

# Full wwPDB X-ray Structure Validation Report (i)

### May 28, 2025 – 04:48 PM EDT

PDB ID	:	$9ML8 / pdb_00009ml8$
Title	:	Crystal structure of the SARS-CoV-2 RBD in complex with the rabbit M8b-B1 $$
		Fab
Authors	:	Fan, C.; Bjorkman, P.J.
Deposited on	:	2024-12-18
Resolution	:	2.40  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	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

# 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 2.40 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	$\begin{array}{c} {\rm Whole \ archive} \\ {\rm (\#Entries)} \end{array}$	${f Similar resolution}\ (\# Entries, resolution range(Å))$			
$R_{free}$	164625	4642 (2.40-2.40)			
Clashscore	180529	5218 (2.40-2.40)			
Ramachandran outliers	177936	5158 (2.40-2.40)			
Sidechain outliers	177891	5159 (2.40-2.40)			
RSRZ outliers	164620	4642 (2.40-2.40)			

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		
			3%		
1	А	212	82%	11%	8%
			5%		
1	В	212	85%	7%	8%
			8%		
1	С	212	83%	10%	8%
			11%		
1	D	212	77%	15%	8%
			19%		
2	Ε	235	87%	ç	9% 5%



Mol	Chain	Longth	Quality of chain	
10101	Ullaili	Length	Quality of Cham	
			13%	
2	H	235	89%	6% 5%
			19%	
2	М	235	84%	11% 5%
			14%	
2	Р	235	88%	7% 5%
			16%	
3	F	217	87%	12%
			9%	
3	L	217	91%	8%
		-	14%	
3	Ν	217	88%	11%
	11		15%	1170
3	0	217	000/	100/
0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	211	00 %	12%
1	C	9	500/	
- 4	G		50% 50%	
4	т	0		
4	1	Z	50% 50%	
	т	0		
4	J	2	50% 50%	
4	K	2	100%	



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20452 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	Δ	106	Total	С	Ν	0	$\mathbf{S}$	0	1	0
	A	190	1560	1000	262	290	8	0	1	0
1	Р	196	Total	С	Ν	0	S	0	1	0
	I D		1560	1000	262	290	8	0	L	0
1	C	106	Total	С	Ν	0	S	0	2	0
	U	190	1568	1004	264	292	8	0		0
1	1 D	106	Total	С	Ν	0	S	0	1	0
	190	1558	999	260	291	8	0		U	

• Molecule 1 is a protein called Spike protein S1.

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	534	HIS	-	expression tag	UNP P0DTC2
А	535	HIS	-	expression tag	UNP P0DTC2
А	536	HIS	-	expression tag	UNP P0DTC2
А	537	HIS	-	expression tag	UNP P0DTC2
А	538	HIS	-	expression tag	UNP P0DTC2
А	539	HIS	-	expression tag	UNP P0DTC2
В	534	HIS	-	expression tag	UNP P0DTC2
В	535	HIS	-	expression tag	UNP P0DTC2
В	536	HIS	-	expression tag	UNP P0DTC2
В	537	HIS	-	expression tag	UNP P0DTC2
В	538	HIS	-	expression tag	UNP P0DTC2
В	539	HIS	-	expression tag	UNP P0DTC2
С	534	HIS	-	expression tag	UNP P0DTC2
С	535	HIS	-	expression tag	UNP P0DTC2
С	536	HIS	-	expression tag	UNP P0DTC2
С	537	HIS	-	expression tag	UNP P0DTC2
С	538	HIS	-	expression tag	UNP P0DTC2
С	539	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2



Contenta	pagan										
Chain	Residue	Modelled	Actual	Comment	Reference						
D	537	HIS	-	expression tag	UNP P0DTC2						
D	538	HIS	-	expression tag	UNP P0DTC2						
D	539	HIS	-	expression tag	UNP P0DTC2						

• Molecule 2 is a protein called M8b-B1 heavy chain.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	F	224	Total	С	Ν	0	S	0	0	0
	Ľ	224	1683	1078	271	325	9	0	0	0
0	ц	224	Total	С	Ν	0	S	0	0	0
	П	224	1683	1078	271	325	9	0	0	0
0	м	224	Total	С	Ν	0	S	0	0	0
	111	224	1683	1078	271	325	9	0	0	0
0	D	224	Total	С	Ν	0	S	0	0	0
	Г	224	1683	1078	271	325	9		U	0

• Molecule 3 is a protein called M8b-B1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Б	216	Total	С	Ν	0	S	0	1	0
0	Г	210	1643	1030	269	339	5	0	1	0
2	т	216	Total	С	Ν	0	S	0	1	0
0		210	1643	1030	269	339	5		L	0
9	N	216	Total	С	Ν	0	S	0	1	0
5	3 N		1643	1030	269	339	5		1	0
3 Q	216	Total	С	Ν	0	S	0	1	0	
		1643	1030	269	339	5				

• Molecule 4 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
4	G	2	Total 28	C 16	N 2	O 10	0	0	0
4	Ι	2	Total 28	C 16	N 2	O 10	0	0	0
4	J	2	Total 28	C 16	N 2	O 10	0	0	0



