Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 06:22 PM EST

PDB ID	:	6DQY
Title	:	Crystal Structure analysis of Superoxide Dismutase from Trichoderma reesei
Authors	:	Mendoza, E.R.; Stelmastchuk, L.B.F.; Ferreira Junior, J.R.S.; Garratt, R.C.
Deposited on	:	2018-06-11
Resolution	:	2.30 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 (i) 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 (1)) were used in the production of this report:

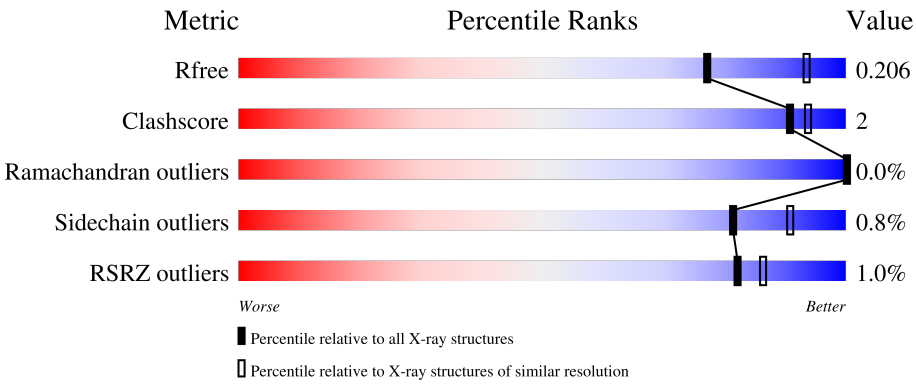
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	212	93% 5% •
1	B	212	96% • •
1	C	212	93% 5% •
1	D	212	96% • •
1	E	212	95% • •

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Mol	Chain	Length	Quality of chain
1	F	212	93% 5%
1	G	212	94%
1	H	212	92% 6%
1	I	212	92% 8%
1	J	212	98%
1	K	212	93% 5%
1	L	212	90% 9%
1	M	212	96%
1	N	212	92% 5%
1	O	212	94%
1	P	212	93% 5%
1	Q	212	92% 5%
1	R	212	92% 6%
1	S	212	94%
1	T	212	90% 8%
1	U	212	92% 5%
1	V	212	90% 7%
1	W	212	93% 5%
1	X	212	94%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41443 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 Superoxide dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1615	1038	271	302	4	0	0	0
1	B	208	1615	1038	271	302	4	0	0	0
1	C	208	1615	1038	271	302	4	0	0	0
1	D	207	1606	1032	269	301	4	0	0	0
1	E	208	1615	1038	271	302	4	0	0	0
1	F	208	1615	1038	271	302	4	0	0	0
1	G	208	1615	1038	271	302	4	0	0	0
1	H	208	1615	1038	271	302	4	0	0	0
1	I	211	1634	1050	274	306	4	0	0	0
1	J	211	1634	1050	274	306	4	0	0	0
1	K	208	1615	1038	271	302	4	0	0	0
1	L	210	1626	1044	273	305	4	0	0	0
1	M	208	1615	1038	271	302	4	0	0	0
1	N	207	1606	1032	269	301	4	0	0	0
1	O	208	1615	1038	271	302	4	0	0	0
1	P	208	1615	1038	271	302	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	206	1600	1029	268	299	4	0	0	0
			Total	C	N	O	S			
1	R	199	1537	987	257	289	4	0	0	0
			Total	C	N	O	S			
1	S	207	1606	1032	269	301	4	0	0	0
			Total	C	N	O	S			
1	T	207	1606	1032	269	301	4	0	0	0
			Total	C	N	O	S			
1	U	207	1606	1032	269	301	4	0	0	0
			Total	C	N	O	S			
1	V	207	1606	1032	269	301	4	0	0	0
			Total	C	N	O	S			
1	W	208	1615	1038	271	302	4	0	0	0
			Total	C	N	O	S			
1	X	208	1615	1038	271	302	4	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	A	1	1	1	0	0
			Total	Mn		
2	B	1	1	1	0	0
			Total	Mn		
2	C	1	1	1	0	0
			Total	Mn		
2	D	1	1	1	0	0
			Total	Mn		
2	E	1	1	1	0	0
			Total	Mn		
2	F	1	1	1	0	0
			Total	Mn		
2	G	1	1	1	0	0
			Total	Mn		
2	H	1	1	1	0	0
			Total	Mn		
2	I	1	1	1	0	0
			Total	Mn		
2	J	1	1	1	0	0
			Total	Mn		
2	K	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
2	L	1	1	1	0	0
2	M	1	1	1	0	0
2	N	1	1	1	0	0
2	O	1	1	1	0	0
2	P	1	1	1	0	0
2	Q	1	1	1	0	0
2	R	1	1	1	0	0
2	S	1	1	1	0	0
2	T	1	1	1	0	0
2	U	1	1	1	0	0
2	V	1	1	1	0	0
2	W	1	1	1	0	0
2	X	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	156	156	156	0	0
3	B	172	172	172	0	0
3	C	151	151	151	0	0
3	D	161	161	161	0	0
3	E	124	124	124	0	0
3	F	146	146	146	0	0

