



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 AM UTC

PDB ID : 1FUU / pdb_00001fuu
Title : YEAST INITIATION FACTOR 4A
Authors : Caruthers, J.M.; Johnson, E.R.; McKay, D.B.
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

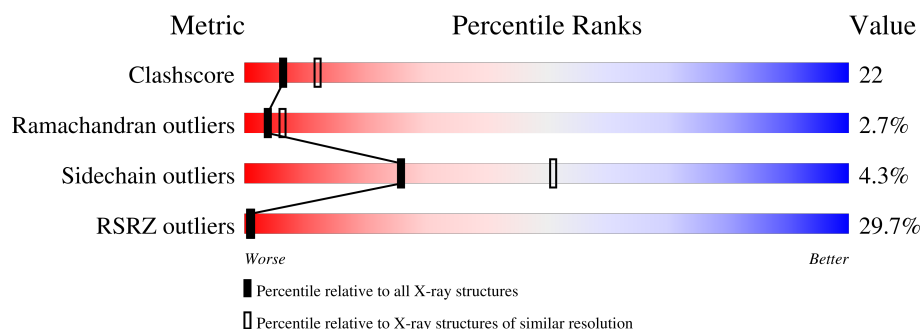
1 Overall quality at a glance

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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 35% 17% 45%
1	B	394	40% 54% 38%

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

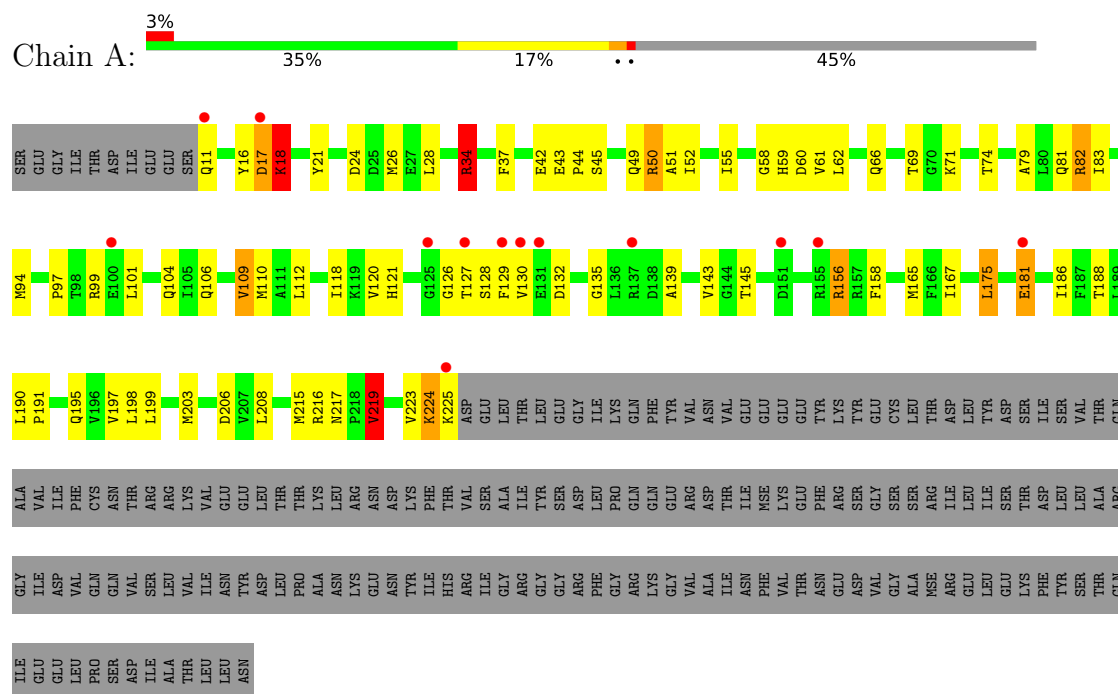
- Molecule 2 is water.