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

• Molecule 5 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	Ν	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	Q	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	58	Total O   58 58	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	63	Total O   63 63	0	0
6	С	31	Total O 31 31	0	0
6	D	24	Total O 24 24	0	0
6	Е	102	Total O   102 102	0	0
6	F	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	0	0
6	Н	105	Total O 105 105	0	0
6	L	51	Total O   51 51	0	0
6	М	94	Total O   94 94	0	0
6	Ν	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0	0
6	Р	81	Total O   81 81	0	0
6	Q	47	$\begin{array}{cc} \text{Total} & \text{O} \\ 47 & 47 \end{array}$	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 2: M8b-B1 heavy chain 19% Chain E: 87% 5% 9% SER LYS SER SER THR SER CYS ASP LYS • Molecule 2: M8b-B1 heavy chain 13% Chain H: 89% 6% 5% SER LYS SER SER SER SER SER CLY GLY V211 E212 P213 P213 K214 SER CYS ASP ASP LYS • Molecule 2: M8b-B1 heavy chain 19% Chain M: 84% 5% 11% LYS SER THR SER P213 K214 SER CYS ASP LYS • Molecule 2: M8b-B1 heavy chain Chain P: 88% 7% 5% LYS SER SER SER GLY GLY SER CYS ASP • Molecule 3: M8b-B1 light chain 16% Chain F: 87% 12%





• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%



#### NAG1 NAG2

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

⊖hain J: 50% 50%			
	Chain J:	50%	50%

#### NAG1 NAG2

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:	100%
NAG2	



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	175.07Å 173.44Å 129.93Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $116.55^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	39.15 - 2.40	Depositor
Resolution (A)	39.15 - 2.40	EDS
% Data completeness	98.4 (39.15-2.40)	Depositor
(in resolution range)	98.4 (39.15-2.40)	EDS
R <sub>merge</sub>	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.51 (at 2.29 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
P. P.	0.223 , $0.247$	Depositor
$n, n_{free}$	0.221 , $0.243$	DCC
$R_{free}$ test set	131265 reflections $(1.32%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , $53.2$	EDS
L-test for $twinning^2$	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20452	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.29% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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, SO4

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	0.10	0/1607	0.31	0/2186
1	В	0.10	0/1607	0.29	0/2186
1	С	0.10	0/1615	0.31	0/2197
1	D	0.12	0/1605	0.33	0/2184
2	Е	0.10	0/1730	0.29	0/2362
2	Н	0.09	0/1730	0.28	0/2362
2	М	0.10	0/1730	0.28	0/2362
2	Р	0.09	0/1730	0.28	0/2362
3	F	0.15	0/1684	0.33	0/2293
3	L	0.09	0/1684	0.30	0/2293
3	Ν	0.10	0/1684	0.31	0/2293
3	Q	0.10	0/1684	0.30	0/2293
All	All	0.10	0/20090	0.30	0/27373

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1560	0	1485	12	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	1560	0	1485	9	0
1	С	1568	0	1490	12	0
1	D	1558	0	1480	21	0
2	Е	1683	0	1630	12	0
2	Н	1683	0	1630	7	0
2	М	1683	0	1630	19	0
2	Р	1683	0	1630	9	0
3	F	1643	0	1576	16	0
3	L	1643	0	1576	11	0
3	Ν	1643	0	1576	16	0
3	Q	1643	0	1576	19	0
4	G	28	0	25	0	0
4	Ι	28	0	25	0	0
4	J	28	0	25	0	0
4	Κ	28	0	25	0	0
5	А	5	0	0	0	0
5	С	5	0	0	0	0
5	D	5	0	0	0	0
5	F	5	0	0	0	0
5	L	5	0	0	0	0
5	Ν	5	0	0	0	0
5	Q	5	0	0	0	0
6	А	58	0	0	0	0
6	В	63	0	0	1	0
6	С	31	0	0	0	0
6	D	24	0	0	0	0
6	Е	102	0	0	0	0
6	F	47	0	0	0	0
6	Н	105	0	0	0	0
6	L	51	0	0	0	0
6	М	94	0	0	1	0
6	N	52	0	0	0	0
6	Р	81	0	0	0	0
6	Q	47	0	0	0	0
All	All	20452	0	18864	155	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 (155) 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:D:366:SER:HA	1:D:369:TYR:CE1	2.21	0.76
3:L:16:GLY:HA3	3:Q:16:GLY:HA3	1.70	0.74
1:D:367:VAL:O	1:D:371:SER:HB3	1.88	0.74
3:F:120:PRO:HD3	3:F:132:VAL:HG22	1.70	0.73
3:Q:123:GLU:OE2	3:Q:123:GLU:N	2.17	0.73
2:M:119:PRO:HB3	2:M:145:TYR:HB3	1.71	0.72
3:F:128:GLY:HA2	3:F:183:LYS:HE3	1.69	0.72
2:E:119:PRO:HB3	2:E:145:TYR:HB3	1.72	0.72
3:F:123:GLU:OE2	3:F:123:GLU:N	2.22	0.70
2:P:119:PRO:HB3	2:P:145:TYR:HB3	1.73	0.70
1:D:387:LEU:HA	1:D:390:LEU:HD12	1.75	0.68
3:N:185:ASP:HA	3:N:188:LYS:HE2	1.75	0.68
3:N:108:ARG:HH21	3:N:111:ALA:HB2	1.59	0.66
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.77	0.66
3:Q:120:PRO:HD3	3:Q:132:VAL:HG22	1.75	0.66
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.78	0.65
3:N:128:GLY:HA2	3:N:183:LYS:HE3	1.78	0.64
2:M:167:PRO:HG2	3:N:162:SER:HB2	1.81	0.61
3:F:2:GLN:HB2	3:F:95(B):TRP:CD1	2.38	0.59
2:E:126:PRO:HG3	2:E:138:LEU:HB3	1.84	0.59
1:A:376:THR:HB	1:A:435:ALA:HB3	1.86	0.58
2:M:126:PRO:HB3	2:M:138:LEU:HB3	1.87	0.57
2:H:171:GLN:OE1	2:H:177:SER:OG	2.18	0.56
3:F:185:ASP:HA	3:F:188:LYS:HE2	1.87	0.56
2:M:43:LYS:NZ	6:M:305:HOH:O	2.36	0.56
2:M:82:MET:HE1	2:M:90:TYR:CE2	2.41	0.56
3:N:188:LYS:HG3	3:N:189:HIS:CD2	2.40	0.56
3:N:120:PRO:HD3	3:N:132:VAL:HG22	1.88	0.55
3:N:123:GLU:O	3:N:126:LYS:N	2.28	0.54
1:D:376:THR:HG23	1:D:378:LYS:HG3	1.90	0.54
1:C:457:ARG:NH1	1:C:459:SER:O	2.41	0.53
1:C:358:ILE:HB	1:C:395:VAL:HB	1.90	0.53
2:H:167:PRO:HG2	3:L:162:SER:HB2	1.90	0.53
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.88	0.53
2:M:35:MET:HE1	2:M:94:ARG:HG3	1.91	0.53
3:F:149:LYS:HB2	3:F:193:ALA:HB3	1.91	0.53
1:D:358:ILE:HB	1:D:395:VAL:HB	1.91	0.53
2:P:167:PRO:HG2	3:Q:162:SER:HB2	1.89	0.53
1:B:376:THR:HB	1:B:435:ALA:HB3	1.91	0.53
2:M:188:SER:HB2	2:M:192:GLN:HG2	1.90	0.52
3:Q:187:GLU:C	3:Q:211:ARG:HH22	2.18	0.52
3:Q:37:GLN:HB2	3:Q:47:LEU:HD11	1.89	0.52



