



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 02:00 pm BST

PDB ID : 5YIM  
Title : Structure of a Legionella effector  
Authors : Feng, Y.; Dong, Y.; Wang, W.  
Deposited on : 2017-10-05  
Resolution : 3.39 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](mailto: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 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	:	2.11
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)	:	2.11

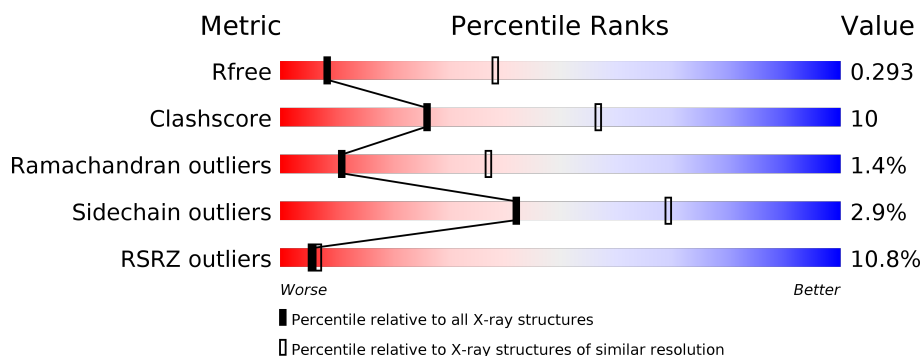
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	960	<div> <div>7%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	C	960	<div> <div>14%</div> <div>67%</div> <div>26%</div> <div>• 7%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14128 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 SdeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	933	Total	C	N	O	S	0	0	0
			7297	4572	1283	1414	28			
1	C	896	Total	C	N	O	S	0	0	0
			6831	4275	1204	1325	27			

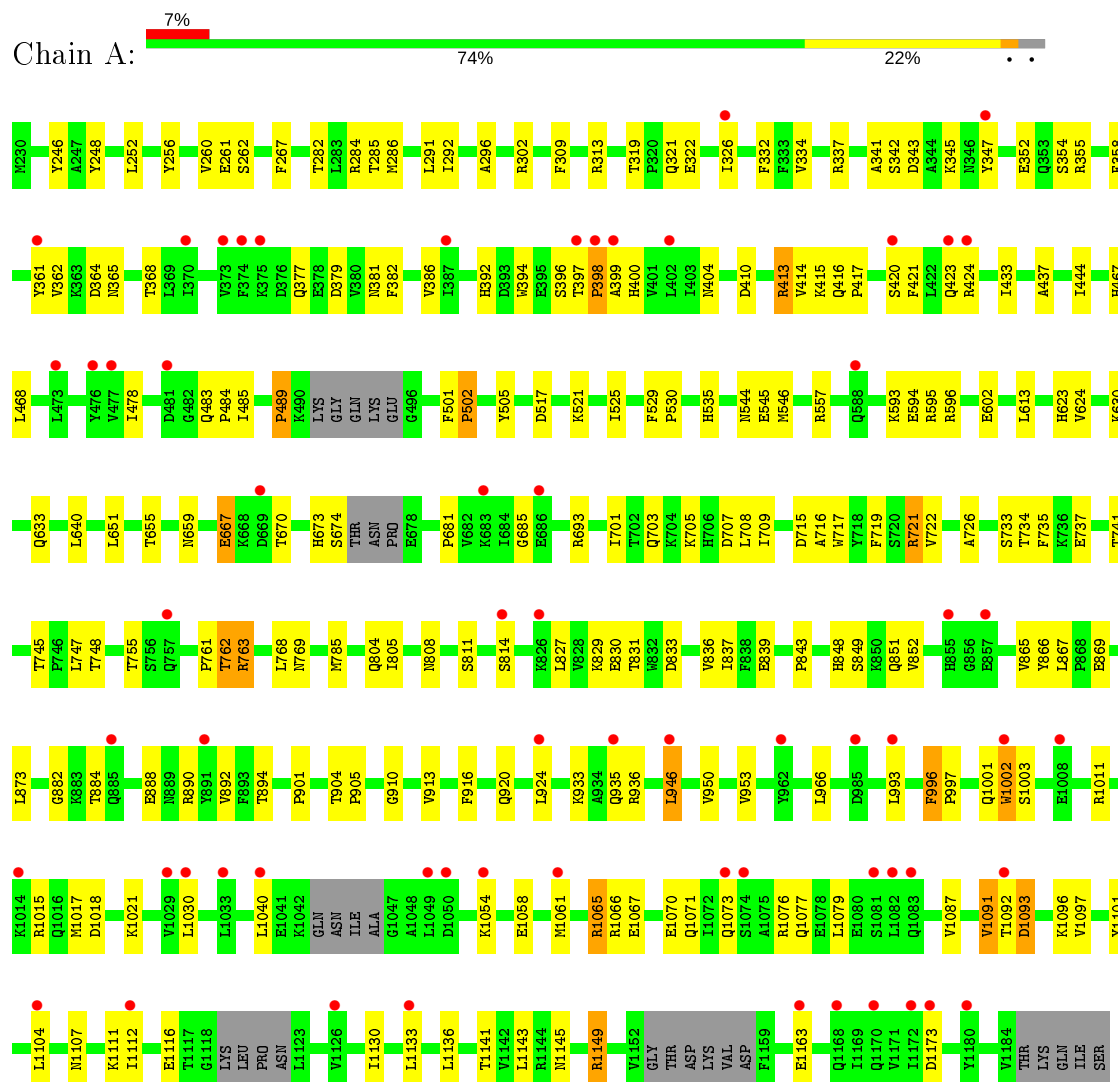
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	-	expression tag	UNP Q6RCR0
C	230	MET	-	expression tag	UNP Q6RCR0

### 3 Residue-property plots [i](#)

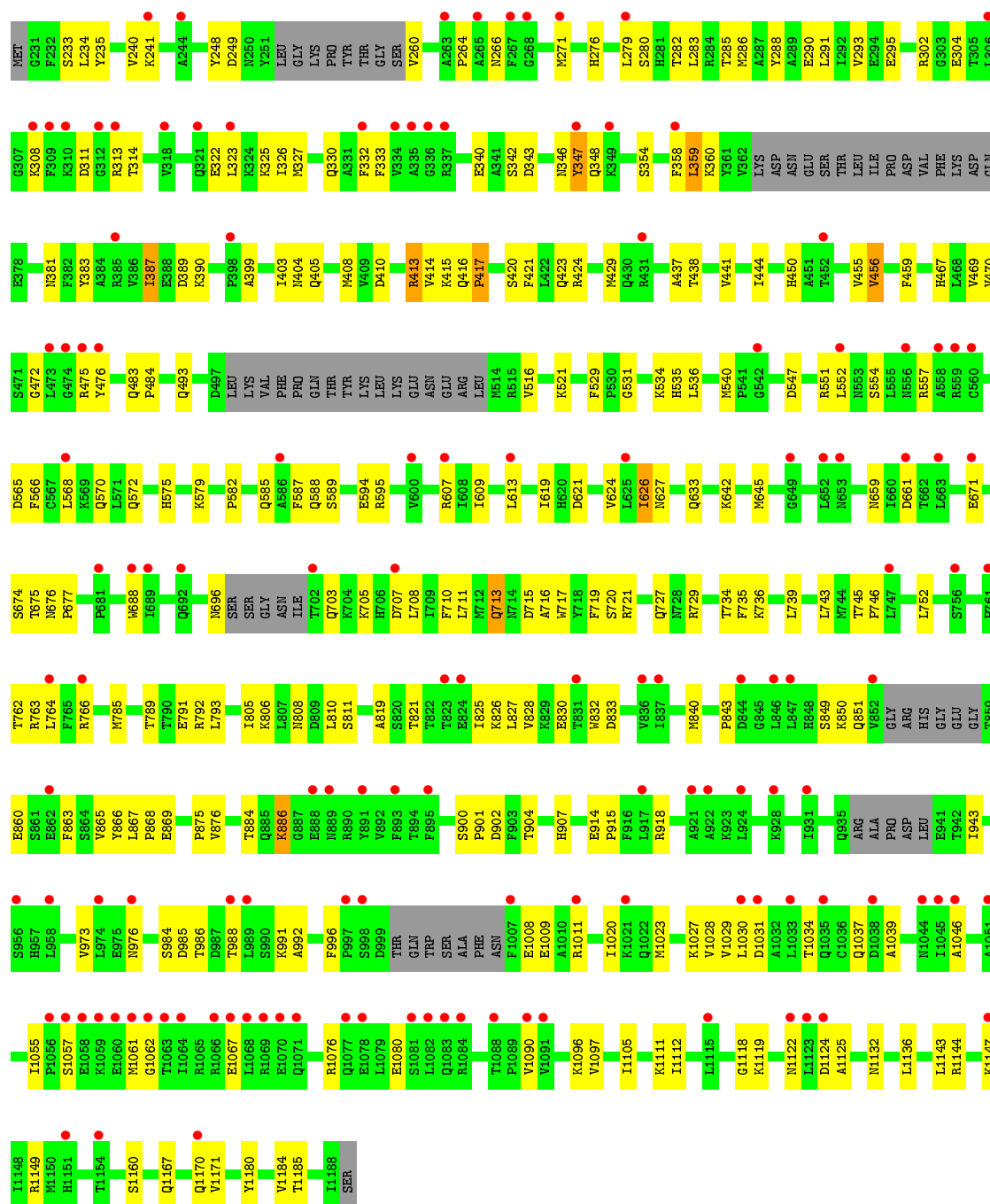
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: SdeA



#### • Molecule 1: SdeA





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.65Å 295.43Å 194.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.39 105.92 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.39) 99.5 (105.92-3.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.251 , 0.287 0.260 , 0.293	Depositor DCC
$R_{free}$ test set	2818 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	125.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 111.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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](#)

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	0.28	0/7419	0.50	4/10012 (0.0%)
1	C	0.26	0/6936	0.49	0/9381
All	All	0.27	0/14355	0.49	4/19393 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	PRO	N-CA-CB	6.19	110.73	103.30
1	A	484	PRO	N-CA-CB	6.16	110.69	103.30
1	A	502	PRO	N-CA-CB	5.87	110.34	103.30
1	A	867	LEU	CA-CB-CG	5.09	127.01	115.30

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	7297	0	7103	134	0
1	C	6831	0	6555	158	0
All	All	14128	0	13658	290	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 (290) 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:755:THR:HG21	1:A:851:GLN:HE21	1.33	0.93
1:A:1130:ILE:HA	1:A:1133:LEU:HD12	1.63	0.81
