



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:36 AM GMT

PDB ID : 2B26  
Title : The crystal structure of the protein complex of yeast Hsp40 Sis1 and Hsp70 Ssa1  
Authors : Li, J.; Wu, Y.; Qian, X.; Sha, B.  
Deposited on : 2005-09-16  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

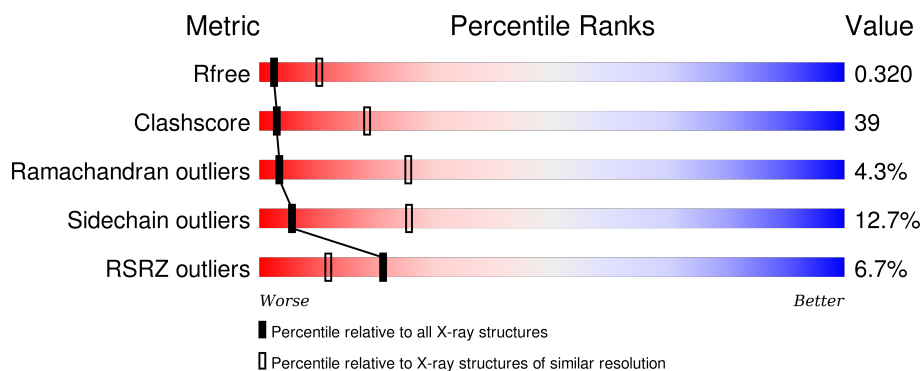
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	173	<div> <div>8%</div> <div>38%</div> <div>43%</div> <div>9%</div> <div>9%</div> </div>
1	B	173	<div> <div>3%</div> <div>40%</div> <div>38%</div> <div>6%</div> <div>15%</div> </div>
1	C	173	<div> <div>5%</div> <div>30%</div> <div>29%</div> <div>11%</div> <div>29%</div> </div>
2	D	7	<div> <div>29%</div> <div>14%</div> <div>71%</div> <div>14%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3428 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 SIS1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1238	789	218	230	1			
1	B	147	Total	C	N	O	S	0	0	0
			1170	750	200	219	1			
1	C	122	Total	C	N	O	S	0	0	0
			965	617	166	181	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	-	CLONING ARTIFACT	UNP P25294
B	180	GLU	-	CLONING ARTIFACT	UNP P25294
C	180	GLU	-	CLONING ARTIFACT	UNP P25294

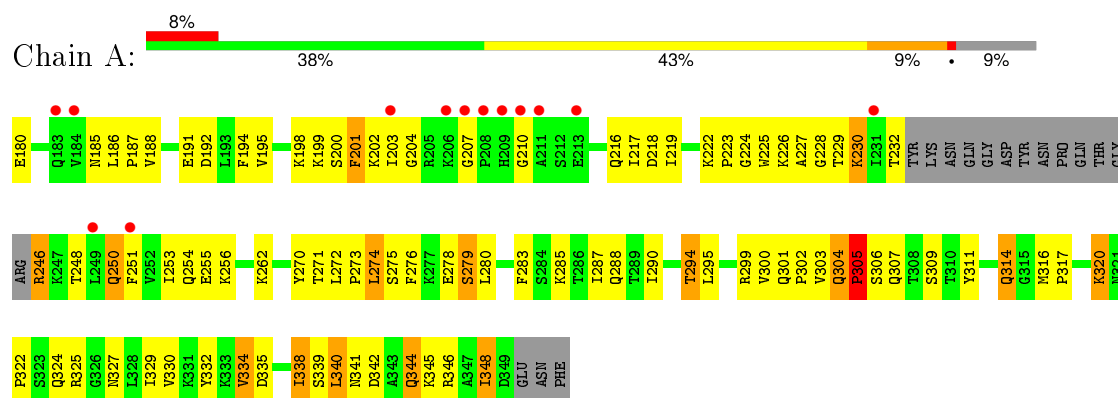
- Molecule 2 is a protein called Heat shock 70 kDa protein cognate 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	7	Total	C	N	O	0	0	0
			55	33	7	15			

