



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:07 AM UTC

PDB ID : 3RW7 / pdb_00003rw7
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 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

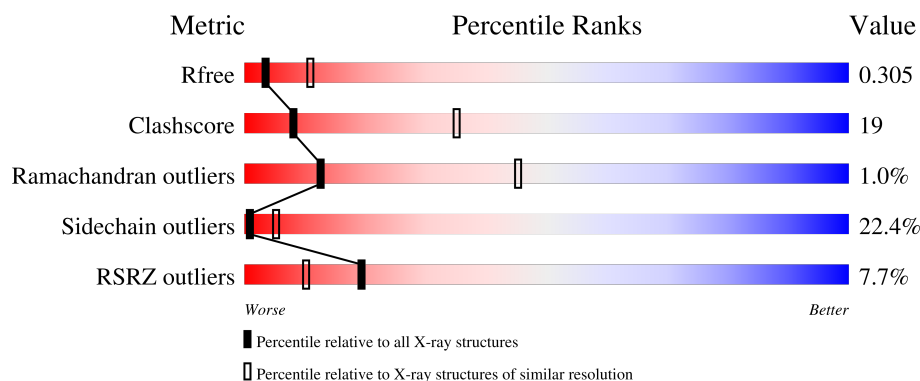
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	267	4% 50% 29% 11% 9%
1	B	267	4% 35% 21% • 40%
1	C	267	10% 46% 33% 11% • 9%
1	D	267	4% 31% 20% 8% 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			

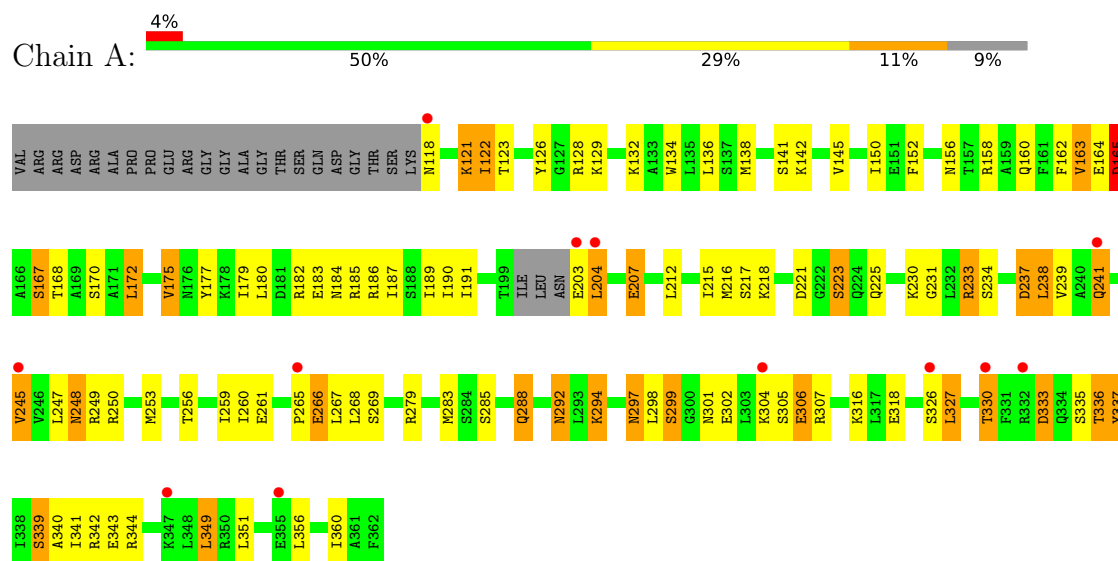
- Molecule 2 is water.