1:C:826:LYS:H	1:C:828:VAL:HG23	1.46	0.79
1:C:424:ARG:HB2	1:C:470:VAL:HG11	1.65	0.79
1:A:910:GLY:HA2	1:A:913:VAL:HG12	1.63	0.78
1:A:1091:VAL:HG12	1:A:1092:THR:H	1.51	0.76
1:C:674:SER:O	1:C:721:ARG:NH2	2.18	0.74
1:C:626:ILE:HG23	1:C:627:ASN:H	1.54	0.73
1:A:829:LYS:HG2	1:A:830:GLU:HG3	1.71	0.73
1:C:727:GLN:OE1	1:C:729:ARG:NH1	2.22	0.72
1:C:266:ASN:HB3	1:C:271:MET:HA	1.71	0.72
1:C:313:ARG:NH1	1:C:322:GLU:OE1	2.22	0.71
1:C:766:ARG:NH2	1:C:840:MET:SD	2.62	0.71
1:A:423:GLN:HE22	1:A:525:ILE:HD12	1.55	0.71
1:C:943:ILE:HG12	1:C:1020:ILE:HG12	1.72	0.70
1:C:806:LYS:NZ	1:C:902:ASP:O	2.22	0.70
1:A:837:ILE:HB	1:A:892:VAL:HG12	1.73	0.70
1:C:785:MET:HE3	1:C:805:ILE:HG23	1.73	0.70
1:A:827:LEU:HB2	1:A:831:THR:HG22	1.73	0.69
1:A:377:GLN:O	1:A:381:ASN:ND2	2.20	0.69
1:A:768:LEU:HB2	1:A:836:VAL:HG23	1.75	0.69
1:A:546:MET:HG3	1:C:455:VAL:HG11	1.76	0.68
1:C:716:ALA:HA	1:C:719:PHE:CE2	2.29	0.68
1:A:248:TYR:HA	1:A:252:LEU:HB2	1.77	0.67
1:C:413:ARG:HG2	1:C:414:VAL:HG13	1.74	0.67
1:C:346:ASN:O	1:C:348:GLN:N	2.29	0.66
1:C:613:LEU:O	1:C:659:ASN:ND2	2.29	0.66
1:C:676:ASN:OD1	1:C:720:SER:OG	2.14	0.66
1:C:1112:ILE:HG12	1:C:1136:LEU:HD13	1.78	0.65
1:A:413:ARG:HD3	1:A:414:VAL:HG13	1.79	0.64
1:A:485:ILE:HA	1:A:501:PHE:H	1.62	0.63
1:C:417:PRO:HD2	1:C:421:PHE:HE2	1.63	0.63
1:C:914:GLU:OE2	1:C:918:ARG:NH2	2.32	0.63
1:A:1093:ASP:HB3	1:A:1096:LYS:HB3	1.81	0.63
1:C:985:ASP:O	1:C:986:THR:OG1	2.17	0.62
1:C:833:ASP:OD1	1:C:884:THR:OG1	2.17	0.62
1:A:904:THR:O	1:A:1149:ARG:NH1	2.32	0.61
1:A:849:SER:HB3	1:A:865:VAL:HG22	1.83	0.60
1:C:901:PRO:O	1:C:1149:ARG:NH2	2.34	0.60
1:A:1011:ARG:HH21	1:A:1015:ARG:HH22	1.47	0.60
1:A:721:ARG:NH1	1:A:733:SER:HB3	2.17	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:OD1	1:A:365:ASN:N	2.35	0.60
1:A:827:LEU:HD22	1:A:831:THR:HA	1.82	0.60
1:C:976:ASN:HB2	1:C:991:LYS:HD2	1.83	0.60
1:A:1058:GLU:OE2	1:A:1071:GLN:NE2	2.35	0.59
1:C:661:ASP:HA	1:C:688:TRP:HZ3	1.66	0.59
1:C:1119:LYS:HB3	1:C:1125:ALA:HB1	1.83	0.59
1:C:291:LEU:HD11	1:C:444:ILE:HD12	1.84	0.59
1:C:671:GLU:HG2	1:C:734:THR:HG21	1.84	0.58
1:C:404:ASN:OD1	1:C:405:GLN:N	2.36	0.58
1:C:469:VAL:HG23	1:C:475:ARG:HA	1.86	0.58
1:A:1040:LEU:HD21	1:A:1077:GLN:HE22	1.68	0.58
1:C:308:LYS:HG2	1:C:314:THR:HB	1.86	0.58
1:A:1141:THR:O	1:A:1145:ASN:ND2	2.36	0.57
1:C:420:SER:HB3	1:C:467:HIS:CD2	2.41	0.56
1:A:1001:GLN:O	1:A:1003:SER:N	2.35	0.56
1:A:613:LEU:HD21	1:A:747:LEU:HD11	1.87	0.56
1:C:589:SER:HB2	1:C:900:SER:HA	1.86	0.56
1:A:670:THR:HB	1:A:681:PRO:HB2	1.89	0.55
1:C:607:ARG:NH1	1:C:1076:ARG:O	2.37	0.55
1:A:769:ASN:ND2	1:A:833:ASP:O	2.32	0.55