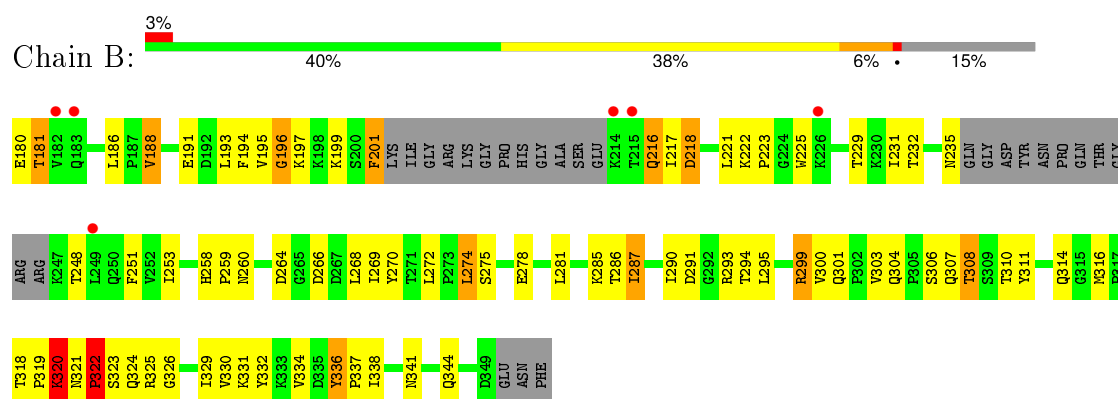
### 3 Residue-property plots [i](#)

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

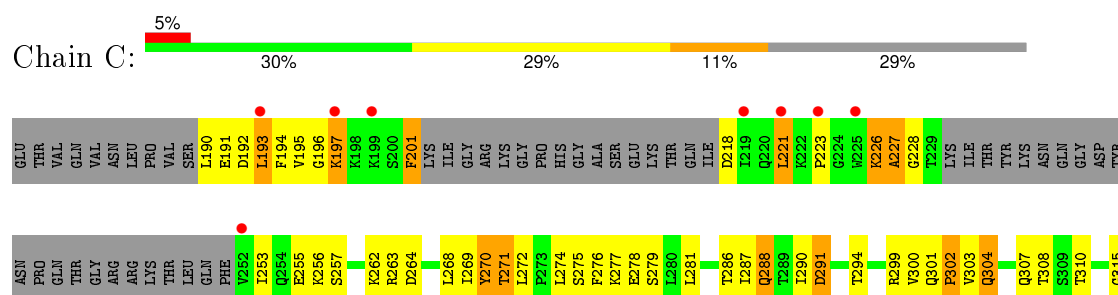
#### • Molecule 1: SIS1 protein



#### • Molecule 1: SIS1 protein

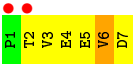


#### • Molecule 1: SIS1 protein





● Molecule 2: Heat shock 70 kDa protein cognate 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.87Å 113.87Å 173.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 48.87 – 3.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 83.9 (48.87-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.276 , 0.339 0.268 , 0.320	Depositor DCC
$R_{free}$ test set	1751 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	104.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 93.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19159 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.41	0/1263	0.71	0/1704
1	B	0.39	0/1193	0.67	0/1611
1	C	0.40	0/985	0.72	0/1329
2	D	0.41	0/55	0.75	0/73
All	All	0.40	0/3496	0.70	0/4717

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

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	1238	0	1285	99	0
1	B	1170	0	1210	92	0
1	C	965	0	987	82	0
2	D	55	0	50	13	0
All	All	3428	0	3532	273	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 39.