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

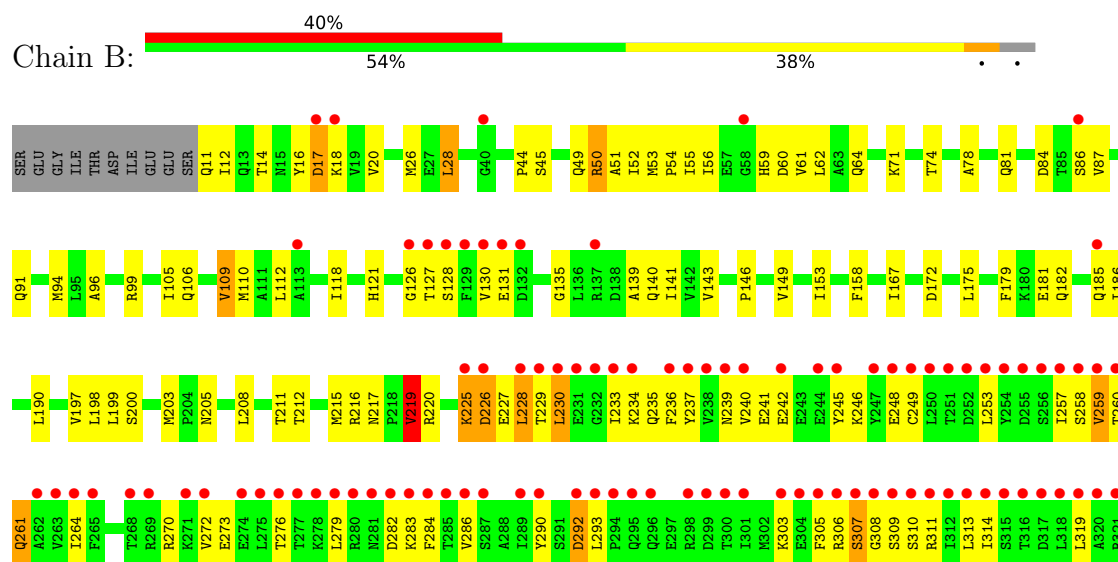
3 Residue-property plots

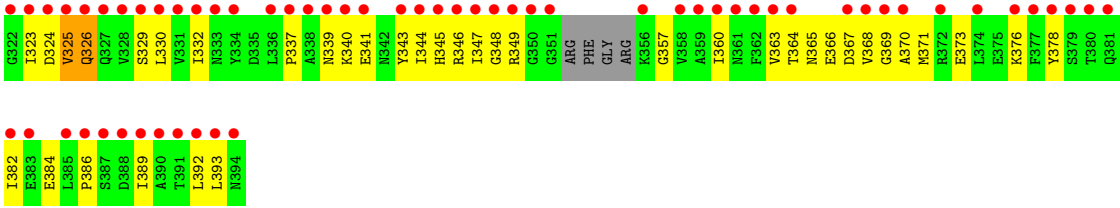
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: YEAST INITIATION FACTOR 4A



• Molecule 1: YEAST INITIATION FACTOR 4A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.80Å 71.20Å 73.20Å 94.00° 89.60° 101.00°	Depositor
Resolution (Å)	40.00 – 2.50 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.50) 84.8 (40.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4800	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.53	0/1678	1.03	10/2258 (0.4%)
1	B	0.43	0/3027	0.88	8/4074 (0.2%)
All	All	0.47	0/4705	0.94	18/6332 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ASP	N-CA-C	-7.42	98.48	110.20
1	A	60	ASP	N-CA-C	-7.37	98.91	109.96
1	A	219	VAL	N-CA-C	-7.03	99.65	109.21
1	A	18	LYS	N-CA-C	-6.89	96.12	110.80
1	B	219	VAL	N-CA-C	-6.80	99.96	109.21
1	A	145	THR	CA-C-N	6.53	126.03	119.24
1	A	145	THR	C-N-CA	6.53	126.03	119.24
1	A	34	ARG	N-CA-C	-6.37	104.34	111.28
1	A	191	PRO	CA-C-N	6.26	127.66	119.84
1	A	191	PRO	C-N-CA	6.26	127.66	119.84
1	B	96	ALA	CA-C-N	6.06	125.95	119.28
1	B	96	ALA	C-N-CA	6.06	125.95	119.28
1	A	52	ILE	N-CA-C	5.65	116.11	110.23
1	B	230	LEU	N-CA-C	-5.60	104.68	112.30
1	A	156	ARG	N-CA-C	5.60	120.06	113.23
1	B	227	GLU	N-CA-C	5.54	117.67	109.69
1	B	376	LYS	N-CA-C	-5.53	106.21	113.12
1	B	225	LYS	CB-CA-C	-5.26	108.98	116.34

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	1660	0	1669	66	0
1	B	2994	0	3000	141	0
2	A	76	0	0	2	0
2	B	70	0	0	2	0
All	All	4800	0	4669	202	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 22.

