



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:39 am GMT

PDB ID : 2A1S
Title : Crystal structure of native PARN nuclease domain
Authors : Wu, M.; Song, H.
Deposited on : 2005-06-21
Resolution : 2.60 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

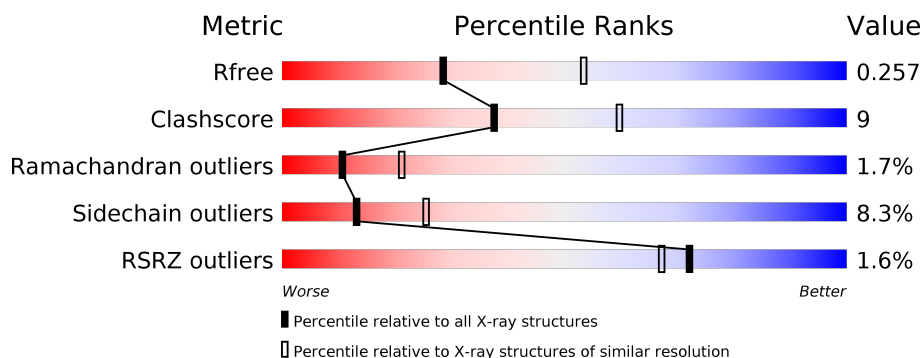
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	430	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>20%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	430	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>20%</div> <div>• •</div> <div>9%</div> </div> </div>
1	C	430	<div> <div></div> <div> <div>65%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	430	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13115 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 Poly(A)-specific ribonuclease PARN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3213	2067	529	602	15			
1	B	390	Total	C	N	O	S	0	0	0
			3210	2064	529	603	14			
1	C	393	Total	C	N	O	S	0	0	0
			3238	2083	532	608	15			
1	D	392	Total	C	N	O	S	0	0	0
			3215	2069	530	601	15			

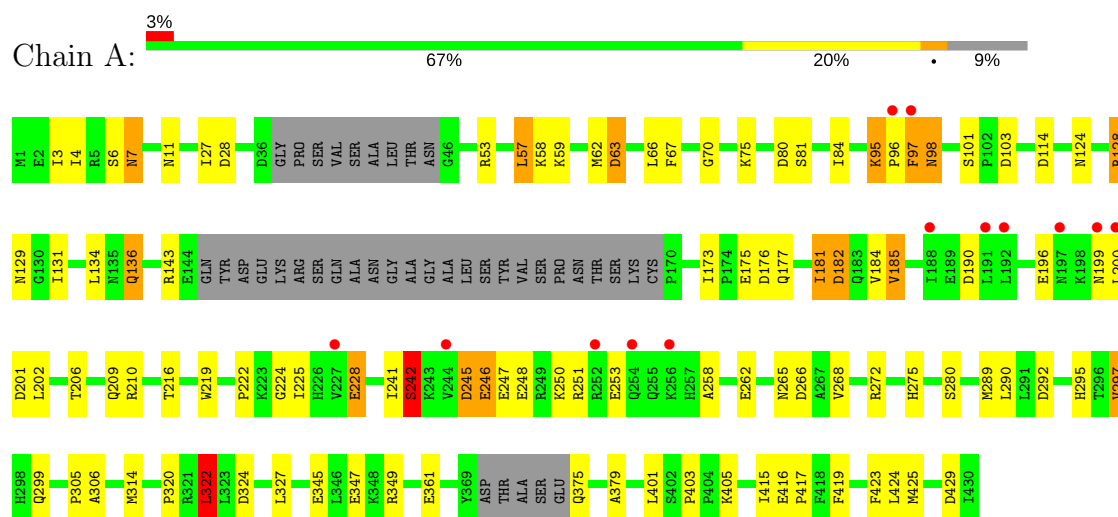
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	B	63	Total	O	0	0
			63	63		
2	C	59	Total	O	0	0
			59	59		
2	D	56	Total	O	0	0
			56	56		

