

Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 04:57 PM EDT

PDB ID	:	2IFG
Title	:	Structure of the extracellular segment of human TRKA in complex with nerve
		growth factor
Authors	:	He, X.; Garcia, K.C.
Deposited on	:	2006-09-20
Resolution	:	3.40 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.40 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	$\begin{array}{c} {\rm Whole \ archive} \\ (\#{\rm Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	Δ	247	5%						
1	A	347	39% 18%	46%	14% •				
1	В	347	45%	43%	12% •				
2	Е	120	55%	27%	7% • 10%				
			3%						
2	F	120	48%	34%	8% 9%				
9	a	0							
3	C	2	50%	50%					



Mol	Chain	Length	Quality of chain						
3	K	2	100%						
4	D	3	67% 33%						
4	Ι	3	100%						
4	L	3	33% 33%	33%					
4	0	3	100%						
5	G	3	33%	67%					
5	Н	3	33%	67%					
5	J	3	33%	67%					
5	М	3	33%	67%					
5	Ν	3	100%						
5	Р	3	67%	33%					

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NDG	Κ	2	-	-	-	Х
4	NDG	D	2	-	-	-	Х
4	MAN	D	3	-	-	-	Х
4	NAG	Ι	1	X	-	-	-
4	NDG	Ι	2	-	-	-	Х
4	MAN	Ι	3	-	-	-	Х
4	MAN	L	3	-	-	-	Х
4	NAG	0	1	X	-	-	Х
4	NDG	0	2	-	-	-	Х
4	MAN	0	3	-	-	-	Х
5	BMA	G	3	-	-	-	Х
5	NAG	Н	1	Х	-	-	-
5	BMA	Н	3	-	-	-	Х
5	NAG	J	1	Х	-	-	-
5	NDG	J	2	-	-	-	Х
5	BMA	J	3	-	-	-	Х
5	BMA	М	3	-	-	-	Х
5	BMA	N	3	-	-	-	Х



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	Р	1	Х	-	-	Х
5	NDG	Р	2	-	-	-	Х
5	BMA	Р	3	-	-	-	Х

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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7483 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called High affinity nerve growth factor receptor.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	347	Total 2659	C 1662	N 479	O 501	S 17	0	0	0
1	В	347	Total 2659	C 1662	N 479	O 501	S 17	0	0	0

• Molecule 2 is a protein called Beta-nerve growth factor.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2 E	F	108	Total	С	Ν	0	S	0	0	0
	Ľ	108	857	540	152	157	8			
9	2 F	109	Total	С	Ν	0	S	0	0	0
			862	543	153	158	8			0

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



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

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	3	Total C N O 39 22 2 15	0	0	0
4	Ι	3	Total C N O 39 22 2 15	0	0	0
4	L	3	Total C N O 39 22 2 15	0	0	0
4	О	3	Total C N O 39 22 2 15	0	0	0

• Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-al pha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	G	3	Total C N O 39 22 2 15	0	0	0
5	Н	3	Total C N O 39 22 2 15	0	0	0
5	J	3	Total C N O 39 22 2 15	0	0	0
5	М	3	Total C N O 39 22 2 15	0	0	0
5	Ν	3	Total C N O 39 22 2 15	0	0	0
5	Р	3	Total C N O 39 22 2 15	0	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: High affinity nerve growth factor receptor



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

Chain C:	50%	50%	

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

Chain K:	100%
MG1 NDG2	

Chain D: 67% 33%

NAG1 NDG2 MAN3

NDG NDG

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



α	•	т
(h	am	1.
UII	am	т.

NAG1 NDG2 MAN3

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

Chain L:	33%	33%	33%
NAG1 NDG2 MAN3			

100%

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

Chain O:	100%
NAG 1 NDG 2 MAN 3	

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:	33%	67%
NAG1 NDG2 BMA3		

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose

Chain H:	33%	67%
NAG1 NDG2 BNA3		

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:	33%	67%
NAG1 NDG2 BMA3		

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M^{\cdot}	330/	67%
	97.66	0778





• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

100%

NAG1 NDG2 BMA3

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

67%

33%

NAG1 NDG2 BMA3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	110.22Å 81.68 Å 115.75 Å	Deperitor
a, b, c, α , β , γ	90.00° 104.15° 90.00°	Depositor
$\mathbf{Posolution} \left(\overset{\circ}{\mathbf{A}} \right)$	12.00 - 3.40	Depositor
Resolution (A)	11.99 - 3.40	EDS
% Data completeness	(Not available) $(12.00-3.40)$	Depositor
(in resolution range)	98.7 (11.99-3.40)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.62 (at 3.43 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
P. P.	0.297 , 0.331	Depositor
n, n_{free}	0.299 , 0.330	DCC
R_{free} test set	1289 reflections (4.83%)	wwPDB-VP
Wilson B-factor $(Å^2)$	66.0	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.24, 86.9	EDS
L-test for twinning ²	$< L >=0.41, < L^2>=0.24$	Xtriage
Estimated twinning fraction	0.063 for l,-k,h	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7483	wwPDB-VP
Average B, all atoms $(Å^2)$	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 12.18% 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: NDG, BMA, NAG, MAN

