



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 AM GMT

PDB ID : 2CWO  
Title : Crystal structure of RNA silencing suppressor p21 from Beet Yellows Virus  
Authors : Ye, K.; Patel, D.J.  
Deposited on : 2005-06-22  
Resolution : 3.30 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

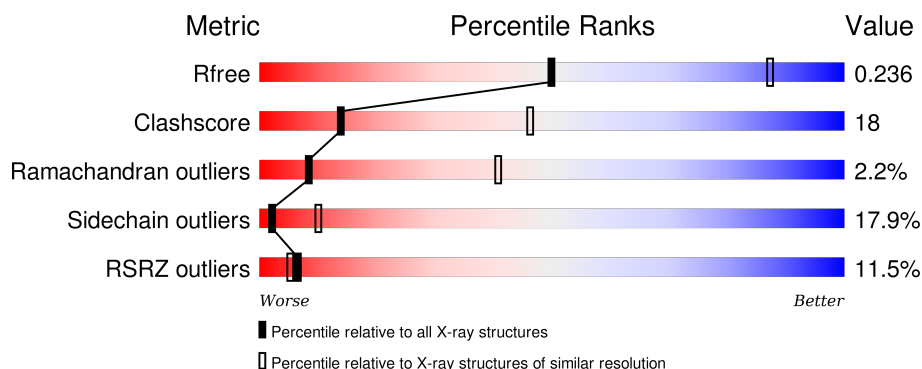
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 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	197	<div> <div>3%</div> <div>42%</div> <div>31%</div> <div>10%</div> <div>16%</div> </div>
1	B	197	<div> <div>9%</div> <div>46%</div> <div>30%</div> <div>8%</div> <div>16%</div> </div>
1	C	197	<div> <div>14%</div> <div>46%</div> <div>32%</div> <div>6%</div> <div>16%</div> </div>
1	D	197	<div> <div>14%</div> <div>49%</div> <div>27%</div> <div>7%</div> <div>16%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5388 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 RNA silencing suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1347	850	236	252	9			
1	B	165	Total	C	N	O	S	0	0	0
			1347	850	236	252	9			
1	C	165	Total	C	N	O	S	0	0	0
			1347	850	236	252	9			
1	D	165	Total	C	N	O	S	0	0	0
			1347	850	236	252	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q08545
A	-18	GLY	-	CLONING ARTIFACT	UNP Q08545
A	-17	SER	-	CLONING ARTIFACT	UNP Q08545
A	-16	SER	-	CLONING ARTIFACT	UNP Q08545
A	-15	HIS	-	CLONING ARTIFACT	UNP Q08545
A	-14	HIS	-	CLONING ARTIFACT	UNP Q08545
A	-13	HIS	-	CLONING ARTIFACT	UNP Q08545
A	-12	HIS	-	CLONING ARTIFACT	UNP Q08545
A	-11	HIS	-	CLONING ARTIFACT	UNP Q08545
A	-10	HIS	-	CLONING ARTIFACT	UNP Q08545
A	-9	SER	-	CLONING ARTIFACT	UNP Q08545
A	-8	SER	-	CLONING ARTIFACT	UNP Q08545
A	-7	GLY	-	CLONING ARTIFACT	UNP Q08545
A	-6	LEU	-	CLONING ARTIFACT	UNP Q08545
A	-5	VAL	-	CLONING ARTIFACT	UNP Q08545
A	-4	PRO	-	CLONING ARTIFACT	UNP Q08545
A	-3	ARG	-	CLONING ARTIFACT	UNP Q08545
A	-2	GLY	-	CLONING ARTIFACT	UNP Q08545
A	-1	SER	-	CLONING ARTIFACT	UNP Q08545
A	0	HIS	-	CLONING ARTIFACT	UNP Q08545
B	-19	MET	-	CLONING ARTIFACT	UNP Q08545

