W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

PDB ID	:	3EQ2
Title	:	Structure of Hexagonal Crystal form of Pseudomonas aeruginosa RssB
Authors	:	Levchenko, I.; Grant, R.A.; Sauer, R.T.; Baker, T.A.
Deposited on	:	2008-09-30
Resolution	:	3.40 Å(reported)

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

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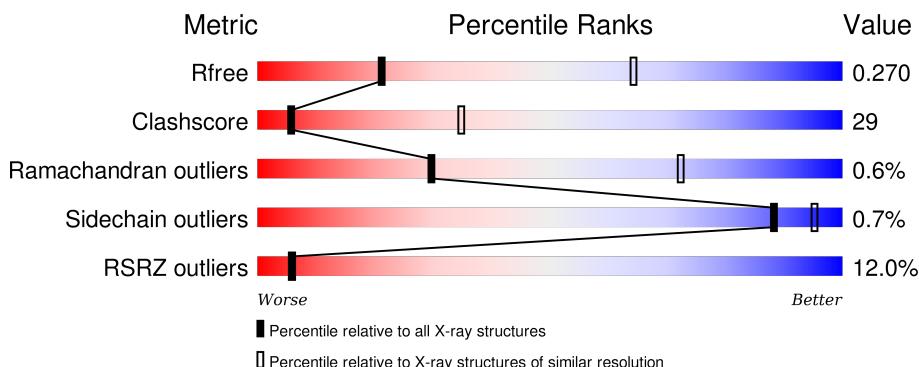
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	394	
1	B	394	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5536 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.
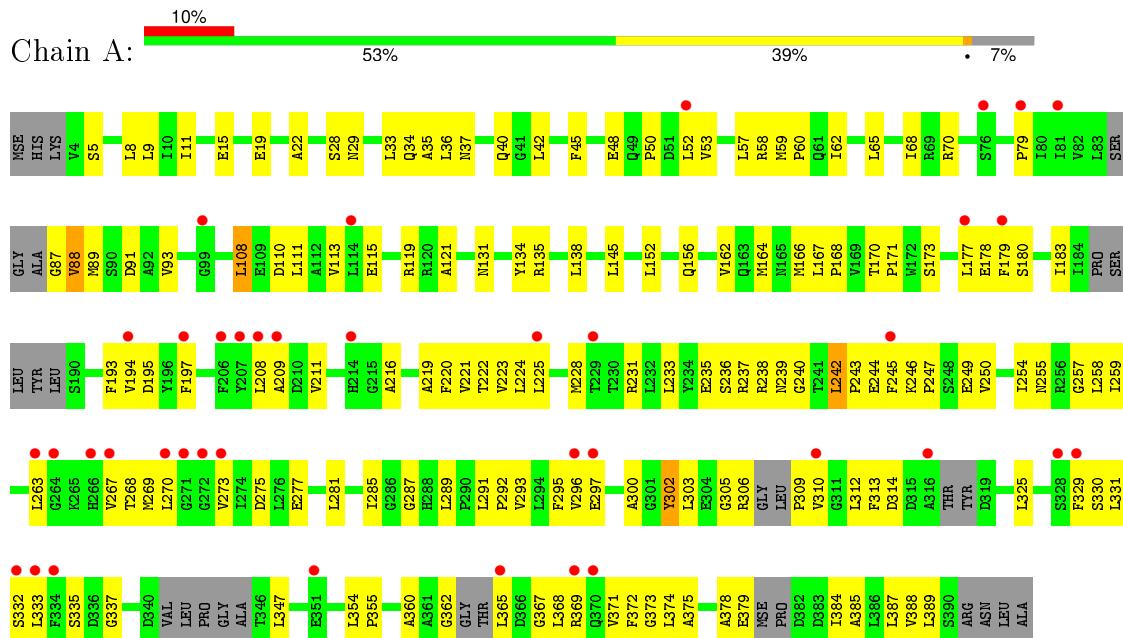
- Molecule 1 is a protein called Probable two-component response regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	Se	0	0	0
			2777	1767	477	525	1	7			
1	B	372	Total	C	N	O	S	Se	0	0	0
			2759	1762	454	535	1	7			
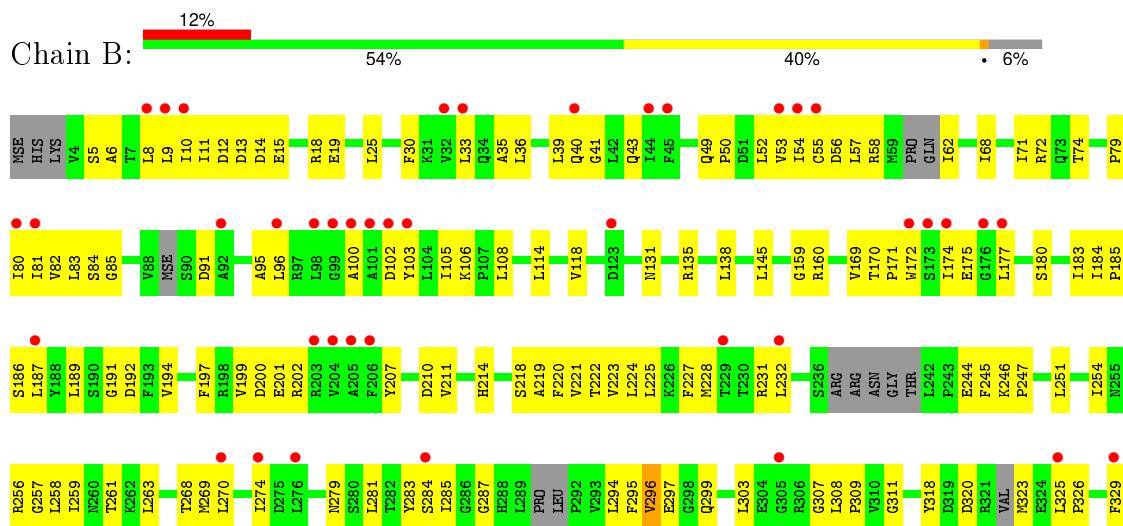
3 Residue-property plots ⓘ

