

Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 06:20 AM JST

PDB ID	:	6L8Q
Title	:	Complex structure of bat CD26 and MERS-RBD
Authors	:	Yuan, Y.
Deposited on	:	2019-11-07
Resolution	:	3.10 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	:	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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	٨	721		1.00/	
1	л	751	80%	18%	••
1	С	731	77%	21%	••
1	Е	731	83%	15%	
1	G	731	80%	18%	••
2	В	246	73% 11%	15%	_
2	D	246	70% 15%	15%	



Mol	Chain	Length	Quality of chain					
2	F	246	% 72%	13%	15%			
2	Н	246	70%	13% •	15%			
3	Ι	2	50%	50%				
3	K	2	100%					
3	L	2	100%					
3	М	2	50%	50%				
3	0	2	100%					
3	Р	2	100%					
3	Q	2	50%	50%				
3	R	2	50%	50%				
3	Т	2	50%	50%				
3	U	2	100%					
3	V	2	50%	50%				
3	Х	2	100%					
3	Y	2	100%					
4	J	3	33%	67%				
4	N	3	67%	33%)			
4	S	3	67%	33%)			
4	W	3	67%	33%)			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30730 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	794	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Л	124	5906	3775	993	1114	24	0	0	U
1	C	794	Total	С	Ν	Ο	S	0	0	0
	U	124	5906	3775	993	1114	24	0	0	0
1	F	794	Total	С	Ν	Ο	S	0	0	0
	124	5906	3775	993	1114	24	0	0	0	
1 G	794	Total	С	Ν	Ο	S	0	0	0	
	(24	5906	3775	993	1114	24		0	0	

• Molecule 1 is a protein called Dipeptidyl peptidase 4.

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
А	762	HIS	-	expression tag	UNP L5LQ33	
А	763	HIS	-	expression tag	UNP L5LQ33	
А	764	HIS	-	expression tag	UNP L5LQ33	
А	765	HIS	-	expression tag	UNP L5LQ33	
А	766	HIS	-	expression tag	UNP L5LQ33	
А	767	HIS	-	expression tag	UNP L5LQ33	
С	762	HIS	-	expression tag	UNP L5LQ33	
С	763	HIS	-	expression tag	UNP L5LQ33	
С	764	HIS	-	expression tag	UNP L5LQ33	
С	765	HIS	-	expression tag	UNP L5LQ33	
С	766	HIS	-	expression tag	UNP L5LQ33	
С	767	HIS	-	expression tag	UNP L5LQ33	
E	762	HIS	-	expression tag	UNP L5LQ33	
Е	763	HIS	-	expression tag	UNP L5LQ33	
E	764	HIS	-	expression tag	UNP L5LQ33	
Е	765	HIS	-	expression tag	UNP L5LQ33	
Е	766	HIS	-	expression tag	UNP L5LQ33	
E	767	HIS	-	expression tag	UNP L5LQ33	
G	762	HIS	-	expression tag	UNP L5LQ33	
G	763	HIS	-	expression tag	UNP L5LQ33	
G	764	HIS	-	expression tag	UNP L5LQ33	



Contentia											
Chain	Residue	Modelled	Actual	Comment	Reference						
G	765	HIS	-	expression tag	UNP L5LQ33						
G	766	HIS	-	expression tag	UNP L5LQ33						
G	767	HIS	-	expression tag	UNP L5LQ33						

• Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	В	208	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	200	1608	1026	256	315	11	0	0	0
0	Л	208	Total	С	Ν	0	S	0	0	0
	D	208	1608	1026	256	315	11	0		0
0	Б	200	Total	С	Ν	0	S	0	0	0
	Г	208	1608	1026	256	315	11	0	0	0
0	9 II	208	Total	С	Ν	0	S	0	0	0
	11	208	1608	1026	256	315	11	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	607	HIS	-	expression tag	UNP A0A0A0Q7F3
В	608	HIS	-	expression tag	UNP A0A0A0Q7F3
В	609	HIS	-	expression tag	UNP A0A0A0Q7F3
В	610	HIS	-	expression tag	UNP A0A0A0Q7F3
В	611	HIS	-	expression tag	UNP A0A0A0Q7F3
В	612	HIS	-	expression tag	UNP A0A0A0Q7F3
D	607	HIS	-	expression tag	UNP A0A0A0Q7F3
D	608	HIS	-	expression tag	UNP A0A0A0Q7F3
D	609	HIS	-	expression tag	UNP A0A0A0Q7F3
D	610	HIS	-	expression tag	UNP A0A0A0Q7F3
D	611	HIS	-	expression tag	UNP A0A0A0Q7F3
D	612	HIS	-	expression tag	UNP A0A0A0Q7F3
F	607	HIS	-	expression tag	UNP A0A0A0Q7F3
F	608	HIS	-	expression tag	UNP A0A0A0Q7F3
F	609	HIS	-	expression tag	UNP A0A0A0Q7F3
F	610	HIS	-	expression tag	UNP A0A0A0Q7F3
F	611	HIS	-	expression tag	UNP A0A0A0Q7F3
F	612	HIS	-	expression tag	UNP A0A0A0Q7F3
Н	607	HIS	-	expression tag	UNP A0A0A0Q7F3
Н	608	HIS	-	expression tag	UNP A0A0A0Q7F3
Н	609	HIS	-	expression tag	UNP A0A0A0Q7F3
Н	610	HIS	-	expression tag	UNP A0A0A0Q7F3
Н	611	HIS	-	expression tag	UNP A0A0A0Q7F3



Chain	Residue	Modelled	Actual	Comment	Reference
Н	612	HIS	-	expression tag	UNP A0A0A0Q7F3

• 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	Ι	2	Total C N O 28 16 2 10	0	0	0
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
3	Ο	2	Total C N O 28 16 2 10	0	0	0
3	Р	2	Total C N O 28 16 2 10	0	0	0
3	Q	2	Total C N O 28 16 2 10	0	0	0
3	R	2	Total C N O 28 16 2 10	0	0	0
3	Т	2	Total C N O 28 16 2 10	0	0	0
3	U	2	Total C N O 28 16 2 10	0	0	0
3	V	2	Total C N O 28 16 2 10	0	0	0
3	Х	2	Total C N O 28 16 2 10	0	0	0
3	Y	2	Total C N O 28 16 2 10	0	0	0

• Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	I	3	Total C N O	0	0	0
1	0	0	39 22 2 15	0	0	0
4	Ν	2	Total C N O	0	0	0
4	IN	5	39 22 2 15	0		
4	C	9	Total C N O	0	0	0
4	G	ა	39 22 2 15			
4	4 117	3	Total C N O	0	0	0
4 W	vv		39 22 2 15			U

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
5	Δ	1	Total C N O	0	0	
0	11	Ĩ	14 8 1 5	0	0	
5	Δ	1	Total C N O	0	0	
0	11	I	14 8 1 5	0	0	
5	В	1	Total C N O	0	0	
0	5 D	1	14 8 1 5	0	0	
5	С	1	Total C N O	0	0	
0	5 0	1	14 8 1 5	0	0	
5	С	1	Total C N O	0	0	
G	C		14 8 1 5		0	



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	Л	1	Total	С	Ν	0	0	0	
0	D	1	14	8	1	5	0	0	
5	F	1	Total	С	Ν	Ο	0	0	
0	Ľ	1	14	8	1	5	0	0	
5	F	1	Total	С	Ν	Ο	0	0	
0	Г	1	14	8	1	5	0	0	
5	C	1	Total	С	Ν	Ο	0	0	
5	G	T	14	8	1	5	0	0	
5	C	1	Total	С	Ν	Ο	0	0	
5 G	1	14	8	1	5	0	0		
5	н	1	Total	C	N	O	0	0	
0	11	1	14	8	1	5		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: Dipeptidyl peptidase 4

