

Full wwPDB X-ray Structure Validation Report (i)

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	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)	:	2.36

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 2.53 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	Similar resolution $(//F)$
	(#Entries)	(#Entries, resolution range(A))
R _{free}	130704	$5743 \ (2.54-2.50)$
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)

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%

Mol	Chain	Length	Quality of chain					
1	А	400	52%	12% · ·	32%			
1	В	400	51%	12% •	35%			
1	С	400	44%	17% • •	35%			
2	D	26	77%		23%			
2	F	26	31%	65%	•			
3	Е	26	58%		38% •			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8033 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	Λ	271	Total	С	Ν	0	\mathbf{S}	0	0	0
1	A	271	2143	1367	389	377	10	0		
1	В	261	Total	С	Ν	0	S	0	0	0
	D	201	2076	1327	381	358	10	0		
1	1 C	C 259	Total	С	Ν	0	S	0	0	0
1			2074	1330	378	356	10	U	0	0

• Molecule 1 is a protein called Endonuclease 8-like 1.

Chain	Residue	Modelled	Actual	Comment	Reference
А	242	ARG	LYS	engineered mutation	UNP Q96FI4
А	391	ALA	-	expression tag	UNP Q96FI4
А	392	ALA	-	expression tag	UNP Q96FI4
А	393	LEU	-	expression tag	UNP Q96FI4
А	394	GLY	-	expression tag	UNP Q96FI4
А	395	HIS	-	expression tag	UNP Q96FI4
А	396	HIS	-	expression tag	UNP Q96FI4
А	397	HIS	-	expression tag	UNP Q96FI4
А	398	HIS	-	expression tag	UNP Q96FI4
А	399	HIS	-	expression tag	UNP Q96FI4
А	400	HIS	-	expression tag	UNP Q96FI4
В	242	ARG	LYS	engineered mutation	UNP Q96FI4
В	391	ALA	-	expression tag	UNP Q96FI4
В	392	ALA	-	expression tag	UNP Q96FI4
В	393	LEU	-	expression tag	UNP Q96FI4
В	394	GLY	-	expression tag	UNP Q96FI4
В	395	HIS	-	expression tag	UNP Q96FI4
В	396	HIS	-	expression tag	UNP Q96FI4
В	397	HIS	-	expression tag	UNP Q96FI4
В	398	HIS	-	expression tag	UNP Q96FI4
В	399	HIS	-	expression tag	UNP Q96FI4
В	400	HIS	-	expression tag	UNP Q96FI4
С	242	ARG	LYS	engineered mutation	UNP Q96FI4

There are 33 discrepancies between the modelled and reference sequences:



Chain

С

С

С

С

С

С

С

С

С

С

Comment

expression tag

expression tag

expression tag

expression tag

expression tag

392	ALA	-	expression tag
393	LEU	-	expression tag
394	GLY	-	expression tag
395	HIS	-	expression tag
396	HIS	-	expression tag

Actual

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Residue

391

397

398

399

400

• Molecule 2 is a DNA chain called DNA (26-MER).

Modelled

ALA

HIS

HIS

HIS

HIS

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	Л	26	Total	С	Ν	0	Р	0	0	0
2	D		516	247	94	151	24	0		
9	Б	26	Total	С	Ν	0	Р	0	0	0
Z	Г	F 20	516	247	94	151	24	0		

• Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	Е	26	Total 514	C 247	N 94	0 149	Р 24	0	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Reference

UNP Q96FI4



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	108	Total O 108 108	0	0
5	В	48	Total O 48 48	0	0
5	С	4	Total O 4 4	0	0
5	D	14	Total O 14 14	0	0
5	Е	6	Total O 6 6	0	0
5	F	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. 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. 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: Endonuclease 8-like 1







