Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 08:12 PM JST

PDB ID	:	8I5Z
Title	:	LDH Mutant P101Q-(An unexpected single-point mutation triggers the unleashing of catalytic potential of a NADH-dependent dehydrogenase)
Authors	:	Liu, J.Q.
Deposited on	:	2023-01-26
Resolution	:	2.65 Å(reported)

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

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

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

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

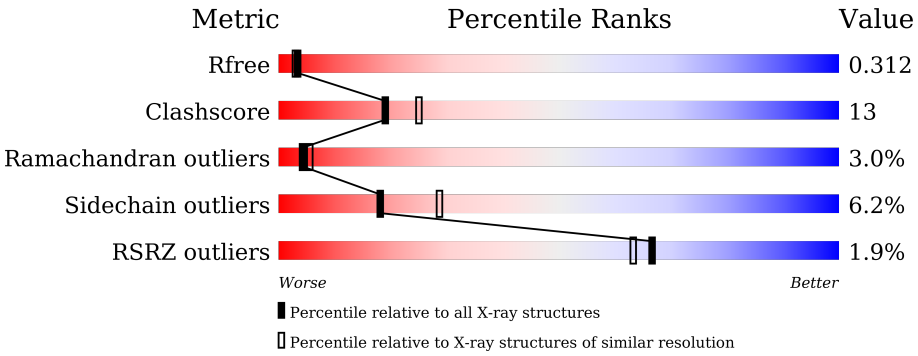
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	339	66% 26% • 5%
1	B	339	2% 65% 29% • •
1	C	339	2% 53% 25% 5% • 16%
1	D	339	2% 55% 22% • 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9638 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 D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2507	1611	427	461	8			
1	B	324	Total	C	N	O	S	0	0	0
			2530	1625	431	465	9			
1	C	284	Total	C	N	O	S	0	0	0
			2229	1436	380	405	8			
1	D	276	Total	C	N	O	S	0	0	0
			2158	1389	370	391	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP F8A9V0
A	-12	GLY	-	expression tag	UNP F8A9V0
A	-11	SER	-	expression tag	UNP F8A9V0
A	-10	SER	-	expression tag	UNP F8A9V0
A	-9	HIS	-	expression tag	UNP F8A9V0
A	-8	HIS	-	expression tag	UNP F8A9V0
A	-7	HIS	-	expression tag	UNP F8A9V0
A	-6	HIS	-	expression tag	UNP F8A9V0
A	-5	HIS	-	expression tag	UNP F8A9V0
A	-4	HIS	-	expression tag	UNP F8A9V0
A	-3	SER	-	expression tag	UNP F8A9V0
A	-2	GLN	-	expression tag	UNP F8A9V0
A	-1	ASP	-	expression tag	UNP F8A9V0
A	0	PRO	-	expression tag	UNP F8A9V0
A	101	GLN	PRO	engineered mutation	UNP F8A9V0
B	-13	MET	-	initiating methionine	UNP F8A9V0
B	-12	GLY	-	expression tag	UNP F8A9V0
B	-11	SER	-	expression tag	UNP F8A9V0
B	-10	SER	-	expression tag	UNP F8A9V0
B	-9	HIS	-	expression tag	UNP F8A9V0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP F8A9V0
B	-7	HIS	-	expression tag	UNP F8A9V0
B	-6	HIS	-	expression tag	UNP F8A9V0
B	-5	HIS	-	expression tag	UNP F8A9V0
B	-4	HIS	-	expression tag	UNP F8A9V0
B	-3	SER	-	expression tag	UNP F8A9V0
B	-2	GLN	-	expression tag	UNP F8A9V0
B	-1	ASP	-	expression tag	UNP F8A9V0
B	0	PRO	-	expression tag	UNP F8A9V0
B	101	GLN	PRO	engineered mutation	UNP F8A9V0
C	-13	MET	-	initiating methionine	UNP F8A9V0
C	-12	GLY	-	expression tag	UNP F8A9V0
C	-11	SER	-	expression tag	UNP F8A9V0
C	-10	SER	-	expression tag	UNP F8A9V0
C	-9	HIS	-	expression tag	UNP F8A9V0
C	-8	HIS	-	expression tag	UNP F8A9V0
C	-7	HIS	-	expression tag	UNP F8A9V0
C	-6	HIS	-	expression tag	UNP F8A9V0
C	-5	HIS	-	expression tag	UNP F8A9V0
C	-4	HIS	-	expression tag	UNP F8A9V0
C	-3	SER	-	expression tag	UNP F8A9V0
C	-2	GLN	-	expression tag	UNP F8A9V0
C	-1	ASP	-	expression tag	UNP F8A9V0
C	0	PRO	-	expression tag	UNP F8A9V0
C	101	GLN	PRO	engineered mutation	UNP F8A9V0
D	-13	MET	-	initiating methionine	UNP F8A9V0
D	-12	GLY	-	expression tag	UNP F8A9V0
D	-11	SER	-	expression tag	UNP F8A9V0
D	-10	SER	-	expression tag	UNP F8A9V0
D	-9	HIS	-	expression tag	UNP F8A9V0
D	-8	HIS	-	expression tag	UNP F8A9V0
D	-7	HIS	-	expression tag	UNP F8A9V0
D	-6	HIS	-	expression tag	UNP F8A9V0
D	-5	HIS	-	expression tag	UNP F8A9V0
D	-4	HIS	-	expression tag	UNP F8A9V0
D	-3	SER	-	expression tag	UNP F8A9V0
D	-2	GLN	-	expression tag	UNP F8A9V0
D	-1	ASP	-	expression tag	UNP F8A9V0
D	0	PRO	-	expression tag	UNP F8A9V0
D	101	GLN	PRO	engineered mutation	UNP F8A9V0

