



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DT9
Title : THE CRYSTAL STRUCTURE OF HUMAN EUKARYOTIC RELEASE
FACTOR ERF1-MECHANISM OF STOP CODON RECOGNITION AND
PEPTIDYL-TRNA HYDROLYSIS
Authors : Frolova, L.
Deposited on : 2000-01-12
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

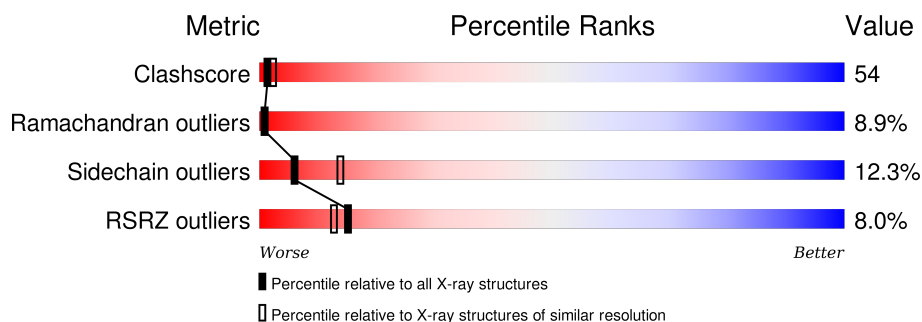
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 $\leq 5\%$. 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	437	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3241 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 PROTEIN (EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3131	2000	533	587	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.08 Å 77.08 Å 194.44 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 24.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-2.70) 99.0 (24.80-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.72 Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.246 , 0.314 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 16675 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3241	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, 0.375 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	0.77	0/3181	0.93	4/4275 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	118	LYS	N-CA-C	7.87	132.26	111.00
1	A	274	VAL	N-CA-C	-5.77	95.41	111.00
1	A	325	ASN	N-CA-C	-5.18	97.01	111.00
1	A	270	LEU	CA-CB-CG	5.11	127.05	115.30

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	3131	0	3194	339	0
2	A	110	0	0	45	0
All	All	3241	0	3194	339	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 54.

All (339) 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:A:279:LYS:HD3	1:A:279:LYS:H	1.05	1.11
1:A:45:ILE:H	1:A:87:LYS:HZ2	1.06	0.97
1:A:349:GLU:HA	2:A:495:HOH:O	1.66	0.96
1:A:218:LYS:HZ2	1:A:219:VAL:H	1.09	0.91
1:A:274:VAL:O	1:A:275:LEU:HB2	1.71	0.89
1:A:159:GLY:HA2	1:A:169:LEU:HG	1.55	0.86
1:A:316:ALA:HB1	1:A:414:ARG:HH21	1.40	0.86
1:A:91:ASN:HA	1:A:118:LYS:HD2	1.59	0.85
1:A:279:LYS:N	1:A:279:LYS:HD3	1.90	0.85
1:A:279:LYS:CD	1:A:279:LYS:H	1.88	0.84
1:A:206:ALA:HB2	1:A:236:LEU:HD11	1.60	0.84
1:A:151:ILE:HG22	1:A:152:ASP:H	1.44	0.83
1:A:100:ILE:HD11	1:A:108:LYS:HB3	1.59	0.82
1:A:193:LEU:HD23	1:A:193:LEU:O	1.79	0.81
