Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:53 AM GMT

PDB ID	:	2BWE
Title	:	The crystal structure of the complex between the UBA and UBL domains of Dsk2
Authors	:	Lowe, E.D.; Hasan, N.; Trempe, J.-F.; Fonso, L.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.; Brown, N.R.
Deposited on	:	2005-07-13
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

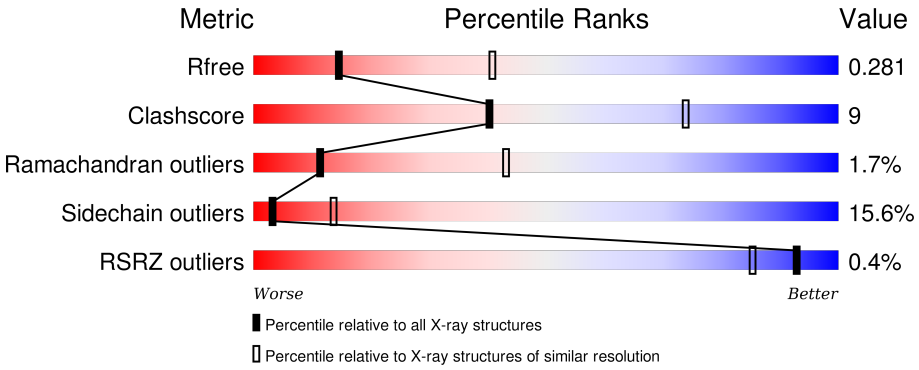
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 <=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	50	70% 18% • 8%
1	B	50	68% 18% 10% •
1	C	50	64% 22% 10% •
1	D	50	66% 20% 6% • 6%
1	E	50	68% 16% 8% 8%

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Mol	Chain	Length	Quality of chain
1	F	50	2% 72% 10% 8% 10%
1	G	50	64% 22% 8%
1	H	50	2% 66% 20% 10%
1	I	50	72% 16% 10%
1	J	50	60% 28% 8%
1	K	50	60% 22% 12% 6%
1	L	50	68% 12% 10% 8%
1	M	50	68% 18% 10%
1	N	50	68% 18% 6% 8%
1	O	50	68% 14% 8% 8%
1	P	50	72% 12% 12%
1	Q	50	66% 22% 6%
1	R	50	70% 18% 8%
2	S	77	65% 27% 5%
2	T	77	66% 26% 5%
2	U	77	3% 69% 22% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8410 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 DSK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			
1	B	48	Total	C	N	O	S	0	0	0
			378	232	71	74	1			
1	C	48	Total	C	N	O	S	0	0	0
			382	233	71	77	1			
1	D	47	Total	C	N	O	S	0	0	0
			374	230	70	73	1			
1	E	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			
1	F	45	Total	C	N	O	S	0	0	0
			358	218	68	71	1			
1	G	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			
1	H	45	Total	C	N	O	S	0	0	0
			358	218	68	71	1			
1	I	45	Total	C	N	O	S	0	0	0
			358	218	68	71	1			
1	J	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			
1	K	47	Total	C	N	O	S	0	0	0
			374	228	70	75	1			
1	L	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			
1	M	45	Total	C	N	O	S	0	0	0
			358	218	68	71	1			
1	N	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			
1	O	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			
1	P	44	Total	C	N	O	S	0	0	0
			354	216	67	70	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	47	Total	C	N	O	S	0	0	0
			374	230	70	73	1			
1	R	46	Total	C	N	O	S	0	0	0
			366	224	69	72	1			

- Molecule 2 is a protein called DSK2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	S	73	Total	C	N	O	0	0	0
			573	360	102	111			
2	T	73	Total	C	N	O	0	0	0
			573	360	102	111			
2	U	72	Total	C	N	O	0	0	0
			567	357	101	109			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	5	Total	O	0	0
			5	5		
3	C	9	Total	O	0	0
			9	9		
3	D	10	Total	O	0	0
			10	10		
3	E	5	Total	O	0	0
			5	5		
3	F	5	Total	O	0	0
			5	5		
3	G	2	Total	O	0	0
			2	2		
3	H	3	Total	O	0	0
			3	3		
3	I	1	Total	O	0	0
			1	1		
3	J	6	Total	O	0	0
			6	6		
3	K	8	Total	O	0	0
			8	8		
3	L	10	Total	O	0	0
			10	10		

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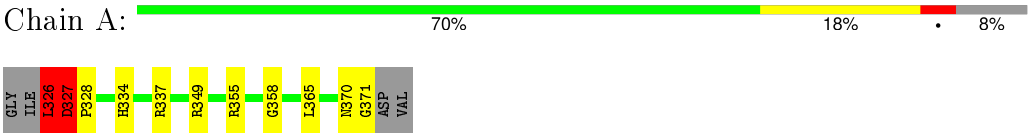
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	3	Total O 3 3	0	0
3	N	1	Total O 1 1	0	0
3	O	2	Total O 2 2	0	0
3	P	4	Total O 4 4	0	0
3	Q	1	Total O 1 1	0	0
3	R	4	Total O 4 4	0	0
3	S	9	Total O 9 9	0	0
3	T	6	Total O 6 6	0	0

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 errors 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.

