

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2022 – 04:55 pm BST

PDB ID	:	7Z4D
Title	:	Crystal structure of SpCas9 bound to a 10 nucleotide complementary DNA
		substrate
Authors	:	Pacesa, M.; Jinek, M.
Deposited on	:	2022-03-03
Resolution	:	3.10 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 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 <=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	А	84	39%	43%	7%	11%
1	F	84	<mark>6%</mark> 35%	44%	13%	8%
2	В	1368	8%	79%	13%	8%
2	Е	1368	7%		14%	15%



Mol	Chain	Length	Quality of chain					
3	С	30	37%	63%				
3	G	30	33%	57%	10%			
4	D	30	10%	23%	27%			
4	Н	30	43%	20%	37%			



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25082 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	75	Total	С	Ν	0	Р	0	0	0
I A	15	1610	723	303	510	74	0	0	0	
1	Б	77	Total	С	Ν	0	Р	0	0	0
1	Г	11	1652	742	310	524	76	0	0	U

• Molecule 1 is a RNA chain called sgRNA.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	1259	Total 10259	C 6549	N 1769	O 1921	S 20	0	0	0
2	Е	1166	Total 9537	C 6102	N 1640	O 1776	S 19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	10	ALA	ASP	engineered mutation	UNP Q99ZW2
В	840	ALA	HIS	engineered mutation	UNP Q99ZW2
Е	10	ALA	ASP	engineered mutation	UNP Q99ZW2
Е	840	ALA	HIS	engineered mutation	UNP Q99ZW2

• Molecule 3 is a DNA chain called Target strand of 10 nucleotide complementary DNA substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	30	Total 606	C 291	N 105	0 181	Р 29	0	0	0
3	G	27	Total 526	C 252	N 90	O 159	Р 25	0	0	1

• Molecule 4 is a DNA chain called Non-target strand of 10 nucleotide complementary DNA substrate.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4		00	Total	С	Ν	0	Р	0	0	1
4 D		429	207	75	127	20	0	0	1	
4	Ц	10	Total	С	Ν	0	Р	0	0	1
4 П	19	359	172	64	106	17	0	0	L	

• Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	6	Total K 6 6	0	0
5	В	3	Total K 3 3	0	0
5	С	1	Total K 1 1	0	0
5	Е	2	Total K 2 2	0	0
5	F	3	Total K 3 3	0	0
5	G	1	Total K 1 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	15	Total O 15 15	0	0
6	В	22	Total O 22 22	0	0
6	С	1	Total O 1 1	0	0
6	D	2	Total O 2 2	0	0
6	Ε	29	Total O 29 29	0	0
6	F	14	Total O 14 14	0	0
6	G	1	Total O 1 1	0	0
6	Н	4	Total O 4 4	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: sgRNA







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	88.64Å 95.51Å 169.80Å	Depositor
a, b, c, α , β , γ	80.83° 78.04° 62.34°	Depositor
Bosolution(A)	66.49 - 3.10	Depositor
Resolution (A)	66.48 - 3.10	EDS
% Data completeness	89.2 (66.49-3.10)	Depositor
(in resolution range)	89.2(66.48-3.10)	EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.86 (at 3.13 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.246 , 0.276	Depositor
II, II free	0.247 , 0.275	DCC
R_{free} test set	3882 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	52.8	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ < L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	25082	wwPDB-VP
Average B, all atoms $(Å^2)$	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 17.13% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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

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	
1VIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.26	0/1807	0.84	0/2816
1	F	0.26	0/1854	0.82	0/2889
2	В	0.25	1/10440~(0.0%)	0.48	0/14026
2	Е	0.25	0/9706	0.47	1/13036~(0.0%)
3	С	0.59	0/677	0.94	0/1042
3	G	0.55	0/586	0.94	0/901
4	D	0.56	0/479	0.95	0/737
4	Н	0.56	0/401	0.95	0/616
All	All	0.29	1/25950~(0.0%)	0.60	1/36063~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1021	MET	CG-SD	5.24	1.94	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	E	666	LEU	CA-CB-CG	5.29	127.47	115.30

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.



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1610	0	809	27	0
1	F	1652	0	830	37	0
2	В	10259	0	10425	102	0
2	Е	9537	0	9689	118	0
3	С	606	0	341	18	0
3	G	526	0	297	18	0
4	D	429	0	242	5	0
4	Н	359	0	201	7	0
5	А	6	0	0	0	0
5	В	3	0	0	0	0
5	С	1	0	0	0	0
5	Е	2	0	0	0	0
5	F	3	0	0	0	0
5	G	1	0	0	0	0
6	А	15	0	0	0	0
6	В	22	0	0	1	0
6	С	1	0	0	0	0
6	D	2	0	0	0	0
6	Е	29	0	0	1	0
6	F	14	0	0	1	0
6	G	1	0	0	0	0
6	Н	4	0	0	0	0
All	All	25082	0	22834	307	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 6.

