



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2021 – 12:08 PM JST

PDB ID : 7F5N
Title : Crystal structure of TCPTP catalytic domain
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Deposited on : 2021-06-22
Resolution : 1.93 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.25
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) : 2.25

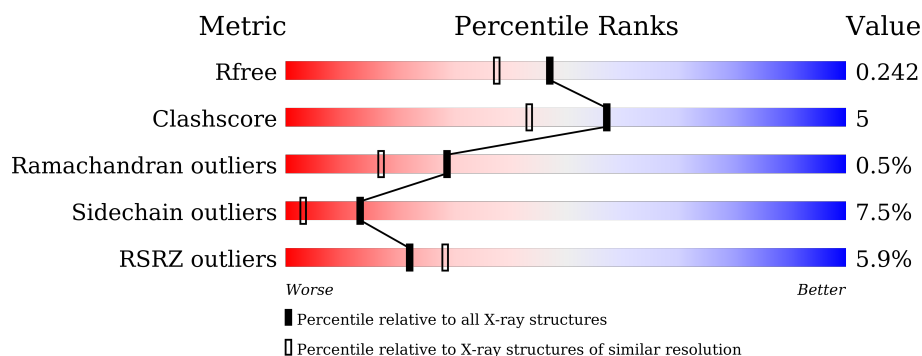
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	317	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	317	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	317	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7601 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 Tyrosine-protein phosphatase non-receptor type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2427	1534	424	455	14			
1	B	287	Total	C	N	O	S	0	0	0
			2367	1499	414	442	12			
1	C	291	Total	C	N	O	S	0	0	0
			2397	1521	419	444	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P17706
A	-1	ASN	-	expression tag	UNP P17706
A	0	ALA	-	expression tag	UNP P17706
B	-2	SER	-	expression tag	UNP P17706
B	-1	ASN	-	expression tag	UNP P17706
B	0	ALA	-	expression tag	UNP P17706
C	-2	SER	-	expression tag	UNP P17706
C	-1	ASN	-	expression tag	UNP P17706
C	0	ALA	-	expression tag	UNP P17706

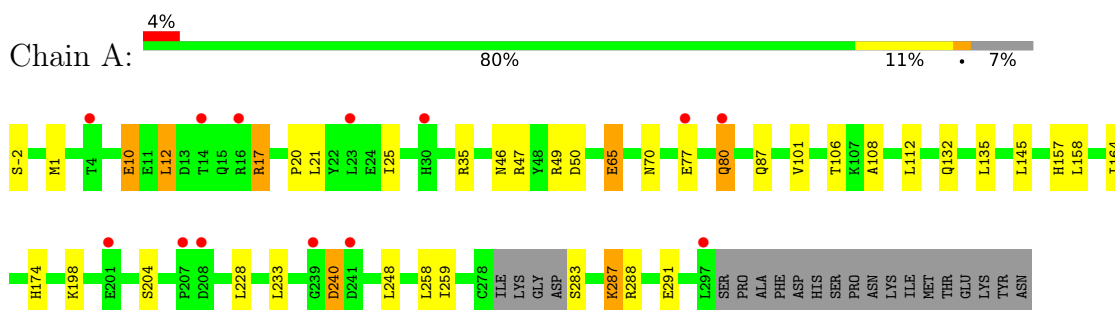
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		
2	B	90	Total	O	0	0
			90	90		
2	C	162	Total	O	0	0
			162	162		

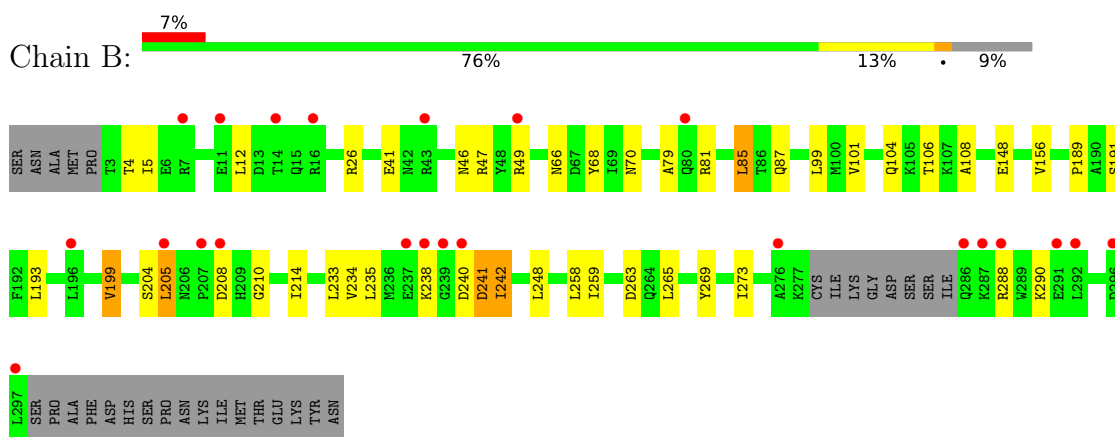
3 Residue-property plots [i](#)

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.