All (273) 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:221:LEU:H	1:C:221:LEU:HD12	1.23	1.03
1:A:287:ILE:HD12	1:A:288:GLN:H	1.17	1.03
2:D:2:THR:HG22	2:D:3:VAL:H	1.25	1.01
1:A:304:GLN:H	1:A:307:GLN:HE21	1.09	0.95
1:A:304:GLN:H	1:A:307:GLN:NE2	1.64	0.94
1:A:207:GLY:HA2	1:A:246:ARG:HH22	1.30	0.94
1:A:345:LYS:O	1:A:348:ILE:HG22	1.74	0.87
1:A:338:ILE:HG22	1:A:339:SER:H	1.40	0.86
1:C:226:LYS:HD3	1:C:226:LYS:N	1.93	0.84
1:A:207:GLY:HA2	1:A:246:ARG:NH2	1.91	0.84
1:B:299:ARG:HH11	1:B:299:ARG:HG2	1.44	0.82
1:A:287:ILE:HD12	1:A:288:GLN:N	1.95	0.81
1:C:226:LYS:H	1:C:226:LYS:HD3	1.44	0.80
1:A:348:ILE:O	1:A:348:ILE:HG23	1.82	0.80
1:A:200:SER:O	2:D:7:ASP:HB3	1.81	0.80
1:A:227:ALA:HB2	1:A:255:GLU:HG3	1.62	0.80
1:B:180:GLU:HG2	1:B:181:THR:H	1.48	0.78
1:A:226:LYS:O	1:A:229:THR:HG23	1.84	0.78
1:C:317:PRO:HA	1:C:325:ARG:HB3	1.66	0.77
1:C:193:LEU:H	1:C:193:LEU:HD13	1.51	0.75
2:D:2:THR:HG22	2:D:3:VAL:N	2.00	0.74
1:C:345:LYS:O	1:C:346:ARG:HB2	1.86	0.73
1:C:263:ARG:HG2	1:C:264:ASP:N	2.02	0.73
1:C:320:LYS:HD3	1:C:321:ASN:HB3	1.69	0.73
1:A:316:MET:HE3	1:A:317:PRO:HD2	1.68	0.73
1:C:221:LEU:CD1	1:C:221:LEU:H	2.02	0.72
1:B:201:PHE:HE2	1:B:217:ILE:HB	1.54	0.72
1:A:348:ILE:HG21	1:B:281:LEU:HD11	1.71	0.72
1:A:304:GLN:N	1:A:307:GLN:HE21	1.88	0.71
1:C:227:ALA:HB2	1:C:255:GLU:HG3	1.72	0.71
1:B:286:THR:HG22	1:B:287:ILE:N	2.05	0.71
1:C:320:LYS:NZ	1:C:321:ASN:HB3	2.05	0.71
1:B:275:SER:H	1:B:278:GLU:HG2	1.56	0.71
1:B:272:LEU:HD21	1:B:274:LEU:HD11	1.73	0.71
1:A:305:PRO:HG2	1:B:334:VAL:HG13	1.73	0.71
1:A:278:GLU:HB2	1:A:283:PHE:HB3	1.72	0.71
1:C:303:VAL:HG23	1:C:307:GLN:CD	2.11	0.70
1:A:180:GLU:O	1:A:248:THR:HB	1.90	0.70
1:C:270:TYR:CE2	1:C:287:ILE:HG12	2.26	0.70
1:C:320:LYS:HZ3	1:C:321:ASN:HB3	1.56	0.70
1:A:287:ILE:CD1	1:A:288:GLN:H	1.99	0.69
1:A:201:PHE:N	1:A:201:PHE:CD2	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:O	2:D:5:GLU:HB3	1.92	0.69
1:B:341:ASN:ND2	1:B:344:GLN:HE21	1.90	0.69
1:C:320:LYS:HD3	1:C:321:ASN:N	2.07	0.68
1:A:340:LEU:HD12	1:A:345:LYS:HG2	1.75	0.67
1:C:197:LYS:O	1:C:221:LEU:HD13	1.94	0.67
1:A:338:ILE:HG22	1:A:339:SER:N	2.09	0.67
1:A:309:SER:HB2	1:A:330:VAL:HG22	1.77	0.66
1:C:288:GLN:HE22	1:C:294:THR:HB	1.61	0.66
1:A:201:PHE:HD1	2:D:6:VAL:HA	1.60	0.66
1:A:201:PHE:HB2	2:D:5:GLU:O	1.96	0.65
1:C:317:PRO:HA	1:C:325:ARG:CB	2.27	0.65
1:C:334:VAL:HG13	1:C:336:TYR:CE1	2.32	0.64
1:B:286:THR:HG22	1:B:287:ILE:H	1.62	0.64
1:A:314:GLN:HA	1:A:325:ARG:NH2	2.13	0.64
1:B:307:GLN:HG2	1:B:308:THR:N	2.13	0.64
1:A:187:PRO:HA	1:A:254:GLN:O	1.97	0.64
1:B:188:VAL:CG2	1:B:193:LEU:HD21	2.28	0.64
1:B:193:LEU:H	1:B:193:LEU:HD22	1.62	0.64
1:A:340:LEU:HD12	1:A:345:LYS:CG	2.28	0.64
1:B:229:THR:HB	1:B:253:ILE:HD12	1.80	0.63
2:D:2:THR:CG2	2:D:3:VAL:H	2.08	0.63
1:C:270:TYR:CZ	1:C:287:ILE:HG12	2.33	0.63
1:B:320:LYS:HD3	1:B:320:LYS:C	2.18	0.63
1:B:299:ARG:NH1	1:B:299:ARG:HG2	2.13	0.62
1:A:272:LEU:HD11	1:A:285:LYS:HD2	1.81	0.62
1:B:320:LYS:HD3	1:B:321:ASN:N	2.14	0.62
1:C:315:GLY:O	1:C:325:ARG:HD2	2.00	0.62