All (202) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:ILE:HD11	1:B:78:ALA:HA	1.83	0.60
1:B:167:ILE:HD13	1:B:197:VAL:HB	1.84	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
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:A:181:GLU:CD	1:A:181:GLU:H	2.14	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:A:216:ARG:O	1:A:217:ASN:C	2.50	0.55
1:B:235:GLN:HB3	1:B:382:ILE:HG12	1.87	0.55
1:B:368:VAL:C	1:B:370:ALA:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:366:GLU:C	1:B:368:VAL:H	2.17	0.53
1:B:259:VAL:HG12	1:B:260:THR:N	2.25	0.52
1:B:84:ASP:OD1	1:B:86:SER:HB3	2.10	0.52
1:B:273:GLU:HG2	1:B:290:TYR:OH	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:82:ARG:HH22	1:A:195:GLN:NE2	2.08	0.51
1:B:253:LEU:CD1	1:B:389:ILE:HD13	2.40	0.51
1:B:253:LEU:HD12	1:B:389:ILE:HD13	1.93	0.51
1:B:216:ARG:O	1:B:217:ASN:C	2.53	0.51
1:A:16:TYR:O	1:A:17:ASP:C	2.52	0.51
1:A:61:VAL:C	1:A:215:MSE:HE1	2.35	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:HA	1:A:104:GLN:HE21	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: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:A:128:SER:C	1:A:130:VAL:H	2.19	0.50
1:B:56:ILE:CD1	1:B:81:GLN:HB3	2.42	0.50
1:B:343:TYR:CZ	1:B:347:ILE:HD11	2.46	0.50
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:A:198:LEU:C	1:A:198:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:198:LEU:HD23	1:B:198:LEU:C	2.38	0.48
1:B:248:GLU:HA	1:B:248:GLU:OE2	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:59:HIS:O	1:A:61:VAL:HG23	2.14	0.48
1:A:199:LEU:N	1:A:199:LEU:HD22	2.28	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:A:128:SER:C	1:A:130:VAL:N	2.71	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:HG23	1:B:325:VAL:O	2.13	0.47
1:A:82:ARG:HH11	1:A:82:ARG:HB3	1.80	0.47
1:A:175:LEU:HD23	1:A:206:ASP:CB	2.45	0.47
1:B:237:TYR:CD2	1:B:371:MSE:HE1	2.50	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:349:ARG:HG3	1:B:349:ARG:HH11	1.78	0.47
1:B:239:ASN:ND2	1:B:241:GLU:HG2	2.30	0.46
1:B:158:PHE:CD1	1:B:158:PHE:C	2.92	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:O	1:B:306:ARG:HG2	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:B:199:LEU:N	1:B:199:LEU:HD22	2.31	0.46
1:A:34:ARG:HH12	1:B:99:ARG:CD	2.28	0.46
1:A:97:PRO:HD2	1:A:101:LEU:HD13	1.96	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:B:392:LEU:C	1:B:393:LEU:HD12	2.42	0.45
1:A:203:MSE:HE3	1:A:208:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:HE	1:B:50:ARG:HB2	1.27	0.45
1:B:276:THR:HG23	1:B:286:VAL:HG13	1.99	0.45
1:B:259:VAL:O	1:B:260:THR:HB	2.17	0.45
1:A:158:PHE:C	1:A:158:PHE:CD1	2.96	0.44
1:B:241:GLU:O	1:B:364:THR:HB	2.16	0.44
1:B:242:GLU:HB2	1:B:245:TYR:HD1	1.82	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: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:B:364:THR:C	1:B:366:GLU:H	2.26	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:94:MSE:CE	1:A:143:VAL:HB	2.47	0.43
1:A:121:HIS:HE1	1:A:132:ASP:OD2	2.01	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:118:ILE:HD12	1:B:118:ILE:C	2.43	0.43
1:B:14:THR:HA	1:B:220:ARG:O	2.19	0.42
1:B:20:VAL:HG21	1:B:53:MSE:HG3	2.00	0.42
1:B:56:ILE:HD12	1:B:81:GLN:CG	2.49	0.42
1:B:59:HIS:HD2	2:B:423:HOH:O	2.01	0.42
1:B:393:LEU:HD12	1:B:393:LEU:N	2.34	0.42
1:B:51:ALA:O	1:B:54:PRO:HG2	2.19	0.42
1:A:156:ARG:HH11	1:A:156:ARG:HG2	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:241:GLU:HG2	1:B:365:ASN:HD21	1.84	0.42
1:B:303:LYS:O	1:B:307:SER:HB3	2.18	0.42
1:B:349:ARG:HG3	1:B:349:ARG:NH1	2.34	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:240:VAL:O	1:B:241:GLU:HB2	2.20	0.41
1:B:305:PHE:C	1:B:307:SER:H	2.28	0.41
1:B:11:GLN:OE1	1:B:11:GLN:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG23	1:A:127:THR:O	2.20	0.41
1:B:237:TYR:CD1	1:B:237:TYR:C	2.98	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:366:GLU:C	1:B:368:VAL:N	2.78	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:368:VAL:C	1:B:370:ALA:N	2.78	0.41
1:B:293:LEU:HD12	1:B:293:LEU:H	1.86	0.40
1:A:223:VAL:O	1:A:224:LYS:C	2.65	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