1:A:149:ILE:HD11	1:A:209:ALA:HB1	1.62	0.80
1:A:325:ASN:O	1:A:326:LEU:HB2	1.81	0.80
1:A:326:LEU:HD22	1:A:328:ILE:HB	1.62	0.80
1:A:87:LYS:HD3	1:A:88:VAL:H	1.46	0.80
1:A:386:GLY:HA3	2:A:505:HOH:O	1.80	0.80
1:A:302:CYS:HB3	1:A:413:LEU:HD21	1.65	0.79
1:A:189:ARG:HD2	2:A:519:HOH:O	1.82	0.79
1:A:80:GLN:HG2	2:A:510:HOH:O	1.82	0.78
1:A:324:GLU:OE2	1:A:393:THR:HG22	1.82	0.78
1:A:45:ILE:H	1:A:87:LYS:NZ	1.83	0.77
1:A:316:ALA:HB1	1:A:414:ARG:NH2	2.00	0.77
1:A:317:VAL:HG13	2:A:484:HOH:O	1.85	0.77
1:A:272:THR:O	1:A:273:GLU:HG2	1.86	0.76
1:A:145:LYS:HD2	1:A:221:VAL:HG13	1.69	0.75
1:A:333:LEU:HA	2:A:506:HOH:O	1.86	0.75
1:A:218:LYS:NZ	1:A:219:VAL:H	1.83	0.74
1:A:118:LYS:NZ	1:A:120:ILE:HD11	2.02	0.74
1:A:293:GLU:OE1	1:A:293:GLU:HA	1.88	0.74
1:A:307:ASP:HB3	1:A:419:PHE:CD1	2.23	0.73
1:A:8:ALA:H	1:A:11:ASN:ND2	1.86	0.73
1:A:69:LEU:O	1:A:69:LEU:HD12	1.89	0.73
1:A:76:THR:HG22	2:A:510:HOH:O	1.88	0.72
1:A:346:LEU:HD12	1:A:350:GLN:HA	1.72	0.71
1:A:218:LYS:HZ2	1:A:219:VAL:N	1.86	0.71
1:A:100:ILE:CD1	1:A:108:LYS:HB3	2.22	0.70
1:A:177:PRO:HB3	1:A:193:LEU:HD22	1.74	0.69
1:A:330:ARG:HH11	1:A:330:ARG:HG2	1.57	0.69
1:A:147:GLY:O	1:A:224:LEU:HA	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:VAL:O	1:A:309:LEU:HD12	1.91	0.69
1:A:151:ILE:HG22	1:A:152:ASP:N	2.07	0.68
1:A:414:ARG:NH2	2:A:505:HOH:O	2.25	0.68
1:A:151:ILE:CD1	1:A:205:VAL:HG11	2.24	0.68
1:A:124:LEU:HD23	1:A:125:TYR:N	2.09	0.67
1:A:176:LEU:HB3	1:A:177:PRO:HD2	1.76	0.67
1:A:391:ILE:HD12	1:A:391:ILE:N	2.09	0.67
1:A:290:TYR:HE2	2:A:538:HOH:O	1.77	0.67
1:A:34:MET:HG3	1:A:129:ASN:O	1.95	0.67
1:A:206:ALA:O	2:A:514:HOH:O	2.13	0.66
1:A:305:VAL:C	1:A:309:LEU:HD12	2.14	0.66
1:A:149:ILE:HD11	1:A:209:ALA:CB	2.24	0.66
1:A:45:ILE:HD12	1:A:87:LYS:HA	1.78	0.66
1:A:157:LEU:HD23	1:A:158:PHE:N	2.11	0.66
1:A:110:VAL:HG23	1:A:112:ILE:HD12	1.77	0.66
1:A:207:GLU:OE1	1:A:207:GLU:HA	1.95	0.66
1:A:110:VAL:HG23	1:A:112:ILE:CD1	2.26	0.66
1:A:374:LEU:HD22	1:A:378:PHE:CE1	2.30	0.66
1:A:214:ILE:HA	1:A:219:VAL:HA	1.76	0.66
1:A:169:LEU:HD12	1:A:212:LEU:HD11	1.78	0.65
1:A:18:LYS:HG3	1:A:140:LEU:HD11	1.78	0.65
1:A:118:LYS:HZ1	1:A:120:ILE:HD11	1.60	0.65
1:A:348:PRO:HA	1:A:350:GLN:NE2	2.11	0.65
1:A:177:PRO:HG2	1:A:194:ARG:HD2	1.78	0.65
1:A:33:SER:HB3	2:A:512:HOH:O	1.97	0.65
1:A:326:LEU:O	1:A:328:ILE:N	2.26	0.65
