



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2021 – 11:08 am BST

PDB ID : 7OX7  
Title : Target-bound SpCas9 complex with TRAC chimeric RNA-DNA guide  
Authors : Donohoue, P.; Pacesa, M.; Lau, E.; Vidal, B.; Irby, M.J.; Nyer, D.B.; Rotstein, T.; Banh, L.; Toh, M.T.; Gibson, J.; Kohrs, B.; Baek, K.; Owen, A.L.G.; Slorach, E.M.; van Overbeek, M.; Fuller, C.K.; May, A.P.; Jinek, M.; Cameron, P.  
Deposited on : 2021-06-22  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

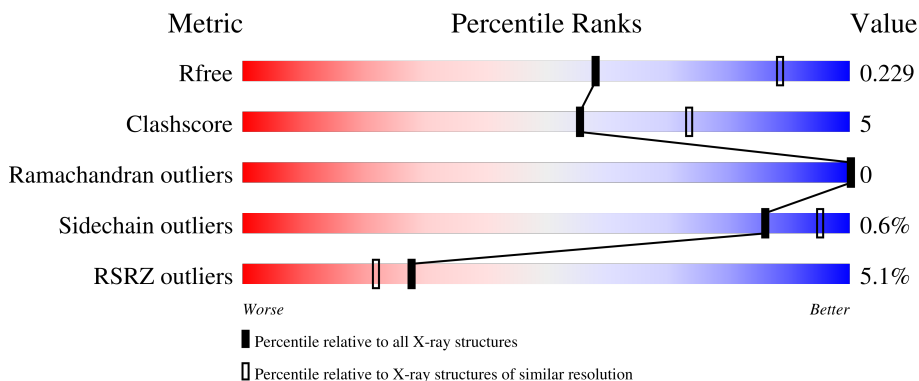
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	81	 2% 58% 42%
2	B	1372	 5% 85% 11% .
3	C	28	 71% 29%
4	D	12	 8% 50% 42% 8%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13729 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 DNA/RNA hybrid called chimeric RNA-DNA guide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	81	1722	779	315	548	80	0	0	0

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1323	10831	6907	1878	2024	22	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q99ZW2
B	-2	ALA	-	expression tag	UNP Q99ZW2
B	-1	ALA	-	expression tag	UNP Q99ZW2
B	0	SER	-	expression tag	UNP Q99ZW2
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called TRAC target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	28	569	272	106	164	27	0	0	0

- Molecule 4 is a DNA chain called TRAC non-target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	11	207	98	37	62	10	0	0	1

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total K 5 5	0	0
6	B	9	Total K 9 9	0	0

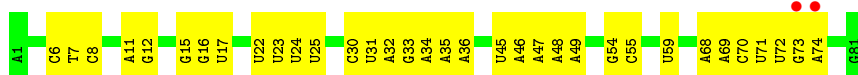
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	117	Total O 117 117	0	0
7	B	241	Total O 241 241	0	0
7	C	20	Total O 20 20	0	0
7	D	6	Total O 6 6	0	0

