Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 09:43 am BST

PDB ID	:	3WY7
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 following versions of software and data (see references ①) were used in the production of this report:

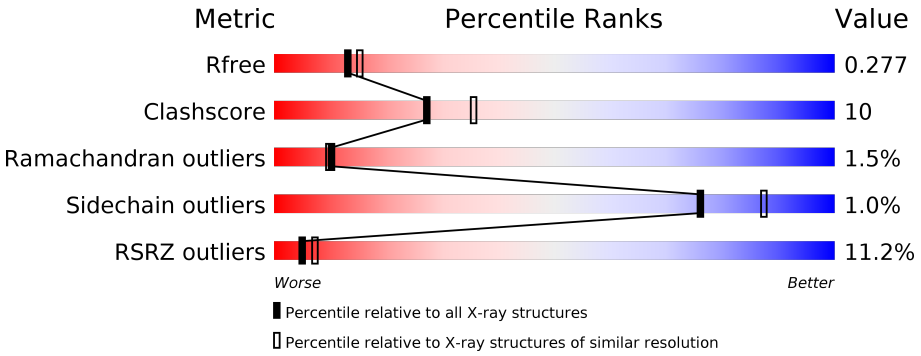
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on 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	404	7% 70% 15% • 14%
1	B	404	16% 71% 19% • 9%
1	C	404	6% 73% 12% 14%
1	D	404	11% 74% 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

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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

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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.

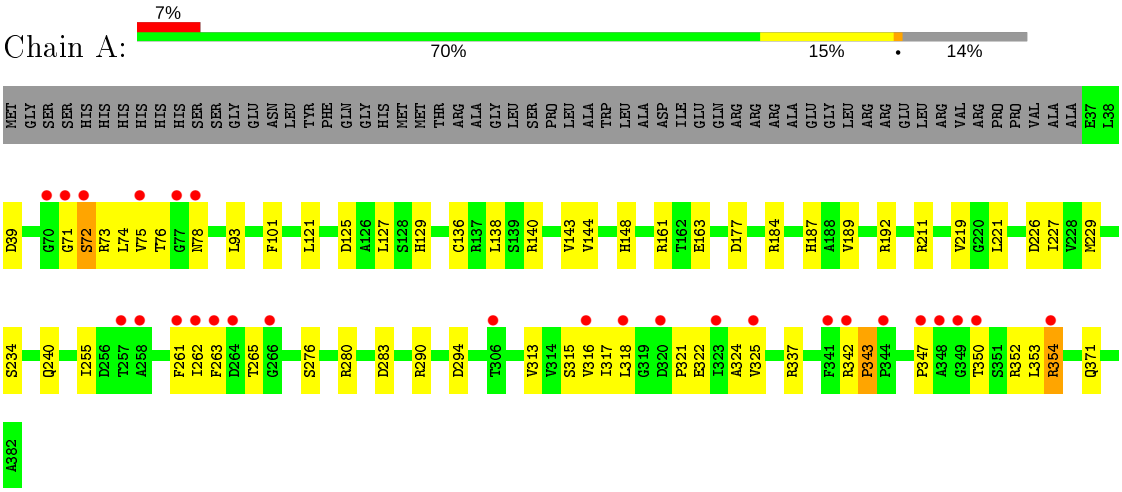
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	B	93	Total O 93 93	0	0
2	C	118	Total O 118 118	0	0
2	D	126	Total O 126 126	0	0