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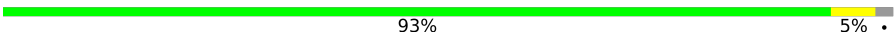
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	G	170	170	170	0	0
			Total	O		
3	H	102	102	102	0	0
			Total	O		
3	I	120	120	120	0	0
			Total	O		
3	J	164	164	164	0	0
			Total	O		
3	K	129	129	129	0	0
			Total	O		
3	L	103	103	103	0	0
			Total	O		
3	M	158	158	158	0	0
			Total	O		
3	N	100	100	100	0	0
			Total	O		
3	O	145	145	145	0	0
			Total	O		
3	P	99	99	99	0	0
			Total	O		
3	Q	54	54	54	0	0
			Total	O		
3	R	41	41	41	0	0
			Total	O		
3	S	79	79	79	0	0
			Total	O		
3	T	89	89	89	0	0
			Total	O		
3	U	70	70	70	0	0
			Total	O		
3	V	64	64	64	0	0
			Total	O		
3	W	93	93	93	0	0
			Total	O		
3	X	67	67	67	0	0

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.

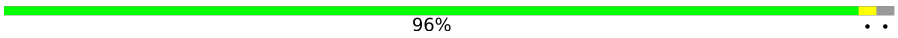
- Molecule 1: Superoxide dismutase

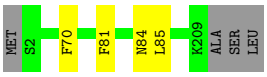
Chain A:



- Molecule 1: Superoxide dismutase

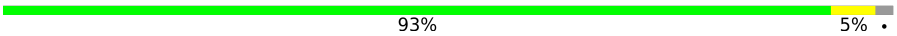
Chain B:

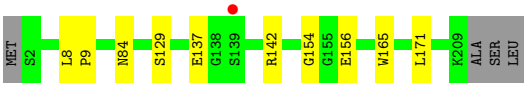




- Molecule 1: Superoxide dismutase

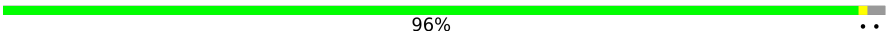
Chain C:

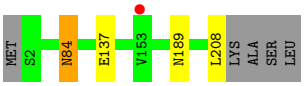




- Molecule 1: Superoxide dismutase

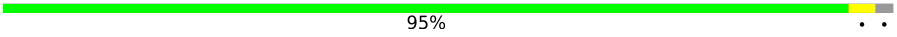
Chain D:





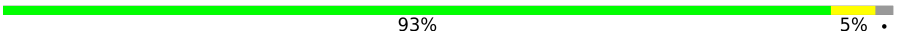
- Molecule 1: Superoxide dismutase

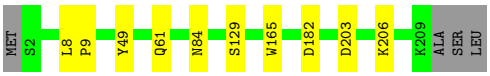
Chain E:



- Molecule 1: Superoxide dismutase

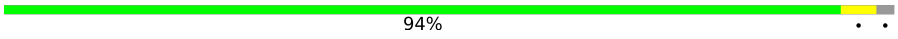
Chain F:





- Molecule 1: Superoxide dismutase

Chain G:

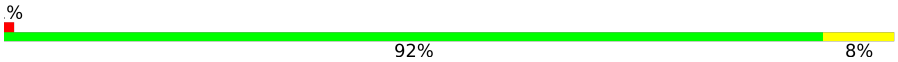


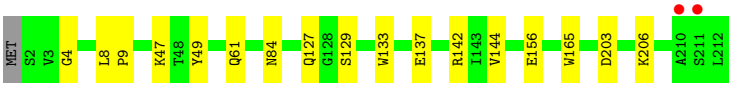
- Molecule 1: Superoxide dismutase

Chain H:

- Molecule 1: Superoxide dismutase

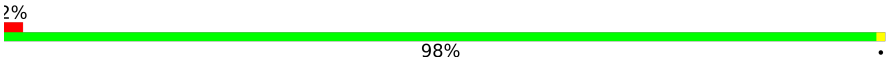
Chain I:

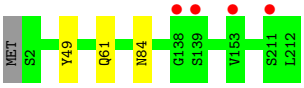




- Molecule 1: Superoxide dismutase

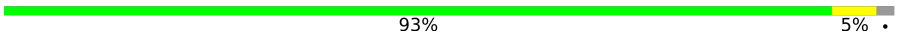
Chain J:





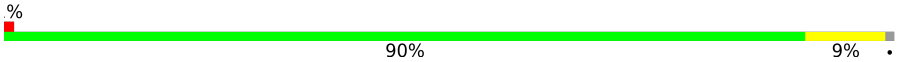
- Molecule 1: Superoxide dismutase

Chain K:



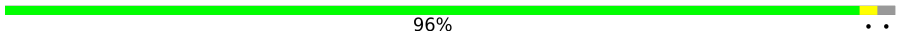
- Molecule 1: Superoxide dismutase

Chain L:



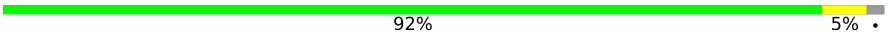
- Molecule 1: Superoxide dismutase

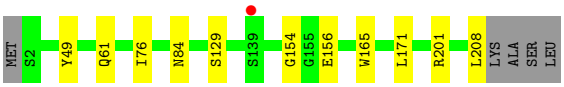
Chain M:



- Molecule 1: Superoxide dismutase

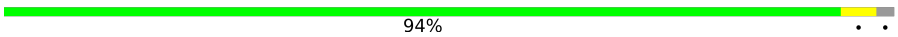
Chain N:





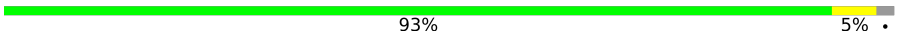
- Molecule 1: Superoxide dismutase

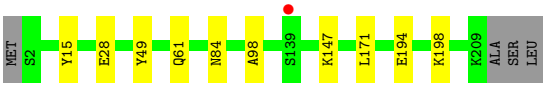
Chain O:



- Molecule 1: Superoxide dismutase

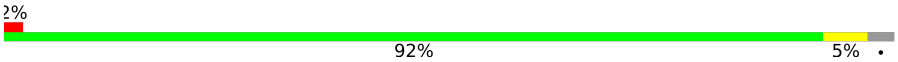
Chain P:

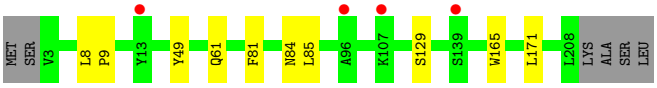




- Molecule 1: Superoxide dismutase

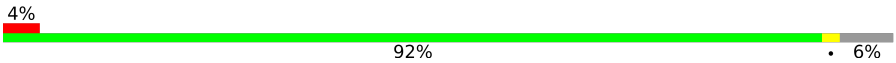
Chain Q:

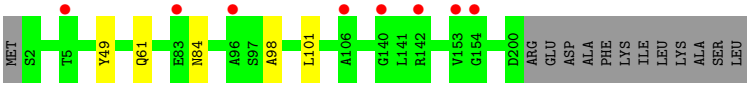




- Molecule 1: Superoxide dismutase

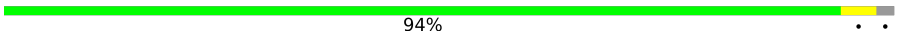
Chain R:





- Molecule 1: Superoxide dismutase

Chain S:

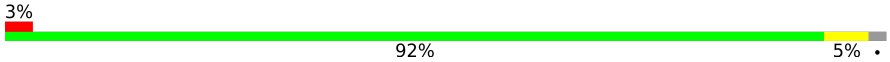


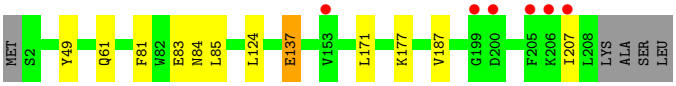
- Molecule 1: Superoxide dismutase

Chain T:

- Molecule 1: Superoxide dismutase

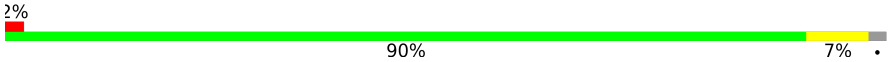
Chain U:

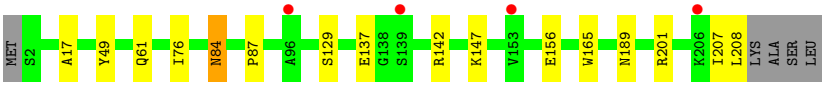




- Molecule 1: Superoxide dismutase

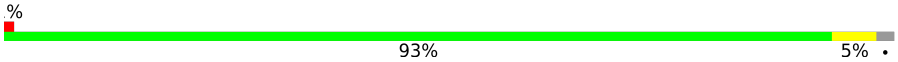
Chain V:





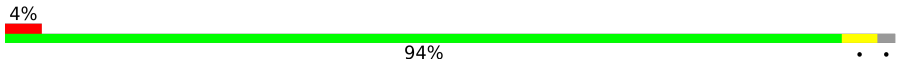
- Molecule 1: Superoxide dismutase

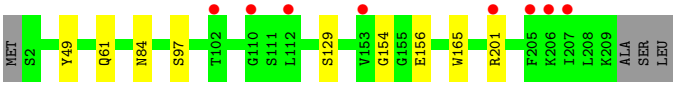
Chain W:



- Molecule 1: Superoxide dismutase

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.77Å 113.06Å 162.71Å 91.59° 93.79° 89.98°	Depositor
Resolution (Å)	81.15 – 2.30 93.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (81.15-2.30) 97.2 (93.98-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.162 , 0.207 0.162 , 0.206	Depositor DCC
R_{free} test set	11462 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.047 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41443	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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 (i)

