

Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2021 - 01:55 pm BST

PDB II) :	70XA
Titl	е:	Target-bound SpCas9 complex with AAVS1 chimeric RNA-DNA guide
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		Р.
Deposited or	n :	2021-06-22
Resolution	n :	2.15 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity Xtriage (Phenix) EDS Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		4.02b-467 1.13 2.23.1 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996) 2.23.1
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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	$1560 \ (2.16-2.16)$
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	81	% 72%	28%	6					
2	В	1372	8%		10% •					
3	С	28	57%	43%						
4	D	12	67%	25%	8%					



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13928 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is DNA/RNA hybrid called chimeric RNA-DNA guide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	81	Total	С	Ν	Ο	Р	0	0	0
		01	1732	781	326	545	80			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	1320	Total 10808	C 6892	N 1875	O 2019	S 22	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

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

• Molecule 3 is a DNA chain called AAVS1 target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	28	Total 559	C 268	N 98	O 166	Р 27	0	0	0

• Molecule 4 is a DNA chain called AAVS1 non-target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total 209	C 100	N 35	0 64	Р 10	0	0	1

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



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	5	Total K 5 5	0	0
6	В	8	Total K 8 8	0	0
6	С	1	Total K 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	164	Total O 164 164	0	0
7	В	394	Total O 394 394	0	0
7	С	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
7	D	12	TotalO1212	0	0



3 Residue-property plots (i)

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



• Molecule 1: chimeric RNA-DNA guide





• Molecule 3: AAVS1 target DNA strand







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	177.93Å 67.57Å 189.23Å	Depositor
a, b, c, α , β , γ	90.00° 112.52° 90.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\mathbf{\hat{A}})$	47.66 - 2.15	Depositor
Resolution (A)	47.66 - 2.15	EDS
% Data completeness	99.9 (47.66 - 2.15)	Depositor
(in resolution range)	99.9 (47.66 - 2.15)	EDS
R_{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 2.16 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D.	0.198 , 0.226	Depositor
Π, Π_{free}	0.198 , 0.226	DCC
R_{free} test set	5666 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	46.8	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 43.7	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13928	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.12% 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, 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).

Mal	Chain	Bond lengths		Bond angles	
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.40	0/1944	0.84	0/3027
2	В	0.26	0/10995	0.43	0/14767
3	С	0.69	0/624	0.97	0/958
4	D	0.63	0/233	1.05	0/360
All	All	0.33	0/13796	0.57	0/19112

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	А	1732	0	876	22	0
2	В	10808	0	10981	88	0
3	С	559	0	316	9	0
4	D	209	0	116	3	0
5	А	2	0	0	0	0
6	А	5	0	0	0	0
6	В	8	0	0	0	0
6	С	1	0	0	0	0
7	А	164	0	0	1	0



0 0 1 0 0 0							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
7	В	394	0	0	7	0	
7	С	34	0	0	0	0	
7	D	12	0	0	0	0	
All	All	13928	0	12289	115	0	

