

Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2024 – 02:23 PM JST

PDB ID	:	8ZES
Title	:	Crystal structure of the Wuhan SARS-CoV-2 RBD (333-541) complexed with
		P2C5 nanobody
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Deposited on	:	2024-05-06
Resolution	:	3.70 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 3.70 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}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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 a	chain	
1	А	221	63%	16%	8% • 12%
1	С	221	56%	22%	8% • 12%
1	D	221	59%	23%	5% • 12%
1	G	221	57%	23%	5% • 13%
1	Ι	221	47%	29%	9% • 12%
2	В	146	59%	15%	8% • 17%



Mol	Chain	Length	Quality of	chain			
2	Е	146	54%	18%	9%	·	17%
2	F	146	59%	14%	7%	•	17%
2	Н	146	55%	18%	8%	•	18%
2	J	146	49%	21%	9%	•	18%
3	K	2	100%				
3	L	2	100%				
3	М	2	100%				



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12398 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		At	oms			ZeroOcc	AltConf	Trace
1	С	104	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	U	194	1530	983	254	285	8	0	0	0
1	Λ	104	Total	С	Ν	Ο	S	0	0	0
1	Л	194	1528	981	253	286	8		0	0
1	С	103	Total	С	Ν	Ο	S	0	0	0
1	G	195	1520	977	251	284	8			0
1	Т	104	Total	С	Ν	Ο	S	0	0	0
1	L	194	1531	982	254	287	8	0	0	0
1	Л	105	Total	С	Ν	0	S	0	0	0
1		199	1540	988	256	288	8	0	0	0

• Molecule 1 is a protein called Spike protein S1.

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
С	542	GLY	-	expression tag	UNP P0DTC2
С	543	SER	-	expression tag	UNP P0DTC2
С	544	HIS	-	expression tag	UNP P0DTC2
С	545	HIS	-	expression tag	UNP P0DTC2
С	546	HIS	-	expression tag	UNP P0DTC2
С	547	HIS	-	expression tag	UNP P0DTC2
С	548	HIS	-	expression tag	UNP P0DTC2
С	549	HIS	-	expression tag	UNP P0DTC2
С	550	HIS	-	expression tag	UNP P0DTC2
С	551	HIS	-	expression tag	UNP P0DTC2
С	552	HIS	-	expression tag	UNP P0DTC2
С	553	HIS	-	expression tag	UNP P0DTC2
А	542	GLY	-	expression tag	UNP P0DTC2
А	543	SER	-	expression tag	UNP P0DTC2
А	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
А	547	HIS	-	expression tag	UNP P0DTC2
А	548	HIS	-	expression tag	UNP P0DTC2



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Chain	Residue	Modelled	Actual	Comment	Reference
А	549	HIS	-	expression tag	UNP P0DTC2
А	550	HIS	-	expression tag	UNP P0DTC2
A	551	HIS	-	expression tag	UNP P0DTC2
А	552	HIS	-	expression tag	UNP P0DTC2
А	553	HIS	-	expression tag	UNP P0DTC2
G	542	GLY	-	expression tag	UNP P0DTC2
G	543	SER	-	expression tag	UNP P0DTC2
G	544	HIS	-	expression tag	UNP P0DTC2
G	545	HIS	-	expression tag	UNP P0DTC2
G	546	HIS	-	expression tag	UNP P0DTC2
G	547	HIS	-	expression tag	UNP P0DTC2
G	548	HIS	-	expression tag	UNP P0DTC2
G	549	HIS	-	expression tag	UNP P0DTC2
G	550	HIS	-	expression tag	UNP P0DTC2
G	551	HIS	-	expression tag	UNP P0DTC2
G	552	HIS	-	expression tag	UNP P0DTC2
G	553	HIS	-	expression tag	UNP P0DTC2
Ι	542	GLY	-	expression tag	UNP P0DTC2
Ι	543	SER	-	expression tag	UNP P0DTC2
Ι	544	HIS	-	expression tag	UNP P0DTC2
Ι	545	HIS	-	expression tag	UNP P0DTC2
Ι	546	HIS	-	expression tag	UNP P0DTC2
Ι	547	HIS	-	expression tag	UNP P0DTC2
Ι	548	HIS	-	expression tag	UNP P0DTC2
Ι	549	HIS	-	expression tag	UNP P0DTC2
Ι	550	HIS	-	expression tag	UNP P0DTC2
Ι	551	HIS	-	expression tag	UNP P0DTC2
Ι	552	HIS	-	expression tag	UNP P0DTC2
Ι	553	HIS	-	expression tag	UNP P0DTC2
D	542	GLY	-	expression tag	UNP P0DTC2
D	543	SER	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2
D	546	HIS	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2
D	548	HIS	-	expression tag	UNP P0DTC2
D	549	HIS	-	expression tag	UNP P0DTC2
D	550	HIS	-	expression tag	UNP P0DTC2
D	551	HIS	-	expression tag	UNP P0DTC2
D	552	HIS	-	expression tag	UNP P0DTC2
D	553	HIS	-	expression tag	UNP P0DTC2

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• Molecule 2 is a protein called Nanobody P2C5.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	F	191	Total	С	Ν	Ο	S	0	0	0
	Ľ	121	931	576	158	190	7	0		0
2	В	191	Total	С	Ν	Ο	S	0	0	0
	D	121	931	576	158	190	7		0	0
0	Б	191	Total	С	Ν	0	S	0	0	0
	Г	121	931	576	158	190	7			0
0	и	190	Total	С	Ν	0	S	0	0	0
	11	120	925	573	157	188	7	0	0	0
0	т	110	Total	С	Ν	0	S	0	0	0
		119	919	570	156	186	7		U	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	K	2	Total C N O 28 16 2 10	0	0	0
3	L	2	Total C N O 28 16 2 10	0	0	0
3	М	2	Total C N O 28 16 2 10	0	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	Δ	1	Total	С	Ν	Ο	0	0		
4	A	1	14	8	1	5	0	0		
4	Л	1	Total	С	Ν	Ο	0	0		
4	D			14	8	1	5	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: Spike protein S1



• Molecule 1: Spike protein S1





E1 q13 L18 L18 R19 R19 R19 R26 C26 C26 V27	128 (320 (320 (331 (331 (332) (333) (33) (333) (R66 R71 K75 B87 E88 B87 B91	M92 K96 897 898 A99	S102 G103 E104 T118 V119	S121 ALA ALA ALA ALA	
GLU GLN CLYS LLEU LLEU SER GLU GLU ASP LEU	ALY ALA ALA ALA HIS HIS HIS HIS HIS RIS SER SER					
• Molecule 2:	Nanobody P2C5					
Chain H:	55%	18%	8% •	18%		
E1 V2 L18 R19 A24 T28 T28	729 732 733 733 733 733 733 733 733 733 740 741 741 833 854 853 853 853 853 854 853 855 855 759	F67 R71 D72 N73 E86 F87 E88	A91 M92 K96 N98 A99	C100 S101 S102 Y105 L106	1118 1119 8120	
SER ALA ALA ALA GLU GLU CYS LYS LVS LEU ILE SER	GLU GLU ASP ASN CELY CELY GLY HIS HIS HIS HIS HIS HIS SER RIS SER SER					
• Molecule 2:	Nanobody P2C5					
Chain J:	49%	21%	9% •	18%		
E1 V2 Q3 C4 V1 S11 V12 Q13 Q13 Q14 A14	817 119 119 119 120 120 221 221 221 225 225 226 226 226 231 231 231 233 233 233 233 233 233 233	r 4 1 E44 R52 R52 R52 R53 D54 T57	T60 D61 K64 F67	R71 D72 N73 A74 K75 F05	887 888 888 A91	
M92 K96 S97 W98 S101 S102 C103 E104 E104	q108 T115 T115 T118 T118 C11 C11 C11 C11 C11 C11 C11 C11 C11	ALAO GLY ALA ALA ALA HIS HIS HIS HIS HIS	GLY SER			
• Molecule 3: opyranose	2-acetamido-2-deoxy-beta-D-	-glucopyranose	e-(1-4)-2-a	acetamido	o-2-deoxy-b	eta-D-gluc
Chain K:	100)%				
NAG1 NAG2						
• Molecule 3: opyranose	2-acetamido-2-deoxy-beta-D-	-glucopyranose	e-(1-4)-2-a	acetamido	o-2-deoxy-b	eta-D-gluc
Chain L:	100'	%				
NAG1 NAG2						
• Molecule 3: opyranose	2-acetamido-2-deoxy-beta-D-	-glucopyranose	e-(1-4)-2-a	acetamido	o-2-deoxy-b	eta-D-gluc

