 N389 V390 K391 T392 G393
T394 P395 A396 A397 Q398 I399 G400 L401 K402 K403 G404 D405 V406 I407 I408 G409 A410 N411 Q412 Q413 A414 V415 K416 N417 I418 A419 E420 L421 R422 K423 V424 L425 D426 S427 K428 P429 S430 V431 L432 A433 L434 N435 I436 Q437 R438 G439 D440 S441 T442 I443 Y444 L445 L446 MET GLN ARG SER HIS HIS HIS
HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.71Å 120.71Å 232.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.07 – 3.10 24.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (24.07-3.10) 97.6 (24.07-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.257 , 0.309 0.242 , 0.295	Depositor DCC
R_{free} test set	957 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	104.4	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 95.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 18452 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5007	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.32	0/2215	0.52	0/2991
1	B	0.30	0/2835	0.49	0/3824
All	All	0.31	0/5050	0.50	0/6815

There are no bond length outliers.

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	2194	0	2270	127	0
1	B	2813	0	2919	137	0
All	All	5007	0	5189	263	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 26.

All (263) 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:409:GLY:HA3	1:B:435:ASN:HB2	1.55	0.88
1:A:318:ILE:HG21	1:A:324:LEU:HG	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG23	1:A:342:LEU:HB3	1.59	0.83
1:A:293:VAL:HG23	1:A:299:ALA:HB1	1.60	0.81
1:A:19:LEU:HD21	1:A:177:VAL:HG21	1.62	0.81
1:A:313:LEU:HD11	1:A:337:LEU:HD12	1.63	0.80
1:B:313:LEU:HD21	1:B:337:LEU:HD12	1.63	0.79
1:B:382:ASP:HB3	1:B:416:LYS:HB2	1.64	0.79
1:B:121:ARG:NH2	1:B:145:LYS:O	2.14	0.79
1:A:298:SER:HA	1:A:301:LYS:HB3	1.65	0.79
1:B:247:VAL:O	1:B:251:THR:HB	1.84	0.78
1:A:29:ILE:HG23	1:A:113:ILE:HD13	1.67	0.76
1:B:276:LEU:HB3	1:B:280:MET:HE2	1.67	0.76
1:A:197:ASN:HD22	1:A:197:ASN:N	1.84	0.74
1:A:262:ARG:HH12	1:A:332:PRO:HG3	1.52	0.73
1:A:273:ASN:HA	1:A:278:LYS:HG2	1.69	0.73
1:A:343:ARG:HH11	1:A:346:LYS:HD2	1.53	0.73
1:B:399:ILE:HG23	1:B:401:LEU:HD13	1.70	0.72
