



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:38 PM UTC

PDB ID : 3WY7 / pdb_00003wy7
Title : Crystal structure of Mycobacterium smegmatis 7-Keto-8-aminopelargonic acid (KAPA) synthase BioF
Authors : Fan, S.H.; Li, D.F.; Wang, D.C.; Chen, G.J.; Zhang, X.E.; Bi, L.J.
Deposited on : 2014-08-20
Resolution : 2.30 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

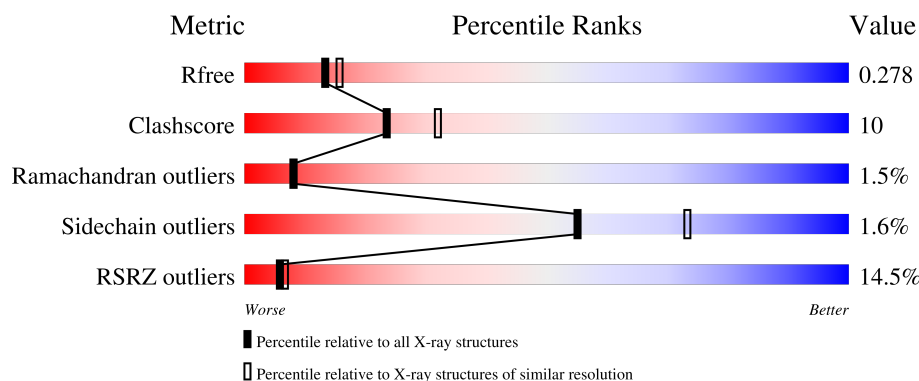
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 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	404	10% 70% 15% • 14%
1	B	404	19% 71% 17% • 9%
1	C	404	7% 73% 11% • 14%
1	D	404	15% 73% 17% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10713 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 8-amino-7-oxononanoate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2477	1533	458	480	6			
1	B	369	Total	C	N	O	S	0	0	0
			2666	1648	500	512	6			
1	C	346	Total	C	N	O	S	0	0	0
			2477	1533	458	480	6			
1	D	371	Total	C	N	O	S	0	0	0
			2682	1657	505	514	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A0QX65
A	-20	GLY	-	expression tag	UNP A0QX65
A	-19	SER	-	expression tag	UNP A0QX65
A	-18	SER	-	expression tag	UNP A0QX65
A	-17	HIS	-	expression tag	UNP A0QX65
A	-16	HIS	-	expression tag	UNP A0QX65
A	-15	HIS	-	expression tag	UNP A0QX65
A	-14	HIS	-	expression tag	UNP A0QX65
A	-13	HIS	-	expression tag	UNP A0QX65
A	-12	HIS	-	expression tag	UNP A0QX65
A	-11	SER	-	expression tag	UNP A0QX65
A	-10	SER	-	expression tag	UNP A0QX65
A	-9	GLY	-	expression tag	UNP A0QX65
A	-8	GLU	-	expression tag	UNP A0QX65
A	-7	ASN	-	expression tag	UNP A0QX65
A	-6	LEU	-	expression tag	UNP A0QX65
A	-5	TYR	-	expression tag	UNP A0QX65
A	-4	PHE	-	expression tag	UNP A0QX65
A	-3	GLN	-	expression tag	UNP A0QX65
A	-2	GLY	-	expression tag	UNP A0QX65
A	-1	HIS	-	expression tag	UNP A0QX65

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP A0QX65
B	-21	MET	-	expression tag	UNP A0QX65
B	-20	GLY	-	expression tag	UNP A0QX65
B	-19	SER	-	expression tag	UNP A0QX65
B	-18	SER	-	expression tag	UNP A0QX65
B	-17	HIS	-	expression tag	UNP A0QX65
B	-16	HIS	-	expression tag	UNP A0QX65
B	-15	HIS	-	expression tag	UNP A0QX65
B	-14	HIS	-	expression tag	UNP A0QX65
B	-13	HIS	-	expression tag	UNP A0QX65
B	-12	HIS	-	expression tag	UNP A0QX65
B	-11	SER	-	expression tag	UNP A0QX65
B	-10	SER	-	expression tag	UNP A0QX65
B	-9	GLY	-	expression tag	UNP A0QX65
B	-8	GLU	-	expression tag	UNP A0QX65
B	-7	ASN	-	expression tag	UNP A0QX65
B	-6	LEU	-	expression tag	UNP A0QX65
B	-5	TYR	-	expression tag	UNP A0QX65
B	-4	PHE	-	expression tag	UNP A0QX65
B	-3	GLN	-	expression tag	UNP A0QX65
B	-2	GLY	-	expression tag	UNP A0QX65
B	-1	HIS	-	expression tag	UNP A0QX65
B	0	MET	-	expression tag	UNP A0QX65
C	-21	MET	-	expression tag	UNP A0QX65
C	-20	GLY	-	expression tag	UNP A0QX65
C	-19	SER	-	expression tag	UNP A0QX65
C	-18	SER	-	expression tag	UNP A0QX65
C	-17	HIS	-	expression tag	UNP A0QX65
C	-16	HIS	-	expression tag	UNP A0QX65
C	-15	HIS	-	expression tag	UNP A0QX65
C	-14	HIS	-	expression tag	UNP A0QX65
C	-13	HIS	-	expression tag	UNP A0QX65
C	-12	HIS	-	expression tag	UNP A0QX65
C	-11	SER	-	expression tag	UNP A0QX65
C	-10	SER	-	expression tag	UNP A0QX65
C	-9	GLY	-	expression tag	UNP A0QX65
C	-8	GLU	-	expression tag	UNP A0QX65
C	-7	ASN	-	expression tag	UNP A0QX65
C	-6	LEU	-	expression tag	UNP A0QX65
C	-5	TYR	-	expression tag	UNP A0QX65
C	-4	PHE	-	expression tag	UNP A0QX65
C	-3	GLN	-	expression tag	UNP A0QX65