All (307) 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:10:A:H62	3:C:11:DG:H1	1.14	0.92
2:E:1051:THR:HG22	2:E:1057:ILE:HG22	1.65	0.78
2:B:847:LEU:HD21	2:B:919:ARG:HH11	1.49	0.76
3:G:-8:DG:H2"	3:G:-7:DT:H5'	1.68	0.75
2:E:1148:LYS:HG2	2:E:1159:SER:HA	1.66	0.75
2:E:174:LEU:HD21	2:E:302:LEU:HD21	1.71	0.73
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.23	0.72
3:C:10:DC:H2'	3:C:11:DG:C8	2.24	0.71
2:E:967:ARG:NH1	2:E:986:ASP:OD1	2.24	0.71
2:B:1018:VAL:HG12	2:B:1022:ILE:HG12	1.73	0.69
2:B:846:PHE:HA	2:B:1040:SER:HB2	1.74	0.69
2:E:949:LEU:HD23	2:E:951:ARG:HE	1.57	0.69



	A compage	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:E:1027:GLN:HE21	2:E:1038:PHE:HD2	1.42	0.68
3:G:12:DT:H2'	3:G:13:DC:C6	2.29	0.68
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.76	0.67
2:E:654:ARG:HE	2:E:655:ARG:H	1.43	0.66
2:E:522:ASN:HA	2:E:683:LEU:HD22	1.76	0.66
1:A:8:A:H2'	1:A:9:A:C8	2.30	0.65
2:E:222:LEU:HD23	2:E:234:LYS:HE3	1.77	0.65
2:E:176:PRO:HG3	2:E:316:PRO:HG3	1.79	0.64
2:B:1042:ILE:HD12	2:B:1043:MET:HG2	1.78	0.64
2:B:1054:ASN:HD22	2:B:1056:GLU:H	1.45	0.64
2:B:1023:ALA:HA	2:B:1035:LYS:HD3	1.79	0.64
3:G:10:DC:H2'	3:G:11:DG:C8	2.33	0.63
3:G:-9:DC:H2'	3:G:-8:DG:C8	2.33	0.63
2:E:936:ASP:OD2	2:E:951:ARG:NH2	2.32	0.62
2:E:499:ASP:HB2	2:E:663:SER:HB3	1.79	0.62
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.32	0.62
2:E:427:GLU:HB2	2:E:434:LYS:HB2	1.82	0.61
3:C:8:DA:H2'	3:C:9:DT:C6	2.35	0.61
2:E:666:LEU:HD21	2:E:693:PHE:HZ	1.65	0.61
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.81	0.61
1:F:10:A:H62	3:G:11:DG:H1	1.49	0.60
2:E:1279:ARG:HG2	2:E:1280:VAL:HG23	1.82	0.60
2:B:258:LEU:HD11	2:B:282:ILE:HD11	1.84	0.60
2:E:189:VAL:HG21	2:E:203:ALA:HB2	1.83	0.60
2:E:691:ARG:HB3	2:E:695:GLN:HB3	1.83	0.59
3:G:-1:DC:H2"	3:G:0:DA:C8	2.38	0.59
4:H:-17:DT:H2'	4:H:-16:DG:C8	2.36	0.59
2:E:522:ASN:OD1	2:E:692:ASN:ND2	2.36	0.59
3:C:9:DT:H2'	3:C:10:DC:C6	2.37	0.59
3:G:8:DA:H2'	3:G:9:DT:C6	2.38	0.59
2:B:505:GLU:HG2	2:B:665:LYS:HB2	1.85	0.59
2:B:1075:ASP:OD2	2:B:1078:ARG:NH2	2.35	0.59
3:C:-1:DC:H2"	3:C:0:DA:C8	2.37	0.59
2:B:427:GLU:HB2	2:B:434:LYS:HB2	1.84	0.58
3:G:9:DT:H2'	3:G:10:DC:C6	2.38	0.58
2:B:222:LEU:HD23	2:B:234:LYS:HE3	1.85	0.58
1:A:46:A:H2'	1:A:47:A:H8	1.67	0.58
2:B:526:LYS:HD3	2:B:692:ASN:HB3	1.85	0.58
1:F:46:A:H2'	1:F:47:A:H8	1.69	0.58
1:F:71:U:H2'	1:F:72:U:C6	2.39	0.58
1:A:22:U:H2'	1:A:23:U:C6	2.39	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.86	0.57
2:E:184:LEU:HD12	2:E:299:ALA:HB2	1.85	0.57
2:E:402:GLN:OE1	1:F:44:U:O2'	2.22	0.57
1:F:46:A:H2'	1:F:47:A:C8	2.40	0.57
2:E:654:ARG:HE	2:E:655:ARG:N	2.02	0.57
1:F:22:U:H2'	1:F:23:U:C6	2.40	0.57
3:C:9:DT:H2'	3:C:10:DC:H6	1.69	0.57
2:E:215:ARG:NH1	2:E:395:ARG:HA	2.19	0.56
2:E:525:THR:HG23	2:E:683:LEU:HA	1.87	0.56
2:E:1151:LYS:HD2	2:E:1158:LYS:HD2	1.86	0.56
1:A:46:A:H2'	1:A:47:A:C8	2.39	0.56
3:C:15:DA:H2'	3:C:16:DC:C6	2.41	0.56
2:E:1163:LEU:HG	2:E:1343:LEU:HD21	1.86	0.56
1:F:10:A:H2'	1:F:11:G:O4'	2.05	0.56
2:B:1279:ARG:HG2	2:B:1280:VAL:HG23	1.88	0.56
2:E:666:LEU:HD21	2:E:693:PHE:CZ	2.40	0.56
2:E:133:PRO:HG2	2:E:137:HIS:CE1	2.41	0.55
1:F:38:A:H2'	1:F:39:G:C8	2.41	0.55
1:F:21:G:N2	6:F:203:HOH:O	2.39	0.55
2:E:305:ILE:HD13	2:E:411:PRO:HD3	1.88	0.55
2:E:324:ARG:NH1	2:E:401:LYS:O	2.40	0.54
1:A:38:A:H2'	1:A:39:G:C8	2.42	0.54
2:B:662:LEU:HD22	2:B:666:LEU:HD23	1.89	0.54
2:B:1245:LEU:HD22	2:B:1255:LYS:HD2	1.89	0.54
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.41	0.54
1:A:53:G:H2'	1:A:54:G:H8	1.72	0.54
1:A:74:A:H3'	1:A:75:A:H8	1.73	0.53
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.37	0.53
1:A:10:A:H2'	1:A:11:G:O4'	2.08	0.53
2:E:489:GLN:HG3	2:E:625:LEU:HD21	1.91	0.53
1:F:8:A:H2'	1:F:9:A:C8	2.42	0.53
2:B:1333:ARG:NH2	4:D:1:DG:O6	2.42	0.53
2:E:1212:ARG:NH2	2:E:1280:VAL:O	2.42	0.53
2:E:499:ASP:HB3	2:E:502:LEU:O	2.08	0.53
2:E:1069:THR:HG23	2:E:1071:GLU:H	1.73	0.53
1:A:70:C:H2'	1:A:71:U:C6	2.44	0.52
2:E:1215:ALA:HB2	2:E:1221:GLN:HG3	1.90	0.52
3:G:-8:DG:H2'	3:G:-7:DT:C6	2.44	0.52
2:B:308:VAL:HG11	2:B:319:ALA:HB3	1.90	0.52
1:F:53:G:H2'	1:F:54:G:H8	1.74	0.52
2:E:215:ARG:HH12	2:E:395:ARG:HA	1.74	0.52