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	73.86Å 108.75Å 171.32Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	81.81 - 2.53	Depositor
	32.54 - 2.53	EDS
% Data completeness	97.9 (81.81-2.53)	Depositor
(in resolution range)	97.9(32.54-2.53)	EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$2.19 (at 2.54 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
B B.	0.210 , 0.278	Depositor
II, II, <i>free</i>	0.265 , 0.302	DCC
R_{free} test set	2318 reflections (5.05%)	wwPDB-VP
Wilson B-factor $(Å^2)$	56.2	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 31.4	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8033	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.48% 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: GOL

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.10	2/2202~(0.1%)	1.11	16/2979~(0.5%)	
1	В	0.94	1/2133~(0.0%)	1.05	10/2885~(0.3%)	
1	С	0.57	2/2129~(0.1%)	0.78	4/2878~(0.1%)	
2	D	0.55	0/577	0.91	1/886~(0.1%)	
2	F	0.42	0/577	0.81	2/886~(0.2%)	
3	Е	0.61	0/575	0.99	1/882~(0.1%)	
All	All	0.83	5/8193~(0.1%)	0.98	34/11396~(0.3%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	2
1	В	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	223	PRO	N-CD	5.52	1.55	1.47
1	А	280	TRP	CE3-CZ3	5.40	1.47	1.38
1	С	64	PRO	N-CD	5.29	1.55	1.47
1	С	68	PRO	N-CD	5.24	1.55	1.47
1	А	68	PRO	N-CD	5.05	1.54	1.47

All (34) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	133	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	А	133	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	А	133	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	А	119	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	В	133	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	В	119	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	А	169	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	А	179	ARG	NE-CZ-NH2	-7.03	116.79	120.30
2	D	22	DT	O5'-P-OP2	-6.72	99.65	105.70
1	С	284	ASP	C-N-CD	6.42	141.88	128.40
1	А	93	LEU	C-N-CD	6.30	141.64	128.40
1	А	169	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	В	119	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	С	61	SER	C-N-CD	6.08	141.16	128.40
1	А	179	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	А	71	GLU	C-N-CD	5.83	140.65	128.40
1	А	90	ARG	NE-CZ-NH1	5.74	123.17	120.30
3	Е	5	DC	C1'-O4'-C4'	-5.71	104.39	110.10
2	F	1	DC	C5'-C4'-O4'	5.70	120.12	109.30
1	А	250	GLU	C-N-CA	-5.66	107.56	121.70
1	В	68	PRO	N-CA-C	-5.55	97.68	112.10
1	А	105	PRO	N-CA-C	5.51	126.42	112.10
1	В	189	PRO	C-N-CD	5.47	139.88	128.40
1	А	277	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	А	95	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	В	122	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	А	119	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	С	63	LEU	C-N-CD	5.25	139.43	128.40
1	В	67	GLN	C-N-CD	-5.24	109.07	120.60
1	В	122	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	В	190	PRO	CA-N-CD	-5.09	104.37	111.50
1	А	67	GLN	C-N-CD	5.08	139.06	128.40
1	С	67	GLN	C-N-CD	5.04	138.99	128.40
2	F	1	DC	C5'-C4'-C3'	5.02	123.13	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	249	GLY	Peptide
1	А	94	PRO	Peptide
1	В	67	GLN	Peptide



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	2143	0	2103	84	0
1	В	2076	0	2061	46	0
1	С	2074	0	2064	80	0
2	D	516	0	290	7	0
2	F	516	0	290	23	0
3	Е	514	0	290	8	0
4	А	6	0	8	1	0
4	В	6	0	8	0	0
5	А	108	0	0	4	0
5	В	48	0	0	2	0
5	С	4	0	0	0	0
5	D	14	0	0	0	0
5	Е	6	0	0	0	0
5	F	2	0	0	0	0
All	All	8033	0	7114	236	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 16.

