Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 01:36 PM EDT

PDB ID	:	8SAP
Title	:	Crystal structure of class III lanthipeptide synthetase ThurKC
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Deposited on	:	2023-04-01
Resolution	:	2.52 Å(reported)

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

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

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

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

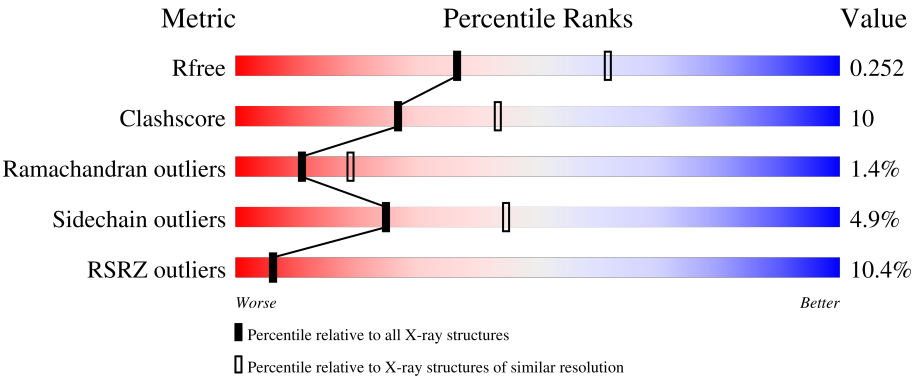
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	875	16% 74% 18% · 5%
1	B	875	4% 73% 21% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13906 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 Class III lanthionine synthetase LanKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6723	4322	1109	1270	22			
1	B	842	Total	C	N	O	S	0	0	0
			6799	4368	1123	1285	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A6H0TJ16
A	-1	ASN	-	expression tag	UNP A0A6H0TJ16
A	0	ALA	-	expression tag	UNP A0A6H0TJ16
B	-2	SER	-	expression tag	UNP A0A6H0TJ16
B	-1	ASN	-	expression tag	UNP A0A6H0TJ16
B	0	ALA	-	expression tag	UNP A0A6H0TJ16

- Molecule 2 is water.

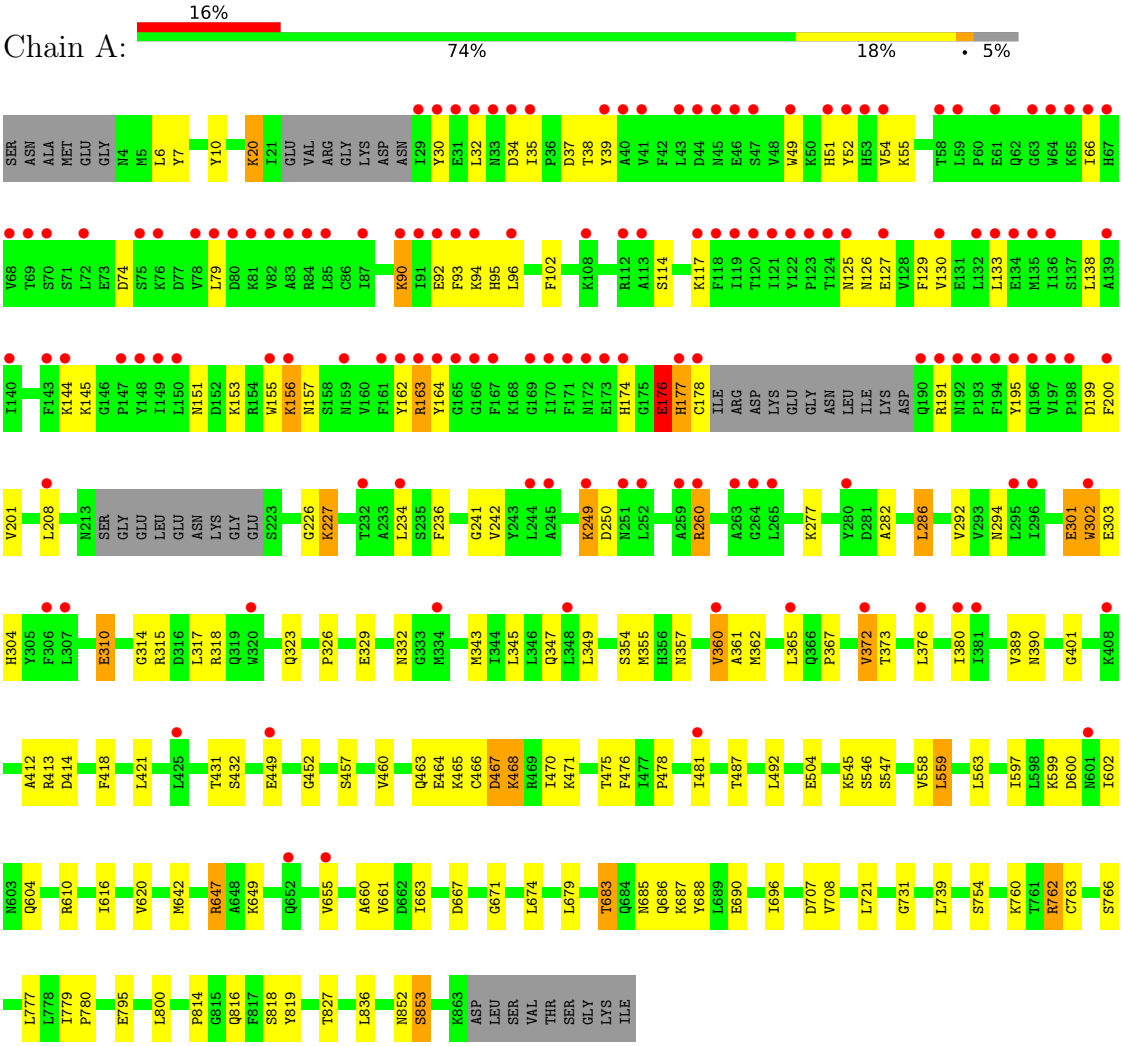
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	224	Total	O	0	0
			224	224		

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.

