



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 PM UTC

PDB ID : 4UN3 / pdb_00004un3
Title : Crystal structure of Cas9 bound to PAM-containing DNA target
Authors : Anders, C.; Niewoehner, O.; Duerst, A.; Jinek, M.
Deposited on : 2014-05-25
Resolution : 2.59 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

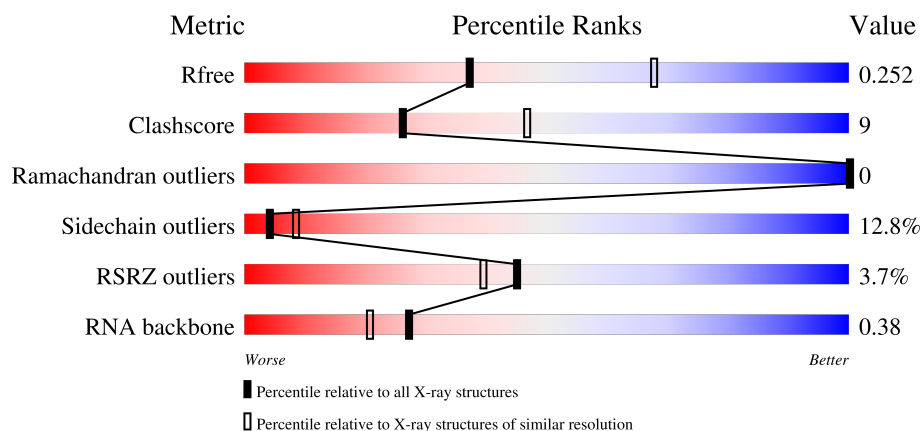
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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 ≥ 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	83	45% 31% 22% •
2	B	1372	4% 67% 25% • 5%
3	C	28	86% 14%
4	D	12	8% 75% 17% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13629 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 RNA chain called SGRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	P	0	0	0
			1732	778	318	555	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1306	Total	C	N	O	S	0	0	0
			10690	6816	1854	1998	22			

There are 5 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	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called TARGET DNA STRAND.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			567	276	96	168	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			227	110	43	64	10			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

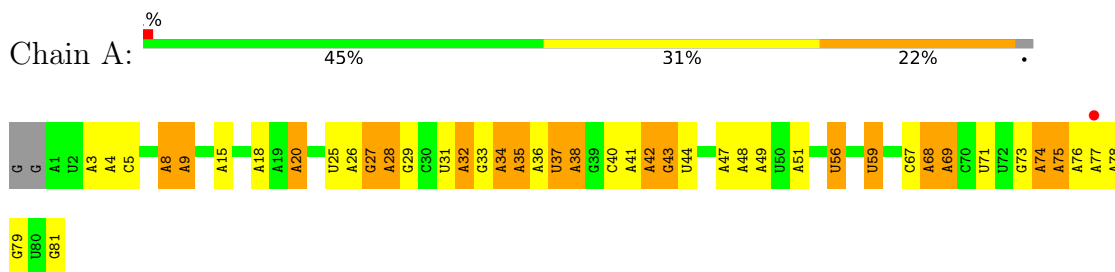
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	146	Total 146	O 146	0	0
6	B	246	Total 246	O 246	0	0
