Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	1STZ
Title	:	Crystal structure of a hypothetical protein at 2.2 A resolution
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Deposited on	:	2004-03-25
Resolution	:	2.20 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 ⓘ) were used in the production of this report:

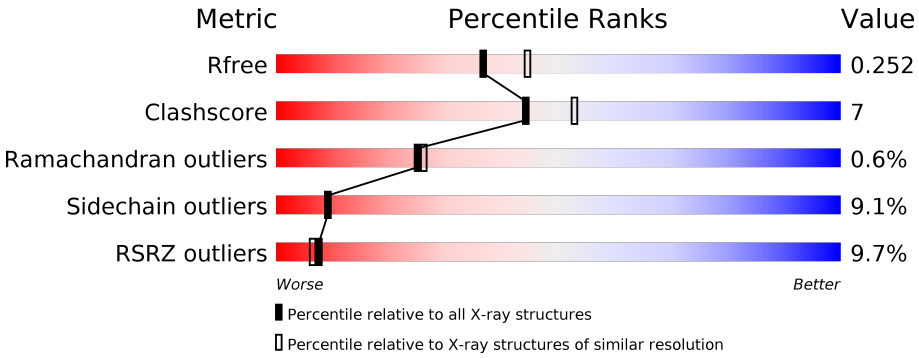
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	338	8% 75% 17%
1	B	338	8% 74% 16% 8%
1	C	338	11% 71% 18% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8166 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 Heat-inducible transcription repressor hrcA homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2634	1690	444	494	6			
1	B	311	Total	C	N	O	S	0	0	0
			2541	1634	431	470	6			
1	C	311	Total	C	N	O	S	0	0	0
			2541	1634	431	470	6			

- Molecule 2 is water.

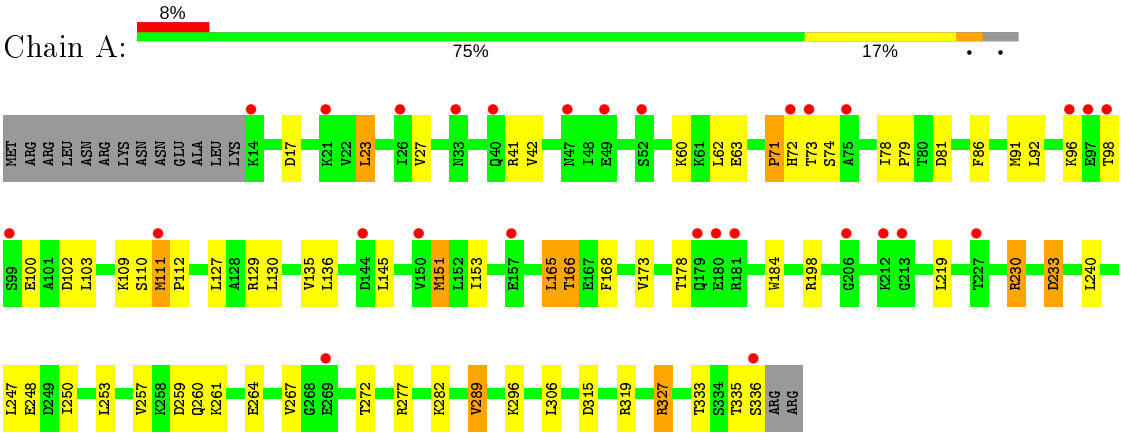
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	184	Total	O	0	0
			184	184		
2	B	131	Total	O	0	0
			131	131		
2	C	135	Total	O	0	0
			135	135		

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.