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	213/394 (54%)	203 (95%)	6 (3%)	4 (2%)	6	11
1	B	376/394 (95%)	328 (87%)	36 (10%)	12 (3%)	3	4
All	All	589/788 (75%)	531 (90%)	42 (7%)	16 (3%)	4	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	B	228	LEU
1	B	325	VAL

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Mol	Chain	Res	Type
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%)	165 (92%)	14 (8%)	11	24
1	B	330/336 (98%)	322 (98%)	8 (2%)	43	70
All	All	509/672 (76%)	487 (96%)	22 (4%)	26	51

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
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

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Mol	Chain	Res	Type
1	A	175	LEU
1	A	181	GLU
1	A	188	THR
1	A	219	VAL
1	B	17	ASP
1	B	28	LEU
1	B	50	ARG
1	B	109	VAL
1	B	112	LEU
1	B	175	LEU
1	B	219	VAL
1	B	270	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	104	GLN
1	A	121	HIS
1	A	195	GLN
1	A	217	ASN
1	B	59	HIS
1	B	106	GLN
1	B	121	HIS
1	B	185	GLN
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
1	B	296	GLN
1	B	326	GLN
1	B	339	ASN
1	B	365	ASN
1	B	381	GLN

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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	206/394 (52%)	0.79	13 (6%) 26 23	8, 26, 48, 77	0
1	B	369/394 (93%)	1.92	158 (42%) 0 0	9, 38, 110, 114	18 (4%)
All	All	575/788 (72%)	1.52	171 (29%) 1 1	8, 30, 108, 114	18 (3%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	VAL	12.6
1	B	257	ILE	7.2
1	B	368	VAL	7.0
1	A	127	THR	6.3
1	B	238	VAL	6.0
1	B	285	THR	6.0
1	B	318	LEU	5.9
1	B	284	PHE	5.8
1	B	129	PHE	5.7
1	B	330	LEU	5.4
1	B	320	ALA	5.4
1	B	322	GLY	5.4
1	B	300	THR	5.3
1	B	374	LEU	5.2
1	B	317	ASP	5.1
1	B	258	SER	4.9
1	B	303	LYS	4.9
1	B	289	ILE	4.9
1	B	313	LEU	4.9
1	B	319	LEU	4.8
1	B	327	GLN	4.8
1	B	254	TYR	4.8
1	B	376	LYS	4.8
1	B	228	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	382	ILE	4.7
1	B	293	LEU	4.7
1	B	338	ALA	4.6
1	B	363	VAL	4.6
1	B	301	ILE	4.6
1	B	377	PHE	4.5
1	B	294	PRO	4.4
1	B	127	THR	4.4
1	B	259	VAL	4.4
1	B	279	LEU	4.3
1	B	351	GLY	4.2
1	B	336	LEU	4.2
1	B	316	THR	4.2
1	B	310	SER	4.1
1	B	323	ILE	4.1
1	B	389	ILE	4.1
1	B	264	ILE	4.1
1	B	361	ASN	4.1
1	B	309	SER	4.1
1	B	332	ILE	4.1
1	B	277	THR	4.1
1	B	268	THR	4.1
1	B	328	VAL	4.1