1:A:187:ARG:HB2	1:A:197:ASN:HB3	1.71	0.72
1:A:267:ILE:HG21	1:A:293:VAL:HA	1.72	0.72
1:A:289:PHE:HA	1:A:309:VAL:HG12	1.73	0.71
1:B:410:ALA:HB1	1:B:424:VAL:HG21	1.72	0.71
1:B:367:ILE:HG23	1:B:368:PHE:H	1.54	0.71
1:B:384:GLY:HA3	1:B:408:ILE:HD13	1.74	0.70
1:B:304:ILE:HG12	1:B:341:LEU:HD11	1.75	0.68
1:B:225:ASN:ND2	1:B:241:ALA:HB2	2.08	0.68
1:B:394:THR:HB	1:B:397:ALA:HB3	1.76	0.67
1:A:293:VAL:HG21	1:A:304:ILE:O	1.95	0.66
1:B:361:GLN:HG3	1:B:375:GLU:HG2	1.77	0.66
1:A:304:ILE:HA	1:A:346:LYS:NZ	2.10	0.65
1:A:341:LEU:HD22	1:A:346:LYS:HD3	1.77	0.65
1:B:402:LYS:HG2	1:B:403:LYS:H	1.61	0.65
1:B:267:ILE:HD11	1:B:321:PHE:HE1	1.61	0.64
1:B:82:GLN:HA	1:B:82:GLN:OE1	1.96	0.64
1:A:126:LYS:HG2	1:A:142:GLN:NE2	2.13	0.64
1:A:272:LEU:O	1:A:273:ASN:HB2	1.98	0.63
1:A:343:ARG:NH1	1:A:346:LYS:HZ2	1.97	0.63
1:A:236:ILE:HG21	1:A:240:PHE:HE1	1.64	0.62
1:A:290:VAL:HG21	1:A:310:ILE:HD13	1.81	0.62
1:A:305:LYS:HG3	1:A:306:ALA:H	1.64	0.62
1:A:304:ILE:HA	1:A:346:LYS:HZ3	1.63	0.61
1:B:367:ILE:HG23	1:B:368:PHE:N	2.15	0.61
1:B:310:ILE:H	1:B:310:ILE:HD12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD12	1:A:297:SER:HB2	1.83	0.61
1:B:354:LEU:HD13	1:B:355:GLN:N	2.17	0.60
1:B:369:ASN:HD22	1:B:396:ALA:HB2	1.66	0.60
1:A:42:MET:HB3	1:A:43:PRO:HA	1.84	0.59
1:A:114:LYS:HE2	1:A:124:ASP:OD1	2.02	0.59
1:A:311:THR:HA	1:A:318:ILE:HB	1.85	0.59
1:B:113:ILE:HG13	1:B:125:ALA:HB3	1.84	0.59
1:A:23:MET:N	1:A:24:PRO:HD2	2.19	0.58
1:B:348:VAL:HG12	1:B:349:ASN:H	1.68	0.58
1:A:267:ILE:O	1:A:268:MET:HB2	2.02	0.58
1:A:293:VAL:HG11	1:A:305:LYS:HD3	1.85	0.58
1:B:313:LEU:HD13	1:B:327:GLN:HE21	1.67	0.58
1:B:410:ALA:C	1:B:412:GLN:H	2.05	0.58
1:A:264:GLU:HA	1:A:329:GLY:HA2	1.84	0.58
1:B:405:ASP:HA	1:B:438:ARG:HB3	1.85	0.58
1:A:200:GLN:HA	1:A:239:GLY:O	2.03	0.58
1:A:18:MET:HA	1:A:21:LYS:HE3	1.85	0.58
1:B:394:THR:N	1:B:395:PRO:HD3	2.19	0.57
1:B:396:ALA:O	1:B:399:ILE:HG22	2.05	0.57
1:B:376:MET:HG3	1:B:387:VAL:HG23	1.86	0.57
1:A:261:LYS:O	1:A:333:VAL:HG23	2.05	0.57
1:A:343:ARG:HH12	1:A:346:LYS:HZ2	1.53	0.56
1:B:303:GLY:O	1:B:304:ILE:HG13	2.05	0.56
1:B:408:ILE:H	1:B:437:GLN:NE2	2.04	0.56
1:B:384:GLY:HA2	1:B:415:VAL:O	2.04	0.56
1:B:141:ILE:O	1:B:144:PRO:HD3	2.05	0.56
