



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:27 AM UTC

PDB ID : 3ER0 / pdb_00003er0
Title : Crystal structure of the full length eIF5A from *Saccharomyces cerevisiae*
Authors : Sanches, M.; Dias, C.A.O.; Aponi, L.H.; Valentini, S.R.; Guimaraes, B.
Deposited on : 2008-10-01
Resolution : 3.35 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
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

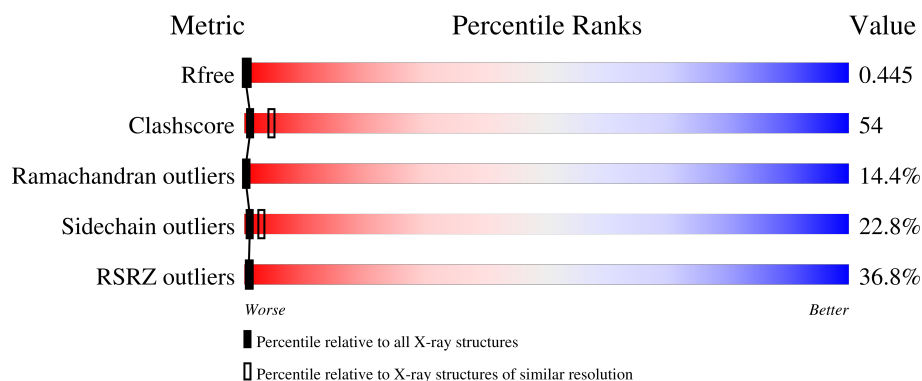
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	167	29% 31% 31% 16% 11% 13%
1	B	167	32% 26% 33% 13% 7% 22%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2105 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 Eukaryotic translation initiation factor 5A-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1104	685	186	224	9			
1	B	131	Total	C	N	O	S	0	0	0
			1001	628	164	200	9			

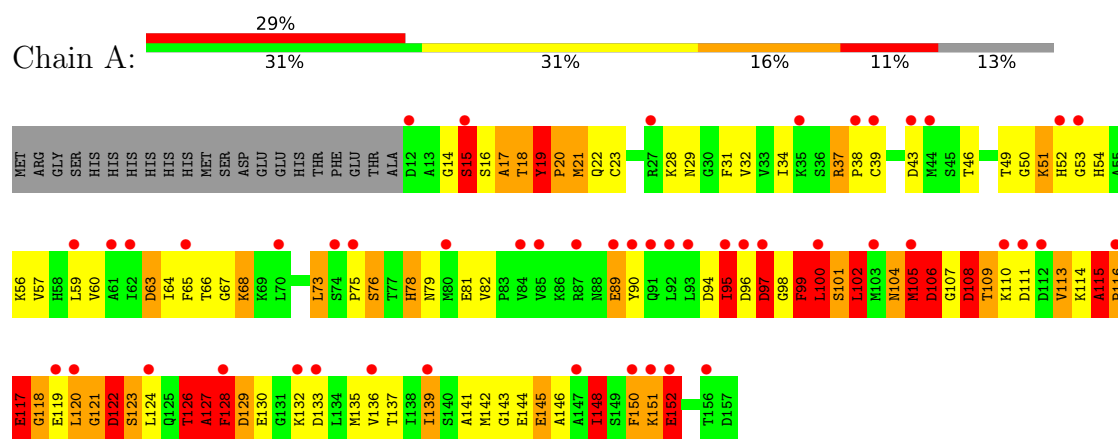
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP P23301
A	-8	ARG	-	expression tag	UNP P23301
A	-7	GLY	-	expression tag	UNP P23301
A	-6	SER	-	expression tag	UNP P23301
A	-5	HIS	-	expression tag	UNP P23301
A	-4	HIS	-	expression tag	UNP P23301
A	-3	HIS	-	expression tag	UNP P23301
A	-2	HIS	-	expression tag	UNP P23301
A	-1	HIS	-	expression tag	UNP P23301
A	0	HIS	-	expression tag	UNP P23301
B	-9	MET	-	expression tag	UNP P23301
B	-8	ARG	-	expression tag	UNP P23301
B	-7	GLY	-	expression tag	UNP P23301
B	-6	SER	-	expression tag	UNP P23301
B	-5	HIS	-	expression tag	UNP P23301
B	-4	HIS	-	expression tag	UNP P23301
B	-3	HIS	-	expression tag	UNP P23301
B	-2	HIS	-	expression tag	UNP P23301
B	-1	HIS	-	expression tag	UNP P23301
B	0	HIS	-	expression tag	UNP P23301