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		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:338:PHE:HE2	1:A:363:ALA:HB1	1.74	0.52	
1:D:369:TYR:HD1	1:D:370:ASN:N	2.07	0.52	
2:P:165:THR:HG23	2:P:180:SER:HB2	1.91	0.52	
2:E:34:TYR:HB2	2:E:100(F):MET:HE1	1.92	0.51	
2:E:38:ARG:HB3	2:E:48:ILE:HD11	1.92	0.51	
2:E:82:MET:HE1	2:E:90:TYR:CE2	2.45	0.51	
2:E:67:PHE:HE2	2:E:82:MET:HE2	1.75	0.51	
2:M:34:TYR:CZ	2:M:100(D):VAL:HG21	2.45	0.51	
3:Q:185:ASP:HA	3:Q:188:LYS:HE2	1.92	0.51	
1:D:457:ARG:NH1	1:D:459:SER:O	2.44	0.51	
3:N:39:LYS:HD3	3:N:84:ALA:HB2	1.93	0.50	
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.42	0.50	
1:D:369:TYR:HA	1:D:377:PHE:CE2	2.47	0.50	
3:F:117:ILE:HG22	3:F:207:LYS:HD2	1.93	0.50	
1:B:456:PHE:CE1	1:B:491:PRO:HA	2.47	0.50	
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.94	0.50	
1:C:527:PRO:O	1:C:528:LYS:HB2	2.12	0.49	
2:E:34:TYR:CZ	2:E:100(D):VAL:HG21	2.47	0.49	
3:Q:121:SER:O	3:Q:124:GLN:N	2.46	0.49	
2:M:67:PHE:CE2	2:M:82:MET:HE2	2.48	0.49	
2:H:34:TYR:CZ	2:H:100(D):VAL:HG21	2.47	0.49	
1:D:444:LYS:NZ	1:D:445:VAL:O	2.46	0.49	
2:E:67:PHE:CE2	2:E:82:MET:HE2	2.48	0.49	
2:H:195:ILE:HG22	2:H:210:ARG:HA	1.95	0.49	
3:L:123:GLU:OE1	3:L:123:GLU:N	2.33	0.48	
1:D:474[B]:GLN:HG2	1:D:480:CYS:SG	2.54	0.48	
1:D:376:THR:HB	1:D:435:ALA:HB3	1.94	0.48	
2:M:38:ARG:HB3	2:M:48:ILE:HD11	1.95	0.48	
3:N:198:HIS:HB3	3:N:201:LEU:HD13	1.95	0.48	
1:C:376:THR:HB	1:C:435:ALA:HB3	1.95	0.48	
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.96	0.48	
2:P:38:ARG:HB3	2:P:48:ILE:HD11	1.95	0.48	
3:Q:189:HIS:H	3:Q:211:ARG:HH21	1.62	0.48	
1:A:456:PHE:CZ	1:A:489:TYR:HB2	2.49	0.47	
1:B:357[A]:ARG:NH2	6:B:603:HOH:O	2.47	0.47	
3:N:145:LYS:HD3	3:N:146:VAL:N	2.29	0.47	
1:A:456:PHE:CE1	1:A:491:PRO:HA	2.49	0.47	
1:B:334:ASN:OD1	1:B:334:ASN:N	2.44	0.47	
1:C:444:LYS:HD2	1:C:445:VAL:H	1.79	0.47	
3:L:145:LYS:HD3	3:L:146:VAL:N	2.30	0.47	
3:Q:121:SER:C	3:Q:125:LEU:HD23	2.40	0.47	



