Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:05 pm BST

PDB ID	:	3RW7
Title	:	Structure of N-terminal domain of nuclear RNA export factor TAP
Authors	:	Teplova, M.; Khin, N.W.; Wohlbold, L.; Izaurralde, E.; Patel, D.J.
Deposited on	:	2011-05-07
Resolution	:	3.00 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 following versions of software and data (see references ①) were used in the production of this report:

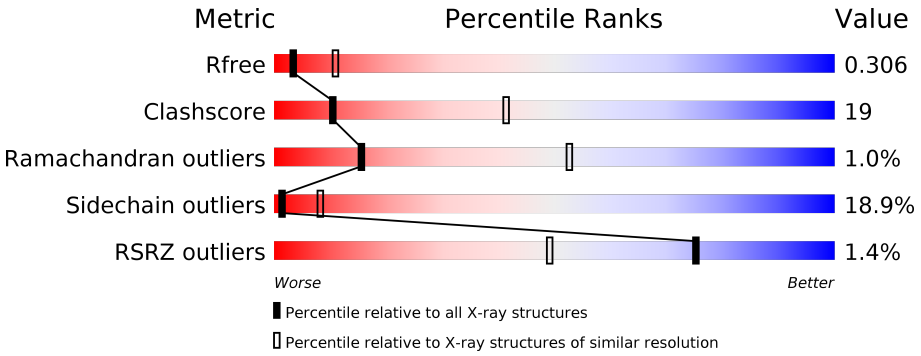
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 <=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	267	52% 28% 9% 9%
1	B	267	38% 18% 40%
1	C	267	49% 33% 9% 9%
1	D	267	32% 21% 7% 40%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6488 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 Nuclear RNA export factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1959	1243	343	366	7			
1	B	160	Total	C	N	O	S	0	0	0
			1285	807	227	246	5			
1	C	242	Total	C	N	O	S	0	0	0
			1961	1245	344	365	7			
1	D	159	Total	C	N	O	S	0	0	0
			1276	802	226	243	5			

- Molecule 2 is water.

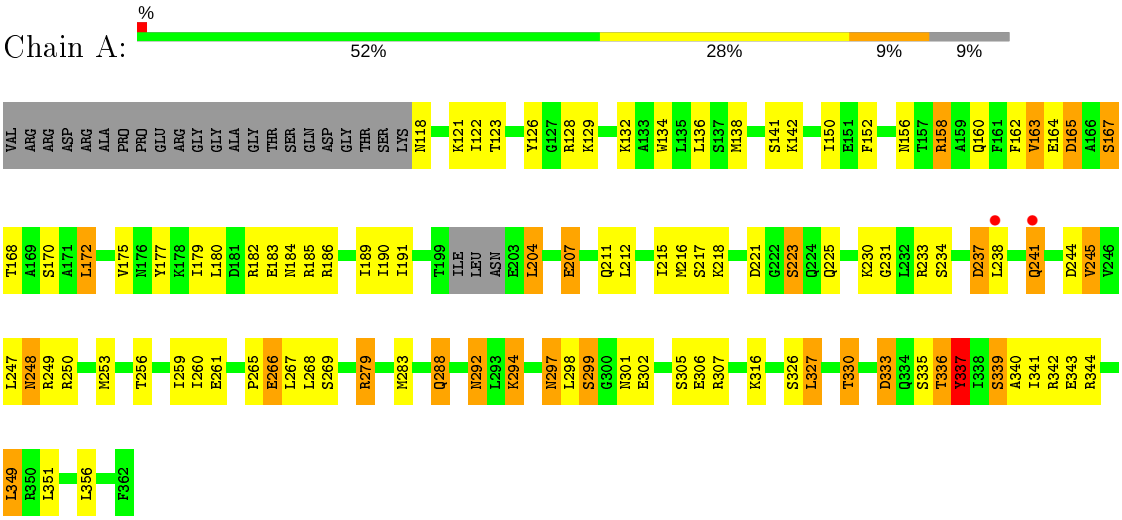
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	O	0	0
			2	2		
2	B	2	Total	O	0	0
			2	2		
2	C	1	Total	O	0	0
			1	1		
2	D	2	Total	O	0	0
			2	2		

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 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.