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:343:LEU:HD13	2:B:346:LYS:HB2	1.33	1.06
2:B:343:LEU:O	2:B:343:LEU:HD12	1.56	1.02
2:B:343:LEU:CD1	2:B:346:LYS:HB2	1.93	0.98
2:B:80:CYS:SG	7:B:1884:HOH:O	2.49	0.70
2:B:1335:ARG:NH2	4:D:2:DG:O6	2.24	0.70
1:A:71:U:H2'	1:A:72:U:C6	2.26	0.69
2:B:343:LEU:HD13	2:B:346:LYS:CB	2.19	0.67
2:B:788:ILE:HG23	2:B:793:SER:HB3	1.77	0.65
2:B:411:PRO:HD2	2:B:414:ILE:HD13	1.79	0.63
3:C:17:DC:H5"	3:C:17:DC:H6	1.63	0.62
2:B:1004:LEU:HD11	2:B:1042:ILE:HD11	1.82	0.62
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.84	0.60
2:B:343:LEU:O	2:B:343:LEU:CD1	2.41	0.60
2:B:1179:ILE:HD11	2:B:1192:LYS:HG2	1.84	0.59
1:A:59:U:OP1	2:B:467:ARG:NH2	2.35	0.58
2:B:558:LYS:HD2	2:B:586:ARG:HH11	1.68	0.58
2:B:434:LYS:NZ	7:B:1508:HOH:O	2.37	0.57
2:B:763:MET:HE1	2:B:931:VAL:HG21	1.86	0.57
2:B:212:LEU:HD21	2:B:225:LEU:HD22	1.87	0.57
2:B:501:ASN:HB3	2:B:708:ILE:HD12	1.85	0.56
1:A:69:A:H2'	1:A:70:C:H6	1.70	0.56
1:A:18:G:N7	2:B:71:ARG:NH1	2.53	0.56
1:A:32:A:H2'	1:A:33:G:O4'	2.06	0.55
2:B:704:PHE:O	2:B:708:ILE:HG12	2.07	0.55
2:B:780:ARG:NH1	2:B:806:LEU:O	2.39	0.55
1:A:72:U:H2'	1:A:73:G:O4'	2.07	0.54
3:C:-6:DA:H2'	3:C:-5:DA:C8	2.43	0.54
1:A:46:A:H2'	1:A:47:A:C8	2.43	0.54
2:B:528:LYS:HE3	2:B:539:PHE:CE1	2.43	0.53
2:B:614:ASP:OD1	2:B:664:ARG:NH2	2.37	0.53



