



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 01:37 AM EDT

PDB ID : 4ZT0 / pdb_00004zt0
Title : Crystal structure of catalytically-active Streptococcus pyogenes Cas9 in complex with single-guide RNA at 2.9 Angstrom resolution
Authors : Jiang, F.; Doudna, J.A.
Deposited on : 2015-05-14
Resolution : 2.90 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

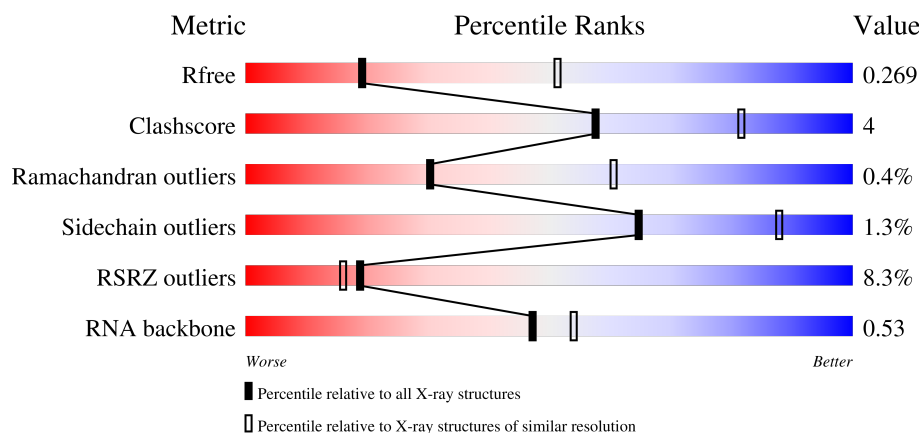
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)
RNA backbone	3690	1039 (3.10-2.70)

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	1369	<div> <div>7%</div> <div>87%</div> <div>12%</div> </div>
1	C	1369	<div> <div>9%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
2	B	85	<div> <div>4%</div> <div>49%</div> <div>31%</div> <div>5%</div> <div>15%</div> </div>
2	D	85	<div> <div>44%</div> <div>36%</div> <div>5%</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23790 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR-associated endonuclease Cas9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1364	Total	C	N	O	S	Se	0	0	0
			10654	6778	1829	2025	2	20			
1	C	1296	Total	C	N	O	S	Se	0	0	0
			10046	6393	1728	1904	2	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A0C6FZC2
A	1	MSE	-	expression tag	UNP A0A0C6FZC2
C	0	SER	-	expression tag	UNP A0A0C6FZC2
C	1	MSE	-	expression tag	UNP A0A0C6FZC2

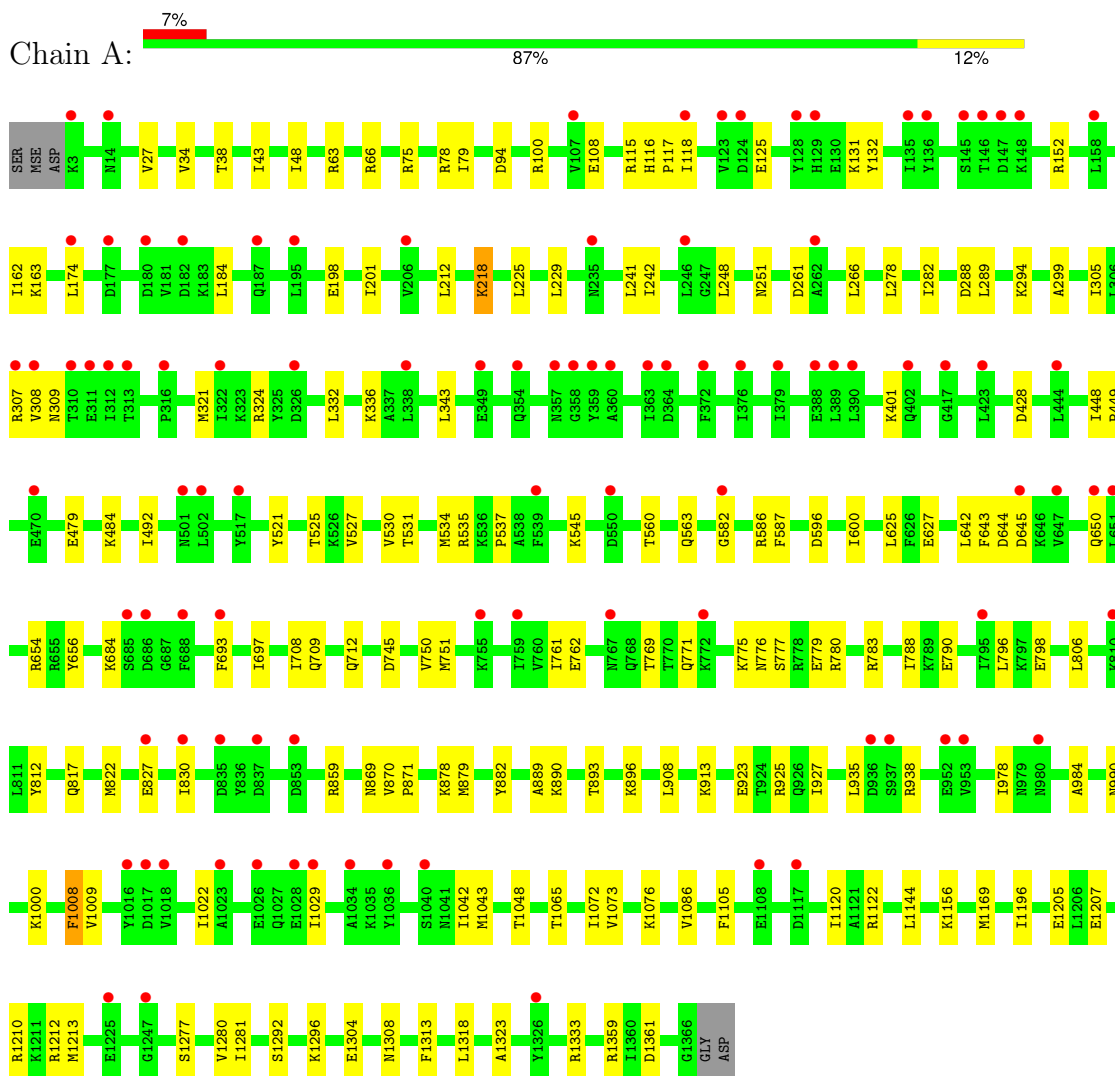
- Molecule 2 is a RNA chain called single-guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	P	0	0	0
			1545	692	285	496	72			
2	D	72	Total	C	N	O	P	0	0	0
			1545	692	285	496	72			