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0QX65
C	-1	HIS	-	expression tag	UNP A0QX65
C	0	MET	-	expression tag	UNP A0QX65
D	-21	MET	-	expression tag	UNP A0QX65
D	-20	GLY	-	expression tag	UNP A0QX65
D	-19	SER	-	expression tag	UNP A0QX65
D	-18	SER	-	expression tag	UNP A0QX65
D	-17	HIS	-	expression tag	UNP A0QX65
D	-16	HIS	-	expression tag	UNP A0QX65
D	-15	HIS	-	expression tag	UNP A0QX65
D	-14	HIS	-	expression tag	UNP A0QX65
D	-13	HIS	-	expression tag	UNP A0QX65
D	-12	HIS	-	expression tag	UNP A0QX65
D	-11	SER	-	expression tag	UNP A0QX65
D	-10	SER	-	expression tag	UNP A0QX65
D	-9	GLY	-	expression tag	UNP A0QX65
D	-8	GLU	-	expression tag	UNP A0QX65
D	-7	ASN	-	expression tag	UNP A0QX65
D	-6	LEU	-	expression tag	UNP A0QX65
D	-5	TYR	-	expression tag	UNP A0QX65
D	-4	PHE	-	expression tag	UNP A0QX65
D	-3	GLN	-	expression tag	UNP A0QX65
D	-2	GLY	-	expression tag	UNP A0QX65
D	-1	HIS	-	expression tag	UNP A0QX65
D	0	MET	-	expression tag	UNP A0QX65

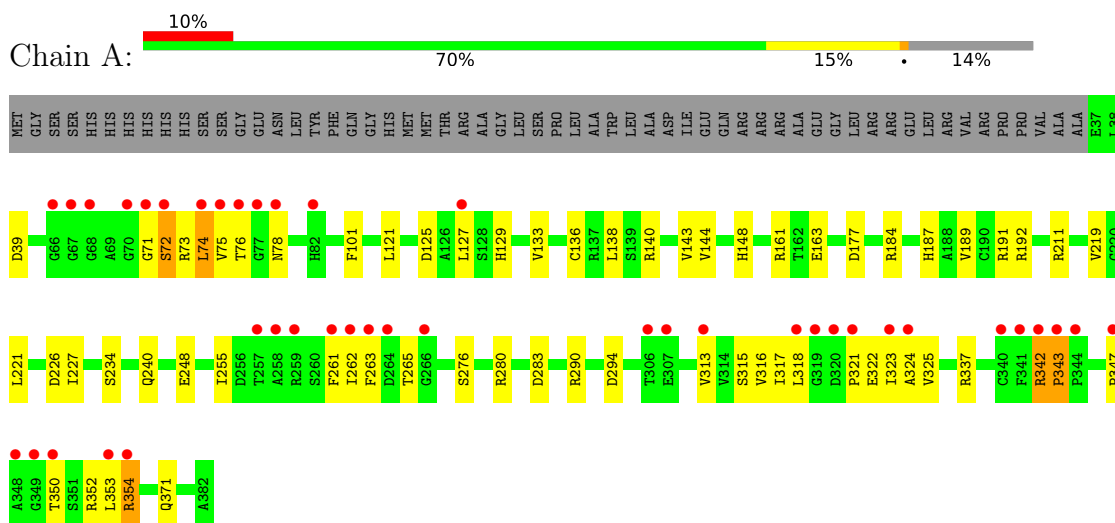
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	B	93	Total O 93 93	0	0
2	C	118	Total O 118 118	0	0
2	D	126	Total O 126 126	0	0

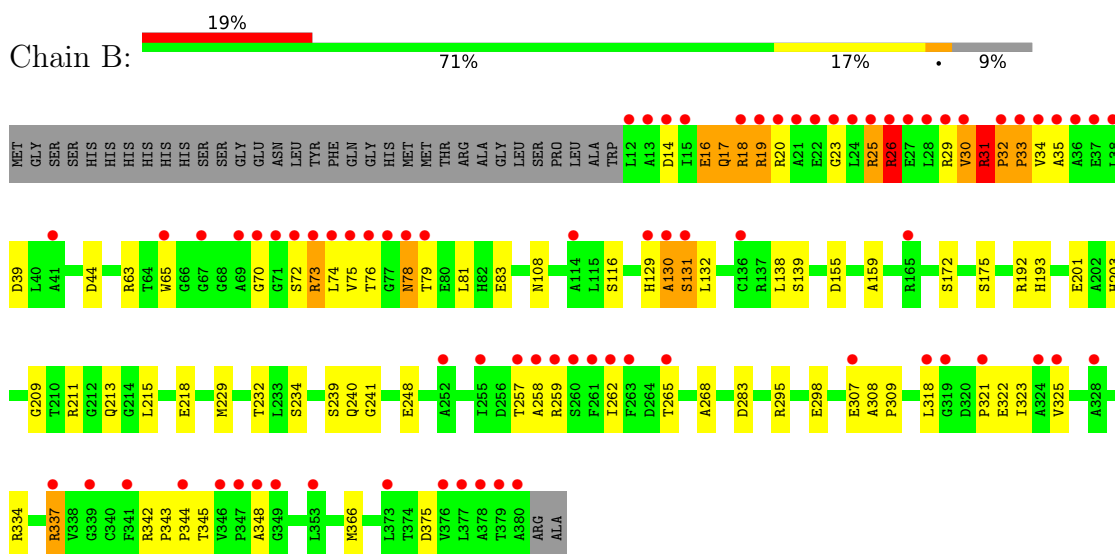
3 Residue-property plots

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.