	A l o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:E:842:VAL:HG22	2:E:846:PHE:HB2	1.92	0.52
1:F:11:G:H2'	1:F:12:A:C8	2.45	0.52
2:E:8:GLY:HA3	2:E:991:ALA:HB2	1.92	0.51
1:A:22:U:H2'	1:A:23:U:H6	1.75	0.51
1:A:44:U:O2'	2:B:402:GLN:OE1	2.28	0.51
1:A:71:U:H2'	1:A:72:U:C6	2.45	0.51
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.92	0.51
2:E:526:LYS:HD2	2:E:692:ASN:HB2	1.91	0.51
3:G:-5:DA:H1'	3:G:-4:DT:H5'	1.93	0.51
2:B:691:ARG:NH1	2:B:699:ASP:OD2	2.38	0.51
2:B:1117:ASP:OD1	2:B:1117:ASP:N	2.44	0.51
2:E:170:ILE:HD11	2:E:301:LEU:HD13	1.93	0.51
1:F:42:A:H2'	1:F:43:G:C8	2.45	0.51
2:E:279:LEU:O	2:E:283:GLY:N	2.44	0.50
2:B:404:THR:H	2:B:407:ASN:ND2	2.09	0.50
2:E:1064:GLU:O	2:E:1073:VAL:HG22	2.11	0.50
1:F:22:U:H2'	1:F:23:U:H6	1.77	0.50
2:B:468:LYS:HG3	2:B:483:ASP:HB2	1.94	0.50
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.94	0.50
2:E:594:TYR:OH	2:E:604:LYS:HG3	2.12	0.50
2:E:500:LYS:HG3	4:H:-17:DT:OP1	2.12	0.50
2:E:1306:ALA:O	2:E:1310:ILE:HG12	2.11	0.49
2:E:951:ARG:NH1	2:E:1010:TYR:O	2.46	0.49
1:A:9:A:H2'	1:A:10:A:N3	2.28	0.49
2:E:521:TYR:O	2:E:683:LEU:HB3	2.13	0.49
2:B:511:HIS:CD2	2:B:656:TYR:HB3	2.47	0.49
2:E:45:LYS:NZ	6:E:1503:HOH:O	2.45	0.49
1:A:74:A:H3'	1:A:75:A:C8	2.48	0.49
2:B:149:ALA:O	2:B:430:TYR:OH	2.23	0.49
1:F:11:G:H2'	1:F:12:A:H8	1.78	0.49
1:F:27:G:H5'	1:F:28:A:O5'	2.12	0.49
2:B:521:TYR:HB3	2:B:683:LEU:HB3	1.95	0.49
2:E:456:ALA:O	2:E:467:ARG:NH1	2.45	0.49
1:F:70:C:H2'	1:F:71:U:C6	2.47	0.49
2:B:1028:GLU:HA	2:B:1031:LYS:HE3	1.95	0.49
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.44	0.49
1:A:27:G:H5'	1:A:28:A:O5'	2.13	0.49
3:C:15:DA:H2'	3:C:16:DC:H6	1.78	0.48
3:G:9:DT:H2'	3:G:10:DC:H6	1.79	0.48
2:B:456:ALA:O	2:B:467:ARG:NH1	2.47	0.48
2:B:560:THR:HA	2:B:586:ARG:HA	1.95	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:H:-17:DT:H2'	4:H:-16:DG:H8	1.79	0.48
4:D:-18:DA:H2'	4:D:-17:DT:C6	2.49	0.48
2:E:78:ARG:NH1	2:E:162:ILE:O	2.45	0.48
2:E:212:LEU:HD13	2:E:300:ILE:HD11	1.95	0.48
2:B:958:LEU:HD22	2:B:962:LEU:HD12	1.96	0.48
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	1.96	0.48
2:E:843:PRO:HD2	2:E:846:PHE:CD2	2.49	0.48
2:E:1108:GLU:HB2	3:G:1:DG:H5"	1.95	0.48
2:B:495:MET:HB3	3:C:9:DT:H1'	1.94	0.47
2:E:391:VAL:HG12	2:E:395:ARG:HD3	1.95	0.47
1:F:68:A:C4	1:F:69:A:C8	3.02	0.47
1:A:18:C:H41	2:B:71:ARG:NH1	2.12	0.47
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.13	0.47
2:E:404:THR:H	2:E:407:ASN:ND2	2.12	0.47
4:D:-19:DT:H2'	4:D:-18:DA:H8	1.78	0.47
2:E:1148:LYS:HG2	2:E:1159:SER:CA	2.40	0.47
2:B:641:HIS:CE1	2:B:642:LEU:HG	2.49	0.47
2:E:975:VAL:HG11	2:E:1310:ILE:HD12	1.96	0.47
2:E:1210:ARG:NH2	2:E:1341:GLU:OE2	2.48	0.47
2:B:3:LYS:HG3	2:B:4:LYS:H	1.80	0.47
3:C:2:DC:H2"	3:C:3:DG:H5"	1.96	0.47
2:E:450:TYR:CE1	3:G:7:DC:H2"	2.50	0.47
2:E:524:LEU:HG	2:E:545:LYS:HD3	1.97	0.47
2:B:619:ILE:O	2:B:623:LEU:HG	2.16	0.46
2:E:71:ARG:NH1	1:F:18:C:H41	2.13	0.46
1:A:48:A:H2'	1:A:49:A:C8	2.50	0.46
2:E:62:THR:HG22	1:F:63:U:O2'	2.16	0.46
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.79	0.46
2:E:495:MET:HB3	3:G:9:DT:H1'	1.97	0.46
1:F:72:U:H2'	1:F:73:G:O4'	2.15	0.46
2:E:842:VAL:HG12	2:E:854:ASN:OD1	2.16	0.46
2:B:665:LYS:O	2:B:669:GLY:N	2.48	0.46
2:B:665:LYS:HG3	2:B:670:ILE:HG23	1.98	0.46
2:E:258:LEU:HD12	2:E:260:GLU:O	2.16	0.46
2:E:526:LYS:HB3	2:E:526:LYS:HE2	1.73	0.46
2:B:178:ASN:OD1	2:B:178:ASN:N	2.48	0.46
2:B:508:LEU:HD21	2:B:664:ARG:HB2	1.98	0.46
2:E:654:ARG:NH1	2:E:655:ARG:O	2.48	0.46
4:D:-16:DG:H2'	4:D:-15:DT:C6	2.50	0.45
2:E:1300:LYS:O	2:E:1305:GLN:NE2	2.49	0.45
2:B:426:GLN:NE2	6:B:1507:HOH:O	2.49	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:225:LEU:HD23	2:E:242:ILE:HG21	1.99	0.45
2:E:619:ILE:O	2:E:623:LEU:HG	2.16	0.45
1:A:68:A:C4	1:A:69:A:C8	3.04	0.45
3:G:-6:DG:H2"	3:G:-5:DA:H8	1.82	0.45
2:E:1143:VAL:HG12	2:E:1145:VAL:HG13	1.98	0.45
2:E:1333:ARG:NH2	4:H:1:DG:O6	2.49	0.45
3:C:8:DA:H2'	3:C:9:DT:H6	1.80	0.45
2:E:165:ARG:O	2:E:412:HIS:HA	2.16	0.45
2:E:518:PHE:HB2	2:E:667:ILE:HG23	1.97	0.45
2:E:956:ILE:HG12	2:E:1009:VAL:HG22	1.98	0.45
1:F:30:C:H2'	1:F:31:U:C6	2.52	0.45
2:E:467:ARG:NH2	1:F:59:U:OP1	2.50	0.45
2:E:845:SER:O	2:E:1041:ASN:HB2	2.16	0.45
2:E:1229:PRO:HD2	2:E:1232:TYR:HD2	1.81	0.45
2:E:77:ASN:ND2	1:F:59:U:H1'	2.32	0.44
2:E:515:TYR:OH	4:H:-16:DG:OP1	2.26	0.44
2:B:170:ILE:HD11	2:B:301:LEU:HD13	1.98	0.44
2:B:1002:PRO:O	2:B:1005:GLU:HG3	2.18	0.44
2:B:936:ASP:OD1	2:B:940:ASN:ND2	2.50	0.44
3:C:2:DC:H2"	3:C:3:DG:H8	1.82	0.44
2:E:1241:HIS:O	2:E:1245:LEU:HD23	2.17	0.44
3:G:-4:DT:H2"	3:G:-3:DT:H5"	2.00	0.44
2:B:165:ARG:O	2:B:412:HIS:HA	2.17	0.44
2:B:451:TYR:CD1	2:B:488:ALA:HB2	2.53	0.44
1:F:73:G:O2'	1:F:76:A:N6	2.51	0.44
2:B:993:VAL:O	2:B:997:LEU:HB2	2.18	0.44
2:E:101:LEU:HD23	2:E:101:LEU:HA	1.79	0.44
2:E:842:VAL:HG12	2:E:854:ASN:HD21	1.82	0.44
1:A:70:C:H2'	1:A:71:U:H6	1.81	0.43
2:B:119:PHE:HE2	2:B:128:TYR:HB2	1.83	0.43
2:E:240:ASN:HB3	2:E:252:PHE:CE1	2.53	0.43
2:E:956:ILE:HA	2:E:1008:PHE:O	2.18	0.43
3:G:12:DT:H2'	3:G:13:DC:H6	1.82	0.43
2:E:245:SER:HA	2:E:297:SER:HB2	2.00	0.43
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.51	0.43
2:E:1060:ARG:NH1	2:E:1064:GLU:OE1	2.51	0.43
4:H:4:DA:C8	4:H:5:DT:H72	2.53	0.43
2:B:1245:LEU:HD21	2:B:1252:ASN:HA	2.01	0.43
2:E:119:PHE:HE2	2:E:128:TYR:HB2	1.83	0.43
3:G:-7:DT:H2"	3:G:-6:DG:H5"	2.00	0.43
1:A:32:A:H2'	1:A:33:G:C8	2.54	0.43