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: Probable two-component response regulator

Chain A:

10%
53%   39%   • 7%

MSE HIS LYS V4 S5 L8 L9 I10 I11 E15 E19 A22 S28 N29 L33 Q34 A35 L36 N37 Q40 G41 L42 F45 E48 Q49 P50 D51 L52 V53 L57 R58 M59 P60 Q61 I62 L65 I68 R69 R70 S76 P79 I80 I81 V82 L83 SER

GLY ALA G87 V88 M89 S90 D91 A92 V93 G99 L108 E109 D110 L111 A112 V113 L114 E115 R119 R120 A121 N131 Y134 R135 L138 L145 L152 Q156 V162 Q163 M164 N165 M166 L167 P168 V169 T170 P171 W172 S173 L177 E178 F179 S180 I183 I184 PRO SER

LEU TYR LEU S190 F193 V194 D195 Y196 F197 P206 Y207 L208 A209 D210 V211 H214 G215 A216 A219 F220 V221 T222 V223 Y234 L225 M228 T229 T230 R231 L232 L233 Y234 E235 S236 R237 R238 N239 Q240 T241 L242 P243 E244 F245 K246 P247 S248 E249 V250 I254 N255 R256 G257 I258 I259

L263 G264 K265 H266 V267 T268 M269 L270 G271 G272 V273 I274 D275 L276 E277 L281 I285 G286 G287 H288 E289 P290 L291 P292 V293 V294 F295 V296 E297 A300 G301 Y302 L303 E304 G305 R306 GLY LEU P309 V310 G311 L312 F313 D314 D315 A316 THR TYR D319 I325 S328 F329 S330 L331

S332 L333 F334 S335 D336 G337 D340 VAL LEU PRO GLY ALA T346 L347 E351 L354 P355 A360 A361 G362 GLY THR L365 D366 G367 L368 R369 Q370 V371 F372 G373 L374 A375 A378 E379 MSE PRO D382 D383 I384 A385 L386 L387 V388 S390 ARG ASN LEU ALA

• Molecule 1: Probable two-component response regulator

Chain B:

12%
54%   40%   • 6%

MSE HIS LYS V4 S5 A6 T7 L8 L9 I10 I11 D12 D13 D14 E15 R18 E19 L25 F30 K31 V32 L33 Q34 A35 L36 L39 Q40 G41 L42 Q43 I44 F45 Q49 P50 D51 L52 V53 I54 C55 D56 L57 R58 M59 PRO GLN I62 I68 I71 R72 Q73 T74 P79

I80 I81 V82 L83 S84 G85 V88 MSE S90 D91 A92 A95 L96 R97 L98 G99 A100 A101 D102 Y103 L104 L105 K106 P107 L108 L114 V118 D123 N131 R135 L138 L145 G159 R160 V169 T170 P171 W172 S173 I174 E175 G176 L177 S180 I183 I184 P185

S186 L187 Y188 L189 S190 G191 D192 F193 V194 F197 R198 V199 D200 E201 R202 R203 V204 A205 F206 Y207 D210 V211 H214 S218 A219 F220 V221 T222 V223 L224 L225 K226 F227 M228 T229 T230 R231 L232 S236 ARG ARG ASN GLY THR L242 P243 E244 F245 K246 P247 L251 I254 N255

R256 G257 I258 I259 N260 T261 K262 L263 T268 M269 L270 I274 D275 L276 N279 S280 L281 T282 Y283 S284 I285 G286 G287 H288 E289 PRO LEU P292 V293 L294 F295 V296 E297 G298 Q299 L303 E304 G305 R306 G307 L308 P309 V310 G311 Y318 D319 D320 R321 VAL M323 E324 L325 P326 F329

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	76.28Å　　76.28Å　　305.08Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	29.05　–　3.40 38.14　–　3.40	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.05-3.40) 98.7 (38.14-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.271　,　0.307 0.269　,　0.270	Depositor DCC
R_{free} test set	679 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	73.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.7	EDS
Estimated twinning fraction	0.509 for k,h,-l 0.438 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.509 for k,h,-l	Depositor
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 13579 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	5536	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.22	0/2806	0.39	0/3789
1	B	0.21	0/2790	0.37	0/3780
All	All	0.21	0/5596	0.38	0/7569

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 (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	2777	0	2759	166	1
1	B	2759	0	2690	160	1
All	All	5536	0	5449	319	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 29.