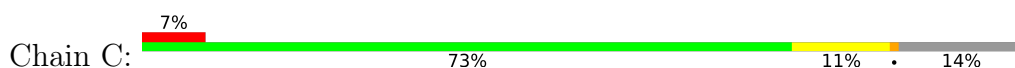
• Molecule 1: 8-amino-7-oxononanoate synthase

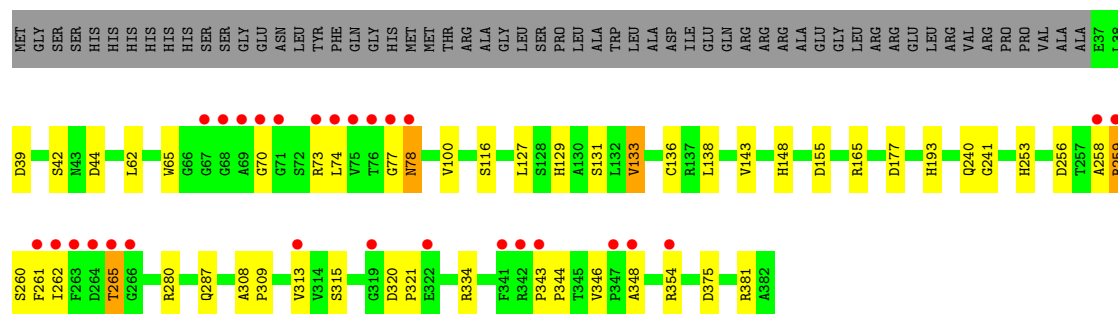


• Molecule 1: 8-amino-7-oxononanoate synthase

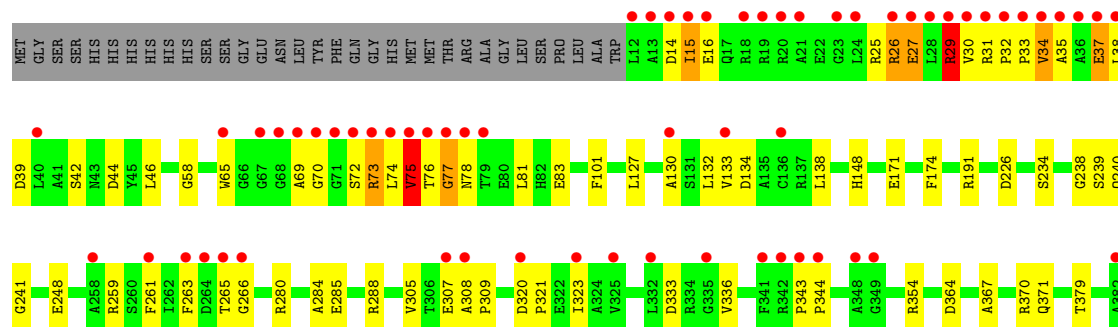
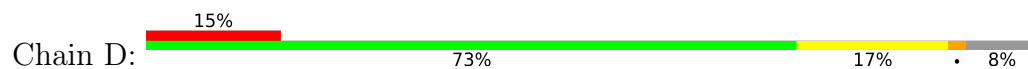


• Molecule 1: 8-amino-7-oxononanoate synthase





• Molecule 1: 8-amino-7-oxononanoate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.88Å 91.68Å 109.84Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	55.75 – 2.30 55.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (55.75-2.30) 97.8 (55.75-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.242 , 0.277 0.246 , 0.278	Depositor DCC
R_{free} test set	2000 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10713	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0923e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.37	0/2510	0.87	3/3421 (0.1%)
1	B	0.38	0/2701	0.99	14/3678 (0.4%)
1	C	0.35	0/2510	0.84	2/3421 (0.1%)
1	D	0.42	0/2717	0.94	8/3699 (0.2%)
All	All	0.39	0/10438	0.91	27/14219 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ARG	CA-C-N	13.52	134.30	120.38
1	B	31	ARG	C-N-CA	13.52	134.30	120.38
1	B	18	ARG	N-CA-C	-9.44	102.35	112.93
1	D	73	ARG	N-CA-C	8.55	122.41	109.41
1	B	19	ARG	N-CA-C	-7.72	103.47	113.12
1	D	75	VAL	N-CA-C	-7.42	106.26	113.53
1	C	259	ARG	N-CA-C	-7.24	103.92	112.89
1	D	26	ARG	N-CA-C	7.09	118.78	110.41
1	B	74	LEU	N-CA-C	-6.97	106.68	114.62
1	C	265	THR	N-CA-C	-6.88	104.88	113.20
1	B	32	PRO	N-CA-C	6.82	119.02	110.70
1	D	37	GLU	N-CA-C	6.37	118.23	109.18
1	A	343	PRO	C-N-CD	-5.97	107.46	120.60
1	A	323	ILE	N-CA-C	-5.84	104.12	112.35
1	D	37	GLU	N-CA-CB	-5.61	102.36	111.22
1	A	74	LEU	N-CA-C	-5.55	105.12	113.89
1	D	73	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	B	79	THR	N-CA-C	5.50	117.55	109.24
1	B	73	ARG	N-CA-C	5.46	118.12	109.50
1	B	130	ALA	CA-C-N	5.41	131.44	121.70
1	B	130	ALA	C-N-CA	5.41	131.44	121.70
1	D	29	ARG	N-CA-C	5.40	118.20	109.40
1	B	130	ALA	N-CA-C	5.38	119.03	107.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	GLU	N-CA-C	5.38	122.26	110.80
1	B	337	ARG	CB-CG-CD	-5.12	99.53	111.30
1	B	16	GLU	CA-C-N	-5.06	114.56	122.65
1	B	16	GLU	C-N-CA	-5.06	114.56	122.65