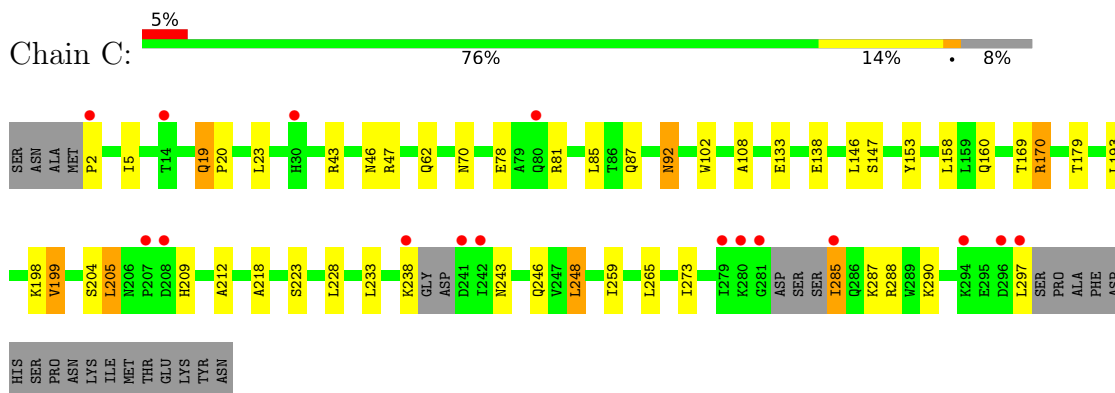
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 2



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 2



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.57Å 68.06Å 73.24Å 112.93° 106.46° 92.46°	Depositor
Resolution (Å)	19.95 – 1.93 19.94 – 1.93	Depositor EDS
% Data completeness (in resolution range)	91.2 (19.95-1.93) 91.3 (19.94-1.93)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.23 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.238 0.192 , 0.242	Depositor DCC
R_{free} test set	3120 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7601	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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 [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	0.73	0/2484	0.89	1/3361 (0.0%)
1	B	0.69	0/2423	0.84	0/3278
1	C	0.76	0/2453	0.89	1/3316 (0.0%)
All	All	0.73	0/7360	0.87	2/9955 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	C	170	ARG	NE-CZ-NH1	-5.24	117.68	120.30

