



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:09 am GMT

PDB ID : 1FUU  
Title : YEAST INITIATION FACTOR 4A  
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Deposited on : 2000-09-15  
Resolution : 2.50 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

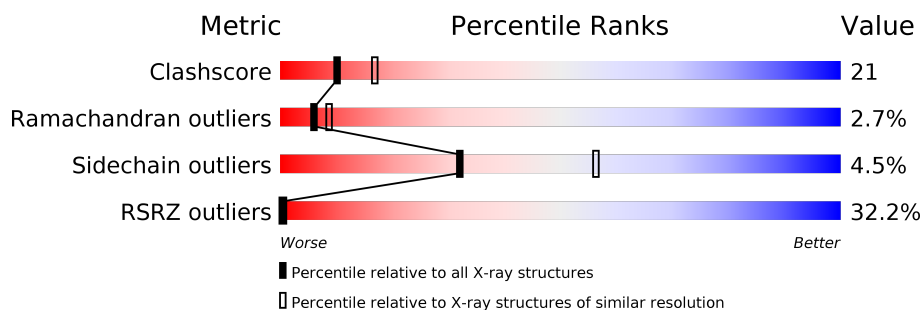
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	394	
1	B	394	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4800 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 YEAST INITIATION FACTOR 4A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	Se	0	0	0
			1660	1060	277	313	1	9			
1	B	380	Total	C	N	O	S	Se	64	0	0
			2994	1898	500	582	3	11			

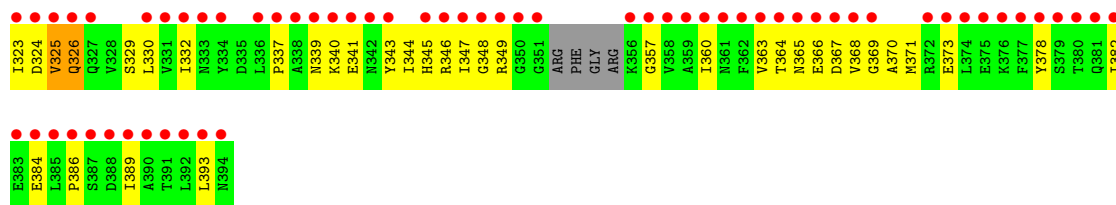
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MSE	MET	modified residue	UNP P10081
A	53	MSE	MET	modified residue	UNP P10081
A	94	MSE	MET	modified residue	UNP P10081
A	110	MSE	MET	modified residue	UNP P10081
A	116	MSE	MET	modified residue	UNP P10081
A	165	MSE	MET	modified residue	UNP P10081
A	174	MSE	MET	modified residue	UNP P10081
A	203	MSE	MET	modified residue	UNP P10081
A	215	MSE	MET	modified residue	UNP P10081
A	302	MSE	MET	modified residue	UNP P10081
A	371	MSE	MET	modified residue	UNP P10081
B	26	MSE	MET	modified residue	UNP P10081
B	53	MSE	MET	modified residue	UNP P10081
B	94	MSE	MET	modified residue	UNP P10081
B	110	MSE	MET	modified residue	UNP P10081
B	116	MSE	MET	modified residue	UNP P10081
B	165	MSE	MET	modified residue	UNP P10081
B	174	MSE	MET	modified residue	UNP P10081
B	203	MSE	MET	modified residue	UNP P10081
B	215	MSE	MET	modified residue	UNP P10081
B	302	MSE	MET	modified residue	UNP P10081
B	371	MSE	MET	modified residue	UNP P10081

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	76	Total 76	O 76	0	0
2	B	70	Total 70	O 70	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.80Å 71.20Å 73.20Å 94.00° 89.60° 101.00°	Depositor
Resolution (Å)	40.00 – 2.50 27.09 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.50) 83.9 (27.09-2.51)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.97 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.273 0.251 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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](#)

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	0/1678	0.66	1/2258 (0.0%)
1	B	0.35	0/3027	0.57	0/4074
All	All	0.37	0/4705	0.61	1/6332 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LYS	N-CA-C	-5.51	96.12	111.00

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	1660	0	1669	64	0
1	B	2994	0	3000	134	0
2	A	76	0	0	2	0
2	B	70	0	0	2	0
All	All	4800	0	4669	193	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 21.

