Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 05:50 AM EDT

PDB ID	:	3ECU
Title	:	Crystal structure of human apo Cu,Zn Superoxide Dismutase (SOD1)
Authors	:	Calderone, V.
Deposited on	:	2008-09-02
Resolution	:	1.90 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:

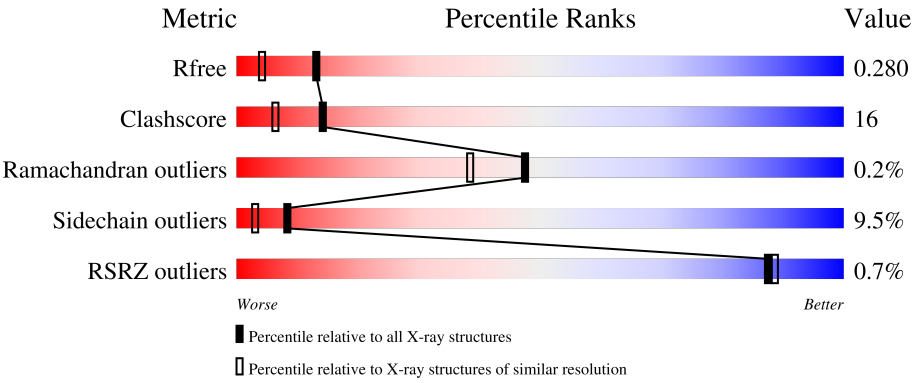
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	153	72% 21% 5%
1	B	153	71% 22% 6%
1	C	153	52% 25% 5% 18%
1	D	153	54% 24% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4326 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	B	153	Total	C	N	O	S	0	0	0
			1110	679	203	224	4			
1	C	126	Total	C	N	O	S	0	0	0
			915	567	165	179	4			
1	D	123	Total	C	N	O	S	0	0	0
			892	553	159	176	4			

- Molecule 2 is water.

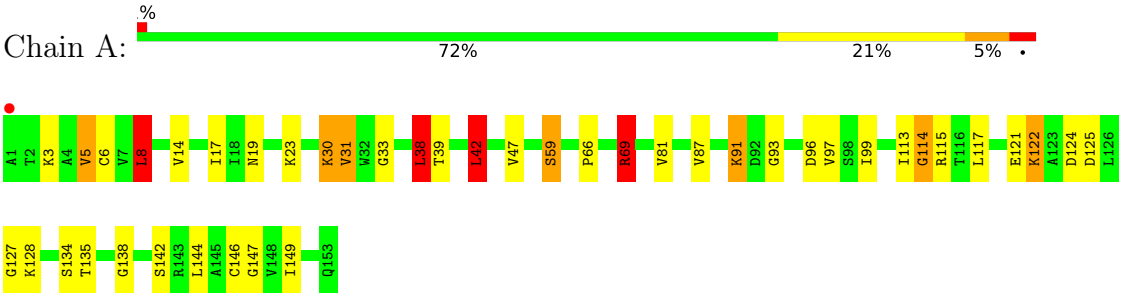
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	105	Total	O	0	0
			105	105		
2	C	62	Total	O	0	0
			62	62		
2	D	48	Total	O	0	0
			48	48		

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.

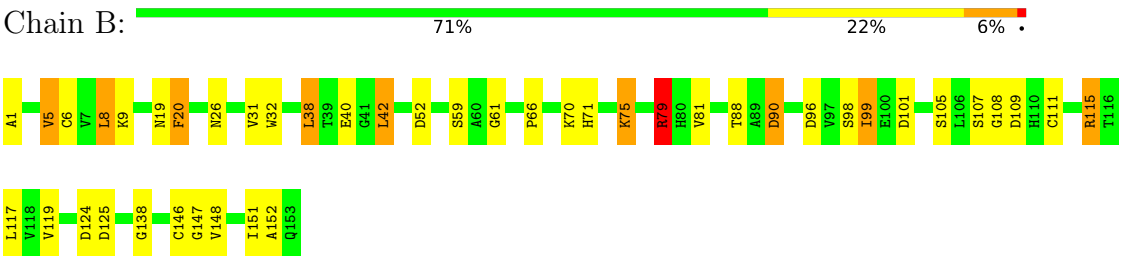
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



