



# Full wwPDB X-ray Structure Validation Report

Sep 26, 2014 – 12:54 PM EDT

PDB ID : 4UN5  
Title : Crystal structure of Cas9 bound to PAM-containing DNA target containing mismatches at positions 1-3  
Authors : Anders, C.; Niewoehner, O.; Duerst, A.; Jinek, M.  
Deposited on : 2014-05-25  
Resolution : 2.40 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>

---

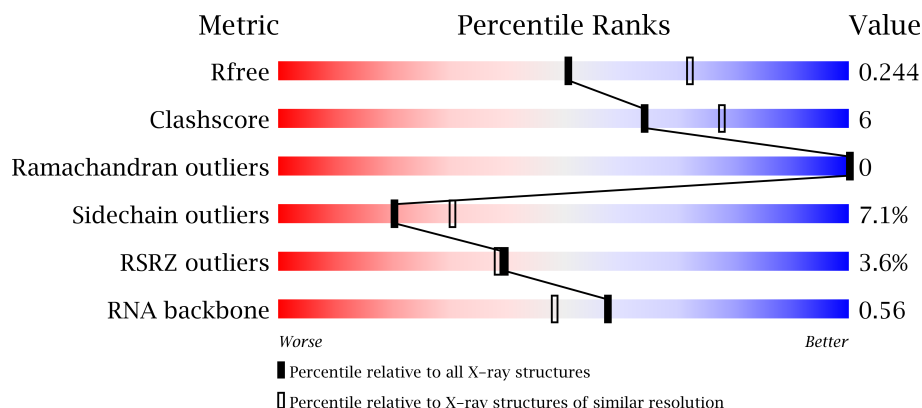
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : trunk23956  
Percentile statistics : 23426  
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) : trunk23956

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	77520	2546 (2.40-2.40)
Clashscore	88313	3035 (2.40-2.40)
Ramachandran outliers	86584	2982 (2.40-2.40)
C $\alpha$ geometry	86677	2981 (2.40-2.40)
Sidechain outliers	86556	2983 (2.40-2.40)
RSRZ outliers	77580	2550 (2.40-2.40)
RNA backbone	2044	1127 (3.00-1.80)

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	83	
2	B	1372	
3	C	11	
4	D	11	
5	E	17	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	MG	A	1082	-	X
6	MG	A	1084	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13943 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 RNA chain called SGRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	P	0	0	1
			1733	778	318	556	81			

- Molecule 2 is a protein called CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1310	Total	C	N	O	S	0	0	0
			10716	6832	1860	2002	22			

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 TARGET DNA STRAND PROXIMAL FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	P	0	0	0
			162	77	31	46	8			

- Molecule 4 is a DNA chain called NON-TARGET DNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			206	100	35	62	9			

- Molecule 5 is a DNA chain called TARGET DNA STRAND DISTAL FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	17	Total	C	N	O	P	0	0	0
			346	169	59	102	16			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	Mg	0	0
			4	4		
6	A	4	Total	Mg	0	0
			4	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	233	Total	O	0	0
			233	233		
7	B	491	Total	O	0	0
			491	491		
7	C	6	Total	O	0	0
			6	6		
7	D	15	Total	O	0	0
			15	15		
7	E	27	Total	O	0	0
			27	27		



LEU  
GLY  
GLY  
ASP

- Molecule 3: TARGET DNA STRAND PROXIMAL FRAGMENT

Chain C: 

  
C1  
A2  
A3  
T4  
C5  
DA  
DA


- Molecule 4: NON-TARGET DNA STRAND

Chain D: 

  
DT  
T3  
G4  
G7  
G12

- Molecule 5: TARGET DNA STRAND DISTAL FRAGMENT

Chain E: 

  
T12  
A17  
A18  
T26

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.18Å 68.07Å 190.26Å 90.00° 111.37° 90.00°	Depositor
Resolution (Å)	48.35 – 2.40 48.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.35-2.40) 99.9 (48.35-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.215 , 0.246 0.213 , 0.244	Depositor DCC
$R_{free}$ test set	4219 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 84391 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.19	0/1943	0.77	0/3026
2	B	0.24	0/10903	0.40	0/14646
3	C	0.48	0/181	1.17	2/277 (0.7%)
4	D	0.46	0/230	1.17	0/355
5	E	0.44	0/387	1.14	0/596
All	All	0.25	0/13644	0.56	2/18900 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	4	DT	C1'-O4'-C4'	-5.56	104.54	110.10
3	C	4	DT	O4'-C1'-C2'	-5.34	101.63	105.90

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	1733	0	869	19	0
2	B	10716	0	10887	123	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	162	0	90	4	0
4	D	206	0	117	3	0
5	E	346	0	197	1	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	A	233	0	0	10	0
7	B	491	0	0	33	0
7	C	6	0	0	1	0
7	D	15	0	0	0	0
7	E	27	0	0	0	0
All	All	13943	0	12160	144	0

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 6.