All (236) 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)
1:B:199:GLU:OE1	1:B:202:GLN:NE2	1.57	1.35
1:A:250:GLU:HG3	1:A:253:PHE:HD1	1.03	1.16
1:A:250:GLU:HG3	1:A:253:PHE:CD1	1.85	1.11
1:A:250:GLU:HB2	1:A:253:PHE:HB3	1.08	1.08
1:C:282:GLN:OE1	1:C:284:ASP:N	1.88	1.07
1:A:250:GLU:HB2	1:A:253:PHE:CB	1.92	0.99
1:A:147:ASN:HD22	1:A:150:ARG:HH12	1.11	0.98
2:D:13:DC:H2"	2:F:1:DC:C6	2.00	0.97
1:B:189:PRO:HB2	1:B:192:GLU:CG	1.96	0.96
1:B:199:GLU:O	1:B:202:GLN:HG3	1.67	0.95
1:A:249:GLY:N	1:A:250:GLU:HB3	1.82	0.94
1:A:250:GLU:CB	1:A:253:PHE:HB3	1.99	0.93
1:A:95:ARG:HG3	1:A:96:HIS:HA	1.51	0.92



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:147:ASN:HD22	1:A:150:ARG:NH1	1.65	0.91
1:A:186:LEU:HD21	1:A:228:LEU:HD11	1.55	0.87
1:B:78:ARG:NH1	3:E:10:DC:OP2	2.08	0.86
1:A:250:GLU:CG	1:A:253:PHE:HD1	1.87	0.85
1:B:199:GLU:O	1:B:202:GLN:CG	2.25	0.85
1:B:189:PRO:O	1:B:192:GLU:HG3	1.77	0.84
1:B:189:PRO:HB2	1:B:192:GLU:HG3	1.58	0.84
1:C:281:PHE:CE2	1:C:285:PRO:HB3	2.16	0.80
1:A:248:SER:HA	1:A:250:GLU:HB3	1.64	0.78
2:F:2:DG:H1	2:F:26:DC:H42	1.31	0.77
1:C:78:ARG:NH1	2:F:10:DC:OP1	2.17	0.77
1:C:195:ARG:O	1:C:199:GLU:HB3	1.84	0.77
1:C:41:GLU:O	1:C:70:GLN:OE1	2.04	0.76
1:A:250:GLU:O	1:A:251:GLU:C	2.16	0.75
1:A:34:ARG:HG2	1:A:34:ARG:HH11	1.52	0.75
1:C:62:PRO:HG2	1:C:70:GLN:O	1.86	0.74
1:C:88:VAL:HG21	1:C:94:PRO:HD3	1.71	0.73
1:A:249:GLY:N	1:A:250:GLU:OE1	2.20	0.72
1:A:143:GLN:NE2	5:A:601:HOH:O	2.21	0.72
1:B:239:LEU:N	1:B:239:LEU:HD23	2.04	0.71
1:A:147:ASN:ND2	1:A:150:ARG:NH1	2.39	0.70
1:A:95:ARG:CG	1:A:96:HIS:HA	2.21	0.70
1:C:186:LEU:O	1:C:187:LYS:C	2.29	0.69
1:B:57:ARG:NH1	1:B:127:GLY:O	2.25	0.69
1:A:248:SER:CA	1:A:250:GLU:HB3	2.23	0.69
1:A:250:GLU:CG	1:A:253:PHE:CD1	2.68	0.69
1:C:46:ARG:HG3	1:C:63:LEU:HD11	1.75	0.69
1:C:281:PHE:CZ	1:C:285:PRO:HB3	2.29	0.68
1:B:130:GLN:NE2	1:B:133:ARG:HD2	2.09	0.68
1:A:95:ARG:CG	1:A:95:ARG:HH11	2.08	0.67
1:C:149:LEU:HD21	1:C:201:LEU:HB3	1.76	0.67
1:C:138:LEU:HD21	1:C:233:PRO:HB2	1.76	0.67
1:C:149:LEU:HD21	1:C:201:LEU:CB	2.24	0.67
1:C:221:GLN:HE21	1:C:221:GLN:CA	2.05	0.66
1:B:158:ASP:HA	1:B:193:LYS:HE3	1.78	0.66
1:A:250:GLU:O	1:A:250:GLU:HG2	1.97	0.65
1:B:194:ALA:O	1:B:197:VAL:HG23	1.96	0.65
1:C:46:ARG:N	1:C:61:SER:O	2.26	0.64
1:A:147:ASN:ND2	1:A:150:ARG:HH12	1.89	0.64
2:F:2:DG:H1	2:F:26:DC:N4	1.94	0.64
1:B:222:ASN:OD1	1:B:222:ASN:N	2.30	0.64