• Molecule 1: Dipeptidyl peptidase 4















F571 T579 D580 D580 D580 D580 D580 C583 C583 C583 C583 C583 C583 C583 C583	11LE ALA ALA CLU CLU CLU CLU CYS CYS CYS CYS CYS HIS HIS	HIS HIS HIS				
• Molecule 2: Spike gly	zcoprotein					
Chain D:	70%		15%	15%		
GLU ALA ALA LYS SER PRD GLY GLU GLU GLU GLY GLY GLY	1392 1394 1394 1394 1394 1394 1400 1402 1402 1402 1402 1402 1402 140	5416 F423 8429 A432 Y438 S439 S439 L443	S447 S447 D455 L456 P463	N468 L479 I480	K493	
R505 [L506 [L506 N553 (N553 [L554 [L554 [L554 [S571 [S571 [S571] [S572] [S523 [S533] [S533] [S533]	K867 K867 L1588 C1588 C1588 A1A A1A A1A A1A A1A A1A A1A A1A A1A A	LEU GLY ASN CYS CYS CYS CYAL TYR HIS HIS HIS	HIS			
• Molecule 2: Spike gly	coprotein					
Chain F:	72%		13%	15%		
GLU ALA ALA LYS LYS PRO GLY GLV GLU GLU GLU GLU GLU GLU	P393 P394 K400 N408 K413 K413 F413 F423 F423	I 428 8429 432 433 8439 5439 1456 L456	P476 L479 K493	S498 N501 K502 V534	8557 8558 8559 8559	
Mees T1663 1564 E565 C566 L667 C566 C565 C585 C585 C585 C585 C585 C585	ASP ASP THR THR LLZ GLN GLN CLN CLN CLN CLN CLN CVS CVS CVS	TYR HIS HIS HIS HIS HIS				
• Molecule 2: Spike gly	vcoprotein					
Chain H:	70%		13% •	15%		
GLU ALA ALA LYS SER SER CLU GLN GLN GLN GLN GLN GLN GLN GLY GLN GLY GLN GLY GLN GLY GLN GLY GLN GLY GLN GLY GLN GLN GLU GLN GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU	R400 R406 R406 R411 L411 R413 R413 R413 R413 R413 R413 R413 R	0422 6423 6430 6431 6432 1433 1433 8439 8439 8440	D455 L456 P463 L479	1480 T483 K493	N501 K502 L507	
8508 D509 D509 D509 D509 8557 8557 8558 8558 8558 8558 8558 855	L <mark>1588</mark> GLU PHE ALM ASN ASN ASN ASN ASN ALM ALM ALM CLU CLU CLU CLU	ASN CYS VAL GLU HIS HIS HIS HIS HIS HIS				
• Molecule 3: 2-acetan opyranose	nido-2-deoxy-beta-D	-glucopyranose-	(1-4)-2-ac	etamido	-2-deoxy-b	eta-D-gluc
Chain I:	50%	50'	%			
• Molecule 3: 2-acetam	nido-2-deoxy-beta-D	-glucopyranose-	(1-4)-2-ac	etamido	-2-deoxy-b	eta-D-gluc

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

NAG1 NAG2 100%



• Molecule 3 opyranose	3: 2-acetamido-2-deoxy-bet	a-D-glucopyranose-(1-4)-2-acetami	do-2-deoxy-beta-D-gluc
Chain L:		100%	-
NAG1 NAG2			
• Molecule 3 opyranose	3: 2-acetamido-2-deoxy-bet	a-D-glucopyranose-(1-4)-2-acetami	do-2-deoxy-beta-D-gluc
Chain M:	50%	50%	-
NAG2 NAG2			
• Molecule 3 opyranose	3: 2-acetamido-2-deoxy-bet	a-D-glucopyranose-(1-4)-2-acetami	do-2-deoxy-beta-D-gluc
Chain O:		100%	-
NAG1 NAG2			
• Molecule 3 opyranose	3: 2-acetamido-2-deoxy-bet	a-D-glucopyranose-(1-4)-2-acetami	do-2-deoxy-beta-D-gluc
Chain P:		100%	-
NAG1 NAG2			
• Molecule 3 opyranose	3: 2-acetamido-2-deoxy-bet	a-D-glucopyranose-(1-4)-2-acetami	do-2-deoxy-beta-D-gluc
Chain Q:	50%	50%	-
NAG2 NAG2			
• Molecule 3 opyranose	3: 2-acetamido-2-deoxy-bet	a-D-glucopyranose-(1-4)-2-acetami	do-2-deoxy-beta-D-gluc
Chain R:	50%	50%	-
NAG1 NAG2			
• Molecule 3 opyranose	3: 2-acetamido-2-deoxy-bet	a-D-glucopyranose-(1-4)-2-acetami	do-2-deoxy-beta-D-gluc
Chain T:	50%	50%	-

PROTEIN DATA BANK

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:	100%	
NAG1 NAG2		
• Molecule 3: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta	mido-2-deoxy-beta-D-gluc
Chain V:	50% 50%	_
NAG1 NAG2		
• Molecule 3: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta	mido-2-deoxy-beta-D-gluc
Chain X:	100%	
NAG1 NAG2		
• Molecule 3: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta	mido-2-deoxy-beta-D-gluc
Chain Y:	100%	
NAG1 NAG2		
• Molecule 4: etamido-2-dec	beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-loxy-beta-D-glucopyranose	D-glucopyranose-(1-4)-2-ac

Chain J:	33%	67%	1
NAG1 NAG2 BMA3			

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

Chain N:	67%	33%
NAG1 BMAG BMAG		



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

Chain S:

NAG1 NAG2 BMA3

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

Chain W:

NAG1 NAG2 BMA3

67%

67%

33%

33%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	114.66Å 273.67Å 115.23Å	Deresiter
a, b, c, α , β , γ	90.00° 119.68° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	49.81 - 3.10	Depositor
Resolution (A)	49.81 - 3.10	EDS
% Data completeness	85.3 (49.81-3.10)	Depositor
(in resolution range)	84.9(49.81-3.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.83 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
D D	0.200 , 0.241	Depositor
n, n_{free}	0.200 , 0.241	DCC
R_{free} test set	4577 reflections $(4.80%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	64.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 12.9	EDS
L-test for $twinning^2$	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
	0.007 for -h-l,k,h	
	0.007 for l,k,-h-l	
Estimated twinning fraction	0.438 for h,-k,-h-l	Xtriage
	0.019 for -h-l,-k,l	
	0.015 for l,-k,h	
F_o, F_c correlation	0.91	EDS
Total number of atoms	30730	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.92% 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, BMA

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/6078	0.47	0/8266	
1	С	0.27	0/6078	0.46	0/8266	
1	Е	0.26	0/6078	0.46	0/8266	
1	G	0.32	0/6078	0.49	0/8266	
2	В	0.25	0/1647	0.45	0/2249	
2	D	0.25	0/1647	0.45	0/2249	
2	F	0.26	0/1647	0.45	0/2249	
2	H	0.25	0/1647	0.45	0/2249	
All	All	0.28	0/30900	0.47	0/42060	

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	5906	0	5607	81	0
1	С	5906	0	5607	97	0
1	Е	5906	0	5607	74	0
1	G	5906	0	5607	90	0
2	В	1608	0	1573	14	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1608	0	1573	21	0
2	F	1608	0	1573	18	0
2	Н	1608	0	1573	24	0
3	Ι	28	0	25	1	0
3	Κ	28	0	25	0	0
3	L	28	0	25	0	0
3	М	28	0	25	1	0
3	0	28	0	25	0	0
3	Р	28	0	25	0	0
3	Q	28	0	25	1	0
3	R	28	0	25	1	0
3	Т	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	1	0
3	Х	28	0	25	0	0
3	Y	28	0	25	0	0
4	J	39	0	34	0	0
4	Ν	39	0	34	0	0
4	S	39	0	34	0	0
4	W	39	0	34	0	0
5	А	28	0	26	1	0
5	В	14	0	13	1	0
5	С	28	0	26	2	0
5	D	14	0	13	0	0
5	Е	14	0	13	0	0
5	F	14	0	13	0	0
5	G	28	0	26	0	0
5	Н	14	0	13	1	0
All	All	30730	0	29324	413	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 7.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:G:472:ILE:HD11	1:G:495:LEU:CD1	1.42	1.46	
1:G:472:ILE:CD1	1:G:495:LEU:HD12	1.50	1.41	
1:A:80:ASP:OD1	1:A:462:TYR:OH	1.59	1.19	
1:E:233:ARG:HH21	1:E:253:PRO:HG3	1.20	1.05	
1:E:233:ARG:NH2	1:E:253:PRO:HG3	1.78	0.97	



	io ao pago	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:472:ILE:HD11	1:G:495:LEU:HD13	1.46	0.97	
1:G:488:LEU:HD21	1:G:491:ASN:HB2	1.53	0.90	
1:G:472:ILE:HD11	1:G:495:LEU:HD12	0.88	0.87	
1:G:597:GLU:OE1	1:G:597:GLU:N	2.08	0.85	
2:F:456:LEU:HB3	2:F:479:LEU:HD21	1.59	0.84	
1:G:466:ARG:HH11	1:G:466:ARG:HB3	1.42	0.84	
1:A:122:TRP:CH2	1:A:252:ILE:HD11	2.16	0.81	
1:C:208:THR:HG22	1:C:210:SER:H	1.47	0.78	
1:G:472:ILE:HD13	1:G:495:LEU:HD12	1.61	0.78	
1:A:383:GLN:HB2	1:A:386:LYS:HB2	1.66	0.77	
1:E:233:ARG:HH21	1:E:253:PRO:CG	1.96	0.77	
1:G:466:ARG:HH11	1:G:466:ARG:CB	1.98	0.76	
1:A:448:ARG:HA	1:A:471:GLN:HG3	1.68	0.75	
1:E:474:ARG:NH1	1:E:485:GLU:OE2	2.20	0.74	
2:H:564:THR:HG22	2:H:565:GLU:N	2.02	0.74	
2:B:394:PRO:HG3	2:B:400:LYS:HG3	1.71	0.73	
1:A:591:ARG:NH2	1:A:673:ASP:OD1	2.22	0.72	
1:C:505:PRO:HD3	1:C:564:SER:HB2	1.71	0.71	
1:G:635:LEU:HD11	1:G:645:GLY:HA3	1.72	0.71	
1:A:188:ARG:HB3	1:A:191:ALA:HB3	1.70	0.71	
1:E:256:LYS:NZ	1:E:709:GLN:OE1	2.24	0.71	
1:G:426:LEU:HD22	1:G:440:LEU:HD12	1.74	0.70	
1:C:240:LEU:HB2	1:C:244:LEU:HD12	1.73	0.69	
1:C:78:ASN:HB3	1:C:83:ASN:HB3	1.75	0.69	
1:C:635:LEU:HD11	1:C:645:GLY:HA3	1.74	0.69	
1:C:591:ARG:NH2	1:C:673:ASP:OD1	2.24	0.68	
1:G:83:ASN:OD1	1:G:84:SER:N	2.25	0.68	
1:G:633:MET:O	1:G:686:ARG:NH1	2.26	0.68	
1:E:153:ILE:HD12	1:E:164:TYR:HB3	1.75	0.68	
2:F:493:LYS:NZ	2:F:565:GLU:O	2.27	0.68	
1:C:312:ARG:NH2	2:D:510:ASP:OD2	2.25	0.68	
1:A:627:GLY:O	1:A:631:THR:N	2.23	0.67	
1:A:688:GLU:OE1	1:A:691:LYS:NZ	2.27	0.67	
1:A:72:ASN:ND2	5:A:809:NAG:O7	2.25	0.67	
1:C:122:TRP:CH2	1:C:252:ILE:HD11	2.29	0.67	
1:A:505:PRO:HD3	1:A:564:SER:HB2	1.77	0.67	
1:C:342:GLU:OE2	1:C:368:LYS:NZ	2.26	0.66	
1:C:625:SER:HB2	1:C:735:HIS:CE1	2.30	0.66	
1:G:448:ARG:HA	1:G:471:GLN:HG3	1.76	0.66	
1:E:635:LEU:HD11	1:E:645:GLY:HA3	1.77	0.65	
1:A:625:SER:HB2	1:A:735:HIS:CE1	2.31	0.65	



