



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:28 AM UTC

PDB ID : 5YIM / pdb_00005yim
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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

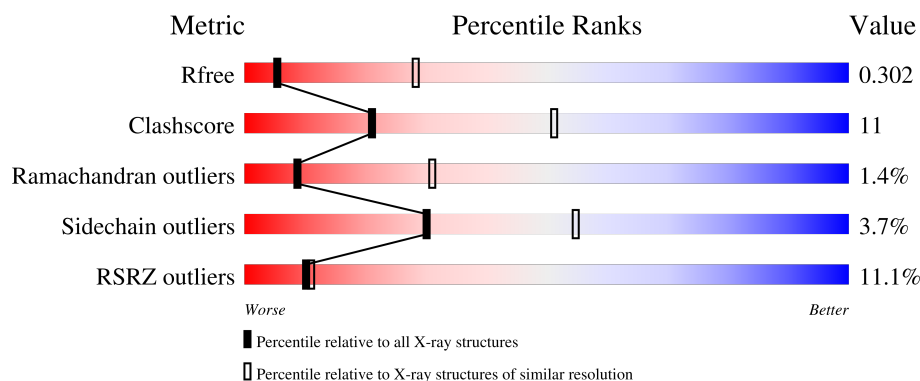
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. 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	8% 72% 23% • •
1	C	960	13% 66% 26% • 7%

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			

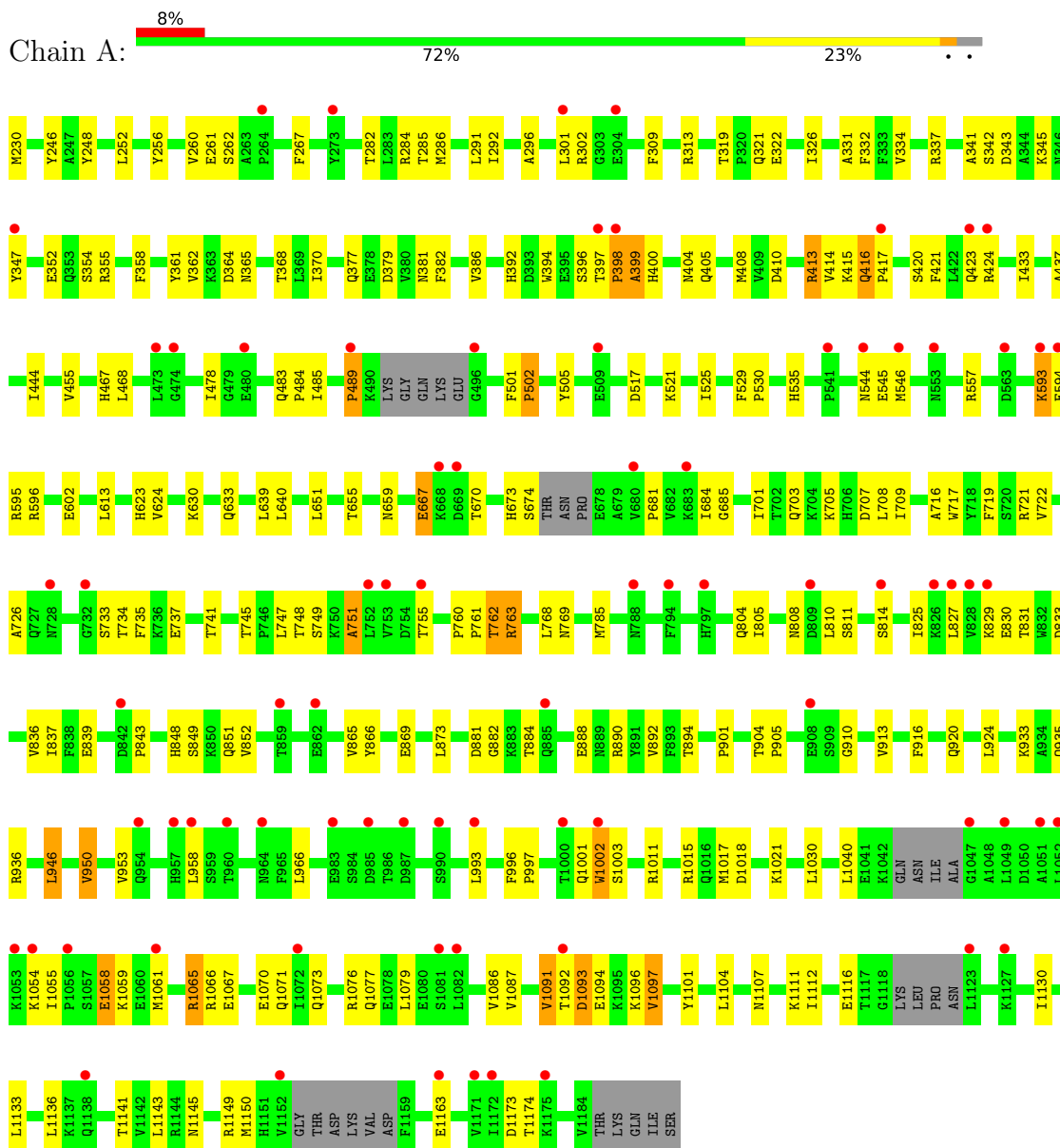
There are 2 discrepancies between the modelled and reference sequences:

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

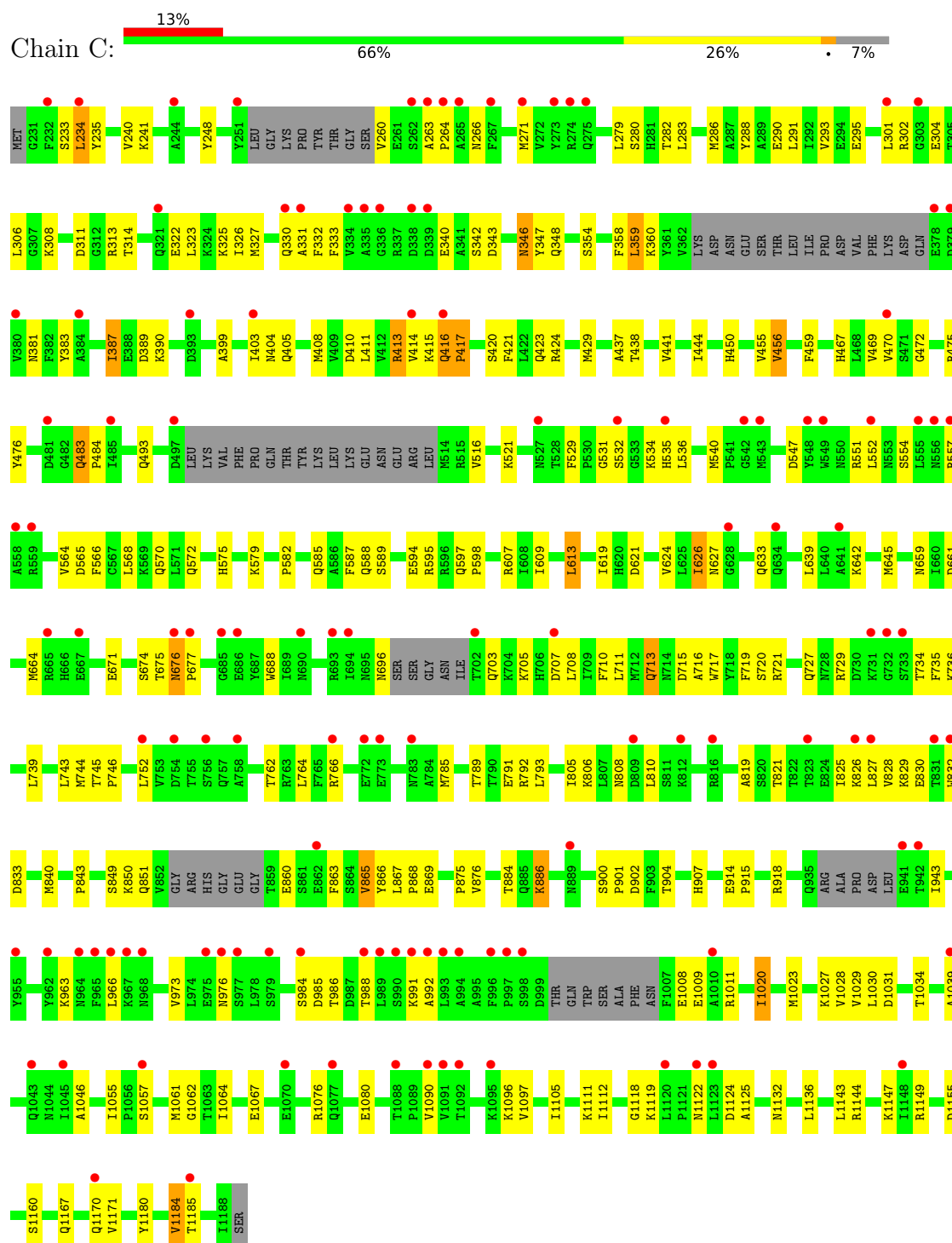
3 Residue-property plots

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: SdeA



• Molecule 1: SdeA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.65Å 295.43Å 194.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.39 50.00 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.39) 99.5 (50.00-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.251 , 0.287 0.269 , 0.302	Depositor DCC
R_{free} test set	2819 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	125.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 105.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.36	0/7419	0.84	14/10012 (0.1%)
1	C	0.36	0/6936	0.85	12/9381 (0.1%)
All	All	0.36	0/14355	0.85	26/19393 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	PRO	N-CA-CB	9.24	110.69	103.30
1	C	1064	ILE	N-CA-C	7.16	117.26	110.53
1	A	489	PRO	N-CA-CB	7.13	110.73	103.25
1	A	502	PRO	N-CA-CB	6.75	110.34	103.25
1	A	416	GLN	CA-C-N	-6.53	113.65	120.38