1:A:716:ALA:HA	1:A:719:PHE:CE2	2.41	0.55
1:A:309:PHE:CZ	1:A:397:THR:HA	2.42	0.55
1:C:582:PRO:HA	1:C:585:GLN:HE21	1.70	0.55
1:C:483:GLN:N	1:C:483:GLN:OE1	2.35	0.55
1:C:283:LEU:HD22	1:C:568:LEU:HD21	1.89	0.55
1:C:293:VAL:HG21	1:C:323:LEU:HD12	1.89	0.54
1:A:415:LYS:HD3	1:A:421:PHE:CE1	2.43	0.54
1:C:1031:ASP:O	1:C:1034:THR:OG1	2.21	0.54
1:C:675:THR:HB	1:C:717:TRP:HA	1.90	0.54
1:A:1104:LEU:HB3	1:A:1143:LEU:HD21	1.89	0.54
1:A:1054:LYS:NZ	1:A:1073:GLN:HG2	2.23	0.54
1:C:884:THR:HG23	1:C:886:LYS:H	1.73	0.54
1:A:1002:TRP:HH2	1:A:1017:MET:HG2	1.73	0.54
1:A:593:LYS:NZ	1:A:593:LYS:O	2.32	0.54
1:C:992:ALA:HB2	1:C:1028:VAL:HG11	1.89	0.54
1:A:1076:ARG:HA	1:A:1079:LEU:HD12	1.90	0.53
1:A:313:ARG:HH22	1:A:398:PRO:HG3	1.74	0.53
1:C:1144:ARG:NH2	1:C:1167:GLN:OE1	2.41	0.53
1:C:399:ALA:O	1:C:403:ILE:HG22	2.08	0.53
1:A:993:LEU:HA	1:A:996:PHE:HD2	1.73	0.53
1:A:1112:ILE:HG12	1:A:1136:LEU:HD13	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HH12	1:A:437:ALA:HB2	1.75	0.52
1:C:414:VAL:HG23	1:C:415:LYS:HE2	1.91	0.52
1:C:417:PRO:HD2	1:C:421:PHE:CE2	2.43	0.52
1:C:675:THR:OG1	1:C:677:PRO:HD2	2.08	0.52
1:C:1029:VAL:HG22	1:C:1057:SER:HB2	1.91	0.52
1:C:830:GLU:HG3	1:C:832:TRP:HD1	1.73	0.52
1:A:703:GLN:NE2	1:A:707:ASP:OD1	2.43	0.52
1:A:1107:ASN:HD21	1:A:1111:LYS:HE2	1.74	0.52
1:A:342:SER:OG	1:A:343:ASP:N	2.43	0.52
1:A:924:LEU:HG	1:A:1073:GLN:OE1	2.10	0.51
1:C:1105:ILE:HA	1:C:1143:LEU:HD21	1.92	0.51
1:A:640:LEU:HD13	1:A:726:ALA:HA	1.92	0.51
1:C:764:LEU:HG	1:C:821:THR:HB	1.91	0.51
1:C:240:VAL:HG11	1:C:327:MET:HE2	1.92	0.51
1:A:655:THR:O	1:A:659:ASN:ND2	2.43	0.51
1:C:330:GLN:HG3	1:C:403:ILE:HD13	1.92	0.51
1:A:309:PHE:CE1	1:A:397:THR:HA	2.46	0.51
1:A:839:GLU:HB3	1:A:894:THR:HG22	1.93	0.51
1:C:342:SER:OG	1:C:343:ASP:N	2.43	0.51
1:A:352:GLU:HB3	1:A:355:ARG:HH21	1.75	0.51
1:C:241:LYS:HE3	1:C:565:ASP:HB3	1.93	0.51
1:C:358:PHE:O	1:C:360:LYS:N	2.43	0.51
1:A:267:PHE:CE2	1:A:557:ARG:HG2	2.46	0.50
1:A:358:PHE:O	1:A:362:VAL:HG23	2.11	0.50
1:A:394:TRP:HE1	1:A:404:ASN:HD22	1.60	0.50
1:C:762:THR:HG22	1:C:843:PRO:HA	1.93	0.50
1:A:291:LEU:HD11	1:A:444:ILE:HD12	1.93	0.50
1:C:661:ASP:HA	1:C:688:TRP:CZ3	2.43	0.50
1:C:260:VAL:HG12	1:C:340:GLU:H	1.77	0.50
1:A:708:LEU:HG	1:A:748:THR:HG22	1.94	0.50
1:C:588:GLN:HG3	1:C:1096:LYS:HE2	1.94	0.50
1:A:673:HIS:CG	1:A:674:SER:H	2.30	0.49
1:C:381:ASN:HB2	1:C:383:TYR:CE2	2.47	0.49
1:A:424:ARG:NH1	1:A:468:LEU:O	2.45	0.49
1:A:667:GLU:O	1:A:685:GLY:HA3	2.12	0.49
1:C:302:ARG:NH1	1:C:304:GLU:OE1	2.45	0.49
1:A:260:VAL:O	1:A:262:SER:N	2.45	0.49
1:A:256:TYR:HD2	1:A:262:SER:HB2	1.77	0.49