All (193) 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:B:211:THR:HA	1:B:215:MSE:HE3	1.46	0.98
1:A:42:GLU:HG3	1:B:127:THR:H	1.36	0.91
1:B:272:VAL:HG13	1:B:314:ILE:HG22	1.58	0.83
1:B:261:GLN:HG2	1:B:311:ARG:HA	1.63	0.80
1:B:118:ILE:HD12	1:B:118:ILE:O	1.85	0.77
1:B:94:MSE:HE3	1:B:143:VAL:HB	1.66	0.77
1:B:52:ILE:HG22	1:B:53:MSE:HE2	1.68	0.75
1:B:11:GLN:HG3	1:B:12:ILE:H	1.51	0.75
1:B:45:SER:O	1:B:49:GLN:HG3	1.86	0.75
1:B:259:VAL:HG22	1:B:311:ARG:NH2	2.03	0.74
1:B:260:THR:HG23	1:B:329:SER:HB3	1.68	0.73
1:B:228:LEU:HG	1:B:344:ILE:HG21	1.71	0.73
1:B:26:MSE:SE	1:B:53:MSE:HE3	2.39	0.72
1:B:344:ILE:HD12	1:B:345:HIS:N	2.04	0.72
1:B:337:PRO:HG3	1:B:346:ARG:NH1	2.06	0.69
1:B:105:ILE:O	1:B:109:VAL:HG12	1.94	0.67
1:B:228:LEU:HD23	1:B:229:THR:N	2.10	0.67
1:B:319:LEU:O	1:B:323:ILE:HG13	1.96	0.66
1:A:58:GLY:HA2	1:A:82:ARG:HH21	1.61	0.66
1:B:344:ILE:HD12	1:B:345:HIS:H	1.61	0.66
1:B:61:VAL:HG13	1:B:219:VAL:CG2	2.26	0.65
1:B:52:ILE:HG22	1:B:53:MSE:CE	2.27	0.65
1:B:292:ASP:OD2	1:B:293:LEU:HD12	1.98	0.64
1:B:340:LYS:HE2	1:B:373:GLU:HB3	1.80	0.63
1:A:44:PRO:HB2	1:A:49:GLN:HG2	1.79	0.63
1:B:128:SER:OG	1:B:130:VAL:HG22	1.99	0.63
1:A:45:SER:O	1:A:49:GLN:HG3	1.97	0.62
1:B:44:PRO:HB2	1:B:49:GLN:HG2	1.80	0.62
1:B:118:ILE:HA	1:B:140:GLN:OE1	2.01	0.61
1:B:146:PRO:HB2	1:B:179:PHE:CD2	2.36	0.61
1:B:337:PRO:HG3	1:B:346:ARG:CZ	2.31	0.61
1:B:279:LEU:O	1:B:284:PHE:HB2	1.99	0.61
1:B:62:LEU:HD11	1:B:203:MSE:SE	2.51	0.61
1:A:203:MSE:HE3	1:A:208:LEU:HD12	1.82	0.60
1:B:167:ILE:HD13	1:B:197:VAL:HB	1.84	0.60
1:B:56:ILE:HD11	1:B:78:ALA:HA	1.83	0.60
1:B:230:LEU:HD21	1:B:344:ILE:HG22	1.83	0.60
1:B:369:GLY:O	1:B:373:GLU:HG2	2.02	0.60
1:B:347:ILE:O	1:B:347:ILE:HG13	2.02	0.59
1:A:42:GLU:HG3	1:B:127:THR:N	2.14	0.59
1:A:82:ARG:NH2	1:A:195:GLN:HE22	2.01	0.59
1:B:16:TYR:CE2	1:B:18:LYS:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:HA	1:B:365:ASN:ND2	2.18	0.58
1:B:228:LEU:CG	1:B:344:ILE:HG21	2.34	0.58
1:B:186:ILE:O	1:B:190:LEU:HD13	2.05	0.57
1:A:175:LEU:HD23	1:A:206:ASP:HB3	1.85	0.57
1:B:94:MSE:CE	1:B:143:VAL:HB	2.34	0.57
1:A:82:ARG:NH2	1:A:195:GLN:NE2	2.52	0.57