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	CLONING ARTIFACT	UNP Q08545
B	-17	SER	-	CLONING ARTIFACT	UNP Q08545
B	-16	SER	-	CLONING ARTIFACT	UNP Q08545
B	-15	HIS	-	CLONING ARTIFACT	UNP Q08545
B	-14	HIS	-	CLONING ARTIFACT	UNP Q08545
B	-13	HIS	-	CLONING ARTIFACT	UNP Q08545
B	-12	HIS	-	CLONING ARTIFACT	UNP Q08545
B	-11	HIS	-	CLONING ARTIFACT	UNP Q08545
B	-10	HIS	-	CLONING ARTIFACT	UNP Q08545
B	-9	SER	-	CLONING ARTIFACT	UNP Q08545
B	-8	SER	-	CLONING ARTIFACT	UNP Q08545
B	-7	GLY	-	CLONING ARTIFACT	UNP Q08545
B	-6	LEU	-	CLONING ARTIFACT	UNP Q08545
B	-5	VAL	-	CLONING ARTIFACT	UNP Q08545
B	-4	PRO	-	CLONING ARTIFACT	UNP Q08545
B	-3	ARG	-	CLONING ARTIFACT	UNP Q08545
B	-2	GLY	-	CLONING ARTIFACT	UNP Q08545
B	-1	SER	-	CLONING ARTIFACT	UNP Q08545
B	0	HIS	-	CLONING ARTIFACT	UNP Q08545
C	-19	MET	-	CLONING ARTIFACT	UNP Q08545
C	-18	GLY	-	CLONING ARTIFACT	UNP Q08545
C	-17	SER	-	CLONING ARTIFACT	UNP Q08545
C	-16	SER	-	CLONING ARTIFACT	UNP Q08545
C	-15	HIS	-	CLONING ARTIFACT	UNP Q08545
C	-14	HIS	-	CLONING ARTIFACT	UNP Q08545
C	-13	HIS	-	CLONING ARTIFACT	UNP Q08545
C	-12	HIS	-	CLONING ARTIFACT	UNP Q08545
C	-11	HIS	-	CLONING ARTIFACT	UNP Q08545
C	-10	HIS	-	CLONING ARTIFACT	UNP Q08545
C	-9	SER	-	CLONING ARTIFACT	UNP Q08545
C	-8	SER	-	CLONING ARTIFACT	UNP Q08545
C	-7	GLY	-	CLONING ARTIFACT	UNP Q08545
C	-6	LEU	-	CLONING ARTIFACT	UNP Q08545
C	-5	VAL	-	CLONING ARTIFACT	UNP Q08545
C	-4	PRO	-	CLONING ARTIFACT	UNP Q08545
C	-3	ARG	-	CLONING ARTIFACT	UNP Q08545
C	-2	GLY	-	CLONING ARTIFACT	UNP Q08545
C	-1	SER	-	CLONING ARTIFACT	UNP Q08545
C	0	HIS	-	CLONING ARTIFACT	UNP Q08545
D	-19	MET	-	CLONING ARTIFACT	UNP Q08545
D	-18	GLY	-	CLONING ARTIFACT	UNP Q08545
D	-17	SER	-	CLONING ARTIFACT	UNP Q08545

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	CLONING ARTIFACT	UNP Q08545
D	-15	HIS	-	CLONING ARTIFACT	UNP Q08545
D	-14	HIS	-	CLONING ARTIFACT	UNP Q08545
D	-13	HIS	-	CLONING ARTIFACT	UNP Q08545
D	-12	HIS	-	CLONING ARTIFACT	UNP Q08545
D	-11	HIS	-	CLONING ARTIFACT	UNP Q08545
D	-10	HIS	-	CLONING ARTIFACT	UNP Q08545
D	-9	SER	-	CLONING ARTIFACT	UNP Q08545
D	-8	SER	-	CLONING ARTIFACT	UNP Q08545
D	-7	GLY	-	CLONING ARTIFACT	UNP Q08545
D	-6	LEU	-	CLONING ARTIFACT	UNP Q08545
D	-5	VAL	-	CLONING ARTIFACT	UNP Q08545
D	-4	PRO	-	CLONING ARTIFACT	UNP Q08545
D	-3	ARG	-	CLONING ARTIFACT	UNP Q08545
D	-2	GLY	-	CLONING ARTIFACT	UNP Q08545
D	-1	SER	-	CLONING ARTIFACT	UNP Q08545
D	0	HIS	-	CLONING ARTIFACT	UNP Q08545

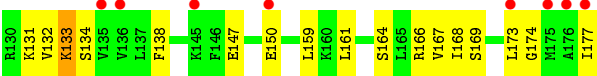
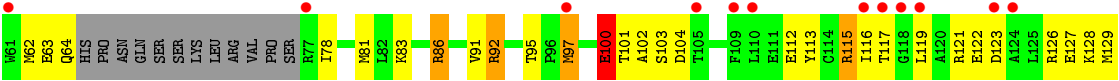