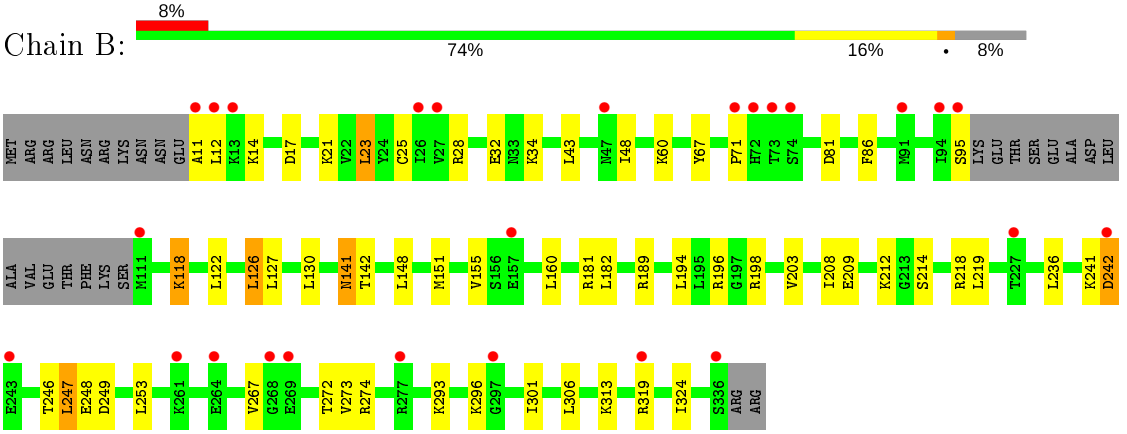
- Molecule 1: Heat-inducible transcription repressor hrcA homolog

Chain A:



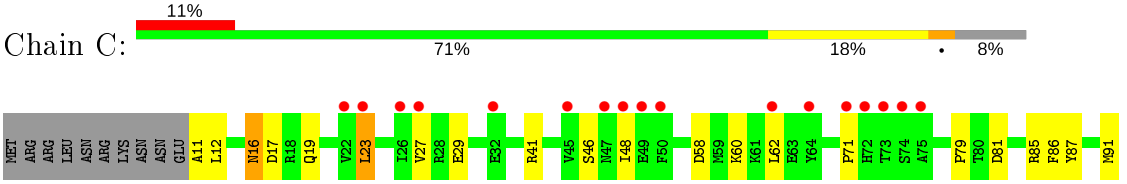
- Molecule 1: Heat-inducible transcription repressor hrcA homolog

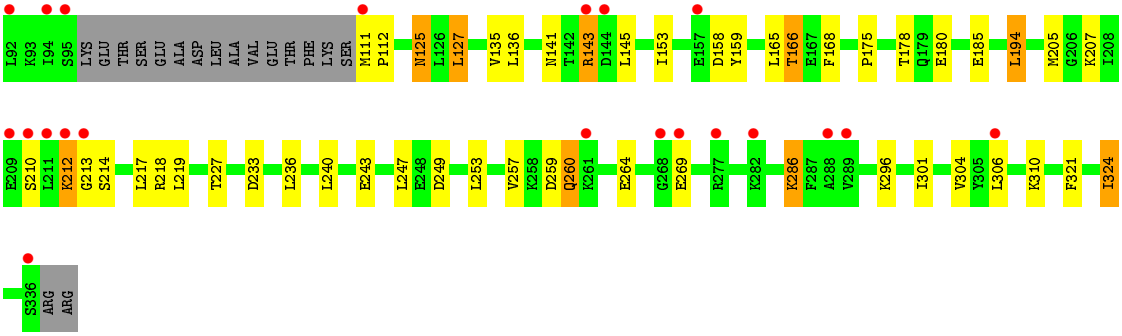
Chain B:



- Molecule 1: Heat-inducible transcription repressor hrcA homolog

Chain C:




L92 K93 I94 S95 LYS GLU THR SER GLU ALA ASP LEU ALA VAL GLU THR PHE LYS SER M111 P112 N125 L126 L127 V135 L136 N141 T142 R143 D144 L145 I153 E157 D158 Y159 L165 T166 E167 F168 P175 T178 Q179 E180 E185 L194 M205 G206 K207 I208
E209 S210 L211 K212 G213 S214 L217 R218 L219 T227 D233 L236 L240 E243 L247 E248 D249 L253 V257 K258 D259 Q260 K261 E264 G268 E269 H277 K282 K286 P287 A288 V289 K296 I301 V304 Y305 L306 K310 F321 I324
S336 ARG ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.30Å 115.30Å 185.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.20) 91.7 (19.95-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.258 0.215 , 0.252	Depositor DCC
R_{free} test set	3405 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8166	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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	0.50	0/2676	0.76	4/3599 (0.1%)
1	B	0.48	0/2581	0.73	4/3469 (0.1%)
1	C	0.44	0/2581	0.72	6/3469 (0.2%)
All	All	0.48	0/7838	0.74	14/10537 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	259	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	233	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	259	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	58	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	81	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	242	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	81	ASP	CB-CG-OD2	5.88	123.60	118.30
1	C	81	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	289	VAL	CB-CA-C	-5.37	101.20	111.40
1	C	17	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	233	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	17	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	249	ASP	CB-CG-OD2	5.09	122.89	118.30
1	C	158	ASP	CB-CG-OD2	5.05	122.85	118.30

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	2634	0	2717	45	0
1	B	2541	0	2634	26	0
1	C	2541	0	2634	41	0
2	A	184	0	0	15	0
2	B	131	0	0	2	0
2	C	135	0	0	11	0
All	All	8166	0	7985	103	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 7.

