

wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 11:07 PM EDT

PDB ID : 3L88

Title: Crystal structure of the human Adenovirus type 21 fiber knob

Authors: Cupelli, K.; Jost, M.; Persson, B.D.; Stehle, T.

Deposited on : 2009-12-30

Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

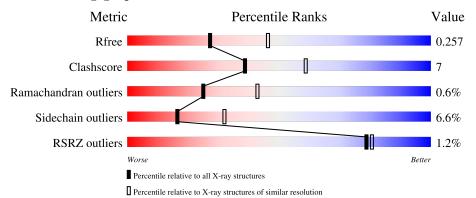
Validation Pipeline (wwPDB-VP) : 2.35

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 2.50 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	A	201	74%	15%	• 9%
1	В	201	76%	13%	• 9%
1	С	201	80%	10%	• 8%
1	D	201	75%	13%	• 9%
1	Е	201	75%	14%	• 9%



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Mol	Chain	Length	Quality of chain			
1	F	201	% 	110/		00/
	I.	201	77%	11%	•	9%
1	G	201	76%	12%	•	9%
1	Н	201	77%	11%	•	9%
1	I	201	78%	11%	•	9%
1	J	201	78%	11%		9%
1	K	201	75%	14%	•	9%
1	L	201	74%	14%		9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	\mathbf{E}	6	-	-	X	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17174 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 Fiber protein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	183	Total	С	N	О	S	0	0	0
1	A	165	1415	898	230	281	6	U	0	U
1	В	183	Total	С	N	О	S	0	0	0
1	D	100	1419	902	230	281	6	0		
1	С	184	Total	С	N	О	S	0	0	0
1		104	1430	906	234	284	6	0	0	U
1	D	183	Total	С	N	О	S	0	0	0
1	Ъ	100	1422	903	230	283	6	0	0	U
1	Е	183	Total	С	N	О	S	0	1	0
1	15	100	1420	898	232	284	6	0	1	U
1	F	183	Total	С	N	О	S	0	1	0
1	Г	100	1431	906	234	285	6	0	1	U
1	G	183	Total	С	N	О	S	0	0	0
1	G	100	1415	898	230	281	6	0	0	U
1	Н	183	Total	С	N	О	S	0	0	0
1	11	100	1415	898	230	281	6	0		U
1	I	183	Total	С	N	О	S	0	0	0
1	1	100	1426	903	233	284	6	0	0	U
1	J	182	Total	С	N	О	S	0	1	0
1	J	102	1424	903	231	284	6	0	1	U
1	K	183	Total	С	N	О	S	0	0	0
1	11/	100	1426	903	233	284	6		U	U
1	L	182	Total	С	N	О	S	0	1	0
1	L	102	1427	904	234	283	6		1	U

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

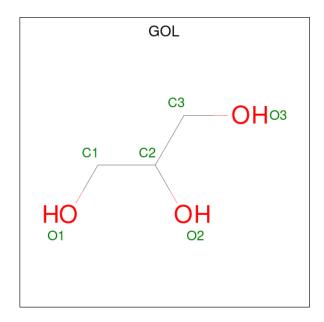
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Na 2 2	0	0
2	F	2	Total Na 2 2	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Н	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	J	2	Total Na 2 2	0	0
2	K	2	Total Na 2 2	0	0
2	L	1	Total Na 1 1	0	0

 \bullet Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	Ε	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	2	Total Cl 2 2	0	0

• Molecule 5 is water.

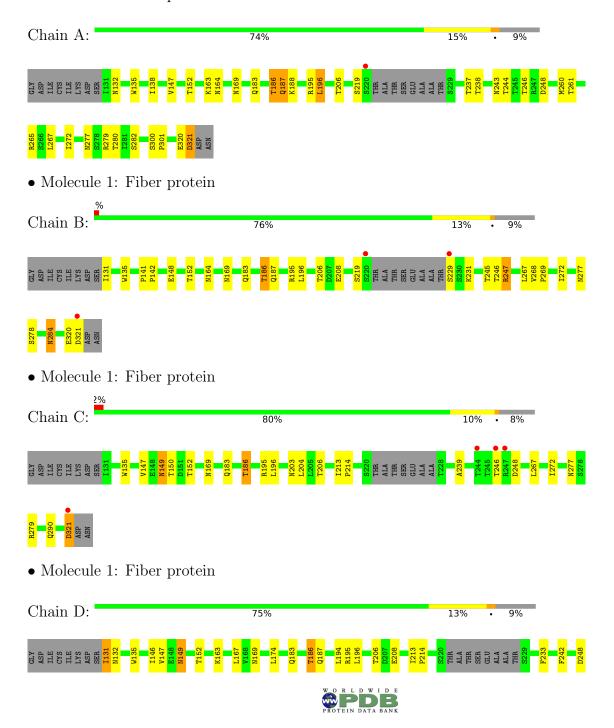
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	В	2	Total O 2 2	0	0
5	С	3	Total O 3 3	0	0
5	D	5	Total O 5 5	0	0
5	Е	6	Total O 6 6	0	0
5	F	6	Total O 6 6	0	0
5	G	8	Total O 8 8	0	0
5	Н	5	Total O 5 5	0	0
5	I	8	Total O 8 8	0	0
5	J	6	Total O 6 6	0	0
5	К	11	Total O 11 11	0	0
5	L	2	Total O 2 2	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: Fiber protein





