



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:24 AM GMT

PDB ID : 2B7J  
Title : Crystal Structure of Yeast Sco1 with Copper Bound  
Authors : Abajian, C.; Rosenzweig, A.C.  
Deposited on : 2005-10-04  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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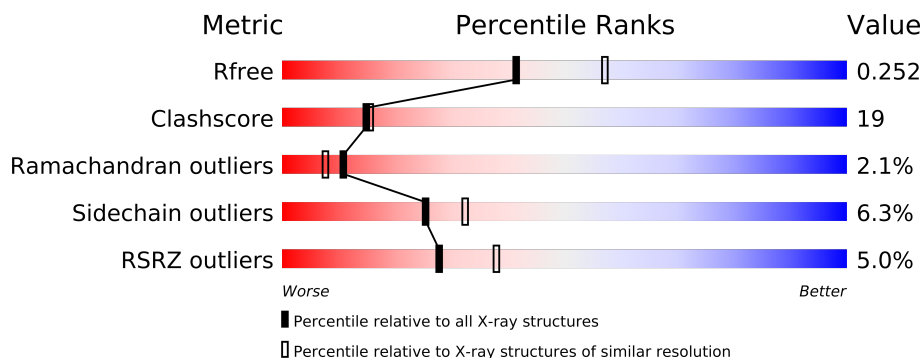
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	200	
1	B	200	
1	C	200	
1	D	200	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CU	A	297	-	X
2	CU	C	296	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5580 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SCO1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1263	818	200	239	6			
1	B	181	Total	C	N	O	S	0	0	0
			1457	948	229	274	6			
1	C	158	Total	C	N	O	S	0	0	0
			1263	818	200	239	6			
1	D	181	Total	C	N	O	S	0	0	0
			1457	948	229	274	6			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cu	0	0
			3	3		
2	C	3	Total	Cu	0	0
			3	3		

- Molecule 3 is water.

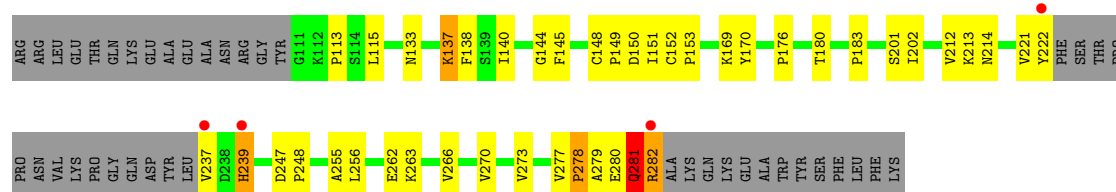
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	33	Total	O	0	0
			33	33		
3	C	33	Total	O	0	0
			33	33		
3	D	36	Total	O	0	0
			36	36		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

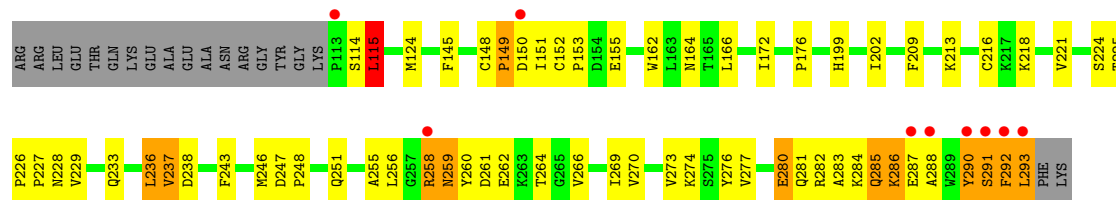
#### • Molecule 1: SCO1 protein

Chain A: 



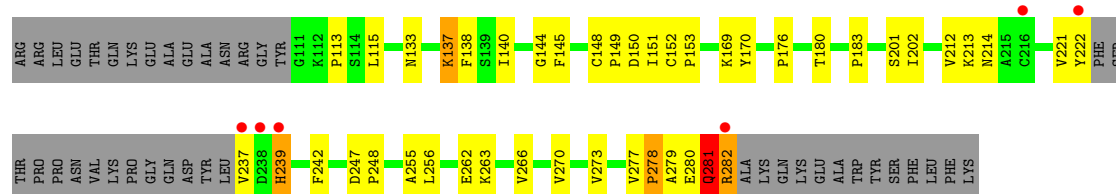
#### • Molecule 1: SCO1 protein

Chain B: 