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:249:GLY:H	1:A:250:GLU:HB3	1.63	0.63
1:B:243:GLY:O	1:B:256:PHE:CD2	2.53	0.62
1:B:105:PRO:O	1:C:222:ASN:ND2	2.32	0.62
2:D:13:DC:C2'	2:F:1:DC:C6	2.80	0.62
2:F:26:DC:H2'	2:F:27:DG:C8	2.35	0.61
1:A:130:GLN:NE2	1:A:133:ARG:HD2	2.16	0.61
1:B:104:ALA:HB1	1:B:105:PRO:HD2	1.82	0.60
1:A:248:SER:C	1:A:250:GLU:HB3	2.20	0.60
1:A:248:SER:HA	1:A:250:GLU:CB	2.30	0.60
1:C:181:GLU:O	1:C:185:ARG:HG2	2.02	0.60
1:A:155:LYS:HD3	2:F:27:DG:OP1	2.01	0.59
1:A:246:SER:OG	1:A:253:PHE:HA	2.02	0.59
1:B:189:PRO:HG2	1:B:192:GLU:CD	2.21	0.59
1:A:30:SER:HB3	1:A:98:HIS:HA	1.85	0.59
1:A:132:GLY:O	1:A:169:ARG:HG2	2.03	0.59
1:A:72:PRO:HG3	5:A:660:HOH:O	2.02	0.59
1:A:30:SER:HB2	1:A:95:ARG:NH2	2.18	0.59
1:C:281:PHE:CE2	1:C:285:PRO:CB	2.86	0.59
1:C:269:SER:HB2	1:C:281:PHE:CE1	2.38	0.58
2:F:17:DA:C8	2:F:17:DA:OP2	2.56	0.58
1:A:250:GLU:HB2	1:A:253:PHE:CG	2.39	0.58
1:B:81:MET:SD	3:E:8:DG:H5"	2.43	0.58
1:C:196:SER:O	1:C:199:GLU:HG2	2.03	0.57
2:F:1:DC:H2'	2:F:1:DC:O2	2.03	0.57
1:A:90:ARG:O	1:A:93:LEU:HD13	2.04	0.57
1:C:198:LEU:C	1:C:200:ALA:H	2.08	0.57
2:D:16:DT:H5"	2:F:28:DG:O3'	2.05	0.57
2:D:17:DA:H2"	2:D:18:DG:H5"	1.87	0.56
1:C:194:ALA:O	1:C:198:LEU:HD12	2.06	0.56
1:C:281:PHE:CE2	1:C:285:PRO:CA	2.88	0.56
1:C:285:PRO:HD2	1:C:286:GLY:H	1.69	0.56
1:B:199:GLU:O	1:B:202:GLN:HG2	2.03	0.56
1:A:275:HIS:HB3	5:A:680:HOH:O	2.06	0.56
2:F:9:DT:H2"	2:F:10:DC:OP1	2.05	0.56
1:C:63:LEU:HB3	1:C:64:PRO:CD	2.36	0.56
2:F:27:DG:H2'	2:F:28:DG:C8	2.40	0.56
1:C:45:TYR:HB2	1:C:61:SER:O	2.06	0.56
1:B:95:ARG:NH1	3:E:23:DG:OP1	2.39	0.56
1:C:281:PHE:CD1	1:C:281:PHE:N	2.72	0.56
1:A:247:GLU:O	1:A:250:GLU:HA	2.07	0.55
1:A:96:HIS:CD2	1:A:96:HIS:N	2.72	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:222:ASN:N	1:B:223:PRO:HD3	2.22	0.55
1:B:188:ILE:HG21	1:B:197:VAL:HG11	1.89	0.54
1:A:34:ARG:HG2	1:A:34:ARG:NH1	2.21	0.54
1:A:246:SER:OG	1:A:253:PHE:CA	2.56	0.54
1:C:260:LEU:HB2	1:C:265:MET:HE2	1.87	0.54
1:A:94:PRO:O	1:A:95:ARG:HD2	2.08	0.54
1:C:79:PHE:O	1:C:80:GLY:C	2.46	0.54
1:C:221:GLN:HE21	1:C:221:GLN:HA	1.72	0.53
1:B:191:PHE:O	1:B:288:LEU:HB2	2.08	0.53
1:B:130:GLN:HE21	1:B:133:ARG:HD2	1.71	0.53
1:C:149:LEU:CD2	1:C:201:LEU:CB	2.87	0.53
1:B:189:PRO:HB2	1:B:192:GLU:HG2	1.86	0.53
1:C:154:ASP:O	1:C:195:ARG:NH2	2.43	0.52
1:B:35:ASN:HB2	1:B:123:TRP:CZ2	2.44	0.52
1:C:190:PRO:HD2	1:C:285:PRO:HA	1.92	0.52
1:C:191:PHE:N	1:C:285:PRO:O	2.33	0.52
1:C:221:GLN:HA	1:C:221:GLN:NE2	2.25	0.52
1:A:130:GLN:HE22	1:A:133:ARG:HH11	1.57	0.52
1:A:250:GLU:O	1:A:252:ASP:N	2.42	0.51
1:C:116:ASP:OD2	1:C:119:ARG:HA	2.10	0.51
1:C:278:THR:CG2	1:C:280:TRP:NE1	2.73	0.51
1:C:281:PHE:HD1	1:C:281:PHE:H	1.58	0.51
1:C:109:ARG:HA	1:C:109:ARG:NE	2.25	0.51
1:C:184:TYR:CE2	1:C:261:ARG:O	2.64	0.51
1:A:247:GLU:O	1:A:250:GLU:CA	2.59	0.51
1:B:199:GLU:OE1	1:B:199:GLU:HA	2.11	0.51
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.75	0.50
1:B:223:PRO:HA	1:B:227:GLU:OE2	2.11	0.50
1:C:48:SER:OG	1:C:59:ILE:HB	2.12	0.50
1:C:281:PHE:CE2	1:C:285:PRO:HA	2.47	0.50
1:A:247:GLU:O	1:A:250:GLU:CB	2.60	0.50
1:C:221:GLN:HE21	1:C:221:GLN:C	2.15	0.50
1:C:221:GLN:CA	1:C:221:GLN:NE2	2.73	0.50
1:C:149:LEU:CD2	1:C:201:LEU:HB2	2.42	0.50
1:B:232:VAL:HB	1:B:233:PRO:CD	2.43	0.49
1:C:19:ARG:O	1:C:46:ARG:NH1	2.45	0.49
1:A:17:ALA:HB1	1:A:87:LEU:HD22	1.93	0.49
1:A:130:GLN:HE21	1:A:133:ARG:HD2	1.78	0.49
1:A:95:ARG:CG	1:A:95:ARG:NH1	2.72	0.49
1:A:249:GLY:CA	1:A:250:GLU:OE1	2.60	0.49
1:A:53:GLY:HA3	1:A:172:ASN:CG	2.33	0.48