All (144) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:859:ARG:NH1	7:B:3316:HOH:O	2.03	0.89
2:B:1332:ASP:OD2	7:B:3481:HOH:O	1.93	0.87
2:B:437:ARG:NH2	7:B:3169:HOH:O	2.10	0.84
2:B:1212:ARG:NH1	7:B:3443:HOH:O	2.13	0.81
7:A:2187:HOH:O	2:B:69:ARG:NH2	2.15	0.79
2:B:977:GLU:OE2	7:B:3353:HOH:O	2.02	0.78
2:B:251:ASN:O	7:B:3131:HOH:O	2.03	0.77
1:A:27:G:H5'	1:A:28:A:H5''	1.67	0.76
2:B:451:TYR:OH	7:B:3177:HOH:O	2.03	0.75
2:B:1043:MET:O	7:B:3372:HOH:O	2.03	0.75
2:B:1308:ASN:ND2	2:B:1326:TYR:O	2.21	0.73
2:B:234:LYS:O	7:B:3129:HOH:O	2.07	0.73
2:B:1286:ASN:ND2	7:B:3469:HOH:O	2.23	0.71
2:B:783:ARG:NH2	7:B:3308:HOH:O	2.23	0.71
2:B:1183:GLU:OE2	7:B:3430:HOH:O	2.08	0.71
1:A:76:A:H5''	7:A:2228:HOH:O	1.92	0.70
2:B:1049:GLU:OE2	7:B:3373:HOH:O	2.12	0.67
2:B:1335:ARG:NH2	4:D:7:DG:O6	2.28	0.67
3:C:2:DA:N3	7:C:2004:HOH:O	2.27	0.67
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.28	0.66
2:B:1207:GLU:O	7:B:3438:HOH:O	2.13	0.66
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.76	0.66
2:B:261:ASP:O	7:B:3133:HOH:O	2.15	0.65
1:A:64:U:OP2	7:A:2188:HOH:O	2.12	0.65
2:B:245:SER:HB3	2:B:296:LEU:HG	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:849:ASP:HB3	2:B:854:ASN:HD22	1.63	0.64
2:B:141:LYS:NZ	7:B:3099:HOH:O	2.30	0.64
3:C:3:DA:H1'	3:C:4:DT:H5'	1.79	0.64
2:B:248:LEU:O	7:B:3132:HOH:O	2.15	0.63
2:B:898:ASP:O	2:B:905:ARG:NH2	2.31	0.63
7:A:2224:HOH:O	2:B:1358:THR:HG21	1.99	0.61
2:B:185:PHE:N	7:B:3116:HOH:O	2.33	0.61
2:B:758:ASN:OD1	2:B:954:LYS:NZ	2.34	0.60
2:B:874:GLU:HG2	2:B:878:LYS:HE3	1.84	0.60
1:A:33:G:N2	1:A:36:A:OP2	2.34	0.60
2:B:405:PHE:O	7:B:3159:HOH:O	2.16	0.60
2:B:629:ARG:HE	2:B:655:ARG:HD3	1.66	0.59
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.83	0.59
2:B:1295:ASN:OD1	2:B:1298:ARG:NH2	2.34	0.59
2:B:1046:PHE:HB2	7:B:3372:HOH:O	2.03	0.59
3:C:1:DC:O2	4:D:12:DG:N2	2.30	0.58
2:B:1180:ASP:OD1	7:B:3428:HOH:O	2.17	0.58
2:B:635:ARG:NH1	7:B:3259:HOH:O	2.36	0.58
7:A:2066:HOH:O	2:B:71:ARG:NH2	2.36	0.58
2:B:780:ARG:NH1	2:B:806:LEU:O	2.35	0.58
2:B:349:GLU:HG3	2:B:356:LYS:HD3	1.85	0.58
1:A:59:U:OP2	2:B:467:ARG:NH2	2.36	0.57
2:B:516:GLU:HA	2:B:519:THR:HG22	1.86	0.57
1:A:62:G:OP1	7:A:2183:HOH:O	2.17	0.57
2:B:525:THR:HG22	2:B:690:ASN:HB3	1.87	0.57
1:A:5:C:OP1	2:B:515:TYR:OH	2.22	0.56
2:B:584:GLU:O	2:B:584:GLU:HG3	2.05	0.56
2:B:790:GLU:HG2	2:B:889:ALA:HA	1.86	0.56
2:B:605:ASP:OD1	7:B:3250:HOH:O	2.17	0.56
2:B:977:GLU:HG3	2:B:1310:ILE:HG23	1.88	0.56
2:B:672:ASP:HA	2:B:703:THR:HG22	1.88	0.56
2:B:442:LYS:HE3	2:B:476:TRP:HA	1.88	0.55
2:B:1300:LYS:O	2:B:1305:GLN:NE2	2.39	0.55
2:B:1037:PHE:O	2:B:1041:ASN:ND2	2.34	0.55
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.89	0.55
2:B:244:LEU:HD11	2:B:264:LEU:HD11	1.88	0.55
2:B:951:ARG:NH1	2:B:1011:GLY:HA3	2.22	0.54
2:B:192:TYR:OH	7:B:3122:HOH:O	2.10	0.54
2:B:139:ARG:HH21	2:B:160:HIS:CE1	2.25	0.54
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.42	0.53
2:B:826:GLN:OE1	7:B:3314:HOH:O	2.19	0.53
2:B:326:ASP:OD2	7:B:3146:HOH:O	2.18	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:450:TYR:OH	2:B:627:GLU:HG2	2.08	0.52
2:B:957:THR:HG23	7:B:3343:HOH:O	2.09	0.52
2:B:564:LEU:HD23	2:B:580:ILE:HD13	1.91	0.52
2:B:893:THR:HG23	2:B:896:LYS:H	1.75	0.52