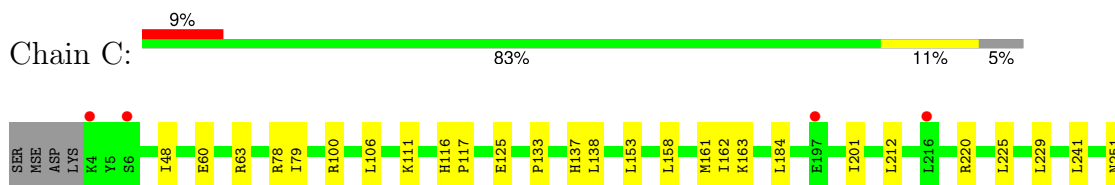
3 Residue-property plots

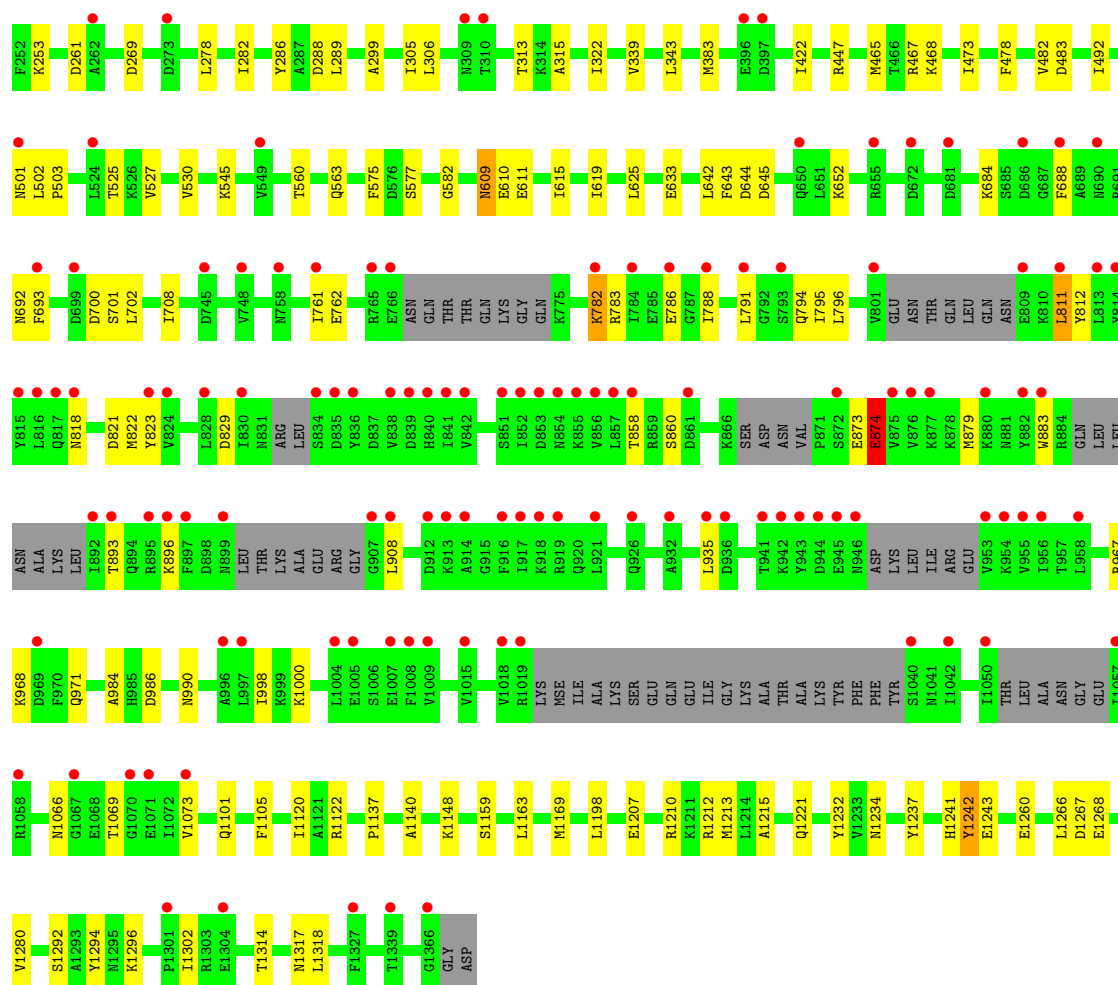
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated endonuclease Cas9