Chain M:

100%

NAG1 NAG2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants	126.64Å 194.24Å 264.37Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	74.10 - 3.70	Depositor
Resolution (A)	74.10 - 3.70	EDS
% Data completeness	98.9 (74.10-3.70)	Depositor
(in resolution range)	98.9 (74.10-3.70)	EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 3.67 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
P. P.	0.207 , 0.269	Depositor
n, n_{free}	0.209 , 0.260	DCC
R_{free} test set	1810 reflections (5.15%)	wwPDB-VP
Wilson B-factor $(Å^2)$	150.3	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 173.8	EDS
L-test for $twinning^2$	$ < L >=0.42, < L^2>=0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12398	wwPDB-VP
Average B, all atoms $(Å^2)$	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.08% 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: NAG

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	Bo	ond lengths	Bond angles		
INIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.93	1/1571~(0.1%)	1.71	38/2139~(1.8%)	
1	С	0.92	1/1574~(0.1%)	1.75	48/2143~(2.2%)	
1	D	0.86	1/1583~(0.1%)	1.62	26/2154~(1.2%)	
1	G	0.94	2/1563~(0.1%)	1.77	49/2128~(2.3%)	
1	Ι	1.01	3/1574~(0.2%)	1.80	47/2143~(2.2%)	
2	В	0.89	0/950	1.75	27/1285~(2.1%)	
2	Ε	0.88	0/950	1.72	24/1285~(1.9%)	
2	F	0.90	1/950~(0.1%)	1.78	26/1285~(2.0%)	
2	Н	0.96	1/944~(0.1%)	1.75	27/1277~(2.1%)	
2	J	0.88	0/938	1.79	29/1269~(2.3%)	
All	All	0.92	10/12597~(0.1%)	1.74	341/17108~(2.0%)	

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	8
1	С	0	18
1	D	0	9
1	G	0	11
1	Ι	0	19
2	В	0	7
2	Ε	0	16
2	F	0	11
2	Н	0	17
2	J	0	16
All	All	0	132

All (10) bond length outliers are listed below:



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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	G	514	SER	CA-CB	8.64	1.66	1.52
1	А	399	SER	CA-CB	7.53	1.64	1.52
1	G	406	GLU	CD-OE1	6.96	1.33	1.25
1	С	399	SER	CA-CB	6.53	1.62	1.52
1	Ι	373	SER	CA-CB	6.44	1.62	1.52
1	Ι	399	SER	CA-CB	6.16	1.62	1.52
2	F	102	SER	CA-CB	5.99	1.61	1.52
1	D	399	SER	CA-CB	5.64	1.61	1.52
2	Н	45	ARG	NE-CZ	5.57	1.40	1.33
1	Ι	406	GLU	CD-OE1	5.04	1.31	1.25

All (341) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	346	ARG	NE-CZ-NH1	14.08	127.34	120.30
1	G	346	ARG	NE-CZ-NH2	-13.18	113.71	120.30
2	Н	45	ARG	CG-CD-NE	13.03	139.16	111.80
2	Е	52	ARG	NE-CZ-NH2	12.78	126.69	120.30
2	F	32	TYR	N-CA-CB	12.60	133.28	110.60
1	G	355	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	G	346	ARG	NE-CZ-NH1	11.75	126.18	120.30
1	А	355	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	D	346	ARG	NE-CZ-NH2	11.52	126.06	120.30
2	Е	71	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	Ι	355	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	С	346	ARG	NE-CZ-NH2	-10.19	115.21	120.30
2	J	27	TYR	CB-CA-C	10.00	130.41	110.40
2	F	92	MET	CG-SD-CE	9.95	116.12	100.20
1	А	505	TYR	CB-CG-CD2	-9.95	115.03	121.00
1	Ι	408	ARG	CA-CB-CG	9.55	134.42	113.40
2	F	32	TYR	CA-CB-CG	9.39	131.24	113.40
1	С	390	LEU	CB-CG-CD1	9.26	126.74	111.00
2	Е	92	MET	CG-SD-CE	9.15	114.84	100.20
2	F	1	GLU	OE1-CD-OE2	-9.06	112.42	123.30
2	F	29	TYR	CB-CG-CD1	8.95	126.37	121.00
2	В	27	TYR	N-CA-CB	8.89	126.60	110.60
1	С	378	LYS	CD-CE-NZ	8.82	131.98	111.70
2	J	54	ASP	CB-CG-OD1	-8.82	110.36	118.30
1	A	505	TYR	CB-CG-CD1	8.78	126.27	121.00
1	D	390	LEU	CB-CG-CD1	8.60	125.62	111.00
2	Е	96	LYS	CD-CE-NZ	8.53	131.33	111.70
2	В	92	MET	CG-SD-CE	8.54	113.86	100.20
2	F	96	LYS	CD-CE-NZ	8.50	131.25	111.70



		i previo	ous page		7	Oh a survey $\mathbf{d}(0)$	$\mathbf{L} = 1(0)$
MOI	Chain	Res	Type	Atoms		Observed(°)	Ideal(°)
1	G	335	LEU	CB-CG-CD2	8.47	125.39	111.00
2	J	45	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	<u> </u>	454	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	<u> </u>	486	PHE	CA-CB-CG	8.36	133.95	113.90
2	F	53	ARG	CG-CD-NE	8.34	129.32	111.80
2	В	96	LYS	CD-CE-NZ	8.20	130.55	111.70
2	Н	52	ARG	CB-CA-C	8.18	126.77	110.40
2	J	52	ARG	CB-CA-C	8.17	126.73	110.40
1	G	408	ARG	N-CA-CB	-8.16	95.91	110.60
1	G	517	LEU	CB-CG-CD1	8.16	124.87	111.00
1	А	417	LYS	CD-CE-NZ	8.15	130.44	111.70
2	Н	71	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	G	441	LEU	CB-CG-CD1	8.08	124.74	111.00
1	А	360	ASN	CB-CA-C	8.07	126.54	110.40
1	С	408	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	G	471	GLU	OE1-CD-OE2	-8.07	113.62	123.30
1	А	444	LYS	N-CA-CB	8.02	125.03	110.60
1	Ι	412	PRO	N-CD-CG	-7.96	91.25	103.20
1	G	337	PRO	N-CA-CB	-7.96	93.75	103.30
1	С	444	LYS	CA-CB-CG	7.95	130.89	113.40
1	Ι	451	TYR	CB-CG-CD1	7.89	125.73	121.00
2	Е	52	ARG	CB-CA-C	7.87	126.14	110.40
2	J	96	LYS	CD-CE-NZ	7.86	129.78	111.70
2	Е	52	ARG	NH1-CZ-NH2	-7.82	110.79	119.40
1	С	355	ARG	NE-CZ-NH1	7.77	124.19	120.30
2	J	34	MET	CG-SD-CE	7.71	112.54	100.20
1	D	465	GLU	CB-CG-CD	7.70	134.99	114.20
2	В	52	ARG	CB-CA-C	7.70	125.79	110.40
2	F	45	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	Н	106	LEU	N-CA-CB	7.60	125.60	110.40
1	D	355	ARG	CD-NE-CZ	7.55	134.17	123.60
1	С	335	LEU	CB-CG-CD2	7.54	123.82	111.00
2	F	52	ARG	CB-CA-C	7.53	125.45	110.40
1	С	360	ASN	CB-CA-C	7.49	125.38	110.40
1	С	474	GLN	CA-CB-CG	7.48	129.85	113.40
1	G	514	SER	CB-CA-C	7.41	124.17	110.10
2	J	38	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	E	45	ARG	NE-CZ-NH1	7.35	123.97	120.30
2	 E	32	TYR	CA-CB-CG	7.33	127.33	113.40
1	 C	389	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	Ă	492	LEU	CB-CG-CD2	7.28	123.38	111.00
2	.J	32	TYR	CB-CG-CD1	7.27	125.36	121.00