- Molecule 2 is water.

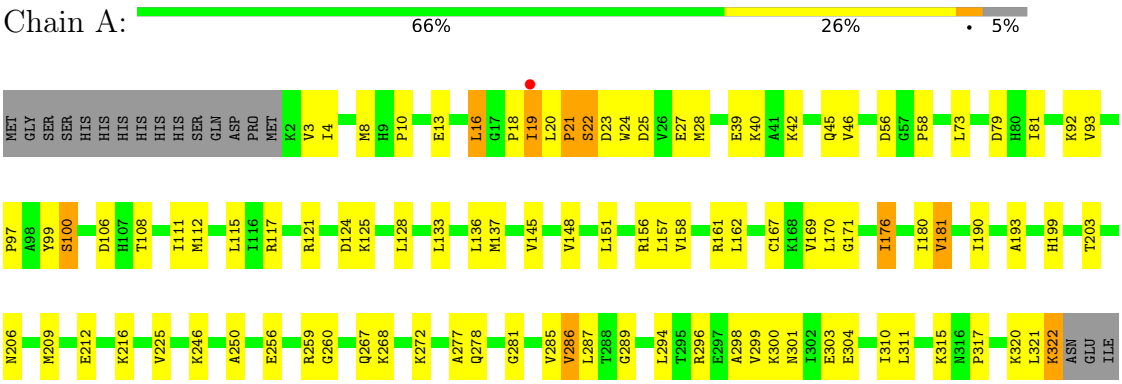
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	54	Total O 54 54	0	0
2	B	56	Total O 56 56	0	0
2	C	56	Total O 56 56	0	0
2	D	48	Total O 48 48	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

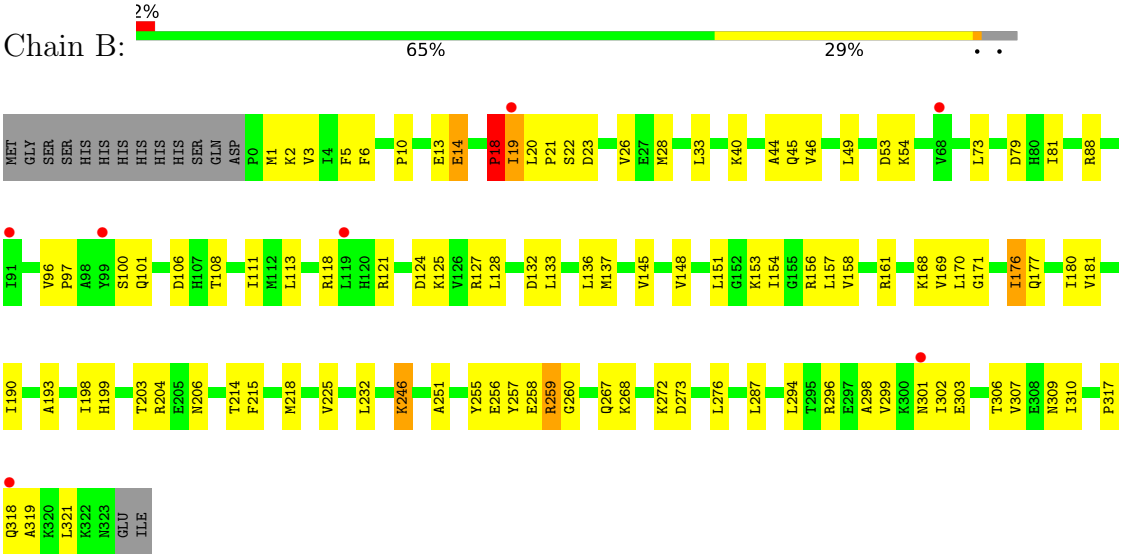
• Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding protein

Chain A:



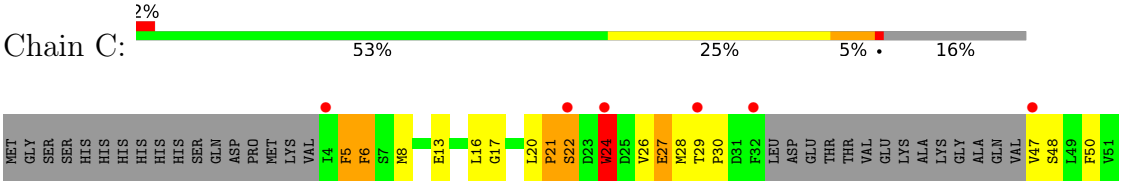
• Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding protein