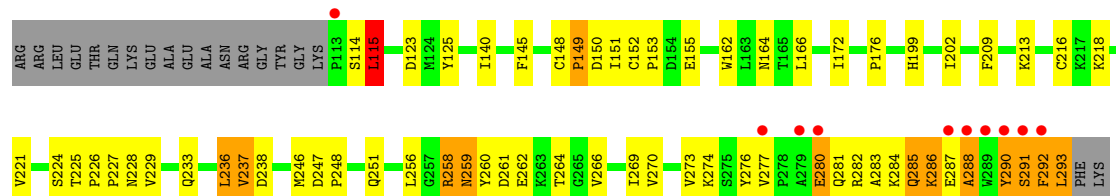
#### • Molecule 1: SCO1 protein

Chain C: 



#### • Molecule 1: SCO1 protein

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.60Å 81.90Å 79.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.30 79.30 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (81.65-2.30) 78.5 (79.30-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.252 0.212 , 0.252	Depositor DCC
$R_{free}$ test set	2490 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.3	EDS
Estimated twinning fraction	0.034 for -h,-l,-k 0.035 for -h,l,k 0.480 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 55233 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	0.40	0/1297	0.57	0/1755
1	B	0.37	0/1501	0.59	0/2036
1	C	0.38	0/1297	0.57	0/1755
1	D	0.37	0/1501	0.59	0/2036
All	All	0.38	0/5596	0.58	0/7582