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:105:PRO:N	1:B:106:PRO:HD2	2.28	0.48
1:C:201:LEU:HD12	1:C:226:LEU:HD12	1.93	0.48
3:E:1:DC:O4'	3:E:1:DC:O2	2.31	0.48
1:A:154:ASP:OD1	1:A:155:LYS:HE2	2.13	0.48
1:B:35:ASN:HB3	1:B:36:PRO:CD	2.42	0.48
1:C:196:SER:C	1:C:199:GLU:HG2	2.33	0.48
1:A:130:GLN:NE2	1:A:133:ARG:HH11	2.12	0.48
1:B:233:PRO:O	1:B:237:VAL:HG23	2.14	0.48
1:C:159:ARG:HB3	1:C:160:PRO:HD2	1.96	0.48
1:C:269:SER:CB	1:C:281:PHE:CE1	2.96	0.48
1:C:41:GLU:H	1:C:70:GLN:HE22	1.61	0.48
1:A:56:LEU:C	1:A:56:LEU:HD23	2.34	0.48
1:A:105:PRO:O	1:A:106:PRO:C	2.48	0.48
3:E:17:DA:H2"	3:E:18:DG:OP2	2.14	0.47
1:A:105:PRO:O	1:A:107:GLY:N	2.47	0.47
1:B:76:VAL:O	1:B:123:TRP:HA	2.14	0.47
1:B:243:GLY:O	1:B:244:TYR:HB2	2.13	0.47
1:A:90:ARG:HD3	1:A:102:TYR:CD1	2.50	0.47
1:B:193:LYS:HA	1:B:288:LEU:CD1	2.45	0.47
1:C:148:VAL:CG1	1:C:198:LEU:HD22	2.45	0.47
1:C:190:PRO:HG3	1:C:281:PHE:CG	2.49	0.47
1:C:281:PHE:N	1:C:281:PHE:HD1	2.11	0.47
3:E:1:DC:H2"	3:E:2:DG:H5'	1.97	0.47
3:E:21:DC:H2'	3:E:22:DT:C6	2.50	0.47
1:C:281:PHE:HE2	1:C:285:PRO:CA	2.28	0.47
1:A:201:LEU:O	1:A:202:GLN:HB2	2.15	0.46
1:C:54:LYS:HB2	1:C:133:ARG:NH2	2.30	0.46
1:A:186:LEU:CD2	1:A:228:LEU:HD11	2.37	0.46
1:C:264:GLY:O	1:C:265:MET:SD	2.73	0.46
1:C:278:THR:HG22	1:C:280:TRP:NE1	2.30	0.46
1:A:88:VAL:HG21	1:A:94:PRO:HD3	1.98	0.46
1:C:186:LEU:O	1:C:187:LYS:O	2.34	0.46
1:B:222:ASN:N	1:B:223:PRO:CD	2.79	0.46
1:C:56:LEU:C	1:C:56:LEU:HD23	2.36	0.45
1:A:186:LEU:HB2	1:A:188:ILE:HG13	1.99	0.45
1:A:250:GLU:CB	1:A:253:PHE:CD1	3.00	0.45
1:C:29:LYS:NZ	1:C:33:SER:O	2.44	0.45
1:B:23:PHE:HA	1:B:103:THR:HA	1.96	0.45
1:A:222:ASN:N	1:A:223:PRO:CD	2.80	0.45
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.63	0.45
1:A:156:ALA:O	1:A:159:ARG:HG2	2.17	0.44



