



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2014 – 03:13 PM GMT

PDB ID : 4OO8  
Title : Crystal structure of Streptococcus pyogenes Cas9 in complex with guide RNA and target DNA  
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Deposited on : 2014-01-31  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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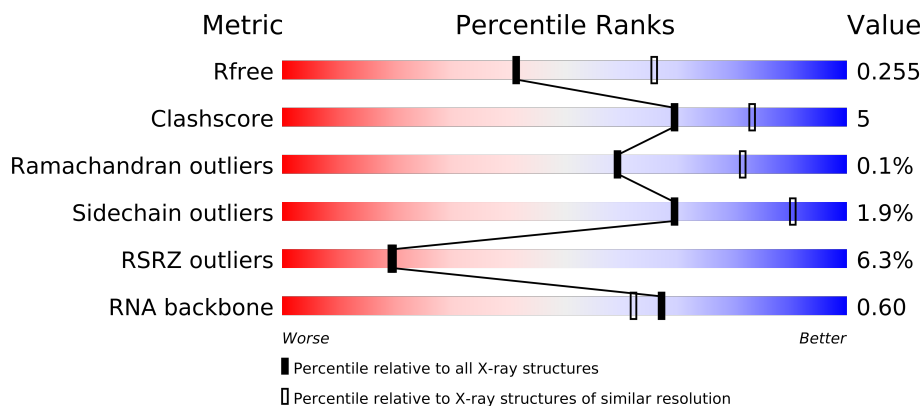
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : trunk22714  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk22714

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)
RNA backbone	1838	1107 (3.10-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1372	
1	D	1372	
2	B	98	
2	E	98	
3	C	23	
3	F	23	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24153 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1301	Total	C	N	O	S	0	0	0
			9999	6388	1708	1883	20			
1	D	1163	Total	C	N	O	S	0	0	0
			8998	5754	1529	1698	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q99ZW2
A	-2	SER	-	EXPRESSION TAG	UNP Q99ZW2
A	-1	GLY	-	EXPRESSION TAG	UNP Q99ZW2
A	0	HIS	-	EXPRESSION TAG	UNP Q99ZW2
A	10	ALA	ASP	ENGINEERED MUTATION	UNP Q99ZW2
A	80	LEU	CYS	ENGINEERED MUTATION	UNP Q99ZW2
A	574	GLU	CYS	ENGINEERED MUTATION	UNP Q99ZW2
A	840	ALA	HIS	ENGINEERED MUTATION	UNP Q99ZW2
D	-3	GLY	-	EXPRESSION TAG	UNP Q99ZW2
D	-2	SER	-	EXPRESSION TAG	UNP Q99ZW2
D	-1	GLY	-	EXPRESSION TAG	UNP Q99ZW2
D	0	HIS	-	EXPRESSION TAG	UNP Q99ZW2
D	10	ALA	ASP	ENGINEERED MUTATION	UNP Q99ZW2
D	80	LEU	CYS	ENGINEERED MUTATION	UNP Q99ZW2
D	574	GLU	CYS	ENGINEERED MUTATION	UNP Q99ZW2
D	840	ALA	HIS	ENGINEERED MUTATION	UNP Q99ZW2

- Molecule 2 is a RNA chain called RNA (97-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	P	0	0	0
			2082	930	380	675	97			
2	E	97	Total	C	N	O	P	0	0	0
			2082	930	380	675	97			

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*CP\*AP\*GP\*CP\*CP\*AP\*AP\*GP\*CP\*GP\*CP\*AP\*CP\*CP\*TP\*AP\*AP\*TP\*TP\*TP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total 404	C 192	N 72	O 120	P 20	0	0	1
3	F	23	Total 444	C 211	N 80	O 131	P 22	0	0	1

- Molecule 4 is water.