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	
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.47	1/2720~(0.0%)	0.83	7/3705~(0.2%)
1	В	0.41	0/2720	0.81	9/3705~(0.2%)
2	Е	0.42	0/875	0.70	0/1178
2	F	0.41	0/880	0.70	1/1185~(0.1%)
All	All	0.43	1/7195~(0.0%)	0.80	17/9773~(0.2%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	114	THR	C-N	5.46	1.44	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	149	PRO	O-C-N	11.90	141.74	122.70
1	В	181	GLY	N-CA-C	-10.42	87.05	113.10
1	А	181	GLY	N-CA-C	-8.85	90.98	113.10
1	В	185	HIS	N-CA-C	-8.80	87.23	111.00
1	А	185	HIS	N-CA-C	-8.55	87.91	111.00
1	В	346	LEU	N-CA-C	-7.85	89.81	111.00
1	А	181	GLY	C-N-CD	-7.50	104.11	120.60
1	А	346	LEU	N-CA-C	-7.44	90.92	111.00



2IFG

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	147	GLY	N-CA-C	-7.41	94.57	113.10
1	В	149	PRO	CA-C-N	-7.36	101.00	117.20
1	А	182	PRO	N-CA-C	7.27	130.99	112.10
1	В	182	PRO	N-CA-C	6.75	129.66	112.10
1	А	345	CYS	CA-CB-SG	5.70	124.26	114.00
1	В	345	CYS	CA-CB-SG	5.69	124.25	114.00
1	А	179	GLY	N-CA-C	-5.68	98.90	113.10
1	В	179	GLY	N-CA-C	-5.28	99.91	113.10
2	F	77	ASN	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	145	LEU	Mainchain

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	2659	0	2573	254	0
1	В	2659	0	2574	227	0
2	Е	857	0	832	46	0
2	F	862	0	837	62	0
3	С	28	0	24	5	0
3	K	28	0	24	0	0
4	D	39	0	33	1	0
4	Ι	39	0	33	0	0
4	L	39	0	33	2	0
4	0	39	0	33	0	0
5	G	39	0	33	6	0
5	Н	39	0	33	2	0
5	J	39	0	33	0	0
5	М	39	0	33	0	0
5	N	39	0	33	0	0
5	Р	39	0	33	0	0
All	All	7483	0	7194	581	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 40.

All (581) 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:A:149:PRO:O	1:A:178:HIS:HB2	1.31	1.25
1:B:149:PRO:O	1:B:178:HIS:HB2	1.38	1.19
1:B:74:GLU:HB3	1:B:99:VAL:HG13	1.33	1.08
1:A:260:ARG:HH22	5:G:1:NAG:H62	1.20	1.06
1:B:149:PRO:O	1:B:178:HIS:CB	2.04	1.05
1:B:185:HIS:O	1:B:186:MET:HB2	1.56	1.02
1:A:185:HIS:O	1:A:186:MET:HB2	1.57	0.97
1:A:181:GLY:N	1:A:182:PRO:HD3	1.79	0.97
3:C:1:NAG:H3	3:C:2:NDG:H2	1.44	0.95
1:B:104:ARG:HA	1:B:127:LEU:HA	1.44	0.95
1:B:196:LEU:HD21	1:B:217:VAL:HG22	1.49	0.95
2:E:14:VAL:HG22	2:E:68:CYS:HB3	1.49	0.94
1:A:176:GLN:HB3	1:A:182:PRO:O	1.67	0.92
1:B:193:VAL:HG12	1:B:194:PRO:HD2	1.51	0.92
2:F:47:SER:HB3	2:F:49:PHE:HE1	1.33	0.92
2:F:46:ASN:C	2:F:46:ASN:HD22	1.73	0.92
1:A:163:GLU:OE1	1:A:184:ALA:HB1	1.71	0.91
1:B:335:PRO:HB3	1:B:342:ARG:HH11	1.35	0.91
1:A:196:LEU:HD21	1:A:217:VAL:HG22	1.54	0.90
1:A:193:VAL:HG12	1:A:194:PRO:HD2	1.51	0.90
1:A:178:HIS:C	1:A:180:GLN:H	1.76	0.89
1:A:149:PRO:O	1:A:178:HIS:CB	2.21	0.88
1:A:178:HIS:O	1:A:180:GLN:N	2.06	0.88
1:A:42:PRO:HD2	1:A:49:ARG:O	1.75	0.86
1:B:42:PRO:HG2	1:B:49:ARG:HB2	1.58	0.86
1:B:163:GLU:OE1	1:B:184:ALA:HB1	1.76	0.86
1:A:180:GLN:HG2	1:A:182:PRO:HG3	1.56	0.85
1:B:176:GLN:HB3	1:B:182:PRO:O	1.75	0.85
1:A:352:THR:HG21	2:F:31:ILE:HD11	1.59	0.85
1:A:212:LEU:HD23	1:A:212:LEU:H	1.42	0.84
1:B:74:GLU:HA	1:B:99:VAL:O	1.77	0.84
1:B:118:SER:O	1:B:141:GLN:N	2.12	0.83
1:B:149:PRO:C	1:B:178:HIS:HB2	1.99	0.83
1:A:74:GLU:HA	1:A:99:VAL:O	1.79	0.83
1:B:262:ASN:ND2	4:L:1:NAG:H61	1.94	0.82
1:A:260:ARG:HG2	1:A:338:ASN:HA	1.61	0.82
1:B:146:SER:C	1:B:148:ASN:N	2.24	0.82