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	2427	0	2376	21	0
1	B	2367	0	2315	18	0
1	C	2397	0	2358	31	0
2	A	158	0	0	5	1
2	B	90	0	0	1	1
2	C	162	0	0	6	0
All	All	7601	0	7049	69	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (69) 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:2:PRO:HD3	2:C:524:HOH:O	1.61	0.99
1:B:235:LEU:HB3	1:B:242:ILE:HD11	1.59	0.84
1:B:148:GLU:OE1	2:B:401:HOH:O	1.99	0.80
1:C:46:ASN:HD22	1:C:70:ASN:HD22	1.30	0.79
1:A:47:ARG:H	1:A:87:GLN:HE22	1.35	0.74
1:C:62:GLN:HG2	2:C:538:HOH:O	1.89	0.73
1:A:80:GLN:HE21	1:A:80:GLN:HA	1.59	0.68
1:A:240:ASP:O	2:A:401:HOH:O	2.11	0.67
1:B:47:ARG:H	1:B:87:GLN:HE22	1.40	0.67
1:C:47:ARG:H	1:C:87:GLN:HE22	1.45	0.65
1:C:46:ASN:ND2	1:C:70:ASN:HD22	1.94	0.64
1:C:92:ASN:H	1:C:92:ASN:HD22	1.46	0.63
1:C:147:SER:HB3	1:C:158:LEU:HB2	1.80	0.63
1:B:85:LEU:HD22	1:B:214:ILE:HB	1.81	0.62
1:C:2:PRO:CD	2:C:524:HOH:O	2.30	0.62
1:A:47:ARG:H	1:A:87:GLN:NE2	1.99	0.60
1:B:47:ARG:H	1:B:87:GLN:NE2	2.01	0.59
1:C:5:ILE:HG22	1:C:273:ILE:HD11	1.83	0.59
1:A:157:HIS:HE1	2:A:507:HOH:O	1.86	0.58
1:B:269:TYR:O	1:B:273:ILE:HG12	2.04	0.57
1:A:108:ALA:CB	1:A:204:SER:HB3	2.36	0.55
1:C:47:ARG:H	1:C:87:GLN:NE2	2.06	0.54
1:A:108:ALA:HB2	1:A:204:SER:HB3	1.89	0.54
1:C:243:ASN:ND2	1:C:246:GLN:HG2	2.24	0.53
1:C:108:ALA:HB2	1:C:204:SER:HB3	1.90	0.52
1:B:189:PRO:O	1:B:193:LEU:HD23	2.10	0.51
1:C:199:VAL:HG23	1:C:205:LEU:HD22	1.92	0.51
1:A:46:ASN:HD22	1:A:70:ASN:HD22	1.59	0.50
1:A:25:ILE:HD13	1:A:248:LEU:HD23	1.95	0.49
1:C:102:TRP:CZ3	1:C:170:ARG:HG3	2.48	0.49
1:A:108:ALA:HB2	1:A:204:SER:CB	2.43	0.48
1:C:138:GLU:OE2	2:C:401:HOH:O	2.20	0.48
1:C:108:ALA:HB2	1:C:204:SER:CB	2.42	0.48
1:C:285:ILE:HG22	1:C:288:ARG:H	1.78	0.48
1:B:46:ASN:HD22	1:B:70:ASN:HD22	1.61	0.47
1:C:153:TYR:HB2	1:C:179:THR:OG1	2.15	0.47
1:A:157:HIS:HD2	1:A:174:HIS:ND1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LEU:HD11	1:C:160:GLN:HB2	1.97	0.46
1:C:108:ALA:CB	1:C:204:SER:HB3	2.45	0.45
1:C:209:HIS:HD2	2:C:437:HOH:O	2.00	0.45
1:B:41:GLU:HG3	1:B:66:ASN:ND2	2.33	0.44
1:B:241:ASP:O	1:B:242:ILE:HD12	2.18	0.44
1:C:205:LEU:HD12	1:C:212:ALA:HB2	1.98	0.44
1:C:85:LEU:HD13	1:C:223:SER:HB3	1.99	0.44
1:A:132:GLN:CG	2:A:528:HOH:O	2.65	0.44
1:B:5:ILE:HG22	1:B:273:ILE:HD11	2.00	0.43
1:C:78:GLU:HG2	2:C:458:HOH:O	2.16	0.43
1:A:10:GLU:HG2	2:A:537:HOH:O	2.19	0.43
1:C:108:ALA:HB2	1:C:204:SER:OG	2.19	0.43
1:A:12:LEU:HD21	1:A:21:LEU:HD22	2.01	0.43
1:B:79:ALA:O	1:B:234:VAL:HG11	2.19	0.43
1:C:19:GLN:CB	1:C:20:PRO:HD3	2.49	0.42
1:C:169:THR:O	1:C:170:ARG:HG2	2.19	0.42
1:B:108:ALA:CB	1:B:204:SER:HB3	2.49	0.42
1:A:65:GLU:HG2	1:C:218:ALA:HB2	2.02	0.42
1:A:132:GLN:HG2	2:A:528:HOH:O	2.18	0.42
1:A:49:ARG:HG3	1:A:50:ASP:OD2	2.20	0.42
1:A:80:GLN:HA	1:A:80:GLN:NE2	2.31	0.42
1:A:287:LYS:O	1:A:291:GLU:HG2	2.20	0.41
1:B:4:THR:CG2	1:B:241:ASP:OD1	2.68	0.41
1:C:285:ILE:HG23	1:C:287:LYS:H	1.86	0.41
1:B:101:VAL:HG13	1:B:106:THR:HB	2.03	0.41
1:B:104:GLN:O	1:B:210:GLY:HA3	2.21	0.41
1:C:248:LEU:HD23	1:C:248:LEU:HA	1.91	0.41
1:C:102:TRP:O	1:C:170:ARG:NH1	2.54	0.41
1:A:17:ARG:C	1:A:20:PRO:HD2	2.41	0.40
1:A:101:VAL:HG13	1:A:106:THR:HB	2.02	0.40
1:B:46:ASN:ND2	1:B:68:TYR:OH	2.49	0.40
1:B:199:VAL:HG22	1:B:205:LEU:HD22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:509:HOH:O	2:B:479:HOH:O[1_445]	2.09	0.11

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	292/317 (92%)	280 (96%)	11 (4%)	1 (0%)	41	32
1	B	283/317 (89%)	267 (94%)	14 (5%)	2 (1%)	22	11
1	C	285/317 (90%)	273 (96%)	11 (4%)	1 (0%)	34	24
All	All	860/951 (90%)	820 (95%)	36 (4%)	4 (0%)	29	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ILE
1	B	259	ILE
1	C	259	ILE
1	B	238	LYS