1:A:263:GLY:O	1:A:265:LEU:HD22	2.06	0.56
1:B:113:ILE:CG1	1:B:125:ALA:HB3	2.36	0.55
1:B:379:LYS:HB2	1:B:386:VAL:HB	1.89	0.55
1:A:113:ILE:HD12	1:A:114:LYS:N	2.22	0.55
1:A:29:ILE:HG23	1:A:113:ILE:CD1	2.37	0.55
1:A:269:GLY:HA2	1:A:291:SER:OG	2.06	0.55
1:A:335:SER:HB2	1:A:352:LEU:HD22	1.89	0.55
1:B:381:LYS:HD3	1:B:381:LYS:H	1.72	0.54
1:A:283:ASP:O	1:A:284:ALA:HB3	2.08	0.54
1:B:348:VAL:HG12	1:B:349:ASN:N	2.22	0.54
1:A:230:ALA:HA	1:A:232:ASP:H	1.73	0.54
1:B:386:VAL:HG22	1:B:406:VAL:HG22	1.90	0.54
1:A:94:ASP:HB3	1:A:99:TYR:HB2	1.88	0.54
1:B:333:VAL:HG13	1:B:353:GLU:HA	1.90	0.54
1:A:23:MET:N	1:A:24:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HD23	1:A:342:LEU:N	2.23	0.54
1:B:160:VAL:HG13	1:B:182:VAL:O	2.08	0.53
1:A:87:LEU:HD23	1:A:87:LEU:C	2.28	0.53
1:B:365:SER:HB3	1:B:367:ILE:HG22	1.90	0.53
1:A:91:VAL:CG2	1:A:213:ALA:HB2	2.39	0.53
1:A:243:PRO:O	1:A:247:VAL:HG23	2.09	0.53
1:B:19:LEU:O	1:B:23:MET:HG2	2.08	0.53
1:A:244:SER:O	1:A:247:VAL:HB	2.09	0.53
1:A:293:VAL:HG11	1:A:305:LYS:HA	1.90	0.52
1:B:225:ASN:HD22	1:B:241:ALA:HB2	1.74	0.52
1:A:214:LEU:HG	1:A:225:ASN:HD21	1.74	0.52
1:B:141:ILE:HD12	1:B:147:LEU:HD21	1.89	0.52
1:A:160:VAL:HG13	1:A:182:VAL:O	2.09	0.52
1:A:337:LEU:HD21	1:A:352:LEU:HD11	1.90	0.52
1:B:272:LEU:HD11	1:B:287:GLY:H	1.75	0.52
1:A:163:TYR:HB2	1:A:217:LEU:CD2	2.40	0.52
1:A:266:GLY:C	1:A:267:ILE:HG13	2.30	0.52
1:B:81:GLN:O	1:B:82:GLN:OE1	2.28	0.52
1:B:286:ARG:O	1:B:286:ARG:HD2	2.10	0.51
1:A:141:ILE:O	1:A:144:PRO:HD3	2.11	0.51
1:A:31:VAL:HG21	1:A:106:VAL:O	2.11	0.51
1:A:304:ILE:HG23	1:A:308:ASP:OD2	2.11	0.50
1:B:310:ILE:N	1:B:310:ILE:HD12	2.27	0.50
1:A:313:LEU:HD11	1:A:337:LEU:CD1	2.39	0.50
1:A:312:SER:HB2	1:A:340:GLY:HA3	1.93	0.50
1:B:367:ILE:HG13	1:B:368:PHE:N	2.26	0.50
1:B:267:ILE:HD11	1:B:321:PHE:CE1	2.46	0.50
1:A:163:TYR:HB2	1:A:217:LEU:HD21	1.94	0.50
1:B:94:ASP:HB3	1:B:99:TYR:HB2	1.93	0.49
1:A:312:SER:HB2	1:A:340:GLY:H	1.78	0.49
1:A:170:PRO:HG3	1:A:205:ILE:HG12	1.93	0.49
1:B:206:ASN:OD1	1:B:207:ARG:HG3	2.13	0.49
1:A:256:GLU:HG2	1:A:257:TYR:CZ	2.48	0.49
1:B:226:THR:HG22	1:B:240:PHE:O	2.13	0.49
1:A:128:VAL:HG13	1:A:138:LEU:O	2.13	0.49