1:A:45:ILE:N	1:A:87:LYS:HZ2	1.85	0.64
1:A:242:PHE:HA	2:A:514:HOH:O	1.96	0.64
1:A:34:MET:HG3	1:A:129:ASN:C	2.18	0.64
1:A:224:LEU:HB3	2:A:507:HOH:O	1.98	0.64
1:A:317:VAL:HG12	1:A:413:LEU:HD22	1.79	0.64
1:A:326:LEU:CD2	1:A:328:ILE:HB	2.27	0.64
1:A:216:GLY:O	1:A:218:LYS:N	2.30	0.63
1:A:272:THR:O	1:A:273:GLU:CB	2.46	0.63
1:A:191:ALA:O	1:A:194:ARG:HB3	1.98	0.63
1:A:333:LEU:HB3	2:A:504:HOH:O	1.98	0.63
1:A:174:VAL:HG11	1:A:201:TYR:CD2	2.33	0.63
1:A:112:ILE:HA	2:A:498:HOH:O	1.97	0.63
1:A:188:LEU:HD21	1:A:192:ARG:NH2	2.14	0.62
1:A:214:ILE:HD12	2:A:477:HOH:O	1.99	0.62
1:A:206:ALA:HB2	1:A:236:LEU:CD1	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASP:HB3	1:A:155:GLY:O	1.99	0.62
1:A:100:ILE:HB	2:A:529:HOH:O	1.99	0.62
1:A:272:THR:O	1:A:273:GLU:CG	2.48	0.62
1:A:169:LEU:CD1	1:A:212:LEU:HD11	2.30	0.62
1:A:64:SER:O	1:A:66:VAL:N	2.33	0.62
1:A:326:LEU:HB3	2:A:540:HOH:O	1.99	0.62
1:A:307:ASP:OD2	1:A:307:ASP:N	2.32	0.62
1:A:157:LEU:HD13	1:A:261:GLU:H	1.66	0.61
1:A:34:MET:HB2	1:A:128:ASP:O	2.00	0.61
1:A:274:VAL:O	1:A:275:LEU:CB	2.45	0.61
1:A:137:THR:O	1:A:140:LEU:HB2	2.01	0.61
1:A:333:LEU:HD12	2:A:506:HOH:O	2.01	0.61
1:A:171:LYS:HG3	1:A:171:LYS:O	2.01	0.61
1:A:347:THR:C	1:A:349:GLU:H	2.04	0.60
1:A:309:LEU:HD22	1:A:345:TYR:CZ	2.36	0.60
1:A:90:PRO:O	1:A:91:ASN:HB2	2.01	0.60
1:A:346:LEU:CD1	1:A:350:GLN:HA	2.32	0.60
1:A:210:VAL:HG13	1:A:214:ILE:HG21	1.84	0.60
1:A:248:SER:O	1:A:249:LYS:HD3	2.01	0.60
1:A:303:PHE:HA	1:A:410:GLY:HA2	1.84	0.60
1:A:31:GLY:O	1:A:33:SER:N	2.35	0.60
1:A:218:LYS:NZ	1:A:219:VAL:HG22	2.17	0.59
1:A:146:PHE:CD2	1:A:223:GLY:HA3	2.37	0.59
1:A:182:ARG:NH1	1:A:182:ARG:HG2	2.17	0.59
1:A:122:THR:O	1:A:123:SER:C	2.38	0.59
1:A:65:ARG:HB3	1:A:65:ARG:NH1	2.17	0.59
1:A:316:ALA:HB1	2:A:505:HOH:O	2.02	0.59
1:A:134:GLU:H	1:A:134:GLU:CD	2.06	0.59
1:A:257:SER:O	1:A:258:TYR:CG	2.55	0.59
1:A:331:TYR:O	1:A:332:VAL:HB	2.02	0.58
1:A:100:ILE:HB	2:A:511:HOH:O	2.02	0.58
1:A:212:LEU:HD12	1:A:213:PHE:CD1	2.37	0.58
1:A:41:PRO:O	1:A:42:LYS:HB2	2.02	0.58
1:A:147:GLY:HA2	1:A:213:PHE:HE2	1.68	0.58
1:A:346:LEU:HD12	1:A:350:GLN:CA	2.33	0.58
1:A:188:LEU:HG	1:A:189:ARG:N	2.17	0.58
1:A:177:PRO:CB	1:A:193:LEU:HD22	2.32	0.58
1:A:101:VAL:HG13	1:A:101:VAL:O	2.04	0.58
1:A:112:ILE:HG23	2:A:498:HOH:O	2.03	0.58
1:A:166:ARG:HG3	1:A:166:ARG:O	2.04	0.58