9ML8
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		Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:Q:122:ASP:HA	3:Q:125:LEU:HB2	1.96	0.47	
3:F:145:LYS:HD3	3:F:146:VAL:N	2.30	0.47	
1:D:366:SER:HA	1:D:369:TYR:CZ	2.50	0.46	
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.98	0.46	
2:P:34:TYR:CZ	2:P:100(D):VAL:HG21	2.50	0.46	
2:E:167:PRO:HG2	3:F:162:SER:HB2	1.96	0.46	
1:B:354:ASN:O	1:B:398:ASP:HA	2.16	0.45	
1:A:362:VAL:HA	1:A:525:CYS:O	2.17	0.45	
1:D:455:LEU:HD11	1:D:493:GLN:HB2	1.99	0.45	
1:A:366:SER:HA	1:A:369:TYR:CZ	2.51	0.45	
1:B:456:PHE:CZ	1:B:489:TYR:HB2	2.52	0.45	
1:B:366:SER:HA	1:B:369:TYR:CZ	2.52	0.45	
3:Q:120:PRO:HG3	3:Q:130:ALA:HB1	1.98	0.44	
3:N:155:GLN:OE1	3:N:158:ASN:ND2	2.47	0.44	
3:L:185:ASP:HA	3:L:188:LYS:HE2	2.00	0.44	
1:D:392:PHE:HA	1:D:517:LEU:HD23	1.99	0.44	
1:B:358:ILE:HB	1:B:395:VAL:HB	1.98	0.43	
1:B:360:ASN:H	1:B:523:THR:HB	1.83	0.43	
3:F:170:ASP:HB3	3:F:172:THR:HG23	2.00	0.43	
3:L:188:LYS:HG3	3:L:189:HIS:CD2	2.52	0.43	
2:M:67:PHE:HE2	2:M:82:MET:HE2	1.83	0.43	
1:C:382:VAL:HG11	1:C:387:LEU:HD21	1.98	0.43	
1:D:454:ARG:HD3	1:D:457:ARG:HG3	2.00	0.43	
2:M:82:MET:HB2	2:M:82(C):LEU:HD21	1.99	0.43	
3:L:149:LYS:HB2	3:L:193:ALA:HB3	2.00	0.43	
2:M:94:ARG:HB3	2:M:101:VAL:HG23	2.00	0.43	
2:M:39:GLN:HB2	2:M:45:LEU:HD23	2.00	0.43	
1:D:354:ASN:O	1:D:398:ASP:HA	2.18	0.43	
2:E:139:GLY:HA3	2:E:181:VAL:HG12	2.01	0.43	
2:E:186:SER:HA	2:E:189:LEU:HG	2.00	0.43	
2:M:154:TRP:CH2	2:M:196:CYS:HB3	2.53	0.43	
3:Q:189:HIS:H	3:Q:211:ARG:NH2	2.17	0.43	
1:C:502:GLY:O	1:C:506:GLN:HG3	2.19	0.43	
1:D:334:ASN:OD1	1:D:334:ASN:N	2.51	0.43	
1:C:388:ASN:HD22	1:C:527:PRO:HD2	1.84	0.42	
1:D:425:LEU:HD21	1:D:512:VAL:HG11	2.02	0.42	
2:H:186:SER:HA	2:H:189:LEU:HG	2.01	0.42	
3:F:188:LYS:HG3	3:F:189:HIS:CE1	2.54	0.42	
3:N:189:HIS:O	3:N:211:ARG:NE	2.38	0.42	
1:A:421:TYR:CD1	1:A:457:ARG:HB2	2.54	0.42	
1:D:379:CYS:SG	1:D:384:PRO:HG3	2.60	0.42	