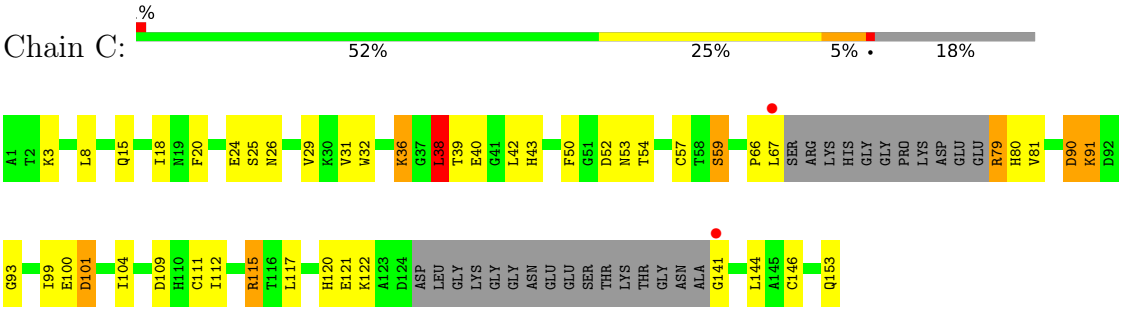
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:



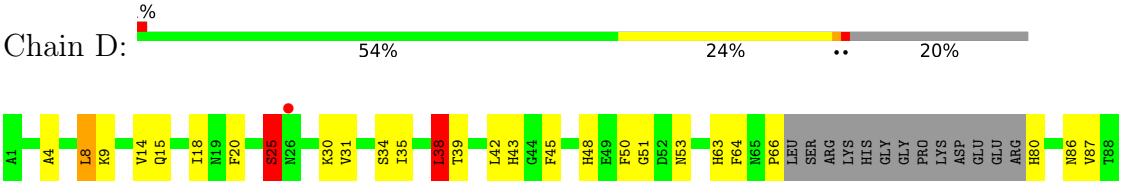
• Molecule 1: Superoxide dismutase [Cu-Zn]

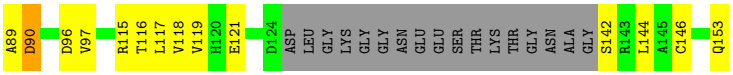
Chain C:



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain D:




A89
D90
D96
V97
R115
T116
L117
V118
V119
H120
E121
D124
ASP
LEU
GLY
LYS
GLY
GLY
ASN
GLU
GLU
SER
THR
LYS
THR
GLY
ASN
ALA
GLY
S142
R143
L144
A145
C146
Q153

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	156.17Å 33.53Å 113.98Å 90.00° 111.64° 90.00°	Depositor
Resolution (Å)	39.01 – 1.90 39.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.01-1.90) 97.0 (39.03-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.239 , 0.279 0.240 , 0.280	Depositor DCC
R_{free} test set	3880 reflections (9.06%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% 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	1.13	4/1128 (0.4%)	1.18	5/1520 (0.3%)
1	B	1.24	4/1128 (0.4%)	1.18	5/1520 (0.3%)
1	C	1.12	1/929 (0.1%)	1.18	6/1253 (0.5%)
1	D	1.00	0/906	1.10	4/1223 (0.3%)
All	All	1.13	9/4091 (0.2%)	1.16	20/5516 (0.4%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	CYS	CB-SG	-7.97	1.68	1.82
1	A	47	VAL	CB-CG2	7.79	1.69	1.52
1	A	5	VAL	CB-CG2	6.92	1.67	1.52
1	B	5	VAL	CB-CG2	6.68	1.66	1.52
1	B	20	PHE	CE1-CZ	-5.79	1.26	1.37
1	B	119	VAL	CA-CB	5.47	1.66	1.54
1	A	114	GLY	C-O	5.12	1.31	1.23
1	C	57	CYS	CB-SG	-5.12	1.73	1.81
1	A	149	ILE	CB-CG2	5.00	1.68	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	LEU	CB-CG-CD1	9.04	126.36	111.00
1	A	8	LEU	CA-CB-CG	8.85	135.65	115.30
1	B	8	LEU	CA-CB-CG	7.29	132.07	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	115	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	90	ASP	CB-CG-OD1	6.97	124.58	118.30
1	D	8	LEU	CA-CB-CG	6.70	130.72	115.30
1	A	69	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	79	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	D	42	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	69	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	C	115	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	C	38	LEU	CA-CB-CG	6.28	129.74	115.30
1	D	38	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	42	LEU	CB-CG-CD2	-6.14	100.57	111.00
1	A	38	LEU	CB-CG-CD1	5.93	121.08	111.00
1	C	90	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	C	101	ASP	CB-CG-OD2	5.84	123.56	118.30
1	C	115	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	42	LEU	CA-CB-CG	5.51	127.98	115.30
1	D	90	ASP	CB-CG-OD2	5.40	123.16	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	99	ILE	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	1110	0	1077	31	0
1	B	1110	0	1077	29	0
1	C	915	0	894	43	0
1	D	892	0	867	26	0
2	A	84	0	0	4	0
2	B	105	0	0	6	0
2	C	62	0	0	12	0
2	D	48	0	0	6	0
All	All	4326	0	3915	124	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 16.