- Molecule 1: RNA silencing suppressor





● Molecule 1: RNA silencing suppressor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.63 Å   199.63 Å   56.12 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 3.30 34.58 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.30) 97.9 (34.58-3.19)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.18 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.210 , 0.244 0.205 , 0.236	Depositor DCC
$R_{free}$ test set	951 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 160.5	EDS
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 21434 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.13	4/1364 (0.3%)	1.07	2/1824 (0.1%)
1	B	0.75	0/1364	0.84	1/1824 (0.1%)
1	C	0.82	0/1364	0.88	1/1824 (0.1%)
1	D	0.77	1/1364 (0.1%)	0.85	0/1824
All	All	0.88	5/5456 (0.1%)	0.91	4/7296 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	100	GLU	CG-CD	7.74	1.63	1.51
1	A	39	CYS	CB-SG	-6.57	1.71	1.82
1	A	100	GLU	CG-CD	5.87	1.60	1.51
1	A	33	GLN	CG-CD	5.63	1.64	1.51
1	A	131	LYS	CD-CE	5.59	1.65	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	CG-SD-CE	6.57	110.70	100.20
1	B	1	MET	CG-SD-CE	6.45	110.52	100.20
1	A	101	THR	CB-CA-C	-5.37	97.09	111.60
1	C	115	ARG	NE-CZ-NH1	-5.32	117.64	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1347	0	1378	65	0
1	B	1347	0	1378	51	0
1	C	1347	0	1378	48	1
1	D	1347	0	1378	49	1
All	All	5388	0	5512	200	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 18.