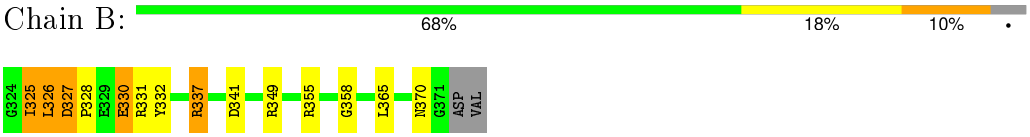
- Molecule 1: DSK2

Chain A:



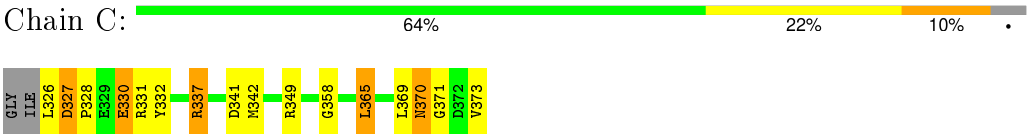
- Molecule 1: DSK2

Chain B:



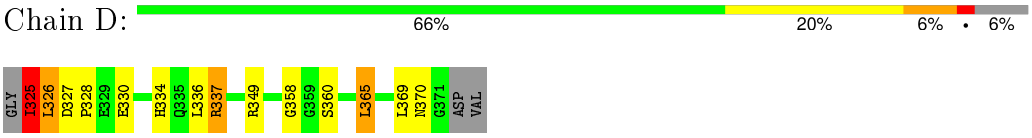
- Molecule 1: DSK2

Chain C:



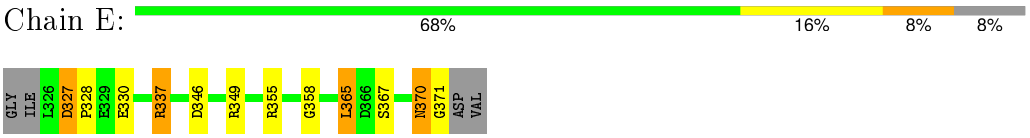
- Molecule 1: DSK2

Chain D:



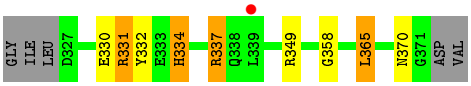
- Molecule 1: DSK2

Chain E:



- Molecule 1: DSK2

Chain F:

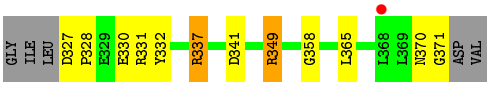


• Molecule 1: DSK2

Chain G:

• Molecule 1: DSK2

Chain H:

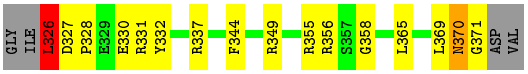


• Molecule 1: DSK2

Chain I:

• Molecule 1: DSK2

Chain J:



• Molecule 1: DSK2

Chain K:

• Molecule 1: DSK2

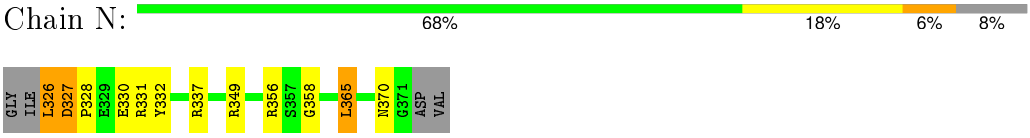
Chain L:

• Molecule 1: DSK2

Chain M:

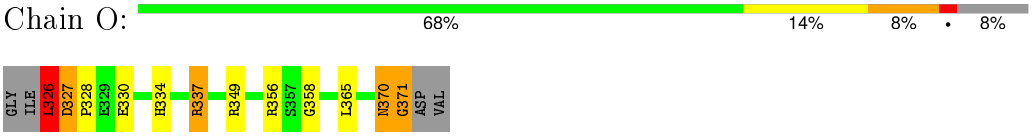
- Molecule 1: DSK2

Chain N:



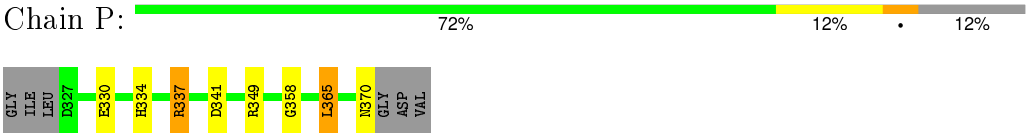
- Molecule 1: DSK2

Chain O:



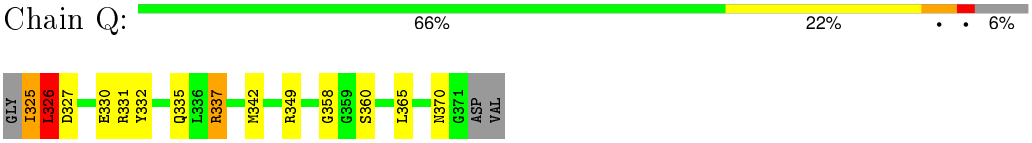
- Molecule 1: DSK2

Chain P:



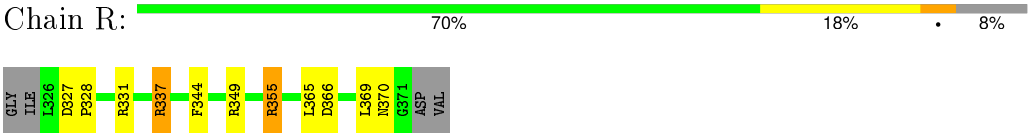
- Molecule 1: DSK2

Chain Q:



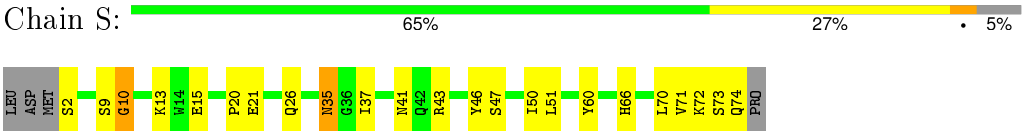
- Molecule 1: DSK2

Chain R:



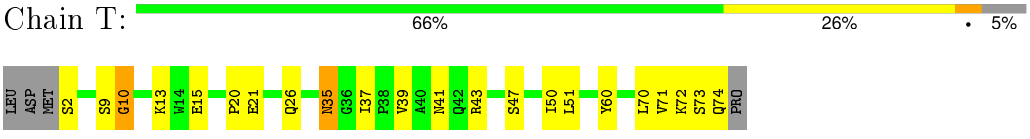
- Molecule 2: DSK2

Chain S:



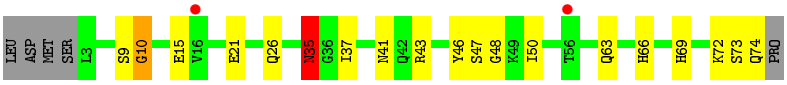
- Molecule 2: DSK2

Chain T:



- Molecule 2: DSK2

Chain U:


LEU
ASP
MET
SER
L3
S9
G10
E15
V16
E21
Q26
N35
G36
I37
N41
Q42
R43
Y46
S47
G48
K49
I50
T56
Q63
H66
H69
K72
S73
Q74
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.36Å 88.85Å 141.50Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	136.08 – 3.10 59.29 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (136.08-3.10) 98.5 (59.29-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.239 , 0.267 0.281 , 0.281	Depositor DCC
R_{free} test set	1707 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	66.1	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.8	EDS
Estimated twinning fraction	0.459 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 33640 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8410	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.79	0/371	0.87	1/497 (0.2%)
1	B	0.78	0/383	0.79	0/513
1	C	0.91	0/387	0.89	0/518
1	D	0.88	0/379	0.89	0/508
1	E	0.71	0/371	0.85	0/497
1	F	0.60	0/363	0.73	0/486
1	G	0.78	0/371	0.89	1/497 (0.2%)
1	H	0.57	0/363	0.63	0/486
1	I	0.74	1/363 (0.3%)	0.67	0/486
1	J	0.80	0/371	0.81	0/497
1	K	0.89	0/379	0.84	0/508
1	L	0.85	0/371	0.83	1/497 (0.2%)
1	M	0.79	0/363	0.78	1/486 (0.2%)
1	N	0.68	0/371	0.78	1/497 (0.2%)
1	O	2.08	2/371 (0.5%)	0.91	2/497 (0.4%)
1	P	0.63	0/359	0.67	0/481
1	Q	0.72	0/379	0.80	1/508 (0.2%)
1	R	0.80	0/371	0.89	2/497 (0.4%)
2	S	0.64	0/583	0.77	0/787
2	T	0.63	0/583	0.76	0/787
2	U	0.44	0/577	0.67	0/779
All	All	0.84	3/8429 (0.0%)	0.80	10/11309 (0.1%)

