Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:27 AM GMT

PDB ID	:	3ER0
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)

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 (i)

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.
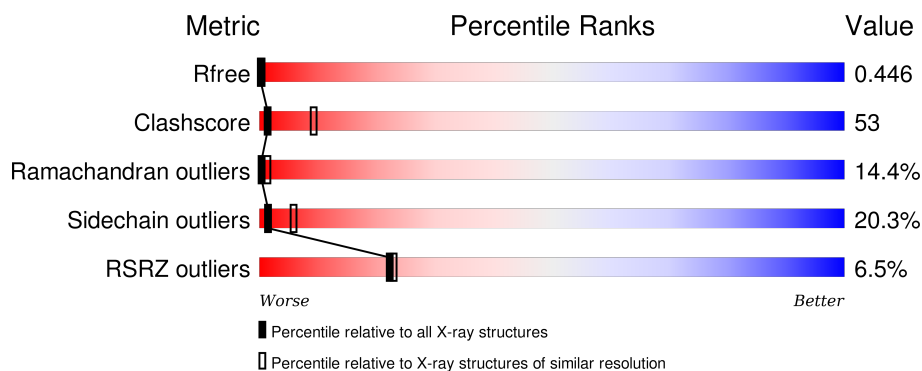
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	
1	B	167	

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 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: Eukaryotic translation initiation factor 5A-2

Chain A:

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

Chain B:
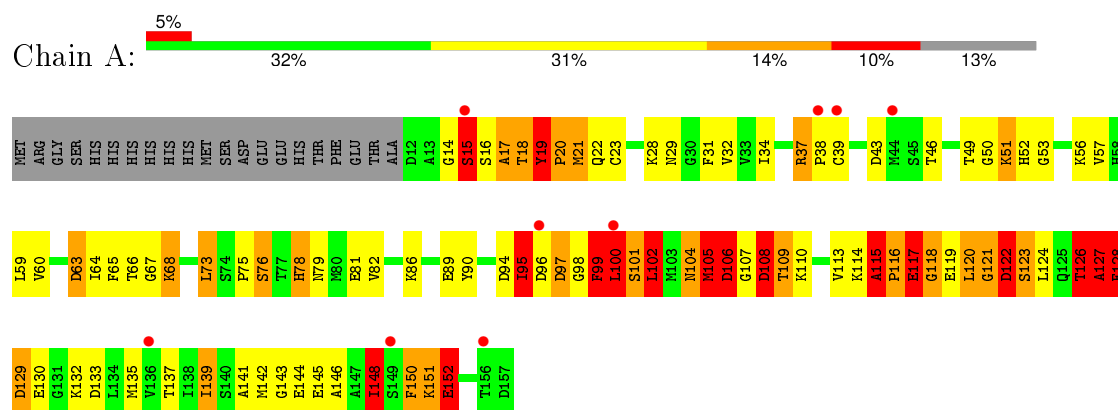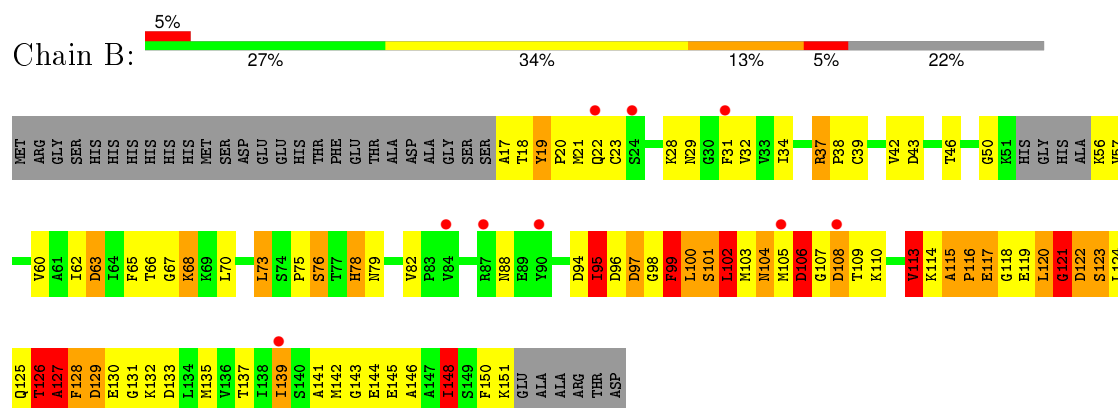
4 Data and refinement statistics ⓘ