6	C	11	Total 11	O 11	0	0
6	D	2	Total 2	O 2	0	0

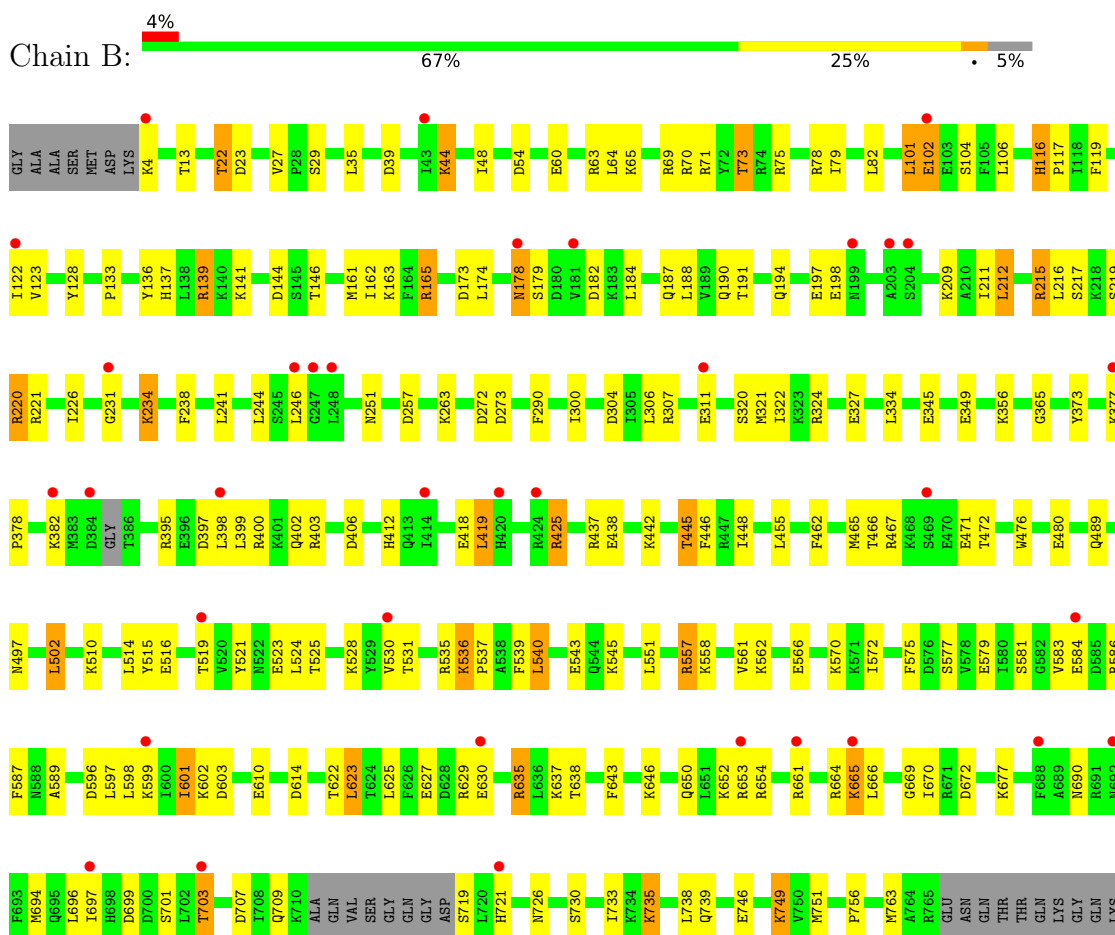
3 Residue-property plots

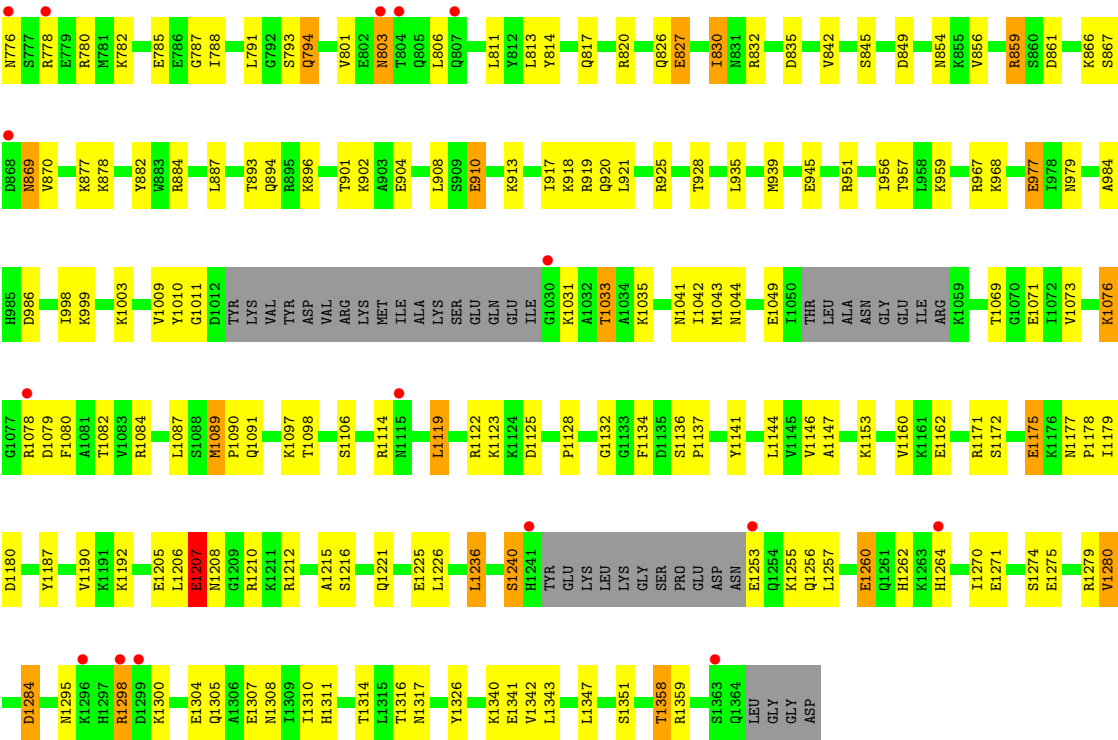
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SGRNA



• Molecule 2: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.72Å 68.14Å 188.23Å 90.00° 111.17° 90.00°	Depositor
Resolution (Å)	48.15 – 2.59 48.15 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.15-2.59) 99.3 (48.15-2.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.252 0.220 , 0.252	Depositor DCC
R_{free} test set	3263 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13629	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.16	0/1942	0.38	0/3023
2	B	0.30	0/10877	0.75	4/14612 (0.0%)
3	C	0.14	0/634	0.69	1/976 (0.1%)
4	D	0.14	0/255	0.65	0/393
All	All	0.27	0/13708	0.70	5/19004 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	DA	C4'-C3'-O3'	7.54	121.30	110.00
2	B	869	ASN	N-CA-C	5.58	115.91	108.38
2	B	1207	GLU	N-CA-C	5.49	117.12	111.03
2	B	116	HIS	CA-C-N	5.22	124.40	118.97
2	B	116	HIS	C-N-CA	5.22	124.40	118.97

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	1732	0	869	39	0
2	B	10690	0	10858	207	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	567	0	322	5	0
4	D	227	0	127	3	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	146	0	0	10	0
6	B	246	0	0	28	1
6	C	11	0	0	0	0
6	D	2	0	0	0	0
All	All	13629	0	12176	238	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 9.