3 Residue-property plots (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.

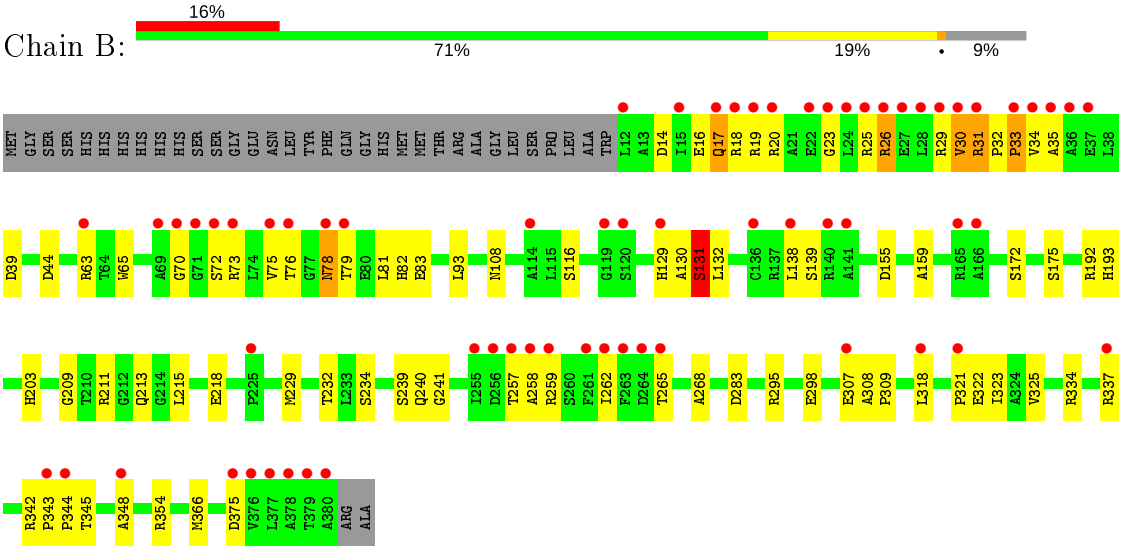
- Molecule 1: 8-amino-7-oxononanoate synthase

Chain A:



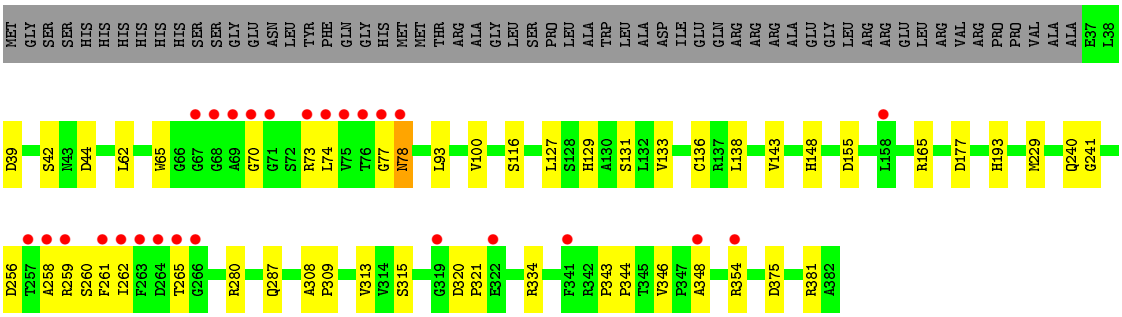
- Molecule 1: 8-amino-7-oxononanoate synthase

Chain B:

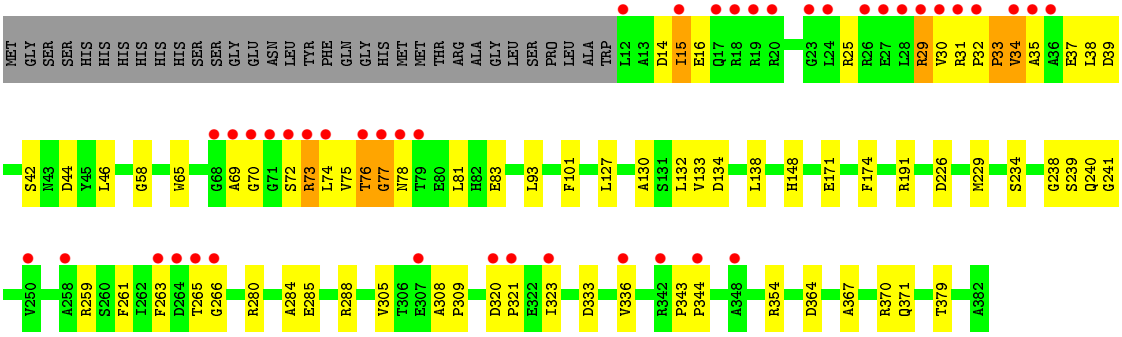


- Molecule 1: 8-amino-7-oxononanoate synthase

Chain C:



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



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.74 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.242 , 0.277 0.244 , 0.277	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)	0.33 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[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	0.27	0/2510	0.52	1/3421 (0.0%)
1	B	0.26	0/2701	0.58	0/3678
1	C	0.25	0/2510	0.50	0/3421
1	D	0.31	0/2717	0.60	2/3699 (0.1%)
All	All	0.27	0/10438	0.55	3/14219 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	73	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	A	343	PRO	C-N-CD	-5.97	107.46	120.60
1	D	73	ARG	NE-CZ-NH2	5.36	122.98	120.30

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	51	1
1	B	2666	0	2699	68	0
1	C	2477	0	2497	46	0
1	D	2682	0	2717	65	0
2	A	74	0	0	2	1
2	B	93	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	118	0	0	4	1
2	D	126	0	0	15	0
All	All	10713	0	10410	209	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 (209) 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
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: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: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:D:73:ARG:HH12	1:D:83:GLU:CD	1.93	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:D:37:GLU:CD	1:D:38:LEU:H	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:93:LEU:HD13	1:B:229:MET:HE1	1.85	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:C:73:ARG:HA	1:C:77:GLY:HA3	1.88	0.56
1:D:76:THR:OG1	1:D:77:GLY:N	2.29	0.56
1:B:31:ARG:HH21	1:B:33:PRO:HD3	1.72	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:A:75:VAL:HG23	1:A:76:THR:N	2.11	0.54
1:B:19:ARG:O	1:B:23:GLY:N	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:240:GLN:HG2	1:C:241:GLY:N	2.23	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:364:ASP:OD2	2:D:441:HOH:O	2.19	0.51
1:D:69:ALA:N	2:D:408:HOH:O	2.43	0.51
1:B:209:GLY:N	1:B:218:GLU:OE1	2.38	0.51
1:D:65:TRP:CD1	1:D:81:LEU:HD22	2.46	0.51
1:D:73:ARG:HG3	1:D:74:LEU:N	2.26	0.51
1:B:334:ARG:HH12	1:B:375:ASP:HB3	1.75	0.51
1:A:211:ARG:NH2	1:A:283:ASP:O	2.44	0.51
1:A:313:VAL:C	1:A:354:ARG:HH21	2.14	0.51
1:D:37:GLU:CD	1:D:38:LEU:N	2.62	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:C:177:ASP:C	1:C:354:ARG:HH22	2.16	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:A:93:LEU:HD13	1:A:229:MET:HE1	1.95	0.49
1:D:46:LEU:HD22	1:D:288:ARG:HG2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	1:A:187:HIS:O	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:C:93:LEU:HD13	1:C:229:MET:HE1	1.97	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
1:B:211:ARG:NH2	1:B:283:ASP:OD1	2.48	0.46
2:A:430:HOH:O	1:C:287:GLN:HB3	2.16	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: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:B:79:THR:OG1	1:B:82:HIS:ND1	2.49	0.44
1:A:316:VAL:HB	1:A:353:LEU:HB2	1.98	0.44
1:A:255:ILE:CG2	1:B:29:ARG:HG2	2.41	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:HA	1:C:262:ILE:HD13	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:343:PRO:HA	1:B:344:PRO:HA	1.66	0.44
1:B:63:ARG:NH1	2:B:492:HOH:O	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:93:LEU:HD13	1:D:229:MET:HE1	2.00	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:HD12	1:C:262:ILE:HG23	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:127:LEU:HD22	1:A:148:HIS:CD2	2.53	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
1:B:65:TRP:CD1	1:B:81:LEU:HD22	2.54	0.43
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:C:65:TRP:HZ3	1:D:34:VAL:HA	1.84	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:C:308:ALA:HA	1:C:309:PRO:HD3	1.87	0.42
1:C:39:ASP:OD2	1:C:42:SER:HB3	2.20	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:D:285:GLU:OE2	1:D:288:ARG:NH2	2.40	0.42
1:A:226:ASP:N	1:A:226:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:343:PRO:HA	1:D:344:PRO:HA	1.77	0.41
1:D:73:ARG:O	1:D:74:LEU:HD23	2.21	0.41
1:C:127:LEU:HD13	1:C:148:HIS:HB2	2.03	0.41
1:B:211:ARG:HB2	1:B:213:GLN:CD	2.41	0.40
1:D:308:ALA:HA	1:D:309:PRO:HD3	1.91	0.40
1:D:73:ARG:NH2	1:D:75:VAL:O	2.54	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%)	25 31
1	B	367/404 (91%)	340 (93%)	18 (5%)	9 (2%)	5 4
1	C	344/404 (85%)	327 (95%)	14 (4%)	3 (1%)	17 20
1	D	369/404 (91%)	346 (94%)	16 (4%)	7 (2%)	8 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1424/1616 (88%)	1345 (94%)	58 (4%)	21 (2%)	10 10