5.1 Standard geometry (i)

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

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	0.40	0/1660	0.53	0/2259
1	B	0.44	0/1660	0.54	0/2259
1	C	0.42	0/1660	0.56	0/2259
1	D	0.42	0/1651	0.54	0/2248
1	E	0.44	1/1660 (0.1%)	0.50	0/2259
1	F	0.41	0/1660	0.53	0/2259
1	G	0.42	0/1660	0.54	0/2259
1	H	0.35	0/1660	0.52	0/2259
1	I	0.39	0/1679	0.52	0/2285
1	J	0.39	0/1679	0.52	0/2285
1	K	0.41	0/1660	0.54	0/2259
1	L	0.36	0/1671	0.50	0/2274
1	M	0.45	0/1660	0.55	0/2259
1	N	0.37	0/1651	0.51	0/2248
1	O	0.41	0/1660	0.52	0/2259
1	P	0.35	0/1660	0.50	0/2259
1	Q	0.34	0/1645	0.49	0/2240
1	R	0.32	0/1581	0.49	0/2155
1	S	0.35	0/1651	0.49	0/2248
1	T	0.35	0/1651	0.50	0/2248
1	U	0.36	1/1651 (0.1%)	0.49	0/2248
1	V	0.34	0/1651	0.51	0/2248
1	W	0.38	0/1660	0.53	0/2259
1	X	0.34	0/1660	0.47	0/2259
All	All	0.39	2/39741 (0.0%)	0.52	0/54094

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	137	GLU	CG-CD	-5.37	1.43	1.51
1	E	137	GLU	CG-CD	-5.21	1.44	1.51

There are no bond angle outliers.

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	1615	0	1574	7	0
1	B	1615	0	1574	2	0
1	C	1615	0	1574	6	0
1	D	1606	0	1561	3	0
1	E	1615	0	1574	8	0
1	F	1615	0	1574	4	0
1	G	1615	0	1574	4	0
1	H	1615	0	1574	8	0
1	I	1634	0	1595	10	0
1	J	1634	0	1595	1	0
1	K	1615	0	1574	7	0
1	L	1626	0	1584	10	0
1	M	1615	0	1574	3	0
1	N	1606	0	1561	6	0
1	O	1615	0	1574	5	0
1	P	1615	0	1574	10	0
1	Q	1600	0	1556	5	0
1	R	1537	0	1489	2	0
1	S	1606	0	1561	15	0
1	T	1606	0	1561	9	0
1	U	1606	0	1561	9	0
1	V	1606	0	1561	10	0
1	W	1615	0	1574	8	0
1	X	1615	0	1574	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	156	0	0	0	0
3	B	172	0	0	0	0
3	C	151	0	0	0	0
3	D	161	0	0	0	0
3	E	124	0	0	0	0
3	F	146	0	0	0	0
3	G	170	0	0	0	0
3	H	102	0	0	0	0
3	I	120	0	0	0	0
3	J	164	0	0	0	0
3	K	129	0	0	1	0
3	L	103	0	0	1	0
3	M	158	0	0	2	0
3	N	100	0	0	0	0
3	O	145	0	0	1	0
3	P	99	0	0	0	0
3	Q	54	0	0	0	0
3	R	41	0	0	0	0
3	S	79	0	0	1	0
3	T	89	0	0	0	0
3	U	70	0	0	0	0
3	V	64	0	0	0	0
3	W	93	0	0	0	0
3	X	67	0	0	0	0
All	All	41443	0	37647	131	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 2.