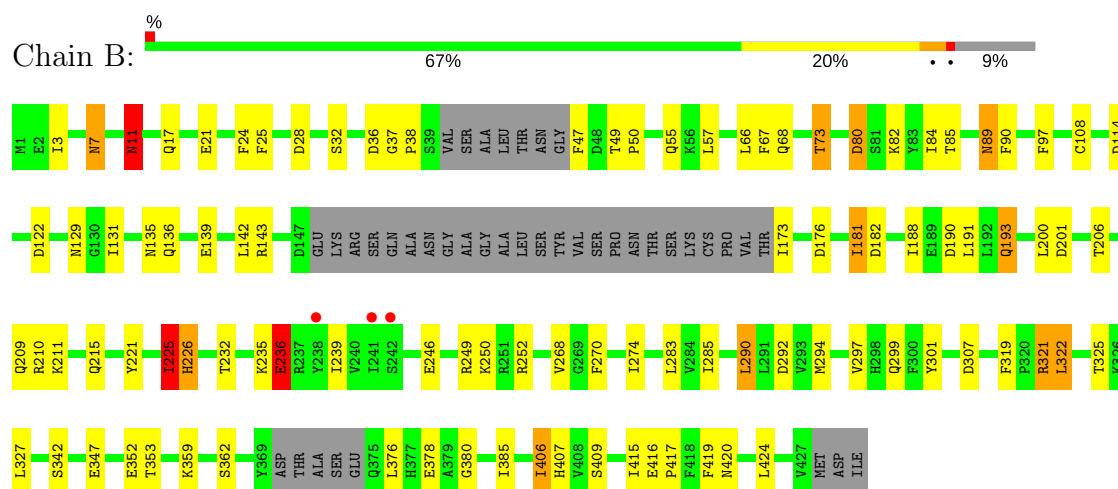
3 Residue-property plots [i](#)

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: Poly(A)-specific ribonuclease PARN

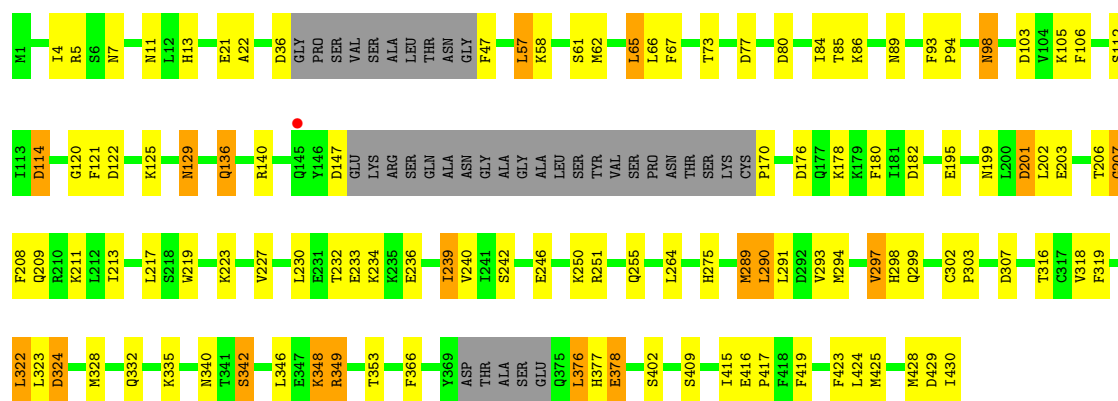


• Molecule 1: Poly(A)-specific ribonuclease PARN

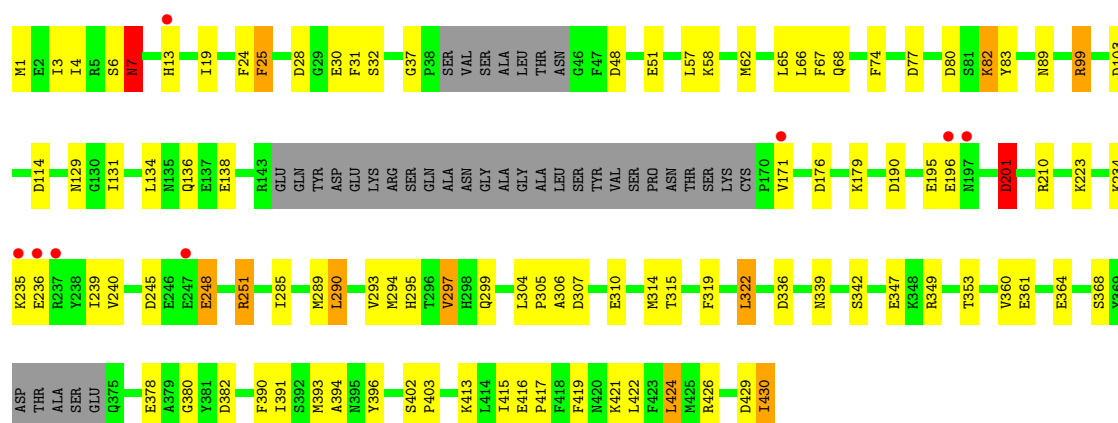


• Molecule 1: Poly(A)-specific ribonuclease PARN





● Molecule 1: Poly(A)-specific ribonuclease PARN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.54Å 123.02Å 82.84Å 90.00° 112.59° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 75.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.60) 99.4 (75.35-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.219 , 0.254 0.225 , 0.257	Depositor DCC
R_{free} test set	1786 reflections (3.17%)	DCC
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13115	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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	0.56	0/3288	0.77	13/4425 (0.3%)
1	B	0.57	0/3286	0.80	11/4423 (0.2%)
1	C	0.60	1/3314 (0.0%)	0.79	9/4461 (0.2%)
1	D	0.59	0/3291	0.79	13/4430 (0.3%)
All	All	0.58	1/13179 (0.0%)	0.79	46/17739 (0.3%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	289	MET	SD-CE	-5.62	1.46	1.77