1:C:607:ARG:NH1	1:C:1080:GLU:HB2	2.28	0.49
1:C:984:SER:OG	1:C:985:ASP:N	2.45	0.49
1:A:382:PHE:O	1:A:386:VAL:HG23	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:NH2	1:A:602:GLU:OE1	2.44	0.49
1:A:884:THR:HG22	1:A:888:GLU:O	2.13	0.49
1:C:282:THR:O	1:C:286:MET:HG3	2.13	0.49
1:C:459:PHE:HB3	1:C:536:LEU:CB	2.43	0.49
1:C:707:ASP:OD1	1:C:708:LEU:N	2.45	0.49
1:C:710:PHE:HA	1:C:713:GLN:HB2	1.95	0.49
1:A:709:ILE:HG22	1:A:852:VAL:HG13	1.94	0.49
1:A:595:ARG:NH1	1:A:866:TYR:O	2.46	0.49
1:A:935:GLN:HE22	1:A:1030:LEU:HD22	1.77	0.49
1:C:1008:GLU:HG3	1:C:1011:ARG:HG3	1.95	0.48
1:A:1054:LYS:HZ3	1:A:1073:GLN:HG2	1.78	0.48
1:C:785:MET:HG2	1:C:805:ILE:HA	1.95	0.48
1:A:478:ILE:HA	1:A:483:GLN:HA	1.94	0.48
1:C:264:PRO:HB2	1:C:271:MET:HB3	1.95	0.48
1:C:291:LEU:HD21	1:C:444:ILE:HB	1.96	0.48
1:C:389:ASP:OD1	1:C:390:LYS:N	2.42	0.48
1:C:645:MET:SD	1:C:746:PRO:HG3	2.54	0.48
1:A:282:THR:O	1:A:285:THR:OG1	2.24	0.48
1:A:705:LYS:O	1:A:709:ILE:HG13	2.13	0.48
1:A:721:ARG:CZ	1:A:733:SER:HB3	2.43	0.48
1:C:438:THR:O	1:C:441:VAL:HG12	2.14	0.48
1:C:444:ILE:HG12	1:C:791:GLU:HG3	1.96	0.48
1:C:595:ARG:NH1	1:C:866:TYR:O	2.45	0.48
1:C:849:SER:HB3	1:C:865:VAL:HB	1.96	0.48
1:A:322:GLU:O	1:A:326:ILE:HG12	2.13	0.47
1:A:593:LYS:HE2	1:A:596:ARG:HA	1.96	0.47
1:A:345:LYS:HA	1:A:347:TYR:CD2	2.48	0.47
1:C:429:MET:SD	1:C:441:VAL:HG11	2.53	0.47
1:C:415:LYS:HB3	1:C:421:PHE:CD2	2.50	0.47
1:A:596:ARG:HG3	1:A:1087:VAL:HG11	1.95	0.47
1:C:633:GLN:HB3	1:C:735:PHE:HD1	1.80	0.47
1:C:1167:GLN:O	1:C:1171:VAL:HG23	2.15	0.47
1:C:808:ASN:O	1:C:810:LEU:N	2.48	0.47
1:A:365:ASN:HB3	1:A:368:THR:HG22	1.96	0.47
1:C:1119:LYS:HD3	1:C:1125:ALA:HB1	1.97	0.46
1:A:319:THR:HG22	1:A:321:GLN:H	1.79	0.46
1:A:920:GLN:HB3	1:A:1073:GLN:NE2	2.29	0.46
1:C:1039:ALA:O	1:C:1046:ALA:HB2	2.15	0.46
1:A:332:PHE:O	1:A:354:SER:HB2	2.16	0.46
1:C:621:ASP:N	1:C:621:ASP:OD1	2.48	0.46
1:A:417:PRO:HD2	1:A:421:PHE:CE2	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:ARG:HG2	1:A:1066:ARG:N	2.31	0.46
1:A:246:TYR:CE2	1:A:361:TYR:HB2	2.51	0.46
1:C:708:LEU:O	1:C:711:LEU:HB3	2.16	0.46
1:C:973:VAL:HA	1:C:976:ASN:HD21	1.81	0.46
1:A:394:TRP:C	1:A:396:SER:H	2.20	0.45
1:C:869:GLU:HG3	1:C:904:THR:HG22	1.98	0.45
1:C:429:MET:HG2	1:C:438:THR:HG22	1.99	0.45
1:C:675:THR:HA	1:C:721:ARG:HG2	1.99	0.45
1:C:752:LEU:HA	1:C:850:LYS:HG3	1.98	0.45
1:C:1030:LEU:O	1:C:1034:THR:HG23	2.16	0.45
1:C:469:VAL:HG22	1:C:476:TYR:CE2	2.51	0.45
1:A:1067:GLU:O	1:A:1070:GLU:HG3	2.16	0.45
1:A:396:SER:HB3	1:A:400:HIS:CG	2.51	0.45
1:A:901:PRO:HG3	1:A:1091:VAL:HG23	1.97	0.45
1:A:633:GLN:HB2	1:A:735:PHE:HD1	1.81	0.45