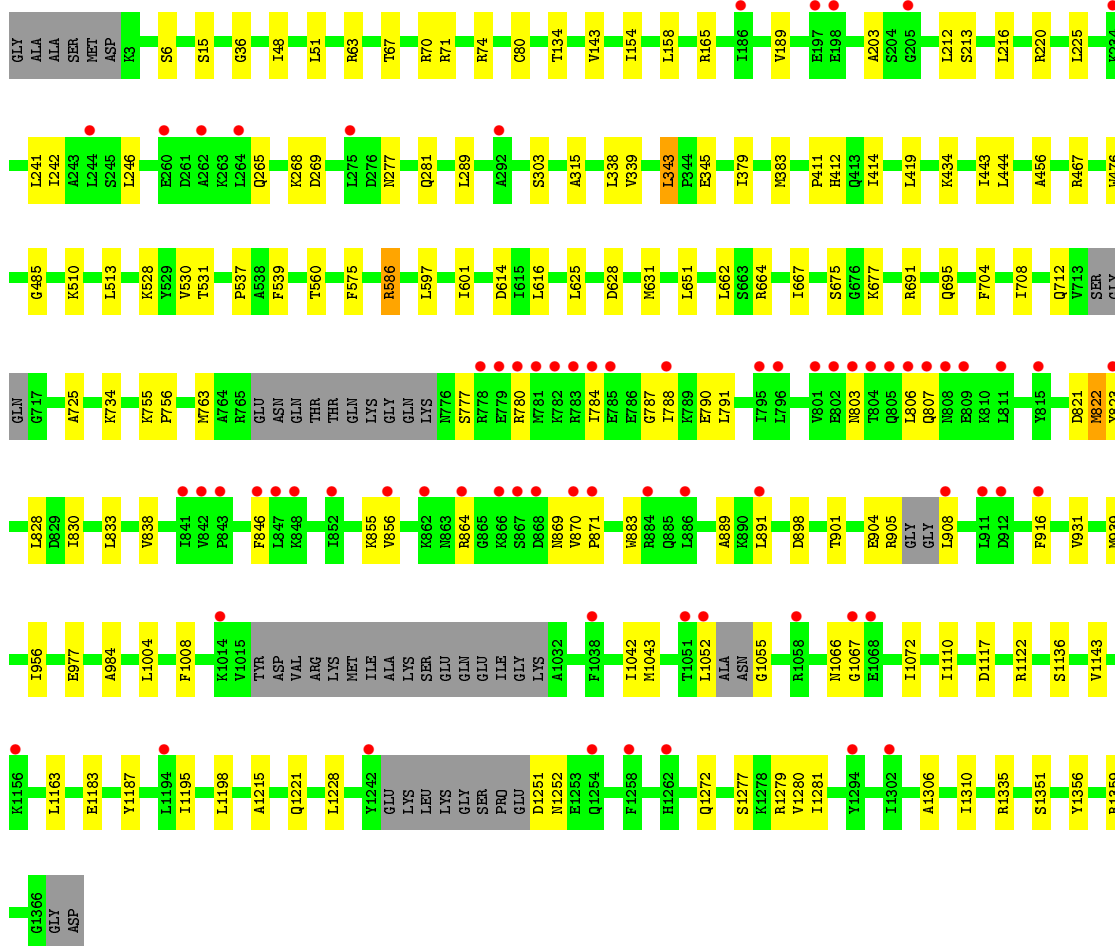
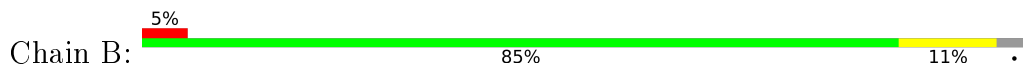
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: chimeric RNA-DNA guide



- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



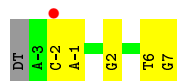
- Molecule 3: TRAC target DNA strand

Chain C:  71% 29%



- Molecule 4: TRAC non-target DNA strand

Chain D:  8% 50% 42% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.54Å 67.41Å 188.14Å 90.00° 112.54° 90.00°	Depositor
Resolution (Å)	42.46 – 2.60 42.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.46-2.60) 99.9 (42.46-2.60)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.209 , 0.229 0.209 , 0.229	Depositor DCC
$R_{free}$ test set	3179 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtrriage
Anisotropy	0.384	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13729	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, 0.333 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: K, MG

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	0.37	0/1930	0.92	0/3003
2	B	0.27	0/11020	0.43	0/14805
3	C	0.65	0/638	1.02	1/982 (0.1%)
4	D	0.62	0/231	0.97	0/356
All	All	0.32	0/13819	0.59	1/19146 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	DG	O4'-C4'-C3'	-6.33	101.97	104.50