1:A:328:ILE:HG22	1:A:374:LEU:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HD23	1:A:268:ILE:HD13	1.86	0.57
1:A:213:PHE:O	1:A:220:ASN:ND2	2.37	0.57
1:A:203:ARG:HB2	1:A:241:MET:SD	2.44	0.57
1:A:215:SER:HB2	1:A:220:ASN:HD22	1.70	0.57
1:A:182:ARG:HH11	1:A:182:ARG:HG2	1.71	0.56
1:A:208:THR:HG22	1:A:208:THR:O	2.06	0.56
1:A:198:ARG:O	1:A:201:TYR:N	2.38	0.56
1:A:257:SER:O	1:A:258:TYR:CD2	2.58	0.56
1:A:317:VAL:CG1	1:A:413:LEU:HD22	2.35	0.56
1:A:8:ALA:O	1:A:12:VAL:HG23	2.06	0.56
1:A:146:PHE:HD2	1:A:223:GLY:HA3	1.71	0.56
1:A:210:VAL:O	1:A:214:ILE:HG23	2.06	0.56
1:A:8:ALA:H	1:A:11:ASN:HD22	1.52	0.56
1:A:120:ILE:O	1:A:122:THR:N	2.39	0.56
1:A:87:LYS:HD3	1:A:88:VAL:N	2.20	0.56
1:A:402:PHE:CD1	1:A:408:GLY:HA2	2.40	0.55
1:A:223:GLY:O	1:A:249:LYS:O	2.23	0.55
1:A:146:PHE:CE1	1:A:275:LEU:HG	2.41	0.55
1:A:279:LYS:HG2	1:A:280:PHE:H	1.70	0.55
1:A:322:VAL:CG1	1:A:326:LEU:HD12	2.36	0.55
1:A:40:PRO:HD3	1:A:123:SER:HA	1.89	0.55
1:A:7:ALA:C	1:A:9:ASP:H	2.10	0.55
1:A:89:PRO:HG2	1:A:92:GLY:O	2.07	0.55
1:A:188:LEU:HD21	1:A:192:ARG:HH22	1.72	0.55
1:A:95:VAL:HG13	2:A:532:HOH:O	2.07	0.55
1:A:30:ASN:OD1	1:A:30:ASN:N	2.39	0.55
1:A:117:PHE:O	1:A:118:LYS:HB2	2.06	0.55
1:A:402:PHE:CE1	1:A:408:GLY:HA2	2.42	0.54
1:A:219:VAL:HG23	1:A:219:VAL:O	2.07	0.54
1:A:91:ASN:O	1:A:119:PRO:HD2	2.07	0.54
1:A:91:ASN:OD1	1:A:118:LYS:HD2	2.08	0.54
1:A:79:GLN:O	1:A:83:LYS:HG3	2.08	0.54
1:A:44:GLN:O	1:A:47:ARG:HB3	2.08	0.54
1:A:218:LYS:NZ	1:A:219:VAL:HG13	2.23	0.53
1:A:378:PHE:O	1:A:382:TYR:HB3	2.08	0.53
1:A:254:VAL:HG13	1:A:270:LEU:HD23	1.90	0.53
1:A:254:VAL:CG1	1:A:270:LEU:HD23	2.38	0.53
1:A:153:GLY:HA2	1:A:232:PHE:CE2	2.43	0.53
1:A:84:LEU:HD23	1:A:84:LEU:N	2.24	0.53
1:A:316:ALA:CB	1:A:414:ARG:HH21	2.18	0.53
1:A:5:PRO:O	1:A:6:SER:CB	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.73	0.53
1:A:138:ALA:HB3	2:A:462:HOH:O	2.09	0.53
1:A:332:VAL:HB	1:A:343:ILE:HA	1.90	0.53
1:A:7:ALA:O	1:A:9:ASP:N	2.34	0.53
1:A:122:THR:O	1:A:123:SER:O	2.27	0.53
1:A:80:GLN:CG	2:A:510:HOH:O	2.50	0.53
1:A:330:ARG:NH1	1:A:330:ARG:HG2	2.23	0.53
1:A:172:PHE:HD2	1:A:173:THR:N	2.06	0.52
1:A:225:VAL:HG13	1:A:252:LYS:HB2	1.91	0.52
1:A:391:ILE:CD1	1:A:391:ILE:N	2.73	0.52
1:A:113:ASP:O	1:A:114:PHE:HB3	2.09	0.52
1:A:184:GLY:O	1:A:185:GLN:HB3	2.10	0.52
1:A:15:TRP:HZ3	2:A:442:HOH:O	1.93	0.52