1:C:288:TYR:HE2	1:C:410:ASP:HB2	1.82	0.45
1:C:867:LEU:HD12	1:C:868:PRO:HD2	1.99	0.45
1:C:642:LYS:HD2	1:C:907:HIS:CG	2.52	0.45
1:A:1011:ARG:HE	1:A:1015:ARG:NH2	2.14	0.45
1:A:377:GLN:HG2	1:A:381:ASN:HD21	1.81	0.45
1:A:785:MET:HG2	1:A:805:ILE:HA	1.98	0.45
1:C:743:LEU:O	1:C:746:PRO:HD2	2.17	0.45
1:A:804:GLN:O	1:A:808:ASN:ND2	2.42	0.45
1:A:361:TYR:O	1:A:361:TYR:CG	2.70	0.44
1:A:722:VAL:HG22	1:A:741:THR:HG22	1.98	0.44
1:C:624:VAL:HG23	1:C:735:PHE:HZ	1.81	0.44
1:C:248:TYR:CD1	1:C:279:LEU:HD23	2.51	0.44
1:C:785:MET:HE1	1:C:875:PRO:HD2	1.98	0.44
1:A:953:VAL:HG21	1:A:966:LEU:HD12	2.00	0.44
1:C:851:GLN:HB3	1:C:863:PHE:CE2	2.52	0.44
1:C:333:PHE:HE1	1:C:389:ASP:HB2	1.83	0.44
1:A:623:HIS:CD2	1:A:630:LYS:HG3	2.53	0.44
1:C:467:HIS:HB2	1:C:516:VAL:HA	2.00	0.44
1:C:529:PHE:CE2	1:C:531:GLY:HA3	2.52	0.44
1:C:575:HIS:ND1	1:C:579:LYS:HE3	2.33	0.44
1:C:1020:ILE:HD12	1:C:1020:ILE:HA	1.80	0.44
1:C:1027:LYS:O	1:C:1030:LEU:HG	2.17	0.44
1:C:381:ASN:HB2	1:C:383:TYR:CD2	2.53	0.44
1:C:810:LEU:O	1:C:811:SER:OG	2.35	0.44
1:C:459:PHE:HB3	1:C:536:LEU:HB2	2.00	0.44
1:C:988:THR:HG21	1:C:1031:ASP:OD2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:ILE:O	1:C:619:ILE:HG13	2.15	0.43
1:A:386:VAL:HG11	1:A:399:ALA:HB1	1.99	0.43
1:C:1180:TYR:O	1:C:1184:VAL:HG23	2.19	0.43
1:A:673:HIS:CG	1:A:674:SER:N	2.87	0.43
1:C:521:LYS:HB3	1:C:521:LYS:HE2	1.74	0.43
1:A:924:LEU:HG	1:A:1073:GLN:CD	2.39	0.43
1:C:582:PRO:HB2	1:C:789:THR:HG23	1.99	0.43
1:C:943:ILE:HD11	1:C:1023:MET:HE1	2.01	0.43
1:A:284:ARG:NH1	1:A:410:ASP:OD2	2.52	0.43
1:A:869:GLU:HB2	1:A:905:PRO:HD3	2.00	0.43
1:C:264:PRO:HG2	1:C:271:MET:SD	2.58	0.43
1:C:327:MET:HE3	1:C:327:MET:HB3	1.64	0.43
1:A:933:LYS:HA	1:A:933:LYS:HD3	1.76	0.43
1:C:266:ASN:OD1	1:C:554:SER:OG	2.35	0.43
1:C:470:VAL:O	1:C:472:GLY:N	2.52	0.43
1:C:914:GLU:HB3	1:C:915:PRO:HD3	2.01	0.43
1:A:1054:LYS:HZ2	1:A:1077:GLN:HG3	1.83	0.43
1:A:882:GLY:O	1:A:890:ARG:HG2	2.18	0.43
1:A:544:ASN:ND2	1:C:416:GLN:O	2.50	0.43
1:C:235:TYR:HB2	1:C:572:GLN:HG3	2.01	0.43
1:A:1011:ARG:HE	1:A:1015:ARG:HH22	1.66	0.42
1:A:651:LEU:HD23	1:A:651:LEU:HA	1.85	0.42
1:C:766:ARG:HE	1:C:819:ALA:HB1	1.84	0.42
1:C:404:ASN:OD1	1:C:405:GLN:HG2	2.19	0.42
1:A:296:ALA:HA	1:A:433:ILE:HG23	2.00	0.42
1:A:624:VAL:HG23	1:A:735:PHE:HZ	1.84	0.42
1:A:420:SER:HB3	1:A:467:HIS:CE1	2.54	0.42
1:A:1018:ASP:O	1:A:1021:LYS:HB2	2.19	0.42
1:C:703:GLN:HG2	1:C:705:LYS:HG3	2.01	0.42
1:C:322:GLU:O	1:C:326:ILE:HG13	2.20	0.42
1:C:405:GLN:HA	1:C:408:MET:HG2	2.02	0.42
1:C:282:THR:O	1:C:285:THR:OG1	2.25	0.42
1:C:534:LYS:O	1:C:536:LEU:N	2.51	0.42