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:C:17:DC:H5"	3:C:17:DC:C6	2.42	0.53	
2:B:1110:ILE:HG23	2:B:1122:ARG:HD2	1.91	0.52	
2:B:870:VAL:HG23	2:B:908:LEU:HG	1.91	0.52	
2:B:58:THR:HA	2:B:731:PRO:HG2	1.91	0.52	
2:B:187:GLN:NE2	7:B:1514:HOH:O	2.42	0.51	
1:A:70:C:H2'	1:A:71:U:C6	2.46	0.51	
2:B:1136:SER:HA	4:D:2:DG:O3'	2.11	0.51	
2:B:343:LEU:HD13	2:B:346:LYS:HD2	1.93	0.50	
1:A:22:U:H2'	1:A:23:U:C6	2.46	0.50	
2:B:1117:ASP:N	2:B:1117:ASP:OD1	2.44	0.50	
1:A:35:A:H2'	1:A:36:A:C8	2.46	0.50	
2:B:939:MET:HE3	2:B:953:VAL:HG21	1.93	0.50	
2:B:708:ILE:O	2:B:712:GLN:HG2	2.11	0.49	
2:B:814:TYR:CZ	2:B:830:ILE:HG12	2.47	0.49	
1:A:69:A:H2'	1:A:70:C:C6	2.46	0.49	
1:A:70:C:H2'	1:A:71:U:H6	1.78	0.49	
2:B:530:VAL:HG22	2:B:537:PRO:HA	1.94	0.49	
2:B:1306:ALA:O	2:B:1310:ILE:HG12	2.12	0.49	
1:A:54:G:H2'	1:A:55:C:C6	2.48	0.49	
1:A:75:A:H8	1:A:75:A:O5'	1.96	0.48	
1:A:79:G:OP2	7:A:201:HOH:O	2.20	0.48	
2:B:898:ASP:O	2:B:905:ARG:NH2	2.47	0.47	
1:A:17:G:H4'	2:B:447:ARG:HD2	1.96	0.47	
2:B:265:GLN:OE1	2:B:268:LYS:HG3	2.15	0.47	
2:B:1122:ARG:HG2	2:B:1134:PHE:CE2	2.50	0.46	
2:B:1277:SER:HA	2:B:1281:ILE:HG12	1.97	0.46	
2:B:1163:LEU:HD21	2:B:1198:LEU:HD12	1.97	0.46	
2:B:585:ASP:HB2	7:B:1851:HOH:O	2.15	0.46	
2:B:1075:ASP:OD2	2:B:1078:ARG:HD2	2.16	0.46	
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.97	0.46	
3:C:8:DC:H2'	3:C:9:DC:C6	2.51	0.46	
2:B:154:ILE:O	2:B:158:LEU:HG	2.15	0.46	
3:C:1:DA:H2"	3:C:2:DT:H5'	1.97	0.46	
2:B:756:PRO:HD2	2:B:939:MET:CE	2.46	0.46	
1:A:49:A:N3	2:B:1122:ARG:NH2	2.60	0.45	
2:B:222:LEU:HD23	2:B:234:LYS:HE3	1.98	0.45	
2:B:394:ASN:HB3	7:B:1806:HOH:O	2.15	0.45	
2:B:1339:THR:O	2:B:1342:VAL:HG22	2.16	0.45	
2:B:901:THR:O	2:B:904:GLU:HG2	2.16	0.45	
2:B:1251:ASP:HB3	2:B:1252:ASN:H	1.61	0.45	
2:B:817:GLN:HE22	2:B:857:LEU:HB3	1.82	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.99	0.45	
2:B:1066:ASN:OD1	2:B:1067:GLY:N	2.50	0.45	
2:B:225:LEU:HD23	2:B:242:ILE:HG21	1.99	0.44	
4:D:3:DT:H2"	4:D:4:DA:C8	2.52	0.44	
2:B:468:LYS:HD2	2:B:483:ASP:HA	2.00	0.44	
3:C:9:DC:H2'	3:C:10:DC:C6	2.53	0.44	
1:A:46:A:H2'	1:A:47:A:H8	1.82	0.44	
2:B:485:GLY:HA2	2:B:631:MET:HE1	1.98	0.44	
2:B:1042:ILE:HG23	2:B:1043:MET:HG2	1.98	0.44	
2:B:560:THR:HA	2:B:586:ARG:HA	1.99	0.44	
1:A:70:C:C2	1:A:71:U:C5	3.05	0.44	
2:B:349:GLU:HG3	2:B:356:LYS:HG3	1.99	0.44	
2:B:976:ARG:HG2	2:B:982:HIS:NE2	2.33	0.44	
2:B:269:ASP:OD1	2:B:269:ASP:N	2.51	0.43	
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.83	0.43	
2:B:1279:ARG:HG2	2:B:1280:VAL:HG23	2.00	0.43	
2:B:1122:ARG:HD3	7:B:1705:HOH:O	2.19	0.43	
2:B:343:LEU:HD22	2:B:346:LYS:HD2	2.00	0.43	
2:B:468:LYS:HG3	2:B:483:ASP:HB2	2.01	0.43	
3:C:9:DC:H2'	3:C:10:DC:H6	1.84	0.43	
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.29	0.43	
2:B:1179:ILE:HG13	2:B:1192:LYS:HE2	2.00	0.43	
2:B:36:GLY:HA3	2:B:1359:ARG:O	2.18	0.42	
2:B:628:ASP:OD1	2:B:631:MET:HG3	2.20	0.42	
2:B:983:HIS:HD2	7:B:1844:HOH:O	2.01	0.42	
2:B:851:SER:O	2:B:855:LYS:HG3	2.20	0.42	
2:B:513:LEU:HD12	2:B:616:LEU:HB3	2.02	0.42	
2:B:15:SER:HA	2:B:51:LEU:O	2.20	0.41	
2:B:502:LEU:HD13	2:B:665:LYS:HD3	2.02	0.41	
3:C:14:DT:H2'	3:C:15:DG:C8	2.56	0.41	
2:B:323:LYS:HE2	2:B:327:GLU:OE2	2.20	0.41	
2:B:838:VAL:HG12	2:B:855:LYS:HE2	2.01	0.41	
2:B:439:LYS:O	2:B:443:ILE:HG13	2.21	0.41	
2:B:939:MET:CE	2:B:953:VAL:HG21	2.51	0.41	
1:A:15:C:P	2:B:70:ARG:HH22	2.44	0.41	
1:A:68:A:C4	1:A:69:A:C8	3.08	0.41	
2:B:795:ILE:HD11	2:B:814:TYR:HE2	1.86	0.41	
2:B:821:ASP:N	2:B:828:LEU:HG	2.36	0.41	
2:B:343:LEU:HD13	2:B:346:LYS:CD	2.51	0.40	
2:B:822:MET:HG3	2:B:856:VAL:HG23	2.03	0.40	
3:C:-1:DC:H2"	3:C:0:DA:C8	2.56	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:G:H2'	1:A:35:A:N7	2.36	0.40
2:B:1268:GLU:O	2:B:1271:GLU:HB3	2.21	0.40
2:B:216:LEU:HB3	2:B:220:ARG:HD3	2.03	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	1302/1372~(95%)	1262 (97%)	40 (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	В	1186/1226~(97%)	1175~(99%)	11 (1%)	78 83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	174	LEU
2	В	264	LEU
2	В	281	GLN