All (238) 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:A:9:A:OP1	6:A:2016:HOH:O	1.83	0.97
2:B:587:PHE:O	6:B:2124:HOH:O	1.86	0.92
2:B:1084:ARG:O	6:B:2182:HOH:O	1.92	0.85
2:B:1225:GLU:OE2	6:B:2230:HOH:O	1.94	0.85
6:A:2121:HOH:O	2:B:69:ARG:NH2	2.11	0.82
2:B:601:ILE:HD12	2:B:603:ASP:H	1.45	0.82
6:B:2032:HOH:O	3:C:9:DT:O4	1.97	0.82
2:B:523:GLU:O	6:B:2119:HOH:O	1.97	0.81
6:A:2078:HOH:O	2:B:102:GLU:O	1.98	0.81
6:A:2141:HOH:O	2:B:1098:THR:O	2.00	0.80
2:B:577:SER:OG	6:B:2127:HOH:O	1.94	0.76
2:B:614:ASP:OD1	6:B:2136:HOH:O	2.02	0.76
1:A:41:A:OP1	6:A:2067:HOH:O	2.04	0.76
2:B:442:LYS:HE3	2:B:476:TRP:HD1	1.50	0.75
2:B:1132:GLY:O	6:B:2202:HOH:O	2.04	0.75
1:A:18:A:OP2	2:B:71:ARG:NH1	2.20	0.74
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.21	0.74
2:B:1316:THR:O	6:B:2229:HOH:O	2.04	0.74
2:B:60:GLU:OE1	6:B:2028:HOH:O	2.06	0.73
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.68	0.73
2:B:263:LYS:NZ	6:B:2072:HOH:O	2.14	0.73
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.22	0.72
2:B:1295:ASN:OD1	2:B:1298:ARG:NH1	2.22	0.71
2:B:307:ARG:NH2	2:B:397:ASP:OD2	2.24	0.70
2:B:1300:LYS:O	2:B:1305:GLN:NE2	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.26	0.69
2:B:1076:LYS:HG3	2:B:1080:PHE:HE2	1.57	0.69
2:B:182:ASP:H	2:B:209:LYS:HE2	1.58	0.69
2:B:1236:LEU:O	2:B:1240:SER:OG	2.10	0.68
2:B:54:ASP:OD2	6:B:2023:HOH:O	2.11	0.68
2:B:1212:ARG:NH1	6:B:2224:HOH:O	2.20	0.68
2:B:212:LEU:HD12	2:B:246:LEU:HD21	1.76	0.67
2:B:184:LEU:O	6:B:2063:HOH:O	2.13	0.67
2:B:516:GLU:HA	2:B:519:THR:HG22	1.76	0.67
2:B:1125:ASP:OD1	6:B:2203:HOH:O	2.14	0.66
2:B:672:ASP:HA	2:B:703:THR:HG22	1.78	0.66
1:A:77:A:OP1	2:B:721:HIS:NE2	2.29	0.65
2:B:165:ARG:NH2	2:B:446:PHE:O	2.30	0.65
2:B:365:GLY:O	6:B:2086:HOH:O	2.14	0.65
2:B:780:ARG:NH1	2:B:806:LEU:O	2.29	0.65
1:A:73:G:H3'	1:A:74:A:H5''	1.80	0.63
1:A:75:A:H2'	1:A:76:A:C8	2.32	0.63
2:B:778:ARG:NH2	3:C:11:DT:OP1	2.31	0.63
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.82	0.62
2:B:179:SER:O	2:B:209:LYS:NZ	2.30	0.61
2:B:1256:GLN:NE2	2:B:1260:GLU:OE2	2.33	0.61
2:B:1304:GLU:O	2:B:1308:ASN:ND2	2.28	0.61
2:B:521:TYR:O	2:B:525:THR:OG1	2.18	0.61
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.34	0.61
2:B:1009:VAL:O	6:B:2176:HOH:O	2.16	0.61
2:B:817:GLN:O	2:B:882:TYR:OH	2.19	0.60
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.34	0.60
1:A:20:A:OP2	2:B:403:ARG:NH1	2.34	0.60
2:B:776:ASN:N	6:B:2154:HOH:O	2.35	0.59
2:B:817:GLN:NE2	6:B:2156:HOH:O	2.10	0.59
2:B:437:ARG:NH1	6:B:2095:HOH:O	2.36	0.59