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	1722	0	876	32	0
2	B	10831	0	11008	93	0
3	C	569	0	316	7	0
4	D	207	0	114	5	0
5	A	2	0	0	0	0
6	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	0	0	0
7	A	117	0	0	1	0
7	B	241	0	0	2	0
7	C	20	0	0	0	0
7	D	6	0	0	0	0
All	All	13729	0	12314	130	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 (130) 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)
3:C:-6:DA:H2'	3:C:-5:DA:C8	2.21	0.74
1:A:16:G:N7	7:A:201:HOH:O	2.24	0.70
2:B:158:LEU:HD22	2:B:419:LEU:HD12	1.73	0.69
2:B:434:LYS:NZ	7:B:1501:HOH:O	2.27	0.68
2:B:241:LEU:HD11	2:B:289:LEU:HD21	1.78	0.65
1:A:71:U:H2'	1:A:72:U:C6	2.31	0.65
2:B:1335:ARG:NH2	4:D:2:DG:O6	2.33	0.61
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.82	0.61
1:A:17:U:OP2	2:B:74:ARG:NH1	2.33	0.60
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.83	0.59
1:A:46:A:H2'	1:A:47:A:C8	2.37	0.59
2:B:339:VAL:HG13	2:B:343:LEU:HD12	1.83	0.58
3:C:17:DC:H5'	3:C:17:DC:H6	1.67	0.58
1:A:54:G:H2'	1:A:55:C:C6	2.38	0.57
2:B:80:CYS:SG	7:B:1658:HOH:O	2.57	0.57
2:B:763:MET:HE1	2:B:931:VAL:HG21	1.87	0.57
2:B:675:SER:HB2	2:B:677:LYS:HD3	1.87	0.56
2:B:628:ASP:OD1	2:B:631:MET:HG3	2.04	0.56
2:B:614:ASP:OD1	2:B:664:ARG:NH2	2.37	0.56
1:A:70:C:H2'	1:A:71:U:H6	1.71	0.56
4:D:6:DT:H1'	4:D:7:DG:H5'	1.87	0.55
1:A:69:A:H2'	1:A:70:C:H6	1.70	0.55
2:B:36:GLY:HA3	2:B:1359:ARG:O	2.07	0.55
2:B:780:ARG:NH1	2:B:806:LEU:O	2.40	0.55
2:B:704:PHE:O	2:B:708:ILE:HG12	2.07	0.54
2:B:708:ILE:O	2:B:712:GLN:HG2	2.07	0.54
1:A:35:A:H2'	1:A:36:A:C8	2.42	0.54
2:B:822:MET:HG3	2:B:883:TRP:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.89	0.54
1:A:22:U:H2'	1:A:23:U:C6	2.43	0.53
2:B:212:LEU:HD22	2:B:246:LEU:HD21	1.90	0.53
3:C:-5:DA:H1'	3:C:-4:DT:H5'	1.92	0.52
1:A:70:C:H2'	1:A:71:U:C6	2.44	0.52
1:A:6:DC:OP2	2:B:510:LYS:NZ	2.31	0.52
2:B:216:LEU:HB3	2:B:220:ARG:HD3	1.91	0.52
1:A:7:DT:H2'	1:A:8:DC:C6	2.45	0.52
2:B:780:ARG:NH1	2:B:807:GLN:HA	2.25	0.52
2:B:898:ASP:O	2:B:905:ARG:NH2	2.43	0.51
2:B:777:SER:HB2	2:B:803:ASN:HB2	1.93	0.51