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	2477	0	2497	53	1
1	B	2666	0	2699	67	0
1	C	2477	0	2497	47	0
1	D	2682	0	2717	65	0
2	A	74	0	0	2	1
2	B	93	0	0	7	0
2	C	118	0	0	4	1
2	D	126	0	0	15	0
All	All	10713	0	10410	211	2

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 (211) 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:D:73:ARG:NH1	1:D:83:GLU:OE2	1.95	1.00
1:A:75:VAL:HG23	1:A:76:THR:H	1.30	0.96
1:B:343:PRO:HG3	1:B:348:ALA:HA	1.56	0.87
1:B:73:ARG:HH12	1:B:83:GLU:HG3	1.42	0.84
1:D:72:SER:HB2	1:D:265:THR:HA	1.61	0.82
1:A:315:SER:OG	1:A:354:ARG:NH1	2.13	0.81
1:B:29:ARG:HG3	1:B:30:VAL:HB	1.63	0.79
1:B:108:ASN:ND2	1:B:131:SER:OG	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:HA	1:A:325:VAL:HG12	1.66	0.78
1:C:260:SER:O	2:C:479:HOH:O	2.01	0.78
1:B:39:ASP:HB2	1:B:337:ARG:HH21	1.50	0.77
1:A:255:ILE:HG22	1:B:29:ARG:HG2	1.67	0.76
1:D:73:ARG:HH12	1:D:83:GLU:CD	1.93	0.76
1:D:305:VAL:O	2:D:419:HOH:O	2.02	0.76
1:B:322:GLU:HA	1:B:325:VAL:HG22	1.68	0.75
1:D:379:THR:O	2:D:499:HOH:O	2.05	0.75
1:D:37:GLU:CD	1:D:38:LEU:H	1.97	0.72
1:C:116:SER:O	1:C:165:ARG:NH1	2.22	0.72
1:C:321:PRO:HB3	1:C:343:PRO:HD2	1.72	0.71
1:A:127:LEU:HD13	1:A:148:HIS:HB2	1.72	0.71
1:B:73:ARG:HD2	1:B:78:ASN:HB2	1.72	0.70
1:A:184:ARG:NH2	1:A:219:VAL:O	2.24	0.69
1:D:354:ARG:NH2	2:D:468:HOH:O	2.24	0.69
1:B:318:LEU:HB3	1:B:323:ILE:HD11	1.73	0.69
1:C:240:GLN:HE22	1:D:240:GLN:HE22	1.41	0.69
1:B:108:ASN:HD22	1:B:131:SER:HG	1.40	0.68
1:D:280:ARG:NH2	2:D:501:HOH:O	2.14	0.68
1:D:333:ASP:OD1	2:D:508:HOH:O	2.12	0.68
1:C:155:ASP:OD1	1:C:193:HIS:NE2	2.28	0.66
1:B:16:GLU:O	1:B:19:ARG:HB3	1.94	0.66
1:D:44:ASP:OD1	2:D:410:HOH:O	2.12	0.66
1:A:74:LEU:HD22	1:B:29:ARG:HD2	1.78	0.66
1:C:313:VAL:HG12	1:C:354:ARG:HD2	1.78	0.66
1:D:31:ARG:NH2	2:D:498:HOH:O	2.28	0.65
1:D:25:ARG:NH2	2:D:434:HOH:O	2.29	0.64
1:A:265:THR:HG21	1:B:234:SER:HB2	1.81	0.63
1:B:130:ALA:HA	1:B:132:LEU:N	2.13	0.63
1:A:72:SER:OG	1:A:73:ARG:N	2.31	0.63
1:D:37:GLU:OE2	1:D:336:VAL:HA	1.98	0.63
1:A:76:THR:HA	1:B:31:ARG:HH22	1.64	0.63
1:C:42:SER:HB2	1:D:70:GLY:HA3	1.80	0.62
1:B:130:ALA:HA	1:B:132:LEU:H	1.63	0.62
1:A:74:LEU:HD11	1:A:262:ILE:HG12	1.81	0.62
1:A:138:LEU:HD13	1:B:138:LEU:HD13	1.81	0.61
1:A:240:GLN:OE1	1:B:268:ALA:N	2.29	0.61
1:B:14:ASP:O	1:B:18:ARG:HG2	2.01	0.61
1:D:371:GLN:OE1	2:D:514:HOH:O	2.16	0.59
1:A:187:HIS:HD1	1:A:221:LEU:HD22	1.67	0.59
1:B:73:ARG:HG2	1:B:78:ASN:H	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:SER:HA	1:C:354:ARG:HD3	1.85	0.59
1:B:44:ASP:OD1	2:B:401:HOH:O	2.15	0.59
1:D:39:ASP:OD2	1:D:42:SER:HB3	2.03	0.58
1:A:276:SER:OG	1:A:280:ARG:NH2	2.37	0.58
1:A:321:PRO:HB3	1:A:342:ARG:HG2	1.85	0.57
1:A:317:ILE:HG12	1:A:352:ARG:HE	1.70	0.57
1:C:315:SER:HB3	1:C:354:ARG:CZ	2.35	0.57
1:C:265:THR:HG21	1:D:234:SER:HB2	1.87	0.57
1:A:127:LEU:HD22	1:A:148:HIS:CG	2.40	0.56
1:C:334:ARG:NH2	1:C:375:ASP:OD2	2.36	0.56
1:D:37:GLU:CD	1:D:38:LEU:N	2.62	0.56
1:C:73:ARG:HA	1:C:77:GLY:HA3	1.88	0.56
1:B:31:ARG:HH21	1:B:33:PRO:HD3	1.72	0.55
1:A:313:VAL:C	1:A:354:ARG:HH21	2.14	0.55
1:A:72:SER:HA	1:A:265:THR:HA	1.86	0.55
1:B:73:ARG:HD2	1:B:78:ASN:CB	2.37	0.54