. C_{α} mtin d fa



	Chain	l preud	Type	Atoms	7	$Observed(^{o})$	Ideal ⁽⁰⁾
1		454		NE CZ NU2	7.95	116.69	100 20
1	A	404	ANG	$\frac{\text{NE-CZ-NHZ}}{\text{CD-CE-NZ}}$	-1.20	110.08	120.30 111.70
	J	04 505		CA CP CC	7.92	120.00 197.12	111.70
1	A	000 456		CR-CD-CG	7.20	127.13	110.40
1		400		CD-CA-C	-1.22	95.90	110.40
1	A	300		NE CZ NU2	-1.10	90.79	111.00
1	G	408	AKG	NE-CZ-NHZ	7.18	123.89	120.30
1	G	402	LIS	UB-UG-UD	(.1)	130.23	111.00
1		355	ARG	NHI-CZ-NH2	-1.15	111.54	119.40
2	E	27	TYR	CB-CA-C	7.14	124.69	110.40
1	D	495	TYR	N-CA-CB	7.14	123.45	110.60
2	B	19	ARG	NE-CZ-NHI	7.13	123.86	120.30
2	B	64	LYS	CB-CG-CD	7.11	130.09	111.60
1	G	360	ASN	CB-CA-C	7.11	124.61	110.40
1	A	454	ARG	NE-CZ-NH1	7.07	123.83	120.30
2	B	53	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	G	355	ARG	NH1-CZ-NH2	-7.03	111.67	119.40
1	С	516	GLU	CB-CA-C	-7.03	96.35	110.40
1	С	455	LEU	CA-C-N	7.02	132.65	117.20
2	J	3	GLN	CB-CA-C	7.00	124.40	110.40
1	D	369	TYR	CA-CB-CG	6.98	126.67	113.40
1	А	369	TYR	CA-CB-CG	6.98	126.66	113.40
1	D	346	ARG	CA-CB-CG	6.97	128.74	113.40
1	G	369	TYR	CA-CB-CG	6.94	126.59	113.40
1	С	444	LYS	N-CA-CB	6.94	123.09	110.60
1	Ι	505	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	А	403	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	С	351	TYR	CB-CG-CD1	6.91	125.14	121.00
1	D	466	ARG	CD-NE-CZ	6.90	133.26	123.60
1	А	466	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	Е	78	LEU	CB-CG-CD1	6.89	122.71	111.00
1	А	355	ARG	NH1-CZ-NH2	-6.87	111.84	119.40
1	G	408	ARG	CA-CB-CG	6.85	128.47	113.40
1	А	509	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	Ι	517	LEU	CB-CG-CD1	6.80	122.57	111.00
2	В	29	TYR	CB-CG-CD1	6.78	125.07	121.00
1	G	365	TYR	CA-CB-CG	6.77	126.26	113.40
2	Н	54	ASP	CB-CG-OD1	-6.77	112.21	118.30
2	Н	106	LEU	CB-CG-CD2	6.75	122.47	111.00
2	J	73	ASN	CB-CA-C	6.75	123.90	110.40
2	J	88	GLU	N-CA-CB	6.75	122.74	110.60
1	D	505	TYR	CA-CB-CG	6.74	126.20	113.40
1	D	365	TYR	CA-CB-CG	6.73	126.19	113.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	29	TYR	CB-CG-CD1	6.73	125.04	121.00
2	F	19	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	Ε	46	GLU	CG-CD-OE1	6.67	131.65	118.30
2	J	27	TYR	N-CA-CB	-6.67	98.60	110.60
2	F	18	LEU	CB-CG-CD2	6.67	122.33	111.00
1	G	454	ARG	NE-CZ-NH1	6.63	123.62	120.30
2	В	1	GLU	CB-CG-CD	6.63	132.11	114.20
1	С	454	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	Н	18	LEU	CB-CG-CD1	6.63	122.27	111.00
2	Н	44	GLU	CB-CG-CD	6.61	132.05	114.20
2	J	92	MET	CG-SD-CE	6.61	110.77	100.20
1	Ι	505	TYR	CA-CB-CG	6.61	125.95	113.40
1	Ι	522	ALA	C-N-CA	6.59	138.17	121.70
2	J	64	LYS	CG-CD-CE	6.58	131.65	111.90
2	J	3	GLN	N-CA-CB	-6.58	98.76	110.60
2	F	75	LYS	CB-CG-CD	6.55	128.63	111.60
1	G	454	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	А	466	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	G	390	LEU	CB-CG-CD1	6.54	122.12	111.00
1	G	335	LEU	CB-CA-C	6.51	122.58	110.20
1	D	408	ARG	CB-CG-CD	6.51	128.54	111.60
2	J	45	ARG	CG-CD-NE	6.51	125.47	111.80
2	В	45	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	Ι	385	THR	CA-CB-CG2	6.50	121.50	112.40
2	В	1	GLU	OE1-CD-OE2	-6.50	115.51	123.30
2	J	88	GLU	CB-CA-C	-6.49	97.43	110.40
1	Ι	393	THR	OG1-CB-CG2	-6.48	95.10	110.00
1	Ι	400	PHE	CB-CG-CD2	-6.44	116.29	120.80
1	А	509	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	Η	92	MET	CG-SD-CE	6.44	110.50	100.20
1	D	495	TYR	CB-CA-C	-6.44	97.53	110.40
1	Ι	356	LYS	CB-CG-CD	6.43	128.32	111.60
2	Ε	102	SER	N-CA-CB	6.42	120.13	110.50
2	В	98	TRP	CB-CG-CD2	-6.42	118.25	126.60
1	G	408	ARG	CG-CD-NE	-6.42	98.31	111.80
2	Η	88	GLU	CB-CA-C	-6.40	97.59	110.40
2	В	75	LYS	CB-CG-CD	6.40	128.24	111.60
1	А	408	ARG	CA-CB-CG	6.39	127.45	113.40
2	Н	34	MET	CG-SD-CE	-6.34	90.06	100.20
1	D	463	PRO	N-CA-CB	-6.33	95.64	102.60
1	Ι	341	VAL	N-CA-CB	6.32	125.40	111.50
1	Ι	369	TYR	N-CA-CB	6.31	121.96	110.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	378	LYS	CA-CB-CG	6.31	127.28	113.40
2	F	88	GLU	CB-CA-C	-6.29	97.82	110.40
1	Ι	350	VAL	CB-CA-C	-6.29	99.45	111.40
1	G	378	LYS	CG-CD-CE	6.28	130.75	111.90
1	С	466	ARG	CD-NE-CZ	6.28	132.39	123.60
1	Ι	495	TYR	CB-CA-C	-6.26	97.87	110.40
2	В	18	LEU	CB-CG-CD2	6.25	121.63	111.00
1	С	454	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	Н	88	GLU	N-CA-CB	6.23	121.81	110.60
2	J	115	THR	OG1-CB-CG2	6.23	124.32	110.00
1	Ι	444	LYS	CB-CA-C	6.22	122.84	110.40
2	Е	61	ASP	CB-CA-C	6.22	122.83	110.40
2	В	45	ARG	CG-CD-NE	6.22	124.86	111.80
1	G	415	THR	CA-CB-OG1	-6.21	95.97	109.00
1	D	408	ARG	CD-NE-CZ	6.20	132.28	123.60
2	В	30	CYS	CA-CB-SG	6.20	125.15	114.00
1	G	495	TYR	CB-CA-C	-6.19	98.02	110.40
2	Н	46	GLU	CA-CB-CG	6.19	127.01	113.40
1	С	365	TYR	CA-CB-CG	6.18	125.14	113.40
2	В	59	TYR	CB-CG-CD2	6.16	124.70	121.00
1	Ι	376	THR	OG1-CB-CG2	6.15	124.15	110.00
2	F	44	GLU	CG-CD-OE1	-6.15	106.00	118.30
2	Н	44	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	А	334	ASN	CB-CA-C	6.13	122.67	110.40
2	Н	27	TYR	CB-CA-C	6.12	122.65	110.40
2	Н	105	TYR	N-CA-CB	6.12	121.61	110.60
1	G	514	SER	N-CA-CB	-6.11	101.33	110.50
1	С	369	TYR	CA-CB-CG	6.11	125.00	113.40
2	F	71	ARG	CG-CD-NE	6.06	124.52	111.80
1	Ι	509	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	J	33	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	G	471	GLU	CG-CD-OE1	6.04	130.37	118.30
1	Ι	462	LYS	CB-CG-CD	6.03	127.29	111.60
1	С	509	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	D	403	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	G	341	VAL	N-CA-CB	5.99	124.68	111.50
1	Ι	444	LYS	CB-CG-CD	5.97	127.12	111.60
2	Н	32	TYR	CA-CB-CG	5.95	124.71	113.40
2	F	1	GLU	CB-CG-CD	5.95	130.27	114.20
1	D	444	LYS	CB-CA-C	5.95	122.29	110.40
1	Ι	369	TYR	CA-CB-CG	5.94	124.69	113.40
1	А	495	TYR	CB-CA-C	-5.92	98.57	110.40