1	A	416	GLN	C-N-CA	-6.53	113.65	120.38
1	C	676	ASN	CA-C-N	-6.35	112.95	120.13
1	C	676	ASN	C-N-CA	-6.35	112.95	120.13
1	C	416	GLN	CA-C-N	-6.31	113.88	120.38
1	C	416	GLN	C-N-CA	-6.31	113.88	120.38
1	C	346	ASN	N-CA-C	-6.20	100.86	110.10
1	A	760	PRO	CA-C-N	6.19	127.58	119.84
1	A	760	PRO	C-N-CA	6.19	127.58	119.84
1	A	751	ALA	N-CA-C	-6.12	105.77	113.18
1	A	1059	LYS	N-CA-C	6.02	117.92	111.36
1	A	1055	ILE	CB-CA-C	-5.98	108.02	114.35
1	A	1058	GLU	N-CA-C	5.95	118.27	111.02
1	A	399	ALA	N-CA-C	5.82	117.49	111.03
1	A	370	ILE	CA-C-N	-5.77	113.73	119.56
1	A	370	ILE	C-N-CA	-5.77	113.73	119.56
1	C	263	ALA	CA-C-N	5.68	125.21	119.19
1	C	263	ALA	C-N-CA	5.68	125.21	119.19
1	C	1155	ASP	CB-CA-C	-5.64	110.05	116.54
1	C	829	LYS	N-CA-C	-5.52	105.27	111.28
1	C	483	GLN	CA-C-N	5.09	126.20	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	483	GLN	C-N-CA	5.09	126.20	119.84

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	7297	0	7103	146	0
1	C	6831	0	6555	162	0
All	All	14128	0	13658	306	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 11.