All (103) 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:136:LEU:O	2:C:431:HOH:O	1.75	1.02
1:A:178:THR:HB	2:A:509:HOH:O	1.76	0.84
1:B:23:LEU:HD13	1:B:86:PHE:CD2	2.14	0.81
1:A:260:GLN:NE2	2:A:502:HOH:O	2.02	0.81
1:A:111:MET:HB2	1:A:112:PRO:HD3	1.62	0.80
1:A:335:THR:C	2:A:460:HOH:O	2.21	0.79
1:B:242:ASP:HB3	2:B:422:HOH:O	1.82	0.77
1:C:136:LEU:C	2:C:431:HOH:O	2.21	0.77
1:A:178:THR:HG21	1:A:184:TRP:HZ2	1.50	0.75
1:C:166:THR:HG23	1:C:168:PHE:H	1.52	0.75
1:A:23:LEU:HD13	1:A:86:PHE:CD2	2.24	0.72
1:A:282:LYS:NZ	2:A:364:HOH:O	2.22	0.71
1:C:321:PHE:HA	2:C:428:HOH:O	1.91	0.70
1:A:71:PRO:HG3	1:A:78:ILE:HD12	1.73	0.69
1:C:23:LEU:HD13	1:C:86:PHE:CD2	2.28	0.68
1:A:166:THR:HG22	1:A:168:PHE:H	1.59	0.67
1:A:173:VAL:HG21	1:C:175:PRO:HG3	1.77	0.66
1:C:212:LYS:NZ	2:C:453:HOH:O	2.29	0.65
1:C:141:ASN:HD21	1:C:143:ARG:HB3	1.61	0.65
1:B:32:GLU:OE2	1:B:313:LYS:NZ	2.30	0.64
1:B:25:CYS:HA	1:B:28:ARG:HG2	1.80	0.62
1:B:296:LYS:CB	1:B:301:ILE:HD11	2.30	0.61
1:C:260:GLN:HE22	1:C:264:GLU:CD	2.05	0.60
1:A:336:SER:N	2:A:460:HOH:O	2.35	0.60
1:C:125:ASN:ND2	2:C:456:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:THR:O	1:A:336:SER:HB3	2.02	0.59
1:A:327:ARG:NH1	2:A:421:HOH:O	2.37	0.57
1:C:111:MET:N	1:C:112:PRO:HD2	2.20	0.57
1:A:178:THR:HG21	1:A:184:TRP:CZ2	2.37	0.57
1:A:63:GLU:OE1	2:A:353:HOH:O	2.18	0.56
1:B:203:VAL:HG22	1:B:208:ILE:HD12	1.86	0.56
1:B:296:LYS:HB2	1:B:301:ILE:HD11	1.88	0.54
1:A:102:ASP:HB2	1:A:319:ARG:HD3	1.90	0.54
1:A:111:MET:HB2	1:A:112:PRO:CD	2.33	0.54
1:A:296:LYS:HD2	2:A:341:HOH:O	2.07	0.53
1:A:151:MET:HB3	1:A:153:ILE:HD11	1.90	0.53
1:A:109:LYS:CD	1:A:111:MET:HB3	2.40	0.52
1:A:111:MET:CB	1:A:112:PRO:CD	2.87	0.52
1:B:296:LYS:HB3	1:B:301:ILE:HD11	1.91	0.51
1:A:109:LYS:HD2	1:A:111:MET:HB3	1.92	0.51
1:C:324:ILE:HB	2:C:428:HOH:O	2.10	0.51
1:A:240:LEU:HD21	1:C:240:LEU:HD21	1.91	0.51
1:B:189:ARG:NH2	1:C:227:THR:OG1	2.44	0.51
1:A:109:LYS:HB3	1:B:214:SER:HB3	1.92	0.50
1:C:178:THR:HG23	1:C:178:THR:O	2.11	0.50
1:B:11:ALA:N	1:B:14:LYS:HB2	2.26	0.50
1:B:126:LEU:HD22	1:B:130:LEU:HD11	1.95	0.49
1:C:249:ASP:OD2	1:C:286:LYS:NZ	2.45	0.48
1:C:210:SER:O	1:C:212:LYS:NZ	2.45	0.48
1:C:296:LYS:CB	1:C:301:ILE:HD11	2.44	0.48
1:C:304:VAL:HG13	2:C:431:HOH:O	2.13	0.47
1:A:336:SER:HA	2:A:341:HOH:O	2.14	0.47
1:A:165:LEU:HD11	1:C:159:TYR:CE1	2.50	0.47
1:B:267:VAL:HG11	1:B:293:LYS:HD2	1.96	0.47
1:C:16:ASN:C	1:C:16:ASN:HD22	2.19	0.47
1:A:96:LYS:HD2	2:A:491:HOH:O	2.14	0.46
1:C:296:LYS:HB2	1:C:301:ILE:HD11	1.96	0.46
1:A:129:ARG:NH2	2:A:343:HOH:O	2.49	0.46
1:C:127:LEU:HG	2:C:428:HOH:O	2.14	0.46
1:C:205:MET:HB2	1:C:207:LYS:HG3	1.97	0.46
1:B:118:LYS:HE3	1:B:122:LEU:HD11	1.98	0.45
1:A:315:ASP:HB3	2:A:425:HOH:O	2.16	0.45
1:C:87:TYR:CZ	1:C:91:MET:SD	3.09	0.45
1:A:230:ARG:HD3	2:A:502:HOH:O	2.17	0.45
1:B:236:LEU:HD13	1:B:236:LEU:C	2.37	0.45
1:B:241:LYS:HA	1:B:241:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PRO:HG3	1:C:219:LEU:HD11	1.97	0.45
1:B:274:ARG:CZ	2:B:368:HOH:O	2.65	0.45
1:A:111:MET:HG3	1:A:112:PRO:HD2	1.98	0.45
1:C:213:GLY:O	1:C:214:SER:OG	2.29	0.45
1:C:23:LEU:HG	1:C:62:LEU:HD22	1.99	0.45
1:C:194:LEU:HD21	1:C:210:SER:HB2	1.99	0.44
1:A:41:ARG:NH2	2:A:470:HOH:O	2.49	0.44
1:A:264:GLU:O	1:A:267:VAL:HG12	2.18	0.44
1:C:27:VAL:HG22	1:C:79:PRO:HB3	1.99	0.44
1:C:46:SER:OG	1:C:48:ILE:HG12	2.18	0.44
1:A:153:ILE:HG21	1:C:153:ILE:HG21	2.00	0.44
1:C:11:ALA:N	2:C:464:HOH:O	2.51	0.44
1:C:85:ARG:NH2	2:C:465:HOH:O	2.50	0.44
1:A:272:THR:HG23	2:A:462:HOH:O	2.18	0.43
1:C:87:TYR:OH	1:C:91:MET:SD	2.69	0.43
1:A:327:ARG:N	1:A:327:ARG:HD2	2.33	0.42
1:C:11:ALA:N	2:C:445:HOH:O	2.52	0.42
1:A:23:LEU:HG	1:A:62:LEU:HD22	2.01	0.42
1:A:240:LEU:HD23	1:A:250:ILE:HD13	2.01	0.42
1:B:141:ASN:HD22	1:B:142:THR:N	2.18	0.42
1:C:16:ASN:ND2	1:C:19:GLN:H	2.17	0.42
1:C:127:LEU:HD13	1:C:135:VAL:HG22	2.01	0.42
1:C:127:LEU:HB3	1:C:135:VAL:HG21	2.02	0.42
1:B:12:LEU:N	1:B:12:LEU:HD22	2.34	0.41
1:A:136:LEU:HD11	1:A:257:VAL:HG13	2.02	0.41
1:B:246:THR:HG22	1:B:248:GLU:H	1.84	0.41
1:A:27:VAL:HG22	1:A:79:PRO:HB3	2.03	0.41
1:B:11:ALA:HA	1:B:67:TYR:OH	2.20	0.41
1:B:196:ARG:O	1:C:218:ARG:NH1	2.54	0.41
1:A:72:HIS:HB2	1:A:73:THR:H	1.72	0.41
1:A:135:VAL:O	1:A:233:ASP:HA	2.21	0.41
1:C:111:MET:N	1:C:112:PRO:CD	2.82	0.41
1:A:109:LYS:HD2	1:A:111:MET:SD	2.61	0.40
1:B:246:THR:HG22	1:B:247:LEU:N	2.37	0.40
1:B:21:LYS:HD2	1:B:48:ILE:HD11	2.03	0.40
1:A:130:LEU:HD21	1:B:182:LEU:HD13	2.04	0.40
1:B:212:LYS:O	1:B:218:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	321/338 (95%)	312 (97%)	6 (2%)	3 (1%)	17	16
1	B	307/338 (91%)	299 (97%)	7 (2%)	1 (0%)	41	46
1	C	307/338 (91%)	294 (96%)	11 (4%)	2 (1%)	22	22
All	All	935/1014 (92%)	905 (97%)	24 (3%)	6 (1%)	25	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	MET
1	C	71	PRO
1	B	71	PRO
1	C	269	GLU
1	A	100	GLU
1	A	71	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	294/308 (96%)	268 (91%)	26 (9%)	10	10
1	B	283/308 (92%)	258 (91%)	25 (9%)	10	10
1	C	283/308 (92%)	256 (90%)	27 (10%)	8	8
All	All	860/924 (93%)	782 (91%)	78 (9%)	9	9