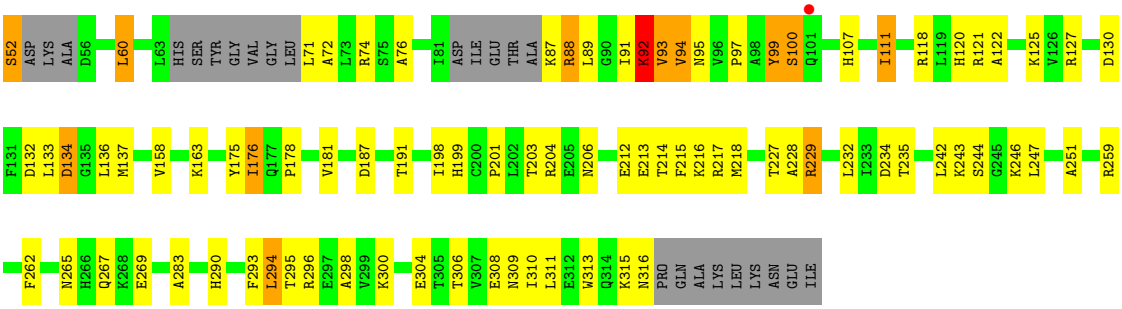
Chain B:



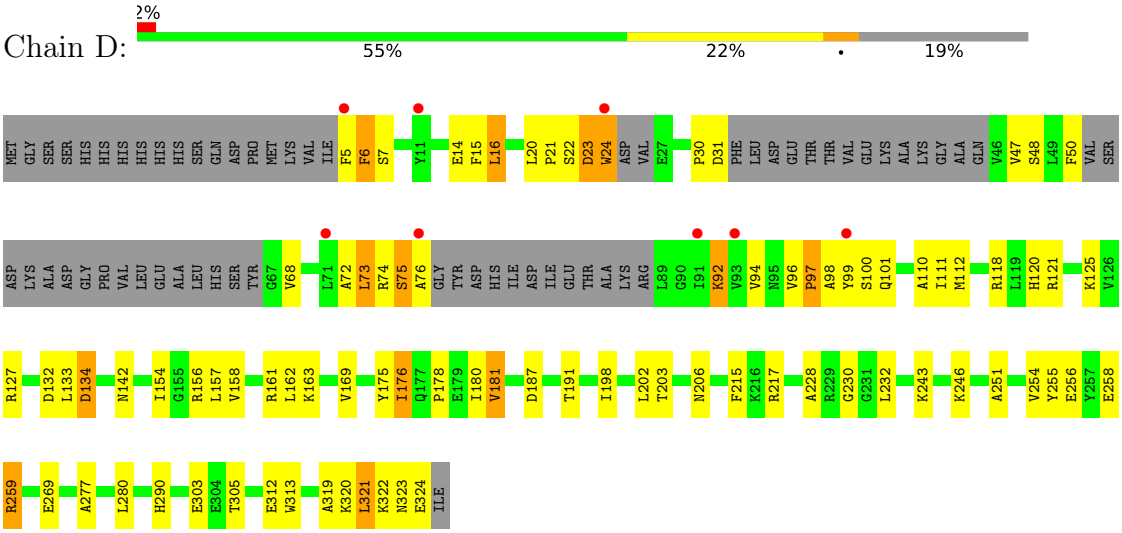
• Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding protein

Chain C:





• Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	92.30Å 92.30Å 380.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.64 – 2.65 49.64 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.64-2.65) 98.1 (49.64-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.36 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.241 , 0.310 0.246 , 0.312	Depositor DCC
R_{free} test set	2739 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.449 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9638	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	0/2556	0.65	0/3458
1	B	0.44	0/2580	0.64	0/3490
1	C	0.42	0/2271	0.67	1/3067 (0.0%)
1	D	0.41	0/2197	0.65	1/2965 (0.0%)
All	All	0.42	0/9604	0.65	2/12980 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	24	TRP	CA-CB-CG	9.15	131.08	113.70
1	D	16	LEU	CA-CB-CG	6.72	130.75	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	18	PRO	Peptide
1	C	21	PRO	Peptide
1	C	22	SER	Peptide

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	2507	0	2549	69	0
1	B	2530	0	2574	67	0
1	C	2229	0	2251	72	0
1	D	2158	0	2192	53	0
2	A	54	0	0	11	0
2	B	56	0	0	6	0
2	C	56	0	0	13	0
2	D	48	0	0	6	0
All	All	9638	0	9566	246	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 13.