A + a 1	A 4 a m 2	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
3:C:-9:DC:H2'	3:C:-8:DG:C8	2.54	0.43	
2:E:678:THR:HG23	2:E:681:ASP:H	1.83	0.43	
1:F:54:G:H2'	1:F:55:C:C6	2.54	0.43	
2:B:174:LEU:HD23	2:B:302:LEU:HD21	2.00	0.43	
1:F:70:C:H2'	1:F:71:U:H6	1.84	0.43	
2:E:148:LYS:HD2	2:E:429:PHE:HB3	2.01	0.43	
1:A:49:A:N3	2:B:1122:ARG:NH2	2.67	0.43	
3:C:11:DG:H2"	3:C:12:DT:H5"	2.01	0.43	
2:E:508:LEU:HD12	2:E:667:ILE:HD12	1.99	0.43	
2:E:746:GLU:HA	2:E:749:LYS:HE3	2.00	0.43	
2:E:116:HIS:NE2	2:E:122:ILE:HD12	2.34	0.42	
2:E:186:ILE:O	2:E:190:GLN:HG3	2.19	0.42	
3:C:-4:DT:H2"	3:C:-3:DT:H5"	2.00	0.42	
2:B:1054:ASN:ND2	2:B:1056:GLU:H	2.14	0.42	
2:E:78:ARG:HG2	2:E:443:ILE:HG23	2.02	0.42	
1:F:74:A:H3'	1:F:75:A:H8	1.83	0.42	
2:B:1204:PHE:HE1	2:B:1214:LEU:HD13	1.85	0.42	
2:B:400:ARG:NH2	2:B:406:ASP:OD2	2.52	0.42	
2:B:1245:LEU:CD2	2:B:1255:LYS:HD2	2.49	0.42	
3:C:-6:DG:H2"	3:C:-5:DA:H8	1.85	0.42	
1:F:47:A:H2'	1:F:48:A:C8	2.55	0.42	
2:B:226:ILE:HD11	2:B:239:GLY:HA2	2.00	0.42	
2:B:501:ASN:HB3	2:B:708:ILE:HD12	2.01	0.42	
2:B:536:LYS:HB3	2:B:536:LYS:HE2	1.79	0.42	
2:E:525:THR:HA	2:E:689:ALA:HA	2.01	0.42	
2:E:1342:VAL:O	2:E:1362:LEU:HD12	2.20	0.42	
2:B:704:PHE:O	2:B:708:ILE:HG12	2.20	0.42	
2:B:935:LEU:O	2:B:939:MET:HG2	2.20	0.42	
2:E:512:SER:OG	2:E:617:GLU:OE1	2.34	0.42	
2:E:1265:TYR:O	2:E:1269:ILE:HG13	2.19	0.42	
2:B:609:ASN:O	2:B:611:GLU:N	2.49	0.42	
2:B:557:ARG:O	2:B:590:SER:HB2	2.19	0.42	
2:B:1228:LEU:HD12	2:B:1272:GLN:HG2	2.00	0.42	
1:A:28:A:OP2	2:B:126:VAL:HG22	2.20	0.42	
2:E:60:GLU:O	2:E:64:LEU:HG	2.19	0.42	
2:E:189:VAL:HG11	2:E:203:ALA:HB2	2.02	0.42	
2:E:492:ILE:O	2:E:496:THR:HG23	2.20	0.42	
2:B:349:GLU:HG3	2:B:356:LYS:HG3	2.02	0.41	
2:E:958:LEU:HD22	2:E:962:LEU:HD12	2.02	0.41	
2:E:1242:TYR:CD2	2:E:1303:ARG:HD2	2.55	0.41	
1:F:27:G:H4'	1:F:28:A:OP2	2.20	0.41	