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 49.43 – 3.35	Depositor EDS
% Data completeness (in resolution range)	91.9 (49.45-3.35) 91.9 (49.43-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.386 , 0.448 0.382 , 0.446	Depositor DCC
R_{free} test set	528 reflections (10.97%)	DCC
Wilson B-factor (Å^2)	114.4	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 102.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 5343 reflections	Xtriage
F_o,F_c correlation	0.83	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.71	3/1119 (0.3%)	1.04	4/1505 (0.3%)
1	B	0.47	0/1013	0.94	1/1360 (0.1%)
All	All	0.61	3/2132 (0.1%)	0.99	5/2865 (0.2%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	GLU	CD-OE1	15.09	1.42	1.25
1	A	152	GLU	CG-CD	6.86	1.62	1.51
1	A	152	GLU	CB-CG	6.11	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	GLU	OE1-CD-OE2	-10.52	110.68	123.30
1	A	152	GLU	CG-CD-OE2	8.19	134.68	118.30
1	A	128	PHE	N-CA-C	-6.59	93.21	111.00
1	B	102	LEU	CB-CA-C	5.79	121.20	110.20
1	A	118	GLY	N-CA-C	-5.37	99.67	113.10

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
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 (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	1104	0	1096	100	1
1	B	1001	0	1011	94	1
All	All	2105	0	2107	194	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 53.

All (194) 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:109:THR:HG23	1:B:110:LYS:HA	1.48	0.93
1:B:42:VAL:HG21	1:B:62:ILE:HD12	1.50	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: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:A:150:PHE:HD2	1:A:150:PHE:C	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:150:PHE:CD2	1:A:150:PHE:C	2.59	0.69
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:109:THR:CG2	1:B:110:LYS:HA	2.24	0.68
1:B:28:LYS:HE3	1:B:42:VAL:O	1.93	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: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: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:128:PHE:N	1:A:130:GLU:H	1.97	0.61
1:A:19:TYR:O	1:A:82:VAL:N	2.24	0.61
1:B:95:ILE:HB	1:B:96:ASP:C	2.21	0.61
1:B:63:ASP:OD2	1:B:66:THR:OG1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HG12	1:B:148:ILE:HG12	1.83	0.59
1:A:105:MET:HB2	1:A:106:ASP:HB2	1.84	0.59
1:A:120:LEU:HD11	1:A:148:ILE:O	2.02	0.59
1:B:119:GLU:O	1:B:123:SER:HB3	2.01	0.59
1:A:95:ILE:HB	1:A:96:ASP:C	2.24	0.58
1:B:122:ASP:O	1:B:126:THR:HB	2.03	0.58
1:A:127:ALA:CB	1:A:128:PHE:HB2	2.33	0.58
1:A:94:ASP:HA	1:A:128:PHE:HZ	1.68	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:A:97:ASP:CG	1:A:98:GLY:HA3	2.26	0.56
1:B:43:ASP:HB3	1:B:60:VAL:HB	1.87	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
1:B:120:LEU:O	1:B:121:GLY:C	2.45	0.54
1:B:94:ASP:HA	1:B:128:PHE:HZ	1.72	0.54
1:A:101:SER:H	1:A:102:LEU:HA	1.72	0.54
1:B:63:ASP:C	1:B:63:ASP:OD1	2.45	0.54
1:B:98:GLY:CA	1:B:99:PHE:CB	2.81	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:118:GLY:HA3	1:A:121:GLY:N	2.12	0.53
1:A:116:PRO:CA	1:A:121:GLY:HA2	2.39	0.53
1:A:21:MET:HE2	1:A:82:VAL:HG21	1.89	0.53
1:B:39:CYS:HA	1:B:63:ASP:HA	1.90	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:ALA:O	1:A:143:GLY:N	2.44	0.50
1:A:96:ASP:HB3	1:A:97:ASP:HB3	1.91	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:67:GLY:O	1:A:68:LYS:C	2.49	0.50
1:A:63:ASP:C	1:A:63:ASP:OD1	2.51	0.49
1:B:32:VAL:HG13	1:B:34:ILE:HG12	1.93	0.49
1:A:56:LYS:HB3	1:A:73:LEU:CD1	2.42	0.49
1:A:43:ASP:HB3	1:A:60:VAL:HB	1.94	0.49
1:B:139:ILE:HD11	1:B:148:ILE:HG23	1.95	0.49
1:B:108:ASP:HB2	1:B:109:THR:OG1	2.13	0.49
1:A:101:SER:O	1:A:110:LYS:O	2.30	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:42:VAL:CG2	1:B:62:ILE:HD12	2.32	0.49
1:B:39:CYS:SG	1:B:70:LEU:HD22	2.53	0.49
1:A:128:PHE:HD2	1:A:129:ASP:H	1.61	0.48
1:B:65:PHE:CE1	1:B:141:ALA:CB	2.95	0.48
1:A:139:ILE:HD11	1:A:148:ILE:HG23	1.94	0.48
1:A:104:ASN:OD1	1:A:104:ASN:N	2.47	0.48
1:B:67:GLY:O	1:B:68:LYS:C	2.51	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:B:17:ALA:HB1	1:B:18:THR:CA	2.37	0.46
1:A:65:PHE:CE1	1:A:141:ALA:CB	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLU:O	1:B:146:ALA:HB2	2.16	0.45
1:B:139:ILE:HD11	1:B:148:ILE:HG21	1.97	0.45
1:A:56:LYS:HB3	1:A:73:LEU:HD11	1.98	0.45
1:B:28:LYS:O	1:B:29:ASN:HB2	2.18	0.44
1:A:98:GLY:N	1:A:99:PHE:CG	2.80	0.44
1:A:31:PHE:O	1:A:82:VAL:HG13	2.15	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:B:56:LYS:HB3	1:B:73:LEU:HD11	2.00	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:124:LEU:HA	1:A:150:PHE:CE1	2.55	0.42
1:A:75:PRO:HG2	1:A:78:HIS:HB2	2.00	0.42
1:B:62:ILE:HG23	1:B:67:GLY:O	2.19	0.42
1:A:64:ILE:HD11	1:A:141:ALA:HB2	2.02	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: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:51:LYS:HB2	1:A:52:HIS:H	1.66	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:B:120:LEU:HA	1:B:120:LEU:HD23	1.90	0.41
1:B:127:ALA:CB	1:B:128:PHE:CA	2.99	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:A:52:HIS:HA	1:A:53:GLY:HA2	1.61	0.40
1:B:98:GLY:CA	1:B:99:PHE:CD2	2.98	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