All (200) 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:D:6:LYS:O	1:D:9:GLU:HB2	1.70	0.91
1:A:18:GLU:HA	1:A:81:MET:HE1	1.54	0.89
1:B:164:SER:OG	1:B:167:VAL:HG23	1.73	0.89
1:A:97:MET:N	1:A:97:MET:HE3	1.88	0.87
1:C:164:SER:OG	1:C:167:VAL:HG23	1.74	0.87
1:A:6:LYS:O	1:A:9:GLU:HB2	1.74	0.86
1:D:164:SER:OG	1:D:167:VAL:HG23	1.75	0.86
1:C:63:GLU:HB3	1:D:138:PHE:HD1	1.41	0.84
1:C:18:GLU:HA	1:C:81:MET:HE1	1.60	0.83
1:A:63:GLU:HB3	1:B:138:PHE:CE1	2.13	0.83
1:C:63:GLU:HB3	1:D:138:PHE:CD1	2.16	0.81
1:C:14:LEU:HD23	1:C:78:ILE:HG12	1.64	0.80
1:D:18:GLU:HA	1:D:81:MET:HE1	1.63	0.79
1:A:14:LEU:HD23	1:A:78:ILE:HG12	1.61	0.79
1:A:86:ARG:NH2	1:A:147:GLU:HB3	1.98	0.79
1:D:14:LEU:HD23	1:D:78:ILE:HG12	1.64	0.79
1:C:112:GLU:O	1:C:116:ILE:HG12	1.83	0.78
1:B:18:GLU:HA	1:B:81:MET:HE1	1.67	0.77
1:A:101:THR:HG22	1:A:103:SER:H	1.51	0.76
1:A:164:SER:OG	1:A:167:VAL:HG23	1.85	0.76
1:A:2:LYS:HE3	1:A:59:ARG:HD3	1.68	0.75
1:A:29:THR:HG23	1:A:92:ARG:HH12	1.52	0.75
1:B:112:GLU:O	1:B:116:ILE:HG12	1.87	0.75
1:C:4:PHE:O	1:D:44:ASN:OD1	2.05	0.75
1:C:2:LYS:HE3	1:C:59:ARG:HD3	1.69	0.75
1:A:63:GLU:HB3	1:B:138:PHE:HE1	1.51	0.74
1:C:9:GLU:HG3	1:C:49:PHE:CE1	2.23	0.74
1:D:29:THR:HG23	1:D:92:ARG:HH12	1.54	0.73
1:C:9:GLU:HG3	1:C:49:PHE:HE1	1.53	0.72
1:D:97:MET:N	1:D:97:MET:HE3	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:O	1:B:9:GLU:HB2	1.90	0.71
1:B:97:MET:HE3	1:B:97:MET:N	2.04	0.71
1:C:6:LYS:O	1:C:9:GLU:HB2	1.90	0.71
1:D:101:THR:HG22	1:D:103:SER:H	1.56	0.71
1:A:121:ARG:HH21	1:A:177:ILE:HG22	1.57	0.70
1:B:14:LEU:HD23	1:B:78:ILE:HG12	1.74	0.70
1:C:121:ARG:HH21	1:C:177:ILE:HG22	1.55	0.69
1:B:2:LYS:HE3	1:B:59:ARG:HD3	1.74	0.69
1:D:9:GLU:HA	1:D:9:GLU:OE1	1.92	0.69
1:D:112:GLU:O	1:D:116:ILE:HG12	1.94	0.68
1:A:112:GLU:O	1:A:116:ILE:HG12	1.93	0.67
1:D:6:LYS:O	1:D:9:GLU:CB	2.43	0.66
1:D:2:LYS:HE3	1:D:59:ARG:HD3	1.75	0.66
1:B:9:GLU:HG3	1:B:49:PHE:HE1	1.60	0.66
1:B:9:GLU:HG3	1:B:49:PHE:CE1	2.30	0.66
1:B:128:LYS:HG3	1:B:131:LYS:NZ	2.11	0.66
1:A:101:THR:HG22	1:A:102:ALA:N	2.10	0.65
1:A:86:ARG:HH21	1:A:147:GLU:HB3	1.61	0.65
1:D:121:ARG:HH21	1:D:177:ILE:HG22	1.61	0.64
1:D:9:GLU:HG3	1:D:49:PHE:CE1	2.33	0.64
1:A:6:LYS:O	1:A:9:GLU:CB	2.45	0.64
1:C:97:MET:HE3	1:C:97:MET:N	2.12	0.64
1:A:133:LYS:HE2	1:A:134:SER:HB3	1.80	0.63
1:A:113:TYR:O	1:A:117:THR:HG23	1.98	0.63
1:A:29:THR:O	1:A:30:ASN:HB3	1.99	0.62
1:D:9:GLU:HG3	1:D:49:PHE:HE1	1.62	0.62
1:C:12:ARG:O	1:C:16:ARG:HB2	1.99	0.62
1:A:6:LYS:HD2	1:A:6:LYS:H	1.64	0.61
1:A:9:GLU:HG3	1:A:49:PHE:CE1	2.36	0.61
1:B:121:ARG:HH21	1:B:177:ILE:HG22	1.66	0.59
1:B:133:LYS:HE2	1:B:134:SER:HB3	1.84	0.59
1:C:101:THR:HG22	1:C:103:SER:H	1.67	0.59
1:C:3:PHE:O	1:C:59:ARG:NH2	2.36	0.58
1:D:86:ARG:NH2	1:D:147:GLU:O	2.36	0.58
1:D:112:GLU:OE2	1:D:115:ARG:NH1	2.33	0.57
1:A:112:GLU:OE2	1:A:115:ARG:NH1	2.34	0.57
1:B:6:LYS:HD2	1:B:6:LYS:H	1.69	0.57