	A la C	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:466:ARG:NH1	1:C:468:SER:OG	2.28	0.65	
1:C:72:ASN:ND2	5:C:809:NAG:O7	2.30	0.65	
1:C:624:TRP:O	1:C:628:GLY:N	2.22	0.65	
1:G:415:ASN:HD22	1:G:421:PRO:HA	1.61	0.65	
1:A:691:LYS:HG2	1:A:723:VAL:HG22	1.77	0.65	
1:C:256:LYS:NZ	1:C:709:GLN:OE1	2.26	0.65	
1:A:240:LEU:HB2	1:A:244:LEU:HD12	1.77	0.65	
1:G:38:ARG:O	1:G:503:GLN:NE2	2.30	0.65	
1:G:448:ARG:HH21	1:G:472:ILE:HG22	1.63	0.64	
1:E:73:ASN:OD1	1:E:90:ASN:N	2.30	0.64	
1:E:38:ARG:O	1:E:503:GLN:NE2	2.31	0.64	
1:A:621:ILE:HG23	1:A:631:THR:HG23	1.79	0.63	
1:G:73:ASN:OD1	1:G:90:ASN:N	2.29	0.63	
1:E:331:LYS:H	1:E:331:LYS:HD2	1.62	0.63	
1:E:593:LEU:O	1:E:677:HIS:NE2	2.26	0.62	
1:E:190:ASP:O	1:E:233:ARG:NH2	2.32	0.62	
1:C:507:LYS:NZ	1:C:553:THR:O	2.24	0.62	
2:D:456:LEU:HB3	2:D:479:LEU:HD21	1.82	0.62	
1:G:625:SER:HB2	1:G:735:HIS:CE1	2.34	0.62	
1:A:359:PHE:HE2	1:A:384:ILE:HD11	1.64	0.62	
1:C:633:MET:O	1:C:686:ARG:NH1	2.33	0.61	
1:E:688:GLU:OE1	1:E:691:LYS:NZ	2.33	0.61	
1:C:635:LEU:HB3	1:C:693:VAL:HG21	1.83	0.61	
1:G:297:ASP:HB3	7:ASP:HB3 1:G:309:GLN:HB2		0.61	
1:E:699:HIS:ND1	1:E:711:SER:OG	2.24	0.61	
1:G:65:GLU:OE2	1:G:109:ARG:NH2	2.26	0.61	
1:A:543:ALA:HB3	1:A:630:VAL:HG21	1.83	0.61	
1:C:110:GLN:OE1	1:C:136:ASN:ND2	2.32	0.61	
1:G:448:ARG:HG3	1:G:471:GLN:HB2	1.81	0.61	
1:E:633:MET:O	1:E:686:ARG:NH1	2.34	0.61	
1:A:635:LEU:HB3	1:A:693:VAL:HG21	1.82	0.60	
5:C:801:NAG:H3	5:C:801:NAG:H83	1.83	0.60	
2:H:463:PRO:HB3	2:H:501:ASN:HA	1.82	0.60	
1:C:688:GLU:OE1	1:C:691:LYS:NZ	2.34	0.60	
1:G:352:PHE:O	:352:PHE:O 1:G:664:ARG:NH1		0.60	
2:H:394:PRO:HG3	2:H:400:LYS:HG3	1.82	0.60	
2:D:394:PRO:HG3	2:D:400:LYS:HG3	1.84	0.60	
2:H:456:LEU:HB3	2:H:479:LEU:HD21	1.84	0.60	
1:C:296:CYS:SG	1:C:311:LEU:HB2	2.42	0.60	
2:H:581:THR:HG22	2:H:581:THR:O	2.03	0.58	
1:G:89:GLU:O	1:G:92:THR:OG1	2.20	0.58	



	, and page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:153:ILE:O	1:G:154:ARG:NH2	2.35	0.58	
1:A:261:ASN:HD22	1:A:262:PRO:HD2	1.68	0.58	
1:C:543:ALA:HB3	1:C:630:VAL:HG21	1.86	0.58	
1:E:316:ASN:HA	1:E:349:VAL:HG23	1.86	0.58	
2:F:501:ASN:ND2	2:F:559:SER:OG	2.37	0.58	
2:B:421:ASN:ND2	2:B:483:THR:OG1	2.36	0.57	
1:A:633:MET:O	1:A:686:ARG:NH1	2.37	0.57	
1:G:351:ARG:NH2	1:G:399:VAL:O	2.25	0.57	
2:H:564:THR:CG2	2:H:565:GLU:N	2.67	0.57	
1:G:256:LYS:NZ	1:G:656:PHE:O	2.33	0.57	
1:C:80:ASP:OD1	1:C:462:TYR:OH	2.23	0.57	
1:E:479:SER:OG	1:E:482:ASN:OD1	2.23	0.57	
2:F:394:PRO:HG3	2:F:400:LYS:HG3	1.87	0.57	
1:E:297:ASP:HB3	1:E:309:GLN:HB2	1.87	0.56	
2:D:463:PRO:HB2	2:D:501:ASN:HA	1.88	0.56	
1:E:233:ARG:CZ	1:E:253:PRO:HG3	2.35	0.56	
1:A:507:LYS:NZ	1:A:553:THR:O	2.32	0.56	
2:D:381:VAL:HG13	2:D:382:GLU:H	1.70	0.56	
1:A:288:VAL:HG22	1:A:293:HIS:CB	2.35	0.56	
2:H:564:THR:HG22	2:H:565:GLU:H	1.69	0.56	
1:C:233:ARG:HH21	1:C:253:PRO:HG3	1.71	0.56	
1:G:153:ILE:HD12	1:G:164:TYR:HB3	1.86	0.56	
1:E:592:ARG:HH11	1:E:595:THR:HG21	1.71	0.55	
1:G:472:ILE:CD1	1:G:495:LEU:CD1	2.32	0.55	
1:E:405:LEU:HD21	1:E:410:LEU:HD12	1.88	0.55	
1:A:385:ASP:HB3	2:H:432:ALA:HB2	1.87	0.55	
1:A:538:LEU:HD23	1:A:620:ALA:HB3	1.88	0.55	
1:A:424:ARG:NH2	1:A:548:GLN:OE1	2.39	0.55	
2:H:421:ASN:OD1	2:H:483:THR:OG1	2.25	0.55	
2:D:402:LEU:HD12	2:D:443:LEU:HD23	1.88	0.55	
1:E:309:GLN:HG2	1:E:320:ILE:HG12	1.88	0.55	
1:G:309:GLN:HG2	1:G:320:ILE:HG12	1.89	0.55	
2:H:493:LYS:NZ	2:H:565:GLU:O	2.28	0.54	
1:A:107:PRO:HG2	1:A:156:SER:O	2.07	0.54	
1:G:316:ASN:HA	:316:ASN:HA 1:G:349:VAL:HG23		0.54	
1:C:621:ILE:HG23	1:C:631:THR:HG23	1.89	0.54	
1:C:131:ASP:OD1	1:C:145:ARG:NH2	2.38	0.54	
1:A:65:GLU:OE1	1:A:109:ARG:NH1	2.33	0.54	
1:G:374:GLU:N	1:G:374:GLU:OE1	2.41	0.54	
1:E:233:ARG:NH2	1:E:253:PRO:CG	2.63	0.54	
1:G:41:TYR:O	1:G:565:THR:OG1	2.25	0.54	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:625:SER:HB2	1:E:735:HIS:CE1	2.43	0.53	
1:E:597:GLU:OE1	1:E:597:GLU:N	2.41	0.53	
1:C:42:THR:N	1:C:45:ASP:OD2	2.40	0.53	
1:C:374:GLU:OE1	1:C:374:GLU:N	2.42	0.53	
2:D:408:ASN:HB3	2:D:587:LYS:HB3	1.91	0.53	
1:A:62:SER:OG	1:A:65:GLU:N	2.40	0.53	
1:A:147:PRO:O	1:A:150:THR:OG1	2.25	0.53	
1:A:244:LEU:HD11	1:A:248:LYS:HE3	1.89	0.53	
1:A:635:LEU:HD11	1:A:645:GLY:HA3	1.91	0.53	
1:C:383:GLN:HG3	1:C:386:LYS:HD2	1.90	0.53	
2:D:480:ILE:HB	2:D:571:PHE:HB2	1.91	0.53	
2:B:413:LYS:HE3	5:B:701:NAG:H62	1.91	0.53	
1:G:643:LYS:NZ	1:G:757:CYS:O	2.28	0.53	
1:G:666:MET:O	1:G:674:ASN:ND2	2.30	0.53	
1:A:312:ARG:NH2	2:B:510:ASP:OD2	2.39	0.52	
1:C:359:PHE:HE2	1:C:384:ILE:HD11	1.73	0.52	
1:A:161:LYS:NZ	1:A:218:GLY:O	2.39	0.52	
1:C:538:LEU:HD23	1:C:620:ALA:HB3	1.92	0.52	
1:E:621:ILE:HG23	1:E:631:THR:HG23	1.91	0.52	
2:F:564:THR:OG1	2:F:566:GLN:O	2.23	0.52	
1:A:131:ASP:OD1	1:A:145:ARG:NH2	2.43	0.52	
1:E:541:VAL:HG21	1:E:621:ILE:HD11	1.91	0.52	
1:A:255:PRO:O	1:A:255:PRO:HG2	2.09	0.52	
3:Q:1:NAG:O7	3:Q:1:NAG:O3	2.25	0.52	
1:A:504:MET:HE3	1:A:505:PRO:HD2	1.92	0.52	
1:A:305:ARG:NE	1:A:324:ASP:OD1	2.36	0.51	
1:C:452:TYR:HD2	1:C:465:LEU:HD22	1.74	0.51	
2:D:432:ALA:HB2	1:E:385:ASP:HB3	1.92	0.51	
1:C:238:VAL:HG12	1:C:240:LEU:HG	1.92	0.51	
1:A:367:TYR:CE2	1:A:381:LEU:HD23	2.46	0.51	
2:B:456:LEU:HD13	2:B:479:LEU:HD11	1.91	0.51	
2:D:392:THR:HG23	2:D:392:THR:O	2.09	0.51	
1:G:147:PRO:O	1:G:150:THR:OG1	2.29	0.51	
1:C:298:VAL:HG22	1:C:308:LEU:HD22	1.93	0.51	
1:C:367:TYR:CE2	1:C:381:LEU:HD23	2.46	0.51	
1:G:449:CYS:HB3	1:G:452:TYR:CZ	2.46	0.51	
1:A:261:ASN:OD1	1:A:313:ARG:NH2	2.44	0.50	
1:C:309:GLN:HG2	1:C:320:ILE:HG12	1.93	0.50	
1:G:367:TYR:CE2	1:G:381:LEU:HD23	2.46	0.50	
1:A:76:LEU:HB2	1:A:87:PHE:HB2	1.94	0.50	
1:C:153:ILE:O	1:C:154:ARG:NH2	2.43	0.50	