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	A	0	1
1	D	0	1
1	E	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	L	0	2
1	O	0	2
1	Q	0	2
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	371	GLY	C-O	37.37	1.83	1.23
1	O	371	GLY	CA-C	7.64	1.64	1.51
1	I	371	GLY	C-O	6.76	1.34	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	371	GLY	CA-C-O	-10.45	101.78	120.60
1	G	341	ASP	CB-CG-OD2	-7.56	111.49	118.30
1	Q	326	LEU	N-CA-C	-6.19	94.28	111.00
1	O	326	LEU	CA-CB-CG	5.75	128.53	115.30
1	M	356	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	L	337	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	R	355	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	R	366	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	327	ASP	N-CA-C	5.05	124.65	111.00
1	N	326	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	LEU	Peptide
1	D	325	ILE	Peptide
1	E	370	ASN	Peptide
1	G	326	LEU	Peptide
1	J	326	LEU	Peptide
1	L	326	LEU	Peptide
1	L	370	ASN	Peptide
1	O	326	LEU	Peptide
1	O	370	ASN	Peptide
1	Q	325	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	Q	326	LEU	Peptide

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	366	0	343	6	0
1	B	378	0	357	9	0
1	C	382	0	356	16	0
1	D	374	0	354	11	0
1	E	366	0	343	10	0
1	F	358	0	332	5	0
1	G	366	0	343	7	0
1	H	358	0	332	7	0
1	I	358	0	332	2	0
1	J	366	0	343	8	0
1	K	374	0	347	13	0
1	L	366	0	343	13	0
1	M	358	0	332	4	0
1	N	366	0	343	5	0
1	O	366	0	343	4	0
1	P	354	0	329	4	0
1	Q	374	0	354	11	0
1	R	366	0	343	6	0
2	S	573	0	570	11	0
2	T	573	0	570	11	0
2	U	567	0	565	10	0
3	A	7	0	0	1	0
3	B	5	0	0	0	0
3	C	9	0	0	0	0
3	D	10	0	0	1	0
3	E	5	0	0	1	0
3	F	5	0	0	1	0
3	G	2	0	0	1	0
3	H	3	0	0	1	0
3	I	1	0	0	0	0
3	J	6	0	0	0	0
3	K	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	10	0	0	1	0
3	M	3	0	0	0	0
3	N	1	0	0	0	0
3	O	2	0	0	0	0
3	P	4	0	0	0	0
3	Q	1	0	0	0	0
3	R	4	0	0	0	0
3	S	9	0	0	0	0
3	T	6	0	0	0	0
All	All	8410	0	7874	140	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 (140) 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:O:371:GLY:C	1:O:371:GLY:O	1.83	1.17
1:E:367:SER:O	1:E:371:GLY:HA3	1.43	1.16
1:L:326:LEU:HA	1:L:327:ASP:HB2	1.37	1.04
1:D:325:ILE:N	1:D:326:LEU:HB3	1.81	0.96
1:C:369:LEU:HD11	1:K:365:LEU:HD13	1.47	0.94
1:L:326:LEU:HA	1:L:327:ASP:CB	2.04	0.87
1:Q:360:SER:HA	1:R:337:ARG:NH1	1.89	0.86
1:N:326:LEU:O	1:N:327:ASP:HB2	1.76	0.84
1:D:334:HIS:HB3	3:D:2002:HOH:O	1.79	0.83
1:C:365:LEU:HD13	1:K:369:LEU:HD11	1.59	0.82
1:E:367:SER:O	1:E:371:GLY:CA	2.26	0.80
1:D:360:SER:HA	1:E:337:ARG:NH1	1.99	0.78
2:U:43:ARG:HG3	2:U:50:ILE:HD11	1.69	0.73
1:L:326:LEU:CA	1:L:327:ASP:HB2	2.18	0.70
1:L:360:SER:HA	1:M:337:ARG:NH1	2.07	0.70
1:A:355:ARG:NH2	1:B:330:GLU:OE1	2.23	0.69
1:G:358:GLY:O	1:H:337:ARG:HG3	1.92	0.69
1:N:358:GLY:O	1:O:337:ARG:HG3	1.93	0.69
1:P:358:GLY:O	1:Q:337:ARG:HG3	1.95	0.67
1:H:358:GLY:O	1:I:337:ARG:HG3	1.95	0.66
1:K:362:GLN:HB2	3:K:2008:HOH:O	1.95	0.66
2:S:73:SER:O	2:S:74:GLN:HB2	1.96	0.65
1:C:373:VAL:HG12	1:C:373:VAL:O	1.97	0.65