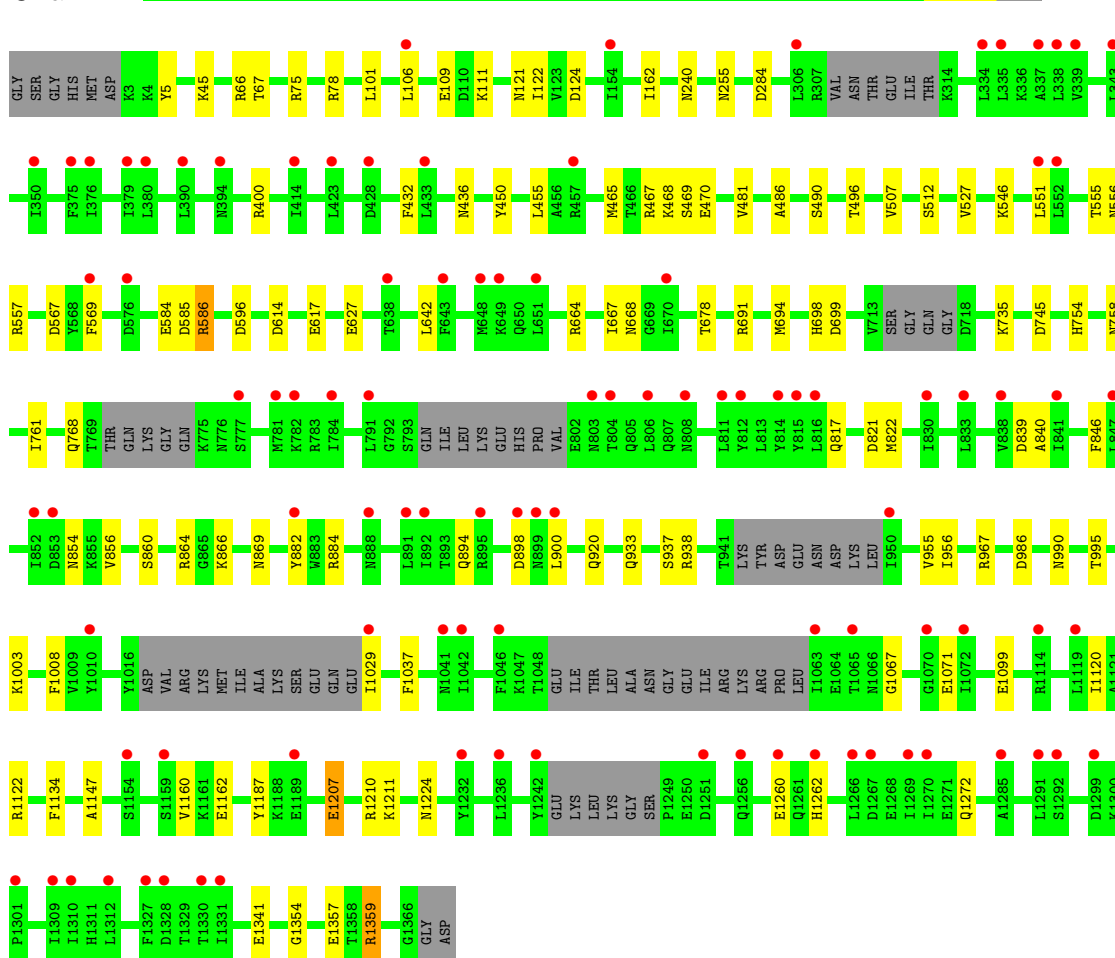
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total 32	O 32	0	0
4	B	28	Total 28	O 28	0	0
4	C	2	Total 2	O 2	0	0
4	D	49	Total 49	O 49	0	0
4	E	32	Total 32	O 32	0	0
4	F	1	Total 1	O 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CRISPR-associated endonuclease Cas9/Csn1