	to ac pagem	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:397:TRP:CE3	1:C:416:GLU:HB2	2.47	0.50	
1:C:510:ASP:HB3	1:C:521:TYR:CZ	2.46	0.50	
1:G:499:LEU:HD23	1:G:502:ILE:HD12	1.94	0.50	
2:B:448:TYR:OH	2:B:452:MET:O	2.25	0.50	
2:B:413:LYS:O	2:B:416:SER:OG	2.29	0.50	
1:C:339:GLN:O	1:C:340:HIS:ND1	2.45	0.50	
2:D:505:ARG:HG3	2:D:554:LEU:HD13	1.93	0.50	
1:G:378:HIS:ND1	1:G:393:THR:OG1	2.35	0.49	
2:H:587:LYS:HG3	5:H:701:NAG:H81	1.94	0.49	
1:A:62:SER:HG	1:A:64:HIS:H	1.60	0.49	
1:A:623:GLY:HA3	1:A:627:GLY:HA3	1.94	0.49	
1:E:635:LEU:HB3	1:E:693:VAL:HG21	1.93	0.49	
1:C:747:TYR:O	1:C:751:THR:OG1	2.26	0.49	
1:A:153:ILE:HG13	1:A:164:TYR:HB3	1.95	0.49	
1:E:643:LYS:NZ	1:E:757:CYS:O	2.26	0.49	
1:E:426:LEU:HD22	1:E:440:LEU:HD12	1.94	0.49	
1:G:338:ARG:NH2	1:G:385:ASP:OD1	2.36	0.49	
1:C:632:SER:OG	1:C:695:TYR:OH	2.25	0.48	
1:C:305:ARG:NH1	1:C:363:GLY:O	2.45	0.48	
1:E:63:ASP:OD1	1:E:63:ASP:N	2.45	0.48	
1:G:217:ASN:ND2	3:V:1:NAG:O7	2.46	0.48	
1:G:515:ASN:O	1:G:515:ASN:ND2	2.46	0.48	
2:H:381:VAL:O	2:H:408:ASN:N	2.46	0.48	
1:C:106:SER:HG	1:C:111:PHE:H	1.58	0.48	
1:G:312:ARG:NH2	2:H:510:ASP:OD2	2.37	0.48	
1:G:623:GLY:HA3	1:G:627:GLY:HA3	1.95	0.48	
1:A:153:ILE:O	1:A:154:ARG:NH2	2.46	0.48	
1:E:330:PRO:HD3	2:F:461:ALA:O	2.14	0.48	
1:G:285:PRO:O	1:G:288:VAL:HG12	2.14	0.48	
1:A:342:GLU:OE2	1:A:368:LYS:NZ	2.42	0.48	
1:G:76:LEU:HD12	1:G:87:PHE:CD1	2.49	0.48	
1:G:244:LEU:HD11	1:G:248:LYS:HE3	1.96	0.48	
1:G:699:HIS:ND1	1:G:711:SER:OG	2.29	0.48	
2:H:564:THR:CG2	2:H:565:GLU:H	2.24	0.48	
2:D:581:THR:O	581:THR:O 2:D:583:SER:N		0.48	
1:G:621:ILE:HG23	1:G:631:THR:HG23	1.96	0.48	
2:H:439:SER:CB	2:H:578:GLY:H	2.26	0.48	
1:E:41:TYR:O	1:E:565:THR:OG1	2.32	0.47	
1:G:96:PHE:HZ	1:G:131:ASP:HB2	1.79	0.47	
1:G:553:THR:HG21	1:G:555:LYS:HE2	1.96	0.47	
1:G:699:HIS:NE2	1:G:706:VAL:O	2.45	0.47	



	A h o	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:288:VAL:HG22	1:C:293:HIS:CB	2.44	0.47	
1:E:356:GLU:CD	1:E:356:GLU:H	2.17	0.47	
1:E:575:GLY:O	1:E:578:SER:OG	2.25	0.47	
1:G:593:LEU:HG	1:G:666:MET:HG2	1.96	0.47	
1:A:426:LEU:HD22	1:A:440:LEU:HD12	1.97	0.47	
2:F:413:LYS:O	2:F:416:SER:OG	2.31	0.47	
2:F:393:PRO:HG2	2:F:567:LEU:HD21	1.97	0.47	
2:F:502:LYS:HB3	2:F:557:SER:HB3	1.97	0.47	
1:A:288:VAL:HG22	1:A:293:HIS:HB2	1.96	0.47	
1:A:539:ILE:HD12	1:A:642:PHE:CE1	2.50	0.47	
2:D:413:LYS:O	2:D:416:SER:OG	2.33	0.47	
2:D:493:LYS:NZ	2:D:565:GLU:O	2.37	0.47	
1:G:466:ARG:HB3	1:G:466:ARG:NH1	2.22	0.47	
2:H:411:LEU:HD22	2:H:434:ALA:HB2	1.97	0.47	
1:A:449:CYS:HA	1:A:469:GLY:O	2.14	0.47	
2:B:419:SER:HB3	2:B:483:THR:HB	1.97	0.47	
1:E:156:SER:HB3	1:E:161:LYS:HB2	1.97	0.47	
1:E:338:ARG:NH2	1:E:385:ASP:OD1	2.29	0.47	
1:G:472:ILE:HG22	1:G:472:ILE:O	2.14	0.47	
1:C:539:ILE:HD12	1:C:642:PHE:CE2	2.50	0.47	
1:C:536:PRO:HB3	1:C:618:ARG:HB3	1.97	0.46	
2:D:393:PRO:HB2	2:D:447:SER:OG	2.15	0.46	
1:E:76:LEU:HD12	1:E:87:PHE:CD1	2.50	0.46	
1:E:456:PHE:CD2	1:E:463:TYR:HB3	2.51	0.46	
1:G:541:VAL:HG21	1:G:621:ILE:HD11	1.97	0.46	
2:H:439:SER:HB3	2:H:578:GLY:H	1.80	0.46	
1:C:736:GLY:C	1:C:738:ALA:H	2.16	0.46	
1:A:539:ILE:HD12	1:A:642:PHE:HE1	1.79	0.46	
1:C:211:ALA:HB1	1:C:224:ALA:HB3	1.98	0.46	
2:F:428:ILE:HB	2:F:476:PRO:HB3	1.98	0.46	
1:G:456:PHE:CD2	1:G:463:TYR:HB3	2.51	0.46	
1:C:373:SER:OG	1:C:374:GLU:OE1	2.22	0.46	
1:E:131:ASP:HB3	1:E:140:LEU:HD11	1.97	0.46	
2:F:439:SER:CB	2:F:578:GLY:H	2.28	0.46	
2:B:463:PRO:HB3	2:B:501:ASN:HA	1.97	0.45	
1:E:92:THR:C	1:E:94:ASP:H	2.20	0.45	
1:A:41:TYR:O	1:A:565:THR:OG1	2.33	0.45	
1:A:285:PRO:O	1:A:288:VAL:HG12	2.16	0.45	
1:C:622:TRP:HB2	1:C:646:ILE:HB	1.98	0.45	
1:A:589:ILE:HD11	1:A:597:GLU:OE1	2.17	0.45	
2:D:397:TYR:HB3	2:D:468:ASN:OD1	2.17	0.45	