9ML8
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A 4 and 1	A + a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:387:LEU:HA	1:A:390:LEU:HD23	2.01	0.42	
1:A:354:ASN:O	1:A:398:ASP:HA	2.19	0.42	
2:P:100(F):MET:HB2	3:Q:96:TYR:CE1	2.54	0.42	
3:F:188:LYS:HG3	3:F:189:HIS:ND1	2.35	0.42	
2:M:122:PHE:CE1	3:N:123:GLU:HG3	2.54	0.42	
3:Q:128:GLY:C	3:Q:183:LYS:HG2	2.45	0.42	
2:E:152:VAL:HG22	2:E:198:VAL:HG22	2.02	0.42	
3:Q:113:PRO:HB3	3:Q:139:PHE:CD2	2.55	0.42	
1:D:377:PHE:CD2	1:D:434:ILE:HG12	2.55	0.41	
3:Q:181:LEU:HD13	3:Q:185:ASP:HB3	2.02	0.41	
3:F:13:ALA:HA	3:F:107:LYS:HE2	2.02	0.41	
1:C:350:VAL:HG22	1:C:422:ASN:HB3	2.02	0.41	
3:F:135:LEU:HD12	3:F:136:LEU:N	2.36	0.41	
2:M:122:PHE:HE1	3:N:123:GLU:HG3	1.86	0.41	
2:M:186:SER:HA	2:M:189:LEU:HG	2.01	0.41	
1:D:366:SER:HA	1:D:369:TYR:CD1	2.54	0.41	
3:F:119:PRO:HB3	3:F:209:PHE:CE1	2.55	0.41	
2:P:52(F):GLY:N	2:P:71:LYS:O	2.49	0.41	
3:Q:188:LYS:HG3	3:Q:189:HIS:CD2	2.56	0.41	
2:P:11:LEU:HD23	2:P:116:PRO:HG3	2.03	0.41	
1:C:461:LEU:HD22	1:C:465:GLU:HB3	2.02	0.40	
2:H:38:ARG:HB3	2:H:48:ILE:HD11	2.02	0.40	
3:L:163:VAL:HG22	3:L:175:LEU:HD12	2.02	0.40	
2:M:154:TRP:CZ3	2:M:196:CYS:HB3	2.56	0.40	
1:A:350:VAL:HG22	1:A:422:ASN:HB3	2.03	0.40	
1:C:444:LYS:C	1:C:499:PRO:HD3	2.46	0.40	
3:N:123:GLU:O	3:N:125:LEU:N	2.54	0.40	
3:L:113:PRO:HB3	3:L:139:PHE:CD2	2.57	0.40	
2:P:186:SER:HA	2:P:189:LEU:HG	2.02	0.40	
3:Q:120:PRO:HB3	3:Q:131:SER:H	1.87	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	195/212~(92%)	190~(97%)	5(3%)	0	100 100
1	В	195/212~(92%)	191~(98%)	4 (2%)	0	100 100
1	С	196/212~(92%)	190~(97%)	6 (3%)	0	100 100
1	D	195/212~(92%)	192 (98%)	3(2%)	0	100 100
2	Ε	220/235~(94%)	217~(99%)	3 (1%)	0	100 100
2	Н	220/235~(94%)	218 (99%)	2(1%)	0	100 100
2	М	220/235~(94%)	217~(99%)	3 (1%)	0	100 100
2	Р	220/235~(94%)	218 (99%)	2(1%)	0	100 100
3	F	215/217~(99%)	209~(97%)	6 (3%)	0	100 100
3	L	215/217~(99%)	209~(97%)	6 (3%)	0	100 100
3	Ν	215/217~(99%)	207~(96%)	8 (4%)	0	100 100
3	Q	215/217 (99%)	207 (96%)	8 (4%)	0	100 100
All	All	2521/2656~(95%)	2465 (98%)	56 (2%)	0	100 100

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Chain Analysed Rotameric Outliers		Outliers	Percentiles	
1	А	170/185~(92%)	169~(99%)	1 (1%)	84	92
1	В	170/185~(92%)	169 (99%)	1 (1%)	84	92
1	С	171/185~(92%)	171 (100%)	0	100	100
1	D	170/185~(92%)	168 (99%)	2 (1%)	67	82
2	Е	186/195~(95%)	185 (100%)	1 (0%)	86	94
2	Н	186/195~(95%)	185 (100%)	1 (0%)	86	94
2	М	186/195~(95%)	185 (100%)	1 (0%)	86	94



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	Р	186/195~(95%)	185 (100%)	1 (0%)	86	94
3	F	187/187~(100%)	187 (100%)	0	100	100
3	L	187/187~(100%)	187 (100%)	0	100	100
3	Ν	187/187~(100%)	187 (100%)	0	100	100
3	Q	187/187~(100%)	186 (100%)	1 (0%)	86	94
All	All	2173/2268~(96%)	2164 (100%)	9~(0%)	89	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	445	VAL
1	В	456	PHE
1	D	369	TYR
1	D	456	PHE
2	Е	101	VAL
2	Н	101	VAL
2	М	101	VAL
2	Р	101	VAL
3	Q	170	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	519	HIS
1	В	360	ASN
1	С	481	ASN
1	D	388	ASN
1	D	414	GLN
1	D	498	GLN
2	Е	171	GLN
2	Е	199	ASN
3	F	158	ASN
3	F	160	GLN
2	М	56	ASN
2	Р	39	GLN
2	Р	115	GLN
3	Q	38	GLN
3	Q	124	GLN



### 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)

8 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	Iol Type Chain Res 1		Tink	Bond lengths			Bond angles			
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	1	1,4	14,14,15	0.79	0	$17,\!19,\!21$	1.22	2 (11%)
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	0.99	0
4	NAG	Ι	1	1,4	14,14,15	0.73	0	$17,\!19,\!21$	0.99	1 (5%)
4	NAG	Ι	2	4	14,14,15	0.70	0	17,19,21	0.87	0
4	NAG	J	1	1,4	14,14,15	0.70	0	$17,\!19,\!21$	1.01	1 (5%)
4	NAG	J	2	4	14,14,15	0.70	0	17,19,21	0.80	0
4	NAG	K	1	1,4	14,14,15	0.75	0	$17,\!19,\!21$	0.98	1(5%)
4	NAG	K	2	4	14,14,15	0.70	0	17,19,21	0.95	1 (5%)