• Molecule 1: Fiber protein

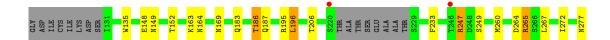
Chain E: 75% 14% • 9%



M260 D264 R265 S266 L267 L267 R271 R271 R271 R271 R281 R282 R282 S283 R283 R3P ASP

• Molecule 1: Fiber protein

Chain F: 77% 11% • 9%



8278 R279 T280 T280 1281 S282 E320 D321 ASP

• Molecule 1: Fiber protein

Chain G: 76% 12% • 9%



1281 5282 5283 N284 (Q290 F313 E320 D321 ASP

• Molecule 1: Fiber protein

Chain H: 77% 11% • 9%

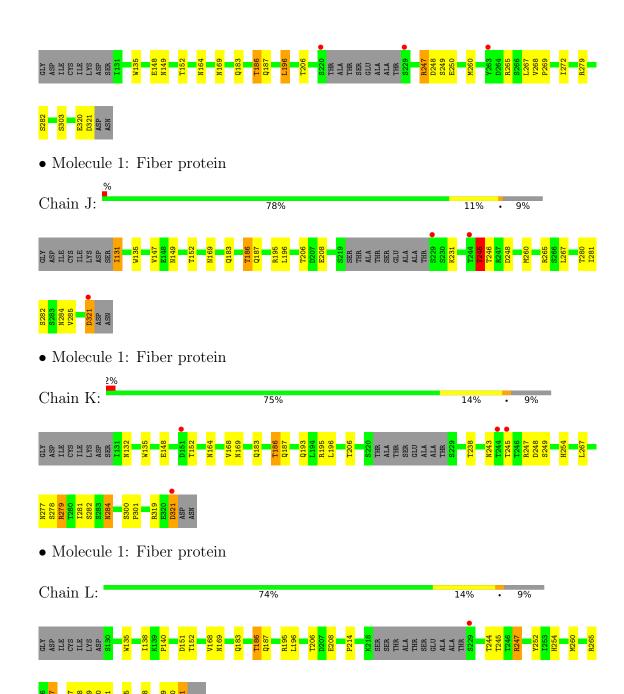


8278 R279 T280 F300 P301 E320 D321

• Molecule 1: Fiber protein

Chain I: 78% 11% • 9%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants	85.00Å 63.92Å 209.35Å	Depositor
a, b, c, α , β , γ	90.00° 91.70° 90.00°	Depositor
Resolution (Å)	49.45 - 2.50	Depositor
Resolution (A)	49.42 - 2.50	EDS
% Data completeness	91.6 (49.45-2.50)	Depositor
(in resolution range)	84.1 (49.42-2.50)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.98 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.234 , 0.259	Depositor
R, R_{free}	0.234 , 0.257	DCC
R_{free} test set	3593 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , -6.1	EDS
L-test for twinning ²	$< L > = 0.41, < L^2> = 0.24$	Xtriage
Estimated twinning fraction	0.187 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17174	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ 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: GOL, NA, CL

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
IVIOI	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.27	0/1444	0.41	0/1970
1	В	0.27	0/1448	0.41	0/1975
1	С	0.27	0/1459	0.41	0/1989
1	D	0.26	0/1451	0.41	0/1979
1	Е	0.32	0/1448	0.42	0/1975
1	F	0.28	0/1460	0.43	0/1990
1	G	0.27	0/1444	0.41	0/1969
1	Н	0.27	0/1444	0.41	0/1970
1	I	0.27	0/1455	0.40	0/1983
1	J	0.27	0/1453	0.41	0/1981
1	K	0.28	0/1455	0.40	0/1983
1	L	0.28	0/1456	0.41	0/1985
All	All	0.28	0/17417	0.41	0/23749