All (319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HB2	1:A:302:TYR:CE1	1.20	1.65
1:A:291:LEU:CB	1:A:302:TYR:CE1	1.83	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:CB	1:A:302:TYR:HE1	1.15	1.42
1:A:330:SER:OG	1:A:365:LEU:HD11	1.25	1.28
1:A:259:ILE:HD12	1:A:314:ASP:OD1	1.34	1.27
1:A:291:LEU:HB3	1:A:302:TYR:CD1	1.69	1.26
1:B:295:PHE:O	1:B:296:VAL:HG12	1.41	1.19
1:A:291:LEU:CB	1:A:302:TYR:CD1	2.26	1.11
1:A:291:LEU:HB3	1:A:302:TYR:CE1	1.76	1.10
1:A:295:PHE:HB3	1:A:330:SER:HB3	1.35	1.08
1:A:259:ILE:CD1	1:A:314:ASP:OD1	2.06	1.04
1:A:57:LEU:HD11	1:A:87:GLY:CA	1.89	1.03
1:B:351:GLU:O	1:B:355:PRO:HD3	1.59	1.02
1:B:295:PHE:O	1:B:296:VAL:CG1	2.11	0.99
1:A:246:LYS:HD3	1:A:249:GLU:HG3	1.47	0.96
1:B:6:ALA:HB3	1:B:30:PHE:HE1	1.32	0.94
1:B:346:THR:O	1:B:351:GLU:HG2	1.68	0.93
1:A:330:SER:OG	1:A:365:LEU:CD1	2.16	0.92
1:A:291:LEU:HB3	1:A:302:TYR:HD1	1.36	0.88
1:B:6:ALA:HB3	1:B:30:PHE:CE1	2.09	0.88
1:A:57:LEU:HD11	1:A:87:GLY:HA3	1.56	0.84
1:A:236:SER:HB2	1:A:240:GLY:HA2	1.59	0.84
1:B:57:LEU:HD23	1:B:57:LEU:O	1.78	0.84
1:A:37:ASN:H	1:A:40:GLN:HE21	1.25	0.84
1:A:57:LEU:HD11	1:A:87:GLY:HA2	1.60	0.82
1:B:295:PHE:CE1	1:B:360:ALA:HA	2.14	0.82
1:B:347:LEU:HD13	1:B:347:LEU:H	1.42	0.82
1:A:281:LEU:HB2	1:A:325:LEU:HD11	1.63	0.81
1:B:296:VAL:HG11	1:B:299:GLN:O	1.82	0.80
1:B:295:PHE:CE1	1:B:363:GLY:HA2	2.15	0.80
1:A:368:LEU:HD12	1:A:369:ARG:N	1.99	0.77
1:A:220:PHE:CE2	1:B:159:GLY:HA2	2.21	0.76
1:A:246:LYS:HD3	1:A:249:GLU:CG	2.14	0.76
1:A:88:VAL:HG12	1:A:89:MSE:H	1.48	0.76
1:B:284:SER:HB3	1:B:320:ASP:HB3	1.68	0.75
1:B:15:GLU:O	1:B:19:GLU:HG2	1.88	0.74
1:A:237:ARG:O	1:A:238:ARG:HG2	1.88	0.73
1:B:311:GLY:HA2	1:B:318:TYR:OH	1.88	0.73
1:B:303:LEU:CD2	1:B:323:MSE:SE	2.86	0.73
1:A:287:GLY:HA3	1:A:309:PRO:O	1.89	0.72
1:A:236:SER:HB2	1:A:240:GLY:CA	2.20	0.72
1:B:14:ASP:H	1:B:58:ARG:NH2	1.88	0.71
1:A:247:PRO:HG3	1:A:273:VAL:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PHE:C	1:B:296:VAL:HG12	2.11	0.71
1:B:36:LEU:H	1:B:40:GLN:HG2	1.56	0.71
1:A:332:SER:OG	1:A:369:ARG:NH2	2.23	0.70
1:B:191:GLY:HA3	1:B:211:VAL:HB	1.71	0.70
1:A:285:ILE:HG13	1:A:305:GLY:HA3	1.72	0.70
1:B:329:PHE:HB3	1:B:391:ARG:HB3	1.73	0.70
1:B:8:LEU:HD22	1:B:52:LEU:HB3	1.72	0.69
1:B:295:PHE:HD2	1:B:297:GLU:H	1.38	0.69
1:A:193:PHE:CE2	1:A:195:ASP:HB2	2.26	0.69
1:B:13:ASP:HB3	1:B:58:ARG:HH12	1.58	0.69
1:A:59:MSE:HE3	1:A:60:PRO:HA	1.76	0.68
1:B:172:TRP:CH2	1:B:174:ILE:HB	2.29	0.68
1:A:374:LEU:HG	1:A:375:ALA:H	1.58	0.68
1:A:373:GLY:O	1:A:374:LEU:HB3	1.94	0.67
1:A:335:SER:HB3	1:A:385:ALA:H	1.58	0.67
1:B:197:PHE:HE2	1:B:207:TYR:HE1	1.43	0.66
1:B:303:LEU:HD22	1:B:323:MSE:SE	2.46	0.66
1:A:378:ALA:O	1:A:379:GLU:HB2	1.96	0.66
1:B:13:ASP:HB3	1:B:58:ARG:HH22	1.61	0.65
1:A:291:LEU:CA	1:A:302:TYR:HE1	2.05	0.65