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	CB-CG-OD2	8.20	125.68	118.30
1	B	182	ASP	CB-CG-OD2	8.16	125.64	118.30
1	C	77	ASP	CB-CG-OD2	7.44	125.00	118.30
1	B	28	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	63	ASP	CB-CG-OD2	6.64	124.28	118.30
1	D	28	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	324	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	176	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	36	ASP	CB-CG-OD2	6.31	123.98	118.30
1	D	201	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	201	ASP	CB-CG-OD2	6.28	123.95	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	429	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	147	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	36	ASP	CB-CG-OD2	6.20	123.88	118.30
1	C	307	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	176	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	190	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	28	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	176	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	114	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	80	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	322	LEU	CA-CB-CG	5.89	128.84	115.30
1	D	77	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	182	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	382	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	190	ASP	CB-CG-OD2	5.67	123.41	118.30
1	D	48	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	292	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	324	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	182	ASP	CB-CG-OD2	5.61	123.34	118.30
1	A	245	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	176	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	429	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	103	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	190	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	114	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	307	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	80	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	307	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	122	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	336	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	245	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	114	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	292	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	114	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	201	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	402	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3213	0	3167	57	0
1	B	3210	0	3151	43	0
1	C	3238	0	3184	72	0
1	D	3215	0	3171	53	0
2	A	61	0	0	4	0
2	B	63	0	0	1	0
2	C	59	0	0	7	0
2	D	56	0	0	2	0
All	All	13115	0	12673	224	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 9.