1:C:287:ILE:HD12	1:C:288:GLN:H	1.64	0.62
1:B:188:VAL:HG21	1:B:193:LEU:HD21	1.82	0.61
1:A:340:LEU:CD1	1:A:345:LYS:HG2	2.30	0.61
1:C:256:LYS:HG2	1:C:257:SER:H	1.65	0.60
1:B:272:LEU:HG	1:B:274:LEU:HD13	1.82	0.60
1:B:197:LYS:NZ	1:B:199:LYS:HE3	2.16	0.60
1:A:202:LYS:HG2	1:A:216:GLN:HA	1.84	0.60
1:B:300:VAL:HG13	1:B:301:GLN:HE21	1.67	0.59
1:C:291:ASP:OD2	1:C:325:ARG:NH2	2.33	0.59
1:B:272:LEU:HD23	1:B:332:TYR:CE1	2.38	0.59
1:B:268:LEU:HD21	1:B:316:MET:CG	2.32	0.59
1:B:195:VAL:HG22	1:B:195:VAL:O	2.03	0.59
1:B:268:LEU:HD21	1:B:316:MET:HG2	1.85	0.59
1:B:191:GLU:O	1:B:194:PHE:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ILE:HG23	1:C:348:ILE:O	2.02	0.58
1:C:321:ASN:OD1	1:C:323:SER:HB2	2.03	0.58
1:A:271:THR:O	1:A:273:PRO:HD3	2.03	0.58
1:B:341:ASN:ND2	1:B:344:GLN:HG3	2.18	0.58
1:A:348:ILE:CG2	1:B:281:LEU:HD11	2.33	0.58
1:B:180:GLU:HG2	1:B:181:THR:N	2.18	0.58
1:B:272:LEU:HD11	1:B:285:LYS:HG3	1.85	0.58
1:A:322:PRO:C	1:A:324:GLN:H	2.07	0.58
1:C:221:LEU:HD12	1:C:221:LEU:N	2.06	0.57
1:A:339:SER:HB2	1:B:301:GLN:OE1	2.04	0.57
1:B:307:GLN:CG	1:B:308:THR:N	2.67	0.57
1:B:216:GLN:HE21	1:B:216:GLN:C	2.07	0.57
1:C:344:GLN:O	1:C:346:ARG:N	2.37	0.57
1:C:256:LYS:HG2	1:C:257:SER:N	2.20	0.57
1:C:276:PHE:O	1:C:279:SER:HB3	2.04	0.56
1:A:230:LYS:HD2	1:A:230:LYS:H	1.69	0.56
1:A:201:PHE:HD2	1:A:201:PHE:H	1.53	0.56
1:C:334:VAL:HG13	1:C:336:TYR:HE1	1.71	0.56
1:A:348:ILE:O	1:A:348:ILE:CG2	2.54	0.56
1:A:219:ILE:N	1:A:219:ILE:HD12	2.21	0.56
1:B:266:ASP:OD1	1:B:319:PRO:HD3	2.06	0.55
1:C:320:LYS:CD	1:C:321:ASN:HB3	2.36	0.55
1:C:341:ASN:OD1	1:C:343:ALA:N	2.40	0.55
1:A:201:PHE:CD1	2:D:6:VAL:HA	2.41	0.55
1:C:290:ILE:HG12	1:C:316:MET:CE	2.37	0.55
1:A:227:ALA:HA	1:A:253:ILE:HG22	1.88	0.55
1:B:299:ARG:NH1	1:B:301:GLN:O	2.40	0.55
1:C:304:GLN:H	1:C:307:GLN:NE2	2.04	0.55
1:B:314:GLN:C	1:B:325:ARG:HH21	2.09	0.55
1:A:194:PHE:HE1	1:A:325:ARG:HH11	1.55	0.54
1:C:327:ASN:HD22	1:C:327:ASN:N	2.03	0.54
1:B:231:ILE:HB	1:B:251:PHE:HB2	1.90	0.54
1:C:191:GLU:O	1:C:194:PHE:HB3	2.08	0.54
1:B:217:ILE:HG22	1:B:218:ASP:N	2.23	0.54
1:A:340:LEU:HD13	1:A:344:GLN:HB3	1.90	0.53
1:B:201:PHE:N	1:B:201:PHE:CD2	2.76	0.53
1:A:305:PRO:HA	1:A:334:VAL:HG12	1.90	0.53
1:B:291:ASP:OD1	1:B:293:ARG:HG2	2.09	0.53
1:A:230:LYS:HD2	1:A:230:LYS:N	2.22	0.53
1:C:303:VAL:HG23	1:C:307:GLN:NE2	2.24	0.53
1:B:235:ASN:H	1:B:248:THR:HA	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:THR:CG2	1:B:331:LYS:HD3	2.38	0.53
1:B:223:PRO:HB2	1:B:322:PRO:CG	2.38	0.53
1:B:286:THR:CG2	1:B:287:ILE:N	2.72	0.52
1:B:321:ASN:ND2	1:B:323:SER:OG	2.41	0.52
1:B:299:ARG:NH1	1:B:303:VAL:HG22	2.24	0.52
1:B:275:SER:H	1:B:278:GLU:CG	2.21	0.52
1:B:222:LYS:HB2	1:B:225:TRP:CE2	2.44	0.52
1:A:320:LYS:C	1:A:320:LYS:HD3	2.30	0.52
1:A:232:THR:CG2	1:A:250:GLN:HA	2.39	0.52
1:A:204:GLY:O	2:D:2:THR:CG2	2.58	0.52
1:A:274:LEU:HG	1:A:278:GLU:HG3	1.92	0.52
1:C:286:THR:HG22	1:C:287:ILE:N	2.24	0.52
1:A:317:PRO:HA	1:A:325:ARG:HA	1.90	0.52
1:B:272:LEU:CD2	1:B:274:LEU:HD11	2.38	0.52
1:B:272:LEU:HD23	1:B:332:TYR:HE1	1.75	0.52