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	272/291 (94%)	251 (92%)	21 (8%)	13	3
1	B	264/291 (91%)	243 (92%)	21 (8%)	12	3
1	C	268/291 (92%)	250 (93%)	18 (7%)	16	4
All	All	804/873 (92%)	744 (92%)	60 (8%)	13	3

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	1	MET
1	A	10	GLU
1	A	12	LEU
1	A	17	ARG
1	A	35	ARG
1	A	65	GLU
1	A	77	GLU
1	A	80	GLN
1	A	112	LEU
1	A	135	LEU
1	A	145	LEU
1	A	158	LEU
1	A	164	ILE
1	A	198	LYS
1	A	228	LEU
1	A	233	LEU
1	A	240	ASP
1	A	258	LEU
1	A	283	SER
1	A	287	LYS
1	B	12	LEU
1	B	26	ARG
1	B	49	ARG
1	B	81	ARG
1	B	85	LEU
1	B	99	LEU
1	B	156	VAL
1	B	191	SER
1	B	199	VAL
1	B	205	LEU
1	B	208	ASP
1	B	233	LEU
1	B	240	ASP
1	B	241	ASP
1	B	242	ILE
1	B	248	LEU
1	B	258	LEU
1	B	263	ASP
1	B	265	LEU
1	B	288	ARG
1	B	290	LYS
1	C	19	GLN

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Mol	Chain	Res	Type
1	C	23	LEU
1	C	43	ARG
1	C	81	ARG
1	C	92	ASN
1	C	133	GLU
1	C	193	LEU
1	C	198	LYS
1	C	199	VAL
1	C	205	LEU
1	C	228	LEU
1	C	233	LEU
1	C	238	LYS
1	C	248	LEU
1	C	265	LEU
1	C	285	ILE
1	C	290	LYS
1	C	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	46	ASN
1	A	80	GLN
1	A	87	GLN
1	A	113	ASN
1	A	125	GLN
1	A	157	HIS
1	A	165	ASN
1	A	209	HIS
1	B	46	ASN
1	B	80	GLN
1	B	87	GLN
1	B	125	GLN
1	B	132	GLN
1	B	165	ASN
1	B	246	GLN
1	C	46	ASN
1	C	80	GLN
1	C	87	GLN
1	C	92	ASN
1	C	113	ASN

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Mol	Chain	Res	Type
1	C	132	GLN
1	C	206	ASN
1	C	209	HIS
1	C	286	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 monosaccharides 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	296/317 (93%)	0.03	13 (4%) 34 41	8, 20, 46, 63	0
1	B	287/317 (90%)	0.33	23 (8%) 12 17	13, 27, 63, 80	0
1	C	291/317 (91%)	0.07	16 (5%) 25 31	7, 20, 54, 85	0
All	All	874/951 (91%)	0.14	52 (5%) 22 28	7, 23, 57, 85	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	LEU	7.7
1	C	297	LEU	7.6
1	C	280	LYS	5.3
1	C	279	ILE	4.7
1	A	297	LEU	4.7
1	A	241	ASP	4.3
1	C	296	ASP	4.0
1	C	281	GLY	4.0
1	A	208	ASP	4.0
1	B	296	ASP	3.6
1	C	2	PRO	3.5
1	C	207	PRO	3.5
1	B	7	ARG	3.5
1	B	16	ARG	3.5
1	A	207	PRO	3.4
1	B	14	THR	3.4
1	B	240	ASP	3.4
1	B	291	GLU	3.3
1	B	292	LEU	3.3
1	C	241	ASP	3.3
1	A	30	HIS	3.2
1	B	287	LYS	3.2
1	C	238	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	201	GLU	3.1
1	B	80	GLN	3.0
1	B	286	GLN	3.0
1	B	207	PRO	2.7
1	B	276	ALA	2.6
1	B	238	LYS	2.6
1	C	14	THR	2.5
1	B	288	ARG	2.5
1	B	11	GLU	2.5
1	A	14	THR	2.4
1	C	294	LYS	2.3
1	B	239	GLY	2.3
1	B	49	ARG	2.3
1	C	285	ILE	2.3
1	C	30	HIS	2.2
1	C	208	ASP	2.2
1	C	242	ILE	2.2
1	B	43	ARG	2.2
1	B	237	GLU	2.2
1	A	239	GLY	2.2
1	B	196	LEU	2.2
1	A	4	THR	2.2
1	B	205	LEU	2.1
1	C	80	GLN	2.1
1	A	16	ARG	2.1
1	A	23	LEU	2.1
1	B	208	ASP	2.1
1	A	80	GLN	2.0
1	A	77	GLU	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 monosaccharides 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.