All (224) 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:D:4:ILE:H	1:D:7:ASN:HD21	1.12	0.93
1:A:62:MET:HE1	1:A:295:HIS:HA	1.53	0.90
1:B:89:ASN:HD21	1:B:380:GLY:H	1.24	0.85
1:B:66:LEU:H	1:B:299:GLN:HE22	1.24	0.81
1:D:66:LEU:H	1:D:299:GLN:HE22	1.27	0.80
1:A:66:LEU:H	1:A:299:GLN:HE22	1.29	0.77
1:B:319:PHE:HB3	1:B:322:LEU:HD11	1.68	0.75
1:A:95:LYS:H	1:A:96:PRO:CD	2.01	0.74
1:D:89:ASN:HD21	1:D:380:GLY:H	1.35	0.74
1:B:319:PHE:HB3	1:B:322:LEU:CD1	2.19	0.72
1:D:89:ASN:HD21	1:D:380:GLY:N	1.89	0.71
1:C:207:GLY:N	2:C:469:HOH:O	2.23	0.70
1:A:177:GLN:HE22	1:A:209:GLN:HE21	1.42	0.68
1:B:235:LYS:O	1:B:236:GLU:HB2	1.92	0.68
1:D:349:ARG:NH2	1:D:353:THR:O	2.27	0.68
1:D:210:ARG:HG3	1:D:239:ILE:HD11	1.74	0.68
1:D:62:MET:HE1	1:D:295:HIS:HA	1.76	0.67
1:D:319:PHE:HB3	1:D:322:LEU:HD13	1.77	0.67
1:D:6:SER:O	1:D:7:ASN:HB3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:NZ	1:A:306:ALA:HA	2.11	0.65
1:C:202:LEU:HD12	1:C:239:ILE:CG1	2.27	0.65
1:A:199:ASN:HA	1:A:242:SER:HA	1.77	0.65
1:A:95:LYS:H	1:A:96:PRO:HD2	1.61	0.64
1:C:62:MET:HB3	1:C:298:HIS:CD2	2.33	0.64
1:A:58:LYS:HZ3	1:A:306:ALA:HA	1.64	0.62
1:D:1:MET:CE	1:D:3:ILE:HD11	2.29	0.62
1:C:323:LEU:HD11	1:C:328:MET:CE	2.30	0.61
1:B:3:ILE:HG22	1:B:131:ILE:HD11	1.83	0.61
1:C:57:LEU:HD23	1:C:294:MET:HE1	1.83	0.61
1:A:265:ASN:HA	1:A:268:VAL:HG12	1.83	0.60
1:D:1:MET:HE3	1:D:3:ILE:HD11	1.82	0.60
1:C:202:LEU:HD12	1:C:239:ILE:HG12	1.83	0.60
1:A:297:VAL:CG2	1:A:314:MET:HE3	2.32	0.60
1:B:139:GLU:O	1:B:143:ARG:HG3	2.01	0.60
1:D:4:ILE:HD12	1:D:129:ASN:HD22	1.66	0.60
1:A:248:GLU:HA	1:A:251:ARG:HB3	1.85	0.59
1:C:136:GLN:NE2	1:C:140:ARG:HH21	2.01	0.59
1:B:232:THR:OG1	1:B:235:LYS:O	2.22	0.58
1:B:221:TYR:O	1:B:225:ILE:HG12	2.03	0.57
1:C:98:ASN:HD22	1:C:98:ASN:C	2.07	0.57
1:D:417:PRO:O	1:D:421:LYS:HE2	2.03	0.57
1:C:298:HIS:ND1	1:C:303:PRO:HA	2.20	0.57
1:D:290:LEU:HD12	2:D:436:HOH:O	2.05	0.56
1:A:327:LEU:HD11	1:A:423:PHE:HB2	1.88	0.56
1:D:394:ALA:HB1	1:D:415:ILE:HD11	1.88	0.56
1:A:375:GLN:N	2:A:435:HOH:O	2.38	0.56
1:D:82:LYS:HE2	1:D:361:GLU:OE1	2.06	0.56
1:D:4:ILE:N	1:D:7:ASN:HD21	1.94	0.56
1:B:17:GLN:O	1:B:21:GLU:HG2	2.07	0.55
1:C:290:LEU:HD12	1:C:294:MET:CE	2.37	0.54
1:A:53:ARG:NH1	1:A:425:MET:HE1	2.23	0.54
1:C:22:ALA:HB2	1:C:73:THR:HG23	1.88	0.54
1:C:323:LEU:HD21	1:C:328:MET:HE3	1.90	0.53
1:D:290:LEU:HD11	1:D:424:LEU:HD13	1.89	0.53
1:D:289:MET:HG3	1:D:422:LEU:HD11	1.91	0.53
1:C:251:ARG:HG3	1:C:255:GLN:NE2	2.23	0.53
1:C:319:PHE:HB3	1:C:322:LEU:CD1	2.39	0.53