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
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 (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	249/296 (84%)	248 (100%)	1 (0%)	91 96
1	B	268/296 (90%)	263 (98%)	5 (2%)	57 73
1	C	249/296 (84%)	248 (100%)	1 (0%)	91 96
1	D	269/296 (91%)	266 (99%)	3 (1%)	73 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1035/1184 (87%)	1025 (99%)	10 (1%)	76 87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ARG
1	B	17	GLN
1	B	31	ARG
1	B	131	SER
1	B	257	THR
1	B	354	ARG
1	C	346	VAL
1	D	15	ILE
1	D	29	ARG
1	D	33	PRO

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

Mol	Chain	Res	Type
1	C	240	GLN
1	D	187	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	346/404 (85%)	0.62	27 (7%) 13 17	23, 34, 70, 86	0
1	B	369/404 (91%)	0.99	65 (17%) 1 1	26, 42, 80, 103	0
1	C	346/404 (85%)	0.45	26 (7%) 14 19	21, 32, 64, 84	0
1	D	371/404 (91%)	0.80	43 (11%) 4 6	20, 35, 81, 103	0
All	All	1432/1616 (88%)	0.72	161 (11%) 5 7	20, 35, 75, 103	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	GLY	9.7
1	D	35	ALA	9.2
1	D	72	SER	9.1
1	B	36	ALA	9.1
1	B	23	GLY	9.0
1	B	28	LEU	8.9
1	D	77	GLY	8.5
1	C	258	ALA	7.8
1	D	70	GLY	7.7
1	B	348	ALA	7.1
1	B	35	ALA	6.8
1	B	258	ALA	6.8
1	D	29	ARG	6.7
1	C	77	GLY	6.7
1	D	74	LEU	6.5
1	A	71	GLY	6.5
1	B	29	ARG	6.2
1	B	71	GLY	6.2
1	B	24	LEU	6.2
1	C	265	THR	6.1
1	B	255	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	70	GLY	5.9
1	B	263	PHE	5.9
1	D	26	ARG	5.9
1	D	266	GLY	5.8
1	C	264	ASP	5.7
1	A	78	ASN	5.3
1	A	77	GLY	5.3
1	C	70	GLY	5.3
1	D	71	GLY	5.3
1	D	69	ALA	5.2
1	A	348	ALA	5.2
1	A	347	PRO	5.0
1	B	265	THR	5.0
1	B	25	ARG	5.0
1	A	264	ASP	4.9
1	C	263	PHE	4.9
1	D	28	LEU	4.8
1	C	73	ARG	4.8
1	B	37	GLU	4.7
1	A	72	SER	4.7
1	B	78	ASN	4.5
1	D	348	ALA	4.4
1	A	75	VAL	4.3
1	B	318	LEU	4.3
1	D	30	VAL	4.2
1	B	76	THR	4.1
1	B	73	ARG	4.0
1	C	76	THR	4.0
1	B	261	PHE	4.0
1	B	165	ARG	4.0
1	D	24	LEU	3.9