1:A:63:GLU:CB	1:B:138:PHE:HE1	2.18	0.56
1:B:101:THR:HG22	1:B:103:SER:H	1.71	0.56
1:A:9:GLU:HG3	1:A:49:PHE:HE1	1.70	0.56
1:C:9:GLU:HA	1:C:9:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASP:N	1:A:7:ASP:OD1	2.36	0.55
1:B:6:LYS:O	1:B:9:GLU:CB	2.53	0.55
1:C:6:LYS:O	1:C:9:GLU:CB	2.54	0.55
1:A:126:ARG:HD2	1:A:166:ARG:HH22	1.72	0.55
1:B:12:ARG:O	1:B:16:ARG:HB2	2.07	0.55
1:B:29:THR:HG23	1:B:92:ARG:HH12	1.72	0.54
1:C:29:THR:HG23	1:C:92:ARG:HH12	1.71	0.54
1:B:8:GLY:O	1:B:12:ARG:HB2	2.08	0.54
1:C:133:LYS:HE2	1:C:134:SER:HB3	1.89	0.54
1:A:6:LYS:CD	1:A:6:LYS:H	2.21	0.53
1:D:91:VAL:O	1:D:91:VAL:HG12	2.08	0.53
1:A:63:GLU:HB3	1:B:138:PHE:CD1	2.42	0.53
1:A:127:GLU:O	1:A:164:SER:HA	2.08	0.53
1:A:29:THR:O	1:A:30:ASN:CB	2.56	0.53
1:A:86:ARG:NH2	1:A:147:GLU:O	2.42	0.53
1:B:128:LYS:HG3	1:B:131:LYS:HZ3	1.73	0.52
1:B:9:GLU:HA	1:B:9:GLU:OE1	2.09	0.52
1:B:24:VAL:HG21	1:B:85:ILE:HG23	1.93	0.51
1:C:29:THR:O	1:C:30:ASN:HB3	2.10	0.51
1:A:29:THR:HG23	1:A:92:ARG:NH1	2.22	0.51
1:B:50:ASN:O	1:B:54:VAL:HG23	2.10	0.51
1:A:8:GLY:O	1:A:12:ARG:HB2	2.11	0.51
1:B:7:ASP:N	1:B:7:ASP:OD1	2.42	0.51
1:B:49:PHE:CD2	1:B:49:PHE:C	2.85	0.51
1:D:12:ARG:O	1:D:16:ARG:HB2	2.11	0.50
1:A:9:GLU:OE1	1:A:9:GLU:HA	2.11	0.50
1:D:6:LYS:H	1:D:6:LYS:HD2	1.76	0.50
1:A:4:PHE:O	1:B:44:ASN:OD1	2.30	0.49
1:B:91:VAL:O	1:B:91:VAL:HG12	2.11	0.49
1:B:129:MET:HB3	1:B:161:LEU:O	2.13	0.49
1:C:91:VAL:O	1:C:91:VAL:HG12	2.13	0.49
1:B:86:ARG:NH2	1:B:147:GLU:O	2.46	0.49
1:D:133:LYS:HE2	1:D:134:SER:HB3	1.95	0.48
1:C:7:ASP:N	1:C:7:ASP:OD1	2.40	0.48
1:D:7:ASP:OD1	1:D:7:ASP:N	2.35	0.48
1:B:128:LYS:HG3	1:B:131:LYS:HZ2	1.78	0.48
1:B:112:GLU:OE2	1:B:115:ARG:NH1	2.41	0.48
1:D:126:ARG:HD2	1:D:166:ARG:HH22	1.79	0.48
1:C:101:THR:HG22	1:C:102:ALA:N	2.28	0.48
1:A:51:HIS:NE2	1:B:55:THR:HG21	2.29	0.48
1:D:86:ARG:NH2	1:D:147:GLU:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:GLY:O	1:D:12:ARG:HB2	2.13	0.47
1:A:5:LEU:HG	1:A:56:VAL:HG21	1.96	0.47
1:C:128:LYS:HG3	1:C:131:LYS:NZ	2.30	0.47
1:B:6:LYS:CD	1:B:6:LYS:H	2.27	0.47
1:A:55:THR:HG21	1:B:51:HIS:NE2	2.29	0.47
1:C:155:TYR:O	1:C:158:LEU:HB3	2.15	0.47
1:C:133:LYS:HG2	1:C:159:LEU:O	2.15	0.47
1:C:5:LEU:HG	1:C:56:VAL:HG21	1.97	0.47
1:A:49:PHE:CD2	1:A:49:PHE:C	2.88	0.46
1:B:113:TYR:O	1:B:117:THR:HG23	2.16	0.46
1:B:95:THR:OG1	1:B:97:MET:HG2	2.15	0.46
1:B:101:THR:HG22	1:B:102:ALA:N	2.31	0.46
1:A:101:THR:CG2	1:A:103:SER:H	2.23	0.46
1:C:8:GLY:O	1:C:12:ARG:HB2	2.17	0.45
1:B:29:THR:O	1:B:30:ASN:HB3	2.16	0.45
1:B:5:LEU:HG	1:B:56:VAL:HG21	1.99	0.45
1:A:29:THR:CG2	1:A:92:ARG:HH12	2.26	0.45
1:C:129:MET:HB3	1:C:161:LEU:O	2.16	0.45
1:A:129:MET:HB3	1:A:161:LEU:O	2.16	0.45
1:C:86:ARG:NH2	1:C:147:GLU:O	2.49	0.45
1:A:12:ARG:O	1:A:16:ARG:HB2	2.17	0.45
1:C:86:ARG:O	1:C:90:LYS:HB2	2.17	0.44
1:A:127:GLU:OE1	1:A:128:LYS:N	2.45	0.44