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1263	0	1219	42	0
1	B	1457	0	1406	63	0
1	C	1263	0	1219	43	0
1	D	1457	0	1406	66	0
2	A	3	0	0	0	0
2	C	3	0	0	0	0
3	A	32	0	0	0	0
3	B	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	33	0	0	2	0
3	D	36	0	0	3	0
All	All	5580	0	5250	204	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (204) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:261:ASP:H	1:D:264:THR:HG22	1.35	0.91
1:B:261:ASP:H	1:B:264:THR:HG22	1.35	0.91
1:D:284:LYS:HE2	1:D:284:LYS:HA	1.54	0.87
1:B:284:LYS:HE2	1:B:284:LYS:HA	1.55	0.86
1:D:247:ASP:HB2	1:D:248:PRO:HD2	1.57	0.85
1:A:282:ARG:H	1:A:282:ARG:HD3	1.41	0.85
1:C:282:ARG:HD3	1:C:282:ARG:H	1.42	0.84
1:B:247:ASP:HB2	1:B:248:PRO:HD2	1.58	0.84
1:D:286:LYS:HD2	1:D:286:LYS:H	1.46	0.80
1:B:286:LYS:HD2	1:B:286:LYS:H	1.46	0.80
1:B:285:GLN:HG2	1:B:286:LYS:N	1.97	0.79
1:D:285:GLN:HG2	1:D:286:LYS:N	1.98	0.78
1:D:277:VAL:HB	1:D:280:GLU:HG2	1.67	0.76
1:B:277:VAL:HB	1:B:280:GLU:HG2	1.67	0.76
1:C:262:GLU:HG2	1:C:263:LYS:HD2	1.72	0.72
1:D:288:ALA:HB1	3:D:311:HOH:O	1.88	0.72
1:A:262:GLU:HG2	1:A:263:LYS:HD2	1.72	0.72
1:D:286:LYS:N	1:D:286:LYS:HD2	2.05	0.71
1:B:286:LYS:N	1:B:286:LYS:HD2	2.05	0.71
1:C:266:VAL:O	1:C:270:VAL:HG23	1.90	0.70
1:A:266:VAL:O	1:A:270:VAL:HG23	1.91	0.70
1:D:172:ILE:CD1	1:D:273:VAL:HG11	2.22	0.68
1:B:172:ILE:CD1	1:B:273:VAL:HG11	2.23	0.68
1:B:172:ILE:HD13	1:B:273:VAL:HG11	1.77	0.67
1:D:172:ILE:HD13	1:D:273:VAL:HG11	1.77	0.66
1:A:282:ARG:CD	1:A:282:ARG:H	2.09	0.65
1:C:282:ARG:CD	1:C:282:ARG:H	2.09	0.65
1:B:286:LYS:HB2	1:B:290:TYR:CG	2.31	0.65
1:D:286:LYS:HB2	1:D:290:TYR:CG	2.31	0.65
1:B:224:SER:HB3	1:B:238:ASP:H	1.63	0.63
1:D:224:SER:HB3	1:D:238:ASP:H	1.63	0.63
1:A:282:ARG:N	1:A:282:ARG:HD3	2.12	0.62
1:C:282:ARG:HD3	1:C:282:ARG:N	2.13	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:262:GLU:H	1:D:262:GLU:CD	2.03	0.62
1:B:262:GLU:CD	1:B:262:GLU:H	2.03	0.62
1:B:209:PHE:O	1:B:213:LYS:HG3	2.00	0.62
1:D:209:PHE:O	1:D:213:LYS:HG3	2.00	0.61
1:D:286:LYS:HD3	1:D:290:TYR:CD2	2.35	0.61
1:B:286:LYS:HD3	1:B:290:TYR:CD2	2.35	0.61
1:A:213:LYS:HE2	1:A:214:ASN:N	2.15	0.61
1:B:152:CYS:HB2	1:B:153:PRO:HD3	1.83	0.60
1:C:213:LYS:HE2	1:C:214:ASN:N	2.16	0.60
1:D:152:CYS:HB2	1:D:153:PRO:HD3	1.84	0.59
1:B:285:GLN:HG2	1:B:286:LYS:H	1.69	0.58
1:D:285:GLN:HG2	1:D:286:LYS:H	1.69	0.57
1:A:247:ASP:HB2	1:A:248:PRO:CD	2.34	0.57
1:B:229:VAL:HB	1:B:233:GLN:HE21	1.69	0.57