A 4 1	A t area D	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:433:LEU:HD23	2:B:433:LEU:HA	1.88	0.41
2:B:1003:LYS:HG3	2:B:1036:TYR:CZ	2.55	0.41
1:A:27:G:H4'	1:A:28:A:OP2	2.21	0.41
2:B:225:LEU:HD23	2:B:242:ILE:HG21	2.01	0.41
2:B:597:LEU:HD13	2:B:616:LEU:HD22	2.01	0.41
2:B:1284:ASP:OD1	2:B:1284:ASP:N	2.53	0.41
2:E:520:VAL:HG11	2:E:591:LEU:HD21	2.01	0.41
2:E:742:LYS:NZ	1:F:67:C:OP1	2.30	0.41
1:A:53:G:H2'	1:A:54:G:C8	2.55	0.41
2:B:1016:TYR:CD1	2:B:1016:TYR:N	2.87	0.41
2:B:1148:LYS:HG2	2:B:1159:SER:HA	2.03	0.41
2:E:256:PHE:HB2	2:E:258:LEU:HD21	2.02	0.41
1:F:32:A:H2'	1:F:33:G:C8	2.55	0.41
2:B:1151:LYS:HD2	2:B:1158:LYS:HD2	2.03	0.41
2:E:31:LYS:HE2	2:E:44:LYS:HB2	2.01	0.41
2:E:761:ILE:HD11	2:E:957:THR:HG22	2.02	0.41
1:F:38:A:H2'	1:F:39:G:H8	1.85	0.41
2:B:60:GLU:O	2:B:64:LEU:HG	2.20	0.41
2:B:240:ASN:HB3	2:B:252:PHE:CE1	2.56	0.41
2:B:450:TYR:CE1	3:C:7:DC:H2"	2.56	0.41
2:B:940:ASN:ND2	2:B:951:ARG:HG3	2.36	0.41
2:B:1000:LYS:HD3	2:B:1045:PHE:CD2	2.56	0.41
4:H:-18:DA:H2'	4:H:-17:DT:C6	2.56	0.41
2:B:137:HIS:HA	2:B:322:ILE:HD11	2.03	0.40
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.57	0.40
3:C:-7:DT:H2"	3:C:-6:DG:H8	1.86	0.40
2:E:250:PRO:HD2	2:E:264:LEU:O	2.21	0.40
1:A:59:U:H1'	2:B:77:ASN:ND2	2.36	0.40
2:B:212:LEU:HD21	2:B:225:LEU:HD22	2.03	0.40
2:B:997:LEU:HD12	2:B:997:LEU:HA	1.95	0.40
2:E:439:LYS:HG2	2:E:476:TRP:NE1	2.36	0.40
2:E:505:GLU:HG3	2:E:665:LYS:HG3	2.02	0.40
1:A:11:G:H2'	1:A:12:A:C8	2.57	0.40
2:B:138:LEU:HD21	2:B:153:LEU:HB3	2.03	0.40
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.88	0.40
2:B:253:LYS:HE2	2:B:258:LEU:O	2.21	0.40
2:E:70:ARG:NH1	1:F:61:C:OP1	2.51	0.40
2:E:468:LYS:HG3	2:E:483:ASP:HB2	2.03	0.40
2:E:679:ILE:O	2:E:683:LEU:HG	2.20	0.40
1:F:53:G:H2'	1:F:54:G:C8	2.56	0.40
2:E:226:ILE:HD11	2:E:239:GLY:HA2	2.03	0.40