2:B:1350:GLN:NE2	7:B:3035:HOH:O	2.23	0.52
2:B:251:ASN:HB2	2:B:263:LYS:HD2	1.93	0.51
1:A:68:A:HO2'	1:A:69:A:P	2.34	0.51
1:A:27:G:N2	1:A:44:U:OP2	2.44	0.51
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.93	0.50
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.92	0.50
2:B:951:ARG:HH12	2:B:1011:GLY:HA3	1.77	0.50
2:B:1117:ASP:N	2:B:1117:ASP:OD1	2.44	0.50
2:B:1146:VAL:HG13	2:B:1191:LYS:HB2	1.92	0.50
2:B:825:ASP:HA	7:B:3312:HOH:O	2.10	0.50
3:C:2:DA:H2'	3:C:3:DA:C8	2.47	0.49
2:B:253:LYS:HA	2:B:258:LEU:HD12	1.95	0.49
2:B:212:LEU:HD12	2:B:246:LEU:HD21	1.94	0.48
2:B:525:THR:HG23	2:B:545:LYS:HE2	1.95	0.48
2:B:817:GLN:O	2:B:882:TYR:OH	2.32	0.47
2:B:216:LEU:HD22	2:B:220:ARG:HG2	1.96	0.47
2:B:777:SER:HB3	2:B:803:ASN:HB2	1.97	0.47
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	1.97	0.47
7:A:2008:HOH:O	2:B:694:MET:HG2	2.14	0.47
2:B:862:LYS:HG3	7:B:3325:HOH:O	2.15	0.46
2:B:814:TYR:CZ	2:B:830:ILE:HG23	2.50	0.46
2:B:245:SER:HA	2:B:297:SER:HB3	1.96	0.46
2:B:508:LEU:HD21	2:B:664:ARG:HB2	1.98	0.46
4:D:3:DT:H2''	4:D:4:DG:C8	2.51	0.46
2:B:63:ARG:NH2	7:B:3056:HOH:O	2.48	0.46
2:B:133:PRO:HG2	2:B:137:HIS:CE1	2.50	0.46
2:B:758:ASN:HD22	2:B:995:THR:HG22	1.81	0.46
2:B:1216:SER:OG	2:B:1217:ALA:N	2.49	0.45
1:A:42:A:O2'	1:A:43:G:OP1	2.31	0.45
2:B:1001:TYR:OH	7:B:3362:HOH:O	2.13	0.45
2:B:158:LEU:HA	2:B:161:MET:HE3	1.98	0.45
2:B:869:ASN:OD1	2:B:870:VAL:N	2.41	0.45
2:B:527:VAL:HA	2:B:582:GLY:HA3	1.99	0.44
1:A:27:G:H4'	1:A:28:A:OP2	2.17	0.44
1:A:74:A:H3'	1:A:75:A:H8	1.81	0.44
2:B:1277:SER:HA	2:B:1281:ILE:HG12	1.99	0.44
1:A:56:U:OP1	7:A:2166:HOH:O	2.21	0.44
2:B:1349:HIS:HB2	2:B:1358:THR:OG1	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.51	0.44
2:B:265:GLN:O	2:B:271:TYR:HB2	2.18	0.43
2:B:187:GLN:O	2:B:191:THR:HG22	2.18	0.43
2:B:877:LYS:HE3	2:B:877:LYS:HB2	1.74	0.43
1:A:27:G:H2'	7:A:2106:HOH:O	2.18	0.43
1:A:8:A:N7	7:A:2034:HOH:O	2.36	0.43
1:A:68:A:O2'	1:A:69:A:OP1	2.27	0.43
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.82	0.43
2:B:1122:ARG:HG3	2:B:1134:PHE:CE2	2.54	0.43
2:B:699:ASP:OD1	2:B:701:SER:OG	2.25	0.43
2:B:918:LYS:HE3	2:B:918:LYS:HB2	1.80	0.42
2:B:1291:LEU:O	2:B:1295:ASN:ND2	2.50	0.42
1:A:18:A:OP1	2:B:165:ARG:HD3	2.20	0.42
2:B:314:LYS:HE2	2:B:314:LYS:HB3	1.75	0.42
2:B:306:LEU:HD22	2:B:316:PRO:HB2	2.00	0.42
2:B:296:LEU:HD13	7:B:3116:HOH:O	2.18	0.42
2:B:398:LEU:HG	2:B:399:LEU:HG	2.02	0.42
1:A:69:A:H5'	2:B:1349:HIS:CE1	2.55	0.42
2:B:22:THR:OG1	2:B:23:ASP:N	2.52	0.42
5:E:17:DA:H2'	5:E:18:DA:C8	2.55	0.42
2:B:122:ILE:HG12	2:B:122:ILE:H	1.45	0.41
1:A:74:A:H3'	1:A:75:A:C8	2.55	0.41
2:B:342:GLN:HB2	2:B:383:MET:HE3	2.03	0.41
2:B:296:LEU:O	2:B:296:LEU:HD12	2.20	0.41
2:B:652:LYS:HB3	2:B:652:LYS:HE2	1.79	0.41
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.54	0.41
2:B:521:TYR:O	2:B:525:THR:OG1	2.36	0.41
2:B:245:SER:CB	2:B:296:LEU:HG	2.46	0.41
2:B:521:TYR:CE1	2:B:684:LYS:HG2	2.56	0.41
2:B:534:MET:HG2	2:B:534:MET:H	1.61	0.41
2:B:901:THR:O	2:B:904:GLU:HG2	2.21	0.40
2:B:1177:ASN:HA	2:B:1178:PRO:HD2	1.92	0.40
2:B:116:HIS:HA	2:B:117:PRO:HD3	1.82	0.40
2:B:234:LYS:HE3	2:B:234:LYS:HB3	1.81	0.40
2:B:796:LEU:HD23	2:B:796:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