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Mol	Chain	\mathbf{Res}	Type			
2	В	625	LEU			
2	В	635	ARG			
2	В	645	ASP			
2	В	853	ASP			
2	В	947	ASP			
2	В	952	GLU			
2	В	1154	SER			
2	В	1284	ASP			

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	240	ASN
2	В	255	ASN
2	В	394	ASN
2	В	511	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	81/81 (100%)	-0.48	1 (1%) 79 83	37, 56, 164, 234	0
2	В	1320/1372~(96%)	0.41	111 (8%) 11 15	34, 60, 133, 200	0
3	С	28/28~(100%)	-0.20	0 100 100	44, 60, 129, 143	0
4	D	11/12~(91%)	0.34	1 (9%) 9 13	53, 75, 133, 150	0
All	All	1440/1493~(96%)	0.35	113 (7%) 13 18	34, 60, 138, 234	0

All (113) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	В	806	LEU	10.7
2	В	788	ILE	10.2
2	В	911	LEU	8.2
2	В	795	ILE	8.0
2	В	784	ILE	7.9
2	В	787	GLY	7.8
2	В	791	LEU	6.4
2	В	823	TYR	6.3
2	В	833	LEU	6.2
2	В	798	GLU	6.0
2	В	811	LEU	5.9
2	В	807	GLN	5.9
2	В	800	PRO	5.9
2	В	814	TYR	5.6
2	В	815	TYR	5.5
2	В	789	LYS	5.5
2	В	781	MET	5.2
2	В	862	LYS	5.2
2	В	846	PHE	5.1
2	В	797	LYS	5.0
2	В	856	VAL	5.0



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Mol	Chain	Res	Res Type F	
2	В	884	ARG	5.0
2	В	778	ARG	5.0
2	В	870	VAL	4.9
2	В	847	LEU	4.9
2	В	908	LEU	4.8
2	В	887	LEU	4.7
2	В	1367	GLY	4.7
2	В	1067	GLY	4.7
2	В	796	LEU	4.6
2	В	805	GLN	4.5
2	В	808	ASN	4.4
2	В	1014	LYS	4.4
2	В	783	ARG	4.2
2	В	883	TRP	4.1
2	B	892	ILE	4.0
2	В	785	GLU	4.0
2	В	803	ASN	3.9
2	В	842	VAL	3.9
2	В	799	HIS	3.9
2	В	850	ASP	3.8
2	В	818	ASN	3.6
2	В	848	LYS	3.6
2	В	804	THR	3.5
2	В	1258	PHE	3.5
2	В	1068	GLU	3.4
2	В	1038	PHE	3.4
2	В	780	ARG	3.4
2	В	813	LEU	3.3
2	В	912	ASP	3.3
2	В	816	LEU	3.3
2	В	843	PRO	3.3
2	В	888	ASN	3.2
2	В	836	TYR	3.2
2	В	782	LYS	3.2
2	В	852	ILE	3.1
2	В	866	LYS	3.1
2	В	790	GLU	3.1
2	В	891	LEU	3.1
2	В	$12\overline{57}$	LEU	3.0
2	В	1039	TYR	3.0
2	В	717	GLY	3.0
2	В	765	ARG	3.0