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	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Ι	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Ι	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Κ	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	G	1	NAG	C1-O5-C5	3.03	116.24	112.19
4	Κ	1	NAG	C1-O5-C5	2.45	115.47	112.19
4	G	1	NAG	C2-N2-C7	2.20	125.85	122.90
4	Ι	1	NAG	C1-O5-C5	2.18	115.11	112.19
4	J	1	NAG	C1-O5-C5	2.10	115.00	112.19
4	Κ	2	NAG	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	Ι	1	NAG	C8-C7-N2-C2
4	Ι	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2

All (8) 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)

7 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	Chain		Link	Bond lengths			Bond angles			
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	SO4	D	601	-	4,4,4	0.68	0	$6,\!6,\!6$	0.08	0
5	SO4	А	601	-	4,4,4	0.68	0	6,6,6	0.08	0
5	SO4	С	601	-	4,4,4	0.68	0	6,6,6	0.10	0



Mal Tura		Chain	Dog		Bond lengths			Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	N	301	-	4,4,4	0.67	0	$6,\!6,\!6$	0.10	0
5	SO4	L	301	-	4,4,4	0.68	0	$6,\!6,\!6$	0.08	0
5	SO4	F	301	-	4,4,4	0.67	0	$6,\!6,\!6$	0.10	0
5	SO4	Q	301	-	4,4,4	0.68	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	196/212~(92%)	0.27	6 (3%) 51 48	24,  45,  65,  92	1 (0%)
1	В	196/212~(92%)	0.39	10 (5%) 34 32	26,  46,  81,  95	1 (0%)
1	С	196/212~(92%)	0.64	18 (9%) 16 14	23, 53, 84, 100	2(1%)
1	D	196/212~(92%)	0.79	23 (11%) 10 9	37, 57, 101, 124	1 (0%)
2	Ε	224/235~(95%)	0.67	44 (19%) 4 3	24, 41, 102, 124	0
2	Н	224/235~(95%)	0.59	30 (13%) 8 7	23, 40, 97, 124	0
2	М	224/235~(95%)	0.74	45 (20%) 3 3	26, 43, 108, 129	0
2	Р	224/235~(95%)	0.67	33 (14%) 7 6	27, 44, 101, 132	0
3	F	216/217~(99%)	0.96	34 (15%) 6 5	30, 56, 108, 129	1 (0%)
3	L	216/217~(99%)	0.78	20 (9%) 16 14	29, 54, 105, 122	1 (0%)
3	Ν	216/217~(99%)	0.96	31 (14%) 7 6	29, 56, 109, 136	1 (0%)
3	Q	$21\overline{6/217}$ (99%)	1.03	$33\ (15\%)\ 6\ 6$	33, 59, 107, 127	1 (0%)
All	All	$254\overline{4/2656}\ (95\%)$	0.71	327 (12%) 9 7	23, 51, 101, 136	9~(0%)

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1	ALA	6.6
3	N	125	LEU	6.3
3	F	1	ALA	6.2
3	Q	1	ALA	5.6
3	Ν	1	ALA	5.4
2	Е	127	SER	5.2
3	F	209	PHE	4.9
2	М	127	SER	4.5
1	D	372	ALA	4.5
2	Н	127	SER	4.4
2	Е	195	ILE	4.3



Mol	Chain	Res	Type	RSRZ
2	М	195	ILE	4.2
1	D	528	LYS	4.2
1	С	333	THR	4.2
1	В	333	THR	4.0
2	М	213	PRO	3.9
1	D	333	THR	3.9
2	М	125	ALA	3.9
2	М	190	GLY	3.9
3	Q	182	SER	3.8
2	Р	2	GLN	3.8
1	С	369	TYR	3.8
2	Е	213	PRO	3.8
1	D	371	SER	3.8
2	Н	190	GLY	3.7
2	М	186	SER	3.7
3	Ν	212	GLY	3.7
2	М	214	LYS	3.7
2	Р	127	SER	3.7
3	F	182	SER	3.7
2	Е	161	SER	3.7
3	L	125	LEU	3.7
2	Н	125	ALA	3.6
2	М	159	LEU	3.6
2	Р	214	LYS	3.6
3	Ν	190	LYS	3.6
2	Р	125	ALA	3.6
2	Е	214	LYS	3.6
3	F	126	LYS	3.6
3	Ν	182	SER	3.6
3	Q	187	GLU	3.5
1	D	368	LEU	3.5
2	Е	159	LEU	3.5
1	А	333	THR	3.5
2	Е	118	ALA	3.5
3	Q	170	ASP	3.5
3	Ν	209	PHE	3.5
3	L	170	ASP	3.4
2	Р	151	THR	3.4
2	Н	208	ASP	3.4
2	Е	194	TYR	3.4
2	Е	186	SER	3.4
1	В	528	LYS	3.4