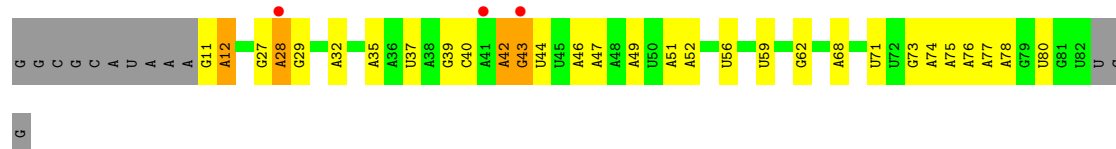


• Molecule 1: CRISPR-associated endonuclease Cas9

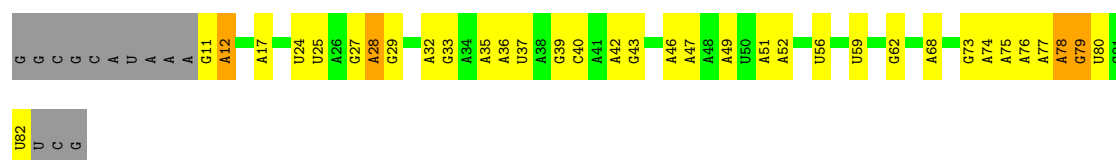




• Molecule 2: single-guide RNA



• Molecule 2: single-guide RNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.24Å 143.00Å 294.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.90 49.15 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.15-2.90) 99.4 (49.15-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.238 , 0.264 0.246 , 0.269	Depositor DCC
R_{free} test set	4812 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23790	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8491e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.25	0/10825	0.37	0/14614
1	C	0.26	0/10200	0.38	0/13759
2	B	0.17	0/1732	0.70	0/2698
2	D	0.17	0/1732	0.70	0/2698
All	All	0.24	0/24489	0.44	0/33769

There are no bond length outliers.

There are no bond angle outliers.

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	10654	0	10330	92	0
1	C	10046	0	9673	84	0
2	B	1545	0	774	15	0
2	D	1545	0	774	13	0
All	All	23790	0	21551	199	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 4.