All (246) 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:C:87:LYS:NZ	2:C:401:HOH:O	1.98	0.95
1:D:156:ARG:NH2	2:D:401:HOH:O	1.93	0.93
1:C:111:ILE:HG23	1:C:251:ALA:HB1	1.52	0.90
1:C:121:ARG:NH1	2:C:402:HOH:O	1.98	0.87
1:A:300:LYS:NZ	2:A:401:HOH:O	1.90	0.84
1:A:128:LEU:HD11	1:B:124:ASP:HB3	1.60	0.81
1:C:88:ARG:HD2	1:C:92:LYS:HD3	1.64	0.80
1:B:19:ILE:HD13	1:B:26:VAL:HG21	1.65	0.79
1:C:316:ASN:ND2	2:C:405:HOH:O	2.15	0.78
1:B:1:MET:HB2	1:B:23:ASP:HB3	1.67	0.77
1:A:203:THR:H	1:A:206:ASN:HB2	1.49	0.76
1:A:256:GLU:OE1	2:A:403:HOH:O	2.04	0.74
1:B:133:LEU:HA	1:B:136:LEU:HD12	1.69	0.74
1:D:121:ARG:NH1	2:D:404:HOH:O	2.17	0.74
1:B:272:LYS:NZ	1:C:243:LYS:O	2.20	0.73
1:A:16:LEU:HB3	1:A:303:GLU:HB3	1.70	0.73
1:C:87:LYS:N	2:C:405:HOH:O	2.21	0.73
1:C:71:LEU:N	1:C:93:VAL:O	2.22	0.73
1:A:287:LEU:O	2:A:405:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:O	2:A:404:HOH:O	2.07	0.71
1:B:257:TYR:N	2:B:405:HOH:O	2.23	0.70
1:B:203:THR:H	1:B:206:ASN:HB2	1.57	0.69
1:A:124:ASP:HB3	1:B:128:LEU:HD11	1.73	0.69
1:C:91:ILE:HD12	1:C:97:PRO:HG3	1.74	0.69
1:B:88:ARG:NH2	2:B:406:HOH:O	2.25	0.69
1:A:272:LYS:NZ	1:D:243:LYS:O	2.22	0.68
1:D:15:PHE:O	2:D:402:HOH:O	2.10	0.68
1:A:281:GLY:O	2:A:406:HOH:O	2.12	0.68
1:D:22:SER:OG	1:D:23:ASP:N	2.26	0.68
1:C:234:ASP:OD2	2:C:403:HOH:O	2.11	0.67
1:C:89:LEU:HD21	1:C:313:TRP:HB2	1.75	0.67
1:B:287:LEU:O	2:B:402:HOH:O	2.14	0.66
1:A:39:GLU:HG3	1:A:42:LYS:HE3	1.76	0.66
1:D:24:TRP:HE3	1:D:24:TRP:H	1.44	0.65
1:B:101:GLN:HG2	1:B:153:LYS:HB3	1.79	0.65
1:B:190:ILE:O	2:B:403:HOH:O	2.14	0.65
1:C:118:ARG:NE	2:C:409:HOH:O	2.29	0.65
1:C:308:GLU:OE1	2:C:404:HOH:O	2.12	0.65
1:C:92:LYS:C	1:C:94:VAL:H	2.00	0.64
1:D:203:THR:H	1:D:206:ASN:HB2	1.63	0.64
1:A:97:PRO:HG3	1:A:320:LYS:HG2	1.79	0.63
1:A:10:PRO:HA	1:A:13:GLU:HG2	1.80	0.63
1:A:27:GLU:OE2	2:A:407:HOH:O	2.15	0.63
1:A:73:LEU:HD21	1:A:81:ILE:HG13	1.79	0.63
1:A:133:LEU:HA	1:A:136:LEU:HD12	1.81	0.63
1:C:215:PHE:O	1:C:246:LYS:NZ	2.32	0.63
1:C:300:LYS:HE2	1:C:304:GLU:OE2	1.99	0.62
1:C:203:THR:H	1:C:206:ASN:HB2	1.64	0.62
1:B:151:LEU:O	1:B:156:ARG:NH1	2.33	0.62
1:C:175:TYR:O	1:C:176:ILE:HG13	1.99	0.61
1:D:73:LEU:HB2	1:D:94:VAL:O	2.00	0.61
1:B:145:VAL:HG13	1:B:170:LEU:HD13	1.81	0.61
1:C:120:HIS:NE2	1:C:283:ALA:O	2.30	0.61
1:D:48:SER:HB3	1:D:74:ARG:HE	1.65	0.61
1:B:158:VAL:HG21	1:B:199:HIS:CE1	2.36	0.61
1:C:52:SER:O	1:C:52:SER:OG	2.14	0.61
1:B:118:ARG:NH1	1:B:137:MET:O	2.33	0.60
1:C:296:ARG:NH2	2:C:408:HOH:O	2.25	0.60
1:B:121:ARG:O	1:B:125:LYS:HG3	2.02	0.60
1:B:106:ASP:OD1	1:B:161:ARG:NH2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:SER:OG	1:D:76:ALA:N	2.35	0.60
1:D:111:ILE:HG23	1:D:251:ALA:HB1	1.83	0.60
1:A:100:SER:HB3	1:A:298:ALA:HB2	1.84	0.59
1:A:112:MET:HG3	1:A:225:VAL:HG21	1.84	0.59
1:B:73:LEU:HD11	1:B:81:ILE:HG13	1.85	0.59
1:B:180:ILE:O	1:B:180:ILE:HG13	2.03	0.59
1:D:97:PRO:HD2	1:D:305:THR:HG21	1.85	0.59
1:C:5:PHE:CD2	1:C:48:SER:HB2	2.38	0.58
1:B:101:GLN:HG3	1:B:154:ILE:HG13	1.84	0.58
1:B:96:VAL:HG21	1:B:302:ILE:HG23	1.85	0.58
1:D:319:ALA:O	2:D:405:HOH:O	2.17	0.58
1:A:317:PRO:HA	1:A:321:LEU:HD22	1.86	0.57
1:C:47:VAL:N	1:C:71:LEU:O	2.38	0.57
1:A:151:LEU:O	1:A:156:ARG:NH1	2.38	0.57
1:A:267:GLN:HG3	1:C:130:ASP:HB2	1.87	0.57
1:B:97:PRO:HG3	1:B:321:LEU:HD22	1.86	0.57
1:D:202:LEU:HD13	1:D:232:LEU:HG	1.87	0.56
1:D:7:SER:HA	1:D:30:PRO:HA	1.87	0.56
1:B:108:THR:O	1:B:111:ILE:HG22	2.06	0.55
1:A:136:LEU:O	2:A:408:HOH:O	2.18	0.55
1:C:5:PHE:CZ	1:C:16:LEU:HD21	2.42	0.55
1:C:5:PHE:HD1	1:C:26:VAL:HG11	1.71	0.55
1:C:100:SER:O	2:C:406:HOH:O	2.18	0.55
1:A:40:LYS:NZ	2:A:407:HOH:O	2.38	0.55
1:C:16:LEU:HD23	1:C:28:MET:HE1	1.89	0.55