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:157:ARG:HE	1:B:160:GLN:HG2	1.44	0.82
1:A:301:ILE:HD12	1:A:346:LEU:HD23	1.59	0.82
1:A:290:LEU:HD23	1:A:374:ILE:HG22	1.62	0.82
1:A:118:SER:O	1:A:141:GLN:N	2.12	0.82
1:A:181:GLY:N	1:A:182:PRO:CD	2.36	0.81
1:A:130:LEU:HD11	1:A:134:THR:HG21	1.63	0.81
1:A:177:CYS:O	1:A:180:GLN:HA	1.81	0.81
1:A:176:GLN:CB	1:A:182:PRO:O	2.27	0.81
1:B:365:ASN:HD21	1:B:367:PHE:HD2	1.29	0.81
1:A:228:ILE:HD11	1:A:266:TRP:HE1	1.46	0.81
1:B:146:SER:H	1:B:148:ASN:HD22	1.29	0.81
1:B:145:LEU:O	1:B:175:LEU:HD21	1.81	0.80
1:B:99:VAL:HA	1:B:123:SER:O	1.82	0.80
1:B:52:ARG:HG2	1:B:53:ASP:H	1.45	0.79
1:B:186:MET:HG2	1:B:187:PRO:HD2	1.64	0.78
1:A:157:ARG:HE	1:A:160:GLN:HG2	1.47	0.78
1:B:178:HIS:C	1:B:180:GLN:H	1.84	0.78
1:A:260:ARG:HB3	1:A:338:ASN:HA	1.66	0.78
1:B:74:GLU:HB3	1:B:99:VAL:CG1	2.14	0.78
2:E:30:ASP:OD2	2:E:34:LYS:HB3	1.84	0.77
1:A:288:VAL:HG22	1:A:305:VAL:HG23	1.66	0.77
1:B:288:VAL:HG22	1:B:305:VAL:HG23	1.66	0.77
1:A:157:ARG:O	1:A:160:GLN:HB3	1.85	0.77
1:A:145:LEU:O	1:A:175:LEU:HD21	1.85	0.76
1:A:178:HIS:C	1:A:180:GLN:N	2.33	0.76
1:B:335:PRO:HD3	1:B:342:ARG:HH12	1.50	0.76
1:A:75:ASN:H	1:A:100:LYS:HB2	1.48	0.76
1:A:353:HIS:HB2	1:A:381:ASN:HB3	1.69	0.75
2:F:95:LYS:CD	2:F:95:LYS:H	1.99	0.75
1:A:180:GLN:C	1:A:182:PRO:HD3	2.06	0.75
1:B:284:PHE:CE1	1:B:308:GLN:HB2	2.22	0.75
1:A:186:MET:HG2	1:A:187:PRO:HD2	1.69	0.74
2:E:104:ILE:HD13	2:E:104:ILE:H	1.52	0.74
1:A:40:CYS:SG	1:A:41:CYS:N	2.57	0.74
1:A:123:SER:HB3	1:A:144:VAL:HG12	1.69	0.74
2:F:46:ASN:C	2:F:46:ASN:ND2	2.41	0.74
2:E:91:THR:OG1	2:E:100:ARG:HG3	1.88	0.73
1:B:228:ILE:HD11	1:B:266:TRP:HE1	1.53	0.73
1:A:176:GLN:CA	1:A:182:PRO:O	2.36	0.73
5:G:1:NAG:H61	5:G:2:NDG:H8C3	1.70	0.73
1:B:146:SER:C	1:B:148:ASN:H	1.90	0.73