1:A:275:SER:OG	1:A:278:GLU:HG2	2.10	0.52
1:B:191:GLU:HA	1:B:290:ILE:HD11	1.92	0.52
1:A:185:ASN:O	1:A:186:LEU:HD12	2.11	0.51
1:A:201:PHE:CB	2:D:5:GLU:O	2.59	0.51
1:A:194:PHE:CE1	1:A:325:ARG:NH1	2.77	0.51
1:A:276:PHE:O	1:A:279:SER:HB3	2.11	0.51
1:A:186:LEU:HG	1:A:201:PHE:CZ	2.45	0.51
1:B:193:LEU:H	1:B:193:LEU:CD2	2.23	0.51
1:A:202:LYS:HG2	1:A:216:GLN:CA	2.41	0.50
1:C:346:ARG:C	1:C:348:ILE:H	2.14	0.50
1:A:322:PRO:C	1:A:324:GLN:N	2.64	0.50
1:C:226:LYS:HB3	1:C:263:ARG:NH1	2.27	0.50
1:B:286:THR:CG2	1:B:287:ILE:H	2.25	0.50
1:A:276:PHE:O	1:A:280:LEU:HD12	2.10	0.50
1:C:329:ILE:HD12	1:C:329:ILE:N	2.27	0.50
1:B:272:LEU:HG	1:B:274:LEU:CD1	2.42	0.50
1:B:193:LEU:HD22	1:B:193:LEU:N	2.26	0.50
1:C:226:LYS:O	1:C:227:ALA:C	2.50	0.50
1:C:263:ARG:CG	1:C:264:ASP:N	2.74	0.50
1:A:188:VAL:O	1:A:256:LYS:HG3	2.13	0.49
1:A:200:SER:HB2	1:A:218:ASP:OD1	2.12	0.49
1:C:304:GLN:H	1:C:307:GLN:HE21	1.60	0.49
1:C:192:ASP:C	1:C:194:PHE:H	2.16	0.49
1:A:203:ILE:CD1	1:A:251:PHE:HZ	2.26	0.49
1:C:290:ILE:HG12	1:C:316:MET:HE1	1.95	0.49
1:B:318:THR:HG23	1:B:324:GLN:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:HIS:CE1	1:B:260:ASN:H	2.31	0.48
1:B:341:ASN:CG	1:B:344:GLN:HG3	2.33	0.48
1:B:222:LYS:HB2	1:B:225:TRP:NE1	2.27	0.48
1:A:311:TYR:O	1:A:327:ASN:HB2	2.12	0.48
1:A:314:GLN:HA	1:A:325:ARG:HH21	1.77	0.48
1:C:346:ARG:C	1:C:348:ILE:N	2.67	0.48
1:C:272:LEU:HD23	1:C:332:TYR:HE1	1.79	0.48
1:A:290:ILE:O	1:A:290:ILE:HG13	2.14	0.48
1:C:190:LEU:C	1:C:192:ASP:N	2.67	0.47
1:B:181:THR:O	1:B:181:THR:HG23	2.14	0.47
1:C:303:VAL:CG2	1:C:307:GLN:HB3	2.44	0.47
1:B:197:LYS:O	1:B:221:LEU:HD13	2.14	0.47
1:B:266:ASP:O	1:B:326:GLY:HA3	2.14	0.47
1:C:270:TYR:CD1	1:C:270:TYR:C	2.87	0.47
1:A:304:GLN:N	1:A:307:GLN:NE2	2.48	0.47
1:C:190:LEU:HA	1:C:193:LEU:CD1	2.44	0.47
1:A:204:GLY:O	2:D:2:THR:HG23	2.14	0.47
1:C:270:TYR:O	1:C:270:TYR:HD1	1.97	0.47
1:C:277:LYS:CG	1:C:281:LEU:HD12	2.45	0.47
1:C:319:PRO:O	1:C:320:LYS:C	2.53	0.47
1:B:321:ASN:O	1:B:323:SER:N	2.48	0.47
1:A:342:ASP:O	1:A:346:ARG:HG3	2.13	0.47
1:B:299:ARG:CG	1:B:299:ARG:NH1	2.76	0.47
2:D:6:VAL:HG12	2:D:7:ASP:H	1.80	0.47
1:C:327:ASN:ND2	1:C:327:ASN:N	2.62	0.47
1:A:300:VAL:O	1:A:300:VAL:HG22	2.14	0.47
1:C:190:LEU:HA	1:C:193:LEU:HD11	1.97	0.46
1:C:253:ILE:O	1:C:253:ILE:HD12	2.14	0.46
1:B:307:GLN:CG	1:B:308:THR:H	2.28	0.46
1:A:228:GLY:O	1:A:230:LYS:HE2	2.15	0.46
1:B:318:THR:HG23	1:B:324:GLN:O	2.14	0.46
1:A:222:LYS:O	1:A:223:PRO:C	2.54	0.46
1:B:264:ASP:HB3	1:B:269:ILE:HD11	1.96	0.46
1:B:194:PHE:CZ	1:B:291:ASP:HB3	2.51	0.46
1:A:192:ASP:OD1	1:A:199:LYS:HE2	2.16	0.46
1:A:288:GLN:OE1	1:A:294:THR:HB	2.15	0.46
1:B:320:LYS:CD	1:B:321:ASN:N	2.79	0.46
1:A:230:LYS:HA	1:A:251:PHE:O	2.16	0.46
1:A:341:ASN:O	1:A:345:LYS:HG3	2.16	0.45
1:A:320:LYS:O	1:A:322:PRO:HD3	2.16	0.45
1:B:258:HIS:CG	1:B:259:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ARG:HH11	1:C:299:ARG:HB2	1.80	0.45
1:C:190:LEU:O	1:C:193:LEU:HD22	2.16	0.45
1:B:217:ILE:HD13	1:B:251:PHE:CZ	2.52	0.45
1:C:343:ALA:O	1:C:346:ARG:HB3	2.16	0.45