1:F:334:HIS:HB3	3:F:2002:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:326:LEU:CA	1:L:327:ASP:CB	2.73	0.64
1:A:358:GLY:O	1:B:337:ARG:HG3	1.98	0.64
1:F:358:GLY:O	1:G:337:ARG:HG3	1.97	0.64
1:L:349:ARG:NH2	1:L:371:GLY:HA2	2.13	0.63
2:S:43:ARG:HG3	2:S:50:ILE:HD11	1.80	0.63
1:O:358:GLY:O	1:P:337:ARG:HG3	1.99	0.62
2:T:43:ARG:HG3	2:T:50:ILE:HD11	1.79	0.62
2:T:73:SER:O	2:T:74:GLN:HB2	1.99	0.61
1:G:361:VAL:HG23	3:G:2001:HOH:O	2.00	0.61
2:U:73:SER:O	2:U:74:GLN:HB2	2.00	0.60
1:H:327:ASP:N	3:H:2001:HOH:O	2.34	0.60
1:Q:358:GLY:O	1:R:337:ARG:HG3	2.02	0.59
2:S:35:ASN:HD21	2:S:37:ILE:HD12	1.68	0.58
1:A:371:GLY:C	3:A:2006:HOH:O	2.41	0.58
2:T:35:ASN:HD21	2:T:37:ILE:HD12	1.67	0.58
1:C:370:ASN:O	1:C:371:GLY:C	2.42	0.57
1:C:337:ARG:HD3	1:C:341:ASP:OD2	2.05	0.56
1:D:365:LEU:CD1	2:T:71:VAL:HG21	2.36	0.56
1:C:371:GLY:C	1:C:373:VAL:H	2.10	0.55
2:S:46:TYR:OH	2:S:66:HIS:ND1	2.38	0.55
1:O:327:ASP:OD1	1:O:328:PRO:HD2	2.08	0.54
1:D:325:ILE:N	1:D:326:LEU:CB	2.64	0.53
1:L:349:ARG:HH22	1:L:371:GLY:HA2	1.73	0.53
1:C:326:LEU:O	1:C:327:ASP:HB2	2.08	0.53
1:G:326:LEU:N	1:G:327:ASP:CB	2.72	0.53
1:G:326:LEU:N	1:G:327:ASP:HB3	2.24	0.53
1:E:358:GLY:O	1:F:337:ARG:HG3	2.10	0.52
1:M:327:ASP:OD1	1:M:328:PRO:HD2	2.10	0.52
1:K:358:GLY:O	1:L:337:ARG:HG3	2.10	0.51
1:J:358:GLY:O	1:K:337:ARG:HG3	2.10	0.51
2:U:35:ASN:HD21	2:U:37:ILE:HD12	1.74	0.51
1:B:358:GLY:O	1:C:337:ARG:HG3	2.11	0.50
1:L:365:LEU:CD1	2:S:71:VAL:HG21	2.41	0.50
1:Q:325:ILE:HG13	1:Q:326:LEU:O	2.12	0.50
1:K:327:ASP:OD1	1:K:328:PRO:HD2	2.11	0.50
1:K:370:ASN:O	1:K:371:GLY:O	2.29	0.49
1:D:365:LEU:HD12	2:T:71:VAL:HG21	1.94	0.49
2:T:9:SER:O	2:T:10:GLY:C	2.50	0.49
1:C:342:MET:O	1:K:342:MET:HE3	2.13	0.49
1:Q:335:GLN:HE21	1:R:337:ARG:NH2	2.11	0.48
2:U:46:TYR:OH	2:U:66:HIS:ND1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:73:SER:O	2:S:74:GLN:CB	2.61	0.47
1:B:331:ARG:HD3	1:B:332:TYR:CZ	2.50	0.47
1:E:327:ASP:OD1	1:E:328:PRO:HD2	2.13	0.47
1:R:327:ASP:OD1	1:R:328:PRO:HD2	2.14	0.47
1:H:349:ARG:NH2	1:H:371:GLY:HA2	2.30	0.46
1:H:337:ARG:HD3	1:H:341:ASP:OD2	2.15	0.46
1:B:326:LEU:O	1:B:327:ASP:HB2	2.15	0.46
1:C:369:LEU:CD1	1:K:365:LEU:HD13	2.32	0.46
1:C:327:ASP:OD1	1:C:328:PRO:HD2	2.14	0.46
1:C:358:GLY:O	1:D:337:ARG:HG3	2.16	0.46
2:T:73:SER:O	2:T:74:GLN:CB	2.63	0.46
1:L:362:GLN:NE2	1:M:341:ASP:O	2.49	0.45
1:A:326:LEU:C	1:A:326:LEU:HD12	2.35	0.45
1:J:327:ASP:OD1	1:J:328:PRO:HD2	2.17	0.45
1:G:327:ASP:OD1	1:G:328:PRO:HD2	2.17	0.45
1:D:358:GLY:O	1:E:337:ARG:HG3	2.17	0.45
1:Q:326:LEU:HD12	1:Q:327:ASP:H	1.81	0.45
1:C:342:MET:HE3	1:K:342:MET:O	2.17	0.45
1:N:365:LEU:HA	1:N:365:LEU:HD23	1.83	0.45
1:K:337:ARG:HD3	1:K:341:ASP:OD2	2.17	0.45
1:P:337:ARG:HD3	1:P:341:ASP:OD2	2.17	0.44
1:B:331:ARG:HD3	1:B:332:TYR:CE2	2.52	0.44
1:A:327:ASP:OD1	1:A:328:PRO:HD2	2.17	0.44
1:Q:326:LEU:HB2	1:Q:327:ASP:CB	2.48	0.44
2:T:35:ASN:ND2	2:T:37:ILE:HD12	2.31	0.44
2:T:2:SER:HA	2:T:20:PRO:HD3	1.98	0.44
1:J:331:ARG:HD3	1:J:332:TYR:CZ	2.51	0.44
2:S:2:SER:HA	2:S:20:PRO:HD3	2.00	0.44
1:R:344:PHE:HZ	1:R:369:LEU:HD21	1.82	0.44