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	1415	0	1369	30	0



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Mol	Chain	Non-H		H(added)	Clashes	Symm-Clashes
1	В	1419	0	1380	25	0
1	С	1430	0	1392	24	0
1	D	1422	0	1382	28	0
1	Ε	1420	0	1371	31	0
1	F	1431	0	1388	26	0
1	G	1415	0	1363	22	0
1	Н	1415	0	1369	18	0
1	I	1426	0	1387	17	0
1	J	1424	0	1381	24	0
1	K	1426	0	1387	22	0
1	L	1427	0	1384	29	0
2	В	2	0	0	0	0
2	F	2	0	0	0	0
2	Н	1	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
3	С	6	0	8	3	0
3	Ε	12	0	16	8	0
3	F	6	0	8	0	0
4	J	2	0	0	1	0
5	A	5	0	0	0	0
5	В	2	0	0	0	0
5	С	3	0	0	0	0
5	D	5	0	0	0	0
5	Е	6	0	0	2	0
5	F	6	0	0	1	0
5	G	8	0	0	2	1
5	Н	5	0	0	0	0
5	I	8	0	0	1	0
5	J	6	0	0	0	0
5	K	11	0	0	1	0
5	L	2	0	0	0	0
All	All	17174	0	16585	251	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 7.

The worst 5 of 251 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:E:214:PRO:HB3	3:E:6:GOL:H32	1.37	1.06
1:J:231:LYS:NZ	4:J:2:CL:CL	2.29	1.03
1:B:247:ARG:HH11	1:B:247:ARG:HG2	1.21	1.02
1:F:247:ARG:HG3	1:F:247:ARG:HH11	1.25	1.00
1:E:204:LEU:H	3:E:6:GOL:H2	1.30	0.97

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		$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
5:G:64:HOH:O	5:G:64:HOH:O[2_555]	2.19	0.01	

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	entiles
1	A	179/201 (89%)	173 (97%)	6 (3%)	0	100	100
1	В	179/201 (89%)	170 (95%)	8 (4%)	1 (1%)	25	43
1	С	180/201 (90%)	170 (94%)	10 (6%)	0	100	100
1	D	179/201 (89%)	170 (95%)	8 (4%)	1 (1%)	25	43
1	E	180/201 (90%)	167 (93%)	10 (6%)	3 (2%)	9	16
1	F	180/201 (90%)	171 (95%)	8 (4%)	1 (1%)	25	43
1	G	179/201 (89%)	170 (95%)	7 (4%)	2 (1%)	14	26
1	Н	179/201 (89%)	167 (93%)	10 (6%)	2 (1%)	14	26
1	Ι	179/201 (89%)	170 (95%)	9 (5%)	0	100	100
1	J	179/201 (89%)	172 (96%)	6 (3%)	1 (1%)	25	43
1	K	179/201 (89%)	174 (97%)	4 (2%)	1 (1%)	25	43
1	L	179/201 (89%)	172 (96%)	7 (4%)	0	100	100
All	All	2151/2412 (89%)	2046 (95%)	93 (4%)	12 (1%)	25	43



5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	230	SER
1	Н	150	THR
1	J	245	THR
1	В	148	GLU
1	F	282	SER

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		
1	A	161/182 (88%)	148 (92%)	13 (8%)	11	23	
1	В	162/182 (89%)	149 (92%)	13 (8%)	12	23	
1	C	164/182 (90%)	156 (95%)	8 (5%)	25	47	
1	D	163/182 (90%)	152 (93%)	11 (7%)	16	31	
1	E	162/182 (89%)	153 (94%)	9 (6%)	21	40	
1	F	164/182 (90%)	152 (93%)	12 (7%)	14	27	
1	G	160/182 (88%)	148 (92%)	12 (8%)	13	26	
1	Н	161/182 (88%)	151 (94%)	10 (6%)	18	35	
1	I	164/182 (90%)	152 (93%)	12 (7%)	14	27	
1	J	164/182 (90%)	155 (94%)	9 (6%)	21	41	
1	K	164/182 (90%)	153 (93%)	11 (7%)	16	31	
1	L	163/182 (90%)	154 (94%)	9 (6%)	21	41	
All	All	1952/2184 (89%)	1823 (93%)	129 (7%)	16	32	