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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
2:E:451:TYR:CD1	2:E:488:ALA:HB2	2.56	0.40
2:B:530:VAL:HA	2:B:534:MET:SD	2.62	0.40
2:B:848:LYS:HE2	2:B:848:LYS:HB2	1.71	0.40
2:B:1136:SER:HA	4:D:2:DG:O3'	2.22	0.40
2:B:1236:LEU:HB3	2:B:1310:ILE:HD11	2.04	0.40
2:E:101:LEU:O	1:F:47:A:O2'	2.38	0.40
2:E:1262:HIS:O	2:E:1265:TYR:HB2	2.22	0.40
1:F:42:A:O2'	1:F:43:G:OP1	2.35	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	Perce	ntiles
2	В	1245/1368~(91%)	1189 (96%)	56 (4%)	0	100	100
2	Е	1144/1368~(84%)	1102 (96%)	42 (4%)	0	100	100
All	All	2389/2736~(87%)	2291 (96%)	98 (4%)	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	В	1125/1225~(92%)	1105~(98%)	20~(2%)	59 82



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntile	S
2	Ε	1045/1225~(85%)	1028~(98%)	17 (2%)	62	84	
All	All	2170/2450 (89%)	2133 (98%)	37 (2%)	60	83	

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	102	GLU
2	В	178	ASN
2	В	272	ASP
2	В	419	LEU
2	В	435	ASP
2	В	644	ASP
2	В	694	MET
2	В	695	GLN
2	В	712	GLN
2	В	713	VAL
2	В	854	ASN
2	В	1008	PHE
2	В	1016	TYR
2	В	1041	ASN
2	В	1054	ASN
2	В	1123	LYS
2	В	1124	LYS
2	В	1207	GLU
2	В	1245	LEU
2	В	1364	GLN
2	Е	122	ILE
2	Е	175	ASN
2	Е	178	ASN
2	E	180	ASP
2	Е	235	ASN
2	Е	258	LEU
2	Е	419	LEU
2	Е	424	ARG
2	Е	951	ARG
2	Е	1012	ASP
2	Е	1017	ASP
2	Е	1041	ASN
2	Е	1115	ASN
2	Е	1144	LEU
2	Е	1207	GLU
2	Е	1242	TYR



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Mol	Chain	\mathbf{Res}	Type
2	Ε	1368	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	281	GLN
2	В	394	ASN
2	В	407	ASN
2	В	426	GLN
2	В	511	HIS
2	В	695	GLN
2	В	712	GLN
2	В	854	ASN
2	В	1044	ASN
2	В	1054	ASN
2	Е	394	ASN
2	Е	407	ASN
2	Е	522	ASN
2	Е	692	ASN
2	Е	1027	GLN
2	Е	1041	ASN
2	Е	1044	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	74/84~(88%)	18 (24%)	2(2%)
1	F	76/84~(90%)	18 (23%)	3~(3%)
All	All	150/168~(89%)	36 (24%)	5(3%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	А	20	С
1	А	28	А
1	А	29	G
1	А	37	U
1	А	51	А
1	А	53	G
1	А	56	U



Mol	Chain	Res	Type
1	А	57	А
1	А	59	U
1	А	63	U
1	А	68	A
1	А	73	G
1	А	74	A
1	А	76	A
1	А	77	A
1	А	78	A
1	А	81	G
1	А	82	A
1	F	8	А
1	F	20	С
1	F	28	A
1	F	29	G
1	F	37	U
1	F	43	G
1	F	51	A
1	F	53	G
1	F	56	U
1	F	57	A
1	F	59	U
1	F	63	U
1	F	68	А
1	F	74	A
1	F	76	А
1	F	78	А
1	F	81	G
1	F	82	А

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All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	А	27	G
1	А	28	А
1	F	27	G
1	F	28	А
1	F	42	А