All (199) 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:C:1120:ILE:HD11	1:C:1137:PRO:HG3	1.66	0.78
2:B:32:A:H61	2:B:37:U:H3	1.31	0.77
1:C:1122:ARG:NH2	2:D:49:A:N3	2.35	0.74
1:A:218:LYS:HG3	1:A:248:LEU:HD21	1.70	0.73
1:A:762:GLU:OE1	1:A:990:ASN:ND2	2.21	0.73
1:C:78:ARG:NH1	1:C:162:ILE:O	2.22	0.72
1:C:116:HIS:HB3	1:C:125:GLU:HG3	1.74	0.70
2:D:27:G:H5''	2:D:28:A:H5'	1.74	0.69
1:C:100:ARG:NH1	1:C:117:PRO:O	2.27	0.68
2:D:33:G:N2	2:D:36:A:OP2	2.27	0.68
1:A:1122:ARG:NH2	2:B:49:A:N3	2.41	0.67
1:A:761:ILE:HD11	1:A:935:LEU:HD12	1.77	0.67
1:C:79:ILE:HD11	1:C:163:LYS:HB2	1.77	0.66
1:A:1304:GLU:O	1:A:1308:ASN:ND2	2.29	0.66
1:A:116:HIS:HB3	1:A:125:GLU:HG3	1.78	0.65
1:C:762:GLU:OE1	1:C:990:ASN:ND2	2.24	0.64
1:A:869:ASN:HD21	1:A:908:LEU:H	1.44	0.63
2:B:27:G:H5''	2:B:28:A:H5'	1.80	0.62
1:A:1205:GLU:OE1	1:A:1359:ARG:NH2	2.30	0.62
1:A:212:LEU:HD21	1:A:225:LEU:HD22	1.83	0.61
2:B:27:G:N2	2:B:44:U:OP2	2.33	0.61
1:C:1212:ARG:NH2	1:C:1280:VAL:O	2.34	0.61
1:A:817:GLN:HG2	1:A:822:MSE:HE2	1.81	0.60
1:A:100:ARG:NH1	1:A:117:PRO:O	2.35	0.60
1:C:822:MSE:HG3	1:C:883:TRP:HE1	1.66	0.60
1:C:343:LEU:HB2	1:C:383:MSE:HE2	1.84	0.60
1:C:971:GLN:O	1:C:1234:ASN:ND2	2.34	0.59
1:A:479:GLU:OE1	1:A:484:LYS:NZ	2.34	0.58
1:A:1105:PHE:HB3	1:A:1169:MSE:HE2	1.84	0.58
1:A:1008:PHE:HD2	1:A:1009:VAL:HG23	1.69	0.58
1:C:1148:LYS:HG2	1:C:1159:SER:HA	1.86	0.57
1:A:1280:VAL:HG23	1:A:1281:ILE:HD12	1.88	0.56
1:A:923:GLU:OE1	1:A:925:ARG:NH1	2.39	0.56
1:A:1048:THR:HG22	1:A:1076:LYS:HD3	1.87	0.56
1:A:94:ASP:OD2	1:A:152:ARG:NH1	2.38	0.56
1:A:307:ARG:O	1:A:309:ASN:N	2.39	0.55
1:A:78:ARG:NH1	1:A:162:ILE:O	2.39	0.55
2:B:52:A:OP2	2:B:62:G:N2	2.38	0.55
1:A:560:THR:HG23	1:A:563:GLN:H	1.72	0.55
1:C:253:LYS:HB2	1:C:261:ASP:HA	1.88	0.55
1:A:251:ASN:HD21	1:A:261:ASP:HB2	1.72	0.55
1:C:158:LEU:HA	1:C:161:MSE:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:VAL:HG22	1:C:383:MSE:HE1	1.89	0.54
1:A:776:ASN:OD1	1:A:777:SER:N	2.41	0.54
1:A:324:ARG:NH1	1:A:401:LYS:O	2.40	0.54
1:A:790:GLU:HG2	1:A:889:ALA:HA	1.89	0.53
1:C:161:MSE:HE1	1:C:422:ILE:HD12	1.90	0.53
1:C:1232:TYR:OH	1:C:1268:GLU:OE2	2.20	0.53
1:A:878:LYS:HG3	1:A:879:MSE:HE2	1.90	0.53
1:A:1065:THR:HG22	1:A:1072:ILE:HG22	1.90	0.53
1:C:1105:PHE:HB3	1:C:1169:MSE:HE2	1.91	0.53
1:C:1215:ALA:HB2	1:C:1221:GLN:HG3	1.91	0.53
2:D:27:G:C5'	2:D:28:A:H5'	2.38	0.53
1:A:108:GLU:OE2	1:A:115:ARG:NH2	2.36	0.52
1:A:201:ILE:HD11	1:A:229:LEU:HD22	1.90	0.52
1:C:138:LEU:HD11	1:C:153:LEU:HB3	1.92	0.52
1:A:266:LEU:HD22	1:A:294:LYS:HD3	1.92	0.52
1:C:501:ASN:HB3	1:C:708:ILE:HD11	1.91	0.52
1:C:811:LEU:HD23	1:C:811:LEU:H	1.75	0.52
1:C:278:LEU:O	1:C:282:ILE:HG13	2.10	0.52
1:A:79:ILE:HD11	1:A:163:LYS:HB2	1.92	0.52
1:A:1000:LYS:HD3	1:A:1073:VAL:HG21	1.92	0.51
1:A:428:ASP:OD1	1:A:428:ASP:N	2.41	0.51
1:A:27:VAL:HG22	1:A:1086:VAL:HG22	1.93	0.51
1:C:761:ILE:HD11	1:C:935:LEU:HD12	1.91	0.51
1:A:492:ILE:HG12	1:A:625:LEU:HD13	1.92	0.51
1:C:465:MSE:HE1	1:C:467:ARG:HG2	1.93	0.50
1:C:465:MSE:HE3	1:C:482:VAL:HG22	1.93	0.50