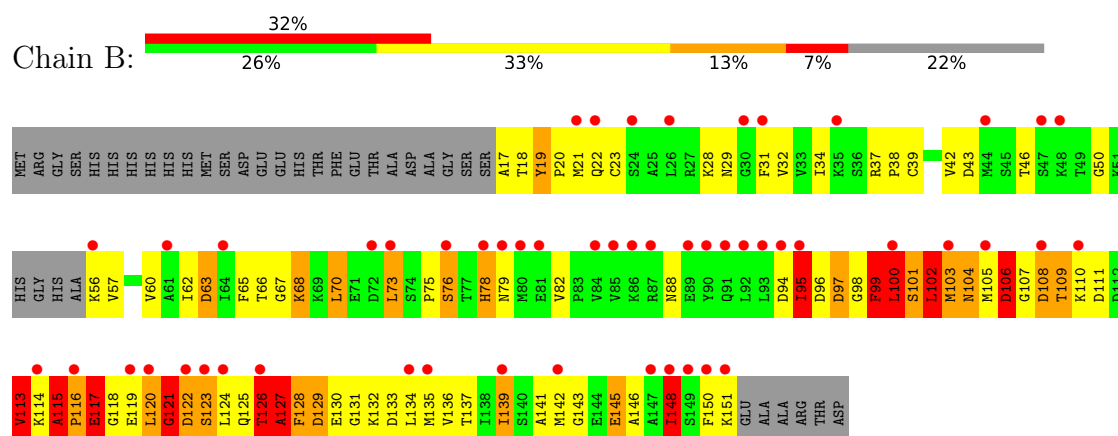
3 Residue-property plots [i](#)

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: Eukaryotic translation initiation factor 5A-2



- Molecule 1: Eukaryotic translation initiation factor 5A-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	59.66Å 59.66Å 339.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 3.35 49.45 – 3.35	Depositor EDS
% Data completeness (in resolution range)	91.9 (49.45-3.35) 91.9 (49.45-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.386 , 0.448 0.381 , 0.445	Depositor DCC
R_{free} test set	528 reflections (9.08%)	wwPDB-VP
Wilson B-factor (Å ²)	114.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 160.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2105	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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

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	0.71	1/1119 (0.1%)	1.36	14/1505 (0.9%)
1	B	0.61	0/1013	1.30	6/1360 (0.4%)
All	All	0.66	1/2132 (0.0%)	1.33	20/2865 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	17
All	All	0	35

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	GLU	CD-OE1	8.89	1.42	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ALA	CA-C-N	12.72	135.75	119.84
1	B	115	ALA	C-N-CA	12.72	135.75	119.84
1	A	19	TYR	CA-C-N	11.20	133.84	119.84
1	A	19	TYR	C-N-CA	11.20	133.84	119.84
1	A	111	ASP	N-CA-C	-9.26	102.56	114.04
1	A	118	GLY	N-CA-C	-9.20	99.67	111.72
1	A	128	PHE	N-CA-C	-8.26	93.21	110.80
1	B	111	ASP	N-CA-C	-8.18	103.89	114.04
1	A	152	GLU	CG-CD-OE2	7.08	134.68	118.40
1	A	108	ASP	N-CA-C	6.74	122.04	113.55
1	B	117	GLU	CB-CA-C	-6.21	108.78	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASP	CA-C-N	6.08	133.16	121.54
1	A	108	ASP	C-N-CA	6.08	133.16	121.54
1	A	54	HIS	N-CA-C	5.67	118.31	109.52
1	A	97	ASP	CA-C-N	5.55	131.69	121.70
1	A	97	ASP	C-N-CA	5.55	131.69	121.70
1	A	19	TYR	CB-CA-C	5.43	117.38	110.16
1	B	102	LEU	CB-CA-C	5.42	121.20	110.42
1	A	152	GLU	OE1-CD-OE2	-5.09	110.68	122.90
1	B	103	MET	N-CA-C	5.06	121.58	110.80

