



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 11:18 PM EDT

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 X-ray Structure 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

<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  
Xtrriage (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

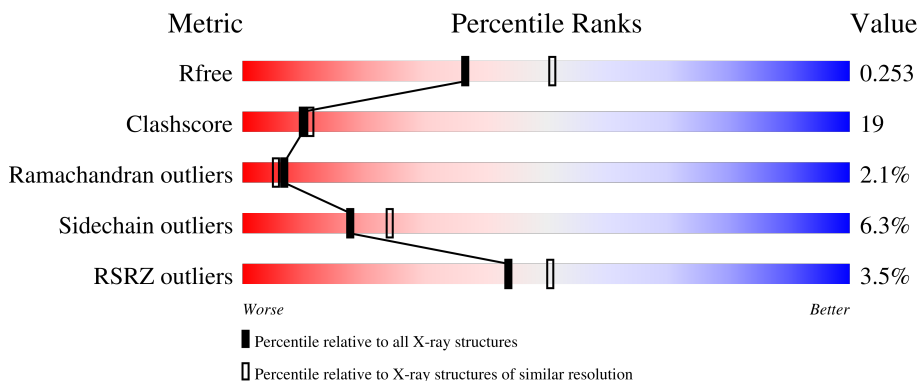
# 1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	200	 2% 58% 19% 21%
1	B	200	 5% 58% 26% 6% 10%
1	C	200	 2% 57% 20% 21%
1	D	200	 4% 58% 26% 6% 10%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5580 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 SCO1 protein.

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

- 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		

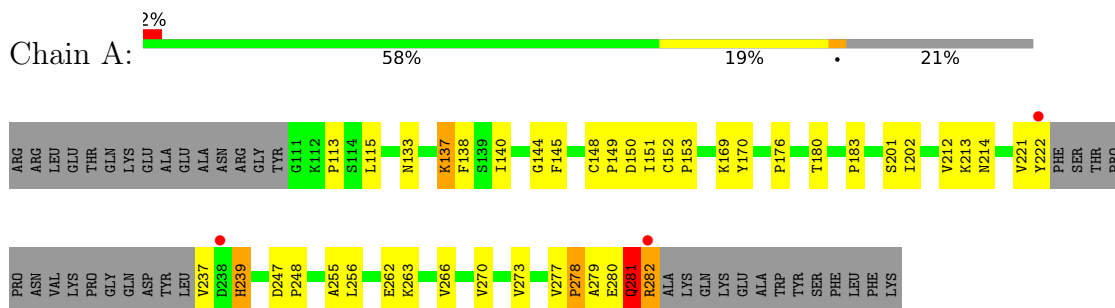
- Molecule 3 is water.

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		

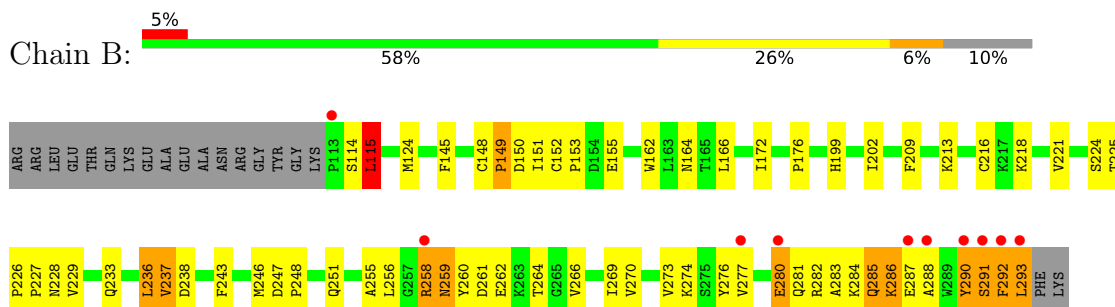
### 3 Residue-property plots [i](#)

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.