1:B:145:VAL:HG12	1:B:193:ALA:HA	1.88	0.54
1:A:13:GLU:HA	1:A:16:LEU:HD23	1.90	0.54
1:B:10:PRO:HA	1:B:13:GLU:HG2	1.90	0.53
1:D:5:PHE:CE2	1:D:16:LEU:HD11	2.44	0.53
1:C:22:SER:OG	1:C:24:TRP:O	2.23	0.53
1:A:115:LEU:HD13	1:A:285:VAL:O	2.08	0.53
1:C:125:LYS:NZ	1:C:132:ASP:O	2.41	0.53
1:A:93:VAL:O	1:A:322:LYS:NZ	2.41	0.53
1:A:137:MET:HG3	1:C:294:LEU:HG	1.90	0.53
1:D:97:PRO:O	1:D:99:TYR:N	2.41	0.53
1:C:21:PRO:HB2	1:C:22:SER:HB2	1.92	0.52
1:A:169:VAL:HG12	1:A:181:VAL:HG22	1.92	0.52
1:B:148:VAL:O	1:B:171:GLY:HA2	2.10	0.52
1:B:214:THR:O	1:B:218:MET:HG3	2.10	0.52
1:D:24:TRP:HE3	1:D:24:TRP:N	2.06	0.52
1:C:158:VAL:HG21	1:C:199:HIS:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ARG:HA	1:D:120:HIS:CE1	2.46	0.51
1:B:113:LEU:HB3	1:D:110:ALA:HB2	1.93	0.51
1:A:46:VAL:HG11	1:A:310:ILE:HG12	1.93	0.51
1:A:79:ASP:OD2	1:A:259:ARG:HD2	2.10	0.51
1:B:14:GLU:OE2	1:B:296:ARG:NH2	2.44	0.50
1:A:145:VAL:HG13	1:A:170:LEU:HD13	1.92	0.50
1:A:180:ILE:HG13	1:A:180:ILE:O	2.11	0.50
1:B:299:VAL:O	1:B:303:GLU:HG2	2.11	0.50
1:A:106:ASP:OD1	1:A:161:ARG:NH2	2.40	0.50
1:A:121:ARG:O	1:A:125:LYS:HG3	2.11	0.50
1:C:187:ASP:O	1:C:191:THR:HG23	2.10	0.50
1:D:198:ILE:HG21	1:D:232:LEU:HD13	1.93	0.50
1:A:250:ALA:O	1:A:285:VAL:O	2.29	0.50
1:C:212:GLU:O	1:C:216:LYS:HG3	2.12	0.50
1:D:320:LYS:O	1:D:324:GLU:HG3	2.12	0.50
1:B:273:ASP:HB3	1:B:276:LEU:HB2	1.94	0.50
1:B:169:VAL:HG12	1:B:181:VAL:HG22	1.94	0.49
1:B:225:VAL:HG22	1:B:251:ALA:HB3	1.94	0.49
1:D:118:ARG:NE	2:D:415:HOH:O	2.46	0.49
1:A:285:VAL:O	1:A:286:VAL:HB	2.12	0.49
1:C:201:PRO:HA	1:C:229:ARG:HH11	1.76	0.49
1:C:227:THR:N	2:C:413:HOH:O	2.37	0.49
1:D:312:GLU:OE2	1:D:321:LEU:HA	2.13	0.49
1:D:72:ALA:HA	1:D:94:VAL:HG23	1.95	0.48
1:B:306:THR:O	1:B:310:ILE:HG13	2.13	0.48
1:C:176:ILE:HD12	1:C:178:PRO:HD3	1.95	0.48
1:B:198:ILE:HG21	1:B:232:LEU:HD13	1.96	0.48
1:A:277:ALA:HB1	1:D:277:ALA:O	2.13	0.48
1:A:289:GLY:N	2:A:402:HOH:O	1.91	0.48
1:C:213:GLU:OE2	1:C:216:LYS:NZ	2.47	0.48
1:D:254:VAL:HG12	1:D:290:HIS:ND1	2.29	0.47
1:C:198:ILE:HG21	1:C:232:LEU:HD13	1.97	0.47
1:B:40:LYS:NZ	2:B:410:HOH:O	2.48	0.47
1:A:294:LEU:HD22	1:C:133:LEU:HB3	1.96	0.47
1:B:294:LEU:HD22	1:D:133:LEU:HB3	1.97	0.47
1:D:142:ASN:HB2	2:D:413:HOH:O	2.13	0.47
1:A:304:GLU:OE1	2:A:409:HOH:O	2.20	0.47
1:C:88:ARG:NH1	1:C:89:LEU:O	2.48	0.47
1:D:178:PRO:HB2	1:D:180:ILE:HG22	1.97	0.47
1:A:18:PRO:O	1:A:20:LEU:N	2.43	0.47
1:A:206:ASN:O	1:A:209:MET:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:HD2	1:A:321:LEU:HD11	1.97	0.46
1:B:33:LEU:HB3	1:B:53:ASP:HB3	1.97	0.46
1:D:24:TRP:N	1:D:24:TRP:CE3	2.83	0.46
1:A:117:ARG:NH1	1:C:107:HIS:HB2	2.31	0.46
1:B:2:LYS:HB3	1:B:44:ALA:HA	1.96	0.46
1:B:20:LEU:HD12	1:B:307:VAL:HG21	1.98	0.46
1:C:94:VAL:HG13	1:C:309:ASN:HD22	1.80	0.46
1:B:3:VAL:HG23	1:B:23:ASP:HB2	1.96	0.46
1:B:73:LEU:HD21	1:B:81:ILE:HD11	1.97	0.46
1:C:47:VAL:O	1:C:48:SER:HB3	2.15	0.46
1:C:293:PHE:O	1:C:295:THR:N	2.49	0.46
1:D:5:PHE:CD2	1:D:47:VAL:HG21	2.51	0.46
1:B:176:ILE:HG13	1:B:177:GLN:N	2.31	0.46
1:A:162:LEU:O	1:A:167:CYS:HB2	2.16	0.46
1:B:100:SER:HB3	1:B:298:ALA:HB2	1.96	0.46
1:C:6:PHE:HB3	2:C:438:HOH:O	2.16	0.45
1:D:175:TYR:O	1:D:176:ILE:HD12	2.15	0.45
1:B:299:VAL:HA	1:B:302:ILE:HD12	1.98	0.45
1:C:100:SER:HB2	1:C:298:ALA:HB2	1.97	0.45
1:A:246:LYS:HA	1:A:246:LYS:HD2	1.80	0.45
1:D:157:LEU:HB3	1:D:161:ARG:NH1	2.32	0.45
1:A:212:GLU:OE2	1:A:216:LYS:NZ	2.37	0.45
1:C:5:PHE:O	1:C:28:MET:HA	2.17	0.45
1:A:108:THR:HG21	1:A:199:HIS:CE1	2.52	0.45
1:B:3:VAL:HG13	1:B:46:VAL:HB	1.98	0.45
1:A:148:VAL:O	1:A:171:GLY:HA2	2.17	0.45
1:A:322:LYS:HB2	1:A:322:LYS:HE2	1.73	0.45