All (306) 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:806:LYS:NZ	1:C:902:ASP:O	2.22	0.70
1:C:943:ILE:HG12	1:C:1020:ILE:HG12	1.72	0.70
1:A:837:ILE:HB	1:A:892:VAL:HG12	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:405:GLN:HG3	1:A:408:MET:HE2	1.79	0.63
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:A:785:MET:HE3	1:A:808:ASN:HB2	1.80	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:C:286:MET:HB3	1:C:327:MET:HE3	1.82	0.62
1:A:904:THR:O	1:A:1149:ARG:NH1	2.32	0.61
1:C:234:LEU:HD22	1:C:327:MET:HE1	1.81	0.61
1:C:785:MET:HE3	1:C:805:ILE:HG23	1.81	0.61
1:A:849:SER:HB3	1:A:865:VAL:HG22	1.83	0.60
1:C:664:MET:HE2	1:C:744:MET:HE3	1.84	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
1:A:364:ASP:OD1	1:A:365:ASN:N	2.35	0.60
1:C:943:ILE:HD11	1:C:1023:MET:HE1	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:613:LEU:HD21	1:A:747:LEU:HD11	1.87	0.56
1:A:1001:GLN:O	1:A:1003:SER:N	2.35	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:283:LEU:HD22	1:C:568:LEU:HD21	1.89	0.55
1:C:483:GLN:N	1:C:483:GLN:OE1	2.35	0.55
1:C:1147:LYS:HZ3	1:C:1160:SER:HA	1.71	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:593:LYS:O	1:A:593:LYS:NZ	2.32	0.54
1:A:1002:TRP:HH2	1:A:1017:MET:HG2	1.73	0.54
1:C:992:ALA:HB2	1:C:1028:VAL:HG11	1.89	0.54
1:A:313:ARG:HH22	1:A:398:PRO:HG3	1.74	0.53
1:A:1076:ARG:HA	1:A:1079:LEU:HD12	1.90	0.53
1:C:399:ALA:O	1:C:403:ILE:HG22	2.08	0.53
1:C:1144:ARG:NH2	1:C:1167:GLN:OE1	2.41	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:785:MET:HE2	1:C:875:PRO:HD2	1.93	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:394:TRP:C	1:A:396:SER:H	2.20	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:256:TYR:HD2	1:A:262:SER:HB2	1.77	0.49
1:A:260:VAL:O	1:A:262:SER:N	2.45	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
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:A:1097:VAL:HG13	1:A:1150:MET:HE3	1.95	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:595:ARG:NH1	1:A:866:TYR:O	2.46	0.49
1:A:709:ILE:HG22	1:A:852:VAL:HG13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:GLN:HE22	1:A:1030:LEU:HD22	1.77	0.49
1:C:832:TRP:H	1:C:832:TRP:CD1	2.31	0.48
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:A:924:LEU:HG	1:A:1073:GLN:CD	2.39	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:C:240:VAL:HG11	1:C:327:MET:HE2	1.96	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:OD1	1:C:621:ASP:N	2.48	0.46
1:A:417:PRO:HD2	1:A:421:PHE:CE2	2.51	0.46
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:C:869:GLU:HG3	1:C:904:THR:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:761:PRO:C	1:A:763:ARG:H	2.25	0.45
1:C:469:VAL:HG22	1:C:476:TYR:CE2	2.51	0.45
1:C:1030:LEU:O	1:C:1034:THR:HG23	2.16	0.45
1:A:396:SER:HB3	1:A:400:HIS:CG	2.51	0.45
1:A:996:PHE:CE1	1:A:1017:MET:HE3	2.50	0.45
1:A:1067:GLU:O	1:A:1070:GLU:HG3	2.16	0.45
1:A:633:GLN:HB2	1:A:735:PHE:HD1	1.81	0.45
1:A:901:PRO:HG3	1:A:1091:VAL:HG23	1.97	0.45
1:C:288:TYR:HE2	1:C:410:ASP:HB2	1.82	0.45
1:C:642:LYS:HD2	1:C:907:HIS:CG	2.52	0.45