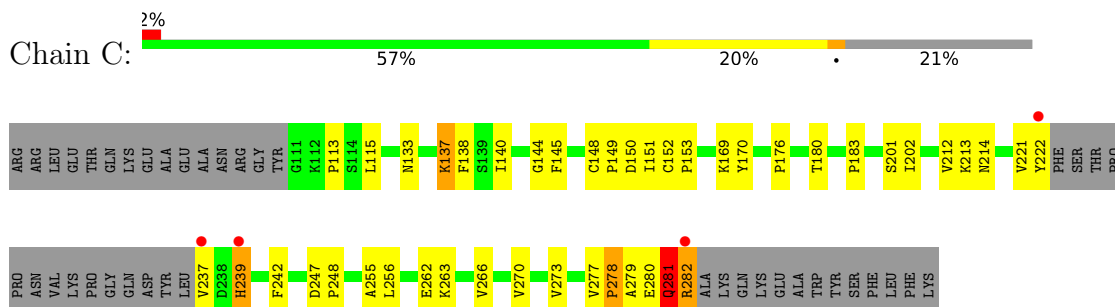
- Molecule 1: SCO1 protein



- Molecule 1: SCO1 protein

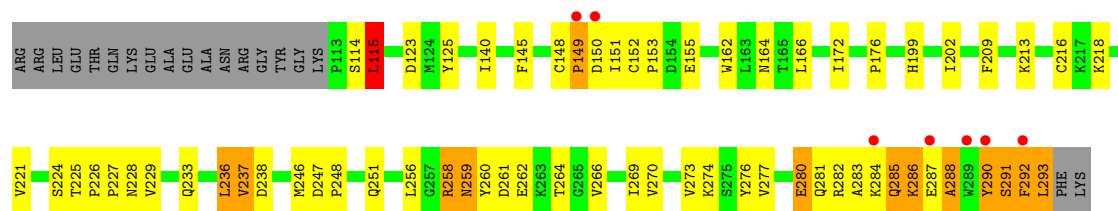


- Molecule 1: SCO1 protein



- Molecule 1: SCO1 protein





## 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)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.252 0.211 , 0.253	Depositor DCC
$R_{free}$ test set	4838 reflections (8.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.9	Xtrriage
Anisotropy	0.611	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.031 for -h,-l,-k 0.033 for -h,l,k 0.479 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage'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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 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	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
3	C	33	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	36	0	0	3	0
All	All	5580	0	5250	204	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 19.