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	SER	Peptide
1	A	102	LEU	Peptide
1	A	105	MET	Peptide
1	A	106	ASP	Peptide
1	A	108	ASP	Peptide
1	A	115	ALA	Peptide
1	A	117	GLU	Peptide
1	A	121	GLY	Peptide
1	A	122	ASP	Peptide
1	A	126	THR	Peptide
1	A	127	ALA	Peptide
1	A	128	PHE	Peptide
1	A	18	THR	Peptide
1	A	19	TYR	Peptide
1	A	49	THR	Peptide
1	A	50	GLY	Peptide
1	A	97	ASP	Peptide
1	A	99	PHE	Peptide
1	B	101	SER	Peptide
1	B	102	LEU	Peptide
1	B	105	MET	Peptide
1	B	106	ASP	Peptide
1	B	108	ASP	Peptide
1	B	115	ALA	Peptide
1	B	117	GLU	Peptide
1	B	121	GLY	Peptide
1	B	122	ASP	Peptide
1	B	126	THR	Peptide

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Mol	Chain	Res	Type	Group
1	B	127	ALA	Peptide
1	B	128	PHE	Peptide
1	B	131	GLY	Peptide
1	B	19	TYR	Peptide
1	B	50	GLY	Peptide
1	B	97	ASP	Peptide
1	B	99	PHE	Peptide

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	1104	0	1096	101	1
1	B	1001	0	1011	95	1
All	All	2105	0	2107	196	1

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 54.