1:A:282:GLN:HG2	2:A:528:HOH:O	2.09	0.52
1:A:357:PHE:N	1:A:357:PHE:CD2	2.78	0.52
1:A:150:VAL:HG21	2:A:513:HOH:O	2.09	0.51
1:A:231:ASP:C	1:A:233:LYS:H	2.14	0.51
1:A:357:PHE:HD2	1:A:357:PHE:N	2.08	0.51
1:A:145:LYS:O	1:A:221:VAL:HG12	2.11	0.51
1:A:149:ILE:HG12	1:A:158:PHE:CD2	2.45	0.51
1:A:8:ALA:N	1:A:11:ASN:HD22	2.09	0.51
1:A:45:ILE:HB	2:A:490:HOH:O	2.10	0.51
1:A:201:TYR:C	1:A:203:ARG:N	2.64	0.51
1:A:15:TRP:HH2	1:A:19:LYS:HZ3	1.56	0.51
1:A:88:VAL:HG12	1:A:89:PRO:O	2.12	0.50
1:A:157:LEU:HD13	1:A:261:GLU:N	2.26	0.50
1:A:332:VAL:HG21	1:A:343:ILE:HG13	1.93	0.50
1:A:271:SER:O	1:A:274:VAL:O	2.29	0.50
1:A:151:ILE:CG2	1:A:152:ASP:H	2.21	0.50
1:A:151:ILE:HD12	1:A:205:VAL:HG11	1.93	0.50
1:A:272:THR:O	1:A:273:GLU:HB2	2.11	0.50
1:A:15:TRP:CZ2	1:A:19:LYS:HD3	2.46	0.50
1:A:40:PRO:HD3	1:A:123:SER:H	1.76	0.50
1:A:146:PHE:CZ	1:A:275:LEU:HG	2.47	0.50
1:A:309:LEU:HD22	1:A:345:TYR:CE2	2.47	0.50
1:A:40:PRO:HD3	1:A:123:SER:CA	2.42	0.50
1:A:245:ARG:HB2	2:A:477:HOH:O	2.11	0.50
1:A:198:ARG:NH2	2:A:509:HOH:O	2.44	0.50
1:A:416:ARG:HH11	1:A:416:ARG:HG3	1.77	0.50
1:A:374:LEU:HD13	1:A:378:PHE:HE1	1.78	0.49
1:A:157:LEU:C	1:A:157:LEU:HD23	2.32	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HA	1:A:227:ALA:O	2.13	0.49
1:A:170:HIS:HB3	2:A:527:HOH:O	2.11	0.49
1:A:226:LEU:HD13	1:A:236:LEU:HD23	1.94	0.49
1:A:323:TYR:CE1	1:A:325:ASN:HB2	2.48	0.49
1:A:104:GLU:HB3	1:A:106:LYS:HE2	1.95	0.49
1:A:118:LYS:HZ3	1:A:120:ILE:HD11	1.76	0.49
1:A:91:ASN:OD1	1:A:118:LYS:HG2	2.12	0.49
1:A:212:LEU:HD12	1:A:213:PHE:CE1	2.47	0.49
1:A:177:PRO:HB3	1:A:193:LEU:CD2	2.40	0.49
1:A:317:VAL:HG23	1:A:317:VAL:O	2.13	0.49
1:A:118:LYS:CA	1:A:118:LYS:HE2	2.42	0.49
1:A:40:PRO:CD	1:A:123:SER:HA	2.43	0.49
1:A:158:PHE:N	1:A:158:PHE:CD1	2.81	0.48
1:A:251:LEU:HD21	1:A:274:VAL:HG12	1.95	0.48
1:A:151:ILE:CG2	1:A:152:ASP:N	2.77	0.48
1:A:189:ARG:HG2	1:A:189:ARG:NH1	2.29	0.48
1:A:239:SER:OG	1:A:242:PHE:HB3	2.13	0.48
1:A:76:THR:C	2:A:510:HOH:O	2.52	0.48
1:A:201:TYR:C	1:A:203:ARG:H	2.16	0.48
1:A:172:PHE:HE2	1:A:201:TYR:HE2	1.62	0.48
1:A:91:ASN:OD1	1:A:118:LYS:CD	2.62	0.48
1:A:149:ILE:HB	1:A:226:LEU:HD22	1.95	0.47
1:A:175:ASP:OD1	1:A:178:LYS:HE2	2.13	0.47
1:A:289:ARG:O	1:A:292:ASP:HB2	2.14	0.47
1:A:124:LEU:HD23	1:A:124:LEU:C	2.35	0.47
1:A:29:GLY:HA2	2:A:511:HOH:O	2.13	0.47