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:43:ASN:HB3	2:E:48:VAL:HG12	1.69	0.73
1:A:82:LEU:HD11	1:A:87:LEU:HD11	1.72	0.72
1:B:176:GLN:HE21	1:B:183:LEU:HD13	1.53	0.72
1:A:264:THR:OG1	1:A:277:SER:HB3	1.89	0.72
1:B:178:HIS:CG	1:B:179:GLY:N	2.57	0.72
2:F:88:LYS:HE2	2:F:99:TRP:O	1.90	0.72
2:F:77:ASN:OD1	2:F:115:LYS:HB3	1.90	0.71
1:B:178:HIS:C	1:B:180:GLN:N	2.40	0.70
1:A:353:HIS:CB	1:A:381:ASN:HB3	2.20	0.70
2:F:47:SER:HB3	2:F:49:PHE:CE1	2.23	0.70
1:B:212:LEU:H	1:B:212:LEU:HD23	1.55	0.70
1:A:281:ASN:HD22	5:G:1:NAG:C7	2.05	0.70
1:B:135:VAL:O	1:B:138:LEU:HG	1.91	0.70
1:B:157:ARG:O	1:B:160:GLN:HB3	1.92	0.69
1:B:176:GLN:CB	1:B:182:PRO:O	2.39	0.69
1:B:283:SER:HA	1:B:308:GLN:HB3	1.75	0.69
2:E:55:GLU:OE2	2:E:104:ILE:HB	1.92	0.69
2:E:14:VAL:CG2	2:E:68:CYS:HB3	2.21	0.69
1:B:181:GLY:N	1:B:182:PRO:CD	2.53	0.68
1:B:284:PHE:N	1:B:308:GLN:O	2.24	0.68
2:F:42:VAL:HG23	2:F:90:LEU:HD22	1.75	0.68
1:B:335:PRO:HB3	1:B:342:ARG:NH1	2.07	0.68
1:B:145:LEU:O	1:B:146:SER:HB3	1.93	0.68
1:B:97:THR:HG22	1:B:99:VAL:HG12	1.74	0.68
1:A:149:PRO:C	1:A:178:HIS:HB2	2.13	0.68
1:B:52:ARG:HG2	1:B:53:ASP:N	2.09	0.68
1:A:103:LEU:HD11	1:A:106:VAL:HG22	1.76	0.67
1:A:260:ARG:NH2	5:G:1:NAG:H62	2.03	0.67
1:A:75:ASN:H	1:A:100:LYS:CB	2.08	0.67
1:B:175:LEU:O	1:B:183:LEU:HB2	1.96	0.66
1:B:183:LEU:HG	1:B:184:ALA:N	2.10	0.66
1:A:178:HIS:CG	1:A:179:GLY:N	2.62	0.66
1:B:185:HIS:O	1:B:186:MET:CB	2.36	0.66
1:B:196:LEU:HB3	1:B:276:VAL:HG11	1.78	0.66
1:A:254:VAL:HG11	1:A:282:VAL:HG11	1.77	0.66
$1:A:260:\overline{ARG:CG}$	1:A:338:ASN:HA	2.25	0.66
2:F:41:GLU:HA	2:F:49:PHE:O	1.96	0.65
1:A:99:VAL:HA	1:A:123:SER:O	1.96	0.65
1:A:180:GLN:CG	1:A:182:PRO:HG3	2.25	0.65
1:A:98:ILE:HB	1:A:122:LEU:HD23	1.78	0.65
1:A:179:GLY:O	1:A:180:GLN:HB2	1.95	0.65



	A L C	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:E:104:ILE:HD13	2:E:104:ILE:N	2.11	0.65
1:B:42:PRO:CG	1:B:49:ARG:HB2	2.27	0.65
2:E:6:ILE:HD13	2:E:10:GLY:HA3	1.77	0.65
1:A:227:TRP:HZ2	1:A:247:LEU:O	1.80	0.64
1:B:98:ILE:HB	1:B:122:LEU:HD23	1.78	0.64
1:A:155:ALA:HA	1:A:271:VAL:HB	1.78	0.64
1:A:185:HIS:O	1:A:186:MET:CB	2.34	0.64
3:C:1:NAG:H5	3:C:2:NDG:N2	2.13	0.64
1:B:148:ASN:CB	1:B:150:LEU:HG	2.27	0.64
1:B:196:LEU:HD13	1:B:276:VAL:HG12	1.79	0.64
1:A:221:GLY:HA3	1:A:269:ASN:HB2	1.80	0.64
1:A:84:LEU:HD13	1:A:112:HIS:HB3	1.80	0.63
1:A:296:MET:CE	2:E:6:ILE:HD12	2.28	0.63
1:A:374:ILE:HD12	1:A:375:MET:H	1.63	0.63
1:A:288:VAL:HG23	1:A:370:ALA:HB3	1.80	0.63
1:B:43:HIS:ND1	1:B:44:GLY:N	2.46	0.63
1:B:104:ARG:CZ	1:B:128:GLU:HB2	2.28	0.63
2:E:14:VAL:HB	2:F:112:LEU:HD11	1.81	0.63
1:A:109:ASP:O	1:A:110:ALA:C	2.36	0.62
1:A:260:ARG:HG2	1:A:338:ASN:CA	2.28	0.62
1:A:260:ARG:CB	1:A:338:ASN:HA	2.28	0.62
1:B:146:SER:N	1:B:148:ASN:HD22	1.98	0.62
1:B:176:GLN:CA	1:B:182:PRO:O	2.47	0.62
1:A:288:VAL:HG21	1:A:363:ALA:HB3	1.81	0.62
2:F:46:ASN:HD22	2:F:47:SER:N	1.96	0.62
1:B:288:VAL:HG21	1:B:363:ALA:HB3	1.82	0.62
1:A:176:GLN:HE21	1:A:183:LEU:HD13	1.64	0.62
1:B:244:LEU:H	1:B:245:PRO:HD2	1.64	0.62
1:A:99:VAL:HG23	1:A:123:SER:C	2.20	0.62
1:B:213:LEU:HD23	1:B:249:LEU:O	2.00	0.62
1:B:288:VAL:HG21	1:B:363:ALA:CB	2.28	0.62
1:A:97:THR:HG22	1:A:99:VAL:HG12	1.79	0.62
1:A:365:ASN:HD21	1:A:367:PHE:HD1	1.48	0.62
1:B:290:LEU:HD23	1:B:374:ILE:HG22	1.82	0.62
1:A:296:MET:HE3	2:E:6:ILE:HD12	1.81	0.61
1:B:70:GLU:HG2	1:B:95:ASN:HD22	1.66	0.61
1:B:146:SER:HB3	1:B:175:LEU:HD21	1.81	0.61
1:B:50:CYS:O	1:B:52:ARG:N	2.35	0.60
1:A:362:LEU:HB3	1:A:369:GLN:HE21	1.65	0.60
2:F:6:ILE:HD13	2:F:10:GLY:HA3	1.82	0.60
1:A:119:ARG:HD3	1:A:142:GLU:OE1	2.00	0.60