All (204) 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: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:HA	1:D:284:LYS:HE2	1.54	0.87
1:B:284:LYS:HA	1:B:284:LYS:HE2	1.55	0.86
1:D:247:ASP:HB2	1:D:248:PRO:HD2	1.57	0.85
1:A:282:ARG:HD3	1:A:282:ARG:H	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:B:286:LYS:HD2	1:B:286:LYS:N	2.05	0.71
1:D:286:LYS:HD2	1:D:286:LYS:N	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:H	1:A:282:ARG:CD	2.09	0.65
1:B:286:LYS:HB2	1:B:290:TYR:CG	2.31	0.65
1:C:282:ARG:H	1:C:282:ARG:CD	2.09	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:HD3	1:A:282:ARG:N	2.12	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ARG:HD3	1:C:282:ARG:N	2.13	0.62
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:A:213:LYS:HE2	1:A:214:ASN:N	2.15	0.61
1:B:286:LYS:HD3	1:B:290:TYR:CD2	2.35	0.61
1:D:286:LYS:HD3	1:D:290:TYR:CD2	2.35	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:145:PHE:CE2	1:B:148:CYS:HB2	2.41	0.55
1:B:261:ASP:OD1	1:B:264:THR:HG22	2.06	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:A:152:CYS:HB2	1:A:153:PRO:HD3	1.89	0.55
1:B:269:ILE:O	1:B:273:VAL:HG12	2.07	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:C:151:ILE:HG23	1:C:152:CYS:H	1.73	0.54
1:D:269:ILE:O	1:D:273:VAL:HG12	2.08	0.54
1:A:247:ASP:HB2	1:A:248:PRO:HD2	1.90	0.53
1:A:113:PRO:HG2	1:A:115:LEU:HG	1.90	0.53
1:C:247:ASP:HB2	1:C:248:PRO:HD2	1.90	0.53
1:C:113:PRO:HG2	1:C:115:LEU:HG	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LYS:O	1:C:169:LYS:HD3	2.08	0.53
1:B:150:ASP:C	1:B:153:PRO:HD2	2.28	0.53
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:A:145:PHE:CE2	1:A:148:CYS:HB2	2.46	0.51
1:B:280:GLU:O	1:B:283:ALA:HB3	2.11	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:B:285:GLN:HE21	1:B:285:GLN:C	2.17	0.49
1:D:285:GLN:C	1:D:285:GLN:HE21	2.17	0.49
1:A:176:PRO:HG2	1:A:202:ILE:HA	1.95	0.49
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:278:PRO:HG2	1:C:282:ARG:NH1	2.28	0.48
1:A:222:TYR:CD2	1:D:228:ASN:HB2	2.48	0.48
1:C:176:PRO:HG2	1:C:202:ILE:HA	1.96	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:216:CYS:HB3	1:B:221:VAL:O	2.15	0.47
1:D:151:ILE:O	1:D:155:GLU:HG2	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:145:PHE:CD2	1:C:148:CYS:HB2	2.51	0.46
1:C:201:SER:O	1:D:290:TYR:HE2	1.99	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:256:LEU:HD12	1:B:256:LEU:N	2.30	0.46
1:B:258:ARG:HD2	3:C:302:HOH:O	2.14	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:B:236:LEU:HD23	1:C:255:ALA:CB	2.46	0.45
1:D:237:VAL:HG21	3:D:299:HOH:O	2.16	0.45
1:D:286:LYS:HB2	1:D:290:TYR:CB	2.47	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:C:277:VAL:O	1:C:279:ALA:N	2.50	0.45
1:A:255:ALA:CB	1:D:236:LEU:HD23	2.47	0.44
1:B:148:CYS:HA	1:B:149:PRO:HD2	1.57	0.44
1:B:172:ILE:HD11	1:B:273:VAL:HG11	1.98	0.44
1:C:140:ILE:HG23	1:C:140:ILE:O	2.17	0.44
1:D:164:ASN:HD21	1:D:199:HIS:HE2	1.65	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:A:140:ILE:O	1:A:140:ILE:HG23	2.17	0.44
1:B:164:ASN:HD21	1:B:199:HIS:HE2	1.65	0.44
1:B:291:SER:OG	1:B:292:PHE:N	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:SER:OG	1:D:292:PHE:N	2.51	0.43
1:A:133:ASN:O	1:A:137:LYS:HE2	2.18	0.43
1:B:292:PHE:HB3	1:B:293:LEU:H	1.62	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
1:C:145:PHE:HZ	1:C:237:VAL:HG12	1.82	0.43
1:B:145:PHE:CD2	1:B:148:CYS:HB2	2.54	0.43
1:D:150:ASP:O	1:D:153:PRO:HD2	2.18	0.43
1:C:221:VAL:HG12	1:C:221:VAL:O	2.19	0.43
1:C:278:PRO:HG2	1:C:282:ARG:CZ	2.49	0.43
1:B:150:ASP:O	1:B:153:PRO:HD2	2.18	0.42
1:C:145:PHE:O	1:C:148:CYS:HB3	2.19	0.42
1:D:145:PHE:CD2	1:D:148:CYS:HB2	2.54	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:114:SER:HA	3:D:325:HOH:O	2.20	0.42
1:D:247:ASP:HB2	1:D:248:PRO:CD	2.40	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:145:PHE:O	1:A:148:CYS:HB3	2.20	0.42
1:A:263:LYS:HD3	1:C:263:LYS:NZ	2.35	0.42
1:C:133:ASN:O	1:C:137:LYS:HE2	2.20	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:144:GLY:O	1:A:180:THR:HA	2.20	0.41
1:D:248:PRO:HG2	1:D:276:TYR:OH	2.19	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:B:262:GLU:O	1:B:266:VAL:HG23	2.20	0.41
1:C:176:PRO:O	1:D:290:TYR:OH	2.38	0.41
1:C:256:LEU:HD12	1:C:256:LEU:N	2.36	0.41
1:A:176:PRO:O	1:B:290:TYR:OH	2.38	0.41
1:A:256:LEU:HD12	1:A:256:LEU:N	2.36	0.41
1:B:247:ASP:HB2	1:B:248:PRO:CD	2.41	0.41
1:B:286:LYS:N	1:B:286:LYS:CD	2.76	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:HIS:CD2	1:C:239:HIS:C	2.92	0.41
1:D:262:GLU:O	1:D:266:VAL:HG23	2.21	0.41
1:B:248:PRO:HG2	1:B:276:TYR:OH	2.21	0.40
1:C:278:PRO:O	1:C:279:ALA:HB3	2.22	0.40
1:D:123:ASP:C	1:D:125:TYR:H	2.24	0.40
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 [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	154/200 (77%)	141 (92%)	10 (6%)	3 (2%)	8	7
1	B	179/200 (90%)	164 (92%)	11 (6%)	4 (2%)	6	5
1	C	154/200 (77%)	141 (92%)	10 (6%)	3 (2%)	8	7
1	D	179/200 (90%)	164 (92%)	11 (6%)	4 (2%)	6	5
All	All	666/800 (83%)	610 (92%)	42 (6%)	14 (2%)	7	5