1	B	278	LYS	4.0
1	B	380	THR	4.0
1	B	286	VAL	4.0
1	B	385	LEU	4.0
1	B	362	PHE	4.0
1	B	229	THR	3.9
1	B	347	ILE	3.9
1	B	248	GLU	3.9
1	B	360	ILE	3.8
1	B	130	VAL	3.8
1	A	129	PHE	3.7
1	B	304	GLU	3.7
1	A	125	GLY	3.7
1	B	326	GLN	3.7
1	B	253	LEU	3.7
1	B	359	ALA	3.7
1	B	372	ARG	3.7
1	B	391	THR	3.6
1	B	392	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	349	ARG	3.5
1	B	312	ILE	3.5
1	B	331	VAL	3.5
1	B	370	ALA	3.5
1	B	231	GLU	3.5
1	B	329	SER	3.5
1	B	337	PRO	3.4
1	B	283	LYS	3.4
1	B	126	GLY	3.4
1	B	232	GLY	3.4
1	A	17	ASP	3.3
1	B	341	GLU	3.3
1	B	132	ASP	3.3
1	B	315	SER	3.3
1	B	386	PRO	3.3
1	B	393	LEU	3.3
1	B	240	VAL	3.3
1	B	296	GLN	3.2
1	B	390	ALA	3.2
1	B	17	ASP	3.2
1	B	356	LYS	3.1
1	B	263	VAL	3.1
1	B	334	TYR	3.1
1	B	236	PHE	3.1
1	B	306	ARG	3.1
1	B	237	TYR	3.1
1	B	262	ALA	3.1
1	B	346	ARG	3.1
1	B	290	TYR	3.0
1	B	311	ARG	3.0
1	B	314	ILE	3.0
1	B	233	ILE	2.9
1	B	307	SER	2.9
1	B	333	ASN	2.9
1	A	11	GLN	2.9
1	B	381	GLN	2.9
1	B	378	TYR	2.9
1	B	321	ARG	2.9
1	A	100	GLU	2.9
1	B	244	GLU	2.9
1	B	287	SER	2.8
1	B	234	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	305	PHE	2.8
1	B	364	THR	2.8
1	A	181	GLU	2.8
1	B	387	SER	2.8
1	B	339	ASN	2.8
1	B	348	GLY	2.7
1	B	275	LEU	2.7
1	B	255	ASP	2.7
1	B	343	TYR	2.7
1	B	256	SER	2.7
1	A	131	GLU	2.7
1	B	252	ASP	2.7
1	B	250	LEU	2.7
1	B	265	PHE	2.6
1	B	281	ASN	2.6
1	B	369	GLY	2.6
1	A	225	LYS	2.6
1	A	130	VAL	2.6
1	B	239	ASN	2.6
1	B	379	SER	2.6
1	B	245	TYR	2.6
1	B	340	LYS	2.5
1	B	247	TYR	2.5
1	B	230	LEU	2.5
1	B	272	VAL	2.5
1	B	350	GLY	2.5
1	B	282	ASP	2.5
1	B	226	ASP	2.4
1	B	269	ARG	2.4
1	B	394	ASN	2.4
1	B	86	SER	2.4
1	B	271	LYS	2.4
1	B	308	GLY	2.4
1	B	131	GLU	2.4
1	B	298	ARG	2.4
1	B	345	HIS	2.4
1	B	249	CYS	2.4
1	B	358	VAL	2.4
1	B	260	THR	2.3
1	B	295	GLN	2.3
1	A	151	ASP	2.3
1	B	383	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	40	GLY	2.3
1	B	113	ALA	2.3
1	B	276	THR	2.3
1	B	299	ASP	2.3
1	A	137	ARG	2.3
1	B	18	LYS	2.2
1	B	292	ASP	2.2
1	B	58	GLY	2.2
1	B	225	LYS	2.2
1	B	251	THR	2.2
1	B	242	GLU	2.2
1	B	344	ILE	2.1
1	B	274	GLU	2.1
1	B	388	ASP	2.1
1	B	324	ASP	2.1
1	B	137	ARG	2.1
1	B	280	ARG	2.1
1	B	128	SER	2.1
1	B	367	ASP	2.0
1	B	185	GLN	2.0
1	A	155	ARG	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 oligosaccharides 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.