1:B:319:ALA:O	1:B:321:LEU:N	2.49	0.44
1:C:311:LEU:O	1:C:315:LYS:HG3	2.16	0.44
1:B:124:ASP:O	1:B:128:LEU:HD13	2.18	0.44
1:C:48:SER:H	1:C:72:ALA:HB3	1.82	0.44
1:A:145:VAL:HG12	1:A:193:ALA:HA	1.99	0.44
1:C:316:ASN:HB3	2:C:412:HOH:O	2.17	0.44
1:C:5:PHE:HB3	1:C:28:MET:HB3	2.00	0.44
1:C:92:LYS:C	1:C:94:VAL:N	2.69	0.44
1:A:108:THR:O	1:A:111:ILE:HG22	2.18	0.44
1:D:158:VAL:HG12	1:D:162:LEU:HD12	1.99	0.44
1:A:3:VAL:HG13	1:A:46:VAL:HB	2.00	0.43
1:B:10:PRO:HD2	1:D:134:ASP:OD1	2.17	0.43
1:C:8:MET:O	1:C:30:PRO:HB3	2.18	0.43
1:C:8:MET:SD	1:C:13:GLU:HG3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HA	1:A:121:ARG:HD2	1.89	0.43
1:A:19:ILE:HG23	1:A:21:PRO:HD3	2.00	0.43
1:B:97:PRO:HD3	1:B:321:LEU:HD13	1.99	0.43
1:B:204:ARG:HA	1:B:204:ARG:HD3	1.68	0.43
1:B:225:VAL:HA	1:B:251:ALA:O	2.18	0.43
1:B:256:GLU:HG3	1:B:257:TYR:CD2	2.53	0.43
1:D:313:TRP:HB2	1:D:321:LEU:HD13	2.00	0.43
1:A:157:LEU:O	1:A:161:ARG:HD2	2.18	0.43
1:A:158:VAL:HG21	1:A:199:HIS:CE1	2.54	0.43
1:B:54:LYS:HD2	1:B:54:LYS:HA	1.81	0.43
1:D:47:VAL:HG13	1:D:72:ALA:HB3	2.00	0.43
1:D:187:ASP:O	1:D:191:THR:HG23	2.19	0.43
1:B:5:PHE:HB2	1:B:28:MET:HG2	2.01	0.43
1:B:97:PRO:CG	1:B:321:LEU:HD22	2.48	0.43
1:B:127:ARG:NH1	1:D:280:LEU:HD22	2.34	0.43
1:C:5:PHE:HA	1:C:48:SER:CB	2.48	0.43
1:A:20:LEU:O	1:A:22:SER:N	2.52	0.42
1:D:23:ASP:OD1	1:D:23:ASP:C	2.57	0.42
1:D:47:VAL:HG13	1:D:72:ALA:O	2.19	0.42
1:A:21:PRO:O	1:A:23:ASP:N	2.51	0.42
1:C:99:TYR:HB3	2:C:406:HOH:O	2.18	0.42
1:B:255:TYR:O	1:B:258:GLU:HB3	2.19	0.42
1:B:309:ASN:OD1	1:B:321:LEU:HD12	2.20	0.42
1:D:121:ARG:HA	1:D:121:ARG:HD2	1.82	0.42
1:A:296:ARG:HG2	1:C:137:MET:HE3	2.01	0.42
1:D:154:ILE:O	1:D:158:VAL:HG23	2.20	0.42
1:B:111:ILE:HD13	1:B:111:ILE:HG21	1.71	0.42
1:C:22:SER:OG	1:C:24:TRP:HE3	2.02	0.42
1:C:262:PHE:HD2	1:C:290:HIS:HB2	1.85	0.42
1:A:278:GLN:O	2:A:410:HOH:O	2.22	0.42
1:B:215:PHE:O	1:B:246:LYS:NZ	2.53	0.42
1:C:306:THR:O	1:C:310:ILE:HG13	2.20	0.42
1:A:24:TRP:HB3	1:A:25:ASP:H	1.73	0.41
1:A:111:ILE:HD13	1:A:111:ILE:HG21	1.76	0.41
1:C:17:GLY:HA2	1:C:21:PRO:HD3	2.02	0.41
1:D:169:VAL:HG12	1:D:181:VAL:HG22	2.02	0.41
1:D:255:TYR:O	1:D:258:GLU:HB3	2.20	0.41
1:C:242:LEU:HD21	1:C:247:LEU:HD23	2.02	0.41
1:A:8:MET:HG2	1:A:28:MET:CG	2.51	0.41
1:A:56:ASP:OD2	1:A:58:PRO:HD2	2.20	0.41
1:D:96:VAL:HG12	1:D:97:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PRO:HD2	1:C:134:ASP:OD1	2.21	0.41
1:B:6:PHE:HB2	1:B:49:LEU:HD23	2.03	0.41
1:B:101:GLN:HB3	1:B:157:LEU:HD12	2.03	0.41
1:B:259:ARG:NH2	2:B:407:HOH:O	2.53	0.41
1:C:122:ALA:HB2	1:C:136:LEU:HD13	2.03	0.41
1:D:112:MET:HE1	1:D:162:LEU:HD11	2.03	0.41
1:A:299:VAL:O	1:A:303:GLU:HG2	2.21	0.41
1:C:87:LYS:HD3	1:C:316:ASN:C	2.40	0.41
1:C:265:ASN:OD1	1:C:267:GLN:HB2	2.21	0.41
1:D:215:PHE:O	1:D:246:LYS:NZ	2.53	0.41
1:D:230:GLY:HA3	1:D:256:GLU:N	2.36	0.41
1:C:48:SER:HA	1:C:72:ALA:O	2.21	0.41
1:D:303:GLU:OE1	1:D:303:GLU:HA	2.20	0.41
1:D:175:TYR:O	1:D:176:ILE:O	2.39	0.40
1:A:19:ILE:HD12	1:A:19:ILE:HA	1.80	0.40
1:B:3:VAL:HG22	1:B:46:VAL:HB	2.03	0.40
1:D:125:LYS:NZ	1:D:132:ASP:O	2.53	0.40
1:C:50:PHE:H	1:C:74:ARG:HH21	1.69	0.40
1:C:76:ALA:HA	1:C:95:ASN:HD22	1.85	0.40
1:C:214:THR:O	1:C:218:MET:HG3	2.20	0.40
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.92	0.40
1:B:18:PRO:HD2	1:B:20:LEU:HD23	2.02	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	319/339 (94%)	293 (92%)	18 (6%)	8 (2%)	5 7
1	B	322/339 (95%)	295 (92%)	21 (6%)	6 (2%)	8 11
1	C	274/339 (81%)	247 (90%)	17 (6%)	10 (4%)	3 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	266/339 (78%)	232 (87%)	22 (8%)	12 (4%)	2 2
All	All	1181/1356 (87%)	1067 (90%)	78 (7%)	36 (3%)	4 5