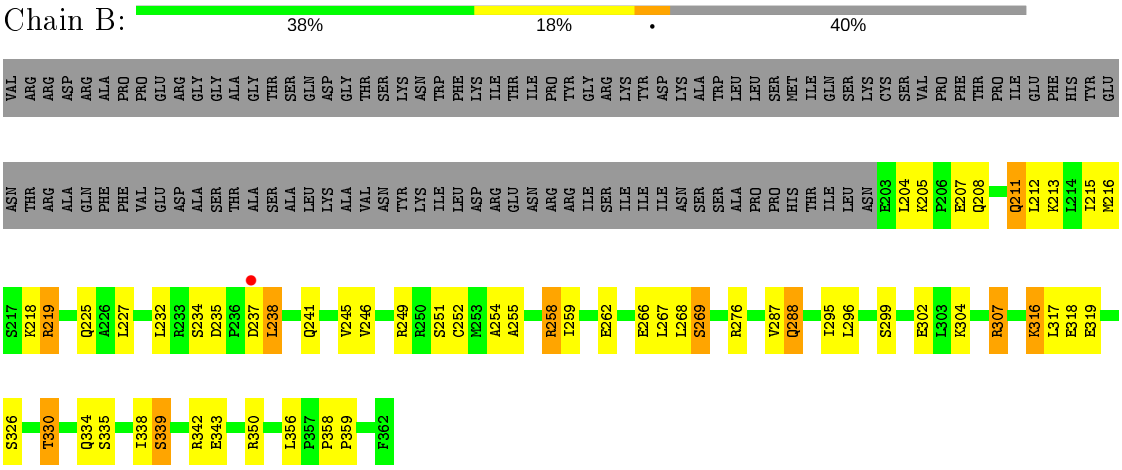
- Molecule 1: Nuclear RNA export factor 1

Chain A:



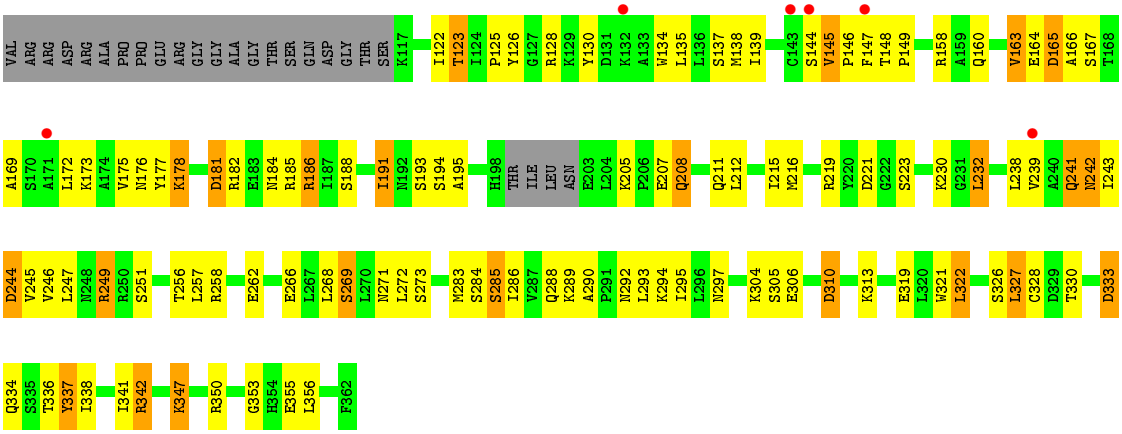
- Molecule 1: Nuclear RNA export factor 1

Chain B:



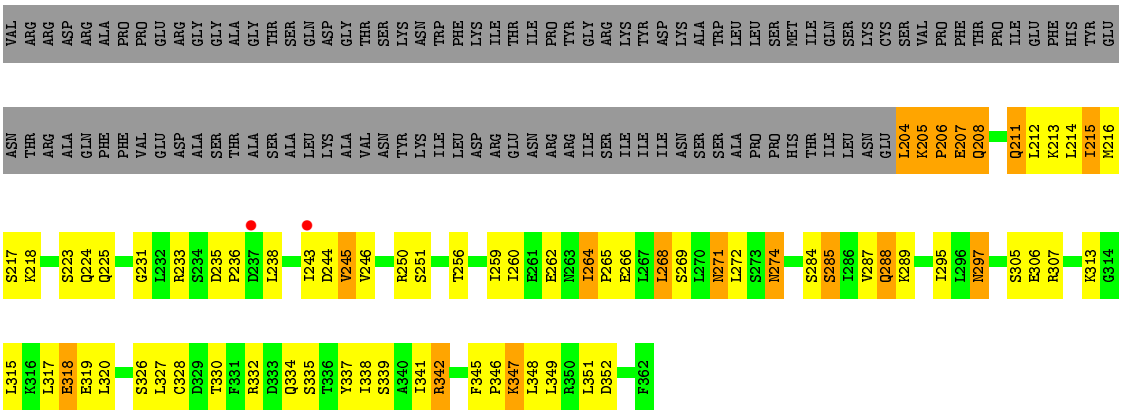
- Molecule 1: Nuclear RNA export factor 1