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		

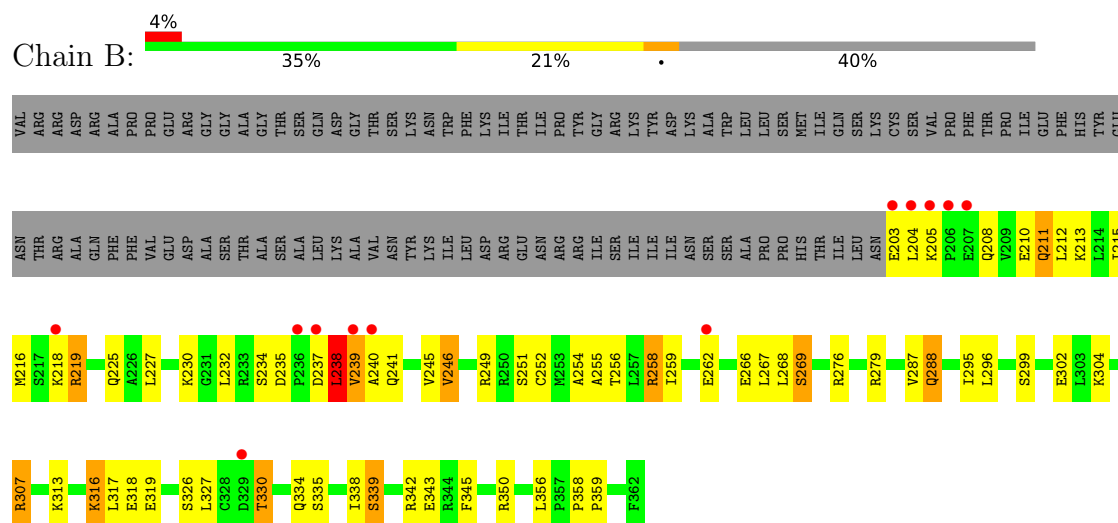
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Nuclear RNA export factor 1

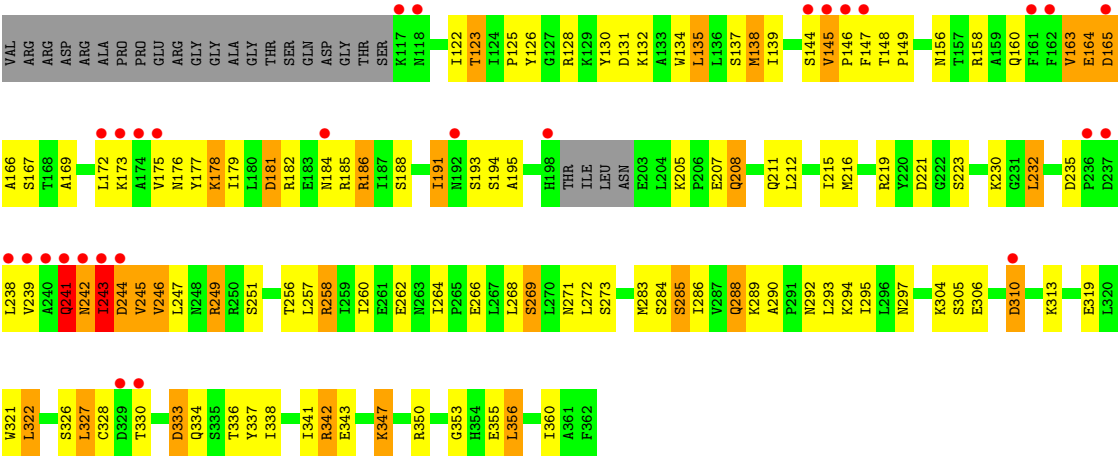


• Molecule 1: Nuclear RNA export factor 1

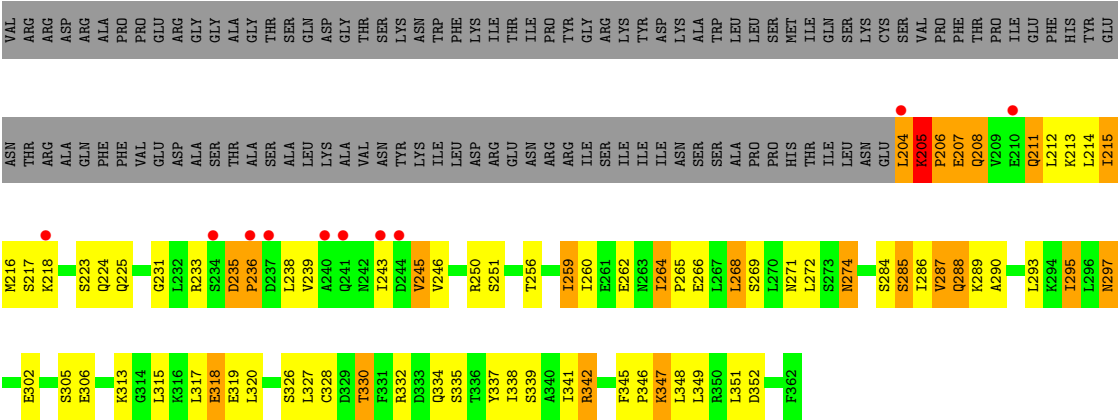
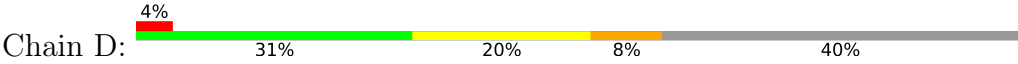