Mol	Chain	Res	Type	RSRZ
2	В	830	ILE	2.9
2	В	1302	ILE	2.8
4	D	7	7 DG 2	
2	В	825 ASP		2.8
2	В	1299	ASP	2.8
2	В	786	GLU	2.7
2	В	1032	ALA	2.7
2	В	810	LYS	2.7
2	В	1259	VAL	2.7
2	В	1251	ASP	2.7
2	В	885	GLN	2.7
1	А	74	А	2.7
2	В	1058	ARG	2.7
2	В	880	LYS	2.7
2	В	387	GLU	2.6
2	В	894	GLN	2.6
2	В	1366	GLY	2.5
2	В	1194	LEU	2.5
2	В	897	PHE	2.4
2	В	831	ASN	2.4
2	В	1036	TYR	2.4
2	В	1035	LYS	2.4
2	В	1263	LYS	2.4
2	В	886	LEU	2.4
2	В	868	ASP	2.4
2	В	1242	TYR	2.4
2	В	1256	GLN	2.3
2	В	343	LEU	2.3
2	В	916	PHE	2.3
2	В	902	LYS	2.3
2	В	832	ARG	2.3
2	В	1052	LEU	2.3
2	В	877	LYS	2.3
2	В	910	GLU	2.2
2	В	841	ILE	2.2
2	В	812	TYR	2.2
2	В	824	VAL	2.2
2	В	794	GLN	2.2
2	В	913	LYS	2.2
2	В	890	LYS	2.2
2	В	777	SER	2.1
2	В	352	PHE	2.1



Mol	Chain	Res	Type	RSRZ
2	В	1254	GLN	2.1
2	В	1013	TYR	2.1
2	В	220	ARG	2.0
2	В	1050	ILE	2.0
2	В	1153	LYS	2.0
2	В	198	GLU	2.0
2	В	779	GLU	2.0
2	В	1151	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
6	K	В	1407	1/1	0.75	0.06	112,112,112,112	0
6	K	В	1402	1/1	0.77	0.24	$102,\!102,\!102,\!102$	0
6	K	А	107	1/1	0.88	0.10	117,117,117,117	0
6	K	В	1404	1/1	0.89	0.09	$68,\!68,\!68,\!68$	0
6	K	А	106	1/1	0.90	0.24	$106,\!106,\!106,\!106$	0
5	MG	А	101	1/1	0.92	0.03	74,74,74,74	0
6	K	В	1401	1/1	0.93	0.14	85,85,85,85	0
6	K	В	1408	1/1	0.94	0.07	84,84,84,84	0
6	K	В	1406	1/1	0.95	0.08	$65,\!65,\!65,\!65$	0
6	K	А	103	1/1	0.98	0.24	$65,\!65,\!65,\!65$	0
6	K	В	1405	1/1	0.98	0.06	$68,\!68,\!68,\!68$	0
6	K	А	105	1/1	0.98	0.10	$46,\!46,\!46,\!46$	0
5	MG	А	102	1/1	0.98	0.07	39,39,39,39	0
6	K	В	1403	1/1	0.98	0.09	$65,\!65,\!65,\!65$	0
6	K	A	104	1/1	0.99	0.08	67,67,67,67	0



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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$\mathbf{Q}{<}0.9$
6	Κ	С	101	1/1	0.99	0.14	$72,\!72,\!72,\!72$	0

6.5 Other polymers (i)

There are no such residues in this entry.