All (131) 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:K:51:THR:OG1	1:S:16:ASP:OD2	1.73	1.05
1:E:137:GLU:OE2	1:S:142:ARG:NH1	1.95	0.98
1:C:142:ARG:NH1	1:D:137:GLU:OE2	2.14	0.80
1:L:16:ASP:OD2	3:L:401:HOH:O	2.00	0.79
1:H:137:GLU:OE2	1:H:142:ARG:NH1	2.19	0.75
1:E:137:GLU:CD	1:S:142:ARG:NH1	2.44	0.71
1:E:137:GLU:CD	1:S:142:ARG:HH12	1.94	0.70
1:P:147:LYS:NZ	1:S:147:LYS:NZ	2.41	0.67
1:M:83:GLU:OE2	3:M:401:HOH:O	2.15	0.64
1:W:83:GLU:HG3	1:W:196:ARG:NH2	2.12	0.63
1:I:133:TRP:HB2	1:I:144:VAL:HG22	1.82	0.62
1:T:100:GLU:OE2	1:T:198:LYS:NZ	2.33	0.62
1:L:83:GLU:OE1	1:L:207:ILE:HG21	2.01	0.61
1:K:206:LYS:HE3	1:K:209:LYS:HE3	1.84	0.60
1:H:142:ARG:HD2	1:W:142:ARG:HD2	1.84	0.58
1:T:103:ALA:O	1:T:107:LYS:HG3	2.03	0.58
1:H:49:TYR:CZ	1:H:61:GLN:HG2	2.39	0.58
1:G:142:ARG:HD2	1:I:142:ARG:NH1	2.20	0.57
1:N:49:TYR:CZ	1:N:61:GLN:HG2	2.39	0.57
1:T:203:ASP:HA	1:T:206:LYS:HE2	1.87	0.56
1:U:137:GLU:OE1	1:V:142:ARG:NH2	2.38	0.56
1:A:137:GLU:HG2	1:A:156:GLU:HG2	1.86	0.56
1:I:137:GLU:OE2	1:I:156:GLU:OE2	2.23	0.56
1:U:83:GLU:OE2	1:U:207:ILE:HG21	2.05	0.56
1:W:49:TYR:CZ	1:W:61:GLN:HG2	2.41	0.55
1:V:49:TYR:CZ	1:V:61:GLN:HG2	2.42	0.55
1:K:171:LEU:HD23	1:Q:171:LEU:HD23	1.88	0.55
1:C:142:ARG:HH12	1:D:137:GLU:CD	2.10	0.55
1:I:203:ASP:HA	1:I:206:LYS:HE2	1.90	0.54
1:E:137:GLU:OE1	1:S:142:ARG:NH1	2.32	0.54
1:P:147:LYS:HZ3	1:S:147:LYS:NZ	2.04	0.54
1:P:147:LYS:NZ	1:S:147:LYS:HZ2	2.06	0.54
1:I:4:GLY:O	1:I:47:LYS:NZ	2.41	0.53
1:L:99:PRO:HD2	1:L:194:GLU:OE2	2.09	0.53
1:P:171:LEU:HD23	1:S:171:LEU:HD23	1.90	0.53
1:W:83:GLU:HG3	1:W:196:ARG:HH21	1.73	0.53
1:I:137:GLU:HG2	1:I:156:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:49:TYR:CZ	1:K:61:GLN:HG2	2.44	0.52
1:P:147:LYS:HZ2	1:S:147:LYS:NZ	2.07	0.52
1:X:49:TYR:CZ	1:X:61:GLN:HG2	2.45	0.52
1:F:49:TYR:CZ	1:F:61:GLN:HG2	2.46	0.51
1:U:49:TYR:CZ	1:U:61:GLN:HG2	2.45	0.51
1:M:49:TYR:CZ	1:M:61:GLN:HG2	2.45	0.50
1:T:49:TYR:CZ	1:T:61:GLN:HG2	2.47	0.50
1:E:137:GLU:O	1:E:137:GLU:HG3	2.11	0.50
1:P:147:LYS:HZ2	1:S:147:LYS:HZ2	1.58	0.50
1:A:171:LEU:HD23	1:C:171:LEU:HD23	1.93	0.50
1:S:154:GLY:HA2	1:S:201:ARG:CZ	2.42	0.50
1:P:194:GLU:O	1:P:198:LYS:HD3	2.12	0.50
1:G:171:LEU:HD23	1:T:171:LEU:HD23	1.94	0.49
1:H:137:GLU:HG2	1:H:156:GLU:HG2	1.95	0.49
1:J:49:TYR:CZ	1:J:61:GLN:HG2	2.48	0.49
1:N:156:GLU:O	1:N:201:ARG:NH2	2.46	0.49
1:L:49:TYR:CZ	1:L:61:GLN:HG2	2.48	0.48
1:P:49:TYR:CZ	1:P:61:GLN:HG2	2.47	0.48
1:O:137:GLU:OE2	1:O:142:ARG:HD3	2.14	0.48
1:Q:81:PHE:CZ	1:Q:85:LEU:HD11	2.48	0.48
1:R:49:TYR:CZ	1:R:61:GLN:HG2	2.48	0.48
1:A:49:TYR:CZ	1:A:61:GLN:HG2	2.49	0.48
1:Q:129:SER:HB3	1:Q:165:TRP:CE2	2.49	0.47
1:W:154:GLY:HA2	1:W:201:ARG:CZ	2.45	0.47
1:H:154:GLY:HA2	1:H:201:ARG:CZ	2.45	0.47
1:N:154:GLY:HA2	1:N:201:ARG:CZ	2.43	0.47
1:Q:49:TYR:CZ	1:Q:61:GLN:HG2	2.49	0.47
1:U:171:LEU:HD23	1:W:171:LEU:HD23	1.96	0.47
1:W:159:VAL:O	1:W:196:ARG:HD2	2.14	0.47
1:K:114:LYS:HE3	3:K:445:HOH:O	2.15	0.46
1:F:203:ASP:HA	1:F:206:LYS:HE2	1.97	0.46
1:N:76:ILE:HG12	1:N:208:LEU:HD11	1.97	0.46
1:X:129:SER:HB3	1:X:165:TRP:CE2	2.50	0.46
1:T:136:LYS:NZ	1:T:199:GLY:O	2.38	0.46
1:K:98:ALA:HA	1:K:194:GLU:HB2	1.97	0.46
1:O:4:GLY:O	1:O:47:LYS:NZ	2.48	0.46
1:V:76:ILE:HG12	1:V:208:LEU:HD11	1.96	0.46
1:C:137:GLU:HG2	1:C:156:GLU:HG2	1.99	0.45
1:D:84:ASN:HA	1:D:189:ASN:HB3	1.98	0.45
1:S:56:ASN:HA	3:S:429:HOH:O	2.16	0.45
1:K:137:GLU:O	1:K:137:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:129:SER:HB3	1:N:165:TRP:CE2	2.51	0.45
1:H:42:LEU:HD22	1:H:72:GLY:HA2	1.99	0.44