1:C:6:LYS:H	1:C:6:LYS:HD2	1.82	0.44
1:A:50:ASN:O	1:A:54:VAL:HG23	2.18	0.44
1:D:15:SER:HA	1:D:18:GLU:HB2	2.00	0.44
1:C:15:SER:HA	1:C:18:GLU:HB2	1.99	0.44
1:C:121:ARG:NH2	1:C:177:ILE:HG22	2.28	0.44
1:C:147:GLU:OE2	1:D:2:LYS:HB3	2.18	0.44
1:A:96:PRO:C	1:A:97:MET:HE3	2.36	0.43
1:D:29:THR:CG2	1:D:92:ARG:HH12	2.26	0.43
1:A:137:LEU:O	1:A:138:PHE:C	2.56	0.43
1:A:17:SER:HB3	1:A:46:LEU:HD22	2.00	0.43
1:A:101:THR:HB	1:A:104:ASP:OD2	2.17	0.43
1:D:101:THR:HG22	1:D:102:ALA:N	2.33	0.43
1:D:12:ARG:HA	1:D:12:ARG:HD3	1.77	0.43
1:A:4:PHE:CD1	1:A:4:PHE:N	2.86	0.43
1:A:5:LEU:H	1:A:5:LEU:HD12	1.82	0.43
1:D:100:GLU:OE1	1:D:100:GLU:HA	2.18	0.43
1:B:86:ARG:HH21	1:B:147:GLU:HB3	1.83	0.43
1:B:86:ARG:NH2	1:B:147:GLU:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:TYR:O	1:D:117:THR:HG23	2.18	0.43
1:A:32:GLN:HB2	1:A:34:SER:OG	2.19	0.43
1:C:29:THR:O	1:C:30:ASN:CB	2.66	0.43
1:D:91:VAL:CG1	1:D:91:VAL:O	2.67	0.43
1:C:113:TYR:O	1:C:117:THR:HG23	2.19	0.43
1:D:51:HIS:O	1:D:55:THR:HG23	2.17	0.43
1:D:29:THR:HG23	1:D:92:ARG:NH1	2.27	0.43
1:A:91:VAL:HG12	1:A:91:VAL:O	2.18	0.43
1:C:18:GLU:HA	1:C:81:MET:CE	2.39	0.43
1:C:50:ASN:O	1:C:54:VAL:HG23	2.18	0.43
1:B:126:ARG:HD2	1:B:166:ARG:HH22	1.84	0.43
1:A:49:PHE:HE2	1:A:53:LEU:HD22	1.84	0.42
1:D:18:GLU:HA	1:D:81:MET:CE	2.43	0.42
1:A:104:ASP:N	1:A:104:ASP:OD2	2.50	0.42
1:C:24:VAL:HG21	1:C:85:ILE:HG23	2.00	0.42
1:C:5:LEU:HD12	1:C:5:LEU:H	1.84	0.42
1:B:157:GLU:HA	1:B:157:GLU:OE2	2.18	0.42
1:A:121:ARG:NH2	1:A:177:ILE:HG22	2.29	0.42
1:A:141:SER:HA	1:A:146:PHE:O	2.19	0.42
1:C:138:PHE:CD1	1:D:63:GLU:HB3	2.55	0.42
1:D:112:GLU:HA	1:D:112:GLU:OE1	2.18	0.42
1:C:12:ARG:HA	1:C:12:ARG:HD3	1.86	0.42
1:C:24:VAL:CG1	1:C:88:PHE:HB3	2.50	0.42
1:C:51:HIS:O	1:C:55:THR:HG23	2.20	0.42
1:D:128:LYS:HG3	1:D:131:LYS:NZ	2.35	0.42
1:A:6:LYS:N	1:A:6:LYS:HD2	2.33	0.41
1:D:95:THR:OG1	1:D:97:MET:HG2	2.20	0.41
1:A:12:ARG:HD3	1:A:12:ARG:HA	1.83	0.41
1:A:138:PHE:CD1	1:B:63:GLU:HB3	2.55	0.41
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.20	0.41
1:A:90:LYS:HG2	1:A:152:MET:CG	2.51	0.41
1:D:6:LYS:H	1:D:6:LYS:CD	2.31	0.41
1:B:15:SER:HA	1:B:18:GLU:HB2	2.02	0.41
1:D:5:LEU:HG	1:D:56:VAL:HG21	2.02	0.41
1:C:9:GLU:CG	1:C:49:PHE:HE1	2.27	0.41
1:D:101:THR:HG22	1:D:103:SER:N	2.31	0.41
1:D:164:SER:O	1:D:168:ILE:HG13	2.21	0.41
1:B:86:ARG:O	1:B:90:LYS:HB2	2.19	0.41
1:D:131:LYS:O	1:D:132:VAL:C	2.59	0.41
1:A:131:LYS:O	1:A:132:VAL:C	2.59	0.41
1:A:32:GLN:CB	1:A:34:SER:OG	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LYS:HG2	1:B:152:MET:HG2	2.03	0.40
1:D:133:LYS:HG2	1:D:159:LEU:O	2.20	0.40
1:B:155:TYR:O	1:B:158:LEU:HB3	2.21	0.40
1:D:129:MET:HB3	1:D:161:LEU:O	2.22	0.40
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.81	0.40
1:A:40:VAL:O	1:A:41:ASP:C	2.60	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ASP:O	1:D:123:ASP:OD2[4_556]	1.90	0.30