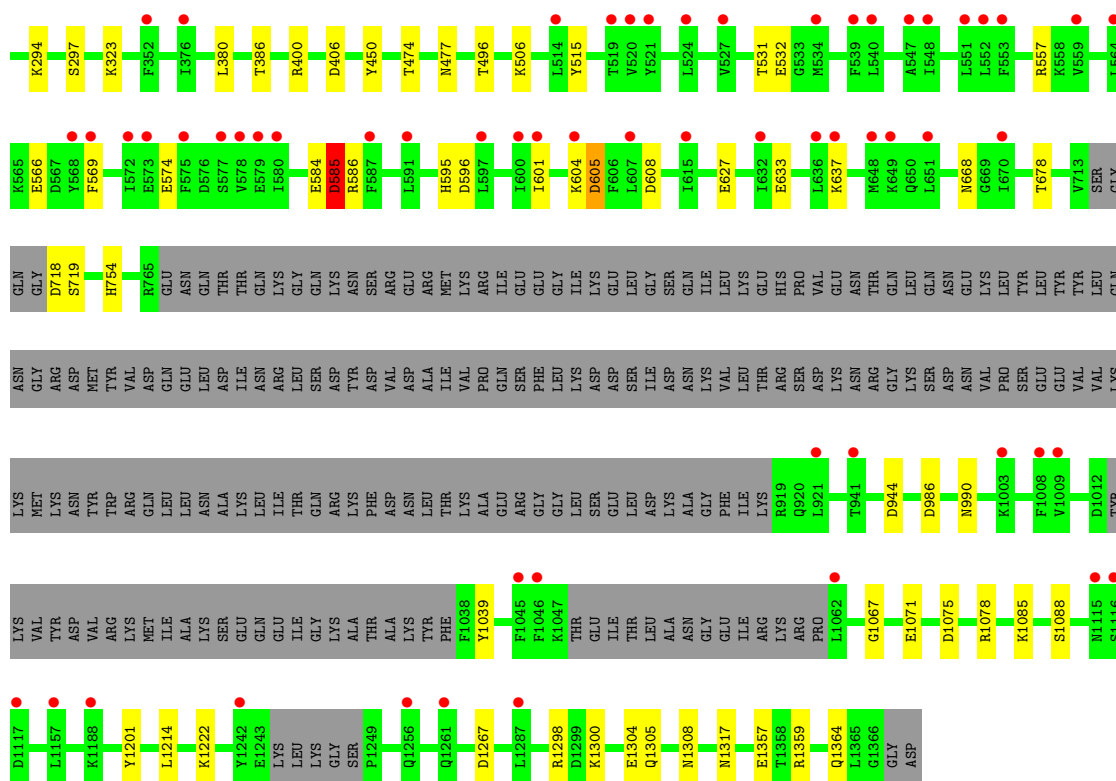
Chain A:



#### • Molecule 1: CRISPR-associated endonuclease Cas9/Csn1

Chain D:





• Molecule 2: RNA (97-MER)

Chain B:



• Molecule 2: RNA (97-MER)

Chain E:



• Molecule 3: DNA (5'-D(\*CP\*CP\*AP\*GP\*CP\*CP\*AP\*AP\*GP\*CP\*GP\*CP\*AP\*CP\*CP\*TP\*AP\*AP\*TP\*TP\*TP\*CP\*C)-3')

Chain C:



• Molecule 3: DNA (5'-D(\*CP\*CP\*AP\*GP\*CP\*CP\*AP\*AP\*GP\*CP\*GP\*CP\*AP\*CP\*CP\*TP\*AP\*AP\*TP\*TP\*TP\*CP\*C)-3')

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.71Å 105.69Å 126.82Å 97.68° 98.43° 100.31°	Depositor
Resolution (Å)	46.70 – 2.50 46.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.70-2.50) 98.6 (46.88-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.222 , 0.254 0.226 , 0.255	Depositor DCC
$R_{free}$ test set	6519 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 130450 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.22	0/10177	0.36	0/13792
1	D	0.22	0/9164	0.37	0/12424
2	B	0.29	1/2332 (0.0%)	0.70	0/3633
2	E	0.30	1/2332 (0.0%)	0.70	0/3633
3	C	0.70	1/451 (0.2%)	0.86	0/693
3	F	0.70	1/496 (0.2%)	0.91	0/762
All	All	0.27	4/24952 (0.0%)	0.48	0/34937