2:B:119:PHE:HE2	2:B:128:TYR:HB2	1.67	0.59
2:B:217:SER:OG	2:B:220:ARG:NH1	2.35	0.59
2:B:525:THR:HG22	2:B:690:ASN:HB3	1.83	0.59
2:B:699:ASP:OD1	2:B:701:SER:OG	2.22	0.58
1:A:67:C:OP2	2:B:1097:LYS:NZ	2.34	0.58
1:A:32:A:H61	1:A:37:U:H3	1.51	0.58
2:B:442:LYS:HE3	2:B:476:TRP:CD1	2.37	0.58
1:A:8:A:H2'	1:A:9:A:C8	2.39	0.58
2:B:22:THR:HG22	2:B:23:ASP:H	1.67	0.57
2:B:849:ASP:HB3	2:B:854:ASN:HD22	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1141:TYR:OH	2:B:1175:GLU:OE1	2.23	0.57
3:C:19:DA:H5''	3:C:19:DA:H8	1.68	0.57
2:B:719:SER:N	6:B:2147:HOH:O	2.37	0.57
1:A:59:U:OP1	2:B:467:ARG:NH2	2.38	0.56
2:B:525:THR:HG23	2:B:545:LYS:HZ1	1.70	0.56
2:B:788:ILE:HG23	2:B:793:SER:HB3	1.87	0.56
1:A:3:A:H2'	1:A:4:A:C8	2.39	0.56
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.86	0.56
6:A:2024:HOH:O	2:B:462:PHE:O	2.18	0.56
2:B:35:LEU:HB2	2:B:1358:THR:HB	1.88	0.56
2:B:75:ARG:HD3	2:B:163:LYS:HG2	1.88	0.55
1:A:33:G:H2'	1:A:34:A:H5''	1.87	0.55
1:A:76:A:C5	1:A:77:A:H1'	2.42	0.55
1:A:27:G:N2	1:A:44:U:OP2	2.38	0.55
2:B:977:GLU:HG3	2:B:1310:ILE:HG23	1.89	0.55
1:A:5:C:OP1	2:B:515:TYR:OH	2.21	0.54
1:A:81:G:N2	6:A:2142:HOH:O	2.29	0.54
2:B:1208:ASN:O	2:B:1279:ARG:NH1	2.39	0.54
1:A:56:U:OP2	6:A:2104:HOH:O	2.18	0.54
1:A:42:A:O2'	1:A:43:G:OP1	2.22	0.54
2:B:1206:LEU:HD11	2:B:1341:GLU:HG3	1.89	0.54
1:A:15:A:OP1	2:B:70:ARG:NH2	2.36	0.54
2:B:832:ARG:NH1	2:B:835:ASP:OD2	2.39	0.53
2:B:1317:ASN:ND2	6:B:2171:HOH:O	2.32	0.53
2:B:519:THR:HG23	2:B:589:ALA:HB1	1.90	0.53
2:B:48:ILE:HG12	2:B:984:ALA:HB1	1.90	0.53
2:B:502:LEU:HD21	2:B:670:ILE:HD11	1.91	0.53
2:B:324:ARG:HB2	2:B:402:GLN:HE22	1.74	0.53
2:B:378:PRO:O	2:B:382:LYS:HG2	2.09	0.53
2:B:597:LEU:O	2:B:601:ILE:HG13	2.08	0.52
2:B:870:VAL:HG23	2:B:908:LEU:HG	1.90	0.52
6:A:2021:HOH:O	2:B:63:ARG:NH1	2.42	0.52
2:B:1119:LEU:HB3	2:B:1128:PRO:HB2	1.91	0.52
2:B:139:ARG:NH1	2:B:418:GLU:OE1	2.43	0.52
2:B:290:PHE:O	6:B:2074:HOH:O	2.19	0.52
2:B:1179:ILE:HD11	2:B:1192:LYS:HD3	1.92	0.52
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.43	0.51
2:B:539:PHE:HB3	2:B:690:ASN:ND2	2.25	0.51
2:B:845:SER:O	2:B:920:GLN:NE2	2.33	0.51
2:B:1340:LYS:HA	2:B:1343:LEU:HD12	1.92	0.51
2:B:1162:GLU:OE2	2:B:1187:TYR:OH	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:A:N7	6:A:2057:HOH:O	2.35	0.50
2:B:908:LEU:O	2:B:913:LYS:NZ	2.41	0.50
2:B:1307:GLU:O	2:B:1310:ILE:HB	2.12	0.50
2:B:215:ARG:NH2	2:B:395:ARG:O	2.42	0.50
2:B:999:LYS:HB3	2:B:1073:VAL:HG12	1.94	0.50
1:A:36:A:H2'	1:A:37:U:H5'	1.92	0.50
2:B:1284:ASP:OD1	2:B:1284:ASP:N	2.23	0.50