1:A:58:GLY:HA2	1:A:82:ARG:NH2	2.18	0.57
1:B:330:LEU:HD22	1:B:393:LEU:HD21	1.86	0.56
1:B:239:ASN:HD21	1:B:241:GLU:HG2	1.71	0.56
1:B:264:ILE:HG12	1:B:332:ILE:HB	1.87	0.56
1:B:339:ASN:ND2	1:B:341:GLU:HB3	2.21	0.55
1:B:205:ASN:HD22	1:B:208:LEU:HD12	1.72	0.55
1:A:26:MSE:HB2	1:A:28:LEU:CD2	2.37	0.55
1:B:235:GLN:HB3	1:B:382:ILE:HG12	1.87	0.55
1:A:121:HIS:CD2	1:A:135:GLY:HA3	2.42	0.54
1:B:240:VAL:HG21	1:B:246:LYS:HG2	1.89	0.54
1:B:240:VAL:HG21	1:B:246:LYS:CG	2.37	0.54
1:B:61:VAL:HG13	1:B:219:VAL:HG22	1.88	0.54
1:A:62:LEU:HD11	1:A:203:MSE:HE1	1.88	0.53
1:B:208:LEU:O	1:B:212:THR:HG22	2.08	0.53
1:A:17:ASP:HB2	2:A:446:HOH:O	2.07	0.53
1:B:259:VAL:HG12	1:B:260:THR:N	2.25	0.52
1:B:273:GLU:HG2	1:B:290:TYR:OH	2.10	0.52
1:B:84:ASP:OD1	1:B:86:SER:HB3	2.10	0.52
1:B:272:VAL:HG13	1:B:314:ILE:CG2	2.35	0.51
1:B:348:GLY:O	1:B:349:ARG:HB3	2.10	0.51
1:A:181:GLU:CD	1:A:181:GLU:H	2.14	0.51
1:A:82:ARG:HH22	1:A:195:GLN:NE2	2.08	0.51
1:B:253:LEU:HD12	1:B:389:ILE:HD13	1.93	0.51
1:B:368:VAL:C	1:B:370:ALA:H	2.14	0.51
1:B:253:LEU:CD1	1:B:389:ILE:HD13	2.40	0.51
1:B:182:GLN:O	1:B:186:ILE:HG13	2.11	0.51
1:B:384:GLU:O	1:B:386:PRO:HD3	2.11	0.51
1:A:104:GLN:HE21	1:A:104:GLN:HA	1.75	0.51
1:A:42:GLU:HB3	1:A:43:GLU:OE2	2.10	0.50
1:B:64:GLN:HA	1:B:200:SER:O	2.10	0.50
1:A:216:ARG:O	1:A:217:ASN:C	2.50	0.50
1:B:87:VAL:HB	1:B:91:GLN:NE2	2.27	0.50
1:A:71:LYS:O	1:A:74:THR:HB	2.11	0.50
1:B:343:TYR:CZ	1:B:347:ILE:HD11	2.46	0.50
1:B:56:ILE:CD1	1:B:81:GLN:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HD3	2:A:400:HOH:O	2.12	0.50
1:B:257:ILE:HG13	1:B:258:SER:N	2.27	0.50
1:A:106:GLN:O	1:A:110:MSE:HG2	2.12	0.50
1:B:233:ILE:HA	1:B:357:GLY:O	2.12	0.49
1:B:234:LYS:HB3	1:B:236:PHE:HE1	1.78	0.49
1:A:26:MSE:HB2	1:A:28:LEU:HD21	1.95	0.49
1:A:79:ALA:O	1:A:83:ILE:HG12	2.13	0.49
1:A:186:ILE:O	1:A:190:LEU:HD13	2.13	0.48
1:B:305:PHE:CD2	1:B:313:LEU:HD22	2.48	0.48
1:A:34:ARG:HH12	1:B:99:ARG:HD2	1.78	0.48
1:B:106:GLN:O	1:B:110:MSE:HG2	2.13	0.48
1:A:61:VAL:HG13	1:A:219:VAL:HG22	1.95	0.48
1:B:11:GLN:HG3	1:B:12:ILE:N	2.26	0.48
1:A:104:GLN:HA	1:A:104:GLN:NE2	2.29	0.48
1:B:181:GLU:O	1:B:185:GLN:HG3	2.13	0.48