1:A:71:GLY:HA3	1:A:75:VAL:HG21	1.89	0.54
1:B:19:ARG:O	1:B:23:GLY:N	2.40	0.54
1:C:177:ASP:C	1:C:354:ARG:HH22	2.16	0.54
1:C:44:ASP:OD1	2:C:401:HOH:O	2.18	0.54
1:B:30:VAL:HG22	1:B:31:ARG:H	1.73	0.54
1:B:307:GLU:OE1	1:B:307:GLU:N	2.37	0.53
1:A:74:LEU:HD12	1:A:262:ILE:HG23	1.89	0.53
1:B:39:ASP:HB2	1:B:337:ARG:NH2	2.23	0.53
1:C:131:SER:HA	1:D:263:PHE:CE2	2.44	0.53
1:D:127:LEU:HD13	1:D:148:HIS:HB2	1.91	0.53
1:B:39:ASP:CB	1:B:337:ARG:HH21	2.21	0.52
1:C:177:ASP:HA	1:C:354:ARG:HH21	1.74	0.52
1:B:25:ARG:NH1	2:B:450:HOH:O	2.43	0.52
1:B:345:THR:N	2:B:472:HOH:O	2.28	0.52
1:C:280:ARG:NH2	2:C:462:HOH:O	2.42	0.52
1:B:72:SER:OG	1:B:262:ILE:O	2.23	0.52
1:B:129:HIS:ND1	1:B:131:SER:HB2	2.25	0.52
1:D:284:ALA:O	2:D:471:HOH:O	2.19	0.52
1:B:17:GLN:HA	1:B:20:ARG:H	1.75	0.52
1:D:69:ALA:N	2:D:408:HOH:O	2.43	0.51
1:D:364:ASP:OD2	2:D:441:HOH:O	2.19	0.51
1:B:209:GLY:N	1:B:218:GLU:OE1	2.38	0.51
1:C:240:GLN:HG2	1:C:241:GLY:N	2.23	0.51
1:D:65:TRP:CD1	1:D:81:LEU:HD22	2.46	0.51
1:B:334:ARG:HH12	1:B:375:ASP:HB3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:NH2	1:A:283:ASP:O	2.44	0.51
1:B:155:ASP:OD1	1:B:193:HIS:NE2	2.40	0.50
1:B:73:ARG:CG	1:B:78:ASN:H	2.25	0.50
1:A:371:GLN:NE2	2:A:473:HOH:O	2.21	0.50
1:A:189:VAL:HG22	1:A:192:ARG:NH2	2.27	0.50
1:D:240:GLN:HG2	1:D:241:GLY:N	2.26	0.50
1:A:318:LEU:HD12	1:A:324:ALA:HA	1.95	0.49
1:B:73:ARG:NH1	1:B:83:GLU:HG3	2.20	0.49
1:D:320:ASP:O	1:D:323:ILE:HG22	2.12	0.49
1:A:263:PHE:HD2	1:B:130:ALA:O	1.96	0.49
1:A:290:ARG:NH2	1:A:294:ASP:OD1	2.46	0.49
1:D:130:ALA:HA	1:D:133:VAL:HG23	1.94	0.49
1:A:177:ASP:HA	1:A:354:ARG:HH12	1.77	0.49
1:D:46:LEU:HD22	1:D:288:ARG:HG2	1.95	0.49
1:A:75:VAL:HG23	1:A:76:THR:N	2.11	0.49
1:D:321:PRO:HB3	1:D:343:PRO:HD2	1.95	0.49
1:C:240:GLN:HE22	1:D:240:GLN:NE2	2.07	0.49
1:C:321:PRO:HD3	1:C:348:ALA:O	2.13	0.49
1:A:136:CYS:HB3	1:A:143:VAL:HG21	1.95	0.48
1:A:75:VAL:CG2	1:A:76:THR:H	2.12	0.48
1:D:83:GLU:N	1:D:83:GLU:OE1	2.47	0.48
1:C:315:SER:HB3	1:C:354:ARG:NE	2.29	0.48
1:C:65:TRP:CZ3	1:D:34:VAL:HA	2.49	0.47
1:A:187:HIS:O	1:A:187:HIS:HD2	1.98	0.47
1:C:138:LEU:HG	1:D:138:LEU:HD13	1.97	0.47
1:A:187:HIS:ND1	1:A:227:ILE:HD11	2.30	0.47
1:C:74:LEU:HD22	1:C:262:ILE:HD11	1.97	0.47
1:A:177:ASP:HA	1:A:354:ARG:NH1	2.29	0.46
1:C:73:ARG:HH21	1:C:261:PHE:HE1	1.62	0.46
1:D:14:ASP:OD1	1:D:15:ILE:N	2.47	0.46
1:C:73:ARG:HB3	1:C:78:ASN:H	1.81	0.46
1:A:347:PRO:HG2	1:A:350:THR:CG2	2.46	0.46
1:B:155:ASP:OD1	1:B:192:ARG:NH2	2.49	0.46
1:D:73:ARG:HH21	1:D:75:VAL:HA	1.80	0.46
1:C:320:ASP:OD1	1:C:321:PRO:HD2	2.15	0.46
2:A:430:HOH:O	1:C:287:GLN:HB3	2.16	0.46
1:B:211:ARG:NH2	1:B:283:ASP:OD1	2.48	0.46
1:C:177:ASP:HA	1:C:354:ARG:NH2	2.31	0.45
1:D:367:ALA:HA	1:D:370:ARG:NH1	2.30	0.45
1:A:101:PHE:CE2	1:A:261:PHE:HB2	2.52	0.45
1:B:201:GLU:HB2	1:B:229:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ARG:HB2	1:B:213:GLN:CD	2.41	0.45
1:D:73:ARG:HG3	1:D:74:LEU:N	2.26	0.45
1:A:234:SER:HB2	1:B:265:THR:HG21	1.98	0.45
1:D:354:ARG:NH1	2:D:495:HOH:O	2.50	0.45
1:A:125:ASP:O	1:A:129:HIS:HB2	2.17	0.45
1:A:187:HIS:HD1	1:A:227:ILE:HD11	1.81	0.45
1:B:31:ARG:HG2	1:B:32:PRO:N	2.30	0.45