1:C:785:MET:CE	1:C:875:PRO:HD2	2.49	0.42
1:A:416:GLN:HB2	1:A:417:PRO:HD3	2.01	0.42
1:C:1124:ASP:OD1	1:C:1124:ASP:N	2.39	0.42
1:C:233:SER:OG	1:C:234:LEU:N	2.53	0.42
1:C:547:ASP:O	1:C:551:ARG:N	2.52	0.42
1:C:566:PHE:O	1:C:570:GLN:HG2	2.20	0.42
1:A:1101:TYR:OH	1:A:1163:GLU:OE2	2.21	0.42
1:A:737:GLU:O	1:A:741:THR:HG23	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:THR:HG23	1:A:843:PRO:HA	2.02	0.42
1:C:325:LYS:HE3	1:C:387:ILE:HD13	2.02	0.42
1:A:256:TYR:CD2	1:A:262:SER:HB2	2.53	0.42
1:C:279:LEU:HD12	1:C:280:SER:N	2.34	0.42
1:C:311:ASP:OD1	1:C:311:ASP:N	2.47	0.42
1:C:1061:MET:HB3	1:C:1067:GLU:OE2	2.20	0.41
1:C:609:ILE:HG23	1:C:743:LEU:HD22	2.02	0.41
1:A:292:ILE:HG23	1:A:433:ILE:HD11	2.02	0.41
1:A:594:GLU:HB3	1:A:848:HIS:CE1	2.55	0.41
1:A:996:PHE:CD1	1:A:997:PRO:HD2	2.54	0.41
1:C:1147:LYS:NZ	1:C:1160:SER:HA	2.35	0.41
1:A:282:THR:O	1:A:286:MET:HG3	2.19	0.41
1:A:517:ASP:O	1:A:521:LYS:HG3	2.21	0.41
1:C:1111:LYS:HA	1:C:1111:LYS:HD3	1.85	0.41
1:C:450:HIS:ND1	1:C:540:MET:SD	2.94	0.41
1:A:1116:GLU:HG3	1:A:1173:ASP:HB3	2.02	0.41
1:C:450:HIS:NE2	1:C:456:VAL:HG11	2.35	0.41
1:C:739:LEU:O	1:C:743:LEU:HG	2.21	0.41
1:C:745:THR:OG1	1:C:746:PRO:HD3	2.20	0.41
1:A:901:PRO:HA	1:A:904:THR:HG23	2.02	0.41
1:A:1091:VAL:HG12	1:A:1092:THR:N	2.27	0.41
1:C:1090:VAL:HG23	1:C:1097:VAL:HG21	2.02	0.41
1:C:621:ASP:HA	1:C:736:LYS:HE3	2.03	0.41
1:A:946:LEU:O	1:A:950:VAL:HG13	2.20	0.41
1:A:415:LYS:HD3	1:A:421:PHE:CD1	2.55	0.41
1:C:594:GLU:HB3	1:C:595:ARG:H	1.72	0.41
1:A:433:ILE:HG22	1:A:437:ALA:HB3	2.03	0.41
1:C:973:VAL:HA	1:C:976:ASN:ND2	2.35	0.41
1:A:337:ARG:NH1	1:A:341:ALA:HB3	2.37	0.40
1:A:761:PRO:C	1:A:763:ARG:H	2.25	0.40
1:C:283:LEU:HD23	1:C:286:MET:HE3	2.02	0.40
1:C:424:ARG:HD3	1:C:470:VAL:HG13	2.02	0.40
1:A:379:ASP:O	1:A:382:PHE:HB3	2.22	0.40
1:A:529:PHE:CD1	1:A:530:PRO:HD2	2.56	0.40
1:A:916:PHE:CZ	1:A:1076:ARG:HD3	2.56	0.40
1:C:1132:ASN:O	1:C:1136:LEU:HG	2.21	0.40
1:C:290:GLU:HA	1:C:323:LEU:HD11	2.03	0.40
1:C:619:ILE:HD12	1:C:736:LYS:HE2	2.03	0.40
1:A:345:LYS:H	1:A:345:LYS:HG2	1.75	0.40
1:A:673:HIS:ND1	1:A:717:TRP:HA	2.37	0.40
1:A:377:GLN:HG2	1:A:381:ASN:ND2	2.37	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:SER:HB2	1:A:873:LEU:HB2	2.03	0.40
1:C:332:PHE:O	1:C:354:SER:HB3	2.21	0.40
1:C:295:GLU:HB3	1:C:437:ALA:HB1	2.03	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	921/960 (96%)	864 (94%)	46 (5%)	11 (1%)	13	41
1	C	880/960 (92%)	803 (91%)	63 (7%)	14 (2%)	9	34
All	All	1801/1920 (94%)	1667 (93%)	109 (6%)	25 (1%)	11	37

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	GLU
1	A	489	PRO