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	B	18	PRO
1	C	20	LEU
1	C	93	VAL
1	D	92	LYS
1	D	100	SER
1	D	176	ILE
1	D	259	ARG
1	A	19	ILE
1	A	176	ILE
1	A	315	LYS
1	B	259	ARG
1	C	92	LYS
1	C	176	ILE
1	C	259	ARG
1	C	294	LEU
1	D	98	ALA
1	D	228	ALA
1	D	321	LEU
1	A	21	PRO
1	A	99	TYR
1	A	286	VAL
1	B	21	PRO
1	C	27	GLU
1	C	60	LEU
1	D	6	PHE
1	D	21	PRO
1	D	322	LYS
1	B	22	SER
1	B	317	PRO
1	C	228	ALA
1	B	260	GLY
1	C	94	VAL
1	D	97	PRO
1	D	269	GLU
1	A	260	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	266/283 (94%)	257 (97%)	9 (3%)	37 53
1	B	269/283 (95%)	257 (96%)	12 (4%)	27 42
1	C	236/283 (83%)	214 (91%)	22 (9%)	9 13
1	D	228/283 (81%)	209 (92%)	19 (8%)	11 16
All	All	999/1132 (88%)	937 (94%)	62 (6%)	18 29

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	16	LEU
1	A	45	GLN
1	A	100	SER
1	A	176	ILE
1	A	181	VAL
1	A	268	LYS
1	A	301	ASN
1	A	322	LYS
1	B	14	GLU
1	B	19	ILE
1	B	45	GLN
1	B	79	ASP
1	B	132	ASP
1	B	168	LYS
1	B	176	ILE
1	B	246	LYS
1	B	267	GLN
1	B	268	LYS
1	B	301	ASN
1	B	318	GLN
1	C	5	PHE
1	C	6	PHE
1	C	24	TRP