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:6:ILE:CD1	2:E:10:GLY:HA3	2.31	0.60
1:A:213:LEU:HD21	1:A:249:LEU:HD12	1.83	0.60
1:B:99:VAL:HG22	1:B:100:LYS:N	2.17	0.60
2:F:67:GLY:HA2	2:F:78:SER:O	2.01	0.60
1:B:180:GLN:C	1:B:182:PRO:HD3	2.22	0.60
2:E:44:ILE:O	2:E:46:ASN:N	2.35	0.60
1:A:249:LEU:HD13	1:A:250:THR:N	2.16	0.59
1:B:177:CYS:O	1:B:180:GLN:HG3	2.03	0.59
1:B:163:GLU:CD	1:B:184:ALA:HB1	2.22	0.59
1:A:244:LEU:H	1:A:245:PRO:HD2	1.66	0.59
1:A:316:LEU:HD23	1:A:321:VAL:HA	1.85	0.59
1:B:97:THR:CG2	1:B:99:VAL:HG12	2.32	0.59
1:A:348:LEU:N	1:A:348:LEU:HD22	2.18	0.59
1:B:149:PRO:O	1:B:178:HIS:CA	2.51	0.59
2:F:47:SER:O	2:F:49:PHE:HD1	1.86	0.59
1:A:43:HIS:ND1	1:A:44:GLY:N	2.51	0.59
1:A:249:LEU:HD13	1:A:249:LEU:C	2.23	0.58
1:B:227:TRP:HZ2	1:B:247:LEU:O	1.86	0.58
1:B:352:THR:HG21	2:E:31:ILE:HD11	1.85	0.58
1:B:353:HIS:HA	1:B:356:ASN:OD1	2.02	0.58
2:F:45:ASN:O	2:F:46:ASN:ND2	2.35	0.58
1:A:42:PRO:HG2	1:A:49:ARG:HB2	1.84	0.58
1:A:316:LEU:HG	1:A:362:LEU:HD21	1.83	0.58
1:B:103:LEU:HD21	1:B:106:VAL:HG22	1.85	0.58
1:B:118:SER:C	1:B:140:LEU:HD12	2.24	0.58
1:B:177:CYS:N	1:B:182:PRO:O	2.36	0.58
2:F:91:THR:OG1	2:F:100:ARG:HG3	2.04	0.58
1:A:99:VAL:HG23	1:A:123:SER:O	2.04	0.58
1:B:269:ASN:HD21	1:B:271:VAL:HG13	1.68	0.58
1:B:99:VAL:HG23	1:B:124:PHE:HB2	1.86	0.58
1:B:123:SER:HB3	1:B:144:VAL:HG12	1.85	0.58
1:B:43:HIS:CD2	1:B:47:GLY:HA3	2.39	0.58
1:B:365:ASN:ND2	1:B:367:PHE:HD2	2.00	0.58
1:B:110:ALA:O	1:B:112:HIS:N	2.37	0.57
1:B:72:TYR:HB3	1:B:74:GLU:OE2	2.03	0.57
1:B:297:HIS:HA	2:F:13:SER:OG	2.03	0.57
1:A:358:ASN:CG	5:H:1:NAG:HN2	2.08	0.57
1:A:98:ILE:HB	1:A:122:LEU:CD2	2.33	0.57
1:A:193:VAL:HG12	1:A:194:PRO:CD	2.31	0.57
1:B:290:LEU:HD13	1:B:372:ALA:HB3	1.87	0.57
1:B:316:LEU:HB2	1:B:360:THR:HB	1.86	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:87:VAL:HG23	2:E:104:ILE:HD11	1.85	0.57
1:A:176:GLN:HA	1:A:182:PRO:O	2.03	0.57
1:A:237:THR:HG22	1:A:251:LEU:CD2	2.35	0.57
1:B:345:CYS:SG	2:F:6:ILE:HG13	2.45	0.57
1:A:215:CYS:HB2	1:A:227:TRP:CH2	2.39	0.57
1:A:98:ILE:O	1:A:98:ILE:HG22	2.05	0.57
1:A:73:ILE:O	1:A:73:ILE:HG22	2.05	0.57
1:B:99:VAL:HG23	1:B:123:SER:C	2.25	0.57
1:B:145:LEU:O	1:B:175:LEU:CD2	2.52	0.57
1:B:99:VAL:CG2	1:B:124:PHE:HB2	2.35	0.56
1:B:237:THR:HG22	1:B:251:LEU:CD2	2.34	0.56
1:B:296:MET:CE	2:F:6:ILE:HD12	2.35	0.56