1	A	502	PRO
1	C	347	TYR
1	C	626	ILE
1	A	398	PRO
1	A	505	TYR
1	C	493	GLN
1	C	1118	GLY
1	A	535	HIS
1	C	535	HIS
1	C	715	ASP
1	C	793	LEU
1	C	860	GLU
1	C	1062	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1122	ASN
1	A	545	GLU
1	A	762	THR
1	A	1093	ASP
1	C	359	LEU
1	A	1061	MET
1	A	1091	VAL
1	C	484	PRO
1	C	825	ILE
1	C	417	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	773/837 (92%)	754 (98%)	19 (2%)	47	72
1	C	702/837 (84%)	678 (97%)	24 (3%)	37	65
All	All	1475/1674 (88%)	1432 (97%)	43 (3%)	42	69

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	VAL
1	A	392	HIS
1	A	413	ARG
1	A	667	GLU
1	A	693	ARG
1	A	701	ILE
1	A	715	ASP
1	A	721	ARG
1	A	734	THR
1	A	745	THR
1	A	763	ARG
1	A	814	SER
1	A	936	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	946	LEU
1	A	996	PHE
1	A	1002	TRP
1	A	1065	ARG
1	A	1097	VAL
1	A	1149	ARG
1	C	249	ASP
1	C	276	HIS
1	C	347	TYR
1	C	359	LEU
1	C	387	ILE
1	C	413	ARG
1	C	423	GLN
1	C	456	VAL
1	C	552	LEU
1	C	557	ARG
1	C	587	PHE
1	C	696	ASN
1	C	713	GLN
1	C	763	ARG
1	C	792	ARG
1	C	827	LEU
1	C	876	VAL
1	C	886	LYS
1	C	996	PHE
1	C	1009	GLU
1	C	1037	GLN
1	C	1055	ILE
1	C	1170	GLN
1	C	1185	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	GLN
1	A	526	GLN
1	A	851	GLN
1	A	935	GLN
1	A	1077	GLN
1	C	695	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	933/960 (97%)	0.75	63 (6%) 17 19	67, 108, 193, 304	0
1	C	896/960 (93%)	0.88	135 (15%) 2 2	74, 143, 235, 328	0
All	All	1829/1920 (95%)	0.81	198 (10%) 5 7	67, 123, 222, 328	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1082	LEU	7.0
1	A	985	ASP	6.0
1	C	1045	ILE	6.0
1	C	1060	GLU	5.7
1	C	889	ASN	5.7
1	C	1062	GLY	5.7
1	C	1091	VAL	5.6
1	C	1067	GLU	5.2
1	C	310	LYS	5.1
1	C	988	THR	5.1
1	C	831	THR	5.0
1	C	335	ALA	5.0
1	C	1083	GLN	4.9
1	C	1068	LEU	4.7
1	C	1007	PHE	4.7
1	C	267	PHE	4.6
1	C	1058	GLU	4.6
1	C	241	LYS	4.6
1	C	358	PHE	4.5
1	C	998	SER	4.5
1	C	1078	GLU	4.4
1	C	1057	SER	4.4
1	C	1061	MET	4.3
1	C	976	ASN	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1081	SER	4.2
1	C	1090	VAL	4.2
1	C	1082	LEU	4.2
1	A	1061	MET	4.1
1	C	1064	ILE	4.1
1	A	398	PRO	4.1
1	A	935	GLN	4.0
1	C	846	LEU	3.9
1	A	757	GLN	3.9
1	C	692	GLN	3.9
1	C	823	THR	3.9
1	C	917	LEU	3.8
1	A	1083	GLN	3.8
1	A	1092	THR	3.8
1	C	1033	LEU	3.8
1	C	560	CYS	3.7
1	C	265	ALA	3.6
1	C	1063	THR	3.6
1	C	1070	GLU	3.6
1	C	766	ARG	3.6
1	A	1073	GLN	3.5
1	C	756	SER	3.5
1	C	558	ALA	3.4
1	C	306	LEU	3.3
1	C	824	GLU	3.3
1	C	347	TYR	3.2
1	A	481	ASP	3.2
1	A	1170	GLN	3.2
1	A	370	ILE	3.2
1	C	559	ARG	3.2
1	A	1172	ILE	3.2
1	C	1151	HIS	3.2
1	A	477	VAL	3.1
1	C	268	GLY	3.1