1:D:229:VAL:HB	1:D:233:GLN:HE21	1.69	0.57
1:C:247:ASP:HB2	1:C:248:PRO:CD	2.34	0.57
1:D:287:GLU:O	1:D:288:ALA:HB3	2.04	0.56
1:D:261:ASP:OD1	1:D:264:THR:HG22	2.06	0.56
1:D:145:PHE:CE2	1:D:148:CYS:HB2	2.41	0.56
1:B:261:ASP:OD1	1:B:264:THR:HG22	2.06	0.55
1:B:145:PHE:CE2	1:B:148:CYS:HB2	2.41	0.55
1:B:227:PRO:HG2	1:B:229:VAL:HG13	1.87	0.55
1:C:152:CYS:HB2	1:C:153:PRO:HD3	1.89	0.55
1:B:269:ILE:O	1:B:273:VAL:HG12	2.07	0.55
1:A:152:CYS:HB2	1:A:153:PRO:HD3	1.89	0.55
1:B:287:GLU:O	1:B:288:ALA:HB3	2.06	0.55
1:B:114:SER:O	1:B:115:LEU:O	2.24	0.54
1:B:258:ARG:HH12	1:B:259:ASN:HD21	1.55	0.54
1:D:227:PRO:HG2	1:D:229:VAL:HG13	1.89	0.54
1:A:169:LYS:HD3	1:A:169:LYS:O	2.07	0.54
1:A:151:ILE:HG23	1:A:152:CYS:H	1.72	0.54
1:A:169:LYS:HD2	1:A:170:TYR:CE1	2.43	0.54
1:D:114:SER:O	1:D:115:LEU:O	2.24	0.54
1:D:258:ARG:HH12	1:D:259:ASN:HD21	1.55	0.54
1:D:269:ILE:O	1:D:273:VAL:HG12	2.08	0.54
1:C:151:ILE:HG23	1:C:152:CYS:H	1.73	0.54
1:A:247:ASP:HB2	1:A:248:PRO:HD2	1.90	0.53
1:C:247:ASP:HB2	1:C:248:PRO:HD2	1.90	0.53
1:A:113:PRO:HG2	1:A:115:LEU:HG	1.90	0.53
1:C:113:PRO:HG2	1:C:115:LEU:HG	1.90	0.53
1:C:169:LYS:HD3	1:C:169:LYS:O	2.08	0.53
1:B:150:ASP:C	1:B:153:PRO:HD2	2.28	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:150:ASP:C	1:D:153:PRO:HD2	2.28	0.53
1:C:169:LYS:HD2	1:C:170:TYR:CE1	2.45	0.52
1:A:151:ILE:HG23	1:A:152:CYS:N	2.24	0.52
1:C:151:ILE:HG23	1:C:152:CYS:N	2.24	0.52
1:A:149:PRO:O	1:A:151:ILE:N	2.43	0.52
1:D:280:GLU:O	1:D:283:ALA:HB3	2.10	0.52
1:D:225:THR:HG23	1:D:226:PRO:HD2	1.91	0.51
1:A:169:LYS:HD2	1:A:170:TYR:CZ	2.46	0.51
1:B:280:GLU:O	1:B:283:ALA:HB3	2.11	0.51
1:A:145:PHE:CE2	1:A:148:CYS:HB2	2.46	0.51
1:C:183:PRO:HB3	1:C:212:VAL:HG21	1.93	0.51
1:C:149:PRO:O	1:C:151:ILE:N	2.44	0.50
1:D:164:ASN:ND2	1:D:199:HIS:HE2	2.08	0.50
1:B:164:ASN:ND2	1:B:199:HIS:HE2	2.09	0.50
1:B:225:THR:HG23	1:B:226:PRO:HD2	1.93	0.50
1:B:258:ARG:NH1	1:B:259:ASN:HD21	2.10	0.50
1:C:242:PHE:HB2	3:C:331:HOH:O	2.11	0.50
1:D:286:LYS:O	1:D:287:GLU:HB2	2.12	0.50
1:C:145:PHE:CE2	1:C:148:CYS:HB2	2.47	0.50
1:B:228:ASN:HB2	1:C:222:TYR:CD2	2.47	0.49
1:D:258:ARG:NH1	1:D:259:ASN:HD21	2.11	0.49
1:A:183:PRO:HB3	1:A:212:VAL:HG21	1.94	0.49
1:B:286:LYS:O	1:B:287:GLU:HB2	2.13	0.49
1:D:285:GLN:C	1:D:285:GLN:HE21	2.17	0.49
1:B:285:GLN:C	1:B:285:GLN:HE21	2.17	0.49
1:A:176:PRO:HG2	1:A:202:ILE:HA	1.95	0.49
1:C:278:PRO:HG2	1:C:282:ARG:NH1	2.28	0.48
1:B:224:SER:HB3	1:B:237:VAL:HG22	1.94	0.48