## 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	
2	B	1296/1372 (94%)	1249 (96%)	47 (4%)	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	
2	B	1175/1226 (96%)	1092 (93%)	83 (7%)	20	30

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	27	VAL
2	B	43	ILE
2	B	73	THR
2	B	82	LEU
2	B	95	ASP
2	B	102	GLU
2	B	112	LYS
2	B	122	ILE
2	B	123	VAL
2	B	165	ARG
2	B	182	ASP
2	B	188	LEU
2	B	191	THR
2	B	195	LEU
2	B	215	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	216	LEU
2	B	234	LYS
2	B	244	LEU
2	B	265	GLN
2	B	377	LYS
2	B	402	GLN
2	B	419	LEU
2	B	425	ARG
2	B	445	THR
2	B	455	LEU
2	B	465	MET
2	B	471	GLU
2	B	507	VAL
2	B	524	LEU
2	B	525	THR
2	B	530	VAL
2	B	534	MET
2	B	540	LEU
2	B	586	ARG
2	B	598	LEU
2	B	599	LYS
2	B	627	GLU
2	B	634	GLU
2	B	635	ARG
2	B	638	THR
2	B	650	GLN
2	B	666	LEU
2	B	696	LEU
2	B	703	THR
2	B	709	GLN
2	B	710	LYS
2	B	712	GLN
2	B	718	ASP
2	B	738	LEU
2	B	751	MET
2	B	776	ASN
2	B	782	LYS
2	B	801	VAL
2	B	803	ASN
2	B	811	LEU
2	B	830	ILE
2	B	842	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	856	VAL
2	B	859	ARG
2	B	868	ASP
2	B	870	VAL
2	B	884	ARG
2	B	887	LEU
2	B	918	LYS
2	B	919	ARG
2	B	921	LEU
2	B	924	THR
2	B	935	LEU
2	B	945	GLU
2	B	1007	GLU
2	B	1031	LYS
2	B	1076	LYS
2	B	1089	MET
2	B	1091	GLN
2	B	1119	LEU
2	B	1207	GLU
2	B	1210	ARG
2	B	1263	LYS
2	B	1266	LEU
2	B	1284	ASP
2	B	1334	LYS
2	B	1342	VAL
2	B	1346	THR