1:B:175:SER:OG	1:B:203:HIS:NE2	2.37	0.45
1:C:136:CYS:HB3	1:C:143:VAL:HG21	1.99	0.45
1:C:381:ARG:NH2	2:C:511:HOH:O	2.45	0.45
1:D:266:GLY:HA2	2:D:417:HOH:O	2.17	0.44
1:A:255:ILE:CG2	1:B:29:ARG:HG2	2.41	0.44
1:A:316:VAL:HB	1:A:353:LEU:HB2	1.98	0.44
1:C:177:ASP:C	1:C:354:ARG:NH2	2.75	0.44
1:B:26:ARG:HG2	1:B:342:ARG:NH2	2.31	0.44
1:C:256:ASP:HB2	1:D:29:ARG:NH2	2.33	0.44
1:C:262:ILE:HD13	1:C:262:ILE:HA	1.82	0.44
1:D:15:ILE:HG22	1:D:16:GLU:HG3	1.99	0.44
1:D:29:ARG:HG2	1:D:29:ARG:HH11	1.82	0.44
1:B:63:ARG:NH1	2:B:492:HOH:O	2.42	0.44
1:B:343:PRO:HA	1:B:344:PRO:HA	1.66	0.44
1:C:259:ARG:HD2	1:D:134:ASP:OD1	2.18	0.44
1:D:191:ARG:NE	1:D:226:ASP:OD2	2.40	0.44
1:B:73:ARG:HH12	1:B:83:GLU:CG	2.22	0.44
1:D:239:SER:OG	1:D:240:GLN:N	2.50	0.44
1:D:73:ARG:HD2	1:D:78:ASN:HB2	2.00	0.44
1:D:307:GLU:H	1:D:307:GLU:CD	2.25	0.44
1:B:75:VAL:HG13	1:B:76:THR:HG22	2.00	0.43
1:D:101:PHE:CE2	1:D:261:PHE:HB2	2.53	0.43
1:B:239:SER:OG	1:B:240:GLN:N	2.51	0.43
1:A:161:ARG:NE	1:A:163:GLU:O	2.51	0.43
1:B:18:ARG:HD3	1:B:18:ARG:N	2.32	0.43
1:C:262:ILE:HG23	1:C:262:ILE:HD12	1.79	0.43
1:D:259:ARG:HG2	1:D:263:PHE:CE2	2.53	0.43
1:C:240:GLN:NE2	1:D:240:GLN:HE22	2.12	0.43
1:A:39:ASP:OD2	1:A:337:ARG:NH2	2.51	0.43
1:A:191:ARG:HH21	1:A:226:ASP:CG	2.26	0.43
1:A:127:LEU:HD22	1:A:148:HIS:CD2	2.53	0.43
1:B:65:TRP:CD1	1:B:81:LEU:HD22	2.54	0.43
1:B:240:GLN:HG2	1:B:241:GLY:N	2.33	0.43
1:B:298:GLU:OE2	2:B:444:HOH:O	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:PRO:HA	1:C:344:PRO:HA	1.72	0.42
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.86	0.42
1:D:127:LEU:HD22	1:D:148:HIS:CG	2.55	0.42
1:A:71:GLY:C	1:A:265:THR:HG23	2.45	0.42
1:C:65:TRP:HZ3	1:D:34:VAL:HA	1.84	0.42
1:C:253:HIS:CD2	1:C:253:HIS:C	2.97	0.42
1:A:313:VAL:HB	1:A:354:ARG:HE	1.84	0.42
1:B:232:THR:N	2:B:449:HOH:O	2.52	0.42
1:C:62:LEU:HD11	1:D:58:GLY:HA3	2.02	0.42
1:D:29:ARG:HG2	1:D:29:ARG:NH1	2.34	0.42
1:B:172:SER:HB2	1:B:215:LEU:HB3	2.02	0.42
1:D:27:GLU:CD	1:D:29:ARG:HH12	2.27	0.42
1:C:39:ASP:OD2	1:C:42:SER:HB3	2.20	0.42
1:C:308:ALA:HA	1:C:309:PRO:HD3	1.87	0.42
1:D:72:SER:O	1:D:77:GLY:HA3	2.19	0.42
1:D:238:GLY:HA2	2:D:409:HOH:O	2.20	0.42
1:A:187:HIS:CD2	1:A:187:HIS:C	2.97	0.42
1:D:285:GLU:OE2	1:D:288:ARG:NH2	2.40	0.42
1:A:226:ASP:OD1	1:A:226:ASP:N	2.53	0.42
1:B:30:VAL:HG13	1:B:31:ARG:N	2.35	0.41
1:B:116:SER:OG	1:B:139:SER:HB2	2.19	0.41
1:A:121:LEU:HD11	1:A:144:VAL:HG22	2.03	0.41
1:A:187:HIS:ND1	1:A:221:LEU:HD22	2.33	0.41
1:B:159:ALA:HB2	1:B:193:HIS:CE1	2.55	0.41
1:B:259:ARG:NH2	2:B:488:HOH:O	2.47	0.41
1:C:313:VAL:CG1	1:C:354:ARG:HD2	2.49	0.41
1:B:26:ARG:NH1	1:B:321:PRO:HG2	2.35	0.41
1:A:342:ARG:HG2	1:A:343:PRO:HD2	2.03	0.41
1:B:31:ARG:HA	1:B:32:PRO:HD3	1.61	0.41
1:C:129:HIS:O	1:C:133:VAL:HG12	2.20	0.41
1:D:171:GLU:OE1	1:D:174:PHE:HA	2.20	0.41
1:C:73:ARG:NH2	1:C:100:VAL:O	2.53	0.41
1:D:73:ARG:O	1:D:74:LEU:HD23	2.21	0.41
1:D:343:PRO:HA	1:D:344:PRO:HA	1.77	0.41
1:C:127:LEU:HD13	1:C:148:HIS:HB2	2.03	0.41
1:D:73:ARG:NH2	1:D:75:VAL:O	2.54	0.40
1:D:308:ALA:HA	1:D:309:PRO:HD3	1.91	0.40
1:B:308:ALA:HA	1:B:309:PRO:HD3	1.91	0.40
1:B:295:ARG:NH1	1:B:366:MET:HG3	2.37	0.40