1:B:89:ASN:HD21	1:B:380:GLY:N	2.00	0.52
1:D:415:ILE:HG22	1:D:419:PHE:CE2	2.43	0.52
1:A:224:GLY:H	1:A:245:ASP:HB3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:LEU:HA	2:C:447:HOH:O	2.10	0.52
1:C:416:GLU:N	1:C:417:PRO:HD2	2.24	0.52
1:B:191:LEU:HD22	1:B:200:LEU:HB2	1.92	0.52
1:C:323:LEU:HD21	1:C:328:MET:CE	2.40	0.52
1:C:93:PHE:CD1	1:C:94:PRO:HD2	2.44	0.52
1:A:219:TRP:O	1:A:222:PRO:HD3	2.10	0.52
1:C:206:THR:O	1:C:208:PHE:N	2.42	0.52
1:B:210:ARG:HG2	1:B:239:ILE:HD11	1.92	0.52
1:C:213:ILE:O	1:C:217:LEU:HG	2.09	0.51
1:C:289:MET:CE	1:C:324:ASP:HA	2.40	0.51
1:C:323:LEU:HD11	1:C:328:MET:HE2	1.92	0.51
1:C:377:HIS:HB3	2:C:431:HOH:O	2.10	0.51
1:D:31:PHE:HA	1:D:65:LEU:O	2.11	0.51
1:C:316:THR:HG23	1:C:430:ILE:HG22	1.92	0.51
1:C:5:ARG:HB3	1:C:129:ASN:ND2	2.26	0.50
1:C:136:GLN:NE2	1:C:140:ARG:NH2	2.59	0.50
1:A:27:ILE:HA	1:A:70:GLY:O	2.12	0.50
1:A:305:PRO:HD3	1:A:314:MET:CE	2.41	0.50
1:D:3:ILE:HG22	1:D:131:ILE:HD11	1.92	0.50
1:A:97:PHE:O	1:A:101:SER:HB2	2.12	0.50
1:B:226:HIS:CD2	1:B:252:ARG:HH12	2.30	0.50
1:A:262:GLU:O	1:A:266:ASP:OD1	2.30	0.50
1:A:416:GLU:N	1:A:417:PRO:HD2	2.27	0.50
1:A:7:ASN:ND2	1:A:11:ASN:ND2	2.59	0.50
1:C:275:HIS:HB3	2:C:443:HOH:O	2.12	0.50
1:D:248:GLU:HA	1:D:251:ARG:HH11	1.76	0.50
1:A:177:GLN:NE2	1:A:209:GLN:HE21	2.07	0.50
1:C:65:LEU:HD22	1:C:106:PHE:CG	2.47	0.50
1:B:84:ILE:HD11	2:B:443:HOH:O	2.11	0.49
1:C:201:ASP:OD1	1:C:240:VAL:HG22	2.12	0.49
1:D:134:LEU:HD22	1:D:138:GLU:HB3	1.93	0.49
1:B:283:LEU:HG	1:B:285:ILE:HD11	1.94	0.49
1:D:293:VAL:O	1:D:297:VAL:HG13	2.13	0.49
1:A:66:LEU:C	1:A:66:LEU:HD23	2.32	0.49
1:C:206:THR:O	1:C:206:THR:OG1	2.26	0.49
1:C:340:ASN:ND2	1:C:342:SER:OG	2.45	0.49
1:D:51:GLU:HB2	2:D:466:HOH:O	2.13	0.48
1:C:290:LEU:HD23	1:C:423:PHE:O	2.13	0.48
1:A:305:PRO:HD3	1:A:314:MET:HE1	1.95	0.48
1:A:75:LYS:HD3	2:A:480:HOH:O	2.13	0.48
1:B:283:LEU:HA	1:B:321:ARG:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:H	1:A:129:ASN:HD21	1.62	0.48
1:A:225:ILE:HB	1:A:241:ILE:HG23	1.96	0.48
1:B:7:ASN:O	1:B:11:ASN:HB2	2.13	0.48
1:C:323:LEU:HD23	1:C:323:LEU:C	2.34	0.48
1:D:58:LYS:NZ	1:D:306:ALA:HA	2.29	0.48
1:C:202:LEU:HD12	1:C:239:ILE:HG13	1.95	0.48
1:C:293:VAL:O	1:C:297:VAL:HG13	2.14	0.48
1:D:394:ALA:CB	1:D:415:ILE:HD11	2.44	0.48
1:A:275:HIS:HB3	2:A:449:HOH:O	2.14	0.47
1:A:182:ASP:O	1:A:185:VAL:HG12	2.15	0.47
1:B:80:ASP:HB2	1:B:82:LYS:HG2	1.96	0.47
1:C:415:ILE:HG22	1:C:419:PHE:CE2	2.49	0.47
1:C:323:LEU:HD11	1:C:328:MET:HE1	1.97	0.47