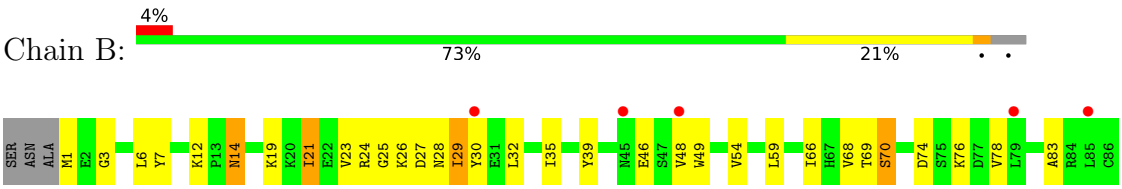
• Molecule 1: Class III lanthionine synthetase LanKC

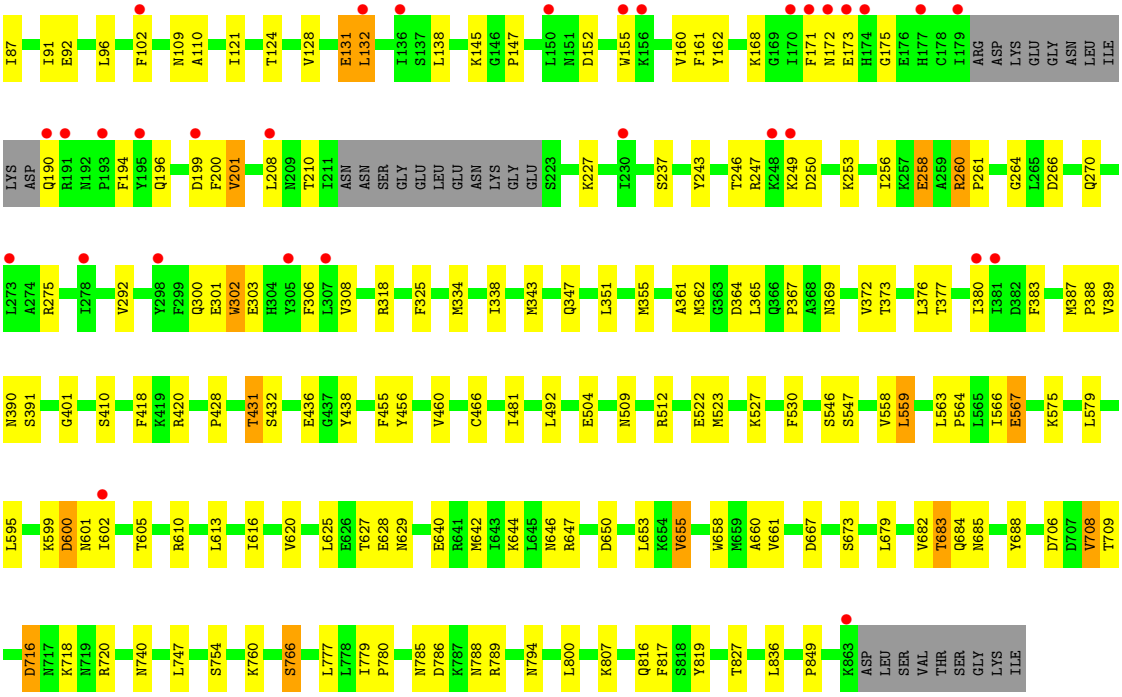
Chain A:



• Molecule 1: Class III lanthionine synthetase LanKC

Chain B:




I87 I91 E92 L96 F102 N109 A110 I121 T124 V128 E131 L132 I136 S137 L138 K145 G146 P147 L150 N151 D152 W155 K156 V160 F161 Y162 K168 G169 I170 F171 N172 E173 H174 G175 E176 H177 C178 I179 ARG ASP LYS GLU GLY ASN LEU ILE
LYS ASP Q190 R191 N192 P193 F194 Y195 Q196 D199 F200 V201 L208 N209 T210 I211 ASN ASN SER GLY GLU LEU GLU ASN LYS GLY GLU S223 K227 I230 S237 Y243 T246 R247 K248 K249 D250 K253 I256 K257 E258 A259 R260 P261 G264 L265 D266 Q270
L273 A274 R275 I278 V292 Y298 F299 Q300 E301 W302 E303 H304 Y305 F306 L307 V308 R318 F325 M334 I338 M343 Q347 L351 M355 A361 M362 G363 D364 L365 Q366 P367 A368 N369 V372 T373 L376 T377 I380 I381 D382 F383 M387 P388 V389
N390 S391 G401 S410 F418 K419 R420 P428 T431 S432 E436 G437 Y438 F455 Y456 V460 C466 I481 L492 E504 N509 R512 E522 M523 K527 F530 S546 S547 V558 L559 L563 P564 L565 I566 E567 K575 L579
L595 K599 D600 N601 I602 T605 R610 L613 I616 V620 L625 E626 T627 E628 N629 E640 R641 M642 I643 K644 L645 N646 R647 D650 L653 K654 V655 W658 M659 A660 V661 D667 S673 L679 V682 T683 Q684 N685 Y688 D706 D707 V708 T709
D716 N717 K718 N719 R720 N740 L747 S754 K760 S766 L777 L778 I779 P780 N785 D786 K787 N788 R789 N794 L800 K807 Q816 F817 S818 Y819 T827 L836 P849 K863 ASP LEU SER VAL THR SER GLY LYS ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.30Å 230.23Å 84.38Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	115.11 – 2.52 115.12 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.9 (115.11-2.52) 98.9 (115.12-2.52)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.250 0.191 , 0.252	Depositor DCC
R_{free} test set	3422 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	61.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13906	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.32	0/6855	0.68	0/9250
1	B	0.33	0/6932	0.68	1/9351 (0.0%)
All	All	0.33	0/13787	0.68	1/18601 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	258	GLU	CB-CA-C	-5.23	99.93	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	ASN	Peptide