1:B:221:LEU:HD12	1:B:221:LEU:N	2.31	0.45
1:B:264:ASP:HB3	1:B:269:ILE:CD1	2.46	0.45
1:C:300:VAL:O	1:C:300:VAL:HG22	2.17	0.45
1:A:287:ILE:CD1	1:A:288:GLN:N	2.70	0.45
1:B:223:PRO:HB2	1:B:322:PRO:HG3	1.99	0.45
1:C:320:LYS:HD3	1:C:321:ASN:CB	2.43	0.45
1:B:308:THR:HG22	1:B:331:LYS:HD3	1.98	0.45
1:A:305:PRO:HG2	1:B:334:VAL:CG1	2.43	0.44
1:A:303:VAL:HG21	1:A:332:TYR:CD2	2.52	0.44
1:B:336:TYR:CD2	1:B:337:PRO:HD2	2.52	0.44
1:A:198:LYS:HG2	1:A:198:LYS:O	2.17	0.44
1:C:201:PHE:CD1	1:C:201:PHE:N	2.85	0.44
2:D:6:VAL:O	2:D:7:ASP:HB2	2.16	0.44
1:B:270:TYR:HE1	1:B:272:LEU:HB2	1.82	0.44
1:C:279:SER:HB2	1:C:334:VAL:HG21	1.99	0.44
1:B:310:THR:HG23	1:B:329:ILE:CD1	2.47	0.44
1:C:193:LEU:HD23	1:C:263:ARG:NH2	2.33	0.44
1:B:186:LEU:HD22	1:B:251:PHE:CD2	2.53	0.44
1:C:299:ARG:CB	1:C:299:ARG:NH1	2.81	0.44
1:C:196:GLY:O	1:C:197:LYS:C	2.56	0.44
1:B:314:GLN:OE1	1:B:314:GLN:HA	2.18	0.44
1:C:271:THR:HG22	1:C:331:LYS:HB3	1.99	0.44
1:A:270:TYR:CE2	1:A:287:ILE:CD1	3.01	0.43
1:A:202:LYS:HG2	1:A:216:GLN:CB	2.48	0.43
1:B:274:LEU:HA	1:B:278:GLU:OE1	2.18	0.43
1:B:188:VAL:HG11	1:B:221:LEU:HD21	1.99	0.43
1:A:299:ARG:HH11	1:A:299:ARG:HG2	1.83	0.43
1:A:201:PHE:N	1:A:201:PHE:HD2	2.09	0.43
1:B:270:TYR:O	1:B:330:VAL:HA	2.18	0.43
1:B:258:HIS:HA	1:B:259:PRO:HD3	1.81	0.43
1:A:194:PHE:CZ	1:A:325:ARG:NH1	2.87	0.43
1:C:308:THR:HG22	1:C:331:LYS:HA	2.01	0.42
1:A:301:GLN:HE21	1:A:302:PRO:HD2	1.83	0.42
1:B:268:LEU:CD2	1:B:316:MET:HG2	2.49	0.42
1:A:232:THR:HG22	1:A:250:GLN:HA	2.02	0.42
1:C:277:LYS:HG2	1:C:281:LEU:HD12	2.01	0.42
1:B:295:LEU:HD21	1:B:311:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:O	1:A:195:VAL:HG12	2.19	0.42
1:A:218:ASP:C	1:A:219:ILE:HD12	2.40	0.42
1:A:309:SER:HB2	1:A:330:VAL:CG2	2.45	0.42
1:C:301:GLN:HE21	1:C:302:PRO:HD2	1.84	0.42
1:A:330:VAL:HG23	1:A:330:VAL:O	2.20	0.42
1:A:224:GLY:O	1:A:225:TRP:C	2.58	0.41
1:A:217:ILE:HG22	1:A:218:ASP:N	2.34	0.41
1:C:226:LYS:HB3	1:C:263:ARG:HH11	1.85	0.41
1:C:268:LEU:HD11	1:C:316:MET:HE3	2.01	0.41
1:C:269:ILE:HD13	1:C:329:ILE:HD13	2.02	0.41
1:A:305:PRO:HA	1:A:334:VAL:CG1	2.50	0.41
1:A:304:GLN:O	1:A:306:SER:N	2.54	0.41
1:C:275:SER:OG	1:C:278:GLU:HG3	2.21	0.41
1:C:195:VAL:HG13	1:C:197:LYS:H	1.86	0.41
1:B:196:GLY:HA2	1:B:221:LEU:O	2.21	0.41
1:B:180:GLU:CG	1:B:181:THR:H	2.17	0.41
1:C:326:GLY:C	1:C:327:ASN:HD22	2.24	0.41
1:C:299:ARG:CB	1:C:299:ARG:HH11	2.34	0.41
1:A:219:ILE:CD1	1:A:219:ILE:N	2.83	0.41
1:B:180:GLU:O	1:B:181:THR:HB	2.20	0.41
1:C:201:PHE:CZ	1:C:218:ASP:N	2.89	0.41
1:C:317:PRO:CA	1:C:325:ARG:HB3	2.45	0.41
1:A:230:LYS:CD	1:A:230:LYS:N	2.83	0.41
1:B:193:LEU:HD12	1:B:225:TRP:HB2	2.03	0.40
1:B:186:LEU:HD22	1:B:251:PHE:HD2	1.86	0.40
1:A:340:LEU:HD12	1:A:345:LYS:HG3	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	153/173 (88%)	128 (84%)	20 (13%)	5 (3%)	5	32
1	B	141/173 (82%)	123 (87%)	13 (9%)	5 (4%)	4	31
1	C	116/173 (67%)	95 (82%)	13 (11%)	8 (7%)	1	10
2	D	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
All	All	415/526 (79%)	350 (84%)	47 (11%)	18 (4%)	3	25