1:A:246:LYS:CD	1:A:249:GLU:HG3	2.23	0.64
1:A:8:LEU:HD22	1:A:52:LEU:HB3	1.78	0.64
1:B:220:PHE:O	1:B:223:VAL:HG22	1.97	0.64
1:B:169:VAL:HG23	1:B:172:TRP:HB2	1.79	0.64
1:A:367:GLY:O	1:A:371:VAL:HG23	1.97	0.64
1:A:310:VAL:HG23	1:A:312:LEU:H	1.62	0.64
1:A:79:PRO:HB3	1:A:121:ALA:HB1	1.80	0.64
1:A:365:LEU:HD13	1:A:388:VAL:HG13	1.80	0.64
1:B:177:LEU:HD21	1:B:391:ARG:HD2	1.81	0.63
1:B:12:ASP:HB3	1:B:18:ARG:HB2	1.80	0.63
1:B:192:ASP:HA	1:B:210:ASP:HA	1.80	0.63
1:A:365:LEU:CD1	1:A:388:VAL:HG13	2.29	0.63
1:A:295:PHE:HE1	1:A:360:ALA:HA	1.63	0.63
1:B:10:ILE:HD11	1:B:25:LEU:HD12	1.81	0.62
1:B:296:VAL:CG1	1:B:299:GLN:O	2.47	0.62
1:A:164:MSE:SE	1:A:183:ILE:HD11	2.49	0.62
1:B:270:LEU:HA	1:B:285:ILE:HG22	1.81	0.62
1:B:279:ASN:OD1	1:B:391:ARG:NH1	2.32	0.62
1:B:85:GLY:H	1:B:106:LYS:HE2	1.64	0.62
1:A:197:PHE:HE1	1:A:233:LEU:HD22	1.62	0.62
1:B:254:ILE:O	1:B:258:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:O	1:B:371:VAL:HG22	2.00	0.62
1:A:231:ARG:HD3	1:A:231:ARG:O	1.99	0.61
1:A:242:LEU:HD12	1:A:242:LEU:O	2.00	0.61
1:A:197:PHE:CE1	1:A:233:LEU:HD22	2.36	0.60
1:B:10:ILE:HA	1:B:54:ILE:O	2.02	0.60
1:B:52:LEU:HD13	1:B:79:PRO:HB2	1.83	0.60
1:B:11:ILE:HG22	1:B:62:ILE:HD12	1.84	0.60
1:A:270:LEU:HD22	1:A:285:ILE:HD12	1.84	0.60
1:B:82:VAL:HG11	1:B:95:ALA:HB1	1.84	0.60
1:A:166:MSE:SE	1:A:223:VAL:HA	2.52	0.59
1:A:368:LEU:HD12	1:A:369:ARG:H	1.65	0.59
1:B:332:SER:HB3	1:B:369:ARG:NH2	2.17	0.59
1:B:341:VAL:HA	1:B:354:LEU:HD13	1.83	0.59
1:A:5:SER:HB3	1:A:29:ASN:O	2.03	0.59
1:A:115:GLU:HB3	1:A:119:ARG:HH12	1.67	0.59
1:B:364:THR:HA	1:B:369:ARG:NH2	2.17	0.59
1:B:39:LEU:HD11	1:B:43:GLN:HE21	1.66	0.59
1:A:291:LEU:CG	1:A:302:TYR:CD1	2.85	0.59
1:A:168:PRO:HG3	1:A:195:ASP:OD2	2.03	0.59
1:B:307:GLY:C	1:B:309:PRO:HD3	2.22	0.59
1:B:363:GLY:O	1:B:364:THR:HG22	2.03	0.59
1:A:52:LEU:HD13	1:A:79:PRO:HB2	1.85	0.59
1:A:108:LEU:HD13	1:A:108:LEU:H	1.68	0.59
1:A:292:PRO:HG2	1:A:303:LEU:HB2	1.85	0.58
1:A:224:LEU:O	1:A:228:MSE:HG2	2.03	0.58
1:A:152:LEU:O	1:A:156:GLN:HG2	2.03	0.58
1:B:244:GLU:HG3	1:B:245:PHE:CD2	2.39	0.58
1:A:57:LEU:HD22	1:A:91:ASP:HB3	1.85	0.58
1:B:224:LEU:HA	1:B:227:PHE:HB3	1.86	0.58
1:A:162:VAL:HG11	1:B:220:PHE:HD1	1.69	0.58
1:A:57:LEU:HD12	1:A:57:LEU:O	2.04	0.57
1:B:189:LEU:O	1:B:214:HIS:HB2	2.03	0.57
1:B:68:ILE:HG23	1:B:80:ILE:HD12	1.86	0.57
1:B:268:THR:HB	1:B:287:GLY:HA3	1.87	0.57
1:B:82:VAL:HG22	1:B:102:ASP:O	2.05	0.57
1:A:108:LEU:O	1:A:108:LEU:HD22	2.05	0.57
1:B:354:LEU:N	1:B:355:PRO:CD	2.67	0.57
1:A:115:GLU:HB3	1:A:119:ARG:NH1	2.20	0.56
1:A:110:ASP:O	1:A:113:VAL:HG22	2.05	0.56
1:A:89:MSE:O	1:A:93:VAL:HG22	2.04	0.56
1:B:295:PHE:HB3	1:B:330:SER:OG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:O	1:A:19:GLU:HB2	2.07	0.55
1:A:387:LEU:HD23	1:A:388:VAL:N	2.22	0.55