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	23	LEU
1	A	42	VAL
1	A	60	LYS
1	A	74	SER
1	A	91	MET
1	A	92	LEU
1	A	98	THR
1	A	103	LEU
1	A	110	SER
1	A	127	LEU
1	A	145	LEU
1	A	151	MET
1	A	165	LEU
1	A	166	THR
1	A	198	ARG
1	A	219	LEU
1	A	230	ARG
1	A	247	LEU
1	A	248	GLU
1	A	253	LEU
1	A	261	LYS
1	A	277	ARG
1	A	289	VAL
1	A	306	LEU
1	A	327	ARG
1	B	23	LEU
1	B	34	LYS
1	B	43	LEU
1	B	60	LYS
1	B	95	SER
1	B	118	LYS
1	B	126	LEU
1	B	127	LEU
1	B	141	ASN
1	B	148	LEU
1	B	151	MET
1	B	155	VAL
1	B	160	LEU
1	B	181	ARG
1	B	194	LEU
1	B	198	ARG

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Mol	Chain	Res	Type
1	B	209	GLU
1	B	219	LEU
1	B	247	LEU
1	B	253	LEU
1	B	272	THR
1	B	273	VAL
1	B	306	LEU
1	B	319	ARG
1	B	324	ILE
1	C	12	LEU
1	C	16	ASN
1	C	23	LEU
1	C	29	GLU
1	C	41	ARG
1	C	60	LYS
1	C	125	ASN
1	C	127	LEU
1	C	143	ARG
1	C	145	LEU
1	C	165	LEU
1	C	166	THR
1	C	180	GLU
1	C	185	GLU
1	C	194	LEU
1	C	212	LYS
1	C	217	LEU
1	C	236	LEU
1	C	243	GLU
1	C	247	LEU
1	C	253	LEU
1	C	257	VAL
1	C	260	GLN
1	C	286	LYS
1	C	306	LEU
1	C	310	LYS
1	C	324	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	70	GLN