2:F:95:LYS:HD2	2:F:96:GLN:HE21	1.70	0.56
2:E:9:ARG:HG2	2:E:9:ARG:HH11	1.71	0.56
1:B:181:GLY:N	1:B:182:PRO:HD3	2.20	0.56
1:B:186:MET:HG2	1:B:187:PRO:CD	2.33	0.56
1:B:306:ASP:OD1	1:B:307:GLY:N	2.39	0.56
1:A:234:GLN:HG2	1:A:257:ASP:HB2	1.88	0.56
1:B:170:VAL:N	1:B:171:PRO:CD	2.69	0.56
1:A:88:ARG:HH11	1:A:113:PHE:HZ	1.54	0.56
1:B:229:LEU:HD12	1:B:229:LEU:N	2.21	0.56
1:A:97:THR:CG2	1:A:99:VAL:HG12	2.36	0.55
1:A:243:GLY:C	1:A:244:LEU:HD22	2.26	0.55
1:A:229:LEU:N	1:A:229:LEU:HD12	2.21	0.55
2:E:6:ILE:HD13	2:E:6:ILE:O	2.06	0.55
1:A:296:MET:HE1	2:E:6:ILE:HG23	1.89	0.55
1:B:296:MET:HE3	2:F:6:ILE:HD12	1.87	0.55
1:A:177:CYS:H	1:A:182:PRO:C	2.09	0.55
1:B:183:LEU:C	1:B:185:HIS:H	2.10	0.55
1:A:288:VAL:CG2	1:A:363:ALA:HB3	2.36	0.55
1:A:352:THR:OG1	1:A:354:VAL:HG22	2.07	0.55
1:B:98:ILE:HG22	1:B:98:ILE:O	2.07	0.55
2:E:85:THR:HG23	2:E:104:ILE:HD11	1.87	0.55
1:A:70:GLU:HG2	1:A:95:ASN:HB2	1.88	0.55
1:A:268:GLU:HG2	1:A:273:ARG:HB2	1.89	0.55
1:B:148:ASN:HB3	1:B:150:LEU:HG	1.89	0.55
2:E:85:THR:HG22	2:E:106:THR:HB	1.88	0.55
1:A:75:ASN:N	1:A:100:LYS:HB2	2.21	0.54
1:B:179:GLY:O	1:B:180:GLN:HB2	2.05	0.54
1:B:264:THR:OG1	1:B:277:SER:HB3	2.07	0.54
1:A:75:ASN:N	1:A:100:LYS:O	2.41	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:362:LEU:HB3	1:B:369:GLN:HE21	1.73	0.54
1:B:42:PRO:HD2	1:B:49:ARG:O	2.08	0.54
1:A:146:SER:O	1:A:147:GLY:C	2.46	0.54
2:F:68:CYS:HB2	2:F:71:ILE:HD13	1.89	0.54
1:A:69:THR:HA	1:A:93:LEU:HA	1.88	0.53
1:B:183:LEU:O	1:B:185:HIS:O	2.26	0.53
1:B:225:ALA:HB1	1:B:247:LEU:HD21	1.89	0.53
2:F:115:LYS:O	2:F:116:ALA:HB3	2.07	0.53
1:A:196:LEU:HD13	1:A:276:VAL:HG12	1.90	0.53
1:B:178:HIS:CG	1:B:179:GLY:H	2.25	0.53
2:F:74:LYS:O	2:F:115:LYS:HD2	2.09	0.53
1:A:165:GLU:HB3	1:A:167:LEU:HG	1.90	0.53
1:A:200:VAL:HB	1:A:201:PRO:HD2	1.89	0.53
1:A:267:ALA:O	1:A:273:ARG:HG3	2.08	0.53
1:A:266:TRP:O	1:A:267:ALA:HB2	2.08	0.53
1:A:333:LEU:HB3	2:E:9:ARG:NH2	2.24	0.53
1:B:290:LEU:HD11	1:B:361:LEU:HB3	1.91	0.53
1:A:43:HIS:CD2	1:A:47:GLY:HA3	2.43	0.53
1:A:186:MET:HG2	1:A:187:PRO:CD	2.37	0.53
1:A:288:VAL:HG21	1:A:363:ALA:CB	2.39	0.53
2:F:42:VAL:HG13	2:F:44:ILE:HD11	1.89	0.53
1:B:155:ALA:HA	1:B:271:VAL:HB	1.89	0.53
1:B:196:LEU:CD2	1:B:217:VAL:HG22	2.32	0.53
1:A:104:ARG:HG2	1:A:104:ARG:HH11	1.73	0.53
1:B:103:LEU:HD21	1:B:106:VAL:CG2	2.38	0.53
2:F:42:VAL:HG13	2:F:44:ILE:CD1	2.38	0.53