1:B:295:PHE:HB2	1:B:364:THR:HB	1.89	0.55
1:A:231:ARG:O	1:A:235:GLU:N	2.39	0.55
1:B:374:LEU:HD23	1:B:375:ALA:N	2.21	0.55
1:A:108:LEU:CD1	1:A:108:LEU:H	2.20	0.55
1:A:183:ILE:HG22	1:A:385:ALA:HB1	1.89	0.55
1:B:308:LEU:N	1:B:309:PRO:HD3	2.21	0.55
1:A:374:LEU:O	1:A:375:ALA:HB3	2.06	0.54
1:A:138:LEU:HD13	1:B:138:LEU:HA	1.88	0.54
1:B:295:PHE:HE1	1:B:360:ALA:HA	1.71	0.54
1:B:159:GLY:HA3	1:B:189:LEU:HD11	1.88	0.54
1:B:14:ASP:H	1:B:58:ARG:HH22	1.56	0.54
1:A:329:PHE:C	1:A:329:PHE:CD1	2.81	0.54
1:A:291:LEU:HB2	1:A:302:TYR:HE1	0.44	0.53
1:B:295:PHE:HD2	1:B:297:GLU:N	2.05	0.53
1:A:291:LEU:HG	1:A:302:TYR:CD1	2.44	0.53
1:A:166:MSE:HE1	1:A:222:THR:HG23	1.90	0.53
1:B:330:SER:CB	1:B:364:THR:HG21	2.38	0.53
1:B:85:GLY:HA2	1:B:106:LYS:H	1.74	0.53
1:B:251:LEU:HA	1:B:254:ILE:HG22	1.91	0.53
1:A:238:ARG:HG3	1:A:239:ASN:N	2.23	0.52
1:B:96:LEU:HD11	1:B:103:TYR:CD2	2.44	0.52
1:B:274:ILE:HG12	1:B:281:LEU:HD13	1.91	0.52
1:B:330:SER:HB2	1:B:364:THR:CB	2.39	0.52
1:B:329:PHE:CE2	1:B:331:LEU:HB2	2.43	0.52
1:A:296:VAL:O	1:A:297:GLU:HG2	2.10	0.52
1:A:368:LEU:O	1:A:372:PHE:HD2	1.93	0.52
1:B:296:VAL:O	1:B:296:VAL:HG22	2.10	0.51
1:A:354:LEU:N	1:A:355:PRO:CD	2.74	0.51
1:B:354:LEU:N	1:B:355:PRO:HD2	2.25	0.50
1:B:177:LEU:CD2	1:B:391:ARG:HD2	2.41	0.50
1:B:294:LEU:HD12	1:B:330:SER:O	2.11	0.50
1:B:71:ILE:O	1:B:74:THR:HG22	2.11	0.50
1:A:173:SER:HB3	1:A:178:GLU:HA	1.93	0.50
1:A:259:ILE:HG13	1:A:312:LEU:HD12	1.93	0.50
1:B:285:ILE:HG13	1:B:308:LEU:HD22	1.94	0.50
1:A:245:PHE:CE2	1:A:250:VAL:HG21	2.46	0.50
1:A:238:ARG:CG	1:A:239:ASN:N	2.74	0.50
1:B:303:LEU:HD21	1:B:323:MSE:SE	2.62	0.50
1:B:279:ASN:OD1	1:B:325:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HG	1:A:375:ALA:N	2.24	0.50
1:B:296:VAL:O	1:B:297:GLU:HB3	2.12	0.50
1:B:367:GLY:O	1:B:371:VAL:HG13	2.12	0.50
1:B:363:GLY:O	1:B:365:LEU:HG	2.11	0.49
1:A:313:PHE:C	1:A:313:PHE:CD2	2.85	0.49
1:B:261:THR:HB	1:B:263:LEU:HD13	1.94	0.49
1:A:178:GLU:OE2	1:A:180:SER:HB2	2.12	0.49
1:A:58:ARG:O	1:A:62:ILE:HB	2.12	0.49
1:B:330:SER:HB2	1:B:364:THR:HG21	1.94	0.49
1:A:242:LEU:C	1:A:242:LEU:HD12	2.33	0.49
1:B:13:ASP:HB3	1:B:58:ARG:NH1	2.26	0.49
1:A:238:ARG:CG	1:A:239:ASN:H	2.26	0.49
1:B:36:LEU:N	1:B:40:GLN:HG2	2.25	0.49
1:B:160:ARG:HH12	1:B:187:LEU:HA	1.77	0.49
1:B:347:LEU:CD1	1:B:347:LEU:H	2.20	0.49
1:A:378:ALA:O	1:A:379:GLU:CB	2.58	0.49
1:A:225:LEU:CD1	1:A:269:MSE:HE1	2.42	0.49
1:B:218:SER:O	1:B:222:THR:HG23	2.12	0.49
1:A:228:MSE:HE2	1:A:254:ILE:HA	1.95	0.48
1:A:193:PHE:CZ	1:A:195:ASP:HB2	2.48	0.48
1:B:160:ARG:NH1	1:B:185:PRO:HB2	2.27	0.48
1:A:228:MSE:HE1	1:A:257:GLY:HA3	1.94	0.48
1:A:242:LEU:CD2	1:A:246:LYS:HE3	2.43	0.48
1:B:367:GLY:O	1:B:370:GLN:HB3	2.14	0.48
1:B:54:ILE:HG12	1:B:81:ILE:HB	1.95	0.48
1:B:323:MSE:O	1:B:323:MSE:HG3	2.13	0.48