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	1
1	B	127/167 (76%)	87 (68%)	23 (18%)	17 (13%)	0	2
All	All	271/334 (81%)	181 (67%)	51 (19%)	39 (14%)	0	1

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

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/142 (87%)	96 (78%)	27 (22%)	1	4
1	B	114/142 (80%)	93 (82%)	21 (18%)	2	9
All	All	237/284 (84%)	189 (80%)	48 (20%)	1	6

All (48) 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

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Mol	Chain	Res	Type
1	A	46	THR
1	A	59	LEU
1	A	63	ASP
1	A	73	LEU
1	A	76	SER
1	A	86	LYS
1	A	95	ILE
1	A	99	PHE
1	A	100	LEU
1	A	104	ASN
1	A	106	ASP
1	A	108	ASP
1	A	120	LEU
1	A	122	ASP
1	A	126	THR
1	A	133	ASP
1	A	135	MET
1	A	139	ILE
1	A	144	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	37	ARG
1	B	46	THR
1	B	63	ASP
1	B	73	LEU
1	B	76	SER
1	B	95	ILE
1	B	99	PHE
1	B	104	ASN
1	B	106	ASP
1	B	113	VAL
1	B	120	LEU
1	B	126	THR
1	B	133	ASP
1	B	135	MET
1	B	139	ILE
1	B	144	GLU
1	B	148	ILE

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Mol	Chain	Res	Type
1	B	150	PHE
1	B	151	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.50	9 (6%)	24	24	82, 84, 87, 91	37 (25%)
1	B	131/167 (78%)	0.32	9 (6%)	20	20	82, 84, 85, 86	29 (22%)
All	All	277/334 (82%)	0.41	18 (6%)	22	23	82, 84, 86, 91	66 (23%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	4.6
1	A	96	ASP	4.1
1	A	136	VAL	3.3
1	B	84	VAL	3.1
1	A	156	THR	3.0
1	A	39	CYS	3.0
1	B	31	PHE	2.6
1	B	22	GLN	2.4
1	A	100	LEU	2.2
1	A	15	SER	2.2
1	B	87	ARG	2.1
1	B	105	MET	2.1
1	B	108	ASP	2.1
1	A	44	MET	2.0
1	B	139	ILE	2.0
1	B	90	TYR	2.0
1	A	149	SER	2.0
1	B	24	SER	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.