1:A:349:GLU:O	1:A:351:GLU:N	2.47	0.47
1:A:374:LEU:HD22	1:A:378:PHE:CD1	2.49	0.47
1:A:101:VAL:O	1:A:101:VAL:CG1	2.62	0.47
1:A:242:PHE:O	1:A:243:ASP:O	2.32	0.47
1:A:193:LEU:HD23	1:A:193:LEU:C	2.35	0.47
1:A:332:VAL:HG21	1:A:343:ILE:CG1	2.45	0.47
1:A:102:THR:OG1	1:A:103:GLU:N	2.48	0.47
1:A:184:GLY:O	1:A:185:GLN:CB	2.61	0.47
1:A:279:LYS:HG2	1:A:280:PHE:N	2.29	0.47
1:A:194:ARG:C	1:A:196:GLU:H	2.18	0.47
1:A:217:ASP:O	1:A:245:ARG:NH1	2.47	0.46
1:A:147:GLY:CA	1:A:213:PHE:CE2	2.97	0.46
1:A:370:GLU:HB3	2:A:506:HOH:O	2.14	0.46
1:A:172:PHE:CD1	1:A:204:LYS:HE2	2.50	0.46
1:A:17:ILE:HD11	2:A:537:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HG12	1:A:214:ILE:O	2.15	0.46
1:A:189:ARG:HH11	1:A:189:ARG:HG2	1.81	0.46
1:A:8:ALA:N	1:A:11:ASN:ND2	2.61	0.46
1:A:145:LYS:C	1:A:221:VAL:HG12	2.36	0.46
1:A:95:VAL:HG22	2:A:532:HOH:O	2.15	0.46
1:A:65:ARG:HB3	1:A:65:ARG:HH11	1.78	0.46
1:A:28:ARG:HB2	2:A:503:HOH:O	2.15	0.46
1:A:347:THR:HB	1:A:348:PRO:HD2	1.98	0.46
1:A:205:VAL:C	1:A:207:GLU:H	2.17	0.46
1:A:90:PRO:C	1:A:92:GLY:H	2.19	0.46
1:A:245:ARG:O	1:A:248:SER:HB2	2.14	0.46
1:A:113:ASP:N	2:A:498:HOH:O	2.40	0.46
1:A:389:LEU:HG	1:A:391:ILE:CD1	2.46	0.46
1:A:37:LEU:HB3	1:A:95:VAL:HB	1.98	0.46
1:A:79:GLN:NE2	2:A:523:HOH:O	2.49	0.46
1:A:149:ILE:HB	1:A:226:LEU:CD2	2.46	0.46
1:A:206:ALA:HB1	1:A:242:PHE:HB2	1.98	0.46
1:A:97:CYS:HA	1:A:110:VAL:O	2.16	0.46
1:A:41:PRO:HD2	1:A:120:ILE:HA	1.96	0.45
1:A:349:GLU:C	1:A:351:GLU:H	2.20	0.45
1:A:172:PHE:CD2	1:A:173:THR:N	2.84	0.45
1:A:331:TYR:N	1:A:331:TYR:CD1	2.84	0.45
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.79	0.45
1:A:7:ALA:C	1:A:9:ASP:N	2.71	0.45
1:A:40:PRO:HD3	1:A:123:SER:N	2.31	0.44
1:A:303:PHE:CD1	1:A:303:PHE:C	2.90	0.44
1:A:5:PRO:O	1:A:6:SER:HB2	2.17	0.44
1:A:15:TRP:CH2	1:A:19:LYS:HD3	2.53	0.44
1:A:347:THR:C	1:A:349:GLU:N	2.71	0.44
1:A:213:PHE:HD2	1:A:221:VAL:HG21	1.81	0.44
1:A:172:PHE:CZ	1:A:204:LYS:HG2	2.53	0.44
1:A:218:LYS:HZ2	1:A:219:VAL:HG22	1.81	0.44
1:A:332:VAL:HG13	1:A:332:VAL:O	2.18	0.44
1:A:416:ARG:NH1	1:A:416:ARG:HG3	2.32	0.44
1:A:354:LYS:O	1:A:356:HIS:N	2.51	0.44
1:A:344:LEU:HB3	1:A:346:LEU:HD23	2.00	0.43
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.83	0.43
1:A:13:GLU:HB3	1:A:117:PHE:CE1	2.53	0.43
1:A:48:VAL:HG12	1:A:82:LEU:HD21	2.00	0.43
1:A:151:ILE:HD11	1:A:205:VAL:HG11	1.99	0.43