1:B:228:LEU:O	1:B:229:THR:HB	2.14	0.48
1:B:343:TYR:CE2	1:B:347:ILE:HD11	2.49	0.48
1:B:228:LEU:CD2	1:B:229:THR:N	2.77	0.48
1:B:240:VAL:HG12	1:B:249:CYS:SG	2.53	0.48
1:B:324:ASP:O	1:B:326:GLN:N	2.47	0.48
1:B:366:GLU:C	1:B:368:VAL:H	2.17	0.48
1:B:248:GLU:OE2	1:B:248:GLU:HA	2.14	0.48
1:B:253:LEU:O	1:B:257:ILE:HG23	2.13	0.48
1:B:363:VAL:HB	1:B:367:ASP:HB2	1.96	0.48
1:A:16:TYR:CE2	1:A:18:LYS:HB3	2.48	0.48
1:A:199:LEU:HD22	1:A:199:LEU:N	2.28	0.48
1:A:59:HIS:O	1:A:61:VAL:HG23	2.14	0.48
1:B:225:LYS:O	1:B:226:ASP:HB3	2.14	0.48
1:A:167:ILE:CD1	1:A:197:VAL:HB	2.44	0.47
1:B:106:GLN:O	1:B:110:MSE:CG	2.62	0.47
1:A:224:LYS:O	1:A:225:LYS:CB	2.62	0.47
1:B:325:VAL:O	1:B:325:VAL:HG23	2.13	0.47
1:B:259:VAL:HA	1:B:311:ARG:CZ	2.44	0.47
1:B:282:ASP:O	1:B:283:LYS:HB2	2.14	0.47
1:B:237:TYR:CD2	1:B:371:MSE:HE1	2.50	0.47
1:A:175:LEU:HD23	1:A:206:ASP:CB	2.45	0.47
1:A:82:ARG:HH11	1:A:82:ARG:HB3	1.80	0.47
1:B:349:ARG:HH11	1:B:349:ARG:HG3	1.78	0.47
1:B:239:ASN:ND2	1:B:241:GLU:HG2	2.30	0.46
1:A:61:VAL:C	1:A:215:MSE:HE1	2.35	0.46
1:B:216:ARG:O	1:B:217:ASN:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:O	1:A:17:ASP:C	2.52	0.46
1:A:50:ARG:HE	1:A:50:ARG:HB2	1.27	0.46
1:A:109:VAL:HG22	1:A:120:VAL:HG21	1.96	0.46
1:B:121:HIS:CD2	1:B:135:GLY:HA3	2.50	0.46
1:B:306:ARG:HG2	1:B:306:ARG:O	2.16	0.46
1:B:344:ILE:HG23	1:B:378:TYR:CE2	2.51	0.46
1:A:21:TYR:O	1:A:44:PRO:HD2	2.16	0.46
1:A:61:VAL:O	1:A:215:MSE:HE1	2.15	0.46
1:B:228:LEU:HD21	1:B:230:LEU:HG	1.98	0.46
1:A:128:SER:C	1:A:130:VAL:H	2.19	0.46
1:B:199:LEU:N	1:B:199:LEU:HD22	2.31	0.46
1:A:97:PRO:HD2	1:A:101:LEU:HD13	1.96	0.46
1:A:34:ARG:HH12	1:B:99:ARG:CD	2.28	0.46
1:A:61:VAL:HG13	1:A:219:VAL:CG2	2.46	0.45
1:B:236:PHE:O	1:B:360:ILE:HA	2.17	0.45
1:A:97:PRO:HD2	1:A:101:LEU:CD1	2.47	0.45
1:A:198:LEU:HD23	1:A:198:LEU:C	2.37	0.45
1:A:203:MSE:HE3	1:A:208:LEU:CD1	2.46	0.45
1:B:276:THR:HG23	1:B:286:VAL:HG13	1.99	0.45
1:B:50:ARG:HE	1:B:50:ARG:HB2	1.27	0.45
1:B:259:VAL:O	1:B:260:THR:HB	2.17	0.45
1:B:242:GLU:HB2	1:B:245:TYR:HD1	1.82	0.44
1:B:241:GLU:O	1:B:364:THR:HB	2.16	0.44
1:A:37:PHE:CE1	1:B:126:GLY:HA3	2.52	0.44