1:C:867:LEU:HD12	1:C:868:PRO:HD2	1.99	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:A:785:MET:HE2	1:A:805:ILE:HA	1.98	0.45
1:C:286:MET:HE2	1:C:331:ALA:HA	1.99	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:A:881:ASP:CG	1:A:882:GLY:H	2.26	0.44
1:C:248:TYR:CD1	1:C:279:LEU:HD23	2.51	0.44
1:A:953:VAL:HG21	1:A:966:LEU:HD12	2.00	0.44
1:A:785:MET:HE1	1:A:810:LEU:H	1.82	0.44
1:C:851:GLN:HB3	1:C:863:PHE:CE2	2.52	0.44
1:A:230:MET:HE3	1:A:892:VAL:HG21	2.00	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:381:ASN:HB2	1:C:383:TYR:CD2	2.53	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: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
1:C:619:ILE:O	1:C:619:ILE:HG13	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:VAL:HG11	1:A:399:ALA:HB1	1.99	0.43
1:A:749:SER:C	1:A:751:ALA:H	2.26	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:C:1061:MET:HB3	1:C:1067:GLU:CD	2.43	0.43
1:C:582:PRO:HB2	1:C:789:THR:HG23	1.99	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: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:544:ASN:ND2	1:C:416:GLN:O	2.50	0.43
1:A:882:GLY:O	1:A:890:ARG:HG2	2.18	0.43
1:A:1054:LYS:HZ2	1:A:1077:GLN:HG3	1.83	0.43
1:C:235:TYR:HB2	1:C:572:GLN:HG3	2.01	0.43
1:A:651:LEU:HD23	1:A:651:LEU:HA	1.85	0.42
1:A:1011:ARG:HE	1:A:1015:ARG:HH22	1.66	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:1092:THR:C	1:A:1094:GLU:H	2.26	0.42
1:A:420:SER:HB3	1:A:467:HIS:CE1	2.54	0.42
1:C:597:GLN:CD	1:C:598:PRO:HD2	2.45	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:534:LYS:O	1:C:536:LEU:N	2.51	0.42
1:A:416:GLN:HB2	1:A:417:PRO:HD3	2.01	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:C:1124:ASP:OD1	1:C:1124:ASP:N	2.39	0.42
1:A:737:GLU:O	1:A:741:THR:HG23	2.19	0.42
1:A:762:THR:HG23	1:A:843:PRO:HA	2.02	0.42
1:A:1101:TYR:OH	1:A:1163:GLU:OE2	2.21	0.42
1:C:325:LYS:HE3	1:C:387:ILE:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:785:MET:CE	1:C:875:PRO:HD2	2.49	0.41
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:A:1150:MET:HE2	1:A:1150:MET:HB3	1.89	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:450:HIS:ND1	1:C:540:MET:SD	2.94	0.41
1:C:1111:LYS:HA	1:C:1111:LYS:HD3	1.85	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:621:ASP:HA	1:C:736:LYS:HE3	2.03	0.41
1:C:1090:VAL:HG23	1:C:1097:VAL:HG21	2.02	0.41
1:A:286:MET:HE2	1:A:331:ALA:HA	2.02	0.41
1:A:415:LYS:HD3	1:A:421:PHE:CD1	2.55	0.41
1:A:946:LEU:O	1:A:950:VAL:HG13	2.20	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: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: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:C:1132:ASN:O	1:C:1136:LEU:HG	2.21	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
1:A:811:SER:HB2	1:A:873:LEU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:GLU:HB3	1:C:437:ALA:HB1	2.03	0.40
1:C:332:PHE:O	1:C:354:SER:HB3	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	921/960 (96%)	864 (94%)	46 (5%)	11 (1%)	10	35
1	C	880/960 (92%)	803 (91%)	63 (7%)	14 (2%)	7	29
All	All	1801/1920 (94%)	1667 (93%)	109 (6%)	25 (1%)	9	31