1:A:97:PHE:CE2	1:A:134:LEU:HD21	2.50	0.47
1:B:246:GLU:HG3	1:B:250:LYS:HE3	1.97	0.47
1:C:57:LEU:HD23	1:C:294:MET:CE	2.45	0.47
1:D:30:GLU:HG3	1:D:68:GLN:OE1	2.14	0.47
1:B:319:PHE:HB3	1:B:322:LEU:HD13	1.97	0.47
1:B:406:ILE:HG13	1:B:407:HIS:N	2.30	0.47
1:C:103:ASP:O	1:C:105:LYS:NZ	2.47	0.47
1:B:32:SER:HB3	1:B:108:CYS:HA	1.96	0.46
1:B:73:THR:O	1:B:85:THR:HA	2.15	0.46
1:C:73:THR:O	1:C:85:THR:HA	2.15	0.46
1:D:201:ASP:HB3	1:D:240:VAL:HG22	1.96	0.46
1:C:415:ILE:N	1:C:415:ILE:HD12	2.30	0.46
1:A:136:GLN:HE21	1:A:136:GLN:HA	1.80	0.46
1:A:4:ILE:O	1:A:7:ASN:HB3	2.16	0.46
1:C:180:PHE:CE1	1:C:209:GLN:HB3	2.50	0.46
1:C:232:THR:HB	1:C:236:GLU:OE1	2.16	0.46
1:B:97:PHE:CD2	1:B:142:LEU:HD11	2.51	0.45
1:D:290:LEU:HD22	1:D:294:MET:SD	2.56	0.45
1:B:415:ILE:HG22	1:B:419:PHE:CE2	2.51	0.45
1:D:24:PHE:CD1	1:D:285:ILE:HD12	2.52	0.45
1:C:206:THR:C	2:C:469:HOH:O	2.55	0.45
1:C:342:SER:O	1:C:346:LEU:HB2	2.17	0.45
1:C:4:ILE:HB	1:C:129:ASN:O	2.16	0.45
1:D:32:SER:HB2	1:D:65:LEU:H	1.82	0.45
1:A:322:LEU:C	1:A:322:LEU:HD23	2.37	0.45
1:B:270:PHE:CE2	1:B:274:ILE:HD11	2.51	0.45
1:C:206:THR:HG23	1:C:209:GLN:OE1	2.15	0.45
1:B:68:GLN:HA	1:B:90:PHE:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:LYS:HE3	1:C:348:LYS:HA	1.97	0.45
1:C:66:LEU:HD23	1:C:66:LEU:C	2.37	0.45
1:D:58:LYS:HZ3	1:D:306:ALA:HA	1.82	0.45
1:A:184:VAL:HG13	1:A:202:LEU:HD21	1.98	0.45
1:A:241:ILE:N	1:A:241:ILE:HD12	2.32	0.45
1:A:401:LEU:HD12	1:A:405:LYS:HG2	1.98	0.45
1:C:290:LEU:HD12	1:C:294:MET:HE1	1.98	0.44
1:A:415:ILE:HG22	1:A:419:PHE:CE2	2.52	0.44
1:A:4:ILE:HB	1:A:129:ASN:HD22	1.83	0.44
1:C:86:LYS:HD3	1:C:366:PHE:CZ	2.53	0.44
1:A:3:ILE:HG22	1:A:131:ILE:HD11	1.99	0.44
1:B:327:LEU:O	1:B:327:LEU:HD12	2.18	0.43
1:C:66:LEU:H	1:C:299:GLN:HE22	1.66	0.43
1:A:403:PRO:HD3	1:C:84:ILE:HG21	2.00	0.43
1:D:305:PRO:HB2	1:D:310:GLU:CD	2.38	0.43
1:D:3:ILE:HD12	1:D:3:ILE:N	2.33	0.43
1:D:4:ILE:H	1:D:7:ASN:ND2	1.96	0.43
1:D:1:MET:HE2	1:D:3:ILE:HD11	2.00	0.43
1:D:390:PHE:CZ	1:D:415:ILE:HD13	2.53	0.43
1:A:250:LYS:HA	1:A:253:GLU:HB3	2.00	0.43
1:B:235:LYS:O	1:B:236:GLU:CB	2.63	0.43
1:D:195:GLU:O	1:D:196:GLU:HB3	2.18	0.43
1:C:234:LYS:HB3	1:C:236:GLU:OE1	2.18	0.43
1:C:61:SER:HB3	2:C:464:HOH:O	2.19	0.43
1:A:175:GLU:HA	1:A:175:GLU:OE2	2.19	0.43
1:B:416:GLU:N	1:B:417:PRO:HD2	2.34	0.43
1:C:298:HIS:HA	1:C:302:CYS:O	2.19	0.43
1:A:70:GLY:HA3	1:A:379:ALA:HB1	2.00	0.43
1:C:120:GLY:O	1:C:121:PHE:C	2.58	0.43
1:D:19:ILE:HG23	1:D:25:PHE:CZ	2.54	0.43
1:B:173:ILE:CD1	1:B:181:ILE:HG21	2.49	0.43