1:A:71:U:H3	1:A:78:A:H61	1.59	0.49
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.94	0.49
2:B:623:LEU:HG	2:B:654:ARG:O	2.13	0.49
2:B:896:LYS:NZ	6:B:2156:HOH:O	2.46	0.49
2:B:584:GLU:O	2:B:586:ARG:N	2.45	0.49
1:A:27:G:H4'	1:A:28:A:OP2	2.12	0.49
1:A:18:A:OP1	2:B:165:ARG:HD3	2.13	0.49
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.45	0.49
2:B:136:TYR:HA	2:B:139:ARG:HG3	1.95	0.49
2:B:951:ARG:NH1	2:B:1011:GLY:HA3	2.28	0.49
2:B:290:PHE:HB3	6:B:2074:HOH:O	2.11	0.49
2:B:1079:ASP:O	2:B:1082:THR:OG1	2.25	0.48
2:B:826:GLN:NE2	2:B:859:ARG:HD3	2.28	0.48
2:B:910:GLU:HG2	2:B:1033:THR:HG23	1.96	0.48
1:A:68:A:O2'	1:A:69:A:OP1	2.30	0.48
1:A:69:A:H1'	2:B:1358:THR:HG21	1.96	0.48
1:A:73:G:C3'	1:A:74:A:H5''	2.43	0.48
1:A:73:G:H3'	1:A:74:A:C5'	2.42	0.48
2:B:465:MET:HE1	2:B:467:ARG:HG3	1.96	0.48
2:B:215:ARG:HG3	2:B:307:ARG:CZ	2.43	0.47
2:B:901:THR:O	2:B:904:GLU:HG2	2.14	0.47
2:B:133:PRO:HG2	2:B:137:HIS:CE1	2.50	0.47
2:B:161:MET:HE1	2:B:419:LEU:HA	1.95	0.47
3:C:19:DA:H5''	3:C:19:DA:C8	2.49	0.47
2:B:814:TYR:CZ	2:B:830:ILE:HG23	2.50	0.47
2:B:1210:ARG:HA	2:B:1280:VAL:HG22	1.97	0.46
2:B:190:GLN:O	2:B:194:GLN:HG2	2.15	0.46
2:B:536:LYS:HG2	2:B:537:PRO:HD2	1.98	0.46
2:B:893:THR:HG23	2:B:896:LYS:H	1.80	0.46
2:B:69:ARG:O	2:B:73:THR:HG23	2.16	0.46
2:B:212:LEU:O	2:B:221:ARG:NE	2.48	0.46
2:B:979:ASN:ND2	2:B:1226:LEU:O	2.47	0.45
2:B:694:MET:HE2	2:B:694:MET:HA	1.97	0.45
2:B:1271:GLU:O	2:B:1275:GLU:HG3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:A:O2'	2:B:101:LEU:O	2.34	0.45
2:B:238:PHE:HA	2:B:241:LEU:HD12	1.97	0.45
2:B:803:ASN:N	2:B:803:ASN:OD1	2.49	0.45
2:B:306:LEU:O	2:B:320:SER:HB3	2.16	0.45
1:A:37:U:H2'	1:A:38:A:O4'	2.17	0.45
2:B:794:GLN:H	2:B:794:GLN:HG2	1.62	0.45
2:B:910:GLU:HA	2:B:913:LYS:HD3	1.99	0.45
2:B:1308:ASN:HB3	2:B:1326:TYR:O	2.16	0.45
2:B:665:LYS:HA	2:B:669:GLY:HA3	1.99	0.45
1:A:28:A:N3	2:B:122:ILE:HG21	2.32	0.44
2:B:78:ARG:NH1	2:B:162:ILE:O	2.50	0.44
2:B:398:LEU:HG	2:B:399:LEU:HG	1.99	0.44
2:B:877:LYS:HE3	2:B:877:LYS:HB2	1.70	0.44
2:B:830:ILE:H	2:B:830:ILE:HG13	1.42	0.44
2:B:231:GLY:N	6:B:2068:HOH:O	2.51	0.44
2:B:756:PRO:HD2	2:B:939:MET:HE2	2.00	0.44
2:B:1153:LYS:HE3	2:B:1153:LYS:HB2	1.69	0.44
2:B:1041:ASN:HB3	2:B:1044:ASN:ND2	2.33	0.44
2:B:178:ASN:O	2:B:178:ASN:ND2	2.47	0.44
2:B:349:GLU:HG2	2:B:356:LYS:HG3	2.00	0.44
1:A:48:A:H2'	1:A:49:A:C8	2.52	0.43
2:B:44:LYS:O	2:B:44:LYS:HG3	2.19	0.43
2:B:652:LYS:HB3	2:B:652:LYS:HE3	1.77	0.43
2:B:1010:TYR:OH	6:B:2177:HOH:O	2.17	0.43
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.82	0.43