1:C:169:LYS:HD2	1:C:170:TYR:CZ	2.48	0.48
1:C:176:PRO:HG2	1:C:202:ILE:HA	1.96	0.48
1:A:222:TYR:CD2	1:D:228:ASN:HB2	2.48	0.48
1:D:260:TYR:HA	1:D:264:THR:CG2	2.43	0.48
1:B:260:TYR:HA	1:B:264:THR:CG2	2.43	0.48
1:D:224:SER:HB3	1:D:237:VAL:HG22	1.95	0.48
1:A:278:PRO:HG2	1:A:282:ARG:NH1	2.29	0.48
1:B:246:MET:HA	1:B:251:GLN:O	2.14	0.47
1:B:270:VAL:O	1:B:274:LYS:HG2	2.13	0.47
1:D:270:VAL:O	1:D:274:LYS:HG2	2.13	0.47
1:D:246:MET:HA	1:D:251:GLN:O	2.14	0.47
1:B:151:ILE:O	1:B:155:GLU:HG2	2.15	0.47
1:B:229:VAL:HB	1:B:233:GLN:NE2	2.29	0.47
1:D:229:VAL:HB	1:D:233:GLN:NE2	2.28	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:151:ILE:O	1:D:155:GLU:HG2	2.15	0.47
1:B:216:CYS:HB3	1:B:221:VAL:O	2.15	0.47
1:C:148:CYS:SG	1:C:151:ILE:HG23	2.55	0.47
1:A:221:VAL:HG12	1:A:239:HIS:CE1	2.50	0.47
1:A:145:PHE:CD2	1:A:148:CYS:HB2	2.51	0.46
1:C:221:VAL:HG12	1:C:239:HIS:CE1	2.51	0.46
1:C:201:SER:O	1:D:290:TYR:HE2	1.99	0.46
1:C:145:PHE:CD2	1:C:148:CYS:HB2	2.51	0.46
1:A:148:CYS:SG	1:A:151:ILE:HG23	2.56	0.46
1:C:280:GLU:O	1:C:281:GLN:C	2.53	0.46
1:A:280:GLU:O	1:A:281:GLN:C	2.53	0.46
1:B:285:GLN:CG	1:B:286:LYS:N	2.72	0.46
1:B:258:ARG:HD2	3:C:302:HOH:O	2.14	0.46
1:B:256:LEU:HD12	1:B:256:LEU:N	2.30	0.46
1:B:176:PRO:HG2	1:B:202:ILE:HA	1.98	0.46
1:D:172:ILE:HD11	1:D:273:VAL:HG11	1.97	0.45
1:D:256:LEU:N	1:D:256:LEU:HD12	2.31	0.45
1:D:216:CYS:HB3	1:D:221:VAL:O	2.17	0.45
1:D:285:GLN:CG	1:D:286:LYS:N	2.72	0.45
1:D:286:LYS:HB2	1:D:290:TYR:CB	2.47	0.45
1:D:237:VAL:HG21	3:D:299:HOH:O	2.16	0.45
1:B:236:LEU:HD23	1:C:255:ALA:CB	2.46	0.45
1:C:277:VAL:O	1:C:279:ALA:N	2.50	0.45
1:A:201:SER:O	1:B:290:TYR:HE2	2.00	0.45
1:B:286:LYS:HB2	1:B:290:TYR:CB	2.47	0.45
1:B:172:ILE:HD11	1:B:273:VAL:HG11	1.98	0.44
1:B:148:CYS:HA	1:B:149:PRO:HD2	1.57	0.44
1:D:164:ASN:HD21	1:D:199:HIS:HE2	1.65	0.44
1:A:255:ALA:CB	1:D:236:LEU:HD23	2.47	0.44
1:C:140:ILE:O	1:C:140:ILE:HG23	2.17	0.44
1:D:176:PRO:HG2	1:D:202:ILE:HA	1.99	0.44
1:A:277:VAL:O	1:A:279:ALA:N	2.50	0.44
1:D:148:CYS:HA	1:D:149:PRO:HD2	1.57	0.44
1:A:138:PHE:CZ	1:A:273:VAL:HA	2.52	0.44
1:C:138:PHE:CZ	1:C:273:VAL:HA	2.52	0.44
1:B:164:ASN:HD21	1:B:199:HIS:HE2	1.65	0.44
1:A:140:ILE:O	1:A:140:ILE:HG23	2.17	0.44
1:D:291:SER:OG	1:D:292:PHE:N	2.51	0.43
1:B:291:SER:OG	1:B:292:PHE:N	2.52	0.43
1:A:133:ASN:O	1:A:137:LYS:HE2	2.18	0.43
1:D:284:LYS:HA	1:D:284:LYS:CE	2.38	0.43
1:D:292:PHE:HB3	1:D:293:LEU:H	1.61	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292:PHE:HB3	1:B:293:LEU:H	1.62	0.43
