Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:36 am BST

PDB ID	:	3QDN
Title	:	Putative thioredoxin protein from Salmonella typhimurium
Authors	:	Osipiuk, J.; Zhou, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2011-01-18
Resolution	:	2.09 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:

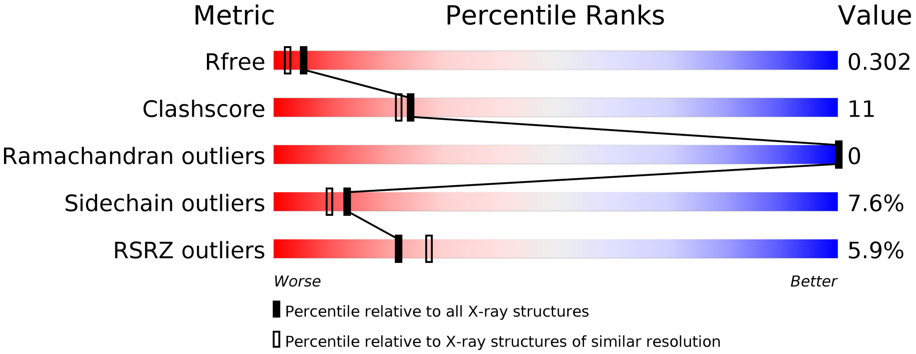
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	287	
1	B	287	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4710 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 Putative thioredoxin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total 2338	C 1479	N 397	O 453	S 2	Se 7	0	17	0
1	B	280	Total 2276	C 1437	N 391	O 442	S 2	Se 4	0	12	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8ZR92
A	-1	ASN	-	EXPRESSION TAG	UNP Q8ZR92
A	0	ALA	-	EXPRESSION TAG	UNP Q8ZR92
B	-2	SER	-	EXPRESSION TAG	UNP Q8ZR92
B	-1	ASN	-	EXPRESSION TAG	UNP Q8ZR92
B	0	ALA	-	EXPRESSION TAG	UNP Q8ZR92

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Ca 2	0	0

- Molecule 3 is water.

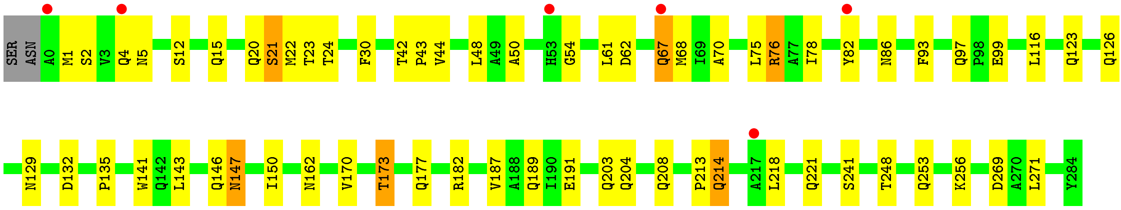
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total 54	O 54	0	0
3	B	40	Total 40	O 40	0	0

3 Residue-property plots ⓘ

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.

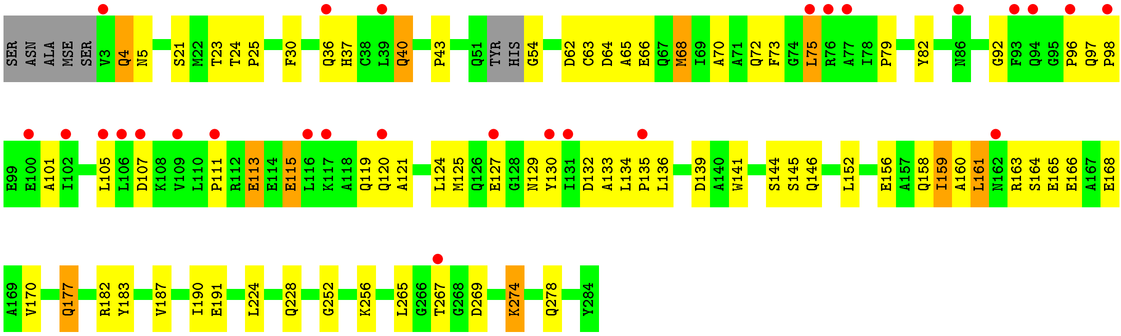
- Molecule 1: Putative thioredoxin protein