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:F:2:DG:H2"	2:F:3:DT:O5'	2.16	0.44
1:C:149:LEU:CD2	1:C:201:LEU:HB3	2.42	0.44
1:B:95:ARG:O	1:B:96:HIS:HB2	2.18	0.44
1:C:185:ARG:NH1	1:C:261:ARG:NH2	2.65	0.44
1:C:219:LYS:HE3	1:C:219:LYS:HA	1.99	0.44
2:F:8:DG:H2"	2:F:9:DT:O5'	2.18	0.44
1:A:159:ARG:NH2	1:A:274:ARG:NE	2.66	0.44
2:F:23:DG:H1'	2:F:24:DG:C8	2.53	0.44
1:A:30:SER:HB2	1:A:95:ARG:HH22	1.82	0.44
1:B:169:ARG:NH1	5:B:606:HOH:O	2.49	0.44
1:A:274:ARG:HG3	1:A:275:HIS:CD2	2.53	0.44
1:B:23:PHE:CD1	1:B:47:ILE:HG13	2.53	0.44
2:F:5:DC:H2"	2:F:6:DA:H5'	1.99	0.43
1:C:198:LEU:C	1:C:200:ALA:N	2.70	0.43
1:B:254:ALA:O	1:B:255:ALA:HB3	2.18	0.43
1:C:63:LEU:HD23	1:C:63:LEU:HA	1.80	0.43
1:C:263:TYR:O	1:C:265:MET:HG2	2.18	0.43
2:F:12:DA:H1'	2:F:13:DC:O5'	2.18	0.43
1:C:46:ARG:HG3	1:C:63:LEU:CD1	2.47	0.43
2:F:8:DG:H1'	2:F:9:DT:C6	2.54	0.43
2:D:12:DA:H2"	2:D:13:DC:OP2	2.18	0.43
3:E:5:DC:H2"	3:E:6:DA:C8	2.54	0.43
1:C:67:GLN:HA	1:C:68:PRO:HA	1.69	0.43
1:A:90:ARG:NH1	1:A:102:TYR:HB3	2.33	0.43
1:C:149:LEU:HD13	1:C:202:GLN:HB3	2.00	0.43
1:A:250:GLU:HB2	1:A:253:PHE:CD1	2.53	0.43
1:B:275:HIS:HB3	5:B:636:HOH:O	2.18	0.43
1:A:159:ARG:NH2	1:A:274:ARG:CZ	2.82	0.43
1:A:63:LEU:HD23	5:A:636:HOH:O	2.19	0.42
1:A:155:LYS:CD	2:F:27:DG:OP1	2.67	0.42
2:F:21:DC:H2'	2:F:22:DT:C6	2.54	0.42
1:A:249:GLY:N	1:A:250:GLU:CB	2.68	0.42
1:A:246:SER:HB2	1:A:252:ASP:CG	2.39	0.42
1:A:29:LYS:HG2	1:A:30:SER:O	2.20	0.42
1:C:278:THR:HG21	1:C:280:TRP:NE1	2.34	0.42
1:A:95:ARG:HG3	1:A:95:ARG:HH11	1.85	0.42
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.84	0.42
1:B:195:ARG:O	1:B:199:GLU:HG2	2.20	0.42
1:B:243:GLY:O	1:B:256:PHE:CG	2.73	0.42
1:C:262:CYS:O	1:C:265:MET:HG2	2.20	0.42
2:D:16:DT:C5'	2:F:28:DG:O3'	2.67	0.42