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ILE
1	C	346	ARG
1	A	210	GLY
1	A	320	LYS
1	B	181	THR
1	A	305	PRO
1	C	197	LYS
1	C	227	ALA
1	C	228	GLY
1	C	345	LYS
1	C	348	ILE
1	B	320	LYS
1	A	348	ILE
1	B	322	PRO
1	B	196	GLY
1	B	287	ILE
1	C	302	PRO
1	C	223	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	141/155 (91%)	124 (88%)	17 (12%)	6	28
1	B	135/155 (87%)	120 (89%)	15 (11%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	110/155 (71%)	94 (86%)	16 (14%)	4	19
2	D	7/7 (100%)	5 (71%)	2 (29%)	0	1
All	All	393/472 (83%)	343 (87%)	50 (13%)	5	25

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	PHE
1	A	230	LYS
1	A	246	ARG
1	A	250	GLN
1	A	262	LYS
1	A	274	LEU
1	A	279	SER
1	A	294	THR
1	A	295	LEU
1	A	304	GLN
1	A	305	PRO
1	A	314	GLN
1	A	329	ILE
1	A	334	VAL
1	A	335	ASP
1	A	340	LEU
1	A	344	GLN
1	B	188	VAL
1	B	201	PHE
1	B	216	GLN
1	B	218	ASP
1	B	232	THR
1	B	274	LEU
1	B	294	THR
1	B	299	ARG
1	B	304	GLN
1	B	306	SER
1	B	308	THR
1	B	320	LYS
1	B	322	PRO
1	B	336	TYR
1	B	338	ILE
1	C	193	LEU
1	C	201	PHE