• Molecule 1: Nuclear RNA export factor 1





● Molecule 1: Nuclear RNA export factor 1



4 Data and refinement statistics

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 49.05 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.05-3.00) 98.3 (49.05-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.260 , 0.310 0.258 , 0.305	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 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.37$	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.*

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	0.61	0/1994	0.99	5/2693 (0.2%)
1	B	0.60	0/1301	0.99	6/1753 (0.3%)
1	C	0.55	0/1996	1.02	9/2694 (0.3%)
1	D	0.62	0/1292	1.05	4/1741 (0.2%)
All	All	0.59	0/6583	1.01	24/8881 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	VAL	N-CA-C	-7.97	102.49	110.62
1	B	238	LEU	N-CA-C	-6.54	107.17	114.62
1	D	205	LYS	CA-C-N	6.33	127.75	119.84
1	D	205	LYS	C-N-CA	6.33	127.75	119.84
1	B	240	ALA	N-CA-C	6.27	117.78	111.07
1	B	345	PHE	CA-C-N	6.14	125.82	119.56
1	B	345	PHE	C-N-CA	6.14	125.82	119.56
1	C	356	LEU	CA-C-N	6.07	126.63	120.38
1	C	356	LEU	C-N-CA	6.07	126.63	120.38
1	A	318	GLU	N-CA-C	-5.59	107.00	113.88
1	A	306	GLU	N-CA-C	-5.44	106.48	113.23
1	A	145	VAL	N-CA-C	5.43	113.64	109.19
1	A	233	ARG	N-CA-C	-5.42	105.47	111.71
1	C	156	ASN	CB-CA-C	-5.27	110.48	116.54
1	A	165	ASP	N-CA-C	5.25	117.17	109.24
1	C	241	GLN	N-CA-C	5.22	116.97	111.28
1	C	243	ILE	CA-C-N	-5.20	115.86	122.77
1	C	243	ILE	C-N-CA	-5.20	115.86	122.77
1	B	279	ARG	N-CA-C	5.15	116.81	108.26
1	D	290	ALA	CA-C-N	5.14	124.94	119.28
1	D	290	ALA	C-N-CA	5.14	124.94	119.28
1	C	246	VAL	N-CA-C	5.13	111.69	106.21
1	C	235	ASP	CA-C-N	5.09	126.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	ASP	C-N-CA	5.09	126.20	119.84