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	Chain	Res	Type	Atoms		Observed(°)	10eal(°)
1	C	457	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	G	517	LEU	CB-CA-C	5.86	121.34	110.20
1	l	500	THR	CA-CB-CG2	5.86	120.61	112.40
1	C	351	TYR	CB-CA-C	-5.86	98.68	110.40
2	F'	88	GLU	N-CA-CB	5.86	121.14	110.60
1	A	365	TYR	CA-CB-CG	5.85	124.52	113.40
1	C	341	VAL	N-CA-CB	5.85	124.38	111.50
1	1	403	ARG	CA-CB-CG	5.84	126.25	113.40
1	D	351	TYR	CB-CA-C	-5.83	98.73	110.40
2	В	59	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	G	417	LYS	CA-CB-CG	5.79	126.14	113.40
1	D	471	GLU	CB-CG-CD	5.79	129.82	114.20
1	G	469	SER	CB-CA-C	-5.78	99.11	110.10
1	G	495	TYR	N-CA-CB	5.77	120.98	110.60
1	С	471	GLU	N-CA-CB	5.76	120.97	110.60
1	С	408	ARG	CB-CA-C	5.76	121.92	110.40
1	G	356	LYS	CA-CB-CG	5.74	126.02	113.40
2	Ε	18	LEU	CB-CG-CD2	5.73	120.73	111.00
2	J	98	TRP	CB-CG-CD2	-5.72	119.17	126.60
2	J	32	TYR	CA-CB-CG	5.71	124.26	113.40
1	А	469	SER	CB-CA-C	-5.70	99.26	110.10
1	С	417	LYS	CB-CG-CD	5.70	126.42	111.60
2	Н	98	TRP	CB-CG-CD2	-5.67	119.22	126.60
1	G	403	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	А	385	THR	CA-CB-OG1	-5.67	97.10	109.00
1	Ι	346	ARG	NE-CZ-NH1	-5.67	117.47	120.30
2	F	66	ARG	CD-NE-CZ	5.66	131.52	123.60
2	J	45	ARG	NH1-CZ-NH2	-5.66	113.18	119.40
1	Ι	408	ARG	CD-NE-CZ	5.65	131.51	123.60
1	С	378	LYS	CA-CB-CG	5.65	125.83	113.40
2	Н	27	TYR	N-CA-CB	-5.63	100.46	110.60
1	Ι	458	LYS	CD-CE-NZ	5.63	124.66	111.70
1	D	341	VAL	N-CA-CB	5.63	123.88	111.50
2	Е	88	GLU	CB-CA-C	-5.61	99.18	110.40
1	А	341	VAL	N-CA-CB	5.61	123.83	111.50
1	А	462	LYS	CB-CG-CD	5.59	126.14	111.60
2	Е	29	TYR	CB-CG-CD1	5.59	124.35	121.00
1	А	441	LEU	CA-CB-CG	5.58	128.14	115.30
2	В	88	GLU	CB-CA-C	-5.58	99.24	110.40
2	J	13	GLN	CB-CA-C	5.57	121.54	110.40
1	G	376	THR	CA-CB-CG2	5.53	120.15	112.40
2	Е	86	GLU	CG-CD-OE2	-5.53	107.24	118.30

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	Chain	Res	Type	Atoms	7	Observed $(^{o})$	Ideal(°)
2	Ц	45	ARC	NF C7 NH1	5 59	117 54	120.30
	C II	40	LVS	$\frac{\text{RE-CZ-RIII}}{\text{CR-CA-C}}$	-0.02	191 44	120.30
1		444	TVR	N CA CB	5.52	121.44	110.40
1		380	VAL	CA CB CC1	5.51	120.00	110.00
$\frac{1}{2}$	E E	45	ARC	CG CD NE	5.51	119.17	110.90
 1	r C	40		CD CE NZ	5.51	123.37	111.00 111.70
1		417	CIU	N CA CB	5.51	124.57	111.70
1	A C	385	U THR	CA CB OC1	5.50	07.46	100.00
1	B	00		CR-CD-OGI	-5.00		109.00 127.00
 1	D I	90 451	TVP	CE1 CZ OH	5.49	134.13	127.00
1	I F	21	SED	N CA CB	5.40	118 79	120.10 110.50
	Ц Ц	51	APC	NF CZ NH1	5.40	110.72	110.30 120.20
2	E II	52	IVG	$\frac{\text{NE-CZ-NIII}}{\text{CP CC CD}}$	5.46	125.03	120.30 111.60
	Г D	105		N CA CD	5.40	120.79	111.00
	D	105	IIR	CD CE NZ	5.40	120.30	110.00 111.70
1	D	417		N CA CD	5.45	124.20	111.70
1		020 205		N-CA-CD	5.45	07.61	110.30
1	D	380		CA-CD-OGI	-0.42	97.01	109.00
		495		CB-CA-C	$\begin{array}{c c c c c c c c c c c c c c c c c c c $		110.40
2	F A	98		UB-UG-UD2	-5.41	119.57	120.00
1	A	417		N-CA-CB	5.40	120.32	110.60
	C	385	THR	CA-CB-OGI	-5.40	97.66	109.00
1	U I	455	LEU	N-CA-CB	-5.40	99.01	110.40
	I C	458	LYS	CB-CG-CD	5.39	125.63	111.60
	C	469	SER	CB-CA-C	-5.39	99.85	110.10
1	l T	505	TYR	CB-CG-CDI	5.39	124.24	121.00
2	F'	99	ALA	CB-CA-C	5.38	118.17	110.10
		421	TYR	CB-CG-CDI	5.37	124.22	121.00
2	В	45	ARG	NHI-CZ-NH2	-5.36	113.50	119.40
1	A	378	LYS	CA-CB-CG	5.36	125.18	113.40
	G	376	THR	OGI-CB-CG2	-5.34	97.72	110.00
1	D	335	LEU	CA-CB-CG	5.34	127.58	115.30
1	G	335	LEU	O-C-N	-5.34	114.16	122.70
2	F'	71	ARG	CB-CG-CD	5.33	125.47	111.60
2	H	73	ASN	CB-CA-C	-5.32	99.76	110.40
2	E	34	MET	CG-SD-CE	-5.32	91.69	100.20
2	F	44	GLU	CB-CA-C	5.31	121.03	110.40
2	E	98	TRP	CB-CG-CD2	-5.30	119.71	126.60
1	Ι	470	THR	CB-CA-C	5.29	125.88	111.60
1	С	380	TYR	CA-CB-CG	5.28	123.44	113.40
1	С	417	LYS	N-CA-CB	5.28	120.09	110.60
2	E	46	GLU	CG-CD-OE2	-5.27	107.75	118.30
1	А	492	LEU	CB-CG-CD1	-5.27	102.04	111.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	517	LEU	CB-CA-C	5.26	120.20	110.20
1	С	441	LEU	CB-CG-CD2	5.26	119.94	111.00
1	А	466	ARG	CD-NE-CZ	5.25	130.96	123.60
2	F	58	ALA	CB-CA-C	5.24	117.97	110.10
1	С	357	ARG	CG-CD-NE	-5.23	100.82	111.80
2	Н	28	THR	CA-C-O	-5.22	109.13	120.10
2	В	88	GLU	N-CA-CB	5.22	119.99	110.60
2	В	32	TYR	CA-CB-CG	5.21	123.30	113.40
1	Ι	405	ASP	CB-CA-C	5.21	120.82	110.40
1	Ι	445	VAL	N-CA-CB	-5.21	100.03	111.50
1	G	352	ALA	N-CA-CB	-5.21	102.81	110.10
1	С	466	ARG	CA-CB-CG	5.20	124.84	113.40
2	J	75	LYS	CB-CA-C	5.20	120.80	110.40
2	В	45	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	Ι	380	TYR	CA-C-N	5.19	126.58	116.20
2	Е	61	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	Н	71	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	G	351	TYR	N-CA-CB	5.15	119.88	110.60
1	С	456	PHE	N-CA-C	5.15	124.90	111.00
2	Н	1	GLU	CB-CA-C	5.15	120.69	110.40
2	В	29	TYR	N-CA-CB	-5.14	101.34	110.60
2	Е	45	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
2	F	30	CYS	N-CA-CB	-5.13	101.37	110.60
1	Ι	346	ARG	CG-CD-NE	-5.12	101.04	111.80
1	G	406	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	G	351	TYR	CB-CA-C	-5.12	100.17	110.40
1	А	417	LYS	CB-CA-C	-5.11	100.17	110.40
1	С	455	LEU	CA-C-O	-5.10	109.39	120.10
1	D	505	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	А	356	LYS	CA-CB-CG	5.10	124.61	113.40
1	С	369	TYR	N-CA-CB	5.09	119.76	110.60
1	С	406	GLU	CG-CD-OE1	5.09	128.48	118.30
1	G	466	ARG	CD-NE-CZ	5.08	130.72	123.60
1	Ι	337	PRO	N-CA-CB	-5.08	97.01	102.60
2	J	104	GLU	CG-CD-OE2	-5.08	108.15	118.30
1	С	451	TYR	N-CA-CB	5.07	119.72	110.60
1	С	351	TYR	CE1-CZ-OH	5.07	133.78	120.10
1	Ι	351	TYR	CB-CA-C	-5.07	100.26	110.40
1	D	454	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	G	527	PRO	N-CA-C	5.07	125.27	112.10
1	D	352	ALA	N-CA-CB	-5.07	103.01	110.10
1	С	518	LEU	CB-CG-CD2	5.06	119.60	111.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Ι	345	THR	CA-CB-OG1	-5.06	98.38	109.00
1	D	415	THR	CA-CB-OG1	-5.06	98.38	109.00
2	J	67	PHE	CB-CG-CD2	-5.05	117.26	120.80
1	Ι	406	GLU	CG-CD-OE1	5.05	128.40	118.30
1	С	489	TYR	CB-CG-CD1	5.05	124.03	121.00
2	Н	67	PHE	CB-CG-CD2	-5.05	117.27	120.80
1	Ι	415	THR	CA-CB-OG1	-5.04	98.41	109.00
2	В	106	LEU	CB-CG-CD2	5.04	119.57	111.00
1	G	448	ASN	CB-CA-C	5.04	120.49	110.40
1	G	471	GLU	CB-CG-CD	5.04	127.81	114.20
1	С	345	THR	CA-CB-OG1	-5.04	98.42	109.00
2	J	60	THR	OG1-CB-CG2	5.04	121.59	110.00
1	Ι	466	ARG	CA-CB-CG	5.04	124.48	113.40
1	Ι	451	TYR	OH-CZ-CE2	-5.02	106.54	120.10
2	Е	71	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	A	403	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	С	368	LEU	CB-CG-CD2	5.00	119.50	111.00
2	J	44	GLU	CG-CD-OE2	-5.00	108.29	118.30