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
1	A	80/83 (96%)	20 (25%)	3 (3%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	28	A
1	A	29	G
1	A	32	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	34	A
1	A	35	A
1	A	37	U
1	A	38	A
1	A	39	G
1	A	42	A
1	A	43	G
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	69	A
1	A	72	U
1	A	74	A
1	A	75	A
1	A	77	A
1	A	78	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	27	G
1	A	42	A
1	A	68	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 ⓘ

Of 8 ligands modelled in this entry, 8 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.

## 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	82/83 (98%)	-0.17	3 (3%) 39 37	16, 32, 109, 144	0
2	B	1310/1372 (95%)	-0.02	48 (3%) 39 37	14, 37, 75, 132	0
3	C	9/11 (81%)	0.08	1 (11%) 5 5	34, 45, 85, 132	0
4	D	10/11 (90%)	-0.10	0 100 100	28, 44, 89, 100	0
5	E	17/17 (100%)	-0.79	0 100 100	23, 28, 35, 38	0
All	All	1428/1494 (95%)	-0.04	52 (3%) 40 38	14, 36, 77, 144	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	ASP	10.4
2	B	293	ALA	6.0
2	B	264	LEU	3.7
2	B	271	TYR	3.7
2	B	291	LEU	3.5
2	B	287	ALA	3.2
2	B	297	SER	3.2
2	B	290	PHE	3.1
2	B	199	ASN	3.1
2	B	184	LEU	3.0
2	B	309	ASN	3.0
2	B	783	ARG	3.0
2	B	286	TYR	3.0
2	B	296	LEU	2.9
2	B	188	LEU	2.9
2	B	1043	MET	2.8
2	B	182	ASP	2.8
2	B	275	LEU	2.8
2	B	1068	GLU	2.8
2	B	268	LYS	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	279	LEU	2.7
2	B	258	LEU	2.6
2	B	215	ARG	2.6
2	B	195	LEU	2.6
2	B	1037	PHE	2.6
1	A	73	G	2.6
2	B	302	LEU	2.5
2	B	191	THR	2.5
1	A	74	A	2.5
2	B	278	LEU	2.5
2	B	356	LYS	2.5
2	B	265	GLN	2.5
2	B	301	LEU	2.5
1	A	76	A	2.4
2	B	1050	ILE	2.4
2	B	198	GLU	2.4
2	B	192	TYR	2.4
2	B	312	ILE	2.4
2	B	1042	ILE	2.4
2	B	284	ASP	2.3
2	B	200	PRO	2.3
2	B	259	ALA	2.3
2	B	850	ASP	2.2
2	B	266	LEU	2.2
3	C	1	DC	2.2
2	B	689	ALA	2.2
2	B	802	GLU	2.2
2	B	260	GLU	2.1
2	B	185	PHE	2.1
2	B	346	LYS	2.1
2	B	776	ASN	2.0
2	B	803	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

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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	A	1084	1/1	0.27	5.58	50,50,50,50	0
6	MG	A	1082	1/1	0.15	2.32	29,29,29,29	0
6	MG	B	2368	1/1	0.21	0.80	31,31,31,31	0
6	MG	B	2365	1/1	0.17	0.42	22,22,22,22	0
6	MG	B	2366	1/1	0.13	-0.25	13,13,13,13	0
6	MG	B	2367	1/1	0.14	-0.47	43,43,43,43	0
6	MG	A	1085	1/1	0.12	-0.85	21,21,21,21	0
6	MG	A	1083	1/1	0.10	-3.38	6,6,6,6	0

## 6.5 Other polymers

There are no such residues in this entry.