1:C:633:GLU:HG2	1:C:652:LYS:HD3	1.92	0.50
1:C:1101:GLN:HB2	1:C:1140:ALA:HA	1.94	0.50
1:A:644:ASP:OD1	1:A:645:ASP:N	2.45	0.50
1:C:184:LEU:HD12	1:C:299:ALA:HB2	1.93	0.50
1:C:282:ILE:HD13	1:C:286:TYR:HD2	1.77	0.50
1:C:1066:ASN:HD22	1:C:1069:THR:HG22	1.76	0.50
2:B:42:A:O2'	2:B:43:G:OP1	2.27	0.49
1:C:644:ASP:OD1	1:C:645:ASP:N	2.44	0.49
2:D:78:A:O2'	2:D:79:G:OP1	2.26	0.49
1:C:313:THR:O	1:C:315:ALA:N	2.41	0.49
1:C:201:ILE:HD11	1:C:229:LEU:HD22	1.95	0.49
1:C:282:ILE:HD13	1:C:286:TYR:CD2	2.47	0.49
1:A:1212:ARG:NH2	1:A:1280:VAL:O	2.45	0.48
1:A:925:ARG:HG2	1:A:927:ILE:HG22	1.95	0.48
1:A:893:THR:HG23	1:A:896:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:LEU:HB3	1:A:1196:ILE:HB	1.95	0.48
1:A:780:ARG:HG3	1:A:806:LEU:HD23	1.95	0.48
1:C:822:MSE:HG3	1:C:883:TRP:NE1	2.28	0.48
1:C:1241:HIS:O	1:C:1243:GLU:N	2.47	0.48
1:C:823:TYR:HD2	1:C:858:THR:HG21	1.79	0.48
1:A:817:GLN:O	1:A:882:TYR:OH	2.31	0.48
1:C:111:LYS:NZ	2:D:25:U:O2'	2.35	0.48
1:A:693:PHE:CZ	1:A:697:ILE:HD11	2.49	0.48
1:C:821:ASP:OD1	1:C:822:MSE:N	2.47	0.48
1:A:278:LEU:O	1:A:282:ILE:HG12	2.14	0.47
1:A:596:ASP:O	1:A:600:ILE:HG12	2.14	0.47
2:B:27:G:H3'	2:B:28:A:H5'	1.95	0.47
1:C:525:THR:HA	1:C:545:LYS:HE2	1.97	0.47
1:C:527:VAL:HA	1:C:582:GLY:HA3	1.96	0.47
1:C:137:HIS:HA	1:C:322:ILE:HD11	1.97	0.47
1:A:654:ARG:HH21	1:A:656:TYR:HE1	1.61	0.47
1:C:492:ILE:HG12	1:C:625:LEU:HD13	1.97	0.47
1:A:116:HIS:HA	1:A:117:PRO:HD3	1.74	0.47
1:C:795:ILE:HD13	1:C:818:ASN:HA	1.96	0.47
1:A:600:ILE:HD12	1:A:650:GLN:HG2	1.96	0.46
1:A:870:VAL:HB	1:A:871:PRO:HD2	1.97	0.46
1:C:560:THR:HG23	1:C:563:GLN:H	1.80	0.46
1:C:1266:LEU:HD11	1:C:1302:ILE:HG23	1.97	0.46
1:A:34:VAL:HG21	1:A:43:ILE:HG13	1.97	0.46
1:A:1207:GLU:OE1	1:A:1210:ARG:NH1	2.48	0.46
2:B:73:G:H21	2:B:76:A:H2	1.61	0.46
1:C:106:LEU:O	1:C:111:LYS:HE3	2.16	0.46
1:C:968:LYS:NZ	1:C:1237:TYR:OH	2.48	0.46
1:C:1000:LYS:HG2	1:C:1073:VAL:HG21	1.96	0.46
2:D:46:A:H2'	2:D:47:A:C8	2.50	0.46
1:A:525:THR:HA	1:A:545:LYS:HE2	1.97	0.46
1:A:531:THR:HG22	1:A:534:MSE:SE	2.66	0.46
1:A:1323:ALA:N	1:A:1333:ARG:HG2	2.31	0.46
1:C:700:ASP:C	1:C:702:LEU:H	2.18	0.46
1:A:780:ARG:HB2	1:A:812:TYR:CE1	2.50	0.46
1:C:967:ARG:NH1	1:C:986:ASP:OD1	2.49	0.46
1:A:535:ARG:HA	1:A:535:ARG:HD2	1.77	0.46
1:A:830:ILE:HD12	1:A:830:ILE:H	1.80	0.46
1:A:1008:PHE:CD2	1:A:1009:VAL:HG23	2.50	0.46
1:A:978:ILE:HG12	1:A:1313:PHE:CE2	2.52	0.45
1:C:212:LEU:HD21	1:C:225:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1120:ILE:HG21	1:C:1169:MSE:HE1	1.97	0.45
1:C:1292:SER:O	1:C:1296:LYS:HG2	2.17	0.45
1:A:305:ILE:HD11	1:A:321:MSE:SE	2.66	0.45
1:A:1213:MSE:HE3	1:A:1318:LEU:HD11	1.97	0.45
1:A:527:VAL:HA	1:A:582:GLY:HA3	1.99	0.45
1:A:241:LEU:HD11	1:A:289:LEU:HD21	1.98	0.45
1:C:783:ARG:NH2	1:C:812:TYR:OH	2.32	0.44
1:A:750:VAL:HG12	1:A:751:MSE:HE3	1.99	0.44
2:D:11:G:O2'	2:D:12:A:O5'	2.35	0.44
1:A:131:LYS:HG2	1:A:132:TYR:CZ	2.52	0.44
1:A:775:LYS:O	1:A:779:GLU:HG2	2.18	0.44
1:A:788:ILE:HG13	1:A:796:LEU:HD13	2.00	0.44
1:C:220:ARG:HD2	1:C:220:ARG:HA	1.73	0.44