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	348	ALA	Peptide
1	А	355	ARG	Peptide
1	А	356	LYS	Peptide
1	А	357	ARG	Sidechain
1	А	372	ALA	Peptide
1	А	466	ARG	Sidechain
1	А	470	THR	Peptide
1	А	525	CYS	Peptide
2	В	119	VAL	Peptide
2	В	2	VAL	Peptide
2	В	24	ALA	Peptide
2	В	40	ALA	Peptide
2	В	41	PRO	Peptide
2	В	52	ARG	Sidechain
2	В	57	THR	Peptide
1	С	343	ASN	Mainchain
1	С	346	ARG	Sidechain
1	С	348	ALA	Peptide
1	С	351	TYR	Sidechain



Mol	Chain	Res	Type	Group
1	С	354	ASN	Sidechain
1	С	355	ARG	Peptide
1	С	356	LYS	Peptide
1	С	357	ARG	Sidechain
1	С	372	ALA	Peptide
1	С	385	THR	Peptide
1	С	390	LEU	Peptide
1	С	403	ARG	Sidechain
1	С	408	ARG	Sidechain
1	С	466	ARG	Sidechain
1	С	518	LEU	Mainchain,Peptide
1	С	520	ALA	Peptide
1	С	525	CYS	Peptide
1	D	346	ARG	Sidechain
1	D	355	ARG	Peptide
1	D	356	LYS	Peptide
1	D	372	ALA	Peptide
1	D	408	ARG	Sidechain
1	D	446	GLY	Peptide
1	D	466	ARG	Sidechain
1	D	476	GLY	Peptide
1	D	525	CYS	Peptide
2	Е	101	SER	Peptide
2	Е	103	GLY	Peptide
2	Е	106	LEU	Mainchain
2	Е	109	GLY	Mainchain
2	Е	2	VAL	Peptide
2	Е	24	ALA	Peptide
2	Е	25	SER	Peptide
2	Е	26	GLY	Peptide
2	Е	29	TYR	Peptide
2	Е	30	CYS	Peptide
2	Е	40	ALA	Peptide
2	Е	41	PRO	Peptide
2	Е	52	ARG	Sidechain
2	Е	53	ARG	Sidechain
2	Е	57	THR	Peptide
2	Е	81	GLN	Sidechain
2	F	19	ARG	Sidechain
2	F	27	TYR	Peptide
2	F	29	TYR	Mainchain,Peptide
2	F	30	CYS	Peptide

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Mol	Chain	Res	Type	Group
2	F	40	ALA	Peptide
2	F	41	PRO	Peptide
2	F	52	ARG	Sidechain
2	F	53	ARG	Sidechain
2	F	57	THR	Peptide
2	F	71	ARG	Sidechain
1	G	335	LEU	Peptide
1	G	346	ARG	Sidechain
1	G	348	ALA	Peptide
1	G	356	LYS	Peptide
1	G	357	ARG	Sidechain
1	G	372	ALA	Peptide
1	G	408	ARG	Sidechain
1	G	446	GLY	Peptide
1	G	466	ARG	Sidechain
1	G	496	GLY	Mainchain
1	G	525	CYS	Peptide
2	Н	101	SER	Peptide
2	Н	102	SER	Peptide
2	Н	106	LEU	Mainchain
2	Н	19	ARG	Sidechain
2	Н	2	VAL	Peptide
2	Н	24	ALA	Peptide
2	Н	28	THR	Mainchain,Peptide
2	Н	29	TYR	Peptide
2	Н	30	CYS	Peptide
2	Н	40	ALA	Peptide
2	Н	41	PRO	Peptide
2	Н	45	ARG	Sidechain
2	Н	52	ARG	Sidechain
2	Н	53	ARG	Sidechain
2	Н	57	THR	Peptide
2	Н	99	ALA	Peptide
1	Ι	346	ARG	Sidechain
1	Ι	355	ARG	Sidechain,Peptide
1	Ι	356	LYS	Peptide
1	Ι	372	ALA	Peptide
1	Ι	381	GLY	Peptide
1	Ι	385	THR	Peptide
1	Ι	388	ASN	Peptide
1	Ι	449	TYR	Peptide
1	Ι	466	ARG	Sidechain

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Mol	Chain	\mathbf{Res}	Type	Group
1	Ι	469	SER	Peptide
1	Ι	471	GLU	Peptide
1	Ι	476	GLY	Peptide
1	Ι	516	GLU	Peptide
1	Ι	518	LEU	Peptide
1	Ι	521	PRO	Peptide
1	Ι	522	ALA	Peptide
1	Ι	525	CYS	Peptide
1	Ι	526	GLY	Peptide
2	J	101	SER	Mainchain,Peptide
2	J	11	SER	Peptide
2	J	17	SER	Peptide
2	J	19	ARG	Sidechain
2	J	24	ALA	Peptide
2	J	25	SER	Peptide
2	J	26	GLY	Peptide
2	J	30	CYS	Peptide
2	J	38	ARG	Sidechain
2	J	40	ALA	Peptide
2	J	41	PRO	Peptide
2	J	53	ARG	Sidechain
2	J	57	THR	Peptide
2	J	71	ARG	Sidechain
2	J	73	ASN	Peptide