1:B:84:LEU:HD13	1:B:112:HIS:HB3	1.91	0.53
1:B:85:ARG:HD2	1:B:85:ARG:O	2.08	0.53
1:B:104:ARG:O	1:B:127:LEU:HD12	2.09	0.53
1:A:85:ARG:HD2	1:A:85:ARG:O	2.07	0.53
1:A:123:SER:O	1:A:124:PHE:C	2.47	0.53
1:A:157:ARG:HE	1:A:160:GLN:CG	2.17	0.53
1:A:163:GLU:CD	1:A:184:ALA:HB1	2.28	0.53
1:A:209:ASP:O	1:A:254:VAL:HG23	2.08	0.53
1:A:165:GLU:CB	1:A:167:LEU:HG	2.40	0.52
1:A:256:SER:C	1:A:258:LEU:H	2.12	0.52
1:A:317:PHE:HE1	1:A:357:GLY:HA3	1.74	0.52
1:B:128:GLU:OE1	1:B:151:HIS:HB2	2.10	0.52
4:D:1:NAG:O3	4:D:1:NAG:H83	2.09	0.52
1:B:73:ILE:HG22	1:B:73:ILE:O	2.09	0.52
1:B:149:PRO:CA	1:B:178:HIS:HB2	2.39	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:123:SER:HB3	1:A:144:VAL:CG1	2.38	0.52
1:B:132:TRP:O	1:B:134:THR:N	2.43	0.52
1:B:348:LEU:N	1:B:348:LEU:HD22	2.24	0.52
1:A:186:MET:O	1:A:187:PRO:C	2.47	0.52
2:E:85:THR:O	2:E:104:ILE:HD13	2.09	0.52
1:B:301:ILE:HD12	1:B:346:LEU:HD23	1.91	0.52
1:A:313:LEU:HD22	1:A:361:LEU:HD11	1.91	0.52
2:F:39:LEU:HD23	2:F:90:LEU:O	2.10	0.52
1:A:170:VAL:N	1:A:171:PRO:CD	2.73	0.51
1:B:178:HIS:O	1:B:180:GLN:N	2.19	0.51
3:C:1:NAG:H5	3:C:2:NDG:C7	2.39	0.51
1:A:103:LEU:O	1:A:127:LEU:HD13	2.11	0.51
1:B:110:ALA:C	1:B:112:HIS:H	2.14	0.51
1:A:89:GLY:O	1:A:90:LEU:C	2.48	0.51
1:A:334:GLU:OE2	1:A:335:PRO:HD2	2.10	0.51
1:B:244:LEU:N	1:B:245:PRO:HD2	2.25	0.51
2:F:95:LYS:H	2:F:95:LYS:HE2	1.76	0.51
1:A:295:GLU:HB2	1:A:299:TRP:CE2	2.45	0.51
2:F:95:LYS:H	2:F:95:LYS:CE	2.22	0.51
1:A:177:CYS:N	1:A:182:PRO:O	2.44	0.51
1:A:332:PHE:HB3	1:A:342:ARG:NH2	2.24	0.51
2:E:14:VAL:HG23	2:E:69:ARG:O	2.11	0.51
1:B:40:CYS:SG	1:B:49:ARG:C	2.89	0.51
1:B:186:MET:O	1:B:187:PRO:C	2.46	0.51
1:B:256:SER:HA	1:B:282:VAL:HG21	1.93	0.51
1:B:308:GLN:HA	1:B:309:PRO:C	2.31	0.51
2:F:48:VAL:HG23	2:F:48:VAL:O	2.10	0.51
1:A:146:SER:C	1:A:148:ASN:N	2.58	0.51
1:A:170:VAL:O	1:A:171:PRO:C	2.49	0.51
1:A:183:LEU:C	1:A:185:HIS:H	2.12	0.51
1:B:48:LEU:HB2	1:B:71:LEU:HD23	1.91	0.51
1:B:75:ASN:O	1:B:76:GLN:HG3	2.11	0.51
1:A:110:ALA:O	1:A:112:HIS:N	2.41	0.50
1:B:40:CYS:O	1:B:41:CYS:SG	2.70	0.50
1:B:271:VAL:HG13	1:B:271:VAL:O	2.11	0.50
2:E:79:TYR:CE1	2:E:111:VAL:HB	2.47	0.50
1:A:317:PHE:CE1	1:A:357:GLY:HA3	2.46	0.50
1:A:308:GLN:HA	1:A:309:PRO:C	2.32	0.50
2:F:2:SER:HA	2:F:7:PHE:CE2	2.46	0.50
1:A:176:GLN:NE2	1:A:183:LEU:HD13	2.25	0.50