All (196) 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:98:GLY:HA2	1:B:99:PHE:CG	1.77	1.19
1:B:100:LEU:H	1:B:101:SER:HA	1.02	1.13
1:A:114:LYS:O	1:A:116:PRO:HD2	1.51	1.10
1:B:17:ALA:CB	1:B:18:THR:HA	1.77	1.09
1:A:17:ALA:CB	1:A:18:THR:HA	1.83	1.06
1:B:17:ALA:HB3	1:B:18:THR:HA	1.38	1.05
1:A:124:LEU:O	1:A:127:ALA:CB	2.05	1.05
1:A:151:LYS:HG2	1:A:152:GLU:H	1.22	1.03
1:B:100:LEU:H	1:B:101:SER:CA	1.72	1.02
1:B:118:GLY:HA3	1:B:121:GLY:H	1.21	1.02
1:B:127:ALA:O	1:B:130:GLU:HB2	1.62	0.99
1:A:118:GLY:HA3	1:A:121:GLY:H	1.28	0.98
1:A:127:ALA:O	1:A:130:GLU:HB2	1.65	0.95
1:B:42:VAL:HG21	1:B:62:ILE:HD12	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:THR:HG23	1:B:110:LYS:HA	1.48	0.93
1:A:17:ALA:HB3	1:A:18:THR:HA	1.50	0.92
1:B:100:LEU:N	1:B:101:SER:HA	1.79	0.91
1:A:124:LEU:O	1:A:127:ALA:HB3	1.69	0.90
1:B:98:GLY:HA2	1:B:99:PHE:CB	2.01	0.88
1:A:151:LYS:CG	1:A:152:GLU:H	1.86	0.85
1:A:150:PHE:HD2	1:A:150:PHE:C	1.84	0.85
1:A:16:SER:HA	1:A:17:ALA:O	1.76	0.84
1:B:127:ALA:HB3	1:B:128:PHE:HB2	1.57	0.84
1:A:89:GLU:HB3	1:A:137:THR:HG22	1.60	0.83
1:A:17:ALA:HB1	1:A:18:THR:HA	1.58	0.83
1:A:14:GLY:HA3	1:A:15:SER:CB	2.09	0.83
1:B:95:ILE:HD13	1:B:125:GLN:NE2	1.94	0.83
1:A:37:ARG:HD3	1:A:38:PRO:HD2	1.62	0.82
1:A:124:LEU:O	1:A:127:ALA:HB2	1.78	0.81
1:B:17:ALA:HB1	1:B:18:THR:HA	1.60	0.80
1:B:17:ALA:CB	1:B:18:THR:CA	2.60	0.79
1:B:37:ARG:HD3	1:B:38:PRO:HD2	1.63	0.78
1:A:90:TYR:HB2	1:A:102:LEU:HD13	1.64	0.78
1:B:96:ASP:HB3	1:B:97:ASP:HB3	1.64	0.77
1:B:115:ALA:HB1	1:B:117:GLU:HG2	1.65	0.77
1:B:100:LEU:HG	1:B:113:VAL:HG22	1.66	0.76
1:A:150:PHE:C	1:A:150:PHE:CD2	2.59	0.76
1:B:98:GLY:HA2	1:B:99:PHE:CD2	2.22	0.75
1:A:109:THR:HG23	1:A:110:LYS:HA	1.69	0.74
1:A:17:ALA:CB	1:A:18:THR:CA	2.64	0.74
1:B:128:PHE:N	1:B:130:GLU:H	1.85	0.74
1:A:104:ASN:HB2	1:A:107:GLY:H	1.52	0.74
1:B:106:ASP:HB3	1:B:107:GLY:CA	2.19	0.73
1:B:96:ASP:HB3	1:B:97:ASP:CB	2.21	0.70
1:B:114:LYS:O	1:B:116:PRO:HD2	1.91	0.69
1:A:38:PRO:HG3	1:A:141:ALA:HB1	1.75	0.69
1:A:96:ASP:HB3	1:A:97:ASP:CB	2.23	0.68
1:B:28:LYS:HE3	1:B:42:VAL:O	1.93	0.68
1:B:109:THR:CG2	1:B:110:LYS:HA	2.24	0.68
1:A:14:GLY:HA3	1:A:15:SER:HB2	1.75	0.67
1:B:124:LEU:O	1:B:127:ALA:HB3	1.94	0.67
1:B:120:LEU:HD11	1:B:148:ILE:O	1.94	0.67
1:A:151:LYS:CG	1:A:152:GLU:N	2.58	0.67
1:A:104:ASN:HD21	1:A:109:THR:HB	1.60	0.66
1:B:95:ILE:HB	1:B:96:ASP:C	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ALA:HB1	1:A:117:GLU:HG2	1.77	0.66
1:A:139:ILE:HG12	1:A:148:ILE:HG12	1.79	0.65
1:A:96:ASP:HB3	1:A:97:ASP:HB2	1.78	0.65
1:A:14:GLY:HA3	1:A:15:SER:OG	1.98	0.64
1:A:65:PHE:HE1	1:A:141:ALA:CB	2.11	0.64
1:B:38:PRO:HG3	1:B:141:ALA:HB1	1.79	0.63
1:B:122:ASP:H	1:B:123:SER:HB3	1.62	0.63
1:B:104:ASN:HD21	1:B:109:THR:HB	1.62	0.63
1:A:95:ILE:HB	1:A:96:ASP:C	2.24	0.63