All (124) 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:36:LYS:HB3	2:C:273:HOH:O	1.50	1.09
1:B:66:PRO:HD2	1:B:81:VAL:HG23	1.35	1.07
1:D:25:SER:HB2	2:D:170:HOH:O	1.60	0.99
1:C:79:ARG:NH2	1:C:101:ASP:OD1	2.06	0.88
1:B:66:PRO:HD2	1:B:81:VAL:CG2	2.05	0.86
1:A:69:ARG:HH11	1:A:69:ARG:HG2	1.41	0.85
1:C:153:GLN:HG3	1:D:50:PHE:CZ	2.13	0.83
1:C:40:GLU:HG3	1:C:90:ASP:C	2.00	0.82
1:D:9:LYS:HE3	2:D:160:HOH:O	1.81	0.80
1:B:109:ASP:HB2	2:B:299:HOH:O	1.83	0.78
1:A:39:THR:HG21	2:A:221:HOH:O	1.85	0.75
1:C:109:ASP:HB2	2:C:241:HOH:O	1.87	0.74
1:C:18:ILE:HG23	2:C:263:HOH:O	1.87	0.74
1:B:6:CYS:SG	1:B:147:GLY:O	2.47	0.73
1:B:52:ASP:O	1:B:59:SER:HB2	1.89	0.71
1:A:6:CYS:SG	1:A:147:GLY:O	2.49	0.70
1:D:90:ASP:OD1	1:D:90:ASP:C	2.26	0.69
1:B:61:GLY:HA2	2:B:330:HOH:O	1.94	0.67
1:B:66:PRO:CD	1:B:81:VAL:CG2	2.74	0.66
1:A:91:LYS:HD3	1:A:91:LYS:H	1.59	0.66
1:B:75:LYS:HG2	2:B:341:HOH:O	1.98	0.64
1:C:36:LYS:CB	2:C:273:HOH:O	2.25	0.63
1:D:9:LYS:HG3	2:D:160:HOH:O	1.99	0.63
1:C:18:ILE:HD12	2:C:263:HOH:O	1.97	0.62
1:C:52:ASP:OD1	1:C:54:THR:HG23	2.00	0.61
1:C:53:ASN:HB3	2:C:251:HOH:O	2.00	0.61
1:B:111:CYS:HB3	2:B:263:HOH:O	2.00	0.60
1:C:32:TRP:C	2:C:263:HOH:O	2.39	0.60
1:A:59:SER:HB3	2:A:180:HOH:O	2.02	0.59
1:B:31:VAL:HB	1:B:99:ILE:HB	1.86	0.58
1:B:40:GLU:HB2	1:B:90:ASP:O	2.04	0.58
1:A:6:CYS:SG	1:A:147:GLY:C	2.82	0.57
1:A:69:ARG:HH11	1:A:69:ARG:CG	2.14	0.57
1:C:52:ASP:O	1:C:59:SER:HB2	2.04	0.57
1:C:66:PRO:HG2	1:C:67:LEU:HD22	1.86	0.56
1:C:99:ILE:HG22	1:C:100:GLU:N	2.20	0.56
1:D:18:ILE:HG13	1:D:45:PHE:HZ	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:N	2:C:283:HOH:O	2.38	0.55
1:D:121:GLU:HA	1:D:144:LEU:HD11	1.89	0.55
1:A:125:ASP:C	1:A:125:ASP:OD1	2.45	0.55
1:A:127:GLY:HA2	1:A:134:SER:O	2.08	0.54
1:A:30:LYS:HE2	1:A:99:ILE:O	2.08	0.54
1:A:114:GLY:O	1:B:151:ILE:HG13	2.07	0.54
1:C:29:VAL:HG21	1:C:104:ILE:HG13	1.90	0.54
1:C:20:PHE:N	1:C:20:PHE:CD1	2.76	0.54
1:D:53:ASN:O	1:D:53:ASN:CG	2.46	0.53
1:C:79:ARG:HD3	1:C:80:HIS:O	2.09	0.53
1:A:38:LEU:O	1:A:93:GLY:HA2	2.08	0.53
1:C:38:LEU:O	1:C:93:GLY:HA2	2.10	0.52
1:C:90:ASP:C	1:C:90:ASP:OD1	2.48	0.52
1:D:38:LEU:HG	1:D:43:HIS:CD2	2.44	0.52
1:C:40:GLU:HG3	1:C:91:LYS:N	2.25	0.51
1:A:31:VAL:O	1:A:31:VAL:HG22	2.11	0.51
1:D:90:ASP:OD1	1:D:90:ASP:O	2.30	0.50
1:B:66:PRO:CD	1:B:81:VAL:HG21	2.40	0.50
1:D:34:SER:HB2	2:D:196:HOH:O	2.09	0.50
1:C:112:ILE:HA	1:C:115:ARG:HG3	1.94	0.50
1:B:5:VAL:HG12	1:B:152:ALA:HB2	1.94	0.50
1:D:4:ALA:HB3	1:D:20:PHE:HB2	1.94	0.49
1:C:39:THR:HG23	2:C:243:HOH:O	2.10	0.49
1:C:18:ILE:CD1	2:C:263:HOH:O	2.59	0.49
1:A:91:LYS:HD3	2:A:208:HOH:O	2.12	0.49
1:B:125:ASP:OD1	1:B:125:ASP:C	2.51	0.49
1:C:117:LEU:O	1:C:146:CYS:HA	2.13	0.48
1:D:15:GLN:HB2	2:D:160:HOH:O	2.13	0.48
1:C:31:VAL:HB	1:C:99:ILE:HB	1.96	0.48