2:B:345:GLU:OE1	2:B:345:GLU:N	2.32	0.50
3:C:-1:DC:H2''	3:C:0:DG:C8	2.46	0.50
2:B:63:ARG:O	2:B:67:THR:HG23	2.12	0.50
2:B:456:ALA:O	2:B:467:ARG:NH1	2.45	0.50
1:A:59:U:OP1	2:B:467:ARG:NH2	2.45	0.50
2:B:528:LYS:HE3	2:B:539:PHE:CE1	2.47	0.49
1:A:71:U:H2'	1:A:72:U:H6	1.77	0.49
2:B:956:ILE:HG23	2:B:1008:PHE:HB3	1.95	0.49
2:B:1163:LEU:HD21	2:B:1198:LEU:HD12	1.94	0.49
3:C:-4:DT:H2''	3:C:-3:DA:C8	2.47	0.49
2:B:411:PRO:HD2	2:B:414:ILE:HD13	1.95	0.49
1:A:32:A:H2'	1:A:33:G:O4'	2.13	0.49
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.12	0.49
2:B:846:PHE:HB3	2:B:916:PHE:CD2	2.47	0.48
2:B:225:LEU:HD23	2:B:242:ILE:HG21	1.95	0.48
2:B:755:LYS:HD3	2:B:939:MET:HE3	1.94	0.48
2:B:977:GLU:N	2:B:977:GLU:OE2	2.47	0.48
2:B:1117:ASP:N	2:B:1117:ASP:OD1	2.45	0.47
2:B:485:GLY:HA2	2:B:631:MET:HE1	1.96	0.47
2:B:691:ARG:HA	2:B:695:GLN:OE1	2.15	0.47
3:C:17:DC:H5''	3:C:17:DC:C6	2.47	0.47
1:A:70:C:C2	1:A:71:U:C5	3.03	0.47
2:B:870:VAL:HG23	2:B:908:LEU:HG	1.96	0.47
1:A:68:A:C4	1:A:69:A:C8	3.02	0.47
2:B:1136:SER:HA	4:D:2:DG:O3'	2.15	0.47
2:B:513:LEU:HD12	2:B:616:LEU:HB3	1.97	0.46
4:D:-2:DC:H2''	4:D:-1:DA:C8	2.49	0.46
1:A:74:A:H8	1:A:74:A:O5'	1.98	0.46
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.98	0.46
2:B:784:ILE:O	2:B:788:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:THR:O	2:B:904:GLU:HG2	2.15	0.46
1:A:46:A:H2'	1:A:47:A:H8	1.78	0.46
2:B:1183:GLU:HA	2:B:1187:TYR:O	2.16	0.46
2:B:530:VAL:HG13	2:B:537:PRO:HA	1.98	0.46
2:B:1279:ARG:HG2	2:B:1280:VAL:HG23	1.97	0.46
1:A:45:U:H4'	2:B:134:THR:HB	1.97	0.46
1:A:69:A:H2'	1:A:70:C:C6	2.50	0.46
2:B:821:ASP:N	2:B:828:LEU:HG	2.30	0.45
1:A:30:C:H2'	1:A:31:U:C6	2.52	0.45
2:B:379:ILE:O	2:B:383:MET:HG3	2.17	0.45
2:B:1066:ASN:OD1	2:B:1067:GLY:N	2.50	0.45
2:B:662:LEU:HD13	2:B:667:ILE:HD11	1.98	0.45
2:B:443:ILE:HD11	2:B:476:TRP:HZ2	1.82	0.45
2:B:1072:ILE:HD12	2:B:1072:ILE:H	1.80	0.45
2:B:560:THR:HA	2:B:586:ARG:HA	1.99	0.45
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.99	0.45
2:B:725:ALA:O	2:B:734:LYS:NZ	2.41	0.45