1:D:289:MET:CG	1:D:422:LEU:HD11	2.49	0.43
1:B:49:THR:HB	1:B:50:PRO:HD2	2.00	0.42
1:C:47:PHE:N	2:C:432:HOH:O	2.50	0.42
1:D:62:MET:HG3	1:D:304:LEU:HD12	2.01	0.42
1:D:83:TYR:HB2	1:D:360:VAL:HG23	2.02	0.42
1:B:210:ARG:CG	1:B:239:ILE:HD11	2.50	0.42
1:C:170:PRO:HA	1:C:219:TRP:CE2	2.54	0.42
1:C:65:LEU:HD21	1:C:94:PRO:CD	2.48	0.42
1:C:232:THR:HG22	1:C:233:GLU:N	2.35	0.42
1:A:124:ASN:O	1:A:128:ARG:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:GLN:HA	1:C:332:GLN:OE1	2.19	0.42
1:C:89:ASN:OD1	1:C:378:GLU:OE1	2.38	0.42
1:A:268:VAL:HG13	1:A:272:ARG:HD2	2.02	0.42
1:B:135:ASN:HB2	1:B:301:TYR:O	2.20	0.42
1:C:227:VAL:HG13	1:C:239:ILE:HD13	2.01	0.42
1:A:173:ILE:CD1	1:A:181:ILE:HG21	2.50	0.42
1:A:84:ILE:HA	1:A:361:GLU:O	2.20	0.42
1:C:234:LYS:HB3	1:C:236:GLU:CD	2.39	0.42
1:B:188:ILE:HD13	1:B:200:LEU:CD2	2.50	0.42
1:B:290:LEU:HD22	1:B:294:MET:HE3	2.02	0.42
1:B:416:GLU:HA	1:B:419:PHE:CD1	2.55	0.42
1:C:7:ASN:OD1	1:C:11:ASN:ND2	2.53	0.42
1:A:297:VAL:HG21	1:A:314:MET:HE3	2.02	0.41
1:D:62:MET:HA	1:D:62:MET:HE3	2.01	0.41
1:A:63:ASP:HB2	2:A:452:HOH:O	2.19	0.41
1:D:393:MET:O	1:D:396:TYR:HB3	2.20	0.41
1:D:74:PHE:CD2	1:D:391:ILE:HD11	2.55	0.41
1:B:206:THR:HG23	1:B:209:GLN:OE1	2.20	0.41
1:B:347:GLU:HG2	1:B:385:ILE:HG23	2.02	0.41
1:A:7:ASN:HD21	1:A:11:ASN:ND2	2.17	0.41
1:B:290:LEU:HD12	1:B:424:LEU:HB2	2.03	0.41
1:C:122:ASP:HB3	1:C:125:LYS:HD2	2.03	0.41
1:D:30:GLU:HB2	1:D:68:GLN:HB3	2.02	0.41
1:D:416:GLU:N	1:D:417:PRO:HD2	2.35	0.41
1:A:228:GLU:O	1:A:228:GLU:HG3	2.20	0.41
1:D:99:ARG:NE	1:D:99:ARG:HA	2.36	0.41
1:A:53:ARG:HG3	1:A:57:LEU:HD22	2.03	0.41
1:A:258:ALA:O	1:A:262:GLU:HB2	2.21	0.41
1:C:232:THR:HG22	1:C:233:GLU:H	1.86	0.41
1:C:424:LEU:O	1:C:425:MET:HB2	2.20	0.41
1:A:173:ILE:HD11	1:A:216:THR:OG1	2.22	0.40
1:C:217:LEU:HD12	1:C:227:VAL:HG21	2.03	0.40
1:D:315:THR:HG21	1:D:430:ILE:HD13	2.04	0.40
1:D:426:ARG:HH11	1:D:426:ARG:HG2	1.85	0.40
1:A:62:MET:CE	1:A:295:HIS:HA	2.38	0.40
1:B:80:ASP:CG	1:B:82:LYS:HE3	2.41	0.40
1:C:223:LYS:HD3	1:C:246:GLU:OE1	2.21	0.40
1:B:7:ASN:HD22	1:B:7:ASN:HA	1.72	0.40
1:A:289:MET:O	1:A:290:LEU:C	2.59	0.40
1:C:349:ARG:NH2	1:C:353:THR:O	2.55	0.40
1:D:402:SER:HA	1:D:403:PRO:HA	1.95	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	383/430 (89%)	355 (93%)	20 (5%)	8 (2%)	8	15
1	B	382/430 (89%)	351 (92%)	22 (6%)	9 (2%)	7	12
1	C	385/430 (90%)	362 (94%)	19 (5%)	4 (1%)	18	37
1	D	384/430 (89%)	358 (93%)	21 (6%)	5 (1%)	14	29
All	All	1534/1720 (89%)	1426 (93%)	82 (5%)	26 (2%)	11	21