1	C	334	VAL	3.1
1	C	893	PHE	3.0
1	C	1059	LYS	3.0
1	A	993	LEU	3.0
1	A	1163	GLU	3.0
1	C	431	ARG	3.0
1	C	844	ASP	3.0
1	C	1011	ARG	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	1122	ASN	3.0
1	C	661	ASP	2.9
1	C	663	LEU	2.9
1	C	312	GLY	2.9
1	C	309	PHE	2.9
1	C	337	ARG	2.9
1	C	837	ILE	2.9
1	C	1038	ASP	2.9
1	A	361	TYR	2.9
1	A	1054	LYS	2.9
1	A	1049	LEU	2.9
1	C	1124	ASP	2.9
1	C	556	ASN	2.8
1	A	399	ALA	2.8
1	A	1050	ASP	2.8
1	C	989	LEU	2.8
1	C	702	THR	2.8
1	A	473	LEU	2.8
1	C	568	LEU	2.8
1	C	1123	LEU	2.7
1	C	997	PRO	2.7
1	C	1035	GLN	2.7
1	A	1040	LEU	2.7
1	C	318	VAL	2.7
1	C	958	LEU	2.7
1	C	852	VAL	2.7
1	A	347	TYR	2.7
1	C	271	MET	2.6
1	C	398	PRO	2.6
1	A	476	TYR	2.6
1	A	1002	TRP	2.6
1	C	1021	LYS	2.6
1	C	922	ALA	2.6
1	C	308	LYS	2.6
1	A	402	LEU	2.6
1	A	683	LYS	2.6
1	C	244	ALA	2.6
1	C	707	ASP	2.6
1	A	1180	TYR	2.6
1	C	681	PRO	2.6
1	C	1084	ARG	2.6
1	C	1069	ARG	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	423	GLN	2.6
1	C	649	GLY	2.6
1	C	1088	THR	2.6
1	C	332	PHE	2.5
1	C	452	THR	2.5
1	C	671	GLU	2.5
1	C	924	LEU	2.5
1	A	885	GLN	2.5
1	C	586	ALA	2.5
1	C	928	LYS	2.5
1	A	1168	GLN	2.5
1	C	921	ALA	2.5
1	C	1031	ASP	2.5
1	C	1046	ALA	2.5
1	C	1170	GLN	2.5
1	A	857	GLU	2.4
1	C	931	ILE	2.4
1	C	1077	GLN	2.4
1	C	1056	PRO	2.4
1	C	974	LEU	2.4
1	C	1051	ALA	2.4
1	C	652	LEU	2.4
1	C	847	LEU	2.4
1	C	613	LEU	2.4
1	C	653	ASN	2.4
1	A	855	HIS	2.4
1	C	607	ARG	2.3
1	C	688	TRP	2.3
1	A	1014	LYS	2.3
1	A	1112	ILE	2.3
1	C	1154	THR	2.3
1	A	1126	VAL	2.3
1	C	473	LEU	2.3
1	A	669	ASP	2.3
1	C	895	PHE	2.3
1	C	313	ARG	2.2
1	A	924	LEU	2.2
1	C	336	GLY	2.2
1	C	956	SER	2.2
1	A	424	ARG	2.2
1	A	946	LEU	2.2
1	C	1081	SER	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	891	TYR	2.2
1	C	1044	ASN	2.2
1	A	1008	GLU	2.2
1	C	888	GLU	2.2
1	A	891	TYR	2.2
1	C	1071	GLN	2.2
1	A	397	THR	2.2
1	A	1173	ASP	2.2
1	C	542	GLY	2.2
1	A	1133	LEU	2.1
1	C	323	LEU	2.1
1	C	1115	LEU	2.1
1	C	600	VAL	2.1
1	C	1147	LYS	2.1
1	A	1033	LEU	2.1
1	A	1074	SER	2.1
1	C	689	ILE	2.1
1	C	836	VAL	2.1
1	C	349	LYS	2.1
1	C	475	ARG	2.1
1	A	962	TYR	2.1
1	A	326	ILE	2.1
1	A	387	ILE	2.1
1	A	1029	VAL	2.1
1	C	385	ARG	2.1
1	C	474	GLY	2.1
1	C	625	LEU	2.1
1	A	420	SER	2.1
1	A	814	SER	2.1
1	C	279	LEU	2.1
1	C	552	LEU	2.1
1	C	321	GLN	2.1
1	C	862	GLU	2.1
1	C	476	TYR	2.0
1	A	1030	LEU	2.0
1	A	588	GLN	2.0
1	A	686	GLU	2.0
1	C	747	LEU	2.0
1	C	764	LEU	2.0
1	C	1030	LEU	2.0
1	A	375	LYS	2.0
1	C	263	ALA	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	1066	ARG	2.0
1	A	826	LYS	2.0
1	A	374	PHE	2.0
1	C	761	PRO	2.0
1	A	373	VAL	2.0
1	A	1104	LEU	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.