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Mol	Chain	Res	Type
1	C	27	GLU
1	C	29	THR
1	C	52	SER
1	C	60	LEU
1	C	88	ARG
1	C	92	LYS
1	C	99	TYR
1	C	100	SER
1	C	111	ILE
1	C	127	ARG
1	C	134	ASP
1	C	163	LYS
1	C	181	VAL
1	C	204	ARG
1	C	217	ARG
1	C	229	ARG
1	C	235	THR
1	C	244	SER
1	C	269	GLU
1	D	6	PHE
1	D	14	GLU
1	D	20	LEU
1	D	23	ASP
1	D	24	TRP
1	D	31	ASP
1	D	50	PHE
1	D	68	VAL
1	D	73	LEU
1	D	75	SER
1	D	92	LYS
1	D	101	GLN
1	D	127	ARG
1	D	134	ASP
1	D	163	LYS
1	D	181	VAL
1	D	217	ARG
1	D	259	ARG
1	D	323	ASN

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

Mol	Chain	Res	Type
1	A	267	GLN
1	C	309	ASN

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 monosaccharides 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	321/339 (94%)	0.10	1 (0%)	94	95	22, 35, 59, 83	0
1	B	324/339 (95%)	0.07	7 (2%)	62	57	21, 35, 57, 88	0
1	C	284/339 (83%)	0.18	7 (2%)	57	53	22, 36, 79, 101	0
1	D	276/339 (81%)	0.15	8 (2%)	51	48	23, 37, 76, 100	0
All	All	1205/1356 (88%)	0.12	23 (1%)	66	63	21, 35, 72, 101	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ILE	5.0
1	C	24	TRP	4.7
1	B	19	ILE	3.9
1	D	76	ALA	3.9
1	B	68	VAL	3.7
1	D	71	LEU	3.6
1	B	91	ILE	3.2
1	D	24	TRP	3.2
1	D	99	TYR	3.2
1	B	99	TYR	3.1
1	C	22	SER	3.0
1	C	29	THR	3.0
1	C	47	VAL	2.8
1	C	32	PHE	2.7
1	C	101	GLN	2.6
1	D	5	PHE	2.6
1	C	4	ILE	2.5
1	B	301	ASN	2.4
1	D	91	ILE	2.3
1	B	318	GLN	2.3
1	D	11	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	93	VAL	2.1
1	B	119	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.