1:B:185:LEU:O	1:B:186:GLY:C	2.51	0.49
1:B:437:GLN:HA	1:B:441:SER:O	2.13	0.49
1:A:205:ILE:O	1:A:235:ASN:ND2	2.45	0.48
1:B:443:ILE:HD12	1:B:445:LEU:HD21	1.94	0.48
1:B:100:VAL:O	1:B:138:LEU:HD23	2.12	0.48
1:B:159:ARG:O	1:B:162:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ALA:HB3	1:B:17:PRO:HD3	1.96	0.48
1:B:301:LYS:C	1:B:301:LYS:HD3	2.32	0.48
1:A:324:LEU:O	1:A:328:VAL:HG22	2.14	0.48
1:A:113:ILE:HG13	1:A:125:ALA:HB3	1.95	0.48
1:A:197:ASN:N	1:A:197:ASN:ND2	2.57	0.48
1:B:313:LEU:HA	1:B:339:LEU:HB3	1.95	0.48
1:B:360:ASN:O	1:B:375:GLU:HA	2.14	0.48
1:B:185:LEU:O	1:B:187:ARG:N	2.47	0.48
1:A:117:LEU:HG	1:A:123:PHE:HE1	1.79	0.47
1:B:200:GLN:HA	1:B:239:GLY:O	2.14	0.47
1:A:312:SER:HB2	1:A:340:GLY:CA	2.44	0.47
1:B:272:LEU:HD23	1:B:289:PHE:HB2	1.96	0.47
1:A:93:ILE:HG13	1:A:152:MET:CE	2.44	0.47
1:A:225:ASN:ND2	1:A:241:ALA:HB2	2.30	0.47
1:A:266:GLY:O	1:A:267:ILE:HG13	2.15	0.47
1:B:185:LEU:O	1:B:187:ARG:HB2	2.15	0.47
1:B:153:ALA:HB2	1:B:220:GLU:HB3	1.96	0.47
1:B:266:GLY:O	1:B:294:LEU:HB2	2.15	0.47
1:B:126:LYS:HG3	1:B:142:GLN:CD	2.34	0.47
1:B:396:ALA:O	1:B:401:LEU:HB2	2.15	0.47
1:A:133:ARG:HD3	1:A:330:THR:O	2.15	0.47
1:A:229:LEU:O	1:A:232:ASP:HB3	2.15	0.47
1:B:18:MET:CE	1:B:165:VAL:HG11	2.45	0.47
1:A:352:LEU:O	1:A:353:GLU:HB2	2.15	0.46
1:A:282:VAL:O	1:A:282:VAL:HG12	2.16	0.46
1:B:337:LEU:HD23	1:B:337:LEU:H	1.81	0.46
1:B:399:ILE:O	1:B:445:LEU:HG	2.16	0.46
1:B:113:ILE:O	1:B:113:ILE:HG13	2.16	0.46
1:A:16:ALA:O	1:A:20:GLU:HG3	2.16	0.46
1:B:355:GLN:HG2	1:B:356:GLN:H	1.81	0.46
1:A:185:LEU:C	1:A:187:ARG:H	2.20	0.45
1:B:413:GLN:HB3	1:B:414:ALA:H	1.46	0.45
1:B:410:ALA:HB2	1:B:415:VAL:HG23	1.98	0.45
1:A:127:MET:HG3	1:A:128:VAL:N	2.31	0.45
1:A:16:ALA:HB3	1:A:17:PRO:HD3	1.98	0.45
1:A:313:LEU:HD23	1:A:327:GLN:HE21	1.82	0.45
1:A:272:LEU:O	1:A:273:ASN:CB	2.64	0.45
1:B:415:VAL:O	1:B:415:VAL:HG12	2.14	0.45
1:B:393:GLY:C	1:B:395:PRO:HD3	2.36	0.45
1:B:420:GLU:O	1:B:423:LYS:HB3	2.17	0.45
1:A:293:VAL:O	1:A:293:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ALA:N	1:A:17:PRO:HD2	2.32	0.45
1:A:342:LEU:HD23	1:A:343:ARG:N	2.32	0.45
1:A:236:ILE:HG21	1:A:240:PHE:CE1	2.46	0.45
1:B:216:ASN:OD1	1:B:218:ASN:N	2.50	0.45