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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	1528	0	1443	12	0
1	С	1530	0	1444	11	0
1	D	1540	0	1460	11	0
1	G	1520	0	1437	16	0
1	Ι	1531	0	1446	25	0
2	В	931	0	864	4	0
2	Ε	931	0	864	3	0
2	F	931	0	864	3	0
2	Н	925	0	859	6	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	919	0	854	6	0
3	Κ	28	0	25	0	0
3	L	28	0	25	0	0
3	М	28	0	25	0	0
4	А	14	0	13	0	0
4	D	14	0	13	0	0
All	All	12398	0	11636	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (90) 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:I:361:CYS:SG	1:I:362:VAL:N	2.45	0.90
1:I:382:VAL:HG11	1:I:387:LEU:HD23	1.61	0.81
1:C:380:TYR:CE2	1:C:412:PRO:HD2	2.25	0.71
1:A:380:TYR:CE2	1:A:412:PRO:HD2	2.24	0.71
1:I:401:VAL:HG11	1:I:451:TYR:CD2	2.27	0.70
1:G:380:TYR:CE2	1:G:412:PRO:HD2	2.27	0.70
1:C:350:VAL:HG23	1:C:400:PHE:CD2	2.29	0.68
2:H:101:SER:HB2	2:H:106:LEU:HA	1.79	0.65
1:G:350:VAL:HG23	1:G:400:PHE:CD2	2.33	0.64
1:G:392:PHE:HA	1:G:517:LEU:HD13	1.83	0.61
1:I:387:LEU:O	1:I:388:ASN:HB2	2.02	0.60
1:A:346:ARG:HH22	1:A:450:ASN:HB3	1.70	0.56
1:C:382:VAL:CG1	1:C:387:LEU:HD23	2.36	0.55
1:G:342:PHE:CE1	1:G:511:VAL:HG21	2.42	0.55
1:A:468:ILE:HG22	1:A:468:ILE:O	2.07	0.54
2:J:87:PRO:HA	2:J:119:VAL:HB	1.90	0.53
1:G:520:ALA:HB1	1:G:521:PRO:HD2	1.91	0.53
1:A:350:VAL:HG23	1:A:400:PHE:CD1	2.44	0.53
1:A:342:PHE:CE1	1:A:511:VAL:HG21	2.44	0.52
2:J:30:CYS:SG	2:J:101:SER:O	2.67	0.52
1:A:492:LEU:HD12	2:B:98:TRP:CZ3	2.45	0.52
1:I:362:VAL:O	1:I:525:CYS:O	2.28	0.52
1:D:402:ILE:HD13	1:D:410:ILE:HD11	1.91	0.52
1:G:342:PHE:CZ	1:G:511:VAL:HG11	2.45	0.51
1:G:354:ASN:HA	2:H:106:LEU:HD12	1.93	0.50
1:I:477:SER:O	1:I:478:THR:HG23	2.11	0.50
2:F:31:SER:CB	2:F:53:ARG:HD2	2.42	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:101:SER:HB2	2:H:106:LEU:HD23	1.94	0.50
1:G:434:ILE:N	1:G:434:ILE:HD12	2.27	0.49
1:I:492:LEU:HD12	2:J:98:TRP:CZ3	2.48	0.49
2:E:53:ARG:NH2	1:D:374:PHE:O	2.45	0.48
1:D:434:ILE:HD12	1:D:434:ILE:N	2.29	0.48
1:D:476:GLY:HA3	1:D:478:THR:HG22	1.95	0.48
1:G:483:VAL:HA	2:H:59:TYR:O	2.13	0.48
1:A:441:LEU:HD12	1:A:509:ARG:NH2	2.29	0.48
1:I:426:PRO:HD3	1:I:464:PHE:CE1	2.49	0.47
1:I:364:ASP:HA	1:I:388:ASN:OD1	2.13	0.47
1:I:434:ILE:HD12	1:I:434:ILE:N	2.29	0.47
2:F:52:ARG:O	2:F:71:ARG:NH2	2.47	0.47
1:I:387:LEU:O	1:I:388:ASN:CB	2.63	0.47
2:E:96:LYS:HE2	2:E:97:SER:O	2.15	0.47
1:A:434:ILE:HD12	1:A:434:ILE:N	2.30	0.47
1:G:380:TYR:CE2	1:G:412:PRO:CD	2.96	0.47
2:B:87:PRO:HA	2:B:119:VAL:HB	1.96	0.47
1:G:468:ILE:HG22	1:G:468:ILE:O	2.14	0.46
1:I:444:LYS:HA	1:I:444:LYS:CE	2.45	0.46
1:I:382:VAL:CG1	1:I:387:LEU:HD23	2.40	0.46
1:D:350:VAL:HG23	1:D:400:PHE:CD1	2.51	0.46
1:D:520:ALA:HB1	1:D:521:PRO:CD	2.46	0.46
2:B:96:LYS:HE2	2:B:97:SER:O	2.16	0.46
1:I:335:LEU:HA	1:I:362:VAL:HG22	1.97	0.46
2:H:87:PRO:HA	2:H:119:VAL:HB	1.98	0.45
1:D:475:ALA:HB3	1:D:487:ASN:HA	1.98	0.45
1:I:410:ILE:HG22	1:I:433:VAL:HG11	1.99	0.45
1:I:461:LEU:HD22	1:I:465:GLU:HG2	1.98	0.45
1:I:520:ALA:HB1	1:I:521:PRO:CD	2.47	0.45
1:D:369:TYR:CE2	1:D:384:PRO:O	2.70	0.45
1:C:377:PHE:CE2	1:C:434:ILE:HD11	2.52	0.45
1:D:461:LEU:HD22	1:D:465:GLU:HG2	1.98	0.44
2:F:87:PRO:HA	2:F:119:VAL:HB	1.99	0.44
1:G:468:ILE:O	1:G:468:ILE:CG2	2.66	0.44
1:G:369:TYR:CE2	1:G:384:PRO:O	2.71	0.44
1:D:335:LEU:O	1:D:361:CYS:HB2	2.18	0.44
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.48	0.43
2:E:87:PRO:HA	2:E:119:VAL:HB	2.01	0.43
1:G:365:TYR:CD1	1:G:387:LEU:HD13	2.54	0.43
1:I:355:ARG:NH2	1:I:464:PHE:CD2	2.87	0.43
1:C:369:TYR:CE2	1:C:384:PRO:O	2.72	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:108:GLN:OE1	2:B:108:GLN:HA	2.18	0.43
1:I:474:GLN:O	1:I:474:GLN:HG3	2.19	0.43
1:I:484:GLU:O	2:J:61:ASP:HB2	2.18	0.42
1:I:352:ALA:O	2:J:108:GLN:NE2	2.52	0.42
1:C:350:VAL:HG23	1:C:400:PHE:CE2	2.54	0.42
1:C:425:LEU:HD21	1:C:512:VAL:HG11	2.02	0.42
1:I:410:ILE:HG22	1:I:433:VAL:CG1	2.49	0.42
1:I:444:LYS:HE2	1:I:445:VAL:HG22	2.02	0.42
1:A:369:TYR:CE2	1:A:384:PRO:O	2.73	0.42
1:A:380:TYR:CE2	1:A:412:PRO:CD	3.00	0.42
1:C:382:VAL:HG13	1:C:387:LEU:HD23	2.02	0.42
1:C:375:SER:OG	1:C:376:THR:N	2.53	0.41
2:J:96:LYS:HE2	2:J:97:SER:O	2.20	0.41
1:D:351:TYR:O	1:D:466:ARG:HG3	2.20	0.41
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.55	0.41
1:C:410:ILE:HD11	1:C:418:ILE:HG21	2.03	0.41
1:I:402:ILE:HD11	1:I:407:VAL:HG12	2.03	0.41
1:G:520:ALA:HB1	1:G:521:PRO:CD	2.50	0.40
1:C:410:ILE:HG22	1:C:433:VAL:HG11	2.04	0.40
1:I:425:LEU:HD21	1:I:512:VAL:HG11	2.02	0.40
1:G:425:LEU:HD21	1:G:512:VAL:HG11	2.04	0.40
2:H:101:SER:CB	2:H:106:LEU:HA	2.49	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	Perc	entiles
1	А	192/221~(87%)	160 (83%)	29 (15%)	3 (2%)	8	37
1	С	192/221~(87%)	163~(85%)	24 (12%)	5 (3%)	4	29
1	D	193/221~(87%)	162 (84%)	25~(13%)	6 (3%)	3	27



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erc	entiles
1	G	191/221~(86%)	161 (84%)	25~(13%)	5 (3%)		4	29
1	Ι	192/221~(87%)	153 (80%)	29 (15%)	10 (5%)		1	18
2	В	119/146~(82%)	107 (90%)	8 (7%)	4 (3%)		3	26
2	E	119/146~(82%)	105 (88%)	9 (8%)	5 (4%)		2	21
2	F	119/146~(82%)	102 (86%)	11 (9%)	6 (5%)		1	18
2	Н	118/146~(81%)	105 (89%)	9 (8%)	4 (3%)		3	26
2	J	117/146~(80%)	104 (89%)	8 (7%)	5 (4%)		2	20
All	All	1552/1835~(85%)	1322 (85%)	177 (11%)	53 (3%)		3	26