Chain C:



• Molecule 1: Nuclear RNA export factor 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.37Å 139.37Å 207.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 3.00 49.04 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.05-3.00) 98.1 (49.04-2.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.260 , 0.310 0.257 , 0.306	Depositor DCC
R_{free} test set	2055 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.52	0/1994	0.63	0/2693
1	B	0.52	0/1301	0.63	0/1753
1	C	0.47	0/1996	0.61	0/2694
1	D	0.50	0/1292	0.69	0/1741
All	All	0.50	0/6583	0.64	0/8881

There are no bond length outliers.

There are no bond angle outliers.

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	1959	0	1999	74	0
1	B	1285	0	1328	37	0
1	C	1961	0	2005	78	0
1	D	1276	0	1322	65	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
All	All	6488	0	6654	244	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 19.

All (244) 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:C:177:TYR:CD2	1:C:186:ARG:HG2	1.56	1.39
1:C:177:TYR:CE2	1:C:186:ARG:HG2	1.95	1.00
1:C:212:LEU:HG	1:C:216:MET:HE3	1.45	0.99
1:C:177:TYR:CD2	1:C:186:ARG:CG	2.51	0.93
1:A:249:ARG:HH12	1:A:279:ARG:HH21	1.16	0.88
1:C:177:TYR:HD2	1:C:186:ARG:HG2	1.42	0.82
1:B:269:SER:HB2	1:B:295:ILE:HB	1.60	0.82
1:D:215:ILE:HG12	1:D:238:LEU:HD21	1.67	0.77
1:A:249:ARG:HH12	1:A:279:ARG:NH2	1.82	0.76
1:C:350:ARG:HG2	1:C:355:GLU:HG3	1.66	0.76
1:A:340:ALA:O	1:A:343:GLU:HB3	1.87	0.75
1:A:216:MET:HE1	1:A:259:ILE:HD12	1.68	0.75
1:D:295:ILE:HG23	1:D:319:GLU:HB3	1.67	0.74
1:C:241:GLN:O	1:C:242:ASN:HB2	1.84	0.74
1:C:232:LEU:HD23	1:C:245:VAL:HG11	1.70	0.74
1:B:330:THR:HG22	1:D:305:SER:HB2	1.69	0.74
1:B:212:LEU:HG	1:B:216:MET:HE3	1.70	0.74
1:D:327:LEU:C	1:D:327:LEU:HD12	2.09	0.73
1:D:212:LEU:HG	1:D:216:MET:HE3	1.70	0.73
1:C:176:ASN:OD1	1:C:188:SER:HA	1.87	0.72
1:C:177:TYR:CE2	1:C:186:ARG:CG	2.71	0.72
1:A:142:LYS:HG3	1:A:179:ILE:HD11	1.70	0.72
1:C:310:ASP:N	1:C:310:ASP:OD2	2.23	0.72
1:B:225:GLN:HE21	1:B:266:GLU:HG3	1.53	0.72
1:B:216:MET:CE	1:B:259:ILE:HD12	2.19	0.71
1:A:122:ILE:HG13	1:A:191:ILE:HD13	1.71	0.71
1:C:288:GLN:NE2	1:D:288:GLN:OE1	2.23	0.71
1:D:347:LYS:HZ2	1:D:347:LYS:H	1.39	0.71
1:D:205:LYS:HB2	1:D:208:GLN:HB2	1.72	0.70
1:D:266:GLU:N	1:D:266:GLU:OE2	2.16	0.70
1:A:216:MET:CE	1:A:259:ILE:HD12	2.22	0.70
1:A:142:LYS:HG3	1:A:179:ILE:CD1	2.22	0.69
1:C:333:ASP:N	1:C:333:ASP:OD2	2.25	0.69
1:A:349:LEU:O	1:A:356:LEU:HB2	1.92	0.68
1:A:177:TYR:CE1	1:A:186:ARG:HG3	2.29	0.68
1:B:295:ILE:HG12	1:B:319:GLU:HB2	1.76	0.68
1:B:219:ARG:NH1	1:B:235:ASP:OD2	2.26	0.68
1:C:158:ARG:NH2	1:C:207:GLU:OE2	2.27	0.67
1:C:212:LEU:CG	1:C:216:MET:HE3	2.23	0.67
1:C:285:SER:HB2	1:C:289:LYS:HE2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:MET:HE1	1:B:259:ILE:HD12	1.77	0.67
1:C:205:LYS:N	1:C:208:GLN:OE1	2.29	0.65
1:D:327:LEU:O	1:D:330:THR:HB	1.97	0.65
1:A:218:LYS:NZ	1:A:237:ASP:OD1	2.30	0.64
1:A:288:GLN:NE2	1:B:288:GLN:OE1	2.30	0.64
1:A:122:ILE:HG13	1:A:191:ILE:CD1	2.27	0.64
