



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2017 – 04:20 PM EST

PDB ID : 4UE1
Title : Structure of the stapled peptide YS-01 bound to MDM2
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Deposited on : 2014-12-14
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

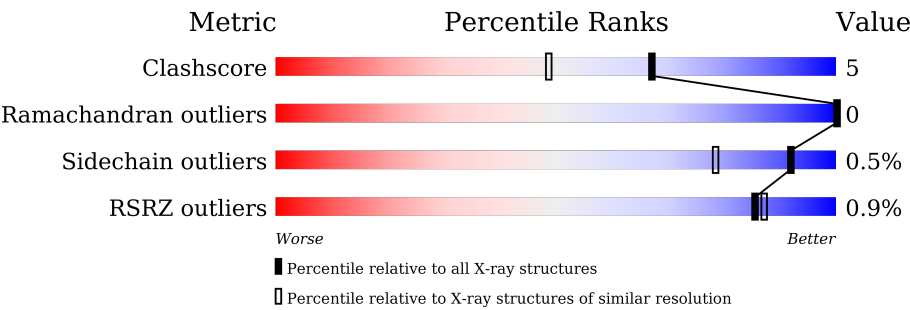
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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))
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	114	<div><div></div><div>82% . . 12%</div></div>
1	B	114	<div><div></div><div>82% 5% 12%</div></div>
1	C	114	<div><div>%</div><div>72% 12% 16%</div></div>
1	D	114	<div><div></div><div>77% 6% . 16%</div></div>
2	F	16	<div><div>13%</div><div>75% 25%</div></div>
2	G	16	<div><div></div><div>75% 13% 6% 6%</div></div>
2	H	16	<div><div>6%</div><div>63% 13% 25%</div></div>

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Mol	Chain	Length	Quality of chain
2	I	16	 75% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4072 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 E3 UBIQUITIN-PROTEIN LIGASE MDM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	7	0
			852	552	141	154	5			
1	B	100	Total	C	N	O	S	0	3	0
			824	534	136	149	5			
1	C	96	Total	C	N	O	S	0	5	0
			818	533	135	146	4			
1	D	96	Total	C	N	O	S	0	5	0
			820	533	136	146	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	EXPRESSION TAG	UNP Q00987
A	13	PRO	-	EXPRESSION TAG	UNP Q00987
A	14	LEU	-	EXPRESSION TAG	UNP Q00987
A	15	GLY	-	EXPRESSION TAG	UNP Q00987
A	16	SER	-	EXPRESSION TAG	UNP Q00987
A	69	ALA	GLU	ENGINEERED MUTATION	UNP Q00987
A	70	ALA	LYS	ENGINEERED MUTATION	UNP Q00987
B	12	GLY	-	EXPRESSION TAG	UNP Q00987
B	13	PRO	-	EXPRESSION TAG	UNP Q00987
B	14	LEU	-	EXPRESSION TAG	UNP Q00987
B	15	GLY	-	EXPRESSION TAG	UNP Q00987
B	16	SER	-	EXPRESSION TAG	UNP Q00987
B	69	ALA	GLU	ENGINEERED MUTATION	UNP Q00987
B	70	ALA	LYS	ENGINEERED MUTATION	UNP Q00987
C	12	GLY	-	EXPRESSION TAG	UNP Q00987
C	13	PRO	-	EXPRESSION TAG	UNP Q00987
C	14	LEU	-	EXPRESSION TAG	UNP Q00987
C	15	GLY	-	EXPRESSION TAG	UNP Q00987
C	16	SER	-	EXPRESSION TAG	UNP Q00987
C	69	ALA	GLU	ENGINEERED MUTATION	UNP Q00987
C	70	ALA	LYS	ENGINEERED MUTATION	UNP Q00987

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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	GLY	-	EXPRESSION TAG	UNP Q00987
D	13	PRO	-	EXPRESSION TAG	UNP Q00987
D	14	LEU	-	EXPRESSION TAG	UNP Q00987
D	15	GLY	-	EXPRESSION TAG	UNP Q00987
D	16	SER	-	EXPRESSION TAG	UNP Q00987
D	69	ALA	GLU	ENGINEERED MUTATION	UNP Q00987
D	70	ALA	LYS	ENGINEERED MUTATION	UNP Q00987

- Molecule 2 is a protein called YS-01.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	16	Total	C	N	O	0	1	1
			140	98	18	24			
2	G	15	Total	C	N	O	0	2	1
			145	100	20	25			
2	H	12	Total	C	N	O	0	0	0
			103	74	12	17			
2	I	12	Total	C	N	O	0	0	0
			103	74	12	17			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	61	Total	O	0	0
			61	61		
3	C	53	Total	O	0	0
			53	53		
3	D	59	Total	O	0	0
			59	59		
3	F	3	Total	O	0	0
			3	3		
3	G	3	Total	O	0	0
			3	3		
3	H	3	Total	O	0	0
			3	3		
3	I	4	Total	O	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.10Å 69.46Å 78.56Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	76.86 – 1.45 45.10 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (76.86-1.45) 94.4 (45.10-1.45)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.140 , 0.184 0.142 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4072	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 46.99 % 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 1.0577e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2JN, ACE, NH2