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	249	SER
1	K	321	ASP
1	Е	167	LEU
1	Ε	152	THR



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Mol	Chain	Res	Type
1	L	151	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	296	ASN
1	K	284	ASN
1	G	290	GLN
1	K	254	HIS
1	L	254	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 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type		Chain	Chain	Chain	Res	Link	Bond lengths			Bond angles				
WIOI	Type	Chain	nes	rtes	rtes	rtes	nes	es Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	GOL	С	2	-	5,5,5	0.40	0	5,5,5	0.15	0				
3	GOL	Е	6	-	5,5,5	0.39	0	5,5,5	0.21	0				
3	GOL	F	3	-	5,5,5	0.35	0	5,5,5	0.24	0				



Mol	Mol Type Chain Res Link				\mathbf{B}_{0}	ond leng	gths	В	ond ang	gles
Moi Type Ch	Chain Res	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
3	GOL	Е	5	-	5,5,5	0.36	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	С	2	-	-	0/4/4/4	-
3	GOL	E	6	-	-	3/4/4/4	-
3	GOL	F	3	-	-	4/4/4/4	-
3	GOL	Ε	5	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	GOL	O1-C1-C2-C3
3	F	3	GOL	C1-C2-C3-O3
3	F	3	GOL	O2-C2-C3-O3
3	Е	5	GOL	C1-C2-C3-O3
3	Е	6	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	2	GOL	3	0
3	Е	6	GOL	6	0
3	Е	5	GOL	2	0

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	183/201 (91%)	-0.24	1 (0%) 91 91	7, 17, 40, 55	0
1	В	183/201 (91%)	-0.32	3 (1%) 72 74	7, 17, 38, 57	0
1	С	184/201 (91%)	-0.24	4 (2%) 62 65	5, 17, 40, 74	0
1	D	183/201 (91%)	-0.25	0 100 100	7, 18, 45, 61	0
1	Е	183/201 (91%)	-0.22	1 (0%) 91 91	7, 18, 48, 61	0
1	F	183/201 (91%)	-0.19	2 (1%) 80 82	7, 18, 44, 65	0
1	G	183/201 (91%)	-0.27	4 (2%) 62 65	7, 17, 45, 55	0
1	Н	183/201 (91%)	-0.25	1 (0%) 91 91	7, 17, 41, 55	0
1	I	183/201 (91%)	-0.30	3 (1%) 72 74	7, 17, 40, 51	0
1	J	182/201 (90%)	-0.18	3 (1%) 72 74	7, 18, 43, 59	0
1	K	183/201 (91%)	-0.25	4 (2%) 62 65	7, 18, 47, 71	0
1	L	182/201 (90%)	-0.26	1 (0%) 91 91	7, 18, 41, 70	0
All	All	2195/2412 (91%)	-0.25	27 (1%) 79 80	5, 18, 46, 74	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	220	SER	4.8
1	J	229	SER	4.7
1	В	220	SER	4.6
1	L	229	SER	4.5
1	K	245	THR	4.4

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	${f B ext{-}factors}({f \AA}^2)$	Q<0.9
3	GOL	Е	6	6/6	0.77	0.22	22,27,30,32	0
2	NA	J	8	1/1	0.84	0.21	52,52,52,52	0
3	GOL	F	3	6/6	0.86	0.19	39,42,44,44	0
2	NA	L	10	1/1	0.87	0.15	29,29,29,29	0
3	GOL	Е	5	6/6	0.87	0.22	22,24,27,28	0
2	NA	В	3	1/1	0.88	0.14	22,22,22,22	0
3	GOL	С	2	6/6	0.89	0.26	23,30,35,35	0
2	NA	Н	6	1/1	0.94	0.15	32,32,32,32	0
2	NA	В	1	1/1	0.95	0.08	23,23,23,23	0
2	NA	K	5	1/1	0.96	0.20	26,26,26,26	0
2	NA	F	2	1/1	0.96	0.15	22,22,22,22	0
2	NA	J	9	1/1	0.96	0.06	20,20,20,20	0
2	NA	F	7	1/1	0.97	0.12	38,38,38,38	0
2	NA	K	4	1/1	0.97	0.15	25,25,25,25	0
4	CL	J	2	1/1	0.98	0.06	33,33,33,33	0
4	CL	J	1	1/1	0.99	0.06	31,31,31,31	0
2	NA	I	11	1/1	0.99	0.06	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.