1:C:145:PHE:HZ	1:C:237:VAL:HG12	1.82	0.43
1:D:150:ASP:O	1:D:153:PRO:HD2	2.18	0.43
1:B:145:PHE:CD2	1:B:148:CYS:HB2	2.54	0.43
1:C:278:PRO:HG2	1:C:282:ARG:CZ	2.49	0.43
1:C:221:VAL:O	1:C:221:VAL:HG12	2.19	0.43
1:B:150:ASP:O	1:B:153:PRO:HD2	2.18	0.42
1:D:145:PHE:CD2	1:D:148:CYS:HB2	2.54	0.42
1:C:145:PHE:O	1:C:148:CYS:HB3	2.19	0.42
1:A:145:PHE:HZ	1:A:237:VAL:HG12	1.82	0.42
1:A:221:VAL:HG12	1:A:221:VAL:O	2.20	0.42
1:A:278:PRO:HG2	1:A:282:ARG:CZ	2.50	0.42
1:B:284:LYS:HA	1:B:284:LYS:CE	2.39	0.42
1:D:247:ASP:HB2	1:D:248:PRO:CD	2.40	0.42
1:D:114:SER:HA	3:D:325:HOH:O	2.20	0.42
1:C:144:GLY:O	1:C:180:THR:HA	2.20	0.42
1:B:227:PRO:O	1:B:229:VAL:N	2.48	0.42
1:B:258:ARG:NE	1:B:258:ARG:H	2.18	0.42
1:A:263:LYS:HD3	1:C:263:LYS:NZ	2.35	0.42
1:D:162:TRP:CD1	1:D:266:VAL:HG23	2.55	0.42
1:D:227:PRO:O	1:D:229:VAL:N	2.49	0.42
1:A:145:PHE:O	1:A:148:CYS:HB3	2.20	0.42
1:C:133:ASN:O	1:C:137:LYS:HE2	2.20	0.42
1:D:248:PRO:HG2	1:D:276:TYR:OH	2.19	0.41
1:A:144:GLY:O	1:A:180:THR:HA	2.20	0.41
1:D:258:ARG:NE	1:D:258:ARG:H	2.18	0.41
1:A:263:LYS:NZ	1:C:263:LYS:HD3	2.36	0.41
1:B:162:TRP:CD1	1:B:266:VAL:HG23	2.56	0.41
1:B:243:PHE:O	1:B:255:ALA:HA	2.21	0.41
1:A:278:PRO:O	1:A:279:ALA:HB3	2.21	0.41
1:C:176:PRO:O	1:D:290:TYR:OH	2.38	0.41
1:B:262:GLU:O	1:B:266:VAL:HG23	2.20	0.41
1:C:256:LEU:N	1:C:256:LEU:HD12	2.36	0.41
1:B:247:ASP:HB2	1:B:248:PRO:CD	2.41	0.41
1:A:176:PRO:O	1:B:290:TYR:OH	2.38	0.41
1:B:286:LYS:N	1:B:286:LYS:CD	2.76	0.41
1:D:262:GLU:O	1:D:266:VAL:HG23	2.21	0.41
1:C:239:HIS:C	1:C:239:HIS:CD2	2.92	0.41
1:A:256:LEU:HD12	1:A:256:LEU:N	2.36	0.41
1:C:278:PRO:O	1:C:279:ALA:HB3	2.22	0.40
1:B:248:PRO:HG2	1:B:276:TYR:OH	2.21	0.40
1:D:123:ASP:C	1:D:125:TYR:H	2.24	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:140:ILE:O	1:D:140:ILE:HG23	2.20	0.40
1:D:145:PHE:O	1:D:148:CYS:HB3	2.21	0.40
1:A:239:HIS:CD2	1:A:239:HIS:C	2.93	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	154/200 (77%)	141 (92%)	10 (6%)	3 (2%)	12	9
1	B	179/200 (90%)	164 (92%)	11 (6%)	4 (2%)	10	7
1	C	154/200 (77%)	141 (92%)	10 (6%)	3 (2%)	12	9
1	D	179/200 (90%)	164 (92%)	11 (6%)	4 (2%)	10	7
All	All	666/800 (83%)	610 (92%)	42 (6%)	14 (2%)	11	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ASP
1	B	149	PRO
1	B	291	SER
1	C	150	ASP
1	D	149	PRO
1	D	291	SER
1	B	115	LEU
1	D	115	LEU
1	A	281	GLN
1	C	278	PRO
1	C	281	GLN
1	A	278	PRO
1	B	124	MET
1	D	288	ALA