1:B:124:LEU:O	1:B:127:ALA:CB	2.47	0.63
1:A:151:LYS:HG2	1:A:152:GLU:N	2.06	0.63
1:B:65:PHE:HE1	1:B:141:ALA:CB	2.11	0.63
1:A:108:ASP:HB2	1:A:109:THR:OG1	1.99	0.62
1:B:42:VAL:HG21	1:B:62:ILE:CD1	2.28	0.62
1:A:19:TYR:O	1:A:82:VAL:N	2.24	0.61
1:A:128:PHE:N	1:A:130:GLU:H	1.97	0.61
1:B:63:ASP:OD2	1:B:66:THR:OG1	2.18	0.61
1:A:97:ASP:CG	1:A:98:GLY:HA3	2.26	0.61
1:A:23:CYS:N	1:A:78:HIS:O	2.27	0.60
1:B:125:GLN:O	1:B:129:ASP:HB2	2.02	0.60
1:A:105:MET:HB2	1:A:106:ASP:HB2	1.84	0.59
1:B:139:ILE:HG12	1:B:148:ILE:HG12	1.83	0.59
1:A:120:LEU:HD11	1:A:148:ILE:O	2.02	0.59
1:B:120:LEU:O	1:B:121:GLY:C	2.45	0.59
1:B:119:GLU:O	1:B:123:SER:HB3	2.01	0.59
1:B:63:ASP:OD1	1:B:63:ASP:C	2.45	0.59
1:B:122:ASP:O	1:B:126:THR:HB	2.03	0.58
1:A:94:ASP:HA	1:A:128:PHE:HZ	1.68	0.58
1:A:127:ALA:CB	1:A:128:PHE:HB2	2.33	0.58
1:B:127:ALA:O	1:B:130:GLU:CB	2.47	0.58
1:B:119:GLU:O	1:B:122:ASP:HB2	2.03	0.57
1:B:43:ASP:HB3	1:B:60:VAL:HB	1.87	0.56
1:A:21:MET:HE2	1:A:82:VAL:HG21	1.85	0.56
1:B:17:ALA:HB3	1:B:18:THR:CA	2.23	0.56
1:B:127:ALA:HB3	1:B:128:PHE:CB	2.31	0.56
1:B:128:PHE:H	1:B:129:ASP:HB2	1.71	0.56
1:A:116:PRO:HA	1:A:121:GLY:HA2	1.87	0.56
1:B:139:ILE:HD11	1:B:148:ILE:CG2	2.35	0.56
1:A:63:ASP:OD2	1:A:66:THR:OG1	2.22	0.56
1:A:95:ILE:HB	1:A:96:ASP:CA	2.36	0.55
1:B:95:ILE:HB	1:B:96:ASP:CA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASP:HA	1:B:128:PHE:HZ	1.72	0.54
1:A:67:GLY:O	1:A:68:LYS:C	2.49	0.54
1:A:63:ASP:OD1	1:A:63:ASP:C	2.51	0.54
1:A:101:SER:H	1:A:102:LEU:HA	1.72	0.54
1:B:141:ALA:O	1:B:143:GLY:N	2.41	0.54
1:A:16:SER:OG	1:A:17:ALA:HA	2.09	0.53
1:B:106:ASP:HB3	1:B:107:GLY:HA2	1.90	0.53
1:A:116:PRO:CA	1:A:121:GLY:HA2	2.39	0.53
1:A:118:GLY:HA3	1:A:121:GLY:N	2.12	0.53
1:B:39:CYS:HA	1:B:63:ASP:HA	1.90	0.53
1:B:67:GLY:O	1:B:68:LYS:C	2.51	0.52
1:B:118:GLY:HA3	1:B:121:GLY:N	2.06	0.52
1:A:139:ILE:HD11	1:A:148:ILE:CG2	2.40	0.52
1:A:32:VAL:HG13	1:A:34:ILE:HG12	1.92	0.52
1:A:119:GLU:O	1:A:123:SER:HB3	2.10	0.52
1:A:17:ALA:HB3	1:A:18:THR:CA	2.33	0.52
1:A:122:ASP:O	1:A:126:THR:HB	2.10	0.52
1:B:23:CYS:HB2	1:B:78:HIS:O	2.09	0.52
1:A:127:ALA:HB1	1:A:128:PHE:HB2	1.92	0.51
1:A:22:GLN:HA	1:A:79:ASN:HA	1.91	0.51
1:A:65:PHE:HE1	1:A:141:ALA:HB3	1.76	0.51
1:A:17:ALA:HB1	1:A:18:THR:CA	2.35	0.51
1:B:23:CYS:N	1:B:78:HIS:O	2.32	0.50
1:A:96:ASP:HB3	1:A:97:ASP:HB3	1.91	0.50
1:A:141:ALA:O	1:A:143:GLY:N	2.44	0.50
1:B:98:GLY:CA	1:B:99:PHE:CB	2.81	0.50
1:B:65:PHE:HE1	1:B:141:ALA:HB3	1.76	0.50
1:A:39:CYS:HA	1:A:63:ASP:HA	1.93	0.50
1:A:43:ASP:HB3	1:A:60:VAL:HB	1.94	0.49
1:A:56:LYS:HB3	1:A:73:LEU:CD1	2.42	0.49
1:B:32:VAL:HG13	1:B:34:ILE:HG12	1.93	0.49
1:B:139:ILE:HD11	1:B:148:ILE:HG23	1.95	0.49
1:A:101:SER:O	1:A:110:LYS:O	2.30	0.49
1:B:108:ASP:HB2	1:B:109:THR:OG1	2.13	0.49
1:B:95:ILE:HG21	1:B:125:GLN:HE22	1.78	0.49
1:A:100:LEU:N	1:A:101:SER:HA	2.27	0.49