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 [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	140/176 (80%)	136 (97%)	4 (3%)	42 58
1	B	161/176 (92%)	146 (91%)	15 (9%)	9 10
1	C	140/176 (80%)	136 (97%)	4 (3%)	42 58
1	D	161/176 (92%)	146 (91%)	15 (9%)	9 10
All	All	602/704 (86%)	564 (94%)	38 (6%)	18 24

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

Sometimes 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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 [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](#)

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.

No monomer is involved in short contacts.

### 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<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%)	-0.37	3 (1%) 66 73	19, 34, 76, 130	0
1	B	181/200 (90%)	-0.23	10 (5%) 25 31	21, 38, 94, 131	0
1	C	158/200 (79%)	-0.30	4 (2%) 57 64	17, 34, 83, 132	0
1	D	181/200 (90%)	-0.18	7 (3%) 39 46	21, 38, 86, 133	0
All	All	678/800 (84%)	-0.26	24 (3%) 44 51	17, 36, 86, 133	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	ARG	6.6
1	B	290	TYR	5.7
1	D	289	TRP	4.0
1	C	237	VAL	3.9
1	D	290	TYR	3.6
1	B	113	PRO	3.5
1	B	258	ARG	3.3
1	D	150	ASP	3.3
1	D	292	PHE	3.1
1	B	287	GLU	2.9
1	D	287	GLU	2.9
1	B	288	ALA	2.8
1	A	282	ARG	2.8
1	B	291	SER	2.6
1	C	239	HIS	2.6
1	D	284	LYS	2.5
1	D	149	PRO	2.5
1	B	280	GLU	2.4
1	B	293	LEU	2.3
1	B	292	PHE	2.2
1	C	222	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	277	VAL	2.2
1	A	222	TYR	2.0
1	A	238	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	C	298	1/1	0.53	0.32	37,37,37,37	1
2	CU	A	298	1/1	0.68	0.17	37,37,37,37	1
2	CU	C	297	1/1	0.87	0.17	37,37,37,37	1
2	CU	A	296	1/1	0.88	0.11	37,37,37,37	1
2	CU	C	296	1/1	0.90	0.55	37,37,37,37	1
2	CU	A	297	1/1	0.95	0.24	37,37,37,37	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.