1:A:147:GLY:HA2	1:A:213:PHE:CE2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:SER:O	1:A:239:SER:N	2.51	0.43
1:A:229:SER:O	1:A:232:PHE:HB2	2.18	0.43
1:A:264:PHE:HB2	2:A:513:HOH:O	2.18	0.43
1:A:319:ILE:HG21	1:A:390:GLU:HG3	2.00	0.43
1:A:149:ILE:HG12	1:A:158:PHE:HD2	1.83	0.43
1:A:187:ALA:O	1:A:190:PHE:HB3	2.17	0.43
1:A:231:ASP:C	1:A:233:LYS:N	2.72	0.43
1:A:205:VAL:C	1:A:207:GLU:N	2.72	0.43
1:A:354:LYS:HE2	1:A:354:LYS:HB3	1.76	0.43
1:A:74:ALA:O	1:A:77:SER:HB3	2.19	0.43
1:A:332:VAL:HG11	1:A:343:ILE:HG12	1.99	0.43
1:A:344:LEU:HD23	2:A:485:HOH:O	2.18	0.43
1:A:56:PHE:CD2	1:A:56:PHE:C	2.92	0.43
1:A:8:ALA:CA	1:A:11:ASN:HD22	2.32	0.43
1:A:45:ILE:HD12	1:A:87:LYS:CA	2.47	0.42
1:A:45:ILE:N	1:A:87:LYS:NZ	2.55	0.42
1:A:347:THR:O	1:A:349:GLU:N	2.52	0.42
1:A:260:GLY:O	1:A:261:GLU:HB3	2.19	0.42
1:A:388:THR:HG21	2:A:539:HOH:O	2.18	0.42
1:A:243:ASP:HA	1:A:247:GLN:HB2	2.01	0.42
1:A:290:TYR:OH	1:A:303:PHE:HB3	2.20	0.42
1:A:322:VAL:O	1:A:391:ILE:HA	2.19	0.42
1:A:420:GLN:O	1:A:421:GLY:O	2.37	0.42
1:A:118:LYS:NZ	1:A:120:ILE:CD1	2.79	0.42
1:A:352:LYS:HG3	1:A:353:ASP:H	1.85	0.42
1:A:36:SER:HG	1:A:96:TYR:HE2	1.64	0.42
1:A:273:GLU:HA	1:A:277:ASN:HD22	1.84	0.41
1:A:147:GLY:CA	1:A:213:PHE:HE2	2.31	0.41
1:A:196:GLU:N	2:A:542:HOH:O	2.53	0.41
1:A:307:ASP:HB3	1:A:419:PHE:CE1	2.56	0.41
1:A:81:ARG:HG2	1:A:81:ARG:NH1	2.33	0.41
1:A:45:ILE:O	1:A:48:VAL:HB	2.21	0.41
1:A:17:ILE:O	1:A:21:ILE:HG13	2.20	0.41
1:A:133:THR:O	1:A:136:LEU:N	2.53	0.41
1:A:243:ASP:HB2	1:A:244:GLN:H	1.56	0.41
1:A:172:PHE:CE1	1:A:204:LYS:HG2	2.55	0.41
1:A:265:ASN:O	1:A:269:GLU:HG3	2.21	0.41
1:A:308:THR:O	1:A:312:LEU:HB2	2.19	0.41
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.93	0.41
1:A:34:MET:O	1:A:127:CYS:HA	2.20	0.41
1:A:40:PRO:HG3	1:A:123:SER:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:HA	1:A:112:ILE:O	2.21	0.40
1:A:27:ALA:HB1	2:A:529:HOH:O	2.20	0.40
1:A:8:ALA:HA	1:A:11:ASN:HD22	1.87	0.40
1:A:7:ALA:O	1:A:8:ALA:HB3	2.22	0.40
1:A:138:ALA:C	1:A:140:LEU:N	2.71	0.40
1:A:294:ILE:HA	1:A:301:TYR:CE2	2.56	0.40
1:A:210:VAL:HG13	1:A:214:ILE:CG2	2.50	0.40
1:A:304:GLY:O	1:A:308:THR:OG1	2.27	0.40
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.85	0.40
1:A:307:ASP:HA	1:A:310:LYS:HB3	2.04	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	392/437 (90%)	282 (72%)	75 (19%)	35 (9%)	1 1