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
1	C	1122	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	749 (97%)	24 (3%)	35	59
1	C	702/837 (84%)	671 (96%)	31 (4%)	25	51
All	All	1475/1674 (88%)	1420 (96%)	55 (4%)	30	55

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	LEU
1	A	334	VAL
1	A	392	HIS
1	A	413	ARG
1	A	455	VAL
1	A	593	LYS
1	A	639	LEU
1	A	667	GLU
1	A	684	ILE
1	A	701	ILE
1	A	734	THR
1	A	745	THR
1	A	763	ARG
1	A	814	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	825	ILE
1	A	936	ARG
1	A	946	LEU
1	A	950	VAL
1	A	958	LEU
1	A	1002	TRP
1	A	1065	ARG
1	A	1086	VAL
1	A	1097	VAL
1	A	1174	THR
1	C	234	LEU
1	C	301	LEU
1	C	306	LEU
1	C	359	LEU
1	C	387	ILE
1	C	411	LEU
1	C	413	ARG
1	C	423	GLN
1	C	456	VAL
1	C	532	SER
1	C	552	LEU
1	C	557	ARG
1	C	564	VAL
1	C	587	PHE
1	C	613	LEU
1	C	639	LEU
1	C	696	ASN
1	C	713	GLN
1	C	792	ARG
1	C	827	LEU
1	C	865	VAL
1	C	876	VAL
1	C	886	LYS
1	C	963	LYS
1	C	966	LEU
1	C	1009	GLU
1	C	1020	ILE
1	C	1055	ILE
1	C	1170	GLN
1	C	1184	VAL
1	C	1185	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	275	GLN
1	A	276	HIS
1	A	404	ASN
1	A	423	GLN
1	A	526	GLN
1	A	550	ASN
1	A	570	GLN
1	A	695	ASN
1	A	788	ASN
1	A	851	GLN
1	A	935	GLN
1	A	1077	GLN
1	A	1135	ASN
1	C	266	ASN
1	C	321	GLN
1	C	467	HIS
1	C	623	HIS
1	C	673	HIS
1	C	804	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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	933/960 (97%)	0.49	78 (8%)	17 15	67, 108, 193, 304	0
1	C	896/960 (93%)	0.81	125 (13%)	6 8	74, 143, 235, 328	0
All	All	1829/1920 (95%)	0.65	203 (11%)	10 11	67, 123, 222, 328	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	979	SER	6.4
1	C	831	THR	6.3
1	C	976	ASN	6.0
1	C	527	ASN	5.7
1	C	497	ASP	5.7
1	C	1091	VAL	5.6
1	A	347	TYR	5.5
1	C	335	ALA	5.2
1	C	988	THR	4.9
1	A	473	LEU	4.9
1	A	755	THR	4.8
1	C	1088	THR	4.7
1	A	1061	MET	4.7
1	C	1123	LEU	4.6
1	A	541	PRO	4.5
1	C	694	ILE	4.5
1	C	303	GLY	4.4
1	A	859	THR	4.3
1	C	816	ARG	4.3
1	C	991	LYS	4.2
1	C	267	PHE	4.1
1	C	832	TRP	3.9
1	A	728	ASN	3.9
1	C	1122	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	994	ALA	3.9
1	C	1090	VAL	3.8
1	C	690	ASN	3.7
1	A	797	HIS	3.7
1	C	380	VAL	3.6
1	A	993	LEU	3.6
1	C	685	GLY	3.6
1	A	828	VAL	3.6
1	A	1172	ILE	3.6
1	C	964	ASN	3.6
1	C	558	ALA	3.5
1	C	984	SER	3.5
1	A	398	PRO	3.5
1	C	941	GLU	3.4
1	C	470	VAL	3.4
1	C	693	ARG	3.4
1	C	766	ARG	3.4
1	C	378	GLU	3.4
1	C	732	GLY	3.4
1	C	542	GLY	3.4
1	C	967	LYS	3.4
1	C	265	ALA	3.3
1	A	1000	THR	3.3
1	C	993	LEU	3.3
1	C	731	LYS	3.2
1	C	275	GLN	3.2
1	C	271	MET	3.2
1	C	321	GLN	3.2
1	C	559	ARG	3.2
1	A	546	MET	3.2
1	C	823	THR	3.2
1	C	989	LEU	3.1
1	A	264	PRO	3.1
1	A	1081	SER	3.1
1	A	417	PRO	3.1
1	A	423	GLN	3.0