1:B:256:ARG:HA	1:B:259:ILE:HD11	1.96	0.48
1:B:185:PRO:HA	1:B:383:ASP:CG	2.34	0.48
1:A:145:LEU:HD13	1:B:145:LEU:HA	1.94	0.48
1:B:283:TYR:CZ	1:B:303:LEU:HB3	2.49	0.48
1:B:13:ASP:HB3	1:B:58:ARG:NH2	2.28	0.48
1:A:275:ASP:OD1	1:A:277:GLU:HG2	2.14	0.48
1:A:220:PHE:HE2	1:B:159:GLY:HA2	1.73	0.48
1:B:174:ILE:HG13	1:B:175:GLU:HG2	1.96	0.48
1:A:293:VAL:HG13	1:A:300:ALA:HB1	1.96	0.48
1:B:131:ASN:O	1:B:135:ARG:HG3	2.14	0.47
1:B:332:SER:HB3	1:B:369:ARG:CZ	2.44	0.47
1:A:52:LEU:HD12	1:A:53:VAL:H	1.79	0.47
1:A:242:LEU:HB2	1:A:243:PRO:HD2	1.95	0.47
1:A:270:LEU:HD12	1:A:333:LEU:HD22	1.95	0.47
1:B:329:PHE:CZ	1:B:331:LEU:HB2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLU:O	1:B:201:GLU:HG3	2.13	0.47
1:B:228:MSE:SE	1:B:231:ARG:HD3	2.64	0.47
1:B:221:VAL:HG22	1:B:263:LEU:HD23	1.97	0.47
1:A:220:PHE:HD1	1:B:220:PHE:CZ	2.33	0.47
1:A:362:GLY:HA3	1:A:368:LEU:CB	2.45	0.47
1:B:224:LEU:HD12	1:B:225:LEU:N	2.30	0.47
1:A:254:ILE:O	1:A:258:LEU:HG	2.15	0.46
1:A:255:ASN:HD21	1:A:313:PHE:H	1.63	0.46
1:B:9:LEU:HD12	1:B:33:LEU:O	2.15	0.46
1:A:221:VAL:HG13	1:A:263:LEU:HD23	1.98	0.46
1:A:246:LYS:O	1:A:250:VAL:HG23	2.15	0.46
1:A:216:ALA:O	1:A:220:PHE:HB2	2.15	0.46
1:A:168:PRO:CG	1:A:195:ASP:HA	2.46	0.46
1:A:179:PHE:CE1	1:A:389:LEU:HD13	2.50	0.46
1:A:65:LEU:O	1:A:68:ILE:HG22	2.16	0.46
1:B:6:ALA:CB	1:B:30:PHE:HE1	2.16	0.46
1:B:186:SER:O	1:B:187:LEU:HB2	2.15	0.46
1:B:231:ARG:HG3	1:B:232:LEU:HD12	1.97	0.46
1:A:347:LEU:O	1:A:347:LEU:HD12	2.16	0.46
1:B:325:LEU:HA	1:B:326:PRO:HD3	1.85	0.46
1:B:183:ILE:O	1:B:185:PRO:HD3	2.16	0.45
1:A:131:ASN:HA	1:A:134:TYR:HD2	1.81	0.45
1:B:171:PRO:HB3	1:B:180:SER:OG	2.16	0.45
1:B:68:ILE:O	1:B:72:ARG:HG2	2.15	0.45
1:A:293:VAL:CG1	1:A:300:ALA:HB1	2.47	0.45
1:A:228:MSE:CE	1:A:254:ILE:HA	2.46	0.45
1:A:331:LEU:HD12	1:A:332:SER:H	1.82	0.45
1:A:368:LEU:O	1:A:372:PHE:CD2	2.69	0.45
1:B:85:GLY:HA2	1:B:106:LYS:N	2.31	0.45
1:A:245:PHE:HE2	1:A:250:VAL:HG21	1.81	0.45
1:B:11:ILE:HG12	1:B:35:ALA:HB3	1.98	0.45
1:B:49:GLN:N	1:B:50:PRO:HD3	2.30	0.45
1:B:369:ARG:NH1	1:B:388:VAL:HG22	2.32	0.45
1:A:9:LEU:HD12	1:A:33:LEU:O	2.17	0.45
1:A:285:ILE:HG13	1:A:305:GLY:CA	2.42	0.45
1:A:374:LEU:CG	1:A:375:ALA:N	2.80	0.45
1:A:242:LEU:C	1:A:242:LEU:CD1	2.85	0.45
1:B:11:ILE:HB	1:B:55:CYS:HB2	1.99	0.45
1:A:362:GLY:HA3	1:A:368:LEU:HB3	1.99	0.45
1:B:106:LYS:HA	1:B:108:LEU:N	2.32	0.44
1:B:353:SER:C	1:B:355:PRO:HD2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:SER:HB3	1:A:385:ALA:N	2.28	0.44
1:A:42:LEU:HD21	1:A:70:ARG:NE	2.31	0.44
1:B:285:ILE:HG13	1:B:308:LEU:CD2	2.48	0.44
1:A:48:GLU:O	1:A:50:PRO:HD3	2.17	0.44
1:A:219:ALA:HA	1:A:222:THR:HG22	1.99	0.44
1:B:184:ILE:N	1:B:184:ILE:HD12	2.33	0.44
1:B:194:VAL:HG21	1:B:387:LEU:HB2	1.99	0.44
1:B:56:ASP:HA	1:B:83:LEU:HB2	2.00	0.44