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	0.54	0/868	0.82	2/1172 (0.2%)
1	B	0.57	0/840	0.74	1/1135 (0.1%)
1	C	0.54	0/833	0.72	0/1126
1	D	0.58	0/835	0.87	4/1128 (0.4%)
2	F	0.61	0/122	0.56	0/165
2	G	0.71	0/129	0.64	0/174
2	H	0.64	0/85	0.62	0/114
2	I	0.65	0/85	0.61	0/114
All	All	0.57	0/3797	0.77	7/5128 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62[A]	MET	CG-SD-CE	-10.09	84.06	100.20
1	D	62[B]	MET	CG-SD-CE	-10.09	84.06	100.20
1	A	62[A]	MET	CG-SD-CE	-9.14	85.58	100.20
1	A	62[B]	MET	CG-SD-CE	-9.14	85.58	100.20
1	B	50	MET	CG-SD-CE	5.60	109.16	100.20
1	D	62[A]	MET	CA-CB-CG	-5.17	104.50	113.30
1	D	62[B]	MET	CA-CB-CG	-5.17	104.50	113.30

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	852	0	884	9	0
1	B	824	0	851	8	0
1	C	818	0	853	12	0
1	D	820	0	852	8	0
2	F	140	0	128	4	0
2	G	145	0	129	2	0
2	H	103	0	96	2	0
2	I	103	0	96	0	0
3	A	81	0	0	3	0
3	B	61	0	0	0	0
3	C	53	0	0	5	0
3	D	59	0	0	2	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	4	0	0	0	0
All	All	4072	0	3889	37	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 5.

All (37) 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:24:GLN:HG2	3:C:2004:HOH:O	1.60	1.02
1:C:29:ARG:NH1	3:C:2012:HOH:O	2.03	0.89
1:C:17:SER:HB3	3:C:2001:HOH:O	1.76	0.85
1:A:105:ARG:HD3	3:A:2063:HOH:O	1.91	0.69
1:B:62[B]:MET:SD	1:B:67:TYR:CE1	2.86	0.69
1:D:96:HIS:HD2	3:D:2030:HOH:O	1.75	0.68
1:D:107[A]:LEU:HD12	1:D:107[A]:LEU:C	2.14	0.67
1:C:102:MET:HG2	3:C:2052:HOH:O	1.95	0.66
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.60	0.65
3:A:2070:HOH:O	2:F:29:ASN:HB3	1.95	0.64
1:C:24:GLN:NE2	3:C:2006:HOH:O	2.34	0.60
1:D:107[A]:LEU:HD12	1:D:107[A]:LEU:O	2.01	0.60
1:D:96:HIS:CD2	3:D:2030:HOH:O	2.55	0.56
1:A:27[A]:LEU:HD12	1:B:27:LEU:HD12	1.88	0.55
1:B:105:ARG:NH1	1:B:105:ARG:HG2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:25:LEU:O	2:G:29[A]:ASN:HB3	2.09	0.53
1:C:43:ALA:HB1	1:C:48:TYR:OH	2.09	0.52
1:A:27[A]:LEU:CD1	1:B:27:LEU:HD12	2.39	0.52
1:C:107[B]:LEU:HD12	1:C:107[B]:LEU:C	2.29	0.52
2:F:23:TRP:HD1	2:F:24:2JN:H11	1.75	0.51
1:A:27[A]:LEU:HD12	1:B:27:LEU:CD1	2.42	0.49
1:A:27[B]:LEU:HD22	1:B:27:LEU:HD12	1.94	0.48
1:A:101[A]:THR:OG1	1:C:76:TYR:HB3	2.16	0.45
1:D:33:LEU:HD21	1:D:84:ASP:HB3	1.99	0.44
2:H:26:LEU:HB2	2:H:27:PRO:CD	2.48	0.43
1:D:107[A]:LEU:CD1	1:D:107[A]:LEU:C	2.84	0.43
1:D:62[B]:MET:CE	1:D:67:TYR:CE1	3.02	0.43
2:H:26:LEU:HB2	2:H:27:PRO:HD3	2.00	0.43
1:B:55:PHE:CE1	2:G:24:2JN:H12	2.54	0.42
1:D:45:LYS:NZ	1:D:52:GLU:OE2	2.53	0.42
1:C:64:LYS:HB3	1:C:64:LYS:HE3	1.79	0.42
1:C:111:ASN:O	1:C:112:GLN:HB2	2.19	0.42
1:A:101[A]:THR:HG23	1:C:78:SER:CB	2.50	0.41
1:A:62[A]:MET:HE2	2:F:20:2JN:H11	2.03	0.41
3:A:2070:HOH:O	2:F:29:ASN:CB	2.63	0.41
1:A:74:ILE:HG21	1:A:76:TYR:CE2	2.56	0.40
1:C:34:LEU:HB2	1:C:85[B]:LEU:HD11	2.04	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	105/114 (92%)	105 (100%)	0	0	100	100
1	B	101/114 (89%)	100 (99%)	1 (1%)	0	100	100
1	C	99/114 (87%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	99/114 (87%)	97 (98%)	2 (2%)	0	100	100
2	F	9/16 (56%)	9 (100%)	0	0	100	100
2	G	9/16 (56%)	9 (100%)	0	0	100	100
2	H	4/16 (25%)	3 (75%)	1 (25%)	0	100	100
2	I	4/16 (25%)	4 (100%)	0	0	100	100
All	All	430/520 (83%)	425 (99%)	5 (1%)	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	97/103 (94%)	97 (100%)	0	100	100
1	B	93/103 (90%)	93 (100%)	0	100	100
1	C	93/103 (90%)	93 (100%)	0	100	100
1	D	93/103 (90%)	91 (98%)	2 (2%)	60	22
2	F	13/12 (108%)	13 (100%)	0	100	100
2	G	14/12 (117%)	12 (86%)	2 (14%)	4	0
2	H	9/12 (75%)	9 (100%)	0	100	100
2	I	9/12 (75%)	9 (100%)	0	100	100
All	All	421/460 (92%)	417 (99%)	4 (1%)	92	56