1:B:355:ARG:NH2	1:C:330:GLU:OE1	2.38	0.44
2:S:35:ASN:ND2	2:S:37:ILE:HD12	2.33	0.43
2:U:9:SER:O	2:U:10:GLY:C	2.56	0.43
1:A:327:ASP:HA	1:A:328:PRO:HD3	1.93	0.43
1:J:326:LEU:HD13	1:J:331:ARG:HB2	2.00	0.43
1:N:327:ASP:OD1	1:N:328:PRO:HD2	2.19	0.43
1:R:355:ARG:HH11	1:R:355:ARG:HD3	1.67	0.43
1:E:337:ARG:NH1	3:E:2002:HOH:O	2.52	0.43
2:T:37:ILE:H	2:T:37:ILE:HG13	1.62	0.43
1:Q:342:MET:O	2:U:48:GLY:N	2.44	0.43
1:B:327:ASP:OD1	1:B:328:PRO:HD2	2.19	0.42
1:J:370:ASN:N	1:J:371:GLY:HA3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:327:ASP:OD1	1:I:328:PRO:HD2	2.19	0.42
1:D:365:LEU:HA	1:D:365:LEU:HD23	1.85	0.42
1:B:325:ILE:HA	1:B:326:LEU:HA	1.91	0.42
2:S:9:SER:O	2:S:10:GLY:C	2.57	0.42
1:C:365:LEU:HD13	1:K:369:LEU:CD1	2.42	0.42
1:J:331:ARG:HD3	1:J:332:TYR:CE2	2.54	0.42
1:C:331:ARG:HD3	1:C:332:TYR:CZ	2.55	0.42
1:G:331:ARG:HD3	1:G:332:TYR:CE2	2.54	0.41
2:T:51:LEU:HD22	2:T:60:TYR:CD2	2.55	0.41
1:P:365:LEU:HA	1:P:365:LEU:HD23	1.84	0.41
2:U:73:SER:O	2:U:74:GLN:CB	2.66	0.41
1:D:327:ASP:OD1	1:D:328:PRO:HD2	2.19	0.41
1:Q:331:ARG:HD3	1:Q:332:TYR:CZ	2.56	0.41
1:K:331:ARG:HD3	1:K:332:TYR:CZ	2.55	0.41
1:E:346:ASP:OD1	1:E:346:ASP:C	2.59	0.41
1:F:365:LEU:HD23	1:F:365:LEU:HA	1.89	0.41
1:H:327:ASP:OD1	1:H:328:PRO:HD2	2.20	0.41
2:U:63:GLN:HB2	2:U:66:HIS:CD2	2.55	0.41
1:H:331:ARG:HD3	1:H:332:TYR:CZ	2.56	0.41
1:Q:342:MET:HE2	2:U:69:HIS:HB2	2.03	0.41
1:M:331:ARG:HD3	1:M:332:TYR:CE2	2.55	0.41
2:S:51:LEU:HD22	2:S:60:TYR:CD2	2.56	0.41
1:E:355:ARG:HH11	1:E:355:ARG:HD3	1.74	0.41
1:L:365:LEU:HD12	2:S:71:VAL:HG21	2.03	0.41
1:N:331:ARG:HD3	1:N:332:TYR:CZ	2.56	0.41
1:L:346:ASP:OD1	1:L:346:ASP:C	2.59	0.40
1:Q:326:LEU:HB2	1:Q:327:ASP:HB2	2.03	0.40
2:U:63:GLN:HB2	2:U:66:HIS:NE2	2.36	0.40
1:J:344:PHE:HZ	1:J:369:LEU:HD21	1.86	0.40
1:J:355:ARG:HD3	1:J:355:ARG:HH11	1.70	0.40
1:F:331:ARG:HD3	1:F:332:TYR:CZ	2.57	0.40
1:L:334:HIS:HB3	3:L:2005:HOH:O	2.20	0.40
1:E:365:LEU:HA	1:E:365:LEU:HD23	1.79	0.40
1:D:336:LEU:HA	1:D:336:LEU:HD23	1.87	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	44/50 (88%)	41 (93%)	2 (4%)	1 (2%)	8 35
1	B	46/50 (92%)	42 (91%)	3 (6%)	1 (2%)	8 36
1	C	46/50 (92%)	44 (96%)	1 (2%)	1 (2%)	8 36
1	D	45/50 (90%)	42 (93%)	3 (7%)	0	100 100
1	E	44/50 (88%)	42 (96%)	1 (2%)	1 (2%)	8 35
1	F	43/50 (86%)	40 (93%)	3 (7%)	0	100 100
1	G	44/50 (88%)	41 (93%)	2 (4%)	1 (2%)	8 35
1	H	43/50 (86%)	42 (98%)	1 (2%)	0	100 100
1	I	43/50 (86%)	41 (95%)	2 (5%)	0	100 100
1	J	44/50 (88%)	43 (98%)	1 (2%)	0	100 100
1	K	45/50 (90%)	42 (93%)	1 (2%)	2 (4%)	3 18
1	L	44/50 (88%)	42 (96%)	1 (2%)	1 (2%)	8 35
1	M	43/50 (86%)	42 (98%)	1 (2%)	0	100 100
1	N	44/50 (88%)	41 (93%)	2 (4%)	1 (2%)	8 35
1	O	44/50 (88%)	41 (93%)	2 (4%)	1 (2%)	8 35
1	P	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
1	Q	45/50 (90%)	42 (93%)	3 (7%)	0	100 100
1	R	44/50 (88%)	43 (98%)	1 (2%)	0	100 100
2	S	71/77 (92%)	62 (87%)	7 (10%)	2 (3%)	6 30
2	T	71/77 (92%)	62 (87%)	6 (8%)	3 (4%)	3 19
2	U	70/77 (91%)	62 (89%)	6 (9%)	2 (3%)	6 29
All	All	1005/1131 (89%)	938 (93%)	50 (5%)	17 (2%)	11 43