1:A:212:LEU:HG	1:A:216:MET:HE3	1.80	0.64
1:D:238:LEU:HD13	1:D:245:VAL:HG21	1.80	0.63
1:A:158:ARG:NH2	1:A:207:GLU:OE2	2.31	0.63
1:A:247:LEU:HB3	1:A:253:MET:HE2	1.81	0.63
1:A:142:LYS:HB2	1:A:175:VAL:HG13	1.81	0.63
1:B:304:LYS:HD2	1:D:332:ARG:NH1	2.14	0.62
1:B:338:ILE:HD13	1:B:356:LEU:HD22	1.80	0.62
1:C:328:CYS:HG	1:C:337:TYR:HH	1.45	0.62
1:A:122:ILE:N	1:A:122:ILE:HD12	2.14	0.61
1:B:255:ALA:O	1:B:259:ILE:HG13	2.01	0.60
1:D:204:LEU:N	1:D:208:GLN:OE1	2.34	0.60
1:D:208:GLN:HA	1:D:211:GLN:HE21	1.67	0.59
1:D:347:LYS:HZ2	1:D:347:LYS:N	2.00	0.59
1:A:212:LEU:HG	1:A:216:MET:CE	2.33	0.59
1:C:268:LEU:O	1:C:293:LEU:HD12	2.01	0.59
1:A:180:LEU:HD12	1:A:185:ARG:O	2.03	0.59
1:D:345:PHE:HB3	1:D:347:LYS:HZ1	1.68	0.59
1:D:342:ARG:HG3	1:D:346:PRO:HA	1.84	0.58
1:A:297:ASN:HD22	1:A:297:ASN:C	2.06	0.58
1:C:212:LEU:HG	1:C:216:MET:CE	2.27	0.58
1:A:247:LEU:HB3	1:A:253:MET:CE	2.33	0.58
1:C:334:GLN:O	1:C:338:ILE:HG13	2.03	0.58
1:C:177:TYR:CE2	1:C:186:ARG:HD3	2.38	0.58
1:D:216:MET:CE	1:D:259:ILE:HD12	2.34	0.58
1:D:351:LEU:O	1:D:352:ASP:HB2	2.03	0.57
1:A:237:ASP:N	1:A:237:ASP:OD2	2.34	0.57
1:C:322:LEU:HD22	1:C:327:LEU:HD21	1.87	0.57
1:A:238:LEU:HD13	1:A:245:VAL:HG21	1.85	0.57
1:A:288:GLN:NE2	1:B:287:VAL:HB	2.20	0.57
1:A:249:ARG:NH1	1:A:279:ARG:HH21	1.96	0.57
1:D:216:MET:HE1	1:D:259:ILE:HD12	1.87	0.57
1:D:231:GLY:HA2	1:D:274:ASN:O	2.05	0.57
1:D:213:LYS:HB2	1:D:259:ILE:HD13	1.86	0.57
1:A:335:SER:O	1:A:339:SER:OG	2.22	0.56
1:D:225:GLN:OE1	1:D:268:LEU:HG	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:GLN:O	1:D:338:ILE:HG13	2.05	0.56
1:C:215:ILE:O	1:C:219:ARG:HG3	2.06	0.56
1:C:230:LYS:HG3	1:C:273:SER:HB2	1.87	0.56
1:A:297:ASN:ND2	1:A:299:SER:H	2.03	0.56
1:D:287:VAL:HG13	1:D:315:LEU:HD23	1.88	0.56
1:D:327:LEU:HD12	1:D:328:CYS:N	2.21	0.55
1:D:238:LEU:HB3	1:D:243:ILE:HB	1.88	0.55
1:D:337:TYR:CE2	1:D:351:LEU:HD21	2.41	0.55
1:A:172:LEU:O	1:A:175:VAL:HG23	2.06	0.55
1:D:318:GLU:O	1:D:349:LEU:N	2.31	0.55
1:B:216:MET:HE3	1:B:259:ILE:HD12	1.86	0.55
1:A:175:VAL:HB	1:A:189:ILE:HD13	1.89	0.54
1:B:334:GLN:HG3	1:C:125:PRO:HB3	1.88	0.54
1:C:175:VAL:O	1:C:178:LYS:HG2	2.07	0.54
1:A:333:ASP:O	1:A:336:THR:OG1	2.25	0.53
1:C:122:ILE:HD12	1:C:191:ILE:HD13	1.90	0.53
1:C:216:MET:CE	1:C:256:THR:HG23	2.39	0.53
1:C:232:LEU:HD23	1:C:245:VAL:CG1	2.38	0.53
1:A:121:LYS:HG3	1:A:162:PHE:CE2	2.44	0.53
1:B:319:GLU:HG2	1:B:350:ARG:HB3	1.91	0.53
1:C:241:GLN:O	1:C:242:ASN:CB	2.56	0.53
1:A:297:ASN:HD21	1:A:299:SER:HG	1.57	0.52
1:A:158:ARG:NH1	1:A:160:GLN:OE1	2.43	0.52
1:C:244:ASP:N	1:C:244:ASP:OD1	2.43	0.52
1:D:264:ILE:N	1:D:265:PRO:HD3	2.25	0.52
1:D:347:LYS:H	1:D:347:LYS:HD3	1.75	0.52
1:A:207:GLU:H	1:A:207:GLU:CD	2.12	0.52
1:B:215:ILE:HG13	1:B:238:LEU:HD22	1.90	0.51
1:D:206:PRO:O	1:D:208:GLN:N	2.43	0.51
1:D:320:LEU:O	1:D:351:LEU:HD12	2.10	0.51
1:C:175:VAL:O	1:C:178:LYS:CG	2.58	0.51
1:A:150:ILE:HB	1:A:162:PHE:HB2	1.91	0.51
1:C:194:SER:OG	1:C:195:ALA:O	2.26	0.51
1:A:248:ASN:OD1	1:A:248:ASN:N	2.44	0.51
1:C:177:TYR:CG	1:C:177:TYR:O	2.64	0.50