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	А	75/84~(89%)	0.39	0 100 100	22, 43, 142, 151	0
1	F	77/84~(91%)	0.63	5 (6%) 18 8	25, 46, 153, 210	0
2	В	1259/1368~(92%)	0.40	108 (8%) 10 4	18, 67, 118, 149	0
2	Е	1166/1368~(85%)	0.44	98 (8%) 11 4	21, 65, 117, 142	0
3	С	30/30~(100%)	0.38	2 (6%) 17 7	36, 61, 129, 140	0
3	G	27/30~(90%)	0.54	4 (14%) 2 1	32, 55, 126, 130	0
4	D	22/30~(73%)	0.71	3(13%) 3 1	32, 89, 137, 141	0
4	Н	$19/30\ (63\%)$	0.64	3(15%) 2 1	33, 83, 122, 141	0
All	All	2675/3024 (88%)	0.43	223 (8%) 11 4	18, 64, 119, 210	0

Mol	Chain	Res	Type	RSRZ
2	Ε	207	ASP	6.2
2	Ε	224	ASN	6.1
2	Ε	281	GLN	5.9
2	Е	216	LEU	5.5
2	Ε	912	ASP	5.5
2	Ε	608	ASP	5.5
2	В	192	TYR	5.3
2	Е	571	LYS	5.1
2	Ε	519	THR	5.1
2	Е	1244	LYS	5.0
2	Ε	551	LEU	4.9
2	В	1246	LYS	4.8
2	В	878	LYS	4.8
2	Е	605	ASP	4.8
2	Е	1024	LYS	4.7
2	Е	290	PHE	4.6



Mol	Chain	Res	Type	RSRZ
2	В	689	ALA	4.6
2	В	688	PHE	4.6
2	Е	574	CYS	4.6
4	D	-3	DT	4.6
2	В	215	ARG	4.4
2	В	537	PRO	4.4
3	G	18	DT	4.3
2	В	716	GLN	4.2
2	В	562	LYS	4.2
2	Е	201	ILE	4.1
2	В	277	ASN	4.1
2	Е	180	ASP	4.0
2	Е	215	ARG	4.0
2	Е	521	TYR	3.9
2	В	530	VAL	3.9
2	В	196	PHE	3.8
2	Е	203	ALA	3.8
2	Е	220	ARG	3.8
2	Е	225	LEU	3.8
2	Е	647	VAL	3.8
1	F	7	U	3.7
2	В	203	ALA	3.7
2	Ε	594	TYR	3.7
2	В	188	LEU	3.6
2	В	290	PHE	3.6
2	Ε	601	ILE	3.6
2	В	199	ASN	3.6
2	В	579	GLU	3.6
1	F	73	G	3.6
2	E	523	GLU	3.6
2	В	872	SER	3.5
2	В	871	PRO	3.5
2	В	583	VAL	3.5
2	В	669	GLY	3.5
2	В	535	ARG	3.5
2	B	$64\overline{4}$	ASP	3.5
2	E	1022	ILE	3.5
2	В	529	TYR	3.4
2	В	679	ILE	3.4
1	F	9	A	3.4
2	E	238	PHE	3.4
2	Е	910	GLU	3.4



7Z4D

Mol	Chain	Res	Type	RSRZ
2	В	1299	ASP	3.4
2	Е	262	ALA	3.3
2	В	894	GLN	3.3
2	Е	223	GLU	3.3
4	D	-4	DT	3.3
2	Е	234	LYS	3.3
2	Е	911	LEU	3.3
1	F	8	А	3.3
2	В	1056	GLU	3.3
2	В	550	ASP	3.3
2	Е	188	LEU	3.3
2	Е	212	LEU	3.3
2	В	1031	LYS	3.3
2	Е	909	SER	3.2
2	Е	1023	ALA	3.2
2	В	198	GLU	3.2
2	Е	916	PHE	3.2
2	В	216	LEU	3.2
2	Ε	257	ASP	3.1
2	Ε	192	TYR	3.1
2	В	554	LYS	3.1
2	Ε	263	LYS	3.1
2	В	195	LEU	3.0
2	Ε	651	LEU	3.0
2	Ε	567	ASP	3.0
2	Ε	1367	GLY	3.0
2	В	224	ASN	3.0
2	В	651	LEU	2.9
3	G	19	DA	2.9
2	В	534	MET	2.9
2	Ε	607	LEU	2.9
2	Ε	222	LEU	2.9
2	Ε	693	PHE	2.9
3	С	16	DC	2.9
2	В	257	ASP	2.9
2	В	594	TYR	2.8
2	В	1244	LYS	2.8
2	Ε	202	ASN	2.8
2	E	1049	GLU	2.8
2	В	1242	TYR	2.8
2	В	580	ILE	2.8
2	В	584	GLU	2.8



2

2

Ŧ	279	LEU	2.6	
Ŧ	1040	SER	2.6	
Ŧ	194	GLN	2.6	
3	899	ASN	2.6	
Ŧ	206	VAL	2.6	
3	869	ASN	2.6	
3	553	PHE	2.6	
3	300	ILE	2.6	
3	637	LYS	2.6	
Ŧ	388	GLU	2.6	
3	212	LEU	2.6	
Ŧ	256	PHE	2.6	
)	-14	DA	2.6	
Ŧ	293	ALA	2.6	
Ŧ	570	LYS	2.6	
Ŧ	1027	GLN	2.6	
3	1193	ASP	2.6	
3	234	LYS	2.5	
	200	TTTC	0.5	