Atom-1	Atom-2	Interatomic $distance (Å)$	Clash
	1 C 200 AT A N		overlap (A)
1:C:198:LEU:O	1:C:200:ALA:N	2.53	0.42
1:B:194:ALA:O	1:B:197:VAL:N	2.47	0.42
1:C:148:VAL:HG11	1:C:198:LEU:HD22	2.01	0.42
1:A:57:ARG:NH1	1:A:127:GLY:O	2.43	0.41
1:C:285:PRO:HD2	1:C:286:GLY:N	2.35	0.41
1:A:274:ARG:HG3	1:A:275:HIS:HD2	1.85	0.41
1:C:81:MET:CE	2:F:6:DA:H2'	2.50	0.41
1:C:197:VAL:C	1:C:199:GLU:N	2.73	0.41
1:A:250:GLU:C	1:A:252:ASP:N	2.72	0.41
1:B:189:PRO:HG2	1:B:192:GLU:OE1	2.21	0.41
1:A:85:PHE:O	4:A:501:GOL:H31	2.20	0.41
1:C:118:ARG:O	1:C:119:ARG:HB2	2.21	0.41
1:C:285:PRO:CD	1:C:286:GLY:H	2.33	0.41
1:A:222:ASN:N	1:A:223:PRO:HD2	2.36	0.40
1:A:234:LYS:O	1:A:235:GLU:C	2.59	0.40
1:C:197:VAL:O	1:C:199:GLU:N	2.55	0.40
2:D:17:DA:H2"	2:D:18:DG:C5'	2.50	0.40
2:F:26:DC:C2'	2:F:27:DG:O5'	2.69	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	entiles
1	А	267/400~(67%)	254~(95%)	13~(5%)	0	100	100
1	В	255/400~(64%)	228~(89%)	25 (10%)	2(1%)	19	33
1	С	249/400~(62%)	215 (86%)	29 (12%)	5 (2%)	7	11
All	All	771/1200~(64%)	697~(90%)	67 (9%)	7 (1%)	17	30