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	6723	0	6717	120	0
1	B	6799	0	6807	157	0
2	A	160	0	0	9	0
2	B	224	0	0	19	0
All	All	13906	0	13524	276	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 10.

All (276) 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:647:ARG:HG2	1:A:647:ARG:HH11	1.20	1.03
1:B:605:THR:HA	1:B:646:ASN:HD21	1.27	0.99
1:B:431:THR:HG21	1:B:436:GLU:OE1	1.63	0.96
1:A:286:LEU:CD1	1:A:292:VAL:HG11	1.98	0.93
1:B:28:ASN:O	1:B:30:TYR:N	2.05	0.90
1:B:683:THR:CG2	1:B:685:ASN:HB3	2.04	0.88
1:A:683:THR:CG2	1:A:685:ASN:HB3	2.06	0.84
1:A:471:LYS:HD3	1:A:476:PHE:O	1.76	0.84
1:B:70:SER:HB2	1:B:78:VAL:HG11	1.63	0.81
1:B:716:ASP:HB3	1:B:718:LYS:H	1.47	0.79
1:B:605:THR:HA	1:B:646:ASN:ND2	1.98	0.78
1:A:647:ARG:HG2	1:A:647:ARG:NH1	1.95	0.75
1:A:226:GLY:HA2	2:A:990:HOH:O	1.86	0.75
1:B:628:GLU:N	2:B:904:HOH:O	2.18	0.74
1:B:760:LYS:HE2	2:B:1025:HOH:O	1.86	0.74
1:B:301:GLU:O	2:B:902:HOH:O	2.05	0.74
1:B:627:THR:O	1:B:627:THR:OG1	2.04	0.74
1:A:365:LEU:HD23	1:A:414:ASP:O	1.88	0.73
1:B:70:SER:CB	1:B:78:VAL:HG11	2.18	0.72
1:A:286:LEU:HD13	1:A:292:VAL:HG21	1.72	0.72
1:B:401:GLY:HA2	1:B:431:THR:O	1.89	0.72
1:B:69:THR:HG22	1:B:70:SER:N	2.05	0.71
1:B:683:THR:HG23	1:B:685:ASN:HB3	1.73	0.70
1:A:286:LEU:HD23	1:A:360:VAL:HG11	1.72	0.70
1:A:487:THR:O	2:A:901:HOH:O	2.10	0.69
1:B:338:ILE:HG23	1:B:455:PHE:CD1	2.28	0.69
1:B:683:THR:HG22	1:B:685:ASN:H	1.58	0.69
1:B:83:ALA:O	1:B:87:ILE:HG12	1.94	0.68
1:A:286:LEU:HD12	1:A:292:VAL:HG11	1.75	0.68
1:A:286:LEU:HD13	1:A:292:VAL:HG11	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:THR:HG23	1:A:685:ASN:HB3	1.73	0.67
1:B:3:GLY:O	1:B:6:LEU:HB2	1.93	0.67
1:A:114:SER:HA	1:A:117:LYS:HE2	1.74	0.67
1:A:421:LEU:HD23	1:A:421:LEU:O	1.95	0.67
1:A:602:ILE:HG23	1:A:642:MET:HE3	1.75	0.67
1:B:74:ASP:O	1:B:78:VAL:HG12	1.94	0.67
1:B:456:TYR:CZ	1:B:460:VAL:HG21	2.30	0.67
1:A:176:GLU:O	1:A:177:HIS:HB2	1.94	0.67
1:A:457:SER:HA	1:A:460:VAL:HG12	1.76	0.67
1:A:545:LYS:NZ	1:B:794:ASN:OD1	2.28	0.66
1:A:163:ARG:HD3	1:A:164:TYR:H	1.60	0.66
1:A:7:TYR:OH	1:A:816:GLN:HG3	1.97	0.65
1:A:401:GLY:HA2	1:A:431:THR:O	1.96	0.65
1:A:683:THR:HG22	1:A:685:ASN:H	1.61	0.65
1:B:504:GLU:HG2	1:B:547:SER:OG	1.97	0.65
1:B:567:GLU:H	1:B:567:GLU:CD	1.97	0.65
1:A:355:MET:HE1	1:A:380:ILE:HD12	1.78	0.65
1:A:655:VAL:HG13	1:A:660:ALA:HB3	1.78	0.64
1:A:465:LYS:O	2:A:902:HOH:O	2.15	0.63
1:A:683:THR:HG21	1:A:688:TYR:CD2	2.34	0.63
1:A:282:ALA:O	1:A:286:LEU:HG	1.98	0.63
1:B:7:TYR:OH	1:B:816:GLN:HG3	1.97	0.63
1:B:12:LYS:HA	1:B:21:ILE:HG22	1.81	0.63
1:B:373:THR:HG22	1:B:377:THR:H	1.64	0.63
1:B:627:THR:C	2:B:904:HOH:O	2.36	0.63
1:A:604:GLN:HG2	1:A:642:MET:HE3	1.81	0.62
1:B:12:LYS:HA	1:B:21:ILE:CG2	2.29	0.62
1:B:69:THR:HG22	1:B:70:SER:H	1.63	0.62
1:B:523:MET:HE2	1:B:658:TRP:CZ3	2.34	0.62
1:B:683:THR:HG21	1:B:688:TYR:CD2	2.35	0.61
1:A:679:LEU:O	1:A:683:THR:HB	2.01	0.60
1:A:286:LEU:HD23	1:A:360:VAL:CG1	2.29	0.60
1:A:176:GLU:OE1	1:A:178:CYS:HB3	2.01	0.59
1:B:343:MET:HG2	1:B:347:GLN:HE21	1.67	0.59
1:A:413:ARG:HD3	2:A:1031:HOH:O	2.02	0.59
1:B:243:TYR:HE2	1:B:258:GLU:HG3	1.66	0.59