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	76	0
1	B	1285	0	1328	38	0
1	C	1961	0	2005	81	0
1	D	1276	0	1322	71	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	256	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 (256) 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:212:LEU:HG	1:C:216:MET:HE3	1.38	1.03
1:C:177:TYR:CE2	1:C:186:ARG:HG2	1.95	1.00
1:C:177:TYR:CD2	1:C:186:ARG:CG	2.51	0.93
1:B:216:MET:HE3	1:B:259:ILE:HD12	1.55	0.88
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:327:LEU:C	1:D:327:LEU:HD12	2.09	0.78
1:C:138:MET:HE3	1:C:179:ILE:HG23	1.66	0.78
1:D:215:ILE:HG12	1:D:238:LEU:HD21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:216:MET:HE3	1:D:259:ILE:HD12	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:OD2	1:C:310:ASP:N	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:212:LEU:HD11	1:D:216:MET:HE2	1.73	0.71
1:D:347:LYS:H	1:D:347:LYS:HZ2	1.39	0.71
1:D:205:LYS:HB2	1:D:208:GLN:HB2	1.72	0.70
1:D:266:GLU:OE2	1:D:266:GLU:N	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:OD2	1:C:333:ASP:N	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:285:SER:HB2	1:C:289:LYS:HE2	1.75	0.67
1:A:216:MET:HE1	1:A:259:ILE:HD12	1.77	0.66
1:C:205:LYS:N	1:C:208:GLN:OE1	2.29	0.65
1:C:212:LEU:CG	1:C:216:MET:HE3	2.20	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:247:LEU:HB3	1:A:253:MET:HE2	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:C:328:CYS:HG	1:C:337:TYR:HH	1.43	0.63
1:A:142:LYS:HB2	1:A:175:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:C	1:A:297:ASN:HD22	2.06	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: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: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:351:LEU:O	1:D:352:ASP:HB2	2.03	0.57
1:A:237:ASP:OD2	1:A:237:ASP:N	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:D:216:MET:CE	1:D:259:ILE:HD12	2.34	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: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
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:D:334:GLN:O	1:D:338:ILE:HG13	2.05	0.56
1:A:212:LEU:HG	1:A:216:MET:HE3	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:A:207:GLU:CD	1:A:207:GLU:H	2.12	0.55
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:212:LEU:HG	1:D:216:MET:HE3	1.89	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:A:175:VAL:HB	1:A:189:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:212:LEU:HG	1:B:216:MET:HE3	1.88	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:D:216:MET:HE1	1:D:256:THR:HA	1.90	0.52
1:A:216:MET:HE3	1:A:259:ILE:HD12	1.92	0.52
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:OD1	1:C:244:ASP:N	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: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:D:214:LEU:O	1:D:217:SER:OG	2.24	0.51
1:A:248:ASN:OD1	1:A:248:ASN:N	2.44	0.51
1:C:165:ASP:C	1:C:167:SER:H	2.18	0.51
1:D:212:LEU:CD1	1:D:216:MET:HE2	2.39	0.51
1:C:177:TYR:CG	1:C:177:TYR:O	2.64	0.50
1:D:327:LEU:C	1:D:327:LEU:CD1	2.80	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:B:304:LYS:HD2	1:D:332:ARG:CZ	2.42	0.49
1:C:177:TYR:CE2	1:C:186:ARG:CD	2.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLU:O	1:D:332:ARG:NH2	2.46	0.48
1:A:216:MET:HE1	1:A:256:THR:HA	1.95	0.48
1:B:212:LEU:HD11	1:B:216:MET:HE2	1.95	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:A:152:PHE:C	1:A:152:PHE:CD2	2.91	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:165:ASP:C	1:C:167:SER:N	2.72	0.47
1:D:271:ASN:C	1:D:271:ASN:HD22	2.22	0.47
1:C:338:ILE:O	1:C:342:ARG:HB2	2.15	0.47
1:D:212:LEU:HG	1:D:216:MET:CE	2.44	0.47
1:C:212:LEU:HG	1:C:216:MET:CE	2.27	0.47
1:C:216:MET:HE1	1:C:256:THR:HA	1.95	0.47
1:A:306:GLU:HG3	1:A:344:ARG:HH12	1.79	0.47
1:C:145:VAL:HG23	1:C:146:PRO:O	2.15	0.47
1:C:290:ALA:HB1	1:C:293:LEU:HB2	1.97	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:A:333:ASP:CG	1:A:335:SER:H	2.23	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:HB3	1:A:294:LYS:HE3	1.60	0.46
1:C:247:LEU:HD23	1:C:247:LEU:HA	1.61	0.46
1:D:297:ASN:C	1:D:297:ASN:HD22	2.23	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:D:205:LYS:HA	1:D:205:LYS:HD3	1.70	0.46
1:C:337:TYR:HD2	1:C:341:ILE:HD13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:TYR:CD2	1:C:341:ILE:HD13	2.50	0.46
1:C:355:GLU:N	1:C:355:GLU:CD	2.74	0.46
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:128:ARG:C	1:C:130:TYR:H	2.23	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:216:MET:HE1	1:B:256:THR:HA	1.99	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: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: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:HE1	1:C:256:THR:HG23	2.01	0.43
1:C:336:THR:OG1	1:C:337:TYR:N	2.52	0.43
1:D:266:GLU:H	1:D:266:GLU:CD	2.18	0.43
1:D:347:LYS:H	1:D:347:LYS:NZ	2.15	0.43
1:B:205:LYS:O	1:B:208:GLN:N	2.48	0.43
1:C:304:LYS:HA	1:C:326:SER:HB2	2.01	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:N	1:D:347:LYS:HD3	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