Chain A:



- Molecule 1: Putative thioredoxin protein

Chain B:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.23Å 62.55Å 79.52Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	35.70 – 2.09 35.68 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.70-2.09) 96.4 (35.68-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.302 0.246 , 0.302	Depositor DCC
R_{free} test set	1629 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4710	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5359e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.76	0/2418	0.78	0/3267
1	B	0.70	0/2338	0.76	0/3156
All	All	0.73	0/4756	0.77	0/6423

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	2338	0	2373	45	1
1	B	2276	0	2309	62	1
2	A	2	0	0	0	0
3	A	54	0	0	3	0
3	B	40	0	0	3	0
All	All	4710	0	4682	102	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 11.

All (102) 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:B:158:GLN:HE21	1:B:166:GLU:HB3	1.29	0.97
1:B:158:GLN:NE2	1:B:166:GLU:HB3	1.83	0.93
1:B:130:TYR:HB2	1:B:161:LEU:HD11	1.49	0.92
1:B:252:GLY:O	1:B:256[B]:LYS:HG3	1.76	0.85
1:A:170:VAL:O	1:A:173:THR:HB	1.79	0.83
1:A:126:GLN:HE21	1:A:126:GLN:HA	1.43	0.82
1:A:20:GLN:HG2	3:A:304:HOH:O	1.80	0.81
1:B:113:GLU:HB2	3:B:309:HOH:O	1.80	0.80
1:B:274[A]:LYS:HE2	1:B:278:GLN:OE1	1.83	0.77
1:A:126:GLN:NE2	1:A:126:GLN:HA	1.99	0.77
1:B:265:LEU:O	1:B:269:ASP:HB2	1.85	0.76
1:B:63:CYS:O	1:B:65:ALA:HA	1.87	0.74
1:A:67[A]:GLN:H	1:A:67[A]:GLN:HE21	1.33	0.74
1:B:119:GLN:HA	1:B:119:GLN:OE1	1.85	0.74
1:B:97:GLN:HG2	1:B:98:PRO:HD2	1.71	0.72
1:B:165:GLU:HB2	3:B:311:HOH:O	1.90	0.71
1:A:187:VAL:O	1:A:191[B]:GLU:HG2	1.90	0.71
1:A:141:TRP:HZ2	1:A:173:THR:HG21	1.58	0.68
1:B:120:GLN:HB3	1:B:136:LEU:HD21	1.74	0.67
1:B:5:ASN:OD1	1:B:54:GLY:HA2	1.94	0.66
1:B:130:TYR:CB	1:B:161:LEU:HD11	2.27	0.63
1:A:1:MSE:SE	1:B:73:PHE:HD1	2.32	0.62
1:A:218:LEU:HA	1:A:221:GLN:HE21	1.64	0.62
1:B:4:GLN:HA	1:B:4:GLN:HE21	1.64	0.62
1:B:265:LEU:O	1:B:269:ASP:CB	2.49	0.61
1:A:147:ASN:OD1	1:A:150:ILE:HG12	2.00	0.60
1:A:93:PHE:CD1	1:A:97:GLN:HG3	2.36	0.60
1:B:121:ALA:O	1:B:125:MSE:HG3	2.00	0.60
1:B:21:SER:HA	1:B:24:THR:O	2.02	0.60
1:A:269:ASP:OD1	1:A:271:LEU:HB3	2.01	0.59
1:A:132:ASP:O	1:A:135:PRO:HD2	2.04	0.58
1:B:152:LEU:HD13	1:B:182[A]:ARG:HD3	1.85	0.57
1:A:44:VAL:O	1:A:48:LEU:HG	2.05	0.56
3:A:311:HOH:O	1:B:72:GLN:HA	2.06	0.56
1:B:115:GLU:O	1:B:119:GLN:HG2	2.06	0.56
1:B:161:LEU:CD1	1:B:161:LEU:N	2.68	0.56
1:A:22[B]:MSE:SE	1:A:86:ASN:HA	2.56	0.56
1:A:93:PHE:CE1	1:A:97:GLN:HG3	2.41	0.56
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.88	0.55