## 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	161/197 (82%)	149 (92%)	8 (5%)	4 (2%)	7	37
1	B	161/197 (82%)	147 (91%)	11 (7%)	3 (2%)	10	45
1	C	161/197 (82%)	147 (91%)	10 (6%)	4 (2%)	7	37
1	D	161/197 (82%)	148 (92%)	10 (6%)	3 (2%)	10	45
All	All	644/788 (82%)	591 (92%)	39 (6%)	14 (2%)	8	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	B	30	ASN
1	C	30	ASN
1	D	30	ASN

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Mol	Chain	Res	Type
1	A	36	ILE
1	A	174	GLY
1	B	174	GLY
1	C	36	ILE
1	C	174	GLY
1	D	36	ILE
1	D	174	GLY
1	A	35	GLU
1	B	36	ILE
1	C	35	GLU

### 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	152/181 (84%)	125 (82%)	27 (18%)	2	10
1	B	152/181 (84%)	124 (82%)	28 (18%)	2	9
1	C	152/181 (84%)	126 (83%)	26 (17%)	2	12
1	D	152/181 (84%)	124 (82%)	28 (18%)	2	9
All	All	608/724 (84%)	499 (82%)	109 (18%)	2	10

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	6	LYS
1	A	7	ASP
1	A	9	GLU
1	A	12	ARG
1	A	14	LEU
1	A	16	ARG
1	A	29	THR
1	A	31	SER
1	A	39	CYS

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Mol	Chain	Res	Type
1	A	44	ASN
1	A	62	MET
1	A	64	GLN
1	A	77	ARG
1	A	83	LYS
1	A	86	ARG
1	A	92	ARG
1	A	97	MET
1	A	100	GLU
1	A	104	ASP
1	A	119	LEU
1	A	122	GLU
1	A	127	GLU
1	A	133	LYS
1	A	150	GLU
1	A	173	LEU
1	B	1	MET
1	B	5	LEU
1	B	6	LYS
1	B	7	ASP
1	B	9	GLU
1	B	12	ARG
1	B	14	LEU
1	B	16	ARG
1	B	29	THR
1	B	31	SER
1	B	39	CYS
1	B	44	ASN
1	B	62	MET
1	B	64	GLN
1	B	83	LYS
1	B	86	ARG
1	B	92	ARG
1	B	97	MET
1	B	100	GLU
1	B	104	ASP
1	B	119	LEU
1	B	122	GLU
1	B	127	GLU
1	B	133	LYS
1	B	143	LEU
1	B	150	GLU