1	C	628	GLY	3.0
1	C	990	SER	3.0
1	A	827	LEU	3.0
1	A	826	LYS	3.0
1	C	1043	GLN	2.9
1	A	964	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	680	VAL	2.9
1	C	1077	GLN	2.9
1	C	414	VAL	2.9
1	A	987	ASP	2.9
1	A	1175	LYS	2.9
1	A	553	ASN	2.9
1	A	985	ASP	2.9
1	C	826	LYS	2.9
1	C	665	ARG	2.8
1	A	829	LYS	2.8
1	C	968	ASN	2.8
1	A	1072	ILE	2.8
1	A	424	ARG	2.8
1	C	336	GLY	2.8
1	A	814	SER	2.8
1	C	1095	LYS	2.8
1	C	234	LEU	2.8
1	C	676	ASN	2.7
1	A	885	GLN	2.7
1	A	908	GLU	2.7
1	C	996	PHE	2.7
1	A	1123	LEU	2.7
1	A	862	GLU	2.7
1	C	772	GLU	2.7
1	C	481	ASP	2.7
1	A	1171	VAL	2.7
1	C	1045	ILE	2.7
1	A	990	SER	2.7
1	C	1039	ALA	2.7
1	C	416	GLN	2.6
1	A	1053	LYS	2.6
1	C	301	LEU	2.6
1	A	273	TYR	2.6
1	A	301	LEU	2.6
1	C	244	ALA	2.6
1	A	752	LEU	2.6
1	A	1051	ALA	2.6
1	C	997	PRO	2.6
1	A	842	ASP	2.6
1	C	889	ASN	2.6
1	C	702	THR	2.6
1	C	535	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	262	SER	2.5
1	C	274	ARG	2.5
1	A	563	ASP	2.5
1	C	485	ILE	2.5
1	C	1148	ILE	2.5
1	A	1056	PRO	2.5
1	C	1120	LEU	2.5
1	C	686	GLU	2.5
1	C	1070	GLU	2.5
1	C	552	LEU	2.5
1	C	384	ALA	2.5
1	A	809	ASP	2.5
1	C	965	PHE	2.5
1	C	733	SER	2.4
1	C	998	SER	2.4
1	A	1082	LEU	2.4
1	A	397	THR	2.4
1	A	1152	VAL	2.4
1	A	1052	LEU	2.4
1	C	827	LEU	2.4
1	C	339	ASP	2.4
1	C	812	LYS	2.4
1	C	1092	THR	2.4
1	C	556	ASN	2.4
1	C	273	TYR	2.4
1	C	809	ASP	2.4
1	C	758	ALA	2.4
1	A	496	GLY	2.3
1	C	752	LEU	2.3
1	C	667	GLU	2.3
1	C	677	PRO	2.3
1	C	942	THR	2.3
1	A	957	HIS	2.3
1	C	232	PHE	2.3
1	C	634	GLN	2.3
1	A	474	GLY	2.3
1	A	960	THR	2.3
1	C	264	PRO	2.3
1	A	1047	GLY	2.3
1	C	756	SER	2.3
1	C	783	ASN	2.3
1	A	669	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	683	LYS	2.3
1	C	773	GLU	2.3
1	A	489	PRO	2.3
1	C	331	ALA	2.3
1	C	1010	ALA	2.3
1	C	379	ASP	2.3
1	A	983	GLU	2.2
1	C	1057	SER	2.2
1	A	788	ASN	2.2
1	A	1138	GLN	2.2
1	C	334	VAL	2.2
1	A	509	GLU	2.2
1	C	1185	THR	2.2
1	C	532	SER	2.2
1	C	977	SER	2.2
1	A	544	ASN	2.2
1	C	543	MET	2.2
1	C	555	LEU	2.2
1	C	992	ALA	2.2
1	A	593	LYS	2.2
1	C	251	TYR	2.2
1	A	958	LEU	2.2
1	A	1127	LYS	2.2
1	C	557	ARG	2.2
1	A	1163	GLU	2.2
1	C	975	GLU	2.2
1	A	732	GLY	2.2
1	A	1002	TRP	2.2
1	C	966	LEU	2.1
1	C	263	ALA	2.1
1	A	794	PHE	2.1
1	C	549	TRP	2.1
1	C	548	TYR	2.1
1	C	962	TYR	2.1
1	C	338	ASP	2.1
1	A	1092	THR	2.1
1	C	641	ALA	2.1
1	A	668	LYS	2.1
1	C	862	GLU	2.1
1	C	955	TYR	2.1
1	A	954	GLN	2.1
1	C	330	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	594	GLU	2.1
1	C	403	ILE	2.0
1	C	1170	GLN	2.0
1	A	480	GLU	2.0
1	A	1049	LEU	2.0
1	C	393	ASP	2.0
1	C	707	ASP	2.0
1	C	754	ASP	2.0
1	A	1054	LYS	2.0
1	A	304	GLU	2.0
1	A	753	VAL	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 oligosaccharides 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.