All (7) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	68	PRO
1	С	199	GLU
1	С	167	ASP
1	С	198	LEU
1	С	262	CYS
1	С	285	PRO
1	В	243	GLY

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	А	222/335~(66%)	205~(92%)	17 (8%)	13 23		
1	В	217/335~(65%)	202~(93%)	15 (7%)	15 28		
1	С	219/335~(65%)	193~(88%)	26 (12%)	5 9		
All	All	658/1005~(66%)	600 (91%)	58 (9%)	10 18		

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	12	GLN
1	А	31	SER
1	А	34	ARG
1	А	56	LEU
1	А	72	PRO
1	А	90	ARG
1	А	93	LEU
1	А	95	ARG
1	А	105	PRO
1	А	125	LEU
1	А	143	GLN
1	А	155	LYS
1	А	201	LEU
1	А	202	GLN
1	A	250	GLU
1	А	253	PHE



Mol	Chain	Res	Type
1	A	274	ARG
1	B	2	PRO
1	B	41	GLU
1	B	81	MET
1	B	92	GLU
1	В	95	ARG
1	В	100	ARG
1	В	109	ARG
1	В	122	ARG
1	В	144	PHE
1	В	155	LYS
1	В	187	LYS
1	В	197	VAL
1	В	222	ASN
1	В	239	LEU
1	В	274	ARG
1	С	12	GLN
1	С	22	VAL
1	С	26	CYS
1	С	46	ARG
1	С	50	SER
1	С	64	PRO
1	С	68	PRO
1	С	69	GLN
1	С	82	SER
1	С	95	ARG
1	С	122	ARG
1	С	130	GLN
1	С	147	ASN
1	С	192	GLU
1	С	198	LEU
1	С	199	GLU
1	С	201	LEU
1	С	219	LYS
1	С	220	LEU
1	С	221	GLN
1	С	239	LEU
1	С	253	PHE
1	С	257	ARG
1	С	262	CYS
1	С	281	PHE
1	С	282	GLN



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

Mol	Chain	Res	Type
1	А	69	GLN
1	А	96	HIS
1	А	130	GLN
1	А	143	GLN
1	А	147	ASN
1	А	275	HIS
1	В	130	GLN
1	В	143	GLN
1	В	222	ASN
1	С	69	GLN
1	С	70	GLN
1	С	221	GLN
1	С	222	ASN

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)

2 ligands are modelled in this entry.

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).



Mal	Tune	Chain	Dec	Tiple	B	ond leng	gths	E	Bond ang	gles
	Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	GOL	A	501	-	5,5,5	0.96	0	$5,\!5,\!5$	1.01	0
4	GOL	В	501	-	5,5,5	0.53	0	$5,\!5,\!5$	0.54	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
4	GOL	А	501	-	-	4/4/4/4	-
4	GOL	В	501	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	501	GOL	C1-C2-C3-O3
4	А	501	GOL	O2-C2-C3-O3
4	А	501	GOL	O1-C1-C2-O2
4	В	501	GOL	O2-C2-C3-O3
4	А	501	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	501	GOL	1	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