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	32	THR
1	A	65	ARG
1	A	118	LYS
1	A	121	ASN
1	A	123	SER
1	A	185	GLN
1	A	217	ASP
1	A	243	ASP
1	A	273	GLU
1	A	326	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	327	ASP
1	A	332	VAL
1	A	350	GLN
1	A	355	SER
1	A	356	HIS
1	A	388	THR
1	A	421	GLY
1	A	260	GLY
1	A	275	LEU
1	A	314	MET
1	A	315	GLY
1	A	116	PRO
1	A	119	PRO
1	A	179	LYS
1	A	28	ARG
1	A	258	TYR
1	A	62	ILE
1	A	223	GLY
1	A	224	LEU
1	A	353	ASP
1	A	372	MET
1	A	192	ARG
1	A	216	GLY
1	A	29	GLY

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	342/376 (91%)	300 (88%)	42 (12%)	6 14

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	TRP
1	A	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	42	LYS
1	A	44	GLN
1	A	50	LYS
1	A	58	THR
1	A	60	SER
1	A	81	ARG
1	A	84	LEU
1	A	86	ASN
1	A	93	LEU
1	A	110	VAL
1	A	117	PHE
1	A	143	ASP
1	A	158	PHE
1	A	182	ARG
1	A	188	LEU
1	A	189	ARG
1	A	198	ARG
1	A	207	GLU
1	A	211	GLN
1	A	217	ASP
1	A	221	VAL
1	A	224	LEU
1	A	232	PHE
1	A	237	SER
1	A	246	LEU
1	A	270	LEU
1	A	275	LEU
1	A	279	LYS
1	A	300	LYS
1	A	302	CYS
1	A	305	VAL
1	A	307	ASP
1	A	327	ASP
1	A	331	TYR
1	A	346	LEU
1	A	357	PHE
1	A	374	LEU
1	A	388	THR
1	A	409	ILE
1	A	416	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	79	GLN
1	A	121	ASN
1	A	162	GLN
1	A	220	ASN
1	A	244	GLN
1	A	247	GLN
1	A	266	GLN
1	A	277	ASN
1	A	350	GLN
1	A	380	ASN
1	A	401	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 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, 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	398/437 (91%)	0.42	32 (8%) 15 13	45, 92, 135, 159	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	GLY	4.6
1	A	321	ILE	4.0
1	A	411	GLY	3.7
1	A	357	PHE	3.7
1	A	353	ASP	3.6
1	A	302	CYS	3.6
1	A	150	VAL	3.4
1	A	216	GLY	3.4
1	A	149	ILE	3.3
1	A	422	MET	3.3
1	A	214	ILE	3.2
1	A	179	LYS	3.1
1	A	121	ASN	3.0
1	A	148	PHE	3.0
1	A	223	GLY	2.9
1	A	242	PHE	2.9
1	A	420	GLN	2.8
1	A	176	LEU	2.8
1	A	387	ALA	2.7
1	A	355	SER	2.6
1	A	409	ILE	2.5
1	A	320	LEU	2.4
1	A	5	PRO	2.4
1	A	185	GLN	2.2
1	A	351	GLU	2.2
1	A	243	ASP	2.2
1	A	258	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	2.1
1	A	261	GLU	2.1
1	A	356	HIS	2.0
1	A	332	VAL	2.0
1	A	177	PRO	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.