1:B:22:GLN:HA	1:B:79:ASN:HA	1.94	0.49
1:B:39:CYS:SG	1:B:70:LEU:HD22	2.53	0.49
1:B:42:VAL:CG2	1:B:62:ILE:HD12	2.32	0.49
1:A:128:PHE:HD2	1:A:129:ASP:H	1.61	0.48
1:A:139:ILE:HD11	1:A:148:ILE:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PHE:CE1	1:B:141:ALA:CB	2.95	0.48
1:A:104:ASN:N	1:A:104:ASN:OD1	2.47	0.48
1:A:14:GLY:CA	1:A:15:SER:CB	2.87	0.47
1:A:90:TYR:CB	1:A:102:LEU:HD13	2.38	0.47
1:A:109:THR:CG2	1:A:110:LYS:HA	2.43	0.47
1:B:75:PRO:HG2	1:B:78:HIS:HB2	1.96	0.47
1:B:56:LYS:HB3	1:B:73:LEU:CD1	2.44	0.47
1:A:127:ALA:HB3	1:A:128:PHE:HB2	1.97	0.47
1:B:102:LEU:HB3	1:B:103:MET:O	2.15	0.47
1:B:95:ILE:HD13	1:B:125:GLN:HE22	1.75	0.47
1:A:20:PRO:HD3	1:A:81:GLU:HG2	1.97	0.46
1:B:31:PHE:O	1:B:82:VAL:HG13	2.15	0.46
1:A:101:SER:N	1:A:102:LEU:HA	2.31	0.46
1:A:65:PHE:CE1	1:A:141:ALA:CB	2.96	0.46
1:B:17:ALA:HB1	1:B:18:THR:CA	2.37	0.46
1:A:89:GLU:N	1:A:89:GLU:OE2	2.49	0.45
1:A:128:PHE:H	1:A:130:GLU:H	1.63	0.45
1:B:125:GLN:O	1:B:128:PHE:HB3	2.17	0.45
1:B:145:GLU:O	1:B:146:ALA:HB2	2.16	0.45
1:A:56:LYS:HB3	1:A:73:LEU:HD11	1.98	0.45
1:B:139:ILE:HD11	1:B:148:ILE:HG21	1.97	0.45
1:A:31:PHE:O	1:A:82:VAL:HG13	2.15	0.44
1:A:98:GLY:N	1:A:99:PHE:CG	2.80	0.44
1:B:28:LYS:O	1:B:29:ASN:HB2	2.18	0.44
1:B:57:VAL:HG23	1:B:76:SER:HA	1.99	0.44
1:B:65:PHE:CE1	1:B:141:ALA:HB3	2.52	0.44
1:B:95:ILE:HB	1:B:96:ASP:HA	2.00	0.44
1:A:28:LYS:O	1:A:29:ASN:HB2	2.18	0.44
1:B:98:GLY:HA2	1:B:99:PHE:HB2	1.96	0.44
1:A:23:CYS:HB2	1:A:78:HIS:O	2.18	0.44
1:A:145:GLU:O	1:A:146:ALA:HB2	2.18	0.44
1:B:99:PHE:HB3	1:B:113:VAL:O	2.19	0.43
1:A:65:PHE:CE1	1:A:141:ALA:HB3	2.53	0.43
1:A:95:ILE:HB	1:A:96:ASP:HA	2.00	0.43
1:A:16:SER:HA	1:A:17:ALA:C	2.43	0.42
1:B:56:LYS:HB3	1:B:73:LEU:HD11	2.00	0.42
1:B:128:PHE:CD2	1:B:128:PHE:C	2.97	0.42
1:B:100:LEU:CG	1:B:113:VAL:HG22	2.44	0.42
1:B:122:ASP:H	1:B:123:SER:CB	2.28	0.42
1:A:75:PRO:HG2	1:A:78:HIS:HB2	2.00	0.42
1:A:124:LEU:HA	1:A:150:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HD11	1:A:141:ALA:HB2	2.02	0.42
1:B:62:ILE:HG23	1:B:67:GLY:O	2.19	0.42
1:B:104:ASN:OD1	1:B:104:ASN:N	2.52	0.42
1:A:63:ASP:OD1	1:A:65:PHE:N	2.48	0.42
1:A:119:GLU:O	1:A:122:ASP:HB2	2.20	0.41
1:A:51:LYS:HB2	1:A:52:HIS:H	1.66	0.41
1:A:94:ASP:HA	1:A:128:PHE:CZ	2.52	0.41
1:B:123:SER:N	1:B:126:THR:HG22	2.36	0.41
1:A:21:MET:CE	1:A:82:VAL:HG21	2.51	0.41
1:A:95:ILE:HG22	1:A:97:ASP:O	2.20	0.41
1:A:57:VAL:HG23	1:A:76:SER:HA	2.02	0.41
1:B:88:ASN:O	1:B:137:THR:HA	2.21	0.41
1:B:120:LEU:HD23	1:B:120:LEU:HA	1.90	0.41
1:B:127:ALA:CB	1:B:128:PHE:CA	2.99	0.41
1:A:52:HIS:HA	1:A:53:GLY:HA2	1.61	0.40
1:A:128:PHE:CD2	1:A:129:ASP:N	2.89	0.40
1:B:65:PHE:HE1	1:B:141:ALA:HB2	1.86	0.40
1:B:98:GLY:CA	1:B:99:PHE:CD2	2.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:OG	1:B:119:GLU:OE1[10_455]	2.06	0.14