1:B:259:VAL:HG12	1:B:260:THR:H	1.83	0.44
1:A:128:SER:C	1:A:130:VAL:N	2.71	0.44
1:B:172:ASP:N	1:B:172:ASP:OD1	2.51	0.44
1:B:51:ALA:O	1:B:55:ILE:HG13	2.17	0.43
1:A:128:SER:O	1:A:130:VAL:N	2.51	0.43
1:A:135:GLY:O	1:A:139:ALA:HB2	2.17	0.43
1:A:51:ALA:O	1:A:55:ILE:HG13	2.18	0.43
1:B:234:LYS:HB3	1:B:236:PHE:CE1	2.53	0.43
1:B:242:GLU:HB2	1:B:245:TYR:CD1	2.53	0.43
1:A:121:HIS:HE1	1:A:132:ASP:OD2	2.01	0.43
1:A:94:MSE:CE	1:A:143:VAL:HB	2.47	0.43
1:B:198:LEU:C	1:B:198:LEU:HD23	2.38	0.43
1:A:83:ILE:HG21	1:A:118:ILE:HD12	2.00	0.43
1:B:71:LYS:O	1:B:74:THR:HB	2.19	0.43
1:B:205:ASN:HA	1:B:208:LEU:HD12	2.01	0.43
1:B:71:LYS:HE2	2:B:418:HOH:O	2.19	0.43
1:B:14:THR:HA	1:B:220:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:VAL:HG21	1:B:53:MSE:HG3	2.00	0.42
1:B:393:LEU:HD12	1:B:393:LEU:N	2.34	0.42
1:B:59:HIS:HD2	2:B:423:HOH:O	2.01	0.42
1:B:56:ILE:HD12	1:B:81:GLN:CG	2.49	0.42
1:B:51:ALA:O	1:B:54:PRO:HG2	2.19	0.42
1:A:156:ARG:HG2	1:A:156:ARG:HH11	1.84	0.42
1:B:198:LEU:HD13	1:B:215:MSE:HE1	2.00	0.42
1:A:28:LEU:HA	1:A:81:GLN:OE1	2.20	0.42
1:B:303:LYS:O	1:B:307:SER:HB3	2.18	0.42
1:B:349:ARG:NH1	1:B:349:ARG:HG3	2.34	0.42
1:B:241:GLU:HG2	1:B:365:ASN:HD21	1.84	0.42
1:B:211:THR:CA	1:B:215:MSE:HE3	2.34	0.42
1:A:62:LEU:HD21	1:A:203:MSE:HE2	2.00	0.42
1:A:165:MSE:SE	1:A:167:ILE:HD11	2.70	0.42
1:B:158:PHE:CD1	1:B:158:PHE:C	2.92	0.41
1:B:240:VAL:O	1:B:241:GLU:HB2	2.20	0.41
1:B:11:GLN:OE1	1:B:11:GLN:HA	2.19	0.41
1:A:127:THR:HG23	1:A:127:THR:O	2.20	0.41
1:B:135:GLY:O	1:B:139:ALA:HB2	2.20	0.41
1:B:290:TYR:H	1:B:293:LEU:HD13	1.86	0.41
1:A:62:LEU:HD21	1:A:203:MSE:CE	2.51	0.41
1:B:130:VAL:HG23	1:B:131:GLU:N	2.36	0.41
1:B:149:VAL:O	1:B:153:ILE:HG13	2.20	0.41
1:A:167:ILE:HD12	1:A:197:VAL:HB	2.03	0.41
1:B:26:MSE:CB	1:B:28:LEU:HD13	2.51	0.41
1:B:94:MSE:HE2	1:B:141:ILE:CG2	2.51	0.41
1:B:293:LEU:H	1:B:293:LEU:HD12	1.86	0.40
1:A:58:GLY:CA	1:A:82:ARG:HH21	2.32	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	213/394 (54%)	203 (95%)	6 (3%)	4 (2%)	9	15
1	B	376/394 (95%)	328 (87%)	36 (10%)	12 (3%)	5	6
All	All	589/788 (75%)	531 (90%)	42 (7%)	16 (3%)	6	9