2:D:32:A:H61	2:D:37:U:H3	1.66	0.44
1:A:48:ILE:HG12	1:A:984:ALA:HB1	1.99	0.44
1:C:575:PHE:O	1:C:577:SER:N	2.46	0.44
1:C:893:THR:HG23	1:C:896:LYS:H	1.83	0.43
1:A:783:ARG:NH2	1:A:890:LYS:O	2.51	0.43
2:D:52:A:OP2	2:D:62:G:N2	2.45	0.43
1:C:251:ASN:HD21	1:C:261:ASP:HB2	1.84	0.43
1:C:873:GLU:O	1:C:874:GLU:HB3	2.17	0.43
1:A:708:ILE:O	1:A:712:GLN:HG2	2.18	0.43
1:A:751:MSE:HA	1:A:751:MSE:HE2	2.01	0.43
1:C:478:PHE:CE1	1:C:482:VAL:HG21	2.54	0.43
1:C:1207:GLU:OE1	1:C:1210:ARG:NH1	2.52	0.43
1:C:1213:MSE:HE3	1:C:1318:LEU:HD11	2.01	0.43
1:C:133:PRO:HD2	1:C:137:HIS:CG	2.54	0.43
1:A:225:LEU:HD23	1:A:242:ILE:HG21	2.01	0.43
1:C:1267:ASP:OD1	1:C:1294:TYR:OH	2.28	0.43
1:A:1120:ILE:HG21	1:A:1169:MSE:HE1	1.99	0.43
1:C:609:ASN:C	1:C:611:GLU:H	2.23	0.43
2:B:71:U:H3	2:B:78:A:H61	1.66	0.42
2:B:46:A:H2'	2:B:47:A:C8	2.54	0.42
1:C:305:ILE:HG22	1:C:306:LEU:H	1.84	0.42
1:A:913:LYS:HB2	1:A:1022:ILE:HD13	2.01	0.42
1:A:1277:SER:HA	1:A:1281:ILE:HD13	2.01	0.42
1:A:1292:SER:O	1:A:1296:LYS:HG3	2.19	0.42
1:C:1163:LEU:HD11	1:C:1198:LEU:HD12	2.01	0.42
1:A:530:VAL:HG22	1:A:537:PRO:HA	2.02	0.42
1:C:269:ASP:OD1	1:C:269:ASP:N	2.51	0.42
1:A:75:ARG:HD3	1:A:163:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:TYR:CE1	1:A:684:LYS:HG2	2.55	0.42
2:D:74:A:H2'	2:D:75:A:O4'	2.19	0.42
1:A:118:ILE:N	1:A:125:GLU:OE2	2.53	0.42
1:A:586:ARG:NH1	1:A:587:PHE:O	2.53	0.42
1:A:869:ASN:OD1	1:A:870:VAL:N	2.47	0.42
1:A:116:HIS:NE2	2:B:27:G:OP1	2.52	0.41
1:C:467:ARG:HH12	1:C:473:ILE:HG13	1.86	0.41
1:A:38:THR:HG22	1:A:1361:ASP:HB2	2.02	0.41
2:B:74:A:H2'	2:B:75:A:O4'	2.20	0.41
1:C:241:LEU:HD11	1:C:289:LEU:HD21	2.03	0.41
1:C:684:LYS:HB2	1:C:684:LYS:HE3	1.85	0.41
1:A:332:LEU:O	1:A:336:LYS:HG3	2.20	0.41
1:A:1042:ILE:HG13	1:A:1043:MSE:HG2	2.02	0.41
1:C:1066:ASN:ND2	1:C:1069:THR:HG22	2.34	0.41
1:C:1314:THR:HA	1:C:1317:ASN:ND2	2.35	0.41
1:C:468:LYS:HB3	1:C:483:ASP:HB2	2.02	0.41
1:C:502:LEU:HA	1:C:503:PRO:HD2	1.97	0.41
1:A:745:ASP:OD2	1:A:938:ARG:NH1	2.53	0.41
2:B:27:G:H3'	2:B:28:A:C5'	2.51	0.41
1:C:788:ILE:HG13	1:C:796:LEU:HD23	2.03	0.41
1:C:782:LYS:HB2	1:C:782:LYS:HE2	1.83	0.41
1:C:615:ILE:O	1:C:619:ILE:HG13	2.21	0.41
1:A:827:GLU:O	1:A:859:ARG:NH2	2.38	0.41
2:B:42:A:HO2'	2:B:43:G:P	2.43	0.41
1:A:448:ILE:HA	1:A:449:PRO:HD3	1.92	0.41
1:C:60:GLU:HG3	1:C:63:ARG:HH22	1.84	0.41
1:C:447:ARG:HG3	2:D:17:A:H5'	2.03	0.41
2:D:73:G:H21	2:D:76:A:H2	1.68	0.40
1:A:63:ARG:HG3	1:A:66:ARG:NH2	2.36	0.40
1:A:769:THR:C	1:A:771:GLN:H	2.25	0.40
2:B:11:G:O2'	2:B:12:A:O5'	2.37	0.40
1:C:48:ILE:HG12	1:C:984:ALA:HB1	2.04	0.40
1:C:986:ASP:O	1:C:990:ASN:ND2	2.40	0.40
1:A:184:LEU:HD22	1:A:299:ALA:HB2	2.03	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	
1	A	1362/1369 (100%)	1301 (96%)	59 (4%)	2 (0%)	48	77
1	C	1276/1369 (93%)	1216 (95%)	51 (4%)	9 (1%)	19	49
All	All	2638/2738 (96%)	2517 (95%)	110 (4%)	11 (0%)	30	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	VAL
1	C	874	GLU
1	C	688	PHE
1	C	1242	TYR
1	C	692	ASN
1	C	860	SER
1	C	908	LEU
1	C	693	PHE
1	C	701	SER
1	A	1029	ILE
1	C	610	GLU