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	144/167 (86%)	94 (65%)	28 (19%)	22 (15%)	0	0
1	B	127/167 (76%)	87 (68%)	23 (18%)	17 (13%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	271/334 (81%)	181 (67%)	51 (19%)	39 (14%)	0 0

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	17	ALA
1	A	20	PRO
1	A	51	LYS
1	A	100	LEU
1	A	102	LEU
1	A	113	VAL
1	A	123	SER
1	A	129	ASP
1	A	132	LYS
1	B	99	PHE
1	B	102	LEU
1	B	106	ASP
1	B	113	VAL
1	B	116	PRO
1	B	127	ALA
1	B	132	LYS
1	B	142	MET
1	A	68	LYS
1	A	109	THR
1	A	117	GLU
1	A	142	MET
1	B	68	LYS
1	B	78	HIS
1	B	100	LEU
1	B	121	GLY
1	B	129	ASP
1	A	78	HIS
1	B	20	PRO
1	A	127	ALA
1	A	95	ILE
1	A	99	PHE
1	A	116	PRO
1	B	95	ILE
1	B	123	SER
1	A	105	MET
1	A	115	ALA

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Mol	Chain	Res	Type
1	B	148	ILE
1	A	148	ILE

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	123/142 (87%)	94 (76%)	29 (24%)	1	2
1	B	114/142 (80%)	89 (78%)	25 (22%)	1	3
All	All	237/284 (84%)	183 (77%)	54 (23%)	1	3

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	19	TYR
1	A	21	MET
1	A	37	ARG
1	A	46	THR
1	A	59	LEU
1	A	63	ASP
1	A	73	LEU
1	A	76	SER
1	A	89	GLU
1	A	95	ILE
1	A	99	PHE
1	A	100	LEU
1	A	104	ASN
1	A	106	ASP
1	A	113	VAL
1	A	120	LEU
1	A	122	ASP
1	A	126	THR
1	A	133	ASP
1	A	135	MET