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	B	228	LEU
1	B	325	VAL
1	B	326	GLN
1	A	17	ASP
1	B	226	ASP
1	B	307	SER
1	B	308	GLY
1	B	310	SER
1	A	126	GLY
1	B	17	ASP
1	B	259	VAL
1	B	261	GLN
1	A	129	PHE
1	B	292	ASP
1	B	309	SER

### 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	179/336 (53%)	163 (91%)	16 (9%)	11	22
1	B	330/336 (98%)	323 (98%)	7 (2%)	59	83
All	All	509/672 (76%)	486 (96%)	23 (4%)	32	56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	17	ASP
1	A	18	LYS
1	A	24	ASP
1	A	34	ARG
1	A	50	ARG
1	A	66	GLN
1	A	69	THR
1	A	82	ARG
1	A	109	VAL
1	A	112	LEU
1	A	129	PHE
1	A	158	PHE
1	A	175	LEU
1	A	181	GLU
1	A	188	THR
1	B	17	ASP
1	B	50	ARG
1	B	109	VAL
1	B	112	LEU
1	B	158	PHE
1	B	175	LEU
1	B	270	ARG

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	66	GLN
1	A	104	GLN
1	A	121	HIS
1	A	152	ASN
1	A	195	GLN
1	A	217	ASN
1	B	59	HIS
1	B	121	HIS
1	B	152	ASN
1	B	195	GLN
1	B	205	ASN
1	B	217	ASN
1	B	239	ASN
1	B	261	GLN
1	B	267	ASN
1	B	281	ASN