1:B:1:MET:HG3	1:B:3:GLY:H	1.68	0.59
1:B:91:ILE:HG13	1:B:132:LEU:HD21	1.84	0.59
1:B:351:LEU:HD21	1:B:380:ILE:HD12	1.85	0.59
1:B:786:ASP:OD1	1:B:789:ARG:NH1	2.35	0.58
1:B:679:LEU:O	1:B:683:THR:HB	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PHE:HB3	1:B:175:GLY:HA2	1.85	0.58
1:A:687:LYS:NZ	2:A:907:HOH:O	2.35	0.58
1:A:130:VAL:HG12	1:A:208:LEU:HD21	1.85	0.58
1:A:354:SER:O	1:A:357:ASN:HB2	2.03	0.58
1:B:785:ASN:OD1	1:B:788:ASN:HB2	2.04	0.58
1:A:343:MET:HG2	1:A:347:GLN:HE21	1.70	0.56
1:B:69:THR:CG2	1:B:70:SER:H	2.19	0.56
1:B:655:VAL:HG13	1:B:660:ALA:HB3	1.88	0.56
1:B:162:TYR:O	2:B:903:HOH:O	2.17	0.55
1:B:355:MET:HE2	1:B:383:PHE:HZ	1.69	0.55
1:B:69:THR:CG2	1:B:70:SER:N	2.69	0.55
1:B:303:GLU:HB3	2:B:921:HOH:O	2.05	0.55
1:B:355:MET:CE	1:B:380:ILE:HD13	2.36	0.55
1:B:523:MET:HE2	1:B:658:TRP:HZ3	1.72	0.55
1:A:294:ASN:H	1:A:310:GLU:HG2	1.72	0.55
1:A:301:GLU:O	1:A:302:TRP:C	2.45	0.55
1:B:388:PRO:O	1:B:391:SER:HB3	2.06	0.54
1:A:610:ARG:HD2	1:A:667:ASP:OD2	2.07	0.54
1:A:816:GLN:HG2	1:A:827:THR:HG21	1.89	0.54
1:B:246:THR:HG22	1:B:253:LYS:HD2	1.90	0.54
1:A:355:MET:CE	1:A:380:ILE:HD12	2.36	0.54
1:B:69:THR:HG23	2:B:1038:HOH:O	2.07	0.54
1:B:683:THR:HG21	1:B:688:TYR:CE2	2.42	0.54
1:B:740:ASN:HD21	1:B:747:LEU:H	1.55	0.54
1:B:373:THR:HG22	1:B:377:THR:HB	1.90	0.54
1:A:683:THR:HG23	1:A:685:ASN:CB	2.37	0.54
1:B:334:MET:O	1:B:338:ILE:HG13	2.08	0.54
1:B:389:VAL:O	1:B:390:ASN:HB2	2.08	0.53
1:B:301:GLU:O	1:B:302:TRP:C	2.45	0.53
1:B:318:ARG:HG2	1:B:367:PRO:HB2	1.91	0.53
1:B:627:THR:O	1:B:629:ASN:N	2.39	0.53
1:A:558:VAL:O	1:A:559:LEU:HB3	2.09	0.53
1:A:10:TYR:CZ	1:A:20:LYS:HE3	2.43	0.52
1:A:777:LEU:HD11	1:A:800:LEU:HD13	1.90	0.52
1:B:683:THR:HG23	1:B:685:ASN:CB	2.40	0.52
1:B:266:ASP:HB2	1:B:270:GLN:H	1.74	0.52
1:B:647:ARG:NE	2:B:901:HOH:O	2.04	0.52
1:A:129:PHE:HZ	1:A:162:TYR:HB2	1.74	0.52
1:B:355:MET:HE3	1:B:380:ILE:HD13	1.91	0.52
1:A:389:VAL:O	1:A:390:ASN:HB2	2.10	0.52
1:B:816:GLN:HG2	1:B:827:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:THR:HG21	1:B:147:PRO:O	2.09	0.52
1:A:760:LYS:HD3	1:A:795:GLU:OE2	2.10	0.52
1:B:6:LEU:HD12	2:B:971:HOH:O	2.10	0.52
1:B:509:ASN:N	2:B:905:HOH:O	2.20	0.51
1:A:683:THR:HG21	1:A:688:TYR:CE2	2.45	0.51
1:A:604:GLN:HG2	1:A:642:MET:CE	2.41	0.51
1:B:264:GLY:O	1:B:275:ARG:NH2	2.43	0.51
1:B:627:THR:CA	2:B:904:HOH:O	2.59	0.51
1:B:194:PHE:HE1	1:B:196:GLN:HE21	1.57	0.51
1:B:610:ARG:HD2	1:B:667:ASP:OD2	2.10	0.51
1:B:24:ARG:O	1:B:26:LYS:N	2.44	0.51
1:B:32:LEU:HB3	1:B:35:ILE:HD11	1.92	0.51
1:B:200:PHE:O	1:B:201:VAL:HG12	2.10	0.51
1:A:153:LYS:HG3	1:A:195:TYR:CZ	2.46	0.50
1:B:76:LYS:HD3	1:B:76:LYS:H	1.75	0.50
1:A:683:THR:HG21	1:A:688:TYR:HD2	1.75	0.50
1:B:39:TYR:CZ	1:B:54:VAL:HG22	2.46	0.50
1:B:145:LYS:NZ	2:B:921:HOH:O	2.43	0.50
1:B:640:GLU:OE2	1:B:644:LYS:HG2	2.12	0.50
1:B:351:LEU:CD2	1:B:380:ILE:CD1	2.89	0.50
1:A:138:LEU:HB3	2:A:921:HOH:O	2.10	0.50
1:A:54:VAL:CG2	1:A:92:GLU:HA	2.42	0.50
1:B:647:ARG:NH1	2:B:915:HOH:O	2.35	0.50
1:A:852:ASN:O	1:A:853:SER:CB	2.60	0.49
1:B:627:THR:C	1:B:629:ASN:H	2.14	0.49