1:A:194:VAL:HB	1:A:208:LEU:HD13	2.00	0.43
1:A:168:PRO:HG3	1:A:195:ASP:HA	1.99	0.43
1:B:307:GLY:O	1:B:308:LEU:HD23	2.18	0.43
1:B:365:LEU:HB2	1:B:368:LEU:HD13	1.99	0.43
1:A:36:LEU:H	1:A:36:LEU:HD12	1.83	0.43
1:B:185:PRO:HA	1:B:383:ASP:HB3	1.99	0.43
1:A:291:LEU:CG	1:A:302:TYR:CE1	2.86	0.43
1:B:352:ALA:C	1:B:355:PRO:HD2	2.38	0.43
1:B:228:MSE:HA	1:B:231:ARG:HG2	2.01	0.43
1:B:105:ILE:N	1:B:105:ILE:HD12	2.33	0.43
1:A:22:ALA:CB	1:A:34:GLN:HE21	2.31	0.43
1:A:45:PHE:CD1	1:A:50:PRO:HD2	2.53	0.43
1:B:57:LEU:HD13	1:B:84:SER:HB3	2.01	0.43
1:B:325:LEU:HD22	1:B:329:PHE:CE1	2.54	0.43
1:A:36:LEU:HB2	1:A:40:GLN:NE2	2.33	0.43
1:A:173:SER:HA	1:A:177:LEU:O	2.18	0.43
1:A:162:VAL:HG11	1:B:220:PHE:CD1	2.49	0.42
1:A:131:ASN:O	1:A:135:ARG:HG3	2.19	0.42
1:B:221:VAL:O	1:B:224:LEU:HG	2.19	0.42
1:A:11:ILE:HG12	1:A:35:ALA:HB3	2.01	0.42
1:A:330:SER:OG	1:A:365:LEU:HD21	2.20	0.42
1:A:57:LEU:HD13	1:A:91:ASP:OD2	2.20	0.42
1:A:268:THR:C	1:A:289:LEU:HD21	2.40	0.42
1:B:341:VAL:HA	1:B:354:LEU:CD1	2.49	0.42
1:B:257:GLY:O	1:B:261:THR:HG23	2.18	0.42
1:A:8:LEU:CD2	1:A:52:LEU:HB3	2.49	0.42
1:A:291:LEU:HD12	1:A:303:LEU:O	2.19	0.42
1:A:36:LEU:N	1:A:36:LEU:HD12	2.35	0.42
1:A:167:LEU:HA	1:A:168:PRO:HD3	1.88	0.42
1:B:96:LEU:HA	1:B:100:ALA:HB3	2.01	0.42
1:B:82:VAL:O	1:B:103:TYR:HA	2.20	0.42
1:B:219:ALA:O	1:B:223:VAL:HG13	2.20	0.42
1:A:295:PHE:N	1:A:330:SER:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLY:HA3	1:A:384:ILE:HG22	2.02	0.41
1:B:330:SER:HB3	1:B:364:THR:HG21	2.02	0.41
1:A:108:LEU:HD23	1:A:110:ASP:O	2.21	0.41
1:B:246:LYS:HA	1:B:247:PRO:HD3	1.86	0.41
1:A:329:PHE:HD1	1:A:330:SER:N	2.17	0.41
1:A:183:ILE:HG22	1:A:385:ALA:CB	2.50	0.41
1:A:246:LYS:HG3	1:A:249:GLU:HB2	2.02	0.41
1:A:36:LEU:HB2	1:A:40:GLN:HE22	1.86	0.41
1:B:52:LEU:HD12	1:B:53:VAL:H	1.85	0.41
1:A:295:PHE:CB	1:A:330:SER:HB3	2.26	0.41
1:A:242:LEU:HD13	1:A:244:GLU:C	2.41	0.41
1:B:199:VAL:O	1:B:200:ASP:HB3	2.21	0.41
1:A:250:VAL:O	1:A:254:ILE:HD13	2.19	0.41
1:B:11:ILE:HA	1:B:35:ALA:HB3	2.03	0.41
1:A:28:SER:O	1:A:29:ASN:HB2	2.21	0.41
1:B:374:LEU:HD23	1:B:375:ALA:H	1.83	0.41
1:A:170:THR:HA	1:A:171:PRO:HA	1.79	0.41
1:B:11:ILE:CD1	1:B:41:GLY:HA3	2.51	0.41
1:B:170:THR:HG23	1:B:180:SER:HA	2.03	0.40
1:B:114:LEU:O	1:B:118:VAL:HG23	2.21	0.40
1:A:374:LEU:O	1:A:375:ALA:CB	2.69	0.40
1:A:211:VAL:HA	1:A:267:VAL:HG22	2.03	0.40
1:B:269:MSE:O	1:B:270:LEU:HD23	2.21	0.40
1:B:57:LEU:CD2	1:B:91:ASP:OD2	2.69	0.40
1:B:57:LEU:HD21	1:B:91:ASP:OD2	2.21	0.40
1:B:174:ILE:C	1:B:175:GLU:HG2	2.42	0.40
1:B:374:LEU:O	1:B:375:ALA:HB3	2.21	0.40
1:A:209:ALA:HB2	1:A:225:LEU:HD21	2.02	0.40
1:B:200:ASP:C	1:B:202:ARG:H	2.25	0.40
1:A:111:LEU:HD12	1:A:111:LEU:N	2.37	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:306:ARG:NH2	1:B:5:SER:OG[1_455]	1.78	0.42