1:C:38:LEU:HB2	1:C:93:GLY:O	2.14	0.48
1:C:122:LYS:HB2	1:C:141:GLY:N	2.28	0.47
1:D:35:ILE:HD12	1:D:87:VAL:HG21	1.95	0.47
1:C:79:ARG:HG2	2:C:285:HOH:O	2.14	0.47
1:A:8:LEU:HD12	1:A:146:CYS:HA	1.96	0.47
1:B:20:PHE:HZ	1:B:117:LEU:HD22	1.80	0.47
1:D:87:VAL:CG1	1:D:97:VAL:HG22	2.45	0.47
1:B:66:PRO:CG	1:B:81:VAL:HG21	2.45	0.47
1:A:121:GLU:HB2	1:A:142:SER:HB2	1.97	0.47
1:B:79:ARG:NH2	1:B:101:ASP:OD1	2.27	0.46
1:B:19:ASN:HB2	1:B:32:TRP:CE2	2.51	0.46
1:C:40:GLU:HG3	1:C:90:ASP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLU:HB2	1:C:144:LEU:HD21	1.98	0.46
1:C:122:LYS:HA	1:C:122:LYS:HD3	1.75	0.46
1:B:108:GLY:HA3	1:C:25:SER:OG	2.16	0.46
1:D:14:VAL:HG21	1:D:144:LEU:HB3	1.98	0.45
1:A:66:PRO:HD2	1:A:81:VAL:HG23	1.96	0.45
1:B:66:PRO:CD	1:B:81:VAL:HG23	2.23	0.45
1:B:115:ARG:O	1:B:148:VAL:HA	2.16	0.45
1:B:42:LEU:CD1	1:B:88:THR:OG1	2.65	0.45
1:B:96:ASP:C	1:B:96:ASP:OD2	2.55	0.44
1:B:1:ALA:N	2:B:281:HOH:O	2.49	0.44
1:A:69:ARG:HG2	1:A:69:ARG:NH1	2.18	0.44
1:C:43:HIS:HB3	1:C:120:HIS:O	2.18	0.44
1:D:51:GLY:HA2	1:D:116:THR:OG1	2.17	0.44
1:D:43:HIS:O	1:D:86:ASN:HA	2.18	0.43
1:A:5:VAL:HG23	1:A:19:ASN:ND2	2.34	0.43
1:A:122:LYS:HE3	1:A:122:LYS:HB3	1.59	0.43
1:A:6:CYS:SG	1:A:147:GLY:CA	3.06	0.43
1:A:17:ILE:O	1:A:33:GLY:HA3	2.19	0.43
1:C:50:PHE:CZ	1:D:153:GLN:HG3	2.53	0.43
1:D:48:HIS:CD2	1:D:118:VAL:CG2	3.02	0.43
1:B:71:HIS:HE2	1:B:124:ASP:CG	2.22	0.42
1:C:18:ILE:HG21	1:C:117:LEU:HD21	2.00	0.42
1:C:50:PHE:C	1:C:52:ASP:H	2.22	0.42
1:C:43:HIS:ND1	1:C:121:GLU:O	2.49	0.42
1:D:64:PHE:CZ	1:D:66:PRO:HG3	2.55	0.42
1:B:124:ASP:OD1	1:B:138:GLY:HA3	2.19	0.42
1:A:69:ARG:N	1:A:69:ARG:HD3	2.34	0.42
1:A:115:ARG:HH11	1:A:115:ARG:HG2	1.85	0.42
1:C:8:LEU:HD23	1:C:146:CYS:HA	2.02	0.42
1:B:26:ASN:HA	1:C:26:ASN:HA	2.01	0.42
1:D:14:VAL:HG13	1:D:38:LEU:HD13	2.01	0.42
1:D:117:LEU:O	1:D:146:CYS:HA	2.20	0.42
1:C:111:CYS:HB3	2:C:266:HOH:O	2.19	0.42
1:A:91:LYS:CD	2:A:208:HOH:O	2.67	0.41
1:C:66:PRO:HD2	1:C:81:VAL:CG2	2.50	0.41
1:D:9:LYS:CG	2:D:160:HOH:O	2.61	0.41
1:A:87:VAL:CG1	1:A:97:VAL:HG22	2.50	0.41
1:A:124:ASP:OD1	1:A:138:GLY:HA3	2.20	0.41
1:D:39:THR:O	1:D:89:ALA:HB3	2.21	0.41
1:A:14:VAL:HG21	1:A:144:LEU:HB3	2.02	0.41
1:A:42:LEU:HA	1:A:87:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HD2	1:A:81:VAL:CG2	2.51	0.41
1:A:117:LEU:O	1:A:146:CYS:HA	2.21	0.41
1:D:63:HIS:ND1	1:D:80:HIS:CD2	2.89	0.41
1:B:6:CYS:SG	1:B:147:GLY:C	3.00	0.40
2:B:250:HOH:O	1:C:24:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	151/153 (99%)	144 (95%)	7 (5%)	0	100 100
1	B	151/153 (99%)	144 (95%)	7 (5%)	0	100 100
1	C	120/153 (78%)	115 (96%)	5 (4%)	0	100 100
1	D	117/153 (76%)	113 (97%)	3 (3%)	1 (1%)	17 7
All	All	539/612 (88%)	516 (96%)	22 (4%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	25	SER