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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: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:N	1:A:122:ILE:CD1	2.82	0.41
1:D:288:GLN:HE21	1:D:288:GLN:HB2	1.70	0.41
1:D:211:GLN:H	1:D:211:GLN:HG2	1.44	0.41
1:D:345:PHE:C	1:D:347:LYS:NZ	2.78	0.41
1:A:327:LEU:O	1:A:330:THR:HB	2.20	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.85	0.41
1:A:297:ASN:C	1:A:297:ASN:ND2	2.76	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:A:123:THR:HB	1:A:190:ILE:HB	2.03	0.41
1:B:227:LEU:HD12	1:B:227:LEU:HA	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:131:ASP:O	1:C:132:LYS:C	2.64	0.41
1:C:163:VAL:HG22	1:C:164:GLU:H	1.86	0.41
1:C:208:GLN:H	1:C:208:GLN:HG3	1.56	0.41
1:C:258:ARG:HH12	1:D:250:ARG:NH2	2.18	0.41
1:C:269:SER:HB2	1:C:295:ILE:HB	2.02	0.41
1:C:286:ILE:O	1:C:286:ILE:HG12	2.20	0.41
1:C:347:LYS:H	1:C:347:LYS:HG3	1.54	0.41
1:D:235:ASP:O	1:D:236:PRO:C	2.63	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: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:C:268:LEU:C	1:C:293:LEU:HD12	2.47	0.40
1:A:122:ILE:HD11	1:A:163:VAL:HB	2.04	0.40
1:A:160:GLN:HE21	1:A:160:GLN:HB2	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

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	238/267 (89%)	209 (88%)	26 (11%)	3 (1%)	9	38
1	B	158/267 (59%)	146 (92%)	12 (8%)	0	100	100
1	C	238/267 (89%)	214 (90%)	23 (10%)	1 (0%)	30	65
1	D	157/267 (59%)	142 (90%)	11 (7%)	4 (2%)	4	23
All	All	791/1068 (74%)	711 (90%)	72 (9%)	8 (1%)	12	45

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

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%)	175 (79%)	46 (21%)	1	7
1	B	147/240 (61%)	117 (80%)	30 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	221/240 (92%)	167 (76%)	54 (24%)	1	4
1	D	146/240 (61%)	111 (76%)	35 (24%)	1	4
All	All	735/960 (77%)	570 (78%)	165 (22%)	1	5

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	121	LYS
1	A	122	ILE
1	A	141	SER
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	175	VAL
1	A	182	ARG
1	A	187	ILE
1	A	203	GLU
1	A	204	LEU
1	A	207	GLU
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	238	LEU
1	A	239	VAL
1	A	241	GLN
1	A	245	VAL
1	A	248	ASN
1	A	266	GLU
1	A	283	MET
1	A	285	SER
1	A	288	GLN
1	A	292	ASN
1	A	294	LYS
1	A	297	ASN

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Mol	Chain	Res	Type
1	A	304	LYS
1	A	316	LYS
1	A	326	SER
1	A	327	LEU
1	A	330	THR
1	A	333	ASP
1	A	336	THR
1	A	339	SER
1	A	342	ARG
1	A	349	LEU
1	A	351	LEU
1	A	360	ILE
1	B	203	GLU
1	B	204	LEU
1	B	210	GLU
1	B	211	GLN
1	B	213	LYS
1	B	218	LYS
1	B	219	ARG
1	B	230	LYS
1	B	234	SER
1	B	237	ASP
1	B	238	LEU
1	B	239	VAL
1	B	246	VAL
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	313	LYS
1	B	316	LYS
1	B	318	GLU
1	B	326	SER
1	B	327	LEU
1	B	330	THR
1	B	335	SER
1	B	339	SER
1	B	342	ARG