1:B:87:LEU:HD23	1:B:87:LEU:O	2.16	0.45
1:B:272:LEU:CD1	1:B:287:GLY:H	2.30	0.45
1:A:133:ARG:HH11	1:A:330:THR:HG23	1.82	0.45
1:A:225:ASN:HD22	1:A:241:ALA:HB2	1.82	0.45
1:B:153:ALA:HB2	1:B:220:GLU:CB	2.47	0.45
1:B:165:VAL:HG12	1:B:215:VAL:O	2.17	0.45
1:B:128:VAL:HG13	1:B:138:LEU:HB3	1.99	0.45
1:A:180:GLY:HA3	1:A:203:ALA:HB2	1.99	0.45
1:A:31:VAL:HB	1:A:86:ALA:HB3	1.99	0.44
1:B:93:ILE:HA	1:B:93:ILE:HD12	1.84	0.44
1:A:337:LEU:HG	1:A:350:VAL:HG22	2.00	0.44
1:B:265:LEU:HD21	1:B:339:LEU:HD21	1.98	0.44
1:A:345:GLY:O	1:A:346:LYS:HB2	2.16	0.44
1:B:217:LEU:HA	1:B:217:LEU:HD12	1.89	0.44
1:A:318:ILE:CG2	1:A:324:LEU:HG	2.40	0.44
1:A:246:MET:HA	1:A:246:MET:HE1	1.99	0.44
1:B:410:ALA:C	1:B:412:GLN:N	2.70	0.43
1:A:271:GLU:HG2	1:A:272:LEU:N	2.31	0.43
1:B:433:ALA:HA	1:B:445:LEU:O	2.18	0.43
1:B:270:THR:HB	1:B:271:GLU:H	1.64	0.43
1:A:337:LEU:HD23	1:A:337:LEU:H	1.84	0.43
1:B:410:ALA:CA	1:B:415:VAL:HG23	2.49	0.43
1:B:184:ALA:HB3	1:B:200:GLN:HB3	2.01	0.43
1:B:381:LYS:HB2	1:B:382:ASP:H	1.60	0.43
1:A:331:MET:HA	1:A:332:PRO:HD3	1.85	0.43
1:B:386:VAL:CG2	1:B:406:VAL:HG22	2.49	0.43
1:A:19:LEU:O	1:A:23:MET:HG2	2.19	0.43
1:B:91:VAL:HG21	1:B:213:ALA:HB2	2.00	0.43
1:B:126:LYS:HG3	1:B:142:GLN:OE1	2.18	0.43
1:B:360:ASN:ND2	1:B:360:ASN:N	2.67	0.43
1:A:18:MET:SD	1:A:18:MET:C	2.97	0.43
1:B:268:MET:HE3	1:B:294:LEU:HD21	2.01	0.43
1:A:93:ILE:HG13	1:A:152:MET:HE1	2.00	0.42
1:B:294:LEU:HA	1:B:295:PRO:HD3	1.87	0.42
1:A:246:MET:HA	1:A:246:MET:CE	2.49	0.42
1:B:424:VAL:C	1:B:426:ASP:H	2.23	0.42
1:A:294:LEU:N	1:A:295:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:HG13	1:A:341:LEU:HG	2.01	0.42
1:B:91:VAL:CG2	1:B:213:ALA:HB2	2.49	0.42
1:B:409:GLY:HA2	1:B:413:GLN:O	2.19	0.42
1:A:262:ARG:HA	1:A:262:ARG:HD3	1.74	0.42
1:B:427:SER:C	1:B:429:PRO:HD3	2.39	0.42
1:B:165:VAL:CG1	1:B:215:VAL:HG12	2.49	0.42
1:B:408:ILE:H	1:B:437:GLN:HE21	1.67	0.42
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.85	0.42
1:B:248:LYS:O	1:B:251:THR:HG22	2.20	0.42
1:B:408:ILE:HG12	1:B:437:GLN:HE21	1.84	0.42
1:A:269:GLY:HA2	1:A:291:SER:H	1.85	0.42
1:A:308:ASP:HB3	1:A:341:LEU:HD21	2.01	0.42
1:B:80:GLN:CD	1:B:82:GLN:HE22	2.23	0.42