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	G	OP3-P	-10.58	1.48	1.61
3	F	-2	DC	O3'-P	-10.56	1.48	1.61
2	B	1	G	OP3-P	-10.56	1.48	1.61
3	C	0	DA	O3'-P	-10.52	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9999	0	0	54	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	8998	0	0	42	1
2	B	2082	0	0	7	0
2	E	2082	0	0	5	0
3	C	404	0	0	0	0
3	F	444	0	0	0	0
4	A	32	0	0	2	0
4	B	28	0	0	0	0
4	C	2	0	0	0	0
4	D	49	0	0	0	0
4	E	32	0	0	0	0
4	F	1	0	0	0	0
All	All	24153	0	0	97	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:100:ARG:NH1	1:D:117:PRO:O	2.26	0.69
1:A:967:ARG:NH1	1:A:986:ASP:OD1	2.26	0.69
1:D:1222:LYS:NZ	1:D:1317:ASN:O	2.26	0.68
1:D:1067:GLY:N	1:D:1071:GLU:O	2.29	0.65
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.28	0.65
1:A:1207:GLU:OE1	1:A:1210:ARG:NH2	2.31	0.63
1:A:400:ARG:NH1	4:A:1417:HOH:O	2.32	0.62
1:D:94:ASP:OD2	1:D:100:ARG:NH2	2.33	0.62
1:A:745:ASP:OD2	1:A:938:ARG:NH2	2.33	0.61
1:A:668:ASN:ND2	1:A:678:THR:OG1	2.33	0.61
1:D:71:ARG:NH1	2:E:18:G:N7	2.49	0.60
1:D:1357:GLU:OE1	1:D:1359:ARG:NE	2.34	0.60
1:D:236:GLY:O	1:D:240:ASN:ND2	2.35	0.60
1:A:1210:ARG:NH1	1:A:1341:GLU:OE1	2.36	0.59
1:A:432:PHE:O	1:A:436:ASN:ND2	2.36	0.58
1:D:39:ASP:O	1:D:41:HIS:ND1	2.36	0.58
1:A:66:ARG:NH1	4:A:1405:HOH:O	2.36	0.57
1:D:986:ASP:O	1:D:990:ASN:ND2	2.38	0.56
1:A:467:ARG:NH1	2:B:59:U:OP1	2.38	0.56
1:A:1162:GLU:OE1	1:A:1187:TYR:OH	2.24	0.55
1:A:1067:GLY:N	1:A:1071:GLU:O	2.40	0.54
1:A:584:GLU:O	1:A:586:ARG:N	2.40	0.54
1:D:604:LYS:NZ	1:D:608:ASP:OD2	2.40	0.54
1:A:450:TYR:OH	1:A:627:GLU:OE2	2.26	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:718:ASP:OD1	1:D:719:SER:N	2.40	0.54
1:A:78:ARG:NH1	1:A:162:ILE:O	2.41	0.54
1:D:450:TYR:OH	1:D:627:GLU:OE2	2.27	0.53
1:D:531:THR:OG1	1:D:532:GLU:OE1	2.27	0.53
1:A:1122:ARG:NH2	2:B:49:A:N3	2.57	0.53
1:D:1300:LYS:O	1:D:1305:GLN:NE2	2.42	0.53
1:A:1272:GLN:NE2	2:B:89:G:O6	2.43	0.52
1:A:894:GLN:NE2	1:A:898:ASP:OD2	2.42	0.52
1:A:614:ASP:OD1	1:A:664:ARG:NH2	2.43	0.52
1:A:512:SER:OG	1:A:617:GLU:OE2	2.28	0.52
1:D:124:ASP:N	1:D:124:ASP:OD2	2.42	0.51
1:D:1085:LYS:O	1:D:1088:SER:OG	2.28	0.51
1:A:1211:LYS:N	1:A:1224:ASN:OD1	2.44	0.51
1:D:633:GLU:O	1:D:637:LYS:NZ	2.44	0.51
1:D:569:PHE:O	1:D:574:GLU:N	2.44	0.51
1:D:31:LYS:NZ	2:E:84:A:N7	2.59	0.50
1:D:532:GLU:N	1:D:532:GLU:OE1	2.44	0.50
1:D:5:TYR:OH	1:D:754:HIS:O	2.30	0.49
1:D:380:LEU:O	1:D:386:THR:OG1	2.30	0.49
1:A:1357:GLU:OE1	1:A:1359:ARG:NH1	2.46	0.49
1:D:585:ASP:OD2	1:D:585:ASP:N	2.45	0.49
1:A:986:ASP:O	1:A:990:ASN:ND2	2.46	0.48