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Mol	Chain	Res	Type
1	B	296	GLN
1	B	326	GLN
1	B	339	ASN
1	B	365	ASN

### 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 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	206/394 (52%)	0.82	24 (11%) <b>5</b> <b>4</b>	8, 26, 48, 77	0
1	B	369/394 (93%)	2.22	161 (43%) <b>0</b> <b>0</b>	9, 38, 110, 114	18 (4%)
All	All	575/788 (72%)	1.72	185 (32%) <b>0</b> <b>0</b>	8, 30, 108, 114	18 (3%)

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	VAL	18.1
1	B	257	ILE	12.6
1	B	318	LEU	9.6
1	B	285	THR	9.0
1	B	381	GLN	8.6
1	B	327	GLN	8.4
1	B	259	VAL	8.1
1	B	309	SER	8.0
1	B	357	GLY	7.9
1	B	391	THR	7.7
1	B	332	ILE	7.5
1	B	319	LEU	7.4
1	B	330	LEU	7.4
1	B	277	THR	7.1
1	B	339	ASN	7.0
1	B	264	ILE	7.0
1	B	256	SER	7.0
1	B	362	PHE	7.0
1	B	284	PHE	6.9
1	B	307	SER	6.8
1	B	258	SER	6.6
1	B	311	ARG	6.6
1	B	321	ARG	6.5
1	B	229	THR	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	320	ALA	6.4
1	B	389	ILE	6.3
1	B	282	ASP	6.1
1	B	333	ASN	6.0
1	B	317	ASP	6.0
1	B	237	TYR	5.9
1	B	380	THR	5.8
1	B	363	VAL	5.7
1	B	300	THR	5.6
1	B	238	VAL	5.6
1	B	338	ALA	5.5
1	B	308	GLY	5.5
1	B	365	ASN	5.5
1	A	129	PHE	5.4
1	B	366	GLU	5.3
1	B	268	THR	5.3
1	B	265	PHE	5.2
1	B	298	ARG	5.2
1	B	263	VAL	5.2
1	B	313	LEU	5.2
1	B	260	THR	5.2
1	B	294	PRO	5.2
1	B	372	ARG	5.2
1	B	130	VAL	5.2
1	B	360	ILE	5.1
1	B	301	ILE	5.1
1	B	255	ASP	4.9
1	A	86	SER	4.9
1	B	291	SER	4.8
1	B	326	GLN	4.8
1	B	286	VAL	4.8
1	B	351	GLY	4.8
1	B	383	GLU	4.7
1	B	228	LEU	4.7
1	B	296	GLN	4.6
1	A	127	THR	4.6
1	B	340	LYS	4.5
1	B	297	GLU	4.5
1	B	314	ILE	4.4
1	B	305	PHE	4.4
1	B	374	LEU	4.4
1	B	281	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	361	ASN	4.4
1	B	306	ARG	4.3
1	B	373	GLU	4.3
1	B	283	LYS	4.2
1	B	382	ILE	4.2
1	B	388	ASP	4.2
1	A	128	SER	4.2
1	B	387	SER	4.2
1	B	310	SER	4.2
1	B	379	SER	4.2
1	B	394	ASN	4.2
1	B	279	LEU	4.1
1	B	290	TYR	4.1
1	A	223	VAL	4.1
1	B	359	ALA	4.1
1	B	295	GLN	4.1
1	B	390	ALA	4.0
1	B	368	VAL	4.0
1	B	253	LEU	3.9
1	B	347	ILE	3.8
1	B	358	VAL	3.8
1	B	376	LYS	3.8
1	B	226	ASP	3.7
1	B	369	GLY	3.7
1	B	191	PRO	3.6
1	B	293	LEU	3.6
1	B	254	TYR	3.6
1	B	232	GLY	3.6
1	B	315	SER	3.5
1	B	367	ASP	3.5
1	B	128	SER	3.5
1	B	280	ARG	3.5
1	B	331	VAL	3.4
1	B	289	ILE	3.4
1	B	364	THR	3.4
1	B	356	LYS	3.4
1	B	378	TYR	3.3
1	A	167	ILE	3.3
1	B	269	ARG	3.3
1	B	292	ASP	3.3
1	B	377	PHE	3.2
1	B	346	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	392	LEU	3.2
1	B	86	SER	3.2
1	B	231	GLU	3.1
1	B	349	ARG	3.1
1	B	236	PHE	3.1
1	B	168	LEU	3.1
1	B	336	LEU	3.1
1	B	225	LYS	3.1
1	B	385	LEU	3.1
1	B	224	LYS	3.0
1	B	234	LYS	3.0
1	A	192	PRO	3.0
1	B	276	THR	3.0
1	B	334	TYR	3.0
1	B	345	HIS	2.9
1	B	262	ALA	2.9
1	B	287	SER	2.9
1	B	384	GLU	2.9
1	B	393	LEU	2.9
1	B	239	ASN	2.9
1	B	127	THR	2.9
1	B	304	GLU	2.9
1	B	129	PHE	2.9
1	B	324	ASP	2.8
1	B	156	ARG	2.8
1	B	251	THR	2.8
1	B	132	ASP	2.8
1	B	131	GLU	2.8
1	B	244	GLU	2.8
1	B	348	GLY	2.8
1	B	252	ASP	2.7
1	A	225	LYS	2.7
1	B	299	ASP	2.7
1	B	249	CYS	2.7
1	B	323	ILE	2.6
1	B	17	ASP	2.6
1	A	79	ALA	2.6
1	A	125	GLY	2.6
1	B	386	PRO	2.6
1	B	167	ILE	2.6
1	B	245	TYR	2.6
1	B	197	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	278	LYS	2.5
1	A	197	VAL	2.5
1	B	312	ILE	2.5
1	A	185	GLN	2.5
1	B	248	GLU	2.5
1	B	350	GLY	2.5
1	A	17	ASP	2.5
1	B	78	ALA	2.5
1	B	343	TYR	2.4
1	B	242	GLU	2.4
1	B	250	LEU	2.4
1	B	375	GLU	2.4
1	B	227	GLU	2.4
1	B	13	GLN	2.4
1	B	337	PRO	2.4
1	A	78	ALA	2.4
1	A	224	LYS	2.4
1	B	316	THR	2.4
1	B	342	ASN	2.4
1	A	181	GLU	2.4
1	B	266	CYS	2.3
1	A	100	GLU	2.3
1	A	168	LEU	2.3
1	B	199	LEU	2.3
1	B	223	VAL	2.3
1	A	196	VAL	2.3
1	A	61	VAL	2.1
1	A	38	GLY	2.1
1	A	92	ALA	2.0
1	B	113	ALA	2.0
1	A	191	PRO	2.0
1	A	130	VAL	2.0
1	B	126	GLY	2.0
1	B	240	VAL	2.0
1	B	341	GLU	2.0

## 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 [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.