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	350/394 (89%)	327 (93%)	22 (6%)	1 (0%)	46	82
1	B	356/394 (90%)	334 (94%)	19 (5%)	3 (1%)	24	67
All	All	706/788 (90%)	661 (94%)	41 (6%)	4 (1%)	30	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	B	296	VAL
1	B	364	THR
1	B	330	SER

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	291/323 (90%)	288 (99%)	3 (1%)	82	93
1	B	285/323 (88%)	284 (100%)	1 (0%)	93	97
All	All	576/646 (89%)	572 (99%)	4 (1%)	88	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	302	TYR
1	B	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	40	GLN
1	A	253	HIS
1	B	34	GLN
1	B	43	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 carbohydrates 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 (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	359/394 (91%)	0.53	39 (10%)	7	7	34, 98, 190, 346	0
1	B	365/394 (92%)	0.72	48 (13%)	4	4	44, 106, 200, 299	0
All	All	724/788 (91%)	0.63	87 (12%)	6	6	34, 102, 198, 346	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	ALA	12.1
1	B	102	ASP	10.3
1	B	204	VAL	9.2
1	B	100	ALA	8.7
1	A	245	PHE	6.3
1	B	173	SER	5.9
1	B	32	VAL	5.7
1	B	229	THR	4.8
1	B	203	ARG	4.8
1	A	197	PHE	4.5
1	A	296	VAL	4.5
1	A	272	GLY	4.4
1	A	310	VAL	4.4
1	A	99	GLY	4.2
1	A	329	PHE	4.2
1	B	346	THR	4.2
1	A	214	HIS	4.1
1	B	187	LEU	4.1
1	A	271	GLY	4.0
1	B	54	ILE	3.9
1	A	177	LEU	3.8
1	A	209	ALA	3.8
1	A	334	PHE	3.8
1	A	225	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	9	LEU	3.6
1	A	333	LEU	3.4
1	B	331	LEU	3.4
1	B	345	ALA	3.4
1	B	99	GLY	3.3
1	B	344	GLY	3.2
1	B	205	ALA	3.2
1	B	55	CYS	3.2
1	A	267	VAL	3.2
1	B	174	ILE	3.2
1	A	76	SER	3.1
1	A	208	LEU	3.1
1	B	176	GLY	3.1
1	B	96	LEU	3.1
1	B	329	PHE	3.1
1	A	328	SER	3.0
1	B	305	GLY	3.0
1	B	81	ILE	3.0
1	B	177	LEU	3.0
1	B	80	ILE	2.9
1	A	206	PHE	2.9
1	A	52	LEU	2.8
1	A	365	LEU	2.8
1	B	232	LEU	2.8
1	A	332	SER	2.8
1	A	229	THR	2.7
1	A	179	PHE	2.7
1	A	370	GLN	2.7
1	A	351	GLU	2.7
1	B	387	LEU	2.7
1	B	381	PRO	2.7
1	B	325	LEU	2.6
1	A	273	VAL	2.6
1	A	207	TYR	2.6
1	A	194	VAL	2.6
1	A	266	HIS	2.6
1	B	92	ALA	2.6
1	B	44	ILE	2.5
1	B	53	VAL	2.5
1	B	206	PHE	2.5
1	B	98	LEU	2.4
1	B	33	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	276	LEU	2.4
1	B	123	ASP	2.4
1	A	297	GLU	2.4
1	B	8	LEU	2.4
1	A	316	ALA	2.4
1	B	274	ILE	2.3
1	B	45	PHE	2.3
1	A	369	ARG	2.2
1	B	10	ILE	2.2
1	A	263	LEU	2.2
1	B	172	TRP	2.2
1	A	81	ILE	2.2
1	A	264	GLY	2.1
1	A	114	LEU	2.1
1	A	270	LEU	2.1
1	A	79	PRO	2.1
1	B	284	SER	2.1
1	B	270	LEU	2.1
1	B	40	GLN	2.0
1	B	347	LEU	2.0
1	B	103	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.