1:B:272:LEU:HD13	1:B:285:GLN:HA	2.01	0.42
1:B:381:LYS:CD	1:B:381:LYS:H	2.30	0.42
1:A:262:ARG:HH12	1:A:332:PRO:CG	2.28	0.42
1:B:402:LYS:HG2	1:B:403:LYS:N	2.32	0.42
1:A:341:LEU:HD13	1:A:346:LYS:HE2	2.02	0.41
1:B:108:ASP:O	1:B:109:ASN:HB2	2.19	0.41
1:B:169:ASN:C	1:B:169:ASN:HD22	2.22	0.41
1:B:333:VAL:HG21	1:B:354:LEU:HD23	2.02	0.41
1:B:387:VAL:CG1	1:B:405:ASP:H	2.33	0.41
1:A:170:PRO:CG	1:A:205:ILE:HG12	2.50	0.41
1:A:321:PHE:HD2	1:A:321:PHE:H	1.60	0.41
1:B:331:MET:SD	1:B:337:LEU:HD13	2.60	0.41
1:B:333:VAL:HG12	1:B:334:GLY:N	2.35	0.41
1:B:238:ILE:HG12	1:B:239:GLY:H	1.84	0.41
1:A:205:ILE:H	1:A:205:ILE:HD12	1.86	0.41
1:A:321:PHE:N	1:A:321:PHE:CD2	2.80	0.41
1:A:290:VAL:HG21	1:A:310:ILE:CD1	2.50	0.41
1:B:415:VAL:CG1	1:B:421:LEU:HB2	2.50	0.41
1:A:142:GLN:HB3	1:B:119:ASP:O	2.20	0.41
1:A:312:SER:HB2	1:A:340:GLY:N	2.34	0.41
1:B:324:LEU:O	1:B:328:VAL:HG22	2.20	0.41
1:A:230:ALA:HA	1:A:232:ASP:N	2.35	0.41
1:A:160:VAL:O	1:A:182:VAL:HB	2.20	0.41
1:A:107:VAL:HG22	1:A:127:MET:HE1	2.03	0.41
1:B:323:ALA:O	1:B:327:GLN:HG3	2.21	0.41
1:B:104:ASN:O	1:B:108:ASP:HB2	2.21	0.41
1:A:125:ALA:HA	1:A:140:GLN:O	2.21	0.41
1:B:407:ILE:HG12	1:B:436:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:O	1:B:398:GLN:HG3	2.21	0.41
1:B:216:ASN:C	1:B:216:ASN:OD1	2.59	0.41
1:A:216:ASN:OD1	1:A:216:ASN:C	2.59	0.41
1:B:214:LEU:O	1:B:222:ILE:HG12	2.21	0.41
1:B:12:MET:HA	1:B:13:PRO:HD3	1.94	0.41
1:B:355:GLN:HG2	1:B:357:SER:H	1.86	0.40
1:B:435:ASN:N	1:B:435:ASN:OD1	2.54	0.40
1:A:343:ARG:HH11	1:A:346:LYS:CD	2.30	0.40
1:B:23:MET:N	1:B:24:PRO:CD	2.84	0.40
1:B:201:THR:O	1:B:238:ILE:HG12	2.21	0.40
1:B:18:MET:HE3	1:B:165:VAL:HG11	2.04	0.40
1:B:377:SER:HA	1:B:418:ILE:HD11	2.03	0.40
1:A:264:GLU:HG2	1:A:264:GLU:H	1.68	0.40
1:A:22:VAL:C	1:A:24:PRO:HD2	2.41	0.40
1:B:39:THR:HA	1:B:40:PRO:HD3	1.90	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	295/456 (65%)	249 (84%)	32 (11%)	14 (5%)	3	17
1	B	373/456 (82%)	319 (86%)	42 (11%)	12 (3%)	5	26
All	All	668/912 (73%)	568 (85%)	74 (11%)	26 (4%)	4	22

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	MET
1	A	281	LYS
1	A	343	ARG

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Mol	Chain	Res	Type