Continued from previous page... Mol Chain

В

Е

Res

600

251

Type

ILE

ASN

RSRZ

2.7

2.7

2	В	650	GLN	2.7
2	Е	646	LYS	2.7
2	В	573	GLU	2.7
2	В	1058	ARG	2.7
2	В	875	VAL	2.7
2	В	274	ASP	2.7
2	В	643	PHE	2.7
2	Е	279	LEU	2.6
2	Ε	1040	SER	2.6
2	Ε	194	GLN	2.6
2	В	899	ASN	2.6
2	Ε	206	VAL	2.6
2	В	869	ASN	2.6
2	В	553	PHE	2.6
2	В	300	ILE	2.6
2	В	637	LYS	2.6
2	Ε	388	GLU	2.6
2	В	212	LEU	2.6
2	Ε	256	PHE	2.6
4	D	-14	DA	2.6
2	Ε	293	ALA	2.6
2	Ε	570	LYS	2.6
2	Ε	1027	GLN	2.6
2	В	1193	ASP	2.6
2	В	234	LYS	2.5
2	В	536	LYS	2.5
2	Ε	685	SER	2.5
2	Ε	1153	LYS	2.5
2	Ε	1242	TYR	2.5
2	В	576	ASP	2.5
2	Ε	1156	LYS	2.5
2	В	208	ALA	2.5
2	В	648	MET	2.5
3	G	14	DT	2.5
2	В	560	THR	2.5
2	Е	604	LYS	2.5
2	В	874	GLU	2.5
2	В	225	LEU	2.5
2	В	230	PRO	2.5
2	Ε	639	TYR	2.5



Mol	Chain	Res	Type	RSRZ
2	Ε	566	GLU	2.5
2	В	194	GLN	2.5
2	Е	243	ALA	2.5
2	Е	525	THR	2.4
2	В	1034	ALA	2.4
2	Е	1058	ARG	2.4
2	Е	676	GLY	2.4
2	Е	565	LYS	2.4
2	В	263	LYS	2.4
2	В	281	GLN	2.4
2	В	897	PHE	2.4
2	В	686	ASP	2.4
2	Е	1021	MET	2.4
2	В	670	ILE	2.4
2	В	571	LYS	2.4
2	В	876	VAL	2.4
2	В	668	ASN	2.4
2	В	304	ASP	2.3
2	Е	261	ASP	2.3
2	Е	385	GLY	2.3
2	Е	919	ARG	2.3
2	В	528	LYS	2.3
2	Е	674	GLN	2.3
2	В	1052	LEU	2.3
2	В	578	VAL	2.3
1	F	10	А	2.3
4	Н	-15	DT	2.3
2	В	202	ASN	2.3
2	В	1028	GLU	2.3
2	В	564	LEU	2.3
2	В	1039	TYR	2.3
3	С	15	DA	2.3
2	В	191	THR	2.3
2	Е	500	LYS	2.3
2	В	910	GLU	2.3
2	Е	668	ASN	2.3
2	В	256	PHE	2.3
2	В	841	ILE	2.3
2	Е	548	ILE	2.2
2	В	1022	ILE	2.2
2	B	552	LEU	2.2

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2.2

Е

2



Mol	Chain	Res	Type	RSRZ	
2	Е	547	ALA	2.2	
2	В	264	LEU	2.2	
2	В	574	CYS	2.2	
2	Е	292	ALA	2.2	
2	В	1032	ALA	2.2	
2	Е	210	ALA	2.2	
2	В	283	GLY	2.2	
2	В	599	LYS	2.2	
2	Е	283	GLY	2.2	
3	G	20	DG	2.2	
4	Н	-16	DG	2.2	
2	В	647	VAL	2.2	
2	В	721	HIS	2.2	
2	Е	852	ILE	2.1	
2	В	1153	LYS	2.1	
2	В	515	TYR	2.1	
2	Е	270	THR	2.1	
2	Е	380	LEU	2.1	
2	В	237	LEU	2.1	
2	В	569	PHE	2.1	
2	Е	1157	LEU	2.1	
2	Е	637	LYS	2.1	
2	Е	654	ARG	2.1	
2	В	303	SER	2.1	
2	В	1194	LEU	2.1	
2	В	1239	ALA	2.1	
2	В	1030	GLY	2.1	
2	E	655	ARG	2.1	
2	Е	670	ILE	2.1	
2	Е	602	LYS	2.1	
2	Е	1036	TYR	2.1	
2	В	343	LEU	2.1	
2	В	282	ILE	2.1	
2	Е	550	ASP	2.1	
4	Н	-2	DA	2.0	
2	Е	680	LEU	2.0	
2	Е	247	GLY	2.0	
2	В	726	ASN	2.0	
2	Е	684	LYS	2.0	

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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^{th} 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	${f B}$ -factors(Å ²)	Q<0.9
5	K	F	103	1/1	0.73	0.19	86,86,86,86	0
5	K	F	101	1/1	0.89	0.19	93,93,93,93	0
5	K	А	106	1/1	0.89	0.24	80,80,80,80	0
5	K	В	1402	1/1	0.90	0.21	60,60,60,60	0
5	K	А	105	1/1	0.92	0.20	73,73,73,73	0
5	K	А	104	1/1	0.93	0.21	68,68,68,68	0
5	K	А	101	1/1	0.94	0.15	98,98,98,98	0
5	K	Е	1401	1/1	0.94	0.16	61,61,61,61	0
5	К	А	103	1/1	0.95	0.18	52,52,52,52	0
5	K	В	1401	1/1	0.95	0.31	53,53,53,53	0
5	K	А	102	1/1	0.96	0.15	69,69,69,69	0
5	К	В	1403	1/1	0.96	0.17	56,56,56,56	0
5	K	С	101	1/1	0.96	0.24	43,43,43,43	0
5	K	Е	1402	1/1	0.97	0.24	47,47,47,47	0
5	K	G	101	1/1	0.97	0.21	48,48,48,48	0
5	К	F	102	1/1	0.99	0.18	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.