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	1106/1206 (92%)	1094 (99%)	12 (1%)	70	90
1	C	1031/1206 (86%)	1015 (98%)	16 (2%)	58	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2137/2412 (89%)	2109 (99%)	28 (1%)	65 88

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	A	198	GLU
1	A	218	LYS
1	A	288	ASP
1	A	343	LEU
1	A	627	GLU
1	A	642	LEU
1	A	643	PHE
1	A	709	GLN
1	A	798	GLU
1	A	1008	PHE
1	A	1156	LYS
1	C	288	ASP
1	C	530	VAL
1	C	609	ASN
1	C	642	LEU
1	C	643	PHE
1	C	782	LYS
1	C	786	GLU
1	C	791	LEU
1	C	794	GLN
1	C	811	LEU
1	C	829	ASP
1	C	874	GLU
1	C	879	MSE
1	C	998	ILE
1	C	1242	TYR
1	C	1260	GLU

Sometimes 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	71/85 (83%)	14 (19%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	71/85 (83%)	16 (22%)	2 (2%)
All	All	142/170 (83%)	30 (21%)	3 (2%)

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	A
2	B	28	A
2	B	29	G
2	B	35	A
2	B	39	G
2	B	40	C
2	B	42	A
2	B	43	G
2	B	51	A
2	B	56	U
2	B	59	U
2	B	68	A
2	B	77	A
2	B	80	U
2	D	12	A
2	D	24	U
2	D	28	A
2	D	29	G
2	D	35	A
2	D	39	G
2	D	40	C
2	D	43	G
2	D	51	A
2	D	56	U
2	D	59	U
2	D	68	A
2	D	77	A
2	D	79	G
2	D	80	U
2	D	82	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	42	A
2	D	42	A