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All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	445	VAL
1	С	456	PHE
2	Е	40	ALA
1	А	445	VAL
2	В	40	ALA
2	F	31	SER
2	F	32	TYR
2	F	40	ALA
1	G	445	VAL
2	Н	40	ALA
1	Ι	445	VAL
2	J	14	ALA
2	J	26	GLY
2	J	40	ALA
2	J	102	SER
1	D	445	VAL
1	D	463	PRO
1	С	375	SER
2	Е	102	SER
1	А	375	SER
2	F	104	GLU
1	G	375	SER
1	G	417	LYS
2	Н	106	LEU
2	Н	107	TYR
1	Ι	363	ALA
1	Ι	375	SER
1	Ι	388	ASN



Mol	Chain	Res	Type
1	Ι	417	LYS
1	Ι	470	THR
1	Ι	523	THR
1	D	375	SER
1	D	417	LYS
2	Е	2	VAL
2	Е	91	ALA
2	В	91	ALA
2	F	91	ALA
2	F	102	SER
2	Н	91	ALA
2	J	91	ALA
1	D	408	ARG
1	С	337	PRO
1	С	455	LEU
2	Е	30	CYS
1	А	337	PRO
2	В	104	GLU
1	Ι	478	THR
1	D	337	PRO
2	В	106	LEU
1	G	408	ARG
1	Ι	475	ALA
1	G	337	PRO
1	Ι	471	GLU

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perc	entiles
1	А	165/193~(86%)	147 (89%)	18 (11%)	5	24
1	С	165/193~(86%)	145 (88%)	20 (12%)	4	20
1	D	167/193~(86%)	141 (84%)	26 (16%)	2	14
1	G	164/193~(85%)	145 (88%)	19~(12%)	4	22
1	Ι	166/193~(86%)	142 (86%)	24 (14%)	2	16



Mol	Chain	Analysed	Rotameric	Outliers	P	erc	entiles
2	В	98/117~(84%)	85 (87%)	13~(13%)		3	18
2	Ε	98/117~(84%)	83~(85%)	15~(15%)		2	14
2	F	98/117~(84%)	84 (86%)	14 (14%)		2	16
2	Н	97/117~(83%)	85 (88%)	12 (12%)		4	20
2	J	96/117~(82%)	81 (84%)	15~(16%)		2	14
All	All	1314/1550~(85%)	1138 (87%)	176 (13%)		3	18

All (176) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	С	334	ASN
1	С	337	PRO
1	С	346	ARG
1	С	347	PHE
1	С	349	SER
1	С	351	TYR
1	С	354	ASN
1	С	359	SER
1	С	375	SER
1	С	380	TYR
1	С	389	ASP
1	С	399	SER
1	С	410	ILE
1	С	417	LYS
1	С	434	ILE
1	С	484	GLU
1	С	494	SER
1	С	513	LEU
1	С	514	SER
1	С	524	VAL
2	Е	1	GLU
2	Е	5	VAL
2	Е	18	LEU
2	Е	27	TYR
2	Е	30	CYS
2	Е	32	TYR
2	Е	33	ASP
2	Е	44	GLU
2	Е	53	ARG
2	Е	54	ASP



Mol	Chain	Res	Type
2	Е	61	ASP
2	Е	86	GLU
2	Е	92	MET
2	Е	106	LEU
2	Е	108	GLN
1	А	337	PRO
1	А	346	ARG
1	А	347	PHE
1	А	351	TYR
1	А	368	LEU
1	А	380	TYR
1	А	389	ASP
1	А	399	SER
1	А	408	ARG
1	А	417	LYS
1	А	441	LEU
1	А	444	LYS
1	А	450	ASN
1	А	462	LYS
1	А	468	ILE
1	А	481	ASN
1	А	484	GLU
1	А	516	GLU
2	В	18	LEU
2	В	30	CYS
2	В	32	TYR
2	В	33	ASP
2	В	53	ARG
2	В	54	ASP
2	В	64	LYS
2	В	71	ARG
2	В	86	GLU
2	В	92	MET
2	В	106	LEU
2	В	108	GLN
2	В	118	THR
2	F	13	GLN
2	F	18	LEU
2	F	25	SER
2	F	27	TYR
2	F	29	TYR
2	F	30	CYS



Mol	Chain	Res	Type
2	F	33	ASP
2	F	41	PRO
2	F	53	ARG
2	F	54	ASP
2	F	71	ARG
2	F	92	MET
2	F	96	LYS
2	F	118	THR
1	G	335	LEU
1	G	337	PRO
1	G	345	THR
1	G	347	PHE
1	G	351	TYR
1	G	354	ASN
1	G	370	ASN
1	G	376	THR
1	G	380	TYR
1	G	389	ASP
1	G	399	SER
1	G	417	LYS
1	G	448	ASN
1	G	450	ASN
1	G	474	GLN
1	G	481	ASN
1	G	484	GLU
1	G	516	GLU
1	G	527	PRO
2	Н	30	CYS
2	Н	32	TYR
2	Н	33	ASP
2	Н	45	ARG
2	Н	53	ARG
2	Н	54	ASP
2	Н	71	ARG
2	Н	86	GLU
2	Н	92	MET
2	Н	96	LYS
2	Н	106	LEU
2	Н	118	THR
1	Ι	334	ASN
1	Ι	337	PRO
1	Ι	338	PHE



Mol	Chain	Res	Type	
1	Ι	347	PHE	
1	Ι	350	VAL	
1	Ι	351	TYR	
1	Ι	354	ASN	
1	Ι	361	CYS	
1	Ι	367	VAL	
1	Ι	371	SER	
1	Ι	389	ASP	
1	Ι	399	SER	
1	Ι	403	ARG	
1	Ι	427	ASP	
1	Ι	444	LYS	
1	Ι	448	ASN	
1	Ι	450	ASN	
1	Ι	458	LYS	
1	Ι	462	LYS	
1	Ι	472	ILE	
1	Ι	478	THR	
1	Ι	505	TYR	
1	Ι	516	GLU	
1	Ι	523	THR	
2	J	3	GLN	
2	J	5	VAL	
2	J	13	GLN	
2	J	21	SER	
2	J	30	CYS	
2	J	32	TYR	
2	J	33	ASP	
2	J	54	ASP	
2	J	60	THR	
2	J	64	LYS	
2	J	73	ASN	
2	J	86	GLU	
2	J	92	MET	
2	J	96	LYS	
2	J	118	THR	
1	D	334	ASN	
1	D	336	CYS	
1	D	337	PRO	
1	D	345	THR	
1	D	347	PHE	
1	D	351	TYR	



Mol	Chain	Res	Type
1	D	358	ILE
1	D	365	TYR
1	D	373	SER
1	D	380	TYR
1	D	386	LYS
1	D	389	ASP
1	D	399	SER
1	D	424	LYS
1	D	427	ASP
1	D	448	ASN
1	D	450	ASN
1	D	463	PRO
1	D	474	GLN
1	D	481	ASN
1	D	484	GLU
1	D	500	THR
1	D	505	TYR
1	D	514	SER
1	D	516	GLU
1	D	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	474	GLN
2	Е	108	GLN
1	А	501	ASN
1	G	501	ASN
1	Ι	501	ASN
2	J	13	GLN
2	J	108	GLN
1	D	501	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)

6 monosaccharides 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	Mol Type Chain	Dec	os Link	Bo	Bond lengths			Bond angles		
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	NAG	К	1	3	14,14,15	2.54	4 (28%)	17,19,21	4.25	6 (35%)
3	NAG	К	2	3	14,14,15	2.16	3 (21%)	17,19,21	4.30	10 (58%)
3	NAG	L	1	3,1	14,14,15	1.89	1 (7%)	17,19,21	<mark>3.64</mark>	8 (47%)
3	NAG	L	2	3	14,14,15	1.24	2 (14%)	17,19,21	1.99	5 (29%)
3	NAG	М	1	3,1	14,14,15	0.77	0	17,19,21	2.70	10 (58%)
3	NAG	М	2	3	14,14,15	0.79	0	17,19,21	1.95	2 (11%)

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	NAG	К	1	3	-	3/6/23/26	0/1/1/1
3	NAG	К	2	3	-	6/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	L	2	3	-	6/6/23/26	0/1/1/1
3	NAG	М	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	М	2	3	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	Κ	1	NAG	O4-C4	7.70	1.61	1.43
3	Κ	2	NAG	C1-C2	6.90	1.62	1.52
3	L	1	NAG	O4-C4	5.14	1.55	1.43
3	L	2	NAG	C1-C2	3.63	1.57	1.52
3	Κ	1	NAG	O5-C5	2.39	1.48	1.43
3	Κ	2	NAG	C2-N2	2.21	1.50	1.46