All (2) 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)
2:C:445:HOH:O	2:C:480:HOH:O[2_656]	1.84	0.36
1:A:140:ARG:NH1	2:A:464:HOH:O[2_655]	2.06	0.14

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	344/404 (85%)	332 (96%)	10 (3%)	2 (1%)	21	27
1	B	367/404 (91%)	340 (93%)	18 (5%)	9 (2%)	4	3
1	C	344/404 (85%)	327 (95%)	14 (4%)	3 (1%)	14	17
1	D	369/404 (91%)	346 (94%)	16 (4%)	7 (2%)	6	5
All	All	1424/1616 (88%)	1345 (94%)	58 (4%)	21 (2%)	8	8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	B	78	ASN
1	C	258	ALA
1	D	77	GLY
1	A	78	ASN
1	B	30	VAL
1	B	34	VAL
1	B	35	ALA
1	B	131	SER
1	C	78	ASN
1	D	30	VAL
1	D	76	THR
1	B	26	ARG
1	B	33	PRO
1	B	70	GLY
1	B	258	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	35	ALA
1	D	32	PRO
1	D	33	PRO
1	D	34	VAL
1	C	70	GLY

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	249/296 (84%)	245 (98%)	4 (2%)	55	73
1	B	268/296 (90%)	262 (98%)	6 (2%)	45	65
1	C	249/296 (84%)	247 (99%)	2 (1%)	73	86
1	D	269/296 (91%)	264 (98%)	5 (2%)	50	69
All	All	1035/1184 (87%)	1018 (98%)	17 (2%)	55	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	VAL
1	A	248	GLU
1	A	342	ARG
1	A	354	ARG
1	B	17	GLN
1	B	25	ARG
1	B	26	ARG
1	B	31	ARG
1	B	248	GLU
1	B	257	THR
1	C	133	VAL
1	C	346	VAL
1	D	15	ILE
1	D	26	ARG
1	D	29	ARG
1	D	75	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	ASN
1	C	240	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 oligosaccharides 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, 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	346/404 (85%)	0.80	41 (11%) 9 10	23, 34, 70, 86	0
1	B	369/404 (91%)	1.21	76 (20%) 2 3	26, 42, 80, 103	0
1	C	346/404 (85%)	0.59	28 (8%) 18 19	21, 32, 64, 84	0
1	D	371/404 (91%)	0.99	62 (16%) 4 5	20, 35, 81, 103	0
All	All	1432/1616 (88%)	0.90	207 (14%) 6 7	20, 35, 75, 103	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	SER	9.6
1	D	74	LEU	7.4
1	D	12	LEU	7.1
1	B	28	LEU	6.9
1	C	258	ALA	6.8
1	C	71	GLY	6.4
1	B	35	ALA	6.3
1	B	258	ALA	6.1
1	C	265	THR	5.8
1	D	77	GLY	5.6
1	B	12	LEU	5.4
1	D	34	VAL	5.3
1	B	318	LEU	5.3
1	D	24	LEU	5.2
1	C	77	GLY	5.2
1	B	70	GLY	5.2
1	A	348	ALA	5.1
1	B	36	ALA	5.0
1	D	348	ALA	5.0
1	D	78	ASN	5.0
1	B	380	ALA	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	34	VAL	4.9
1	D	75	VAL	4.9
1	D	70	GLY	4.9
1	D	266	GLY	4.9
1	B	74	LEU	4.9
1	B	71	GLY	4.8
1	C	264	ASP	4.7
1	D	35	ALA	4.7
1	A	77	GLY	4.6
1	A	264	ASP	4.6
1	A	263	PHE	4.6
1	C	70	GLY	4.5
1	B	23	GLY	4.5
1	D	28	LEU	4.5
1	A	75	VAL	4.5
1	D	30	VAL	4.4
1	A	78	ASN	4.3
1	A	72	SER	4.3
1	B	24	LEU	4.3
1	B	263	PHE	4.2
1	B	78	ASN	4.2
1	B	378	ALA	4.1
1	D	69	ALA	4.1
1	D	71	GLY	4.1
1	B	29	ARG	4.1
1	D	29	ARG	4.1
1	C	263	PHE	4.1
1	B	348	ALA	4.0
1	B	377	LEU	4.0
1	D	68	GLY	4.0