1:A:432:SER:HB3	1:A:819:TYR:HA	1.94	0.49
1:A:260:ARG:HB3	1:A:304:HIS:CD2	2.47	0.49
1:A:852:ASN:O	1:A:853:SER:HB3	2.12	0.49
1:A:616:ILE:O	1:A:620:VAL:HG23	2.12	0.49
1:B:152:ASP:HB3	1:B:161:PHE:HB3	1.94	0.49
1:A:349:LEU:HD21	1:A:465:LYS:HE3	1.94	0.49
1:B:19:LYS:HE3	1:B:512:ARG:NH2	2.27	0.49
1:A:314:GLY:HA3	1:A:373:THR:HA	1.94	0.48
1:A:260:ARG:HB3	1:A:304:HIS:NE2	2.28	0.48
1:B:109:ASN:HB3	1:B:237:SER:HB2	1.96	0.48
1:B:602:ILE:HD11	1:B:616:ILE:HD13	1.93	0.48
1:B:616:ILE:O	1:B:620:VAL:HG23	2.15	0.47
1:A:39:TYR:CZ	1:A:54:VAL:HG22	2.49	0.47
1:A:504:GLU:HG2	1:A:547:SER:OG	2.15	0.47
1:B:355:MET:HE2	1:B:383:PHE:CZ	2.49	0.47
1:B:563:LEU:HB3	1:B:564:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD11	1:B:92:GLU:HG3	1.97	0.47
1:B:96:LEU:HD13	1:B:102:PHE:HA	1.97	0.47
1:B:23:VAL:HG11	2:B:952:HOH:O	2.15	0.46
1:A:125:ASN:O	1:A:127:GLU:N	2.47	0.46
1:B:563:LEU:HA	1:B:566:ILE:HD12	1.97	0.46
1:B:256:ILE:HG12	1:B:308:VAL:HG22	1.98	0.46
1:A:30:TYR:HB3	1:A:79:LEU:HD22	1.96	0.46
1:A:343:MET:O	1:A:347:GLN:HG3	2.16	0.46
1:B:355:MET:CE	1:B:383:PHE:HZ	2.29	0.46
1:A:779:ILE:HB	1:A:780:PRO:HD3	1.98	0.46
1:B:27:ASP:HB3	1:B:29:ILE:HB	1.97	0.46
1:A:602:ILE:CG2	1:A:642:MET:HE3	2.45	0.46
1:A:731:GLY:HA3	2:A:976:HOH:O	2.15	0.46
1:B:301:GLU:HB2	1:B:306:PHE:CE1	2.51	0.46
1:B:683:THR:HG21	1:B:688:TYR:HD2	1.80	0.45
1:A:372:VAL:HG13	1:A:376:LEU:HA	1.98	0.45
1:A:647:ARG:HH11	1:A:647:ARG:CG	2.07	0.45
1:B:124:THR:HG22	1:B:128:VAL:HG11	1.98	0.45
1:B:128:VAL:HA	1:B:131:GLU:HB3	1.97	0.45
1:B:777:LEU:HD11	1:B:800:LEU:HD13	1.98	0.45
1:A:52:TYR:HB2	1:A:93:PHE:O	2.16	0.45
1:A:418:PHE:HD2	1:A:466:CYS:SG	2.39	0.45
1:B:559:LEU:O	1:B:563:LEU:N	2.49	0.45
1:B:610:ARG:NH2	2:B:925:HOH:O	2.46	0.45
1:B:625:LEU:HD21	1:B:682:VAL:HG12	1.97	0.45
1:B:779:ILE:HB	1:B:780:PRO:HD3	1.98	0.45
1:B:716:ASP:HB2	1:B:720:ARG:H	1.82	0.45
1:A:599:LYS:O	1:A:600:ASP:C	2.54	0.45
1:B:766:SER:HG	1:B:817:PHE:H	1.63	0.45
1:A:558:VAL:O	1:A:559:LEU:CB	2.65	0.45
1:A:671:GLY:O	1:A:674:LEU:HB2	2.17	0.45
1:B:708:VAL:HB	1:B:709:THR:H	1.68	0.45
1:A:117:LYS:NZ	1:A:151:ASN:HD22	2.15	0.45
1:A:144:LYS:HB3	1:A:144:LYS:HE2	1.81	0.45
1:A:464:GLU:HA	1:A:467:ASP:HB2	1.98	0.45
1:B:456:TYR:CE1	1:B:460:VAL:HG21	2.51	0.44
1:B:512:ARG:HG2	1:B:527:LYS:HG2	1.99	0.44
1:B:558:VAL:O	1:B:559:LEU:HB3	2.17	0.44
1:B:420:ARG:HE	1:B:431:THR:HG22	1.82	0.44
1:A:176:GLU:OE1	1:A:178:CYS:CB	2.65	0.44
1:A:686:GLN:O	1:A:690:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:HG2	1:B:306:PHE:CE2	2.52	0.44
1:B:351:LEU:CD2	1:B:380:ILE:HD12	2.47	0.44
1:B:418:PHE:HD2	1:B:466:CYS:SG	2.40	0.44
1:B:613:LEU:HD13	1:B:642:MET:HB3	2.00	0.44
1:A:176:GLU:O	1:A:177:HIS:CB	2.62	0.44
1:A:201:VAL:O	1:A:201:VAL:HG13	2.18	0.44
1:A:452:GLY:N	2:A:919:HOH:O	2.50	0.44
1:A:162:TYR:O	1:A:163:ARG:HB2	2.18	0.44
1:A:52:TYR:O	1:A:92:GLU:HG3	2.18	0.44
1:B:128:VAL:HG22	1:B:132:LEU:HD22	2.00	0.44
1:A:389:VAL:O	1:A:390:ASN:CB	2.65	0.43
1:B:647:ARG:NH2	2:B:901:HOH:O	2.51	0.43
1:B:653:LEU:HD21	2:B:915:HOH:O	2.18	0.43
1:B:68:VAL:HG22	1:B:160:VAL:HG22	2.00	0.43
1:B:558:VAL:O	1:B:559:LEU:CB	2.66	0.43