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$				
3	K	2	NAG	C3-C2	2.20	1.57	1.52				
3	K	1	NAG	C3-C2	2.16	1.57	1.52				
3	K	1	NAG	C1-C2	2.13	1.55	1.52				
3	L	2	NAG	C3-C2	2.02	1.56	1.52				

All (41) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	K	1	NAG	C1-O5-C5	12.48	129.10	112.19
3	K	2	NAG	C1-C2-N2	11.53	130.19	110.49
3	L	1	NAG	C2-N2-C7	8.95	135.65	122.90
3	L	1	NAG	C1-O5-C5	8.43	123.61	112.19
3	К	1	NAG	C2-N2-C7	8.01	134.31	122.90
3	K	2	NAG	C1-O5-C5	6.85	121.47	112.19
3	K	2	NAG	C2-N2-C7	6.63	132.35	122.90
3	К	1	NAG	C4-C3-C2	5.71	119.38	111.02
3	М	2	NAG	C2-N2-C7	5.67	130.97	122.90
3	К	2	NAG	O3-C3-C2	5.55	120.95	109.47
3	М	1	NAG	C1-O5-C5	5.48	119.61	112.19
3	L	1	NAG	C4-C3-C2	4.70	117.91	111.02
3	М	1	NAG	C1-C2-N2	4.43	118.06	110.49
3	K	1	NAG	O4-C4-C3	4.34	120.39	110.35
3	K	1	NAG	O3-C3-C2	-3.93	101.34	109.47
3	L	2	NAG	C2-N2-C7	3.88	128.43	122.90
3	М	1	NAG	O5-C1-C2	-3.78	105.31	111.29
3	L	1	NAG	O3-C3-C2	-3.70	101.82	109.47
3	K	2	NAG	O5-C1-C2	-3.64	105.53	111.29
3	L	1	NAG	C1-C2-N2	3.50	116.47	110.49
3	K	2	NAG	O5-C5-C6	-3.46	101.77	107.20
3	L	2	NAG	O5-C1-C2	-3.41	105.91	111.29
3	K	1	NAG	O5-C5-C4	3.36	119.00	110.83
3	L	2	NAG	O3-C3-C2	3.36	116.41	109.47
3	М	2	NAG	O3-C3-C2	3.32	116.33	109.47
3	L	2	NAG	C1-C2-N2	3.05	115.69	110.49
3	М	1	NAG	O3-C3-C2	-3.04	103.19	109.47
3	М	1	NAG	C2-N2-C7	-2.92	118.75	122.90
3	L	1	NAG	O5-C5-C4	2.85	117.77	110.83
3	K	2	NAG	O7-C7-C8	-2.74	116.97	122.06
3	М	1	NAG	C3-C4-C5	2.71	115.08	110.24
3	М	1	NAG	O5-C5-C6	-2.71	102.96	107.20
3	М	1	NAG	O7-C7-C8	2.66	126.99	122.06
3	L	2	NAG	C1-O5-C5	2.64	115.77	112.19



8ZES

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
3	Κ	2	NAG	C6-C5-C4	2.62	119.14	113.00
3	М	1	NAG	O3-C3-C4	2.48	116.09	110.35
3	Κ	2	NAG	C8-C7-N2	2.45	120.25	116.10
3	М	1	NAG	O6-C6-C5	2.44	119.67	111.29
3	L	1	NAG	O5-C5-C6	-2.18	103.79	107.20
3	L	1	NAG	O4-C4-C3	2.13	115.28	110.35
3	Κ	2	NAG	O4-C4-C5	2.06	114.40	109.30

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
3	Κ	1	NAG	C8-C7-N2-C2
3	Κ	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	L	2	NAG	C1-C2-N2-C7
3	М	1	NAG	C8-C7-N2-C2
3	М	1	NAG	O7-C7-N2-C2
3	М	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C1-C2-N2-C7
3	Κ	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	М	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	C4-C5-C6-O6
3	L	2	NAG	O7-C7-N2-C2
3	М	1	NAG	C3-C2-N2-C7
3	М	1	NAG	C1-C2-N2-C7
3	М	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C1-C2-N2-C7
3	L	2	NAG	C3-C2-N2-C7
3	Κ	2	NAG	C4-C5-C6-O6
3	К	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7

All (25) torsion outliers are listed below:

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,





bond angles, torsion angles, and ring geometry for oligosaccharide.









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).

Mol Type	Trune	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Tinle	Bo	ond leng	\mathbf{ths}	B	ond ang	les
IVIOI	туре	Chain	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2												
4	NAG	А	601	-	14,14,15	1.75	3 (21%)	17,19,21	2.65	7 (41%)												
4	NAG	D	601	1	14,14,15	1.26	1 (7%)	17,19,21	2.82	6 (35%)												



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	NAG	А	601	-	-	4/6/23/26	0/1/1/1
4	NAG	D	601	1	-	2/6/23/26	0/1/1/1

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	601	NAG	C1-C2	4.02	1.58	1.52
4	А	601	NAG	O5-C5	2.79	1.49	1.43
4	А	601	NAG	C3-C2	2.69	1.58	1.52
4	D	601	NAG	C3-C2	2.29	1.57	1.52

All (4) bond length outliers are listed below:

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	D	601	NAG	C1-O5-C5	6.95	121.60	112.19
4	А	601	NAG	O3-C3-C2	6.55	123.02	109.47
4	А	601	NAG	C1-O5-C5	6.49	120.99	112.19
4	D	601	NAG	C2-N2-C7	5.66	130.97	122.90
4	D	601	NAG	C4-C3-C2	3.96	116.83	111.02
4	D	601	NAG	C1-C2-N2	-3.39	104.69	110.49
4	D	601	NAG	O4-C4-C5	2.91	116.52	109.30
4	D	601	NAG	O3-C3-C4	-2.51	104.54	110.35
4	А	601	NAG	O6-C6-C5	2.34	119.31	111.29
4	А	601	NAG	O5-C1-C2	-2.20	107.82	111.29
4	A	601	NAG	07-C7-N2	-2.18	117.94	121.95
4	А	601	NAG	O5-C5-C4	2.15	116.05	110.83
4	A	601	NAG	C2-N2-C7	2.12	125.92	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	601	NAG	C8-C7-N2-C2
4	А	601	NAG	O7-C7-N2-C2
4	А	601	NAG	O5-C5-C6-O6
4	А	601	NAG	C4-C5-C6-O6
4	D	601	NAG	O5-C5-C6-O6



Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	601	NAG	C4-C5-C6-O6

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	194/221~(87%)	-0.99	0 100 100	108, 191, 268, 314	0
1	С	194/221~(87%)	-0.85	1 (0%) 87 72	126, 200, 265, 299	0
1	D	195/221~(88%)	-0.99	0 100 100	120, 190, 253, 284	0
1	G	193/221~(87%)	-1.01	1 (0%) 87 72	130, 195, 266, 329	0
1	Ι	194/221~(87%)	-0.94	0 100 100	108, 191, 245, 285	0
2	В	121/146~(82%)	-0.96	0 100 100	147, 196, 244, 302	0
2	Ε	121/146~(82%)	-1.08	0 100 100	150, 208, 252, 293	0
2	F	121/146~(82%)	-1.12	0 100 100	133, 181, 228, 255	0
2	Н	120/146~(82%)	-0.96	0 100 100	133, 190, 235, 255	0
2	J	119/146~(81%)	-1.03	0 100 100	140, 199, 248, 277	0
All	All	1572/1835~(85%)	-0.98	2 (0%) 92 89	108, 195, 254, 329	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	335	LEU	3.1
1	С	518	LEU	2.2

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)

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,



Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
3	NAG	М	2	14/15	0.59	0.08	161,292,339,373	0
3	NAG	K	2	14/15	0.71	0.08	151,267,342,348	0
3	NAG	L	2	14/15	0.79	0.08	135,256,330,342	0
3	NAG	L	1	14/15	0.93	0.05	118,180,228,241	0
3	NAG	М	1	14/15	0.94	0.04	118,210,251,254	0
3	NAG	K	1	14/15	0.96	0.04	137,213,244,256	0

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.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.











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	$B-factors(Å^2)$	Q<0.9
4	NAG	А	601	14/15	0.91	0.07	145,224,264,268	0
4	NAG	D	601	14/15	0.92	0.07	116,180,245,254	0

6.5 Other polymers (i)

There are no such residues in this entry.