2:B:651:LEU:HD23	2:B:651:LEU:HA	1.85	0.44
2:B:787:GLY:O	2:B:791:LEU:HB2	2.17	0.44
2:B:265:GLN:OE1	2:B:268:LYS:HG3	2.18	0.44
1:A:11:A:H2'	1:A:12:G:H8	1.83	0.44
2:B:1277:SER:HA	2:B:1281:ILE:HG12	1.99	0.44
2:B:15:SER:HA	2:B:51:LEU:O	2.17	0.44
1:A:7:DT:H2''	1:A:8:DC:O5'	2.17	0.43
2:B:830:ILE:O	2:B:833:LEU:HG	2.19	0.43
3:C:-4:DT:H2''	3:C:-3:DA:H8	1.83	0.43
2:B:213:SER:HB2	2:B:303:SER:HB2	2.00	0.43
2:B:763:MET:HE3	2:B:763:MET:HB2	1.81	0.43
1:A:15:G:P	2:B:70:ARG:HH22	2.41	0.43
2:B:71:ARG:HB3	2:B:71:ARG:CZ	2.48	0.43
2:B:154:ILE:O	2:B:158:LEU:HG	2.18	0.43
2:B:338:LEU:HB3	2:B:383:MET:HE2	2.01	0.42
1:A:33:G:H2'	1:A:35:A:N7	2.34	0.42
2:B:821:ASP:OD1	2:B:822:MET:N	2.51	0.42
1:A:7:DT:H4'	1:A:8:DC:OP1	2.19	0.42
2:B:419:LEU:HD22	2:B:444:LEU:HD13	2.00	0.42
2:B:1052:LEU:C	2:B:1055:GLY:HA3	2.40	0.42
2:B:597:LEU:O	2:B:601:ILE:HG12	2.19	0.42
2:B:48:ILE:HG12	2:B:984:ALA:HB1	2.02	0.42
2:B:531:THR:HG21	2:B:575:PHE:CD2	2.55	0.42
1:A:72:U:H2'	1:A:73:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:O	2:B:412:HIS:HA	2.20	0.41
1:A:48:A:H2'	1:A:49:A:C8	2.55	0.41
1:A:24:U:H2'	1:A:25:U:C6	2.56	0.41
2:B:790:GLU:HG2	2:B:889:ALA:HA	2.01	0.41
2:B:1228:LEU:HD12	2:B:1272:GLN:HG2	2.01	0.41
2:B:1251:ASP:HB3	2:B:1252:ASN:H	1.66	0.41
2:B:870:VAL:HG13	2:B:871:PRO:HD2	2.03	0.41
2:B:756:PRO:HD2	2:B:939:MET:HE2	2.02	0.41
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	2.03	0.41
4:D:-2:DC:H1'	4:D:-1:DA:H5'	2.03	0.41
2:B:869:ASN:ND2	2:B:908:LEU:HB2	2.36	0.41
2:B:838:VAL:HG12	2:B:855:LYS:HE2	2.03	0.40
2:B:864:ARG:NH2	2:B:871:PRO:HD3	2.37	0.40
1:A:34:A:OP1	1:A:34:A:H8	2.05	0.40
2:B:1351:SER:HB3	2:B:1356:TYR:HB2	2.03	0.40
1:A:71:U:O2'	1:A:72:U:H5'	2.21	0.40
2:B:189:VAL:HG11	2:B:203:ALA:HB2	2.02	0.40
2:B:269:ASP:OD1	2:B:269:ASP:N	2.50	0.40
2:B:823:TYR:OH	2:B:856:VAL:HG11	2.21	0.40
2:B:143:VAL:HG11	2:B:315:ALA:HB2	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
2	B	1309/1372 (95%)	1268 (97%)	41 (3%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