	t i c	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:625:SER:HB2	1:G:735:HIS:HE1	1.82	0.45	
1:G:704:ASP:OD1	1:G:704:ASP:N	2.43	0.45	
1:C:107:PRO:HG2	1:C:156:SER:O	2.15	0.45	
1:C:472:ILE:HD13	1:C:495:LEU:HB3	1.98	0.45	
2:D:439:SER:HB3	2:D:578:GLY:H	1.81	0.45	
1:A:157:PRO:HD3	1:A:214:TRP:HB3	1.99	0.45	
1:C:448:ARG:HA	1:C:471:GLN:HB2	1.99	0.45	
1:C:625:SER:HB2	1:C:735:HIS:NE2	2.32	0.45	
1:A:448:ARG:HG3	1:A:471:GLN:HB2	1.99	0.45	
1:C:267:TYR:CE2	1:C:281:GLN:HB2	2.51	0.45	
1:C:288:VAL:HG22	1:C:293:HIS:HB3	1.98	0.45	
1:G:465:LEU:HD23	1:G:465:LEU:HA	1.72	0.45	
1:G:313:ARG:NH2	1:G:663:GLU:OE2	2.36	0.45	
2:H:413:LYS:O	2:H:416:SER:OG	2.33	0.45	
1:A:42:THR:N	1:A:45:ASP:OD2	2.48	0.44	
1:A:397:TRP:CE3	1:A:416:GLU:HB2	2.53	0.44	
1:C:53:MET:SD	1:C:473:PRO:HG2	2.57	0.44	
1:E:217:ASN:ND2	3:R:1:NAG:O7	2.49	0.44	
2:F:439:SER:HB3	2:F:578:GLY:H	1.82	0.44	
2:F:563:MET:SD	2:F:564:THR:N	2.90	0.44	
1:G:132:ILE:HB	1:G:141:ILE:HD12	2.00	0.44	
1:A:595:THR:O	1:A:599:GLU:HG3	2.17	0.44	
1:G:68:TYR:HB3	1:G:77:PHE:CE2	2.52	0.44	
1:G:338:ARG:HH21	1:G:385:ASP:CG	2.20	0.44	
1:G:538:LEU:HD23	1:G:620:ALA:HB3	2.00	0.44	
1:A:359:PHE:CE2	1:A:384:ILE:HD11	2.50	0.44	
1:A:362:ASP:O	1:A:364:ASN:ND2	2.51	0.44	
1:C:125:SER:HB3	1:C:209:HIS:CD2	2.52	0.44	
1:C:261:ASN:HD22	1:C:262:PRO:HD2	1.83	0.44	
1:C:539:ILE:HD12	1:C:642:PHE:HE2	1.83	0.44	
1:E:244:LEU:CD1	1:E:246:TYR:O	2.66	0.44	
1:A:382:PHE:CE2	1:A:389:CYS:HB3	2.52	0.44	
1:E:198:ASP:OD2	1:E:262:PRO:HG3	2.17	0.44	
1:G:526:PRO:HD3	G:526:PRO:HD3 1:G:569:ILE:HG12		0.44	
1:A:121:LYS:HB3	1:A:125:SER:OG	2.17	0.44	
1:A:351:ARG:HD3	1:A:546:CYS:SG	2.58	0.44	
2:B:493:LYS:NZ	2:B:565:GLU:O	2.46	0.44	
1:G:589:ILE:HG23	1:G:593:LEU:HD23	1.99	0.44	
1:C:368:LYS:HG2	1:C:382:PHE:HE1	1.82	0.43	
1:C:617:LYS:HE2	1:C:617:LYS:HB2	1.73	0.43	
1:C:677:HIS:NE2	1:C:681:SER:HB3	2.34	0.43	



	A la C	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:F:382:GLU:HG3	2:F:408:ASN:O	2.18	0.43	
2:F:498:SER:HB3	2:F:534:VAL:HG23	2.00	0.43	
2:H:413:LYS:HE3	2:H:413:LYS:HB2	1.88	0.43	
1:A:384:ILE:HD13	1:A:384:ILE:HA	1.81	0.43	
1:C:297:ASP:OD2	1:C:299:THR:OG1	2.36	0.43	
1:E:48:LYS:HD3	1:E:48:LYS:HA	1.86	0.43	
1:E:515:ASN:ND2	1:E:515:ASN:O	2.49	0.43	
1:C:121:LYS:HB2	1:C:126:TYR:HA	2.00	0.43	
1:G:543:ALA:HB3	1:G:630:VAL:HG21	2.00	0.43	
1:G:668:LEU:HB3	1:G:670:THR:HG23	2.00	0.43	
1:A:96:PHE:CE2	1:A:140:LEU:HD13	2.54	0.43	
1:C:575:GLY:O	1:C:578:SER:OG	2.27	0.43	
1:C:78:ASN:OD1	1:C:80:ASP:HB2	2.18	0.43	
1:C:382:PHE:CE2	1:C:389:CYS:HB3	2.54	0.43	
1:E:400:ILE:HG13	1:E:424:ARG:HD2	2.01	0.43	
1:C:65:GLU:CD	1:C:109:ARG:HH22	2.22	0.43	
1:C:233:ARG:NH2	1:C:253:PRO:HG3	2.32	0.43	
1:E:424:ARG:NH2	1:E:548:GLN:OE1	2.52	0.43	
1:C:65:GLU:OE1	1:C:109:ARG:NH1	2.51	0.43	
1:C:538:LEU:O	1:C:570:VAL:HA	2.19	0.43	
1:E:622:TRP:HB2	1:E:646:ILE:HB	2.01	0.43	
1:C:650:PRO:HG3	1:C:697:LEU:HD11	2.01	0.43	
2:D:456:LEU:HD13	2:D:479:LEU:HD11	2.00	0.43	
1:G:326:ASN:HB3	1:G:330:PRO:O	2.19	0.43	
1:A:123:ARG:HD2	1:A:203:GLU:OE1	2.19	0.42	
1:A:622:TRP:HB2	1:A:646:ILE:HB	2.01	0.42	
1:C:217:ASN:ND2	3:M:1:NAG:O7	2.52	0.42	
1:C:384:ILE:HD13	1:C:384:ILE:HA	1.91	0.42	
1:E:405:LEU:HA	1:E:405:LEU:HD23	1.78	0.42	
1:G:68:TYR:HB3	1:G:77:PHE:HE2	1.84	0.42	
1:C:631:THR:O	1:C:635:LEU:HG	2.19	0.42	
1:E:68:TYR:HB3	1:E:77:PHE:CE2	2.54	0.42	
1:G:183:VAL:HG22	1:G:274:LEU:HD11	2.00	0.42	
1:G:288:VAL:HG22	1:G:293:HIS:CB	2.48	0.42	
1:G:356:GLU:OE1	G:356:GLU:OE1 1:G:356:GLU:N		0.42	
1:G:538:LEU:HD11	1:G:622:TRP:CD1	2.54	0.42	
1:A:309:GLN:HG2	1:A:320:ILE:HG12	2.01	0.42	
1:A:452:TYR:HD2	1:A:465:LEU:HD22	1.84	0.42	
2:B:581:THR:O	2:B:583:SER:N	2.52	0.42	
1:C:81:HIS:HB2	1:C:83:ASN:HB2	2.00	0.42	
1:C:197:THR:OG1	1:C:202:GLU:HB2	2.19	0.42	