Mol	Chain	Res	Type	RSRZ
2	М	194	TYR	3.4
2	Н	2	GLN	3.4
2	Е	125	ALA	3.3
3	N	188	LYS	3.3
3	F	122	ASP	3.3
1	В	369	TYR	3.3
2	М	193	THR	3.3
1	D	369	TYR	3.3
2	М	151	THR	3.3
2	Е	135	THR	3.3
3	F	170	ASP	3.3
3	Ν	128	GLY	3.3
2	М	211	VAL	3.2
3	Ν	15	VAL	3.2
2	Н	151	THR	3.2
3	F	188	LYS	3.2
3	F	95(B)	TRP	3.2
2	Р	118	ALA	3.2
2	Н	213	PRO	3.2
2	Е	177	SER	3.2
2	М	188	SER	3.2
1	D	527	PRO	3.1
3	F	184	ALA	3.1
3	L	154	LEU	3.1
3	Ν	194	CYS	3.1
2	М	118	ALA	3.1
2	Р	126	PRO	3.1
2	Р	158	ALA	3.1
3	F	125	LEU	3.1
3	N	130	ALA	3.1
3	Ν	213	GLU	3.1
2	М	121	VAL	3.0
2	Н	207	VAL	3.0
2	М	135	THR	3.0
2	Р	193	THR	3.0
2	Н	138	LEU	3.0
3	Q	209	PHE	3.0
1	В	367	VAL	3.0
1	D	367	VAL	3.0
3	L	129	THR	3.0
3	F	194	CYS	3.0
2	Р	195	ILE	3.0



Mol	Chain	Res	Type	RSRZ
1	А	389	ASP	3.0
1	D	382	VAL	3.0
3	N	129	THR	3.0
1	С	528	LYS	2.9
2	Н	214	LYS	2.9
2	Е	192	GLN	2.9
1	С	381	GLY	2.9
2	Е	185	PRO	2.9
1	D	370	ASN	2.9
1	D	385	THR	2.9
2	М	172	SER	2.9
2	Е	115	GLN	2.9
1	D	365	TYR	2.8
3	L	188	LYS	2.8
2	Е	193	THR	2.8
2	М	187	SER	2.8
2	М	189	LEU	2.8
3	F	127	SER	2.8
3	Q	185	ASP	2.8
3	Ν	154	LEU	2.8
2	Н	135	THR	2.8
2	Р	100(B)	HIS	2.8
3	N	208	SER	2.8
2	М	140	CYS	2.8
3	F	189	HIS	2.7
3	L	209	PHE	2.7
3	Q	2	GLN	2.7
2	М	177	SER	2.7
2	М	161	SER	2.7
3	N	127	SER	2.7
3	Q	123	GLU	2.7
1	А	456	PHE	2.7
1	D	387	LEU	2.7
3	Q	186	TYR	2.7
3	F	179	LEU	2.6
2	Р	208	ASP	2.6
2	Е	188	SER	2.6
3	Ν	156	SER	2.6
2	Р	101	VAL	2.6
2	М	191	THR	2.6
2	Р	119	PRO	2.6
3	Q	113	PRO	2.6



Mol	Chain	Res	Type	RSRZ
3	L	2	GLN	2.6
1	В	372	ALA	2.6
1	С	385	THR	2.6
2	Р	135	THR	2.6
3	F	185	ASP	2.6
3	Q	129	THR	2.6
2	Е	190	GLY	2.6
1	D	390	LEU	2.6
2	Е	158	ALA	2.6
2	М	158	ALA	2.6
2	М	185	PRO	2.6
3	Ν	170	ASP	2.6
3	Q	79	GLN	2.6
2	Н	195	ILE	2.5
2	Р	190	GLY	2.5
2	Е	138	LEU	2.5
3	L	95(B)	TRP	2.5
3	Ν	95(B)	TRP	2.5
2	Е	211	VAL	2.5
2	Н	126	PRO	2.5
2	Е	183	THR	2.5
2	М	115	GLN	2.5
2	Е	140	CYS	2.5
2	М	196	CYS	2.5
2	Р	211	VAL	2.5
2	Ε	191	THR	2.5
3	Ν	2	GLN	2.5
3	Q	126	LYS	2.5
1	С	456	PHE	2.5
2	М	138	LEU	2.5
3	Ν	181	LEU	2.5
1	С	367	VAL	2.5
3	F	133	VAL	2.5
3	Q	95(B)	TRP	2.5
2	Е	120	SER	2.5
3	Q	121	SER	2.5
3	F	181	LEU	2.4
3	N	133	VAL	2.4
2	Е	123	PRO	2.4
1	D	373	SER	2.4
2	М	154	TRP	2.4
1	А	528	LYS	2.4



Mol	Chain	Res	Type	RSRZ
2	Р	160	THR	2.4
3	F	151	ASP	2.4
2	Р	184	VAL	2.4
2	Н	118	ALA	2.4
3	Q	143	GLU	2.4
3	F	208	SER	2.4
2	Е	157	GLY	2.4
3	L	122	ASP	2.4
3	N	122	ASP	2.4
3	Q	122	ASP	2.4
2	Е	189	LEU	2.4
3	Q	181	LEU	2.4
2	М	126	PRO	2.4
3	Q	133	VAL	2.4
2	М	2	GLN	2.4
3	Q	60	SER	2.4
2	Н	189	LEU	2.4
2	Н	123	PRO	2.4
1	С	445	VAL	2.4
3	Q	208	SER	2.4
1	В	382	VAL	2.3
3	Q	111	ALA	2.3
3	Q	130	ALA	2.3
3	Ν	121	SER	2.3
2	Н	193	THR	2.3
3	Q	179	LEU	2.3
2	Е	122	PHE	2.3
2	Н	209	LYS	2.3
3	Ν	183	LYS	2.3
3	Q	211	ARG	2.3
2	Н	211	VAL	2.3
2	М	163	VAL	2.3
3	L	150	VAL	2.3
2	E	136	ALA	2.3
3	F	192	TYR	2.3
3	Q	150	VAL	2.3
2	Р	120	SER	2.3
3	F	121	SER	2.3
1	C	481	ASN	2.3
2	P	194	TYR	2.3
3	F	186	TYR	2.3
2	Р	207	VAL	2.3