1:B:111:PRO:CB	1:B:115:GLU:HG2	2.37	0.54
1:B:97:GLN:CD	1:B:101:ALA:CB	2.75	0.54
1:A:67[A]:GLN:H	1:A:67[A]:GLN:NE2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PRO:HB3	1:B:115:GLU:HG2	1.89	0.53
1:B:37:HIS:CE1	1:B:96:PRO:HG3	2.44	0.53
1:B:63:CYS:C	1:B:65:ALA:HA	2.28	0.53
1:A:30:PHE:HD1	1:A:61:LEU:HD23	1.75	0.52
1:B:166:GLU:O	1:B:170:VAL:HG23	2.10	0.52
1:B:92:GLY:HA2	1:B:105:LEU:HD21	1.92	0.51
1:B:224:LEU:O	1:B:228:GLN:HG2	2.11	0.51
1:B:164:SER:HB2	1:B:190:ILE:HG23	1.93	0.50
1:A:123:GLN:O	1:A:126:GLN:HB2	2.12	0.50
1:A:15[B]:GLN:H	1:A:15[B]:GLN:CD	2.15	0.50
1:A:76:ARG:HG2	3:A:308:HOH:O	2.12	0.49
1:A:4:GLN:HG3	1:A:50:ALA:HA	1.94	0.48
1:A:213:PRO:O	1:A:214:GLN:HG2	2.13	0.47
1:B:129:ASN:ND2	1:B:132:ASP:OD2	2.43	0.47
1:B:30:PHE:O	1:B:79:PRO:HA	2.14	0.47
1:B:37:HIS:ND1	1:B:96:PRO:HG3	2.29	0.47
1:A:1:MSE:HB2	1:B:73:PHE:O	2.15	0.46
1:A:70:ALA:HB1	1:A:75:LEU:HD22	1.98	0.46
1:B:187:VAL:O	1:B:191[A]:GLU:HG2	2.15	0.46
1:B:70:ALA:O	1:B:75:LEU:HD11	2.15	0.46
1:A:147:ASN:OD1	1:A:150:ILE:CG1	2.64	0.46
1:A:208:GLN:O	1:A:218:LEU:HD23	2.15	0.46
1:B:119:GLN:OE1	1:B:119:GLN:CA	2.56	0.46
1:B:68:MSE:HA	1:B:68:MSE:HE3	1.97	0.45
1:B:4:GLN:CA	1:B:4:GLN:HE21	2.30	0.45
1:B:75:LEU:HD12	1:B:75:LEU:H	1.80	0.45
1:A:141:TRP:CD1	1:A:146[A]:GLN:HA	2.52	0.45
1:A:253:GLN:HE22	1:A:256:LYS:HD3	1.82	0.44
1:B:177:GLN:H	1:B:177:GLN:HG3	1.19	0.44
1:A:1:MSE:SE	1:B:73:PHE:HB3	2.68	0.44
1:B:121:ALA:HB1	1:B:133:ALA:HB1	2.00	0.44
1:A:182:ARG:HD2	1:A:182:ARG:HA	1.65	0.44
1:B:159:ILE:HG22	1:B:160:ALA:N	2.32	0.43
1:B:121:ALA:HB2	1:B:136:LEU:HD23	2.00	0.43
1:B:183:TYR:C	1:B:183:TYR:CD1	2.92	0.43
1:B:62:ASP:OD1	1:B:64:ASP:C	2.57	0.43
1:A:2:SER:HB2	1:A:5:ASN:HA	2.01	0.43
1:A:129:ASN:ND2	1:A:132:ASP:OD2	2.46	0.43
1:A:30:PHE:CD1	1:A:61:LEU:HD23	2.52	0.43
1:A:21:SER:HA	1:A:24:THR:O	2.19	0.43
1:A:62:ASP:OD1	1:A:62:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:NE2	1:A:256:LYS:HD3	2.34	0.42
1:A:218:LEU:HA	1:A:221:GLN:NE2	2.34	0.42
1:A:42:THR:HB	1:A:43:PRO:HD3	2.02	0.42
1:A:1:MSE:SE	1:B:73:PHE:O	2.87	0.42
1:B:125:MSE:HE1	1:B:156:GLU:HB3	2.00	0.42
1:B:163:ARG:HB3	1:B:166:GLU:HB2	2.00	0.42
1:A:5:ASN:ND2	1:A:54:GLY:N	2.67	0.42
1:A:48:LEU:HD21	1:A:99:GLU:HG3	2.01	0.42
1:B:121:ALA:HA	1:B:124:LEU:HD12	2.01	0.42
1:A:1:MSE:SE	1:B:73:PHE:CD1	3.19	0.42
1:B:40:GLN:O	1:B:43:PRO:HD2	2.20	0.42
1:B:62:ASP:O	1:B:66:GLU:N	2.52	0.42
1:A:75:LEU:HD23	1:A:78:ILE:HD11	2.02	0.41
1:B:144:SER:O	1:B:145[B]:SER:HB3	2.20	0.41
1:B:141:TRP:CD1	1:B:146:GLN:HA	2.55	0.41
1:B:182[A]:ARG:NH1	3:B:286:HOH:O	2.54	0.41
1:B:161:LEU:N	1:B:161:LEU:HD13	2.36	0.41
1:A:141:TRP:CD1	1:A:146[B]:GLN:HA	2.56	0.41