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Mol	Chain	Res	Type
1	C	123	THR
1	C	135	LEU
1	C	137	SER
1	C	138	MET
1	C	144	SER
1	C	145	VAL
1	C	148	THR
1	C	163	VAL
1	C	164	GLU
1	C	165	ASP
1	C	172	LEU
1	C	173	LYS
1	C	178	LYS
1	C	181	ASP
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	243	ILE
1	C	244	ASP
1	C	245	VAL
1	C	249	ARG
1	C	251	SER
1	C	258	ARG
1	C	260	ILE
1	C	262	GLU
1	C	264	ILE
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	288	GLN
1	C	292	ASN
1	C	294	LYS

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Mol	Chain	Res	Type
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	342	ARG
1	C	343	GLU
1	C	347	LYS
1	C	360	ILE
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
1	D	235	ASP
1	D	239	VAL
1	D	245	VAL
1	D	246	VAL
1	D	251	SER
1	D	259	ILE
1	D	262	GLU
1	D	264	ILE
1	D	268	LEU
1	D	274	ASN
1	D	284	SER
1	D	285	SER
1	D	286	ILE
1	D	287	VAL
1	D	288	GLN
1	D	293	LEU
1	D	295	ILE
1	D	297	ASN
1	D	302	GLU
1	D	318	GLU
1	D	326	SER

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Mol	Chain	Res	Type
1	D	330	THR
1	D	335	SER
1	D	339	SER
1	D	342	ARG
1	D	347	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	263	ASN
1	A	274	ASN
1	A	288	GLN
1	A	297	ASN
1	B	225	GLN
1	B	274	ASN
1	B	288	GLN
1	C	274	ASN
1	C	288	GLN
1	D	208	GLN
1	D	263	ASN
1	D	271	ASN
1	D	288	GLN
1	D	292	ASN
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 oligosaccharides 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, 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	242/267 (90%)	0.29	12 (4%) 34 18	40, 73, 103, 119	0
1	B	160/267 (59%)	0.18	12 (7%) 20 10	45, 65, 113, 126	0
1	C	242/267 (90%)	0.77	28 (11%) 9 5	55, 89, 123, 135	0
1	D	159/267 (59%)	0.29	10 (6%) 26 13	47, 70, 117, 130	0
All	All	803/1068 (75%)	0.41	62 (7%) 19 10	40, 74, 118, 135	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	243	ILE	6.6
1	C	240	ALA	5.2
1	D	204	LEU	4.5
1	C	174	ALA	4.3
1	C	173	LYS	4.3
1	C	145	VAL	4.1
1	C	192	ASN	4.0
1	C	144	SER	3.8
1	C	117	LYS	3.7
1	C	241	GLN	3.6
1	C	330	THR	3.5
1	D	236	PRO	3.4
1	D	240	ALA	3.4
1	C	236	PRO	3.4
1	B	204	LEU	3.3
1	C	175	VAL	3.3
1	D	244	ASP	3.3
1	C	198	HIS	3.3
1	A	204	LEU	3.2
1	C	244	ASP	3.2
1	C	172	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	218	LYS	3.0
1	A	241	GLN	3.0
1	C	146	PRO	3.0
1	A	332	ARG	2.9
1	B	207	GLU	2.9
1	B	262	GLU	2.8
1	A	326	SER	2.8
1	C	239	VAL	2.8
1	C	184	ASN	2.7
1	D	237	ASP	2.7
1	B	237	ASP	2.7
1	B	206	PRO	2.6
1	C	238	LEU	2.6
1	A	330	THR	2.6
1	A	265	PRO	2.6
1	C	310	ASP	2.5
1	C	242	ASN	2.5
1	D	210	GLU	2.4
1	B	240	ALA	2.4
1	C	147	PHE	2.4
1	B	239	VAL	2.4
1	A	355	GLU	2.4
1	C	237	ASP	2.4
1	B	203	GLU	2.3
1	C	329	ASP	2.3
1	B	329	ASP	2.2
1	D	234	SER	2.2
1	A	203	GLU	2.2
1	A	347	LYS	2.2
1	B	205	LYS	2.1
1	D	243	ILE	2.1
1	D	241	GLN	2.1
1	C	165	ASP	2.1
1	C	162	PHE	2.1
1	A	304	LYS	2.1
1	B	236	PRO	2.1
1	A	245	VAL	2.0
1	A	118	ASN	2.0
1	D	218	LYS	2.0
1	C	118	ASN	2.0
1	C	161	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.