Mol	Chain	Res	Type	RSRZ	
3	L	191	VAL	2.3	
3	Q	78	VAL	2.3	
2	Р	137	ALA	2.3	
3	Q	184	ALA	2.3	
1	D	381	GLY	2.2	
1	С	470	THR	2.2	
2	Н	210	ARG	2.2	
2	Е	126	PRO	2.2	
3	Q	120	PRO	2.2	
2	М	192	GLN	2.2	
2	Н	150	VAL	2.2	
2	Р	121	VAL	2.2	
3	N	205	VAL	2.2	
2	Е	100(B)	HIS	2.2	
2	Р	159	LEU	2.2	
3	F	154	LEU	2.2	
3	Q	188	LYS	2.2	
2	Е	151	THR	2.2	
2	М	120	SER	2.2	
2	М	210	ARG	2.2	
2	Р	212	GLU	2.2	
3	F	213 GLU		2.2	
2	Е	184	VAL	2.2	
2	М	157	GLY	2.2	
3	Q	41	GLY	2.2	
1	А	477	SER	2.2	
1	С	373	SER	2.2	
1	D	477	SER	2.2	
1	С	357[A]	ARG	2.2	
1	С	408	ARG	2.2	
2	Н	122	PHE	2.2	
2	М	101	VAL	2.2	
3	L	133	VAL	2.2	
3	F	190	LYS	2.2	
3	L	126	LYS	2.2	
3	F	211	ARG	2.2	
2	М	122	PHE	2.2	
2	Н	185	PRO	2.2	
2	Е	208	ASP	2.2	
2	М	209	LYS	2.2	
1	В	365	TYR	2.1	
1 B		373	SER	2.1	



Mol	Chain	Res	Type	RSRZ
1	С	371	SER	2.1
2	Н	177	SER	2.1
1	С	444	LYS	2.1
2	М	182	VAL	2.1
1	С	387	LEU	2.1
2	Е	178	LEU	2.1
3	F	180	THR	2.1
2	Р	122	PHE	2.1
2	Е	172	SER	2.1
2	Р	213	PRO	2.1
2	М	204	ASN	2.1
3	N	151	ASP	2.1
1	D	362	VAL	2.1
2	Е	121	VAL	2.1
3	F	150	VAL	2.1
1	D	435	ALA	2.1
2	Н	159	LEU	2.1
2	Р	102	LEU	2.1
3	Q	125	LEU	2.1
1	D	526	GLY	2.1
3	L	128	GLY	2.1
1	D	374	PHE	2.1
2	М	153	SER	2.1
2	М	212	GLU	2.1
2	Р	187	SER	2.1
1	D	480	CYS	2.1
2	Н	140	CYS	2.1
2	Р	204	ASN	2.1
3	L	185	ASP	2.1
3	N	210	ASN	2.1
2	E	175	LEU	2.1
3	F	15	VAL	2.1
3	F	132	VAL	2.1
3	L	15	VAL	2.1
3	Q	15	VAL	2.1
2	Р	154	TRP	2.1
3	N	184	ALA	2.1
1	D	431	GLY	2.1
2	М	174	GLY	2.1
3	N	157	GLY	2.1
1	A	470	THR	2.1
2	P P	185	PRO	2.1



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Mol	Chain	Res	Type	RSRZ
3	F	183	LYS	2.1
3	L	123	GLU	2.1
2	Е	156	SER	2.1
3	F	174	SER	2.1
3	F	152	ASN	2.1
2	Н	102	LEU	2.0
2	Н	137	ALA	2.0
2	Н	194	TYR	2.0
3	N	116	PHE	2.0
2	Н	212	GLU	2.0
3	F	155	GLN	2.0
2	Е	179	SER	2.0
2	Е	187	SER	2.0
2	Е	152	VAL	2.0
2	Е	207	VAL	2.0
1	В	381	GLY	2.0
2	М	114	GLY	2.0
3	L	212	GLY	2.0
3	L	190	LYS	2.0
1	В	527	PRO	2.0
1	С	365	TYR	2.0
1	С	505	TYR	2.0

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

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

### 6.3 Carbohydrates (i)

SUGAR-RSR INFOmissingINFO

### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	SO4	Q	301	5/5	0.61	0.15	$91,\!91,\!97,\!102$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	SO4	F	301	5/5	0.62	0.13	81,86,92,100	0
5	SO4	N	301	5/5	0.64	0.16	80,84,96,98	0
5	SO4	L	301	5/5	0.72	0.12	77,79,90,93	0
5	SO4	С	601	5/5	0.80	0.21	62,62,80,80	0
5	SO4	D	601	5/5	0.86	0.16	66,69,82,82	0
5	SO4	А	601	5/5	0.89	0.13	48,53,69,73	0

Continued from previous page...

## 6.5 Other polymers (i)

There are no such residues in this entry.