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Mol	Chain	Res	Type
1	B	169	SER
1	B	173	LEU
1	C	1	MET
1	C	5	LEU
1	C	6	LYS
1	C	7	ASP
1	C	12	ARG
1	C	14	LEU
1	C	29	THR
1	C	31	SER
1	C	39	CYS
1	C	44	ASN
1	C	62	MET
1	C	64	GLN
1	C	83	LYS
1	C	86	ARG
1	C	90	LYS
1	C	92	ARG
1	C	97	MET
1	C	100	GLU
1	C	104	ASP
1	C	119	LEU
1	C	122	GLU
1	C	127	GLU
1	C	133	LYS
1	C	150	GLU
1	C	169	SER
1	C	173	LEU
1	D	1	MET
1	D	5	LEU
1	D	6	LYS
1	D	7	ASP
1	D	9	GLU
1	D	12	ARG
1	D	14	LEU
1	D	16	ARG
1	D	29	THR
1	D	31	SER
1	D	39	CYS
1	D	44	ASN
1	D	62	MET
1	D	64	GLN

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Mol	Chain	Res	Type
1	D	83	LYS
1	D	86	ARG
1	D	92	ARG
1	D	97	MET
1	D	100	GLU
1	D	104	ASP
1	D	115	ARG
1	D	119	LEU
1	D	122	GLU
1	D	127	GLU
1	D	133	LYS
1	D	150	GLU
1	D	169	SER
1	D	173	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	B	64	GLN
1	C	64	GLN
1	C	107	ASN
1	D	64	GLN

### 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	165/197 (83%)	0.27	5 (3%) 54 47	128, 132, 136, 143	0
1	B	165/197 (83%)	0.59	17 (10%) 9 7	128, 132, 136, 142	0
1	C	165/197 (83%)	0.89	27 (16%) 2 2	128, 132, 136, 143	0
1	D	165/197 (83%)	0.83	27 (16%) 2 2	128, 132, 136, 142	0
All	All	660/788 (83%)	0.64	76 (11%) 6 5	128, 132, 136, 143	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	ILE	8.2
1	D	176	ALA	6.5
1	C	177	ILE	6.3
1	B	177	ILE	5.9
1	C	88	PHE	5.6
1	C	33	GLN	5.6
1	B	176	ALA	5.5
1	C	64	GLN	5.2
1	B	61	TRP	4.9
1	B	30	ASN	4.9
1	C	34	SER	4.7
1	D	124	ALA	4.7
1	D	117	THR	4.6
1	D	175	MET	4.5
1	D	119	LEU	4.4
1	D	17	SER	4.3
1	C	7	ASP	4.1
1	B	39	CYS	4.1
1	D	109	PHE	4.1
1	D	136	VAL	4.0
1	C	25	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	61	TRP	3.8
1	B	113	TYR	3.7
1	D	135	VAL	3.7
1	A	62	MET	3.6
1	D	116	ILE	3.5
1	C	89	LEU	3.5
1	B	92	ARG	3.3
1	D	77	ARG	3.3
1	C	24	VAL	3.3
1	C	20	LEU	3.2
1	C	1	MET	3.2
1	B	175	MET	3.1
1	B	62	MET	3.1
1	D	118	GLY	3.0
1	A	33	GLN	3.0
1	C	146	PHE	3.0
1	C	172	ILE	2.9
1	C	6	LYS	2.9
1	B	124	ALA	2.9
1	B	64	GLN	2.9
1	C	78	ILE	2.8
1	D	173	LEU	2.8
1	C	5	LEU	2.8
1	D	110	LEU	2.8
1	C	87	ALA	2.7
1	A	57	GLU	2.6
1	B	10	THR	2.6
1	D	97	MET	2.6
1	B	36	ILE	2.5
1	C	40	VAL	2.4
1	D	49	PHE	2.4
1	D	10	THR	2.4
1	D	44	ASN	2.4
1	D	123	ASP	2.3
1	B	9	GLU	2.3
1	C	4	PHE	2.3
1	C	13	ALA	2.3
1	C	91	VAL	2.3
1	C	175	MET	2.2
1	C	61	TRP	2.2
1	D	48	SER	2.2
1	B	116	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	61	TRP	2.2
1	D	150	GLU	2.2
1	A	177	ILE	2.2
1	D	15	SER	2.2
1	C	11	SER	2.1
1	C	17	SER	2.1
1	C	46	LEU	2.1
1	C	21	LEU	2.1
1	D	105	THR	2.1
1	D	145	LYS	2.1
1	D	53	LEU	2.0
1	B	32	GLN	2.0
1	B	131	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 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.