1:A:165:ASP:OD2	1:A:167:SER:OG	2.27	0.50
1:C:246:VAL:HG11	1:C:249:ARG:HG3	1.94	0.50
1:A:134:TRP:CZ2	1:A:138:MET:HG3	2.46	0.50
1:A:215:ILE:O	1:A:218:LYS:HB2	2.11	0.49
1:B:211:GLN:OE1	1:B:241:GLN:NE2	2.29	0.49
1:C:177:TYR:CE2	1:C:186:ARG:CD	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:HD2	1:D:332:ARG:CZ	2.42	0.49
1:B:338:ILE:HD13	1:B:356:LEU:CD2	2.42	0.49
1:D:285:SER:O	1:D:289:LYS:HG3	2.12	0.49
1:C:321:TRP:CH2	1:C:353:GLY:HA3	2.48	0.49
1:D:213:LYS:HG3	1:D:259:ILE:HG23	1.95	0.49
1:C:257:LEU:HB3	1:C:289:LYS:HE3	1.95	0.49
1:D:327:LEU:C	1:D:327:LEU:CD1	2.80	0.48
1:B:302:GLU:O	1:D:332:ARG:NH2	2.46	0.48
1:D:212:LEU:HD11	1:D:216:MET:HE2	1.94	0.48
1:B:215:ILE:O	1:B:219:ARG:HG2	2.13	0.48
1:C:221:ASP:OD1	1:C:223:SER:OG	2.31	0.48
1:B:246:VAL:HB	1:B:249:ARG:HG3	1.96	0.48
1:C:125:PRO:O	1:C:126:TYR:HB2	2.14	0.48
1:A:333:ASP:OD2	1:A:336:THR:N	2.47	0.48
1:D:266:GLU:O	1:D:268:LEU:HD23	2.13	0.48
1:C:355:GLU:OE2	1:C:355:GLU:N	2.47	0.48
1:A:306:GLU:HA	1:A:327:LEU:HD13	1.95	0.47
1:C:319:GLU:OE1	1:C:350:ARG:NH1	2.43	0.47
1:C:338:ILE:O	1:C:342:ARG:HB2	2.15	0.47
1:A:306:GLU:HG3	1:A:344:ARG:HH12	1.79	0.47
1:C:290:ALA:HB1	1:C:293:LEU:HB2	1.97	0.47
1:C:145:VAL:HG23	1:C:146:PRO:O	2.15	0.47
1:B:267:LEU:HD11	1:B:269:SER:O	2.15	0.47
1:A:128:ARG:NH1	1:A:156:ASN:O	2.42	0.47
1:B:251:SER:O	1:B:254:ALA:HB3	2.15	0.47
1:D:347:LYS:H	1:D:347:LYS:CD	2.28	0.47
1:D:212:LEU:O	1:D:216:MET:HG3	2.14	0.47
1:A:126:TYR:O	1:A:129:LYS:HB2	2.15	0.46
1:C:164:GLU:HB2	1:C:165:ASP:OD1	2.14	0.46
1:A:168:THR:HG22	1:A:172:LEU:CD2	2.45	0.46
1:A:305:SER:OG	1:A:307:ARG:HB2	2.15	0.46
1:C:181:ASP:OD2	1:C:185:ARG:HB2	2.16	0.46
1:D:271:ASN:HD22	1:D:272:LEU:N	2.14	0.46
1:A:294:LYS:HE3	1:A:294:LYS:HB3	1.60	0.46
1:C:247:LEU:HA	1:C:247:LEU:HD23	1.61	0.46
1:A:292:ASN:OD1	1:A:292:ASN:N	2.47	0.46
1:B:232:LEU:HD23	1:B:245:VAL:HG11	1.96	0.46
1:C:165:ASP:C	1:C:167:SER:H	2.18	0.46
1:D:205:LYS:HD3	1:D:205:LYS:HA	1.70	0.46
1:C:337:TYR:HD2	1:C:341:ILE:HD13	1.81	0.46
1:C:337:TYR:CD2	1:C:341:ILE:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:PHE:HE1	1:C:149:PRO:HG3	1.80	0.46
1:C:238:LEU:N	1:C:238:LEU:HD23	2.30	0.46
1:D:238:LEU:CD1	1:D:245:VAL:HG21	2.45	0.46
1:A:267:LEU:HD11	1:A:269:SER:O	2.16	0.45
1:A:301:ASN:HB3	1:A:302:GLU:H	1.53	0.45
1:C:123:THR:HG23	1:C:160:GLN:CG	2.46	0.45
1:D:269:SER:HB2	1:D:295:ILE:HD12	1.98	0.45
1:C:169:ALA:HB1	1:C:191:ILE:HG21	1.98	0.45
1:A:225:GLN:HB2	1:A:268:LEU:HD12	1.98	0.45
1:B:258:ARG:HH12	1:B:262:GLU:HB2	1.82	0.45
1:D:213:LYS:CB	1:D:259:ILE:HD13	2.47	0.44
1:C:216:MET:HE1	1:C:256:THR:HA	2.00	0.44
1:C:271:ASN:ND2	1:C:273:SER:OG	2.50	0.44
1:C:338:ILE:HD13	1:C:356:LEU:HD22	1.99	0.44
1:D:295:ILE:HG23	1:D:319:GLU:CB	2.41	0.44
1:A:204:LEU:HD13	1:A:204:LEU:HA	1.84	0.44
1:B:258:ARG:HH22	1:B:262:GLU:HG2	1.83	0.44
1:C:347:LYS:HE3	1:C:347:LYS:HB2	1.80	0.44
1:B:317:LEU:HD23	1:B:317:LEU:HA	1.85	0.43
1:A:152:PHE:CD2	1:A:152:PHE:C	2.91	0.43
1:C:135:LEU:O	1:C:139:ILE:HG13	2.19	0.43
1:A:212:LEU:HD13	1:A:245:VAL:HG11	2.00	0.43