1:A:8:LEU:HD12	1:A:9:PRO:HD2	1.99	0.44
1:I:8:LEU:HD12	1:I:9:PRO:HD2	1.98	0.44
1:L:8:LEU:HD12	1:L:9:PRO:HD2	1.99	0.44
1:W:83:GLU:CG	1:W:196:ARG:HH21	2.30	0.44
1:X:156:GLU:O	1:X:201:ARG:NH2	2.51	0.44
1:L:17:ALA:HB1	1:L:87:PRO:HG3	1.99	0.44
1:V:137:GLU:HG2	1:V:156:GLU:HG2	2.00	0.43
1:E:129:SER:HB3	1:E:165:TRP:CE2	2.53	0.43
1:U:137:GLU:O	1:U:137:GLU:HG3	2.18	0.43
1:L:129:SER:HB3	1:L:165:TRP:CE2	2.54	0.43
1:B:70:PHE:CE1	1:I:127:GLN:HB3	2.53	0.43
1:Q:8:LEU:HD12	1:Q:9:PRO:HD2	2.00	0.43
1:T:154:GLY:HA2	1:T:201:ARG:CZ	2.49	0.43
1:I:129:SER:HB3	1:I:165:TRP:CE2	2.54	0.43
1:L:124:LEU:HD22	1:L:177:LYS:HG3	2.01	0.43
1:E:142:ARG:HD2	1:S:142:ARG:HD2	2.01	0.43
1:S:154:GLY:HA2	1:S:201:ARG:NH1	2.34	0.43
1:A:129:SER:HB3	1:A:165:TRP:CE2	2.54	0.43
1:X:154:GLY:HA2	1:X:201:ARG:CZ	2.49	0.43
1:V:147:LYS:HE2	1:V:147:LYS:HB3	1.77	0.42
1:C:8:LEU:HD12	1:C:9:PRO:HD2	2.00	0.42
1:T:129:SER:HB3	1:T:165:TRP:CE2	2.54	0.42
1:H:129:SER:HB3	1:H:165:TRP:CE2	2.54	0.42
1:L:171:LEU:HD23	1:N:171:LEU:HD23	2.01	0.42
1:F:8:LEU:HD12	1:F:9:PRO:HD2	2.00	0.42
1:M:207:ILE:HG13	3:M:496:HOH:O	2.19	0.42
1:V:17:ALA:HB1	1:V:87:PRO:HG3	2.01	0.42
1:F:129:SER:HB3	1:F:165:TRP:CE2	2.54	0.42
1:U:137:GLU:CD	1:V:142:ARG:NH2	2.73	0.42
1:P:15:TYR:CE1	1:P:28:GLU:HA	2.54	0.42
1:U:124:LEU:HD22	1:U:177:LYS:HG3	2.01	0.42
1:O:207:ILE:HG23	3:O:511:HOH:O	2.20	0.42
1:L:103:ALA:O	1:L:107:LYS:HG3	2.20	0.41
1:O:129:SER:HB3	1:O:165:TRP:CE2	2.55	0.41
1:G:116:LYS:HE3	1:G:185:TRP:CD2	2.56	0.41
1:I:49:TYR:CZ	1:I:61:GLN:HG2	2.54	0.41
1:V:84:ASN:HA	1:V:189:ASN:HB3	2.01	0.41
1:B:81:PHE:CZ	1:B:85:LEU:HD11	2.56	0.41
1:R:98:ALA:HB1	1:R:101:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:81:PHE:CZ	1:U:85:LEU:HD11	2.56	0.41
1:E:49:TYR:CZ	1:E:61:GLN:HG2	2.55	0.41
1:G:159:VAL:O	1:G:196:ARG:HD2	2.21	0.41
1:H:159:VAL:O	1:H:196:ARG:HD2	2.21	0.41
1:A:137:GLU:OE2	1:A:156:GLU:OE2	2.38	0.41
1:V:129:SER:HB3	1:V:165:TRP:CE2	2.56	0.41
1:A:142:ARG:HD2	1:O:142:ARG:NH1	2.37	0.40
1:P:98:ALA:CB	1:P:194:GLU:HB2	2.52	0.40
1:V:137:GLU:CG	1:V:156:GLU:HG2	2.51	0.40
1:C:129:SER:HB3	1:C:165:TRP:CE2	2.56	0.40
1:T:136:LYS:HB3	1:T:157:VAL:HB	2.03	0.40
1:U:85:LEU:HA	1:U:187:VAL:O	2.22	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	206/212 (97%)	200 (97%)	6 (3%)	0	100	100
1	B	206/212 (97%)	201 (98%)	5 (2%)	0	100	100
1	C	206/212 (97%)	200 (97%)	5 (2%)	1 (0%)	29	35
1	D	205/212 (97%)	199 (97%)	6 (3%)	0	100	100
1	E	206/212 (97%)	199 (97%)	7 (3%)	0	100	100
1	F	206/212 (97%)	201 (98%)	5 (2%)	0	100	100
1	G	206/212 (97%)	201 (98%)	5 (2%)	0	100	100
1	H	206/212 (97%)	202 (98%)	4 (2%)	0	100	100
1	I	209/212 (99%)	202 (97%)	7 (3%)	0	100	100
1	J	209/212 (99%)	203 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	206/212 (97%)	202 (98%)	4 (2%)	0	100	100
1	L	208/212 (98%)	201 (97%)	7 (3%)	0	100	100
1	M	206/212 (97%)	202 (98%)	4 (2%)	0	100	100
1	N	205/212 (97%)	199 (97%)	6 (3%)	0	100	100
1	O	206/212 (97%)	199 (97%)	7 (3%)	0	100	100
1	P	206/212 (97%)	199 (97%)	7 (3%)	0	100	100
1	Q	204/212 (96%)	198 (97%)	6 (3%)	0	100	100
1	R	197/212 (93%)	191 (97%)	6 (3%)	0	100	100
1	S	205/212 (97%)	198 (97%)	7 (3%)	0	100	100
1	T	205/212 (97%)	198 (97%)	7 (3%)	0	100	100
1	U	205/212 (97%)	198 (97%)	7 (3%)	0	100	100
1	V	205/212 (97%)	199 (97%)	6 (3%)	0	100	100
1	W	206/212 (97%)	198 (96%)	8 (4%)	0	100	100
1	X	206/212 (97%)	198 (96%)	8 (4%)	0	100	100
All	All	4935/5088 (97%)	4788 (97%)	146 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	154	GLY