1	C	78	ASN	4.0
1	C	67	GLY	3.9
1	C	76	THR	3.9
1	D	23	GLY	3.8
1	D	15	ILE	3.8
1	D	79	THR	3.7
1	B	21	ALA	3.7
1	B	130	ALA	3.7
1	D	73	ARG	3.7
1	B	30	VAL	3.7
1	A	349	GLY	3.6
1	A	344	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	262	ILE	3.6
1	B	19	ARG	3.6
1	C	73	ARG	3.6
1	B	76	THR	3.6
1	A	347	PRO	3.6
1	C	261	PHE	3.5
1	B	255	ILE	3.5
1	B	328	ALA	3.5
1	D	335	GLY	3.5
1	B	75	VAL	3.4
1	A	323	ILE	3.4
1	D	13	ALA	3.4
1	B	262	ILE	3.4
1	B	69	ALA	3.3
1	D	382	ALA	3.3
1	B	257	THR	3.3
1	C	75	VAL	3.3
1	D	307	GLU	3.3
1	B	349	GLY	3.3
1	A	257	THR	3.3
1	D	36	ALA	3.2
1	A	74	LEU	3.2
1	D	263	PHE	3.2
1	A	318	LEU	3.2
1	B	321	PRO	3.2
1	A	261	PHE	3.1
1	A	71	GLY	3.1
1	A	258	ALA	3.1
1	B	347	PRO	3.1
1	B	341	PHE	3.1
1	B	32	PRO	3.1
1	D	344	PRO	3.1
1	D	26	ARG	3.1
1	B	15	ILE	3.1
1	B	73	ARG	3.1
1	B	27	GLU	3.1
1	A	342	ARG	3.1
1	B	72	SER	3.0
1	A	341	PHE	3.0
1	A	354	ARG	3.0
1	D	14	ASP	3.0
1	B	37	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	259	ARG	3.0
1	B	265	THR	3.0
1	D	32	PRO	2.9
1	C	74	LEU	2.9
1	A	266	GLY	2.9
1	D	343	PRO	2.9
1	D	341	PHE	2.9
1	C	319	GLY	2.9
1	D	264	ASP	2.9
1	A	343	PRO	2.8
1	B	261	PHE	2.8
1	B	22	GLU	2.8
1	A	76	THR	2.8
1	B	319	GLY	2.8
1	B	38	LEU	2.8
1	C	354	ARG	2.8
1	B	344	PRO	2.8
1	D	21	ALA	2.8
1	A	306	THR	2.8
1	D	265	THR	2.8
1	B	33	PRO	2.8
1	B	65	TRP	2.7
1	D	33	PRO	2.7
1	C	69	ALA	2.7
1	B	25	ARG	2.7
1	D	31	ARG	2.7
1	B	79	THR	2.7
1	D	76	THR	2.7
1	D	323	ILE	2.7
1	B	77	GLY	2.6
1	C	68	GLY	2.6
1	A	321	PRO	2.6
1	B	114	ALA	2.6
1	A	127	LEU	2.6
1	D	38	LEU	2.6
1	A	70	GLY	2.6
1	B	379	THR	2.6
1	B	129	HIS	2.6
1	D	37	GLU	2.6
1	D	19	ARG	2.6
1	B	13	ALA	2.6
1	B	67	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	67	GLY	2.5
1	B	260	SER	2.5
1	A	66	GLY	2.5
1	A	262	ILE	2.5
1	C	322	GLU	2.5
1	D	27	GLU	2.5
1	C	259	ARG	2.5
1	D	18	ARG	2.5
1	D	20	ARG	2.5
1	A	320	ASP	2.5
1	B	324	ALA	2.5
1	B	337	ARG	2.4
1	D	320	ASP	2.4
1	A	319	GLY	2.4
1	D	325	VAL	2.4
1	C	266	GLY	2.4
1	D	258	ALA	2.4
1	D	136	CYS	2.4
1	D	261	PHE	2.4
1	D	130	ALA	2.3
1	B	307	GLU	2.3
1	D	349	GLY	2.3
1	B	131	SER	2.3
1	B	165	ARG	2.3
1	A	313	VAL	2.3
1	B	376	VAL	2.3
1	C	313	VAL	2.3
1	D	16	GLU	2.3
1	A	67	GLY	2.3
1	A	307	GLU	2.3
1	B	325	VAL	2.3
1	A	340	CYS	2.2
1	B	14	ASP	2.2
1	B	136	CYS	2.2
1	B	18	ARG	2.2
1	B	20	ARG	2.2
1	B	26	ARG	2.2
1	D	40	LEU	2.2
1	D	332	LEU	2.2
1	C	341	PHE	2.2
1	C	347	PRO	2.2
1	A	324	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	350	THR	2.1
1	A	82	HIS	2.1
1	D	65	TRP	2.1
1	B	41	ALA	2.1
1	D	308	ALA	2.1
1	A	353	LEU	2.1
1	D	133	VAL	2.1
1	B	339	GLY	2.1
1	B	252	ALA	2.0
1	B	353	LEU	2.0
1	B	373	LEU	2.0
1	A	259	ARG	2.0
1	B	346	VAL	2.0
1	C	342	ARG	2.0
1	A	68	GLY	2.0
1	C	348	ALA	2.0
1	C	343	PRO	2.0
1	D	342	ARG	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.