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Mol	Chain	Res	Type
1	C	221	LEU
1	C	226	LYS
1	C	262	LYS
1	C	270	TYR
1	C	271	THR
1	C	274	LEU
1	C	288	GLN
1	C	291	ASP
1	C	304	GLN
1	C	310	THR
1	C	320	LYS
1	C	321	ASN
1	C	334	VAL
1	C	344	GLN
2	D	4	GLU
2	D	6	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	250	GLN
1	A	301	GLN
1	A	304	GLN
1	A	307	GLN
1	A	314	GLN
1	A	321	ASN
1	B	216	GLN
1	B	254	GLN
1	B	307	GLN
1	B	321	ASN
1	B	344	GLN
1	C	288	GLN
1	C	301	GLN
1	C	307	GLN
1	C	327	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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<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	157/173 (90%)	0.33	13 (8%) 14 7	55, 90, 176, 201	0
1	B	147/173 (84%)	0.10	6 (4%) 41 27	58, 99, 168, 190	0
1	C	122/173 (70%)	0.36	8 (6%) 22 12	54, 94, 175, 194	0
2	D	7/7 (100%)	1.16	2 (28%) 1 0	126, 154, 175, 189	0
All	All	433/526 (82%)	0.27	29 (6%) 21 12	54, 97, 176, 201	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	PRO	6.6
1	A	249	LEU	5.3
1	A	183	GLN	4.1
2	D	1	PRO	3.8
1	A	210	GLY	3.4
1	C	219	ILE	3.3
1	A	203	ILE	3.3
1	A	231	ILE	3.2
1	A	207	GLY	3.2
1	B	215	THR	3.2
1	C	199	LYS	3.0
1	A	251	PHE	3.0
1	A	209	HIS	2.8
1	B	182	VAL	2.8
1	B	214	LYS	2.7
1	C	197	LYS	2.7
1	C	221	LEU	2.6
1	A	184	VAL	2.6
1	A	206	LYS	2.5
1	B	183	GLN	2.5
1	C	193	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	252	VAL	2.4
1	C	223	PRO	2.3
1	B	249	LEU	2.3
1	C	225	TRP	2.2
1	A	213	GLU	2.2
2	D	2	THR	2.1
1	B	226	LYS	2.1
1	A	211	ALA	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.