	to do pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:424:ARG:NH2	1:C:548:GLN:OE1	2.53	0.42	
1:G:267:TYR:CE2	1:G:281:GLN:HB2	2.54	0.42	
2:B:425:CYS:HA	2:B:478:CYS:HA	2.00	0.42	
1:E:448:ARG:HG3	1:E:471:GLN:HB3	2.02	0.42	
1:G:417:TYR:CE1	1:G:442:CYS:HB3	2.55	0.42	
1:A:267:TYR:CE2	1:A:281:GLN:HB2	2.54	0.42	
1:C:504:MET:HE3	1:C:505:PRO:HD2	2.01	0.42	
1:E:488:LEU:HD21	1:E:491:ASN:HB2	2.02	0.42	
1:G:589:ILE:CD1	1:G:596:PHE:HB2	2.50	0.42	
1:A:367:TYR:HD1	1:A:405:LEU:HD11	1.84	0.42	
1:A:542:TYR:HB2	1:A:549:LYS:HD3	2.01	0.42	
1:C:542:TYR:HB2	1:C:549:LYS:HD3	2.01	0.42	
1:A:53:MET:SD	1:A:473:PRO:HG2	2.60	0.42	
1:E:704:ASP:OD1	1:E:704:ASP:N	2.39	0.42	
1:G:108:ASP:N	1:G:108:ASP:OD1	2.53	0.42	
1:G:453:SER:OG	1:G:466:ARG:HB2	2.19	0.42	
1:C:385:ASP:HB3	2:F:432:ALA:HB2	2.01	0.42	
1:E:666:MET:HB3	1:E:666:MET:HE3	1.88	0.42	
1:E:623:GLY:HA3	1:E:627:GLY:HA3	2.02	0.41	
1:E:591:ARG:HH11	1:E:591:ARG:HD3	1.69	0.41	
2:H:502:LYS:HB3	2:H:557:SER:HB3	2.01	0.41	
2:D:506:LEU:HB3	2:D:553:TRP:HB2	2.03	0.41	
2:F:408:ASN:HA	2:F:585:CYS:O	2.20	0.41	
1:G:288:VAL:HG22	1:G:293:HIS:HB3	2.01	0.41	
1:G:305:ARG:NH1	1:G:363:GLY:O	2.54	0.41	
1:G:383:GLN:HB2	1:G:386:LYS:HB2	2.02	0.41	
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.77	0.41	
1:C:121:LYS:HB3	1:C:125:SER:OG	2.21	0.41	
1:C:173:LYS:HE3	1:C:178:SER:O	2.20	0.41	
1:C:405:LEU:HD23	1:C:405:LEU:HA	1.80	0.41	
1:E:215:SER:HB3	1:E:220:PHE:HB2	2.02	0.41	
1:E:244:LEU:HD13	1:E:246:TYR:O	2.20	0.41	
1:E:280:ALA:HB1	1:E:331:LYS:HD3	2.02	0.41	
1:G:448:ARG:HA	1:G:471:GLN:CG	2.49	0.41	
1:G:630:VAL:O	1:G:634:VAL:N	2.46	0.41	
2:H:423:PHE:CD1	2:H:480:ILE:HG12	2.56	0.41	
1:A:370:MET:HE3	1:A:370:MET:HB3	2.00	0.41	
1:A:703:ASP:OD1	1:A:706:VAL:N	2.46	0.41	
1:E:147:PRO:O	1:E:150:THR:OG1	2.37	0.41	
1:E:382:PHE:CE1	1:E:389:CYS:HB3	2.56	0.41	
1:E:448:ARG:HA	1:E:471:GLN:HB2	2.02	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:G:529:PHE:HE1	1:G:569:ILE:HD11	1.85	0.41	
1:C:285:PRO:O	1:C:288:VAL:HG12	2.21	0.41	
1:C:297:ASP:HB3	1:C:309:GLN:HB2	2.03	0.41	
1:A:298:VAL:HG22	1:A:308:LEU:HD22	2.02	0.41	
1:A:541:VAL:HG21	1:A:621:ILE:HD11	2.03	0.41	
1:C:605:ALA:HA	1:C:608:PHE:HD2	1.86	0.41	
1:E:68:TYR:HB3	1:E:77:PHE:HE2	1.85	0.41	
1:E:101:SER:N	1:E:115:GLU:O	2.47	0.41	
1:E:307:SER:HA	1:E:321:ASP:O	2.20	0.41	
1:E:331:LYS:H	1:E:331:LYS:CD	2.25	0.41	
1:A:255:PRO:O	1:A:255:PRO:CG	2.69	0.41	
1:A:400:ILE:HG13	1:A:424:ARG:CD	2.51	0.41	
1:C:495:LEU:HA	1:C:495:LEU:HD23	1.81	0.41	
2:D:392:THR:O	2:D:392:THR:CG2	2.69	0.41	
2:D:429:SER:OG	1:E:385:ASP:OD1	2.32	0.41	
1:E:666:MET:O	1:E:674:ASN:ND2	2.36	0.41	
1:G:654:TRP:HB3	1:G:662:THR:CG2	2.50	0.41	
1:C:556:LEU:HD23	1:C:556:LEU:HA	1.90	0.41	
1:A:538:LEU:O	1:A:570:VAL:HA	2.21	0.40	
2:B:480:ILE:HB	2:B:571:PHE:HB2	2.02	0.40	
1:C:385:ASP:OD1	2:F:429:SER:OG	2.25	0.40	
1:A:513:HIS:O	1:A:514:LEU:HD23	2.22	0.40	
1:C:76:LEU:HB2	1:C:87:PHE:HB2	2.03	0.40	
1:C:506:ARG:O	1:C:525:LEU:N	2.42	0.40	
1:C:734:ASP:OD1	1:C:734:ASP:N	2.43	0.40	
2:H:423:PHE:CZ	2:H:430:PRO:HB3	2.56	0.40	
2:H:507:LEU:HA	2:H:507:LEU:HD23	1.83	0.40	
1:C:456:PHE:CD2	1:C:463:TYR:HB3	2.55	0.40	
1:E:312:ARG:HD2	1:E:317:TYR:HB3	2.04	0.40	
1:E:326:ASN:HB3	1:E:330:PRO:O	2.21	0.40	
1:E:431:LEU:HD23	1:E:431:LEU:HA	1.91	0.40	
1:E:439:CYS:SG	39:CYS:SG 1:E:442:CYS:N		0.40	
2:H:501:ASN:ND2	2:H:501:ASN:ND2 2:H:559:SER:OG		0.40	
2:B:505:ARG:HG3	2:B:554:LEU:HD13	2.03	0.40	
1:C:351:ARG:HB3	1:C:546:CYS:SG	2.62	0.40	
1:C:621:ILE:O	1:C:645:GLY:HA2	2.22	0.40	
1:G:491:ASN:HD22	1:G:493:THR:HG23	1.87	0.40	
1:G:512:LEU:HD23	1:G:521:TYR:CD2	2.55	0.40	
3:I:1:NAG:O4	3:I:2:NAG:O7	2.40	0.40	

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	722/731~(99%)	682 (94%)	39~(5%)	1 (0%)	51	83
1	С	722/731~(99%)	682 (94%)	40 (6%)	0	100	100
1	Е	722/731~(99%)	688~(95%)	34~(5%)	0	100	100
1	G	722/731~(99%)	685~(95%)	37~(5%)	0	100	100
2	В	206/246~(84%)	197~(96%)	9 (4%)	0	100	100
2	D	206/246~(84%)	193 (94%)	13~(6%)	0	100	100
2	F	206/246~(84%)	199~(97%)	7 (3%)	0	100	100
2	Н	206/246~(84%)	199 (97%)	7(3%)	0	100	100
All	All	3712/3908~(95%)	3525 (95%)	186 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	97	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percer	ntiles
1	А	641/649~(99%)	628~(98%)	13~(2%)	55	80
1	С	641/649~(99%)	619 (97%)	22 (3%)	37	69
1	Ε	641/649~(99%)	624 (97%)	17 (3%)	44	74
1	G	641/649~(99%)	623~(97%)	18 (3%)	43	73



Mol	Chain	Analysed Rotameric Outliers		Perce	ntiles	
2	В	190/221~(86%)	185~(97%)	5(3%)	46	74
2	D	190/221~(86%)	186 (98%)	4 (2%)	53	79
2	F	190/221~(86%)	188~(99%)	2(1%)	73	89
2	Н	190/221~(86%)	183 (96%)	7 (4%)	34	66
All	All	3324/3480~(96%)	3236 (97%)	88 (3%)	46	74

Continued from previous page...