1:A:240:ASN:ND2	1:A:255:ASN:OD1	2.46	0.48
1:A:106:LEU:O	1:A:111:LYS:NZ	2.46	0.48
1:D:496:THR:OG1	1:D:506:LYS:NZ	2.45	0.48
1:A:735:LYS:NZ	1:A:1099:GLU:OE2	2.46	0.48
1:A:5:TYR:OH	1:A:754:HIS:O	2.32	0.48
1:D:557:ARG:NH2	1:D:596:ASP:OD1	2.47	0.48
1:A:121:ASN:ND2	1:A:124:ASP:OD2	2.47	0.48
1:A:821:ASP:OD1	1:A:822:MET:N	2.47	0.47
1:A:45:LYS:NZ	1:A:1357:GLU:OE2	2.48	0.47
1:D:294:LYS:O	1:D:297:SER:OG	2.32	0.47
1:D:400:ARG:NH2	1:D:406:ASP:OD2	2.47	0.47
1:A:551:LEU:O	1:A:555:THR:OG1	2.33	0.47
2:E:27:G:N2	2:E:44:U:OP2	2.48	0.47
1:A:1272:GLN:OE1	2:B:89:G:N1	2.48	0.46
1:A:1147:ALA:O	1:A:1160:VAL:N	2.48	0.46
1:D:1267:ASP:OD1	1:D:1298:ARG:NH1	2.49	0.46
1:A:839:ASP:OD2	1:A:840:ALA:N	2.48	0.46
1:A:817:GLN:O	1:A:882:TYR:OH	2.34	0.46
1:A:864:ARG:NH2	1:A:866:LYS:O	2.49	0.46
1:D:515:TYR:OH	2:E:5:A:OP1	2.34	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:933:GLN:NE2	1:A:937:SER:OG	2.48	0.46
1:A:854:ASN:O	1:A:854:ASN:ND2	2.48	0.45
1:D:269:ASP:N	1:D:269:ASP:OD1	2.49	0.45
1:D:30:LYS:NZ	2:E:83:C:OP1	2.50	0.45
1:A:468:LYS:N	1:A:481:VAL:O	2.49	0.45
1:D:103:GLU:OE2	1:D:112:LYS:N	2.49	0.45
1:D:668:ASN:ND2	1:D:678:THR:OG1	2.50	0.45
1:D:1304:GLU:O	1:D:1308:ASN:ND2	2.49	0.45
1:A:45:LYS:NZ	1:A:1354:GLY:O	2.50	0.44
1:D:209:LYS:O	1:D:213:SER:OG	2.35	0.44
1:D:605:ASP:N	1:D:605:ASP:OD1	2.50	0.44
1:D:474:THR:N	1:D:477:ASN:OD1	2.51	0.43
1:D:584:GLU:O	1:D:586:ARG:N	2.51	0.43
1:D:1075:ASP:OD1	1:D:1078:ARG:N	2.52	0.43
1:A:694:MET:O	1:A:698:HIS:ND1	2.50	0.43
1:A:1120:ILE:N	1:A:1134:PHE:O	2.51	0.43
1:A:691:ARG:NH1	1:A:699:ASP:OD2	2.52	0.43
1:A:109:GLU:OE2	1:A:109:GLU:N	2.52	0.42
1:A:66:ARG:NH2	2:B:15:C:OP2	2.52	0.42
1:A:846:PHE:O	1:A:920:GLN:NE2	2.53	0.42
1:A:839:ASP:O	1:A:856:VAL:N	2.52	0.42
1:A:469:SER:OG	1:A:470:GLU:N	2.53	0.42
1:A:75:ARG:NH2	2:B:50:U:O4	2.53	0.41
1:A:761:ILE:N	1:A:956:ILE:O	2.53	0.41
1:A:101:LEU:O	2:B:47:A:O2'	2.38	0.41
1:A:955:VAL:O	1:A:1008:PHE:N	2.54	0.41
1:D:1201:TYR:N	1:D:1214:LEU:O	2.53	0.41
1:D:406:ASP:N	1:D:406:ASP:OD1	2.54	0.41
1:A:758:ASN:ND2	1:A:995:THR:OG1	2.54	0.40
1:A:486:ALA:O	1:A:490:SER:OG	2.39	0.40
1:D:1364:GLN:OE1	1:D:1364:GLN:N	2.54	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	Distance(Å)	Clash(Å)
1:A:860:SER:OG	1:D:944:ASP:O[1_454]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1283/1372 (94%)	1252 (98%)	30 (2%)	1 (0%)	59	81
1	D	1151/1372 (84%)	1108 (96%)	42 (4%)	1 (0%)	59	81
All	All	2434/2744 (89%)	2360 (97%)	72 (3%)	2 (0%)	59	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	585	ASP
1	A	585	ASP