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	62[A]	MET
1	D	62[B]	MET
2	G	29[A]	ASN
2	G	29[B]	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	24	GLN
2	F	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2JN	F	20	2	6,8,9	0.51	0	3,10,12	1.42	1 (33%)
2	2JN	F	24	2	6,8,9	0.40	0	3,10,12	1.16	0
2	2JN	G	20	2	6,8,9	0.63	0	3,10,12	0.92	0
2	2JN	G	24	2	6,8,9	1.71	1 (16%)	3,10,12	1.58	1 (33%)
2	2JN	H	20	2	6,8,9	0.82	0	3,10,12	0.91	0
2	2JN	H	24	2	6,8,9	1.04	1 (16%)	3,10,12	1.01	0
2	2JN	I	20	2	6,8,9	0.52	0	3,10,12	1.35	1 (33%)
2	2JN	I	24	2	6,8,9	0.99	1 (16%)	3,10,12	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2JN	F	20	2	-	0/6/8/11	0/0/0/0
2	2JN	F	24	2	-	0/6/8/11	0/0/0/0
2	2JN	G	20	2	-	0/6/8/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2JN	G	24	2	-	0/6/8/11	0/0/0/0
2	2JN	H	20	2	-	0/6/8/11	0/0/0/0
2	2JN	H	24	2	-	0/6/8/11	0/0/0/0
2	2JN	I	20	2	-	0/6/8/11	0/0/0/0
2	2JN	I	24	2	-	0/6/8/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	24	2JN	CAO-CAQ	-3.99	1.50	1.55
2	I	24	2JN	CAO-CAQ	-2.16	1.52	1.55
2	H	24	2JN	CAO-CAQ	-2.03	1.52	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	24	2JN	CAO-CAM-CAK	-2.65	106.34	112.86
2	F	20	2JN	CAO-CAM-CAK	-2.40	106.97	112.86
2	I	20	2JN	CAO-CAM-CAK	-2.23	107.37	112.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	20	2JN	1	0
2	F	24	2JN	1	0
2	G	24	2JN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	100/114 (87%)	-0.30	0 100 100	11, 17, 34, 39	0
1	B	100/114 (87%)	-0.37	0 100 100	12, 17, 33, 43	0
1	C	96/114 (84%)	-0.21	1 (1%) 84 85	11, 20, 39, 56	0
1	D	96/114 (84%)	-0.24	0 100 100	10, 18, 34, 44	0
2	F	12/16 (75%)	0.15	2 (16%) 2 2	12, 23, 38, 46	0
2	G	12/16 (75%)	-0.10	0 100 100	12, 19, 29, 37	0
2	H	9/16 (56%)	0.24	1 (11%) 7 6	14, 20, 35, 49	0
2	I	9/16 (56%)	0.05	0 100 100	14, 21, 38, 38	0
All	All	434/520 (83%)	-0.25	4 (0%) 85 87	10, 19, 36, 56	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	27	PRO	3.2
1	C	112	GLN	3.1
2	F	28	GLU	2.4
2	F	29	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	2JN	F	20	9/10	0.97	0.07	-	13,15,18,21	0
2	2JN	F	24	9/10	0.96	0.08	-	19,22,28,28	0
2	2JN	I	24	9/10	0.96	0.06	-	19,22,24,30	0
2	2JN	I	20	9/10	0.96	0.07	-	14,16,22,23	0
2	2JN	G	20	9/10	0.96	0.08	-	12,14,28,31	0
2	2JN	H	20	9/10	0.98	0.07	-	15,18,25,30	0
2	2JN	G	24	9/10	0.97	0.08	-	15,19,26,28	0
2	2JN	H	24	9/10	0.95	0.07	-	21,25,33,35	0

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.