1:A:249:ARG:NE	1:A:250:ARG:H	2.16	0.43
1:C:216:MET:HE2	1:C:256:THR:HG23	2.00	0.43
1:C:336:THR:OG1	1:C:337:TYR:N	2.52	0.43
1:D:347:LYS:NZ	1:D:347:LYS:H	2.15	0.43
1:B:205:LYS:O	1:B:208:GLN:N	2.48	0.43
1:C:165:ASP:C	1:C:167:SER:N	2.72	0.43
1:C:304:LYS:HA	1:C:326:SER:HB2	2.01	0.43
1:D:271:ASN:C	1:D:271:ASN:HD22	2.22	0.43
1:D:337:TYR:O	1:D:341:ILE:HD13	2.18	0.43
1:A:221:ASP:OD1	1:A:223:SER:OG	2.37	0.42
1:D:215:ILE:HD12	1:D:218:LYS:HE3	2.01	0.42
1:C:175:VAL:HA	1:C:178:LYS:HG3	2.00	0.42
1:D:205:LYS:HB3	1:D:206:PRO:HD2	2.01	0.42
1:A:337:TYR:HD1	1:A:341:ILE:HD13	1.85	0.42
1:B:307:ARG:NE	1:D:306:GLU:OE1	2.52	0.42
1:D:347:LYS:HD3	1:D:347:LYS:N	2.34	0.42
1:A:183:GLU:O	1:A:184:ASN:HB2	2.18	0.42
1:B:339:SER:O	1:B:343:GLU:HG3	2.19	0.42
1:D:214:LEU:O	1:D:217:SER:OG	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:LEU:HD12	1:D:345:PHE:CE2	2.55	0.42
1:A:256:THR:O	1:A:260:ILE:HG13	2.20	0.42
1:B:225:GLN:HE21	1:B:266:GLU:CG	2.28	0.42
1:C:271:ASN:HA	1:C:297:ASN:HB3	2.01	0.42
1:A:297:ASN:HD22	1:A:298:LEU:N	2.18	0.42
1:A:333:ASP:CG	1:A:335:SER:H	2.23	0.42
1:A:132:LYS:HG2	1:A:136:LEU:HD12	2.02	0.41
1:A:261:GLU:O	1:A:265:PRO:HG3	2.19	0.41
1:D:215:ILE:HG12	1:D:238:LEU:CD2	2.45	0.41
1:A:122:ILE:CD1	1:A:122:ILE:N	2.82	0.41
1:D:288:GLN:HB2	1:D:288:GLN:HE21	1.70	0.41
1:D:297:ASN:C	1:D:297:ASN:HD22	2.23	0.41
1:D:211:GLN:HG2	1:D:211:GLN:H	1.44	0.41
1:A:327:LEU:O	1:A:330:THR:HB	2.20	0.41
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.85	0.41
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.87	0.41
1:B:316:LYS:H	1:B:316:LYS:HG2	1.75	0.41
1:C:355:GLU:CD	1:C:355:GLU:N	2.74	0.41
1:A:123:THR:HB	1:A:190:ILE:HB	2.03	0.41
1:B:227:LEU:HA	1:B:227:LEU:HD12	1.91	0.41
1:B:358:PRO:HA	1:B:359:PRO:HD3	1.94	0.41
1:D:256:THR:O	1:D:260:ILE:HG13	2.21	0.41
1:C:128:ARG:C	1:C:130:TYR:H	2.23	0.41
1:C:208:GLN:HG3	1:C:208:GLN:H	1.56	0.41
1:C:269:SER:HB2	1:C:295:ILE:HB	2.02	0.41
1:C:347:LYS:H	1:C:347:LYS:HG3	1.54	0.41
1:C:163:VAL:HG22	1:C:164:GLU:H	1.86	0.41
1:C:258:ARG:HH12	1:D:250:ARG:NH2	2.18	0.41
1:C:286:ILE:O	1:C:286:ILE:HG12	2.20	0.41
1:A:225:GLN:O	1:A:267:LEU:HD12	2.21	0.41
1:C:165:ASP:O	1:C:167:SER:N	2.54	0.41
1:A:216:MET:HE1	1:A:256:THR:HA	2.03	0.40
1:D:342:ARG:NH1	1:D:348:LEU:O	2.54	0.40
1:C:134:TRP:CZ2	1:C:138:MET:HG3	2.56	0.40
1:A:122:ILE:HD11	1:A:163:VAL:HB	2.04	0.40
1:A:160:GLN:HB2	1:A:160:GLN:HE21	1.60	0.40
1:A:237:ASP:O	1:A:241:GLN:NE2	2.55	0.40
1:A:266:GLU:H	1:A:266:GLU:HG2	1.42	0.40
1:C:211:GLN:HG2	1:C:243:ILE:HD12	2.04	0.40
1:D:271:ASN:ND2	1:D:297:ASN:HB3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	238/267 (89%)	209 (88%)	26 (11%)	3 (1%)	12 45
1	B	158/267 (59%)	146 (92%)	12 (8%)	0	100 100
1	C	238/267 (89%)	214 (90%)	23 (10%)	1 (0%)	34 72
1	D	157/267 (59%)	142 (90%)	11 (7%)	4 (2%)	5 28
All	All	791/1068 (74%)	711 (90%)	72 (9%)	8 (1%)	15 53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	206	PRO
1	A	299	SER
1	D	207	GLU
1	D	313	LYS
1	A	337	TYR
1	C	166	ALA
1	A	231	GLY
1	D	236	PRO