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	95	LYS
1	A	98	ASN
1	B	225	ILE
1	B	236	GLU
1	B	420	ASN
1	C	80	ASP
1	D	7	ASN
1	A	247	GLU
1	A	280	SER
1	B	193	GLN
1	C	195	GLU
1	C	207	GLY
1	A	97	PHE
1	A	242	SER
1	B	11	ASN
1	D	236	GLU
1	A	246	GLU
1	B	37	GLY
1	D	235	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	314	MET
1	B	24	PHE
1	B	226	HIS
1	D	37	GLY
1	C	318	VAL
1	B	38	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	360/391 (92%)	335 (93%)	25 (7%)	18	36
1	B	359/391 (92%)	326 (91%)	33 (9%)	11	20
1	C	363/391 (93%)	330 (91%)	33 (9%)	11	21
1	D	360/391 (92%)	332 (92%)	28 (8%)	15	29
All	All	1442/1564 (92%)	1323 (92%)	119 (8%)	13	25

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	59	LYS
1	A	67	PHE
1	A	81	SER
1	A	98	ASN
1	A	128	ARG
1	A	136	GLN
1	A	143	ARG
1	A	181	ILE
1	A	185	VAL
1	A	196	GLU
1	A	200	LEU
1	A	201	ASP
1	A	206	THR
1	A	210	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	228	GLU
1	A	242	SER
1	A	246	GLU
1	A	297	VAL
1	A	320	PRO
1	A	322	LEU
1	A	345	GLU
1	A	347	GLU
1	A	349	ARG
1	A	424	LEU
1	B	7	ASN
1	B	11	ASN
1	B	25	PHE
1	B	47	PHE
1	B	55	GLN
1	B	57	LEU
1	B	67	PHE
1	B	73	THR
1	B	89	ASN
1	B	129	ASN
1	B	136	GLN
1	B	181	ILE
1	B	193	GLN
1	B	211	LYS
1	B	215	GLN
1	B	225	ILE
1	B	236	GLU
1	B	249	ARG
1	B	268	VAL
1	B	290	LEU
1	B	297	VAL
1	B	321	ARG
1	B	322	LEU
1	B	325	THR
1	B	342	SER
1	B	352	GLU
1	B	353	THR
1	B	359	LYS
1	B	362	SER
1	B	376	LEU
1	B	378	GLU
1	B	406	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	409	SER
1	C	13	HIS
1	C	21	GLU
1	C	57	LEU
1	C	58	LYS
1	C	65	LEU
1	C	67	PHE
1	C	98	ASN
1	C	112	SER
1	C	114	ASP
1	C	129	ASN
1	C	136	GLN
1	C	178	LYS
1	C	199	ASN
1	C	203	GLU
1	C	211	LYS
1	C	230	LEU
1	C	239	ILE
1	C	242	SER
1	C	250	LYS
1	C	264	LEU
1	C	290	LEU
1	C	291	LEU
1	C	297	VAL
1	C	322	LEU
1	C	335	LYS
1	C	342	SER
1	C	348	LYS
1	C	349	ARG
1	C	376	LEU
1	C	378	GLU
1	C	409	SER
1	C	428	MET
1	C	429	ASP
1	D	7	ASN
1	D	13	HIS
1	D	25	PHE
1	D	57	LEU
1	D	67	PHE
1	D	80	ASP
1	D	82	LYS
1	D	99	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	136	GLN
1	D	171	VAL
1	D	179	LYS
1	D	201	ASP
1	D	223	LYS
1	D	234	LYS
1	D	248	GLU
1	D	251	ARG
1	D	290	LEU
1	D	297	VAL
1	D	322	LEU
1	D	339	ASN
1	D	342	SER
1	D	347	GLU
1	D	364	GLU
1	D	368	SER
1	D	378	GLU
1	D	413	LYS
1	D	424	LEU
1	D	430	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	11	ASN
1	A	17	GLN
1	A	55	GLN
1	A	98	ASN
1	A	129	ASN
1	A	136	GLN
1	A	177	GLN
1	A	183	GLN
1	A	299	GLN
1	B	7	ASN
1	B	89	ASN
1	B	129	ASN
1	B	136	GLN
1	B	193	GLN
1	B	265	ASN
1	B	279	ASN
1	B	299	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	89	ASN
1	C	98	ASN
1	C	129	ASN
1	C	136	GLN
1	C	199	ASN
1	C	215	GLN
1	C	255	GLN
1	C	299	GLN
1	C	340	ASN
1	D	7	ASN
1	D	89	ASN
1	D	98	ASN
1	D	129	ASN
1	D	136	GLN
1	D	183	GLN
1	D	193	GLN
1	D	275	HIS
1	D	299	GLN
1	D	420	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, 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	391/430 (90%)	0.15	13 (3%) 47 39	35, 54, 101, 117	0
1	B	390/430 (90%)	0.07	3 (0%) 86 83	31, 53, 88, 103	0
1	C	393/430 (91%)	-0.05	1 (0%) 93 93	31, 49, 78, 92	0
1	D	392/430 (91%)	0.02	8 (2%) 65 59	28, 50, 81, 98	0
All	All	1566/1720 (91%)	0.05	25 (1%) 72 67	28, 51, 90, 117	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLN	4.8
1	D	197	ASN	4.6
1	A	97	PHE	4.5
1	D	235	LYS	4.3
1	B	238	TYR	3.6
1	A	191	LEU	3.3
1	D	171	VAL	3.1
1	A	256	LYS	3.1
1	A	188	ILE	3.1
1	A	192	LEU	3.1
1	B	241	ILE	2.9
1	D	247	GLU	2.7
1	D	236	GLU	2.7
1	B	242	SER	2.6
1	A	199	ASN	2.6
1	A	197	ASN	2.5
1	A	252	ARG	2.4
1	D	237	ARG	2.4
1	C	145	GLN	2.3
1	D	196	GLU	2.3
1	A	200	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	PRO	2.0
1	A	244	VAL	2.0
1	D	13	HIS	2.0
1	A	227	VAL	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.