### 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
2	B	1189/1226 (97%)	1182 (99%)	7 (1%)	<a href="#">86</a> <a href="#">95</a>

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	6	SER
2	B	277	ASN
2	B	281	GLN
2	B	343	LEU
2	B	586	ARG
2	B	625	LEU
2	B	822	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	240	ASN
2	B	255	ASN
2	B	277	ASN
2	B	394	ASN
2	B	807	GLN
2	B	826	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	81/81 (100%)	-0.30	2 (2%) 57 51	38, 60, 172, 232	0
2	B	1323/1372 (96%)	0.19	71 (5%) 25 20	38, 71, 140, 186	0
3	C	28/28 (100%)	-0.56	0 100 100	49, 65, 128, 137	0
4	D	11/12 (91%)	0.02	1 (9%) 9 6	51, 80, 149, 159	0
All	All	1443/1493 (96%)	0.14	74 (5%) 28 22	38, 70, 141, 232	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	778	ARG	6.4
2	B	807	GLN	6.0
2	B	806	LEU	5.8
2	B	804	THR	5.0
2	B	802	GLU	4.8
2	B	784	ILE	4.6
1	A	74	A	4.5
2	B	803	ASN	4.3
2	B	1058	ARG	3.9
2	B	847	LEU	3.9
2	B	908	LEU	3.8
2	B	788	ILE	3.8
2	B	846	PHE	3.7
2	B	1052	LEU	3.6
2	B	275	LEU	3.6
2	B	186	ILE	3.6
2	B	781	MET	3.5
2	B	244	LEU	3.5
2	B	868	ASP	3.4
2	B	779	GLU	3.4
2	B	805	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	891	LEU	3.3
2	B	866	LYS	3.3
2	B	811	LEU	3.2
2	B	292	ALA	3.2
2	B	870	VAL	3.2
2	B	1068	GLU	3.2
2	B	205	GLY	3.2
2	B	867	SER	3.2
2	B	815	TYR	3.1
2	B	912	ASP	3.1
2	B	916	PHE	3.1
2	B	852	ILE	3.0
2	B	871	PRO	3.0
2	B	1302	ILE	3.0
2	B	785	GLU	3.0
2	B	841	ILE	3.0
2	B	1051	THR	2.9
2	B	795	ILE	2.9
2	B	856	VAL	2.9
2	B	911	LEU	2.9
2	B	264	LEU	2.9
2	B	842	VAL	2.9
2	B	886	LEU	2.6
2	B	801	VAL	2.6
2	B	198	GLU	2.6
2	B	843	PRO	2.6
2	B	1014	LYS	2.5
2	B	783	ARG	2.5
2	B	848	LYS	2.5
2	B	1038	PHE	2.4
2	B	260	GLU	2.4
2	B	262	ALA	2.4
2	B	1242	TYR	2.4
2	B	782	LYS	2.4
2	B	809	GLU	2.4
2	B	862	LYS	2.4
2	B	808	ASN	2.3
2	B	1294	TYR	2.3
2	B	1156	LYS	2.3
2	B	197	GLU	2.2
1	A	73	G	2.2
2	B	823	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1262	HIS	2.2
4	D	-2	DC	2.2
2	B	1067	GLY	2.2
2	B	1194	LEU	2.2
2	B	1254	GLN	2.2
2	B	884	ARG	2.1
2	B	234	LYS	2.1
2	B	864	ARG	2.1
2	B	1258	PHE	2.1
2	B	796	LEU	2.0
2	B	780	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	K	B	1402	1/1	0.62	0.24	138,138,138,138	0
6	K	B	1408	1/1	0.62	0.39	153,153,153,153	0
6	K	B	1409	1/1	0.67	0.17	141,141,141,141	0
6	K	B	1407	1/1	0.70	0.09	103,103,103,103	0
6	K	B	1406	1/1	0.81	0.15	93,93,93,93	0
6	K	A	105	1/1	0.83	0.20	79,79,79,79	0
6	K	B	1401	1/1	0.87	0.12	119,119,119,119	0
6	K	A	106	1/1	0.88	0.13	88,88,88,88	0
6	K	A	107	1/1	0.88	0.17	89,89,89,89	0
6	K	B	1403	1/1	0.89	0.10	87,87,87,87	0
6	K	A	104	1/1	0.90	0.21	82,82,82,82	0
6	K	A	103	1/1	0.93	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	A	101	1/1	0.94	0.13	70,70,70,70	0
6	K	B	1405	1/1	0.95	0.07	82,82,82,82	0
5	MG	A	102	1/1	0.96	0.11	45,45,45,45	0
6	K	B	1404	1/1	0.97	0.13	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.