### 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	140/176 (80%)	136 (97%)	4 (3%)	55	71
1	B	161/176 (92%)	146 (91%)	15 (9%)	13	14
1	C	140/176 (80%)	136 (97%)	4 (3%)	55	71
1	D	161/176 (92%)	146 (91%)	15 (9%)	13	14
All	All	602/704 (86%)	564 (94%)	38 (6%)	25	32

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LYS
1	A	239	HIS
1	A	281	GLN
1	A	282	ARG
1	B	115	LEU
1	B	166	LEU
1	B	218	LYS
1	B	236	LEU
1	B	237	VAL
1	B	258	ARG
1	B	259	ASN
1	B	280	GLU
1	B	281	GLN
1	B	282	ARG
1	B	285	GLN
1	B	286	LYS
1	B	290	TYR
1	B	292	PHE
1	B	293	LEU
1	C	137	LYS
1	C	239	HIS
1	C	281	GLN
1	C	282	ARG
1	D	115	LEU
1	D	166	LEU
1	D	218	LYS

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Mol	Chain	Res	Type
1	D	236	LEU
1	D	237	VAL
1	D	258	ARG
1	D	259	ASN
1	D	280	GLU
1	D	281	GLN
1	D	282	ARG
1	D	285	GLN
1	D	286	LYS
1	D	290	TYR
1	D	292	PHE
1	D	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	175	GLN
1	A	214	ASN
1	A	239	HIS
1	B	120	HIS
1	B	164	ASN
1	B	175	GLN
1	B	233	GLN
1	B	259	ASN
1	B	285	GLN
1	C	120	HIS
1	C	175	GLN
1	C	214	ASN
1	C	239	HIS
1	D	120	HIS
1	D	164	ASN
1	D	175	GLN
1	D	233	GLN
1	D	259	ASN
1	D	285	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	158/200 (79%)	-0.06	4 (2%) 54 65	19, 34, 76, 130	0
1	B	181/200 (90%)	0.06	9 (4%) 28 38	21, 38, 94, 131	0
1	C	158/200 (79%)	-0.08	6 (3%) 38 49	17, 34, 83, 132	0
1	D	181/200 (90%)	0.07	10 (5%) 24 33	21, 38, 86, 133	0
All	All	678/800 (84%)	0.00	29 (4%) 28 44	17, 36, 86, 133	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	290	TYR	6.2
1	B	290	TYR	5.3
1	A	282	ARG	4.8
1	C	282	ARG	4.4
1	D	291	SER	4.2
1	B	150	ASP	3.9
1	D	292	PHE	3.8
1	B	258	ARG	3.7
1	A	222	TYR	3.6
1	B	113	PRO	3.5
1	D	288	ALA	3.4
1	A	237	VAL	3.4
1	D	277	VAL	3.4
1	B	292	PHE	3.4
1	D	287	GLU	3.2
1	B	288	ALA	2.9
1	D	280	GLU	2.9
1	B	291	SER	2.8
1	A	239	HIS	2.7
1	B	293	LEU	2.7
1	D	289	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	239	HIS	2.5
1	D	113	PRO	2.4
1	C	216	CYS	2.4
1	D	279	ALA	2.3
1	C	222	TYR	2.2
1	C	237	VAL	2.2
1	B	287	GLU	2.1
1	C	238	ASP	2.1

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	A	297	1/1	0.84	10.30	37,37,37,37	1
2	CU	C	296	1/1	0.39	3.72	37,37,37,37	1
2	CU	A	298	1/1	0.34	1.80	37,37,37,37	1
2	CU	C	298	1/1	0.26	1.57	37,37,37,37	1
2	CU	C	297	1/1	0.27	1.56	37,37,37,37	1
2	CU	A	296	1/1	0.19	0.20	37,37,37,37	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.