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Mol	Chain	Res	Type
2	D	78	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1343/1369 (98%)	0.54	99 (7%) 22 19	37, 96, 152, 216	0
1	C	1276/1369 (93%)	0.65	127 (9%) 14 12	39, 93, 181, 232	0
2	B	72/85 (84%)	0.19	3 (4%) 41 35	46, 78, 221, 260	0
2	D	72/85 (84%)	-0.12	0 100 100	47, 65, 156, 194	0
All	All	2763/2908 (95%)	0.56	229 (8%) 19 16	37, 94, 170, 260	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	954	LYS	6.3
1	C	1019	ARG	5.8
1	C	852	ILE	5.7
1	A	376	ILE	5.0
1	A	310	THR	4.8
1	A	767	ASN	4.7
1	C	758	ASN	4.6
2	B	28	A	4.6
1	C	854	ASN	4.5
1	C	1009	VAL	4.4
1	C	943	TYR	4.3
1	C	814	TYR	4.2
1	A	177	ASP	4.1
1	C	912	ASP	4.1
1	C	908	LEU	4.1
1	C	856	VAL	4.1
1	A	1018	VAL	4.0
1	A	1036	TYR	4.0
1	A	755	LYS	4.0
1	A	174	LEU	3.9
1	C	936	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	946	ASN	3.8
1	A	128	TYR	3.8
1	A	180	ASP	3.7
1	A	953	VAL	3.7
1	C	748	VAL	3.7
1	C	916	PHE	3.7
1	C	851	SER	3.7
1	C	273	ASP	3.7
1	A	364	ASP	3.6
1	A	1016	TYR	3.6
1	C	838	VAL	3.6
1	C	811	LEU	3.6
1	C	997	LEU	3.6
1	C	823	TYR	3.5
1	C	872	SER	3.5
1	A	360	ALA	3.5
1	A	827	GLU	3.5
1	C	944	ASP	3.4
1	C	818	ASN	3.4
1	C	1040	SER	3.4
1	C	809	GLU	3.4
1	C	932	ALA	3.4
1	C	1304	GLU	3.4
1	C	1301	PRO	3.4
1	A	517	TYR	3.3
1	C	686	ASP	3.3
1	C	815	TYR	3.3
1	A	1028	GLU	3.3
1	C	899	ASN	3.2
1	C	855	LYS	3.2
1	C	841	ILE	3.2
1	A	107	VAL	3.2
1	C	688	PHE	3.2
1	C	1070	GLY	3.2
1	A	145	SER	3.2
1	A	936	ASP	3.2
1	C	917	ILE	3.1
1	C	1057	ILE	3.1
1	C	896	LYS	3.1
1	A	470	GLU	3.1
1	C	907	GLY	3.1
1	C	921	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1073	VAL	3.0
1	A	402	GLN	3.0
1	C	1042	ILE	3.0
1	A	379	ILE	3.0
1	C	958	LEU	3.0
1	C	857	LEU	3.0
1	A	358	GLY	3.0
1	C	524	LEU	3.0
1	C	1058	ARG	2.9
1	A	322	ILE	2.9
1	A	359	TYR	2.9
1	C	1007	GLU	2.9
1	C	1015	VAL	2.9
1	C	942	LYS	2.9
1	C	953	VAL	2.9
1	A	1225	GLU	2.9
1	C	786	GLU	2.9
1	A	937	SER	2.8
1	C	813	LEU	2.8
1	C	956	ILE	2.8
1	A	686	ASP	2.8
1	A	688	PHE	2.8
1	C	309	ASN	2.8
1	C	861	ASP	2.8
1	C	693	PHE	2.8
1	A	148	LYS	2.8
1	C	262	ALA	2.8
1	A	349	GLU	2.8
1	A	837	ASP	2.8
1	C	918	LYS	2.8
1	A	308	VAL	2.7
1	C	914	ALA	2.7
1	A	685	SER	2.7
1	A	952	GLU	2.7
1	C	941	THR	2.7
1	A	1040	SER	2.7
1	C	791	LEU	2.7
1	C	839	ASP	2.7
1	C	1008	PHE	2.7
1	A	357	ASN	2.7
1	C	830	ILE	2.7
1	C	969	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	955	VAL	2.7
1	C	875	VAL	2.6
1	C	883	TRP	2.6
1	C	6	SER	2.6
1	C	882	TYR	2.6
1	A	853	ASP	2.6
1	A	1117	ASP	2.6
1	A	158	LEU	2.6
1	A	1029	ILE	2.6
1	C	1050	ILE	2.6
1	C	216	LEU	2.6
1	A	539	PHE	2.6
1	C	892	ILE	2.6
1	C	690	ASN	2.6
1	A	311	GLU	2.6
1	A	326	ASP	2.6
1	A	388	GLU	2.5
1	C	766	GLU	2.5
1	A	206	VAL	2.5
1	A	389	LEU	2.5
1	C	836	TYR	2.5
1	A	1034	ALA	2.5
1	A	3	LYS	2.5
1	C	996	ALA	2.5
1	A	502	LEU	2.5
1	A	1023	ALA	2.5
1	A	135	ILE	2.5
1	A	759	ILE	2.5
1	C	926	GLN	2.5
1	C	396	GLU	2.5
1	C	784	ILE	2.5
1	A	1017	ASP	2.4
1	A	129	HIS	2.4
1	A	647	VAL	2.4
1	C	858	THR	2.4
1	C	897	PHE	2.4
1	C	853	ASP	2.4
1	C	935	LEU	2.4
1	A	312	ILE	2.4
1	A	795	ILE	2.4
1	A	830	ILE	2.4
1	C	919	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	187	GLN	2.4
1	A	354	GLN	2.4
1	A	835	ASP	2.4
1	C	816	LEU	2.4
1	A	1026	GLU	2.4
2	B	43	G	2.4
1	A	235	ASN	2.4
1	A	246	LEU	2.3
1	A	651	LEU	2.3
1	C	876	VAL	2.3
1	A	313	THR	2.3
1	C	828	LEU	2.3
1	C	1004	LEU	2.3
1	C	397	ASP	2.3
1	C	1018	VAL	2.3
1	A	14	ASN	2.3
1	C	4	LYS	2.3
1	A	650	GLN	2.3
1	A	262	ALA	2.3
1	C	1071	GLU	2.3
1	A	444	LEU	2.3
1	C	893	THR	2.3
1	A	550	ASP	2.2
1	C	835	ASP	2.2
1	A	1247	GLY	2.2
1	C	840	HIS	2.2
1	A	372	PHE	2.2
1	C	655	ARG	2.2
1	C	834	SER	2.2
1	A	316	PRO	2.2
1	C	761	ILE	2.2
1	C	1366	GLY	2.2
1	C	945	GLU	2.2
1	C	782	LYS	2.2
1	C	549	VAL	2.2
1	C	501	ASN	2.2
1	C	765	ARG	2.2
1	C	1005	GLU	2.2
1	C	913	LYS	2.1
1	C	824	VAL	2.1
1	C	310	THR	2.1
1	C	817	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	TYR	2.1
1	A	772	LYS	2.1
1	C	880	LYS	2.1
1	A	363	ILE	2.1
1	A	124	ASP	2.1
1	A	147	ASP	2.1
1	A	645	ASP	2.1
1	C	681	ASP	2.1
1	C	1339	THR	2.1
1	A	423	LEU	2.1
1	A	1326	TYR	2.1
1	C	197	GLU	2.1
1	A	118	ILE	2.1
1	C	788	ILE	2.1
1	C	895	ARG	2.1
1	A	182	ASP	2.1
1	A	810	LYS	2.1
1	A	501	ASN	2.1
2	B	41	A	2.1
1	A	417	GLY	2.1
1	C	877	LYS	2.1
1	A	693	PHE	2.1
1	C	1327	PHE	2.1
1	A	146	THR	2.0
1	C	745	ASP	2.0
1	A	1108	GLU	2.0
1	A	980	ASN	2.0
1	A	123	VAL	2.0
1	A	307	ARG	2.0
1	C	801	VAL	2.0
1	C	842	VAL	2.0
1	A	390	LEU	2.0
1	C	650	GLN	2.0
1	C	672	ASP	2.0
1	C	699	ASP	2.0
1	C	793	SER	2.0
1	A	195	LEU	2.0
1	A	338	LEU	2.0
1	A	582	GLY	2.0
1	C	1067	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.