1:B:325:PHE:CE1	1:B:428:PRO:HD3	2.53	0.43
1:B:372:VAL:HG13	1:B:376:LEU:HA	2.01	0.43
1:A:66:ILE:HG12	1:A:133:LEU:HD12	2.01	0.43
1:A:476:PHE:O	1:A:478:PRO:HD3	2.18	0.43
1:B:208:LEU:C	1:B:210:THR:H	2.22	0.43
1:B:128:VAL:HG22	1:B:132:LEU:CD2	2.48	0.43
1:A:49:TRP:CD2	1:A:94:LYS:HE3	2.53	0.43
1:B:387:MET:HE2	1:B:410:SER:HB2	2.01	0.43
1:A:318:ARG:HG3	1:A:367:PRO:HB2	2.00	0.43
1:A:361:ALA:HB2	1:A:389:VAL:HG12	2.00	0.42
1:A:814:PRO:HB2	1:A:818:SER:HA	2.01	0.42
1:B:361:ALA:HB2	1:B:389:VAL:HG12	2.01	0.42
1:B:456:TYR:O	1:B:460:VAL:HG23	2.20	0.42
1:B:530:PHE:CD1	1:B:849:PRO:HB3	2.54	0.42
1:B:706:ASP:HB3	1:B:709:THR:O	2.19	0.42
1:B:373:THR:HG22	1:B:377:THR:CB	2.48	0.42
1:B:432:SER:HB3	1:B:819:TYR:HA	2.00	0.42
1:B:492:LEU:HD22	1:B:836:LEU:HD22	2.01	0.42
1:A:52:TYR:HE2	1:A:95:HIS:HE1	1.68	0.42
1:B:389:VAL:O	1:B:390:ASN:CB	2.68	0.42
1:B:28:ASN:OD1	1:B:28:ASN:N	2.53	0.42
1:B:492:LEU:CD2	1:B:836:LEU:HD22	2.50	0.42
1:A:227:LYS:HD3	1:A:227:LYS:HA	1.90	0.42
1:B:227:LYS:NZ	1:B:247:ARG:HD2	2.35	0.42
1:B:438:TYR:OH	1:B:807:LYS:HE2	2.19	0.42
1:A:236:PHE:HA	1:A:241:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:HD3	1:A:249:LYS:HA	1.85	0.42
1:A:421:LEU:HD23	1:A:421:LEU:C	2.40	0.42
1:A:163:ARG:HG3	1:A:195:TYR:CE1	2.55	0.42
1:B:600:ASP:HB3	1:B:601:ASN:H	1.49	0.42
1:A:55:LYS:NZ	1:A:90:LYS:HD3	2.36	0.41
1:A:292:VAL:HG22	1:A:355:MET:HE2	2.02	0.41
1:B:48:VAL:HG23	1:B:49:TRP:CD1	2.55	0.41
1:B:343:MET:O	1:B:347:GLN:HG3	2.20	0.41
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.97	0.41
1:A:54:VAL:HG21	1:A:92:GLU:HA	2.03	0.41
1:A:492:LEU:HD22	1:A:836:LEU:HD22	2.01	0.41
1:A:326:PRO:O	1:A:762:ARG:NH1	2.53	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.92	0.41
1:A:96:LEU:HD13	1:A:102:PHE:HA	2.03	0.41
1:B:46:GLU:HG3	1:B:46:GLU:O	2.19	0.41
1:A:234:LEU:HB3	1:A:242:VAL:HG23	2.01	0.41
1:A:362:MET:HE3	1:A:380:ILE:HD13	2.02	0.41
1:A:362:MET:HG3	1:A:380:ILE:HG21	2.02	0.41
1:B:132:LEU:HD13	1:B:132:LEU:HA	1.90	0.41
1:B:563:LEU:N	1:B:564:PRO:CD	2.84	0.41
1:B:6:LEU:HD23	1:B:522:GLU:HG3	2.03	0.41
1:A:647:ARG:NH1	2:A:924:HOH:O	2.54	0.41
1:A:412:ALA:HB1	1:A:470:ILE:HG23	2.02	0.41
1:A:468:LYS:HB3	1:A:471:LYS:HG3	2.01	0.41
1:A:563:LEU:HD23	1:A:563:LEU:HA	1.90	0.41
1:A:696:ILE:HD12	1:A:739:LEU:HD22	2.02	0.41
1:B:168:LYS:NZ	2:B:934:HOH:O	2.51	0.41
1:B:684:GLN:HA	1:B:684:GLN:NE2	2.36	0.41
1:A:20:LYS:HA	1:A:20:LYS:HD3	1.96	0.41
1:A:329:GLU:HA	1:A:762:ARG:NH2	2.36	0.41
1:B:420:ARG:HH21	1:B:431:THR:HB	1.86	0.41
1:B:401:GLY:O	1:B:420:ARG:HG2	2.20	0.40
1:B:292:VAL:HG22	1:B:355:MET:HE2	2.04	0.40
1:B:19:LYS:HE3	1:B:512:ARG:HH22	1.86	0.40
1:B:364:ASP:O	1:B:369:ASN:ND2	2.45	0.40
1:A:32:LEU:HB2	1:A:35:ILE:HD11	2.04	0.40
1:B:260:ARG:HA	1:B:261:PRO:HD3	1.97	0.40
1:B:28:ASN:C	1:B:30:TYR:H	2.00	0.40
1:B:66:ILE:HB	1:B:121:ILE:HB	2.03	0.40
1:B:190:GLN:N	2:B:939:HOH:O	2.53	0.40
1:B:575:LYS:O	1:B:579:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	825/875 (94%)	763 (92%)	49 (6%)	13 (2%)	9 16
1	B	836/875 (96%)	782 (94%)	43 (5%)	11 (1%)	12 20
All	All	1661/1750 (95%)	1545 (93%)	92 (6%)	24 (1%)	11 19