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	ASP
1	G	327	ASP
1	L	327	ASP
1	N	327	ASP
1	A	327	ASP
1	B	327	ASP
1	K	371	GLY
2	S	10	GLY
2	T	10	GLY
2	U	10	GLY
1	O	327	ASP
2	S	35	ASN
2	T	35	ASN
2	U	35	ASN
1	K	327	ASP
1	E	327	ASP
2	T	39	VAL

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	38/41 (93%)	32 (84%)	6 (16%)	3 13
1	B	39/41 (95%)	31 (80%)	8 (20%)	1 6
1	C	40/41 (98%)	35 (88%)	5 (12%)	6 22
1	D	39/41 (95%)	31 (80%)	8 (20%)	1 6
1	E	38/41 (93%)	33 (87%)	5 (13%)	5 20
1	F	37/41 (90%)	30 (81%)	7 (19%)	2 8
1	G	38/41 (93%)	31 (82%)	7 (18%)	2 9
1	H	37/41 (90%)	32 (86%)	5 (14%)	5 20
1	I	37/41 (90%)	31 (84%)	6 (16%)	3 12
1	J	38/41 (93%)	31 (82%)	7 (18%)	2 9
1	K	39/41 (95%)	31 (80%)	8 (20%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	38/41 (93%)	33 (87%)	5 (13%)	5 20
1	M	37/41 (90%)	31 (84%)	6 (16%)	3 12
1	N	38/41 (93%)	32 (84%)	6 (16%)	3 13
1	O	38/41 (93%)	30 (79%)	8 (21%)	1 6
1	P	37/41 (90%)	31 (84%)	6 (16%)	3 12
1	Q	39/41 (95%)	33 (85%)	6 (15%)	3 14
1	R	38/41 (93%)	33 (87%)	5 (13%)	5 20
2	S	64/69 (93%)	56 (88%)	8 (12%)	6 22
2	T	64/69 (93%)	56 (88%)	8 (12%)	6 22
2	U	63/69 (91%)	56 (89%)	7 (11%)	8 29
All	All	876/945 (93%)	739 (84%)	137 (16%)	3 14

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	LEU
1	A	334	HIS
1	A	337	ARG
1	A	349	ARG
1	A	365	LEU
1	A	370	ASN
1	B	325	ILE
1	B	326	LEU
1	B	330	GLU
1	B	337	ARG
1	B	341	ASP
1	B	349	ARG
1	B	365	LEU
1	B	370	ASN
1	C	330	GLU
1	C	337	ARG
1	C	349	ARG
1	C	365	LEU
1	C	370	ASN
1	D	325	ILE
1	D	326	LEU
1	D	330	GLU
1	D	337	ARG

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Mol	Chain	Res	Type
1	D	349	ARG
1	D	365	LEU
1	D	369	LEU
1	D	370	ASN
1	E	330	GLU
1	E	337	ARG
1	E	349	ARG
1	E	365	LEU
1	E	370	ASN
1	F	330	GLU
1	F	331	ARG
1	F	334	HIS
1	F	337	ARG
1	F	349	ARG
1	F	365	LEU
1	F	370	ASN
1	G	326	LEU
1	G	330	GLU
1	G	337	ARG
1	G	349	ARG
1	G	356	ARG
1	G	365	LEU
1	G	370	ASN
1	H	330	GLU
1	H	337	ARG
1	H	349	ARG
1	H	365	LEU
1	H	370	ASN
1	I	330	GLU
1	I	337	ARG
1	I	349	ARG
1	I	356	ARG
1	I	365	LEU
1	I	370	ASN
1	J	326	LEU
1	J	330	GLU
1	J	337	ARG
1	J	349	ARG
1	J	356	ARG
1	J	365	LEU
1	J	370	ASN
1	K	330	GLU