### 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	1013/1227 (83%)	987 (97%)	26 (3%)	59	84
1	D	921/1227 (75%)	911 (99%)	10 (1%)	84	96
All	All	1934/2454 (79%)	1898 (98%)	36 (2%)	69	90

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	122	ILE
1	A	284	ASP
1	A	455	LEU
1	A	465	MET
1	A	496	THR
1	A	507	VAL

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Mol	Chain	Res	Type
1	A	527	VAL
1	A	546	LYS
1	A	556	ASN
1	A	567	ASP
1	A	569	PHE
1	A	586	ARG
1	A	642	LEU
1	A	667	ILE
1	A	768	GLN
1	A	869	ASN
1	A	884	ARG
1	A	900	LEU
1	A	1003	LYS
1	A	1029	ILE
1	A	1037	PHE
1	A	1207	GLU
1	A	1260	GLU
1	A	1262	HIS
1	A	1359	ARG
1	D	31	LYS
1	D	124	ASP
1	D	228	GLN
1	D	323	LYS
1	D	566	GLU
1	D	585	ASP
1	D	595	HIS
1	D	601	ILE
1	D	605	ASP
1	D	1039	TYR

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/98 (97%)	15 (15%)	1 (1%)
2	E	96/98 (97%)	17 (17%)	0
All	All	192/196 (97%)	32 (16%)	1 (0%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	A
2	B	9	G
2	B	28	A
2	B	37	U
2	B	39	G
2	B	40	C
2	B	51	A
2	B	59	U
2	B	63	U
2	B	68	A
2	B	72	U
2	B	77	A
2	B	87	G
2	B	89	G
2	B	91	C
2	E	28	A
2	E	34	A
2	E	37	U
2	E	39	G
2	E	40	C
2	E	51	A
2	E	56	U
2	E	57	A
2	E	59	U
2	E	68	A
2	E	76	A
2	E	77	A
2	E	79	G
2	E	89	G
2	E	91	C
2	E	93	G
2	E	96	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	38	A