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	176	GLU
1	A	250	ASP
1	A	763	CYS
1	B	14	ASN
1	B	25	GLY
1	B	29	ILE
1	B	110	ALA
1	B	250	ASP
1	A	177	HIS
1	A	200	PHE
1	A	559	LEU
1	A	708	VAL
1	A	853	SER
1	B	172	ASN
1	B	559	LEU
1	B	708	VAL
1	A	156	LYS
1	A	302	TRP
1	A	34	ASP
1	B	302	TRP
1	B	600	ASP

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Mol	Chain	Res	Type
1	A	155	TRP
1	B	249	LYS

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	741/778 (95%)	695 (94%)	46 (6%)	18	33
1	B	750/778 (96%)	723 (96%)	27 (4%)	35	59
All	All	1491/1556 (96%)	1418 (95%)	73 (5%)	25	45

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	20	LYS
1	A	37	ASP
1	A	38	THR
1	A	51	HIS
1	A	74	ASP
1	A	90	LYS
1	A	145	LYS
1	A	156	LYS
1	A	157	ASN
1	A	163	ARG
1	A	174	HIS
1	A	176	GLU
1	A	191	ARG
1	A	199	ASP
1	A	227	LYS
1	A	249	LYS
1	A	260	ARG
1	A	277	LYS
1	A	286	LEU
1	A	301	GLU

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Mol	Chain	Res	Type
1	A	303	GLU
1	A	310	GLU
1	A	315	ARG
1	A	323	GLN
1	A	332	ASN
1	A	360	VAL
1	A	372	VAL
1	A	449	GLU
1	A	463	GLN
1	A	467	ASP
1	A	468	LYS
1	A	475	THR
1	A	481	ILE
1	A	546	SER
1	A	597	ILE
1	A	647	ARG
1	A	649	LYS
1	A	661	VAL
1	A	663	ILE
1	A	683	THR
1	A	707	ASP
1	A	721	LEU
1	A	754	SER
1	A	762	ARG
1	A	766	SER
1	B	21	ILE
1	B	70	SER
1	B	131	GLU
1	B	132	LEU
1	B	138	LEU
1	B	155	TRP
1	B	173	GLU
1	B	199	ASP
1	B	201	VAL
1	B	260	ARG
1	B	300	GLN
1	B	362	MET
1	B	365	LEU
1	B	431	THR
1	B	481	ILE
1	B	546	SER
1	B	567	GLU