1	D	23	GLY	3.9
1	C	341	PHE	3.9
1	B	379	THR	3.9
1	A	349	GLY	3.9
1	D	15	ILE	3.9
1	A	323	ILE	3.8
1	B	69	ALA	3.7
1	B	114	ALA	3.7
1	C	75	VAL	3.7
1	D	79	THR	3.7
1	A	306	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	258	ALA	3.6
1	D	78	ASN	3.6
1	B	75	VAL	3.6
1	A	318	LEU	3.5
1	D	19	ARG	3.5
1	B	26	ARG	3.5
1	A	263	PHE	3.4
1	D	20	ARG	3.4
1	D	34	VAL	3.4
1	D	76	THR	3.4
1	B	375	ASP	3.4
1	C	78	ASN	3.4
1	D	73	ARG	3.4
1	C	261	PHE	3.3
1	D	321	PRO	3.2
1	B	17	GLN	3.2
1	C	69	ALA	3.2
1	B	376	VAL	3.1
1	B	259	ARG	3.1
1	B	79	THR	3.1
1	D	32	PRO	3.1
1	B	12	LEU	3.1
1	B	257	THR	3.1
1	D	307	GLU	3.0
1	C	74	LEU	3.0
1	A	262	ILE	3.0
1	B	27	GLU	3.0
1	D	36	ALA	2.9
1	A	70	GLY	2.9
1	B	31	ARG	2.9
1	B	344	PRO	2.9
1	D	320	ASP	2.9
1	B	19	ARG	2.9
1	D	336	VAL	2.8
1	B	166	ALA	2.8
1	A	266	GLY	2.8
1	D	265	THR	2.8
1	B	307	GLU	2.8
1	B	378	ALA	2.8
1	B	20	ARG	2.8
1	C	67	GLY	2.7
1	B	377	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	18	ARG	2.7
1	C	259	ARG	2.7
1	B	22	GLU	2.6
1	C	354	ARG	2.6
1	A	344	PRO	2.6
1	D	344	PRO	2.6
1	B	136	CYS	2.6
1	A	350	THR	2.6
1	B	129	HIS	2.6
1	A	342	ARG	2.6
1	A	341	PHE	2.6
1	D	263	PHE	2.5
1	B	72	SER	2.5
1	B	33	PRO	2.5
1	B	321	PRO	2.5
1	D	250	VAL	2.5
1	C	348	ALA	2.5
1	A	354	ARG	2.5
1	B	18	ARG	2.5
1	D	12	LEU	2.5
1	B	34	VAL	2.4
1	B	120	SER	2.4
1	A	261	PHE	2.4
1	B	337	ARG	2.4
1	B	380	ALA	2.4
1	D	264	ASP	2.4
1	A	257	THR	2.4
1	B	63	ARG	2.3
1	A	325	VAL	2.3
1	A	258	ALA	2.3
1	D	323	ILE	2.3
1	D	17	GLN	2.3
1	B	138	LEU	2.2
1	B	140	ARG	2.2
1	B	225	PRO	2.2
1	C	257	THR	2.2
1	B	256	ASP	2.2
1	B	343	PRO	2.2
1	D	68	GLY	2.2
1	B	141	ALA	2.2
1	B	264	ASP	2.2
1	C	319	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	320	ASP	2.1
1	B	262	ILE	2.1
1	C	262	ILE	2.1
1	C	158	LEU	2.1
1	A	316	VAL	2.1
1	B	30	VAL	2.1
1	D	27	GLU	2.1
1	B	119	GLY	2.1
1	B	15	ILE	2.1
1	D	31	ARG	2.0
1	C	322	GLU	2.0
1	C	266	GLY	2.0
1	D	342	ARG	2.0
1	C	68	GLY	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.