1	B	367	ILE
1	B	381	LYS
1	A	267	ILE
1	A	282	VAL
1	A	285	GLN
1	A	293	VAL
1	B	186	GLY
1	B	412	GLN
1	A	210	ALA
1	B	197	ASN
1	B	281	LYS
1	A	264	GLU
1	A	271	GLU
1	A	319	SER
1	B	304	ILE
1	B	345	GLY
1	A	186	GLY
1	A	346	LYS
1	B	210	ALA
1	B	284	ALA
1	B	286	ARG
1	A	211	GLY
1	B	211	GLY

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	238/364 (65%)	210 (88%)	28 (12%)	6 25
1	B	309/364 (85%)	277 (90%)	32 (10%)	9 32
All	All	547/728 (75%)	487 (89%)	60 (11%)	8 30

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	18	MET
1	A	25	SER
1	A	41	ARG
1	A	93	ILE
1	A	113	ILE
1	A	114	LYS
1	A	128	VAL
1	A	133	ARG
1	A	138	LEU
1	A	147	LEU
1	A	165	VAL
1	A	177	VAL
1	A	197	ASN
1	A	198	PHE
1	A	205	ILE
1	A	214	LEU
1	A	217	LEU
1	A	251	THR
1	A	265	LEU
1	A	267	ILE
1	A	268	MET
1	A	272	LEU
1	A	275	GLU
1	A	305	LYS
1	A	309	VAL
1	A	337	LEU
1	A	343	ARG
1	B	12	MET
1	B	18	MET
1	B	42	MET
1	B	87	LEU
1	B	104	ASN
1	B	113	ILE
1	B	128	VAL
1	B	138	LEU
1	B	164	THR
1	B	169	ASN
1	B	177	VAL
1	B	185	LEU
1	B	205	ILE
1	B	214	LEU
1	B	215	VAL

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Mol	Chain	Res	Type
1	B	217	LEU
1	B	251	THR
1	B	261	LYS
1	B	267	ILE
1	B	286	ARG
1	B	304	ILE
1	B	313	LEU
1	B	316	LYS
1	B	339	LEU
1	B	351	ASN
1	B	352	LEU
1	B	354	LEU
1	B	360	ASN
1	B	381	LYS
1	B	405	ASP
1	B	435	ASN
1	B	437	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	140	GLN
1	A	142	GLN
1	A	169	ASN
1	A	225	ASN
1	A	235	ASN
1	A	245	ASN
1	A	327	GLN
1	A	347	GLN
1	B	80	GLN
1	B	82	GLN
1	B	104	ASN
1	B	140	GLN
1	B	169	ASN
1	B	225	ASN
1	B	245	ASN
1	B	292	GLN
1	B	296	ASN
1	B	327	GLN
1	B	347	GLN
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	360	ASN
1	B	383	GLN
1	B	388	ASN
1	B	413	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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	301/456 (66%)	0.95	63 (20%) 1 0	66, 107, 226, 235	0
1	B	383/456 (83%)	0.82	67 (17%) 2 1	67, 143, 211, 220	0
All	All	684/912 (75%)	0.87	130 (19%) 2 1	66, 125, 218, 235	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	GLY	9.1
1	A	292	GLN	8.9
1	B	439	GLY	8.6
1	A	349	ASN	8.6
1	A	287	GLY	8.4
1	A	274	SER	8.4
1	B	337	LEU	8.1
1	B	43	PRO	7.3