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	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	B	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	C	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	D	166/170 (98%)	164 (99%)	2 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	F	167/170 (98%)	165 (99%)	2 (1%)	71	84
1	G	167/170 (98%)	165 (99%)	2 (1%)	71	84
1	H	167/170 (98%)	165 (99%)	2 (1%)	71	84
1	I	169/170 (99%)	168 (99%)	1 (1%)	86	94
1	J	169/170 (99%)	168 (99%)	1 (1%)	86	94
1	K	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	L	168/170 (99%)	166 (99%)	2 (1%)	71	84
1	M	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	N	166/170 (98%)	165 (99%)	1 (1%)	86	94
1	O	167/170 (98%)	165 (99%)	2 (1%)	71	84
1	P	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	Q	165/170 (97%)	164 (99%)	1 (1%)	86	94
1	R	159/170 (94%)	158 (99%)	1 (1%)	86	94
1	S	166/170 (98%)	165 (99%)	1 (1%)	86	94
1	T	166/170 (98%)	165 (99%)	1 (1%)	86	94
1	U	166/170 (98%)	165 (99%)	1 (1%)	86	94
1	V	166/170 (98%)	163 (98%)	3 (2%)	59	75
1	W	167/170 (98%)	166 (99%)	1 (1%)	86	94
1	X	167/170 (98%)	165 (99%)	2 (1%)	71	84
All	All	3997/4080 (98%)	3964 (99%)	33 (1%)	81	91