2:B:1171:ARG:O	2:B:1175:GLU:HG2	2.17	0.43
2:B:211:ILE:O	2:B:221:ARG:HD2	2.17	0.43
2:B:216:LEU:O	2:B:221:ARG:NH1	2.50	0.43
2:B:869:ASN:OD1	2:B:870:VAL:N	2.48	0.43
2:B:1136:SER:HA	4:D:7:DG:O3'	2.18	0.43
2:B:551:LEU:HD22	2:B:572:ILE:HD11	2.01	0.43
2:B:925:ARG:HB3	2:B:928:THR:HG23	2.00	0.43
2:B:373:TYR:O	2:B:377:LYS:HG3	2.19	0.43
2:B:561:VAL:HG22	2:B:583:VAL:HG13	2.01	0.43
2:B:746:GLU:OE2	2:B:1351:SER:HB3	2.17	0.43
2:B:161:MET:HB2	2:B:161:MET:HE3	1.78	0.42
2:B:566:GLU:O	2:B:570:LYS:HB3	2.19	0.42
2:B:977:GLU:HG3	2:B:1310:ILE:CG2	2.48	0.42
2:B:1262:HIS:HA	2:B:1264:HIS:CE1	2.54	0.42
2:B:956:ILE:HD11	2:B:998:ILE:HD13	2.00	0.42
2:B:1076:LYS:HG3	2:B:1080:PHE:CE2	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ILE:HD11	2:B:163:LYS:HG3	2.02	0.42
2:B:234:LYS:H	2:B:234:LYS:HG2	1.50	0.42
4:D:7:DG:C8	4:D:7:DG:H5'	2.55	0.42
1:A:74:A:C2'	1:A:75:A:H5'	2.49	0.42
2:B:497:ASN:HD21	3:C:19:DA:P	2.43	0.42
2:B:144:ASP:O	2:B:425:ARG:NH2	2.53	0.42
2:B:646:LYS:HE2	2:B:650:GLN:HG3	2.02	0.42
2:B:730:SER:O	2:B:733:ILE:HG22	2.19	0.42
2:B:1206:LEU:HD13	2:B:1210:ARG:HH12	1.85	0.42
2:B:400:ARG:NH2	2:B:406:ASP:OD2	2.53	0.42
2:B:787:GLY:O	2:B:791:LEU:HB2	2.19	0.42
1:A:27:G:H5'	1:A:28:A:C5'	2.50	0.41
2:B:273:ASP:OD1	2:B:653:ARG:NH2	2.52	0.41
2:B:870:VAL:HG21	2:B:902:LYS:HB3	2.00	0.41
2:B:1177:ASN:HA	2:B:1178:PRO:HD2	1.92	0.41
2:B:1210:ARG:HH22	2:B:1341:GLU:CD	2.28	0.41
2:B:187:GLN:O	2:B:191:THR:HG23	2.20	0.41
2:B:448:ILE:HD13	2:B:455:LEU:HD13	2.01	0.41
2:B:1206:LEU:HB3	2:B:1207:GLU:H	1.63	0.41
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	2.02	0.41
2:B:525:THR:HG23	2:B:545:LYS:NZ	2.33	0.41
2:B:1308:ASN:O	2:B:1311:HIS:HB2	2.19	0.41
2:B:442:LYS:HA	2:B:445:THR:HB	2.01	0.41
2:B:535:ARG:H	2:B:535:ARG:HG2	1.74	0.41
2:B:1255:LYS:H	2:B:1255:LYS:HG2	1.62	0.41
2:B:586:ARG:NH1	6:B:2129:HOH:O	2.53	0.41
2:B:1122:ARG:HG3	2:B:1134:PHE:CE2	2.55	0.41
2:B:524:LEU:HD22	2:B:540:LEU:HD23	2.02	0.41
2:B:531:THR:HG21	2:B:575:PHE:CZ	2.56	0.41
2:B:813:LEU:O	2:B:817:GLN:HG3	2.20	0.41
2:B:820:ARG:NH1	2:B:827:GLU:HG3	2.36	0.41
2:B:1106:SER:HB3	2:B:1137:PRO:HA	2.02	0.41
2:B:4:LYS:HB2	2:B:4:LYS:HE2	1.86	0.41
2:B:629:ARG:CZ	2:B:653:ARG:HA	2.50	0.41
2:B:272:ASP:HB2	2:B:653:ARG:NH2	2.35	0.41
1:A:35:A:H2'	1:A:36:A:C8	2.55	0.40
2:B:165:ARG:O	2:B:412:HIS:HA	2.21	0.40
2:B:251:ASN:HB2	2:B:263:LYS:HG2	2.02	0.40
2:B:749:LYS:HE2	2:B:749:LYS:HB3	1.84	0.40
1:A:25:U:H1'	2:B:104:SER:O	2.20	0.40
2:B:116:HIS:HA	2:B:117:PRO:HD3	1.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:LYS:HE3	2:B:539:PHE:CE1	2.56	0.40