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	141	ASN
1	B	318	HIS
1	C	16	ASN
1	C	125	ASN
1	C	141	ASN
1	C	179	GLN
1	C	260	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 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	323/338 (95%)	0.52	28 (8%)	10	8	15, 22, 34, 57	0
1	B	311/338 (92%)	0.38	26 (8%)	11	9	13, 21, 31, 56	0
1	C	311/338 (92%)	0.72	38 (12%)	4	3	10, 22, 30, 49	0
All	All	945/1014 (93%)	0.54	92 (9%)	7	6	10, 22, 32, 57	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	LEU	8.6
1	C	73	THR	6.3
1	C	209	GLU	5.8
1	B	13	LYS	5.4
1	B	73	THR	5.3
1	B	95	SER	5.1
1	C	269	GLU	5.0
1	C	210	SER	5.0
1	C	75	ALA	4.8
1	A	97	GLU	4.7
1	C	49	GLU	4.7
1	C	47	ASN	4.6
1	B	269	GLU	4.6
1	A	179	GLN	4.4
1	B	268	GLY	4.4
1	C	50	PHE	4.4
1	A	144	ASP	4.3
1	C	261	LYS	4.1
1	B	277	ARG	4.0
1	B	227	THR	4.0
1	C	268	GLY	3.9
1	B	336	SER	3.8
1	C	72	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	336	SER	3.8
1	A	98	THR	3.7
1	A	180	GLU	3.7
1	C	26	ILE	3.7
1	C	32	GLU	3.6
1	B	12	LEU	3.5
1	C	45	VAL	3.5
1	C	48	ILE	3.4
1	C	212	LYS	3.4
1	A	181	ARG	3.3
1	B	72	HIS	3.3
1	A	73	THR	3.3
1	C	71	PRO	3.3
1	B	91	MET	3.3
1	A	227	THR	3.3
1	C	213	GLY	3.2
1	C	288	ALA	3.2
1	B	242	ASP	3.1
1	A	14	LYS	3.1
1	C	111	MET	3.1
1	B	27	VAL	3.1
1	A	336	SER	3.1
1	A	99	SER	3.0
1	B	261	LYS	3.0
1	C	23	LEU	2.9
1	A	72	HIS	2.9
1	A	47	ASN	2.8
1	C	94	ILE	2.7
1	B	264	GLU	2.7
1	B	74	SER	2.6
1	C	143	ARG	2.6
1	A	49	GLU	2.6
1	C	289	VAL	2.6
1	A	75	ALA	2.6
1	A	26	ILE	2.6
1	B	319	ARG	2.5
1	C	74	SER	2.5
1	C	92	LEU	2.5
1	C	306	LEU	2.5
1	A	111	MET	2.5
1	C	22	VAL	2.5
1	C	157	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	40	GLN	2.5
1	C	144	ASP	2.5
1	B	111	MET	2.5
1	A	33	ASN	2.5
1	A	157	GLU	2.4
1	C	277	ARG	2.4
1	C	282	LYS	2.4
1	C	27	VAL	2.4
1	A	96	LYS	2.4
1	C	95	SER	2.3
1	B	11	ALA	2.3
1	C	64	TYR	2.3
1	B	47	ASN	2.3
1	A	21	LYS	2.3
1	B	297	GLY	2.2
1	B	71	PRO	2.2
1	A	269	GLU	2.2
1	B	94	ILE	2.1
1	B	243	GLU	2.1
1	B	157	GLU	2.1
1	A	213	GLY	2.1
1	A	206	GLY	2.1
1	A	150	VAL	2.0
1	A	212	LYS	2.0
1	B	26	ILE	2.0
1	C	62	LEU	2.0
1	A	52	SER	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.