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	118/118 (100%)	103 (87%)	15 (13%)	4 1
1	B	118/118 (100%)	108 (92%)	10 (8%)	10 4
1	C	98/118 (83%)	91 (93%)	7 (7%)	14 6
1	D	96/118 (81%)	87 (91%)	9 (9%)	8 3
All	All	430/472 (91%)	389 (90%)	41 (10%)	8 3

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	8	LEU
1	A	23	LYS
1	A	30	LYS
1	A	31	VAL
1	A	38	LEU
1	A	42	LEU
1	A	59	SER
1	A	69	ARG
1	A	91	LYS
1	A	96	ASP
1	A	113	ILE
1	A	122	LYS
1	A	128	LYS
1	A	135	THR
1	B	8	LEU
1	B	9	LYS
1	B	38	LEU
1	B	42	LEU
1	B	70	LYS
1	B	75	LYS
1	B	79	ARG
1	B	98	SER
1	B	105	SER
1	B	107	SER
1	C	3	LYS
1	C	15	GLN
1	C	36	LYS
1	C	38	LEU
1	C	59	SER
1	C	79	ARG
1	C	91	LYS
1	D	8	LEU

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Mol	Chain	Res	Type
1	D	25	SER
1	D	30	LYS
1	D	31	VAL
1	D	38	LEU
1	D	96	ASP
1	D	115	ARG
1	D	119	VAL
1	D	142	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	B	53	ASN
1	C	46	HIS
1	C	53	ASN
1	C	63	HIS
1	D	46	HIS
1	D	53	ASN
1	D	80	HIS

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 monosaccharides 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, 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	153/153 (100%)	-0.16	1 (0%) 87 88	3, 17, 31, 39	0
1	B	153/153 (100%)	-0.34	0 100 100	2, 14, 25, 31	0
1	C	126/153 (82%)	-0.08	2 (1%) 72 74	6, 18, 31, 42	2 (1%)
1	D	123/153 (80%)	-0.00	1 (0%) 86 87	8, 22, 34, 44	0
All	All	555/612 (90%)	-0.16	4 (0%) 87 88	2, 17, 31, 44	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	141	GLY	5.6
1	A	1	ALA	2.9
1	C	67	LEU	2.4
1	D	26	ASN	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.