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Mol	Chain	Res	Type
1	B	595	LEU
1	B	599	LYS
1	B	650	ASP
1	B	655	VAL
1	B	661	VAL
1	B	673	SER
1	B	683	THR
1	B	716	ASP
1	B	754	SER
1	B	766	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	151	ASN
1	A	190	GLN
1	A	323	GLN
1	A	497	ASN
1	A	686	GLN
1	A	719	ASN
1	B	33	ASN
1	B	109	ASN
1	B	190	GLN
1	B	300	GLN
1	B	646	ASN
1	B	684	GLN
1	B	686	GLN
1	B	740	ASN
1	B	816	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	833/875 (95%)	0.99	139 (16%) 1 1	38, 88, 181, 238	0
1	B	842/875 (96%)	0.43	36 (4%) 35 39	37, 76, 126, 196	0
All	All	1675/1750 (95%)	0.71	175 (10%) 6 6	37, 80, 168, 238	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	PHE	12.6
1	A	170	ILE	12.3
1	A	30	TYR	10.7
1	A	124	THR	10.5
1	A	68	VAL	10.4
1	A	197	VAL	10.1
1	A	164	TYR	9.4
1	A	171	PHE	8.7
1	A	80	ASP	8.2
1	A	82	VAL	8.0
1	A	165	GLY	7.8
1	A	123	PRO	7.7
1	A	198	PRO	7.6
1	A	59	LEU	7.1
1	A	64	TRP	7.0
1	A	119	ILE	6.9
1	B	172	ASN	6.8
1	A	125	ASN	6.7
1	A	35	ILE	6.7
1	A	178	CYS	6.6
1	A	75	SER	6.6
1	A	32	LEU	6.5
1	A	173	GLU	6.5
1	A	174	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	140	ILE	6.2
1	A	194	PHE	6.2
1	A	134	GLU	6.1
1	A	96	LEU	5.9
1	A	66	ILE	5.5
1	A	118	PHE	5.4
1	A	67	HIS	5.3
1	A	148	TYR	5.3
1	A	122	TYR	5.2
1	A	264	GLY	5.1
1	A	252	LEU	5.1
1	A	139	ALA	5.0
1	A	193	PRO	5.0
1	A	120	THR	5.0
1	A	44	ASP	4.9
1	A	84	ARG	4.9
1	A	144	LYS	4.9
1	B	191	ARG	4.8
1	A	41	VAL	4.7
1	A	76	LYS	4.7
1	A	192	ASN	4.6
1	A	195	TYR	4.6
1	A	133	LEU	4.6
1	A	45	ASN	4.5
1	A	65	LYS	4.5
1	A	54	VAL	4.4
1	A	72	LEU	4.3
1	A	51	HIS	4.3
1	A	79	LEU	4.2
1	A	46	GLU	4.2
1	A	163	ARG	4.2
1	A	149	ILE	4.2
1	A	132	LEU	4.2
1	A	376	LEU	4.2
1	A	53	HIS	4.2
1	A	34	ASP	4.2
1	A	306	PHE	4.1
1	A	481	ILE	4.1
1	A	381	ILE	4.0
1	A	295	LEU	3.9
1	A	49	TRP	3.9
1	A	127	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	161	PHE	3.8
1	A	136	ILE	3.7
1	A	191	ARG	3.7
1	A	147	PRO	3.7
1	B	173	GLU	3.7
1	A	113	ALA	3.6
1	A	162	TYR	3.5
1	A	87	ILE	3.5
1	A	83	ALA	3.5
1	B	174	HIS	3.4
1	B	230	ILE	3.3
1	A	150	LEU	3.3
1	A	52	TYR	3.3
1	A	260	ARG	3.3
1	B	208	LEU	3.3
1	A	39	TYR	3.3
1	A	40	ALA	3.2
1	A	232	THR	3.2
1	A	380	ILE	3.2
1	A	94	LYS	3.2
1	A	85	LEU	3.2
1	A	117	LYS	3.2
1	B	170	ILE	3.2
1	A	307	LEU	3.2
1	A	263	ALA	3.2
1	A	169	GLY	3.2
1	A	69	THR	3.1
1	A	135	MET	3.1
1	A	425	LEU	3.1
1	A	81	LYS	3.1
1	A	91	ILE	3.0
1	A	655	VAL	3.0
1	B	307	LEU	3.0
1	B	177	HIS	3.0
1	A	177	HIS	2.9
1	A	78	VAL	2.9
1	B	195	TYR	2.9
1	B	150	LEU	2.9
1	A	93	PHE	2.9
1	A	70	SER	2.9
1	A	302	TRP	2.9
1	A	196	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	121	ILE	2.8
1	A	43	LEU	2.8
1	A	155	TRP	2.8
1	A	167	PHE	2.8
1	B	136	ILE	2.8
1	A	90	LYS	2.7
1	A	251	ASN	2.7
1	A	92	GLU	2.7
1	B	79	LEU	2.7
1	A	244	LEU	2.7
1	B	305	TYR	2.7
1	B	380	ILE	2.6
1	B	298	TYR	2.6
1	A	47	SER	2.6
1	A	372	VAL	2.5
1	A	249	LYS	2.5
1	A	159	ASN	2.5
1	A	449	GLU	2.4
1	A	190	GLN	2.4
1	B	190	GLN	2.4
1	A	208	LEU	2.4
1	B	863	LYS	2.4
1	A	112	ARG	2.4
1	A	652	GLN	2.4
1	A	58	THR	2.4
1	B	30	TYR	2.4
1	A	31	GLU	2.4
1	A	29	ILE	2.4
1	A	348	LEU	2.4
1	A	280	TYR	2.3
1	B	132	LEU	2.3
1	A	360	VAL	2.3
1	B	602	ILE	2.3
1	B	45	ASN	2.3
1	B	155	TRP	2.3
1	B	278	ILE	2.3
1	A	172	ASN	2.3
1	B	248	LYS	2.2
1	B	249	LYS	2.2
1	B	179	ILE	2.2
1	A	63	GLY	2.2
1	A	130	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLY	2.2
1	B	381	ILE	2.2
1	A	234	LEU	2.2
1	A	365	LEU	2.2
1	B	273	LEU	2.2
1	A	259	ALA	2.1
1	A	296	ILE	2.1
1	A	61	GLU	2.1
1	A	33	ASN	2.1
1	A	108	LYS	2.1
1	A	245	ALA	2.1
1	A	265	LEU	2.1
1	A	334	MET	2.1
1	B	102	PHE	2.1
1	B	48	VAL	2.1
1	A	156	LYS	2.1
1	B	199	ASP	2.0
1	A	601	ASN	2.0
1	B	171	PHE	2.0
1	A	320	TRP	2.0
1	B	85	LEU	2.0
1	A	200	PHE	2.0
1	B	193	PRO	2.0
1	A	408	LYS	2.0
1	B	156	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.