1	A	293	VAL	7.3
1	A	307	GLY	6.6
1	A	276	LEU	6.6
1	A	188	SER	6.5
1	A	232	ASP	6.3
1	B	42	MET	6.1
1	A	329	GLY	6.0
1	B	38	ASN	5.9
1	A	266	GLY	5.9
1	B	274	SER	5.8
1	B	323	ALA	5.6
1	A	206	ASN	5.5
1	A	283	ASP	5.4
1	B	230	ALA	5.2
1	B	431	VAL	5.0
1	B	236	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	392	THR	4.9
1	B	278	LYS	4.8
1	B	79	GLY	4.6
1	A	342	LEU	4.5
1	B	385	VAL	4.4
1	B	438	ARG	4.4
1	A	317	PRO	4.4
1	A	277	ALA	4.3
1	A	272	LEU	4.3
1	B	443	ILE	4.3
1	B	338	THR	4.3
1	A	323	ALA	4.3
1	A	294	LEU	4.2
1	A	285	GLN	4.1
1	B	333	VAL	4.1
1	A	231	PRO	4.0
1	B	402	LYS	4.0
1	A	234	GLY	4.0
1	B	391	LYS	4.0
1	A	233	GLY	3.9
1	B	440	ASP	3.9
1	B	388	ASN	3.9
1	A	286	ARG	3.9
1	B	410	ALA	3.8
1	B	275	GLU	3.8
1	A	236	ILE	3.8
1	B	413	GLN	3.8
1	A	273	ASN	3.8
1	A	343	ARG	3.7
1	B	228	ILE	3.7
1	B	271	GLU	3.7
1	B	273	ASN	3.6
1	A	90	GLY	3.6
1	B	389	ASN	3.5
1	B	320	SER	3.4
1	B	444	TYR	3.4
1	B	394	THR	3.4
1	B	269	GLY	3.4
1	B	314	ASN	3.4
1	A	265	LEU	3.4
1	B	39	THR	3.3
1	B	330	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLU	3.3
1	A	344	ASP	3.3
1	A	281	LYS	3.2
1	B	339	LEU	3.2
1	B	212	GLY	3.2
1	B	426	ASP	3.1
1	B	196	GLU	3.1
1	A	315	GLY	3.1
1	A	291	SER	3.0
1	B	427	SER	3.0
1	B	390	VAL	3.0
1	B	211	GLY	3.0
1	A	228	ILE	3.0
1	A	271	GLU	3.0
1	B	360	ASN	2.9
1	B	306	ALA	2.9
1	B	335	SER	2.9
1	A	89	SER	2.9
1	B	171	PHE	2.8
1	A	306	ALA	2.8
1	A	229	LEU	2.8
1	B	342	LEU	2.8
1	A	38	ASN	2.8
1	A	259	GLN	2.7
1	A	350	VAL	2.7
1	B	412	GLN	2.7
1	A	211	GLY	2.7
1	B	393	GLY	2.6
1	B	285	GLN	2.6
1	A	264	GLU	2.6
1	B	259	GLN	2.6
1	B	356	GLN	2.6
1	A	102	THR	2.6
1	A	187	ARG	2.5
1	B	292	GLN	2.5
1	A	348	VAL	2.5
1	A	169	ASN	2.5
1	A	319	SER	2.4
1	B	291	SER	2.4
1	B	41	ARG	2.4
1	A	325	ARG	2.4
1	B	364	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	80	GLN	2.4
1	A	212	GLY	2.3
1	B	276	LEU	2.3
1	B	305	LYS	2.3
1	A	207	ARG	2.3
1	B	313	LEU	2.3
1	B	403	LYS	2.3
1	A	237	GLY	2.3
1	A	330	THR	2.2
1	A	320	SER	2.2
1	B	446	LEU	2.2
1	A	43	PRO	2.2
1	A	267	ILE	2.2
1	A	42	MET	2.2
1	A	224	ILE	2.2
1	A	336	LYS	2.1
1	B	378	ASN	2.1
1	B	237	GLY	2.1
1	B	270	THR	2.1
1	B	326	ALA	2.1
1	A	333	VAL	2.1
1	B	357	SER	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.