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	221/240 (92%)	180 (81%)	41 (19%)	1 8
1	B	147/240 (61%)	123 (84%)	24 (16%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	221/240 (92%)	177 (80%)	44 (20%)	1 7
1	D	146/240 (61%)	116 (80%)	30 (20%)	1 6
All	All	735/960 (77%)	596 (81%)	139 (19%)	1 8

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	141	SER
1	A	158	ARG
1	A	163	VAL
1	A	164	GLU
1	A	165	ASP
1	A	167	SER
1	A	170	SER
1	A	172	LEU
1	A	182	ARG
1	A	204	LEU
1	A	207	GLU
1	A	211	GLN
1	A	217	SER
1	A	223	SER
1	A	230	LYS
1	A	233	ARG
1	A	234	SER
1	A	237	ASP
1	A	241	GLN
1	A	244	ASP
1	A	245	VAL
1	A	248	ASN
1	A	266	GLU
1	A	279	ARG
1	A	283	MET
1	A	288	GLN
1	A	292	ASN
1	A	294	LYS
1	A	297	ASN
1	A	316	LYS
1	A	326	SER
1	A	327	LEU
1	A	330	THR

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Mol	Chain	Res	Type
1	A	333	ASP
1	A	336	THR
1	A	337	TYR
1	A	339	SER
1	A	342	ARG
1	A	349	LEU
1	A	351	LEU
1	B	204	LEU
1	B	207	GLU
1	B	211	GLN
1	B	213	LYS
1	B	218	LYS
1	B	219	ARG
1	B	234	SER
1	B	237	ASP
1	B	238	LEU
1	B	252	CYS
1	B	258	ARG
1	B	268	LEU
1	B	269	SER
1	B	276	ARG
1	B	288	GLN
1	B	299	SER
1	B	307	ARG
1	B	316	LYS
1	B	318	GLU
1	B	326	SER
1	B	330	THR
1	B	335	SER
1	B	339	SER
1	B	342	ARG
1	C	123	THR
1	C	137	SER
1	C	144	SER
1	C	145	VAL
1	C	148	THR
1	C	163	VAL
1	C	165	ASP
1	C	172	LEU
1	C	173	LYS
1	C	178	LYS
1	C	181	ASP