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Mol	Chain	Res	Type
1	K	331	ARG
1	K	337	ARG
1	K	349	ARG
1	K	356	ARG
1	K	365	LEU
1	K	370	ASN
1	K	372	ASP
1	L	330	GLU
1	L	337	ARG
1	L	349	ARG
1	L	365	LEU
1	L	370	ASN
1	M	330	GLU
1	M	331	ARG
1	M	337	ARG
1	M	349	ARG
1	M	365	LEU
1	M	370	ASN
1	N	330	GLU
1	N	337	ARG
1	N	349	ARG
1	N	356	ARG
1	N	365	LEU
1	N	370	ASN
1	O	326	LEU
1	O	330	GLU
1	O	334	HIS
1	O	337	ARG
1	O	349	ARG
1	O	356	ARG
1	O	365	LEU
1	O	370	ASN
1	P	330	GLU
1	P	334	HIS
1	P	337	ARG
1	P	349	ARG
1	P	365	LEU
1	P	370	ASN
1	Q	326	LEU
1	Q	330	GLU
1	Q	337	ARG
1	Q	349	ARG

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Mol	Chain	Res	Type
1	Q	365	LEU
1	Q	370	ASN
1	R	331	ARG
1	R	337	ARG
1	R	349	ARG
1	R	365	LEU
1	R	370	ASN
2	S	13	LYS
2	S	15	GLU
2	S	21	GLU
2	S	26	GLN
2	S	41	ASN
2	S	47	SER
2	S	70	LEU
2	S	72	LYS
2	T	13	LYS
2	T	15	GLU
2	T	21	GLU
2	T	26	GLN
2	T	41	ASN
2	T	47	SER
2	T	70	LEU
2	T	72	LYS
2	U	15	GLU
2	U	21	GLU
2	U	26	GLN
2	U	35	ASN
2	U	41	ASN
2	U	47	SER
2	U	72	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	D	362	GLN
1	E	334	HIS
1	E	338	GLN
1	L	338	GLN
1	L	362	GLN
1	M	338	GLN
1	O	338	GLN

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Mol	Chain	Res	Type
1	Q	370	ASN
1	R	334	HIS
1	R	338	GLN
2	S	35	ASN
2	S	74	GLN
2	T	32	ASN
2	T	35	ASN
2	T	63	GLN
2	U	32	ASN
2	U	35	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, 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	46/50 (92%)	0.22	0 100 100	79, 83, 86, 89	0
1	B	48/50 (96%)	0.25	0 100 100	81, 83, 87, 89	0
1	C	48/50 (96%)	0.43	0 100 100	81, 83, 86, 88	1 (2%)
1	D	47/50 (94%)	0.45	0 100 100	81, 83, 85, 88	0
1	E	46/50 (92%)	0.29	0 100 100	80, 83, 85, 88	0
1	F	45/50 (90%)	0.17	1 (2%) 65 42	81, 83, 86, 88	0
1	G	46/50 (92%)	0.05	0 100 100	81, 83, 86, 88	0
1	H	45/50 (90%)	0.08	1 (2%) 65 42	81, 83, 86, 88	0
1	I	45/50 (90%)	0.13	0 100 100	81, 83, 85, 88	0
1	J	46/50 (92%)	0.36	0 100 100	81, 83, 86, 88	0
1	K	47/50 (94%)	0.35	0 100 100	72, 83, 85, 88	1 (2%)
1	L	46/50 (92%)	0.36	0 100 100	81, 83, 86, 88	0
1	M	45/50 (90%)	0.27	0 100 100	80, 83, 86, 88	0
1	N	46/50 (92%)	0.09	0 100 100	81, 83, 85, 88	0
1	O	46/50 (92%)	0.16	0 100 100	81, 83, 86, 88	0
1	P	44/50 (88%)	0.04	0 100 100	81, 83, 85, 88	1 (2%)
1	Q	47/50 (94%)	0.13	0 100 100	51, 83, 87, 91	0
1	R	46/50 (92%)	0.30	0 100 100	79, 83, 86, 88	0
2	S	73/77 (94%)	0.06	0 100 100	72, 81, 85, 86	0
2	T	73/77 (94%)	0.11	0 100 100	72, 81, 85, 86	0
2	U	72/77 (93%)	0.37	2 (2%) 56 32	72, 81, 85, 86	0
All	All	1047/1131 (92%)	0.22	4 (0%) 93 85	51, 83, 86, 91	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	368	LEU	2.2
2	U	16	VAL	2.2
2	U	56	THR	2.1
1	F	339	LEU	2.1

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.