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	52	ARG
1	А	93	PHE
1	А	96	PHE
1	А	101	SER
1	А	160	HIS
1	А	228	ASP
1	А	244	LEU
1	А	338	ARG
1	А	368	LYS
1	А	370	MET
1	А	380	CYS
1	А	433	ASN
1	А	467	CYS
2	В	423	PHE
2	В	438	TYR
2	В	455	ASP
2	В	510	ASP
2	В	580	ASP
1	С	52	ARG
1	С	84	SER
1	С	91	SER
1	С	93	PHE
1	С	98	HIS
1	С	139	GLN
1	С	210	SER
1	С	228	ASP
1	С	233	ARG
1	С	244	LEU
1	С	278	GLU
1	С	338	ARG
1	С	368	LYS
1	С	380	CYS



Mol	Chain	Res	Type
1	С	405	LEU
1	С	426	LEU
1	С	433	ASN
1	С	467	CYS
1	С	495	LEU
1	С	561	TYR
1	С	624	TRP
1	С	625	SER
2	D	423	PHE
2	D	438	TYR
2	D	455	ASP
2	D	510	ASP
1	Е	62	SER
1	Е	95	GLN
1	Е	210	SER
1	Е	217	ASN
1	Е	233	ARG
1	Е	241	ASP
1	Е	278	GLU
1	Е	296	CYS
1	Е	309	GLN
1	Е	331	LYS
1	Е	370	MET
1	Е	380	CYS
1	Е	405	LEU
1	Е	433	ASN
1	Е	465	LEU
1	Е	467	CYS
1	Е	471	GLN
2	F	423	PHE
2	F	438	TYR
1	G	38	ARG
1	G	52	ARG
1	G	188	ARG
1	G	217	ASN
1	G	230	ASP
1	G	233	ARG
1	G	261	ASN
1	G	278	GLU
1	G	380	CYS
1	G	465	LEU
1	G	466	ARG



Mol	Chain	Res	Type
1	G	472	ILE
1	G	473	PRO
1	G	476	SER
1	G	488	LEU
1	G	589	ILE
1	G	592	ARG
1	G	617	LYS
2	Н	406	ASN
2	Н	423	PHE
2	Н	438	TYR
2	Н	440	SER
2	H	455	ASP
2	Н	509	ASP
2	Н	510	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	64	HIS
1	А	110	GLN
1	А	136	ASN
1	А	364	ASN
1	А	503	GLN
1	С	209	HIS
1	С	364	ASN
1	С	425	ASN
1	Е	72	ASN
1	Е	383	GLN
2	F	501	ASN
1	G	500	GLN
1	G	726	GLN
2	Н	408	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)

38 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	Turne	Chain	Dec	Tink	LinkBond lengthsBond angles			les		
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	NAG	Ι	1	3,1	14,14,15	0.35	0	17,19,21	0.64	1 (5%)
3	NAG	Ι	2	3	14,14,15	0.36	0	17,19,21	0.39	0
4	NAG	J	1	4,1	14,14,15	0.56	1 (7%)	17,19,21	0.61	0
4	NAG	J	2	4	14,14,15	0.55	0	17,19,21	0.65	0
4	BMA	J	3	4	11,11,12	1.22	1 (9%)	15,15,17	1.16	1 (6%)
3	NAG	K	1	3,1	14,14,15	0.39	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	L	1	3,1	14,14,15	0.29	0	17,19,21	0.42	0
3	NAG	L	2	3	14,14,15	0.35	0	17,19,21	0.40	0
3	NAG	М	1	3,1	14,14,15	0.35	0	17,19,21	0.63	1 (5%)
3	NAG	М	2	3	14,14,15	0.34	0	17,19,21	0.36	0
4	NAG	N	1	4,1	14,14,15	0.45	0	17,19,21	0.63	0
4	NAG	N	2	4	14,14,15	0.51	0	17,19,21	0.67	0
4	BMA	Ν	3	4	11,11,12	1.25	1 (9%)	15,15,17	1.14	2 (13%)
3	NAG	0	1	3,1	14,14,15	0.38	0	17,19,21	0.57	0
3	NAG	0	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	NAG	Р	1	3,1	$14,\!14,\!15$	0.32	0	17,19,21	0.47	0
3	NAG	Р	2	3	$14,\!14,\!15$	0.22	0	17,19,21	0.44	0
3	NAG	Q	1	3,1	14,14,15	0.58	0	17,19,21	0.86	0
3	NAG	Q	2	3	$14,\!14,\!15$	0.48	0	17,19,21	0.52	0
3	NAG	R	1	3,1	14,14,15	0.38	0	17,19,21	0.66	1 (5%)
3	NAG	R	2	3	14,14,15	0.17	0	17,19,21	0.40	0
4	NAG	S	1	4,1	14,14,15	0.44	0	17,19,21	0.62	0
4	NAG	S	2	4	$14,\!14,\!15$	0.33	0	17,19,21	0.61	0
4	BMA	S	3	4	11,11,12	1.20	1 (9%)	$15,\!15,\!17$	1.20	2 (13%)
3	NAG	Т	1	3,1	14,14,15	0.32	0	17,19,21	0.48	0
3	NAG	Т	2	3	14,14,15	0.14	0	17,19,21	0.74	1 (5%)
3	NAG	U	1	3,1	14,14,15	0.48	0	17,19,21	0.51	0
3	NAG	U	2	3	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	V	1	3,1	14,14,15	0.34	0	17,19,21	0.65	1 (5%)



Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
WIOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	NAG	V	2	3	$14,\!14,\!15$	0.19	0	17,19,21	0.48	0
4	NAG	W	1	4,1	14,14,15	0.40	0	17,19,21	0.55	0
4	NAG	W	2	4	$14,\!14,\!15$	0.21	0	17,19,21	0.51	0
4	BMA	W	3	4	11,11,12	1.19	1 (9%)	$15,\!15,\!17$	1.27	3 (20%)
3	NAG	Х	1	3,1	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	Х	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	Y	1	3,1	14,14,15	0.37	0	17,19,21	0.42	0
3	NAG	Y	2	3	14,14,15	0.17	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Ι	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Ι	2	3	_	1/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
3	NAG	К	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	К	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	М	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	М	2	3	-	0/6/23/26	0/1/1/1
4	NAG	Ν	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Ν	2	4	-	3/6/23/26	0/1/1/1
4	BMA	N	3	4	-	1/2/19/22	0/1/1/1
3	NAG	Ο	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	0	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Р	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Р	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1



6L8Q

Mol		Chain	Res	Link	Chirals	Torsions	Rings
WIOI	турс	Cham	ICCS	LIIIK	Cimais	101310113	Tungs
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	1/2/19/22	0/1/1/1
3	NAG	Т	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Т	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	3/6/23/26	0/1/1/1
4	BMA	W	3	4	-	2/2/19/22	0/1/1/1
3	NAG	Х	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Х	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	Ν	3	BMA	C1-C2	3.57	1.60	1.52
4	J	3	BMA	C1-C2	3.35	1.59	1.52
4	S	3	BMA	C1-C2	2.50	1.57	1.52
4	W	3	BMA	C1-C2	2.47	1.57	1.52
4	J	1	NAG	O5-C1	-2.00	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	S	3	BMA	O2-C2-C3	-2.72	104.69	110.14
4	W	3	BMA	O2-C2-C3	-2.65	104.83	110.14
4	W	3	BMA	C1-C2-C3	-2.62	106.45	109.67
3	Т	2	NAG	C1-O5-C5	2.56	115.67	112.19
3	R	1	NAG	C1-O5-C5	2.26	115.26	112.19
3	V	1	NAG	C1-O5-C5	2.25	115.23	112.19
3	Ι	1	NAG	C1-O5-C5	2.24	115.23	112.19
3	М	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	Ν	3	BMA	O2-C2-C3	-2.15	105.82	110.14
4	J	3	BMA	O2-C2-C3	-2.14	105.85	110.14
4	S	3	BMA	C1-C2-C3	-2.07	107.12	109.67



001100													
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$						
4	N	3	BMA	C1-O5-C5	-2.04	109.43	112.19						
4	W	3	BMA	O5-C1-C2	-2.01	107.67	110.77						

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
3	Р	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C1-C2-N2-C7
3	0	2	NAG	O5-C5-C6-O6
3	Х	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	Х	2	NAG	O5-C5-C6-O6
3	0	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	Р	2	NAG	C4-C5-C6-O6
3	Р	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
4	W	3	BMA	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	Х	1	NAG	C4-C5-C6-O6
3	Х	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	Ν	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2



Mol	Chain	Res	Type	Atoms
3	U	2	NAG	C4-C5-C6-O6
3	М	1	NAG	O5-C5-C6-O6
3	0	1	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
4	Ν	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	Р	1	NAG	C4-C5-C6-O6
3	Ι	1	NAG	O5-C5-C6-O6
3	0	1	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	Κ	2	NAG	O5-C5-C6-O6
3	М	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	Ι	1	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
4	Ν	3	BMA	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
4	Ν	2	NAG	O5-C5-C6-O6
3	Ι	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	W	3	BMA	C4-C5-C6-O6
3	Т	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C3-C2-N2-C7
3	L	1	NAG	O5-C5-C6-O6
3	Т	2	NAG	O5-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6

Continued from previous page...