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Mol	Chain	Res	Type
1	A	136	VAL
1	A	139	ILE
1	A	144	GLU
1	A	145	GLU
1	A	148	ILE
1	A	150	PHE
1	A	151	LYS
1	A	152	GLU
1	B	19	TYR
1	B	21	MET
1	B	46	THR
1	B	63	ASP
1	B	70	LEU
1	B	73	LEU
1	B	76	SER
1	B	95	ILE
1	B	99	PHE
1	B	100	LEU
1	B	104	ASN
1	B	106	ASP
1	B	109	THR
1	B	113	VAL
1	B	120	LEU
1	B	126	THR
1	B	133	ASP
1	B	134	LEU
1	B	135	MET
1	B	136	VAL
1	B	139	ILE
1	B	145	GLU
1	B	148	ILE
1	B	150	PHE
1	B	151	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	88	ASN
1	B	88	ASN
1	B	125	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 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	146/167 (87%)	1.78	49 (33%)	1 1	36, 84, 87, 91	37 (25%)
1	B	131/167 (78%)	1.96	53 (40%)	0 0	32, 84, 85, 86	29 (22%)
All	All	277/334 (82%)	1.86	102 (36%)	1 1	32, 84, 86, 91	66 (23%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	MET	8.2
1	A	96	ASP	8.0
1	B	135	MET	6.8
1	A	52	HIS	6.7
1	A	91	GLN	6.1
1	B	90	TYR	5.9
1	A	90	TYR	5.8
1	A	136	VAL	5.5
1	A	87	ARG	5.4
1	B	151	LYS	5.4
1	B	24	SER	5.2
1	A	27	ARG	5.1
1	B	150	PHE	4.8
1	B	56	LYS	4.8
1	B	48	LYS	4.7
1	A	93	LEU	4.6
1	A	152	GLU	4.6
1	B	139	ILE	4.5
1	A	103	MET	4.5
1	A	133	ASP	4.4
1	B	80	MET	4.3
1	A	80	MET	4.3
1	B	119	GLU	4.3
1	B	31	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	149	SER	4.3
1	B	103	MET	4.1
1	B	84	VAL	4.1
1	A	75	PRO	4.0
1	A	100	LEU	4.0
1	B	120	LEU	3.8
1	B	108	ASP	3.8
1	B	94	ASP	3.7
1	A	65	PHE	3.7
1	A	61	ALA	3.7
1	B	22	GLN	3.7
1	A	132	LYS	3.6
1	B	86	LYS	3.5
1	B	91	GLN	3.5
1	B	47	SER	3.5
1	B	122	ASP	3.5
1	A	62	ILE	3.5
1	A	44	MET	3.4
1	A	43	ASP	3.3
1	B	76	SER	3.2
1	B	61	ALA	3.2
1	B	85	VAL	3.1
1	A	97	ASP	3.1
1	B	73	LEU	3.0
1	B	72	ASP	3.0
1	A	35	LYS	3.0
1	A	39	CYS	3.0
1	A	15	SER	2.9
1	A	85	VAL	2.9
1	A	150	PHE	2.8
1	A	38	PRO	2.8
1	A	151	LYS	2.8
1	B	89	GLU	2.8
1	B	123	SER	2.8
1	A	111	ASP	2.7
1	B	100	LEU	2.7
1	A	110	LYS	2.7
1	B	78	HIS	2.7
1	A	74	SER	2.7
1	B	147	ALA	2.7
1	A	89	GLU	2.6
1	A	156	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	2.6
1	B	81	GLU	2.6
1	A	95	ILE	2.6
1	A	53	GLY	2.6
1	B	21	MET	2.6
1	A	105	MET	2.5
1	A	119	GLU	2.5
1	B	26	LEU	2.5
1	B	95	ILE	2.5
1	A	139	ILE	2.4
1	B	30	GLY	2.4
1	B	110	LYS	2.4
1	A	59	LEU	2.4
1	B	116	PRO	2.3
1	B	44	MET	2.3
1	B	93	LEU	2.3
1	A	124	LEU	2.3
1	A	112	ASP	2.3
1	A	116	PRO	2.3
1	B	105	MET	2.3
1	A	147	ALA	2.3
1	A	92	LEU	2.2
1	A	128	PHE	2.2
1	B	35	LYS	2.2
1	B	92	LEU	2.2
1	B	114	LYS	2.2
1	A	120	LEU	2.2
1	B	124	LEU	2.2
1	A	12	ASP	2.2
1	B	126	THR	2.2
1	B	87	ARG	2.2
1	A	84	VAL	2.1
1	B	64	ILE	2.1
1	B	148	ILE	2.1
1	B	79	ASN	2.0
1	A	70	LEU	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 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.