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)
1:A:177:GLN:NE2	1:B:160:ALA:O[1_455]	2.08	0.12

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	300/287 (104%)	289 (96%)	11 (4%)	0	100	100
1	B	288/287 (100%)	271 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	588/574 (102%)	560 (95%)	28 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	255/235 (108%)	234 (92%)	21 (8%)	11	8
1	B	246/235 (105%)	227 (92%)	19 (8%)	13	9
All	All	501/470 (107%)	461 (92%)	40 (8%)	13	8

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	21	SER
1	A	23	THR
1	A	67[A]	GLN
1	A	67[B]	GLN
1	A	68[A]	MSE
1	A	68[B]	MSE
1	A	76	ARG
1	A	82	TYR
1	A	116	LEU
1	A	143	LEU
1	A	147	ASN
1	A	162	ASN
1	A	173	THR
1	A	189	GLN
1	A	203	GLN
1	A	204[A]	GLN
1	A	204[B]	GLN
1	A	214	GLN
1	A	241	SER

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Mol	Chain	Res	Type
1	A	248	THR
1	B	4	GLN
1	B	23	THR
1	B	36	GLN
1	B	40	GLN
1	B	68	MSE
1	B	75	LEU
1	B	82	TYR
1	B	107	ASP
1	B	113	GLU
1	B	115	GLU
1	B	127	GLU
1	B	139	ASP
1	B	159	ILE
1	B	161	LEU
1	B	168	GLU
1	B	177	GLN
1	B	267	THR
1	B	274[A]	LYS
1	B	274[B]	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	5	ASN
1	A	126	GLN
1	A	214	GLN
1	A	221	GLN
1	A	253	GLN
1	B	4	GLN
1	B	40	GLN
1	B	146	GLN
1	B	189	GLN
1	B	242	HIS

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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	280/287 (97%)	0.14	6 (2%)	63	68	23, 40, 56, 65	0
1	B	276/287 (96%)	0.61	27 (9%)	7	10	25, 48, 85, 98	0
All	All	556/574 (96%)	0.38	33 (5%)	22	27	23, 43, 78, 98	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	93	PHE	7.8
1	B	130	TYR	4.4
1	B	36	GLN	4.2
1	B	75	LEU	4.0
1	B	100	GLU	3.9
1	A	0	ALA	3.8
1	B	98	PRO	3.3
1	B	267	THR	2.9
1	A	82	TYR	2.9
1	B	76	ARG	2.9
1	B	131	ILE	2.9
1	B	107	ASP	2.8
1	B	105	LEU	2.7
1	B	111	PRO	2.7
1	B	120	GLN	2.7
1	B	127	GLU	2.6
1	B	162	ASN	2.6
1	B	106	LEU	2.6
1	B	116	LEU	2.6
1	B	102	ILE	2.5
1	A	4	GLN	2.5
1	B	94	GLN	2.4
1	B	96	PRO	2.3
1	B	39	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	86	ASN	2.3
1	A	53	HIS	2.2
1	B	77	ALA	2.2
1	A	217	ALA	2.2
1	B	135	PRO	2.1
1	A	67[A]	GLN	2.0
1	B	109	VAL	2.0
1	B	3	VAL	2.0
1	B	117	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	502	1/1	0.96	0.21	41,41,41,41	0
2	CA	A	501	1/1	0.98	0.20	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.