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	B	84	ASN
1	C	84	ASN
1	D	84	ASN
1	D	208	LEU
1	E	84	ASN
1	F	84	ASN
1	F	182	ASP
1	G	84	ASN
1	G	153	VAL

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Mol	Chain	Res	Type
1	H	84	ASN
1	H	201	ARG
1	I	84	ASN
1	J	84	ASN
1	K	84	ASN
1	L	84	ASN
1	L	201	ARG
1	M	84	ASN
1	N	84	ASN
1	O	84	ASN
1	O	100	GLU
1	P	84	ASN
1	Q	84	ASN
1	R	84	ASN
1	S	84	ASN
1	T	84	ASN
1	U	84	ASN
1	V	84	ASN
1	V	201	ARG
1	V	207	ILE
1	W	84	ASN
1	X	84	ASN
1	X	97	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 24 ligands modelled in this entry, 24 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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	208/212 (98%)	-0.46	0	100	100	11, 21, 45, 65	0
1	B	208/212 (98%)	-0.48	0	100	100	11, 18, 38, 59	0
1	C	208/212 (98%)	-0.48	1 (0%)	91	94	12, 21, 41, 78	0
1	D	207/212 (97%)	-0.44	1 (0%)	91	94	13, 19, 48, 70	0
1	E	208/212 (98%)	-0.37	1 (0%)	91	94	12, 25, 51, 74	0
1	F	208/212 (98%)	-0.42	0	100	100	13, 23, 43, 62	0
1	G	208/212 (98%)	-0.47	0	100	100	12, 20, 35, 57	0
1	H	208/212 (98%)	-0.37	1 (0%)	91	94	18, 29, 51, 75	0
1	I	211/212 (99%)	-0.34	2 (0%)	84	88	14, 28, 50, 84	0
1	J	211/212 (99%)	-0.39	4 (1%)	66	73	13, 22, 50, 82	0
1	K	208/212 (98%)	-0.42	0	100	100	14, 25, 41, 61	0
1	L	210/212 (99%)	-0.24	3 (1%)	75	80	18, 31, 65, 90	0
1	M	208/212 (98%)	-0.42	0	100	100	10, 18, 41, 69	0
1	N	207/212 (97%)	-0.38	1 (0%)	91	94	16, 28, 53, 76	0
1	O	208/212 (98%)	-0.47	0	100	100	12, 24, 45, 65	0
1	P	208/212 (98%)	-0.31	1 (0%)	91	94	17, 31, 55, 86	0
1	Q	206/212 (97%)	-0.04	4 (1%)	66	73	20, 42, 71, 79	0
1	R	199/212 (93%)	0.33	8 (4%)	38	45	28, 51, 77, 101	0
1	S	207/212 (97%)	-0.12	1 (0%)	91	94	16, 39, 66, 85	0
1	T	207/212 (97%)	-0.29	1 (0%)	91	94	17, 36, 55, 63	0
1	U	207/212 (97%)	-0.14	6 (2%)	51	58	20, 37, 80, 95	0
1	V	207/212 (97%)	-0.12	4 (1%)	66	73	18, 38, 65, 77	0
1	W	208/212 (98%)	-0.32	3 (1%)	75	80	17, 28, 55, 81	0
1	X	208/212 (98%)	-0.07	8 (3%)	40	47	20, 38, 69, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	4983/5088 (97%)	-0.30	50 (1%) 82 86	10, 28, 62, 101	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	209	LYS	4.1
1	U	206	LYS	3.8
1	J	153	VAL	3.8
1	J	139	SER	3.7
1	U	199	GLY	3.6
1	Q	96	ALA	3.2
1	X	206	LYS	3.2
1	U	207	ILE	3.0
1	X	207	ILE	3.0
1	R	153	VAL	3.0
1	U	205	PHE	3.0
1	N	139	SER	2.9
1	V	139	SER	2.9
1	E	153	VAL	2.9
1	X	153	VAL	2.9
1	H	209	LYS	2.9
1	U	153	VAL	2.8
1	S	110	GLY	2.7
1	W	153	VAL	2.7
1	V	206	LYS	2.6
1	Q	13	TYR	2.6
1	X	112	LEU	2.6
1	X	102	THR	2.6
1	I	210	ALA	2.6
1	J	138	GLY	2.5
1	R	140	GLY	2.5
1	C	139	SER	2.5
1	P	139	SER	2.5
1	X	201	ARG	2.5
1	R	96	ALA	2.4
1	R	83	GLU	2.4
1	L	209	LYS	2.3
1	R	142	ARG	2.3
1	U	200	ASP	2.3
1	W	2	SER	2.3
1	R	5	THR	2.3
1	R	154	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	Q	139	SER	2.2
1	J	211	SER	2.2
1	X	205	PHE	2.2
1	X	110	GLY	2.2
1	I	211	SER	2.1
1	Q	107	LYS	2.1
1	V	96	ALA	2.1
1	L	207	ILE	2.1
1	V	153	VAL	2.1
1	R	106	ALA	2.1
1	L	211	SER	2.0
1	D	153	VAL	2.0
1	T	107	LYS	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)

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	MN	R	301	1/1	0.96	0.05	33,33,33,33	0
2	MN	J	301	1/1	0.99	0.06	22,22,22,22	0
2	MN	K	301	1/1	0.99	0.07	22,22,22,22	0
2	MN	L	301	1/1	0.99	0.05	27,27,27,27	0
2	MN	M	301	1/1	0.99	0.09	17,17,17,17	0
2	MN	N	301	1/1	0.99	0.06	23,23,23,23	0
2	MN	P	301	1/1	0.99	0.08	24,24,24,24	0
2	MN	Q	301	1/1	0.99	0.04	28,28,28,28	0
2	MN	F	301	1/1	0.99	0.05	20,20,20,20	0
2	MN	S	301	1/1	0.99	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	T	301	1/1	0.99	0.05	25,25,25,25	0
2	MN	U	301	1/1	0.99	0.06	23,23,23,23	0
2	MN	V	301	1/1	0.99	0.05	25,25,25,25	0
2	MN	X	301	1/1	0.99	0.04	26,26,26,26	0
2	MN	O	301	1/1	1.00	0.06	21,21,21,21	0
2	MN	G	301	1/1	1.00	0.08	18,18,18,18	0
2	MN	H	301	1/1	1.00	0.05	26,26,26,26	0
2	MN	I	301	1/1	1.00	0.05	17,17,17,17	0
2	MN	B	301	1/1	1.00	0.12	21,21,21,21	0
2	MN	C	301	1/1	1.00	0.05	16,16,16,16	0
2	MN	D	301	1/1	1.00	0.09	21,21,21,21	0
2	MN	E	301	1/1	1.00	0.11	20,20,20,20	0
2	MN	W	301	1/1	1.00	0.07	22,22,22,22	0
2	MN	A	301	1/1	1.00	0.09	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.