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	NAG	1	0
3	М	1	NAG	1	0
3	Ι	1	NAG	1	0



Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	1	NAG	1	0
3	Ι	2	NAG	1	0
3	Q	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





























Rings



Torsions

















































5.6 Ligand geometry (i)

11 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	Mol Type Chain		Dog	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
MOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	701	2	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	Н	701	2	14,14,15	0.22	0	17,19,21	0.37	0
5	NAG	В	701	2	$14,\!14,\!15$	0.20	0	$17,\!19,\!21$	0.49	0
5	NAG	G	801	1	14,14,15	0.17	0	17,19,21	1.02	1 (5%)
5	NAG	F	701	2	14,14,15	0.19	0	17,19,21	0.37	0
5	NAG	G	809	1	$14,\!14,\!15$	0.32	0	$17,\!19,\!21$	0.45	0
5	NAG	Е	810	1	$14,\!14,\!15$	0.28	0	$17,\!19,\!21$	0.42	0
5	NAG	С	809	1	$14,\!14,\!15$	0.25	0	$17,\!19,\!21$	0.46	0
5	NAG	А	809	1	14,14,15	0.24	0	$17,\!19,\!21$	0.44	0
5	NAG	A	801	1	14,14,15	0.40	0	17,19,21	0.58	0
5	NAG	C	801	1	14,14,15	0.74	1 (7%)	17,19,21	1.38	3 (17%)

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
5	NAG	D	701	2	-	2/6/23/26	0/1/1/1
5	NAG	Н	701	2	-	1/6/23/26	0/1/1/1
5	NAG	В	701	2	-	2/6/23/26	0/1/1/1
5	NAG	G	801	1	-	3/6/23/26	0/1/1/1
5	NAG	F	701	2	-	2/6/23/26	0/1/1/1
5	NAG	G	809	1	-	0/6/23/26	0/1/1/1
5	NAG	Е	810	1	-	2/6/23/26	0/1/1/1
5	NAG	С	809	1	-	2/6/23/26	0/1/1/1
5	NAG	А	809	1	-	2/6/23/26	0/1/1/1
5	NAG	А	801	1	-	2/6/23/26	0/1/1/1
5	NAG	С	801	1	-	4/6/23/26	0/1/1/1



All ((1)	bond	length	outliers	are	listed	below:
1 TII (<u> </u>	bond	1011S011	outilitit	arc	moucu	DC10W.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	С	801	NAG	C1-C2	2.36	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	С	801	NAG	C2-N2-C7	4.25	128.96	122.90
5	G	801	NAG	C1-O5-C5	3.83	117.38	112.19
5	С	801	NAG	C1-O5-C5	2.57	115.67	112.19
5	С	801	NAG	C1-C2-N2	2.08	114.04	110.49

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	701	NAG	C4-C5-C6-O6
5	В	701	NAG	C4-C5-C6-O6
5	А	809	NAG	O5-C5-C6-O6
5	С	809	NAG	O5-C5-C6-O6
5	D	701	NAG	O5-C5-C6-O6
5	В	701	NAG	O5-C5-C6-O6
5	А	809	NAG	C4-C5-C6-O6
5	G	801	NAG	O5-C5-C6-O6
5	F	701	NAG	C4-C5-C6-O6
5	С	801	NAG	C8-C7-N2-C2
5	С	801	NAG	O7-C7-N2-C2
5	С	801	NAG	O5-C5-C6-O6
5	А	801	NAG	O5-C5-C6-O6
5	G	801	NAG	C4-C5-C6-O6
5	Е	810	NAG	C4-C5-C6-O6
5	А	801	NAG	C4-C5-C6-O6
5	С	809	NAG	C4-C5-C6-O6
5	F	701	NAG	O5-C5-C6-O6
5	Е	810	NAG	O5-C5-C6-O6
5	Н	701	NAG	O5-C5-C6-O6
5	G	801	NAG	C1-C2-N2-C7
5	С	801	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Н	701	NAG	1	0
5	В	701	NAG	1	0
5	С	809	NAG	1	0
5	А	809	NAG	1	0
5	С	801	NAG	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)

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			$OWAB(Å^2)$	Q < 0.9
1	А	724/731~(99%)	-0.11	2 (0%)	94	88	28, 54, 90, 147	0
1	С	724/731~(99%)	-0.10	2(0%)	94	88	30, 53, 89, 154	0
1	Ε	724/731~(99%)	-0.09	5 (0%)	87	75	31, 63, 105, 188	0
1	G	724/731~(99%)	-0.09	5 (0%)	87	75	29, 62, 105, 161	0
2	В	208/246~(84%)	-0.06	1 (0%)	91	81	35, 58, 94, 166	0
2	D	208/246~(84%)	-0.08	0 100) 1	00	37, 58, 98, 173	0
2	F	208/246~(84%)	-0.07	3(1%)	75	56	37, 60, 102, 219	0
2	Н	208/246~(84%)	-0.10	1 (0%)	91	81	38, 62, 104, 196	0
All	All	3728/3908~(95%)	-0.09	19 (0%)	91	81	28, 58, 98, 219	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	579	THR	5.4
1	Е	277	LEU	5.2
1	Е	276	ASP	5.1
1	С	276	ASP	3.2
1	С	277	LEU	3.0
1	G	276	ASP	3.0
1	А	760	LEU	2.7
2	F	580	ASP	2.7
2	В	579	THR	2.6
1	Е	278	GLU	2.4
1	Е	172	VAL	2.4
1	G	277	LEU	2.3
1	G	274	LEU	2.3
2	F	411	LEU	2.2
1	Е	275	THR	2.2
1	G	133	TYR	2.1



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	Н	579	THR	2.1
1	G	137	LYS	2.1
1	А	137	LYS	2.0

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

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

6.3 Carbohydrates (i)

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	$B-factors(A^2)$	Q<0.9
3	NAG	Q	1	14/15	0.69	0.26	36,70,77,78	0
3	NAG	М	2	14/15	0.71	0.24	87,112,129,131	0
3	NAG	Ι	2	14/15	0.72	0.19	97,119,133,133	0
3	NAG	K	2	14/15	0.72	0.29	120,135,140,146	0
4	BMA	S	3	11/12	0.72	0.20	78,88,93,94	0
3	NAG	0	2	14/15	0.75	0.28	108,126,133,137	0
3	NAG	Т	2	14/15	0.76	0.21	104,122,132,135	0
4	BMA	N	3	11/12	0.78	0.29	71,81,88,92	0
4	BMA	J	3	11/12	0.78	0.25	70,82,89,89	0
3	NAG	R	2	14/15	0.79	0.22	65,93,105,107	0
4	BMA	W	3	11/12	0.79	0.21	70,74,83,83	0
3	NAG	L	2	14/15	0.81	0.19	80,91,95,96	0
3	NAG	U	2	14/15	0.84	0.15	93,100,106,109	0
3	NAG	Р	2	14/15	0.86	0.18	75,86,92,94	0
3	NAG	Х	2	14/15	0.86	0.19	101,115,126,127	0
3	NAG	V	2	14/15	0.87	0.18	72,99,108,109	0
3	NAG	Y	2	14/15	0.89	0.18	89,97,105,109	0
3	NAG	М	1	14/15	0.92	0.15	70,83,88,99	0
3	NAG	R	1	14/15	0.92	0.20	91,96,105,109	0
3	NAG	Q	2	14/15	0.93	0.21	35,47,65,78	0
3	NAG	V	1	14/15	0.93	0.18	84,96,107,114	0
3	NAG	K	1	14/15	0.93	0.17	71,80,98,109	0
4	NAG	N	2	14/15	0.94	0.19	55,63,75,76	0
3	NAG	Ι	1	14/15	0.94	0.14	73,84,91,102	0
4	NAG	J	1	14/15	0.94	0.18	43,49,58,60	0



001111											
Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9			
3	NAG	L	1	14/15	0.94	0.15	$65,\!75,\!83,\!85$	0			
4	NAG	S	1	14/15	0.95	0.21	$59,\!63,\!67,\!68$	0			
4	NAG	S	2	14/15	0.95	0.15	51,68,77,80	0			
3	NAG	Т	1	14/15	0.95	0.11	60,74,85,91	0			
4	NAG	W	2	14/15	0.95	0.15	52,70,79,80	0			
3	NAG	Х	1	14/15	0.95	0.14	59,71,80,85	0			
4	NAG	N	1	14/15	0.96	0.17	38,45,54,57	0			
3	NAG	Р	1	14/15	0.96	0.16	59,72,80,81	0			
4	NAG	W	1	14/15	0.96	0.19	$53,\!60,\!63,\!65$	0			
4	NAG	J	2	14/15	0.96	0.15	51,59,69,71	0			
3	NAG	0	1	14/15	0.96	0.22	62,76,89,102	0			
3	NAG	Y	1	14/15	0.97	0.12	69,76,80,86	0			
3	NAG	U	1	14/15	0.98	0.15	67,73,80,89	0			

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	$B-factors(A^2)$	Q<0.9
5	NAG	G	809	14/15	0.61	0.23	77,113,119,120	0
5	NAG	Е	810	14/15	0.71	0.23	114,123,133,137	0
5	NAG	С	809	14/15	0.71	0.26	105,110,113,118	0
5	NAG	G	801	14/15	0.73	0.27	$39,\!69,\!83,\!85$	0
5	NAG	А	801	14/15	0.75	0.20	81,92,99,99	0
5	NAG	А	809	14/15	0.75	0.19	104,112,117,119	0
5	NAG	D	701	14/15	0.78	0.23	90,110,115,123	0
5	NAG	В	701	14/15	0.81	0.29	93,101,106,113	0
5	NAG	С	801	14/15	0.84	0.25	54,83,97,98	0
5	NAG	Н	701	14/15	0.85	0.17	82,89,94,99	0
5	NAG	F	701	14/15	0.86	0.19	69,84,89,90	0

6.5 Other polymers (i)

There are no such residues in this entry.