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Mol	Chain	Res	Type
1	C	182	ARG
1	C	184	ASN
1	C	186	ARG
1	C	191	ILE
1	C	193	SER
1	C	208	GLN
1	C	232	LEU
1	C	239	VAL
1	C	241	GLN
1	C	242	ASN
1	C	244	ASP
1	C	249	ARG
1	C	251	SER
1	C	262	GLU
1	C	266	GLU
1	C	269	SER
1	C	272	LEU
1	C	283	MET
1	C	284	SER
1	C	285	SER
1	C	292	ASN
1	C	294	LYS
1	C	305	SER
1	C	306	GLU
1	C	310	ASP
1	C	313	LYS
1	C	322	LEU
1	C	327	LEU
1	C	330	THR
1	C	333	ASP
1	C	337	TYR
1	C	342	ARG
1	C	347	LYS
1	D	204	LEU
1	D	205	LYS
1	D	207	GLU
1	D	208	GLN
1	D	211	GLN
1	D	215	ILE
1	D	223	SER
1	D	224	GLN
1	D	233	ARG

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Mol	Chain	Res	Type
1	D	235	ASP
1	D	244	ASP
1	D	245	VAL
1	D	246	VAL
1	D	251	SER
1	D	262	GLU
1	D	264	ILE
1	D	268	LEU
1	D	271	ASN
1	D	274	ASN
1	D	284	SER
1	D	285	SER
1	D	288	GLN
1	D	297	ASN
1	D	307	ARG
1	D	318	GLU
1	D	326	SER
1	D	335	SER
1	D	339	SER
1	D	342	ARG
1	D	347	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	288	GLN
1	A	297	ASN
1	B	225	GLN
1	B	288	GLN
1	C	288	GLN
1	D	208	GLN
1	D	271	ASN
1	D	288	GLN
1	D	297	ASN

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	242/267 (90%)	-0.19	2 (0%)	86	65	40, 73, 103, 119	0
1	B	160/267 (59%)	-0.17	1 (0%)	89	72	45, 65, 113, 126	0
1	C	242/267 (90%)	0.12	6 (2%)	57	29	55, 89, 123, 135	0
1	D	159/267 (59%)	-0.14	2 (1%)	77	51	47, 70, 117, 130	0
All	All	803/1068 (75%)	-0.08	11 (1%)	75	49	40, 74, 118, 135	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	VAL	3.1
1	D	243	ILE	3.0
1	B	237	ASP	2.7
1	D	237	ASP	2.6
1	A	238	LEU	2.5
1	C	144	SER	2.5
1	A	241	GLN	2.3
1	C	147	PHE	2.1
1	C	143	CYS	2.0
1	C	171	ALA	2.0
1	C	132	LYS	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.