2:B:558:LYS:HE2	2:B:586:ARG:HH12	1.86	0.40
1:A:33:G:N2	1:A:36:A:OP2	2.54	0.40
2:B:635:ARG:HG3	2:B:635:ARG:HH11	1.86	0.40
2:B:735:LYS:O	2:B:739:GLN:HG2	2.22	0.40
2:B:614:ASP:OD1	2:B:664:ARG:NH2	2.52	0.40
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.80	0.40
1:A:71:U:H3	1:A:78:A:N6	2.19	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)
6:B:2016:HOH:O	6:B:2092:HOH:O[3_445]	2.18	0.02

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	1292/1372 (94%)	1249 (97%)	43 (3%)	0	100	100

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	1174/1227 (96%)	1024 (87%)	150 (13%)	4 8

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	13	THR
2	B	22	THR
2	B	27	VAL
2	B	29	SER
2	B	39	ASP
2	B	44	LYS
2	B	64	LEU
2	B	65	LYS
2	B	73	THR
2	B	82	LEU
2	B	101	LEU
2	B	102	GLU
2	B	106	LEU
2	B	123	VAL
2	B	139	ARG
2	B	141	LYS
2	B	146	THR
2	B	165	ARG
2	B	173	ASP
2	B	174	LEU
2	B	178	ASN
2	B	188	LEU
2	B	197	GLU
2	B	198	GLU
2	B	212	LEU
2	B	215	ARG
2	B	219	SER
2	B	220	ARG
2	B	226	ILE
2	B	234	LYS
2	B	244	LEU
2	B	257	ASP
2	B	300	ILE
2	B	304	ASP
2	B	311	GLU
2	B	321	MET
2	B	327	GLU
2	B	334	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	345	GLU
2	B	419	LEU
2	B	425	ARG
2	B	438	GLU
2	B	445	THR
2	B	466	THR
2	B	471	GLU
2	B	472	THR
2	B	480	GLU
2	B	502	LEU
2	B	510	LYS
2	B	514	LEU
2	B	530	VAL
2	B	536	LYS
2	B	540	LEU
2	B	543	GLU
2	B	557	ARG
2	B	562	LYS
2	B	579	GLU
2	B	581	SER
2	B	598	LEU
2	B	599	LYS
2	B	601	ILE
2	B	602	LYS
2	B	610	GLU
2	B	622	THR
2	B	623	LEU
2	B	627	GLU
2	B	630	GLU
2	B	635	ARG
2	B	637	LYS
2	B	638	THR
2	B	643	PHE
2	B	661	ARG
2	B	665	LYS
2	B	666	LEU
2	B	677	LYS
2	B	696	LEU
2	B	697	ILE
2	B	703	THR
2	B	707	ASP
2	B	709	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	726	ASN
2	B	735	LYS
2	B	738	LEU
2	B	749	LYS
2	B	751	MET
2	B	763	MET
2	B	782	LYS
2	B	785	GLU
2	B	794	GLN
2	B	801	VAL
2	B	803	ASN
2	B	811	LEU
2	B	827	GLU
2	B	830	ILE
2	B	842	VAL
2	B	856	VAL
2	B	859	ARG
2	B	861	ASP
2	B	866	LYS
2	B	867	SER
2	B	878	LYS
2	B	884	ARG
2	B	887	LEU
2	B	894	GLN
2	B	910	GLU
2	B	917	ILE
2	B	918	LYS
2	B	919	ARG
2	B	921	LEU
2	B	935	LEU
2	B	945	GLU
2	B	957	THR
2	B	959	LYS
2	B	968	LYS
2	B	977	GLU
2	B	1003	LYS
2	B	1031	LYS
2	B	1033	THR
2	B	1035	LYS
2	B	1049	GLU
2	B	1069	THR
2	B	1071	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1076	LYS
2	B	1078	ARG
2	B	1087	LEU
2	B	1089	MET
2	B	1091	GLN
2	B	1119	LEU
2	B	1123	LYS
2	B	1144	LEU
2	B	1146	VAL
2	B	1160	VAL
2	B	1172	SER
2	B	1175	GLU
2	B	1207	GLU
2	B	1216	SER