## 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<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	1301/1372 (94%)	0.56	98 (7%) 14 14	36, 82, 120, 160	0
1	D	1163/1372 (84%)	0.48	70 (6%) 21 21	40, 75, 117, 166	0
2	B	97/98 (98%)	0.39	1 (1%) 79 81	40, 75, 146, 168	0
2	E	97/98 (98%)	0.39	2 (2%) 60 63	44, 77, 173, 189	0
3	C	21/23 (91%)	0.23	0 100 100	49, 65, 102, 108	0
3	F	23/23 (100%)	0.18	0 100 100	53, 64, 131, 152	0
All	All	2702/2986 (90%)	0.51	171 (6%) 19 19	36, 78, 121, 189	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	552	LEU	5.9
1	A	643	PHE	5.7
1	A	806	LEU	5.7
1	D	564	LEU	5.5
1	A	852	ILE	5.4
1	D	1256	GLN	5.3
1	A	1312	LEU	4.9
1	D	568	TYR	4.8
1	D	597	LEU	4.8
1	D	1116	SER	4.6
1	D	607	LEU	4.5
1	D	651	LEU	4.4
1	D	648	MET	4.3
1	D	587	PHE	4.3
1	A	1330	THR	4.3
1	A	335	LEU	4.2
1	D	1242	TYR	4.0
1	A	950	ILE	4.0
1	D	600	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1063	ILE	3.9
1	A	1042	ILE	3.8
1	A	812	TYR	3.8
1	A	784	ILE	3.8
1	A	1267	ASP	3.8
1	A	1292	SER	3.8
1	A	895	ARG	3.7
1	D	579	GLU	3.7
1	A	1309	ILE	3.6
1	A	803	ASN	3.6
1	A	1301	PRO	3.5
1	D	601	ILE	3.5
1	A	1266	LEU	3.5
1	A	1046	PHE	3.5
1	D	1115	ASN	3.4
1	A	1310	ILE	3.4
1	A	833	LEU	3.4
1	D	569	PHE	3.4
1	A	433	LEU	3.4
1	A	338	LEU	3.4
1	A	350	ILE	3.4
1	A	390	LEU	3.4
1	A	552	LEU	3.3
1	D	1045	PHE	3.3
1	A	1029	ILE	3.3
1	D	577	SER	3.3
1	D	229	LEU	3.3
1	D	559	VAL	3.3
1	D	551	LEU	3.3
1	D	1157	LEU	3.3
1	A	1242	TYR	3.3
1	A	423	LEU	3.3
1	A	891	LEU	3.3
1	A	569	PHE	3.3
1	D	575	PHE	3.3
1	A	791	LEU	3.2
1	D	225	LEU	3.2
1	A	888	ASN	3.2
1	A	841	ILE	3.2
1	D	1062	LEU	3.2
1	A	1270	ILE	3.2
1	A	1327	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	376	ILE	3.2
1	A	811	LEU	3.1
1	D	376	ILE	3.1
1	A	900	LEU	3.1
1	D	941	THR	3.1
1	A	1291	LEU	3.0
1	A	899	ASN	3.0
1	A	804	THR	3.0
1	A	1285	ALA	3.0
1	D	615	ILE	3.0
1	A	651	LEU	3.0
1	D	580	ILE	2.9
1	D	636	LEU	2.9
1	A	781	MET	2.9
1	A	1299	ASP	2.9
1	A	1072	ILE	2.9
1	A	782	LYS	2.9
1	D	1009	VAL	2.8
1	A	638	THR	2.8
1	A	337	ALA	2.8
1	A	1189	GLU	2.8
1	A	1331	ILE	2.8
1	D	352	PHE	2.8
1	D	203	ALA	2.7
1	A	1041	ASN	2.7
1	A	816	LEU	2.7
1	A	1236	LEU	2.7
1	D	572	ILE	2.7
1	D	527	VAL	2.7
1	D	548	ILE	2.7
1	A	1328	ASP	2.7
1	A	1232	TYR	2.7
1	A	1070	GLY	2.6
1	A	106	LEU	2.6
1	A	853	ASP	2.6
1	D	1287	LEU	2.6
1	A	838	VAL	2.6
1	D	519	THR	2.6
1	A	898	ASP	2.6
1	A	815	TYR	2.6
1	D	1003	LYS	2.5
1	A	847	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	553	PHE	2.5
2	B	74	A	2.5
1	D	573	GLU	2.5
1	D	591	LEU	2.5
1	A	1256	GLN	2.5
1	A	154	ILE	2.5
1	A	1269	ILE	2.5
1	A	814	TYR	2.5
1	D	632	ILE	2.5
1	A	808	ASN	2.5
1	A	1251	ASP	2.5
1	D	204	SER	2.5
1	A	339	VAL	2.5
1	A	1010	TYR	2.4
1	D	520	VAL	2.4
1	D	189	VAL	2.4
2	E	74	A	2.4
2	E	97	U	2.4
1	D	1046	PHE	2.4
1	D	637	LYS	2.4
1	A	1154	SER	2.4
1	D	521	TYR	2.4
1	D	539	PHE	2.4
1	D	649	LYS	2.3
1	D	1261	GLN	2.3
1	D	231	GLY	2.3
1	A	428	ASP	2.3
1	A	670	ILE	2.3
1	A	379	ILE	2.3
1	A	830	ILE	2.3
1	A	1065	THR	2.3
1	D	182	ASP	2.3
1	D	524	LEU	2.3
1	D	540	LEU	2.3
1	A	334	LEU	2.2
1	A	380	LEU	2.2
1	A	892	ILE	2.2
1	D	921	LEU	2.2
1	A	576	ASP	2.2
1	D	1117	ASP	2.2
1	A	343	LEU	2.2
1	A	1260	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	375	PHE	2.2
1	A	1159	SER	2.2
1	D	195	LEU	2.2
1	D	205	GLY	2.2
1	D	1008	PHE	2.2
1	A	394	ASN	2.1
1	D	670	ILE	2.1
1	D	547	ALA	2.1
1	A	457	ARG	2.1
1	D	222	LEU	2.1
1	A	648	MET	2.1
1	A	882	TYR	2.1
1	A	1114	ARG	2.1
1	A	1262	HIS	2.1
1	A	1119	LEU	2.1
1	D	514	LEU	2.1
1	D	534	MET	2.1
1	A	777	SER	2.1
1	A	306	LEU	2.1
1	D	604	LYS	2.1
1	A	414	ILE	2.1
1	A	551	LEU	2.0
1	A	649	LYS	2.0
1	D	1188	LYS	2.0
1	D	578	VAL	2.0
1	D	224	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.