2	B	1236	LEU
2	B	1240	SER
2	B	1253	GLU
2	B	1257	LEU
2	B	1260	GLU
2	B	1270	ILE
2	B	1274	SER
2	B	1280	VAL
2	B	1284	ASP
2	B	1298	ARG
2	B	1314	THR
2	B	1342	VAL
2	B	1347	LEU
2	B	1358	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	46	ASN
2	B	240	ASN
2	B	255	ASN
2	B	402	GLN
2	B	863	ASN
2	B	980	ASN
2	B	1093	ASN
2	B	1101	GLN
2	B	1115	ASN
2	B	1177	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1256	GLN
2	B	1286	ASN
2	B	1349	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/83 (96%)	21 (26%)	4 (5%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	20	A
1	A	28	A
1	A	29	G
1	A	31	U
1	A	32	A
1	A	34	A
1	A	35	A
1	A	37	U
1	A	38	A
1	A	40	C
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	74	A
1	A	75	A
1	A	79	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	27	G
1	A	42	A
1	A	68	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	81/83 (97%)	-0.37	1 (1%) 76 73	16, 38, 96, 112	0
2	B	1306/1372 (95%)	0.28	51 (3%) 43 38	12, 43, 76, 100	0
3	C	28/28 (100%)	-0.37	0 100 100	24, 38, 66, 85	0
4	D	11/12 (91%)	0.34	1 (9%) 15 11	37, 47, 86, 97	0
All	All	1426/1495 (95%)	0.23	53 (3%) 45 39	12, 43, 77, 112	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	377	LYS	3.7
2	B	688	PHE	3.6
2	B	178	ASN	3.6
2	B	424	ARG	3.6
2	B	584	GLU	3.3
2	B	1241	HIS	3.3
2	B	469	SER	3.2
2	B	1363	SER	3.1
2	B	776	ASN	3.1
2	B	247	GLY	3.0
2	B	199	ASN	3.0
2	B	868	ASP	2.9
2	B	420	HIS	2.9
2	B	204	SER	2.9
2	B	1253	GLU	2.9
2	B	181	VAL	2.8
2	B	1299	ASP	2.8
2	B	203	ALA	2.8
2	B	778	ARG	2.8
2	B	1078	ARG	2.8
2	B	43	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	2	DA	2.7
2	B	1115	ASN	2.7
2	B	661	ARG	2.6
2	B	803	ASN	2.6
2	B	248	LEU	2.6
2	B	721	HIS	2.6
2	B	653	ARG	2.5
2	B	231	GLY	2.5
2	B	414	ILE	2.4
2	B	530	VAL	2.4
1	A	77	A	2.4
2	B	665	LYS	2.4
2	B	1264	HIS	2.3
2	B	102	GLU	2.3
2	B	246	LEU	2.3
2	B	692	ASN	2.2
2	B	697	ILE	2.2
2	B	382	LYS	2.2
2	B	1296	LYS	2.2
2	B	519	THR	2.1
2	B	804	THR	2.1
2	B	311	GLU	2.1
2	B	122	ILE	2.1
2	B	703	THR	2.1
2	B	599	LYS	2.1
2	B	384	ASP	2.1
2	B	807	GLN	2.0
2	B	1298	ARG	2.0
2	B	398	LEU	2.0
2	B	630	GLU	2.0
2	B	4	LYS	2.0
2	B	1030	GLY	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	2365	1/1	0.30	0.22	53,53,53,53	0
5	MG	B	2368	1/1	0.63	0.16	36,36,36,36	0
5	MG	A	1085	1/1	0.74	0.36	53,53,53,53	0
5	MG	B	2367	1/1	0.76	0.11	15,15,15,15	0
5	MG	B	2366	1/1	0.76	0.10	25,25,25,25	0
5	MG	A	1084	1/1	0.79	0.10	27,27,27,27	0
5	MG	A	1082	1/1	0.93	0.10	27,27,27,27	0
5	MG	A	1083	1/1	0.96	0.05	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.