1:A:176:GLN:HA	1:A:183:LEU:HA	1.92	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:135:VAL:O	1:B:136:GLN:C	2.50	0.50
1:B:295:GLU:HB2	1:B:299:TRP:CE2	2.46	0.50
1:A:178:HIS:CG	1:A:179:GLY:H	2.27	0.50
1:B:69:THR:HA	1:B:93:LEU:HA	1.94	0.50
2:F:68:CYS:HB2	2:F:71:ILE:CD1	2.42	0.50
1:A:43:HIS:HB2	1:A:49:ARG:HG3	1.94	0.49
1:B:300:CYS:SG	1:B:302:PRO:HG3	2.52	0.49
2:E:59:ARG:O	2:E:60:ASP:C	2.50	0.49
2:F:13:SER:O	2:F:69:ARG:NH1	2.45	0.49
1:B:152:CYS:HA	1:B:156:LEU:HD12	1.93	0.49
2:E:112:LEU:N	2:E:112:LEU:HD12	2.27	0.49
1:A:133:LYS:O	1:A:134:THR:C	2.51	0.49
1:B:93:LEU:C	1:B:93:LEU:HD23	2.33	0.49
1:A:93:LEU:C	1:A:93:LEU:HD23	2.31	0.49
1:A:237:THR:HG22	1:A:251:LEU:HD23	1.94	0.49
1:A:353:HIS:CG	1:A:381:ASN:HB3	2.47	0.49
1:B:223:GLU:HB2	1:B:268:GLU:O	2.11	0.49
2:F:93:ASP:O	2:F:96:GLN:HB2	2.11	0.49
1:B:213:LEU:HD21	1:B:249:LEU:HD12	1.95	0.49
1:B:88:ARG:HA	:B:88:ARG:HA 1:B:113:PHE:CE2		0.49
2:E:88:LYS:HE3	2:E:99:TRP:C	2.32	0.49
1:A:104:ARG:HG3	1:A:126:ALA:O	2.13	0.49
1:B:353:HIS:CD2	1:B:381:ASN:HB3	2.47	0.49
1:A:43:HIS:CD2	1:A:49:ARG:HE	2.30	0.48
1:A:284:PHE:CE1	1:A:308:GLN:HB3	2.47	0.48
1:B:283:SER:CA	1:B:308:GLN:O	2.61	0.48
3:C:2:NDG:H6C2	3:C:2:NDG:O3	2.13	0.48
1:B:40:CYS:SG	1:B:49:ARG:O	2.71	0.48
1:A:254:VAL:CG1	1:A:282:VAL:HG11	2.43	0.48
1:A:284:PHE:HB2	1:A:285:PRO:HD2	1.95	0.48
1:B:108:PRO:CB	1:B:133:LYS:HB3	2.43	0.48
1:A:109:ASP:O	1:A:112:HIS:N	2.47	0.48
1:A:40:CYS:SG	1:A:49:ARG:O	2.72	0.48
1:B:238:VAL:N	1:B:250:THR:O	2.47	0.48
1:A:74:GLU:HG2	1:A:99:VAL:CG1	2.44	0.48
1:B:264:THR:HG22	1:B:265:CYS:N	2.29	0.48
2:F:6:ILE:HD13	2:F:10:GLY:CA	2.44	0.48
1:A:104:ARG:HD3	1:A:105:PHE:HE1	1.79	0.48
1:B:43:HIS:CD2	1:B:49:ARG:HE	2.32	0.47
1:B:93:LEU:HD21	1:B:95:ASN:C	2.34	0.47
1:B:182:PRO:O	1:B:183:LEU:HB3	2.14	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:288:VAL:CG2	1:B:363:ALA:HB3	2.43	0.47
1:A:315:TRP:CZ2	1:A:346:LEU:HB2	2.47	0.47
1:B:246:SER:C	1:B:247:LEU:HD12	2.34	0.47
1:A:135:VAL:O	1:A:138:LEU:HG	2.15	0.47
1:A:259:ASN:ND2	1:A:282:VAL:HG23	2.30	0.47
2:F:47:SER:O	2:F:49:PHE:CD1	2.67	0.47
1:B:99:VAL:CG2	1:B:100:LYS:N	2.77	0.47
1:B:149:PRO:O	1:B:178:HIS:N	2.47	0.47
1:B:183:LEU:O	1:B:185:HIS:N	2.33	0.47
2:E:42:VAL:HG22	2:E:43:ASN:N	2.30	0.47
1:A:106:VAL:HG23	1:A:127:LEU:HD11	1.97	0.47
1:A:107:ALA:O	1:A:109:ASP:N	2.47	0.47
1:B:74:GLU:O	1:B:75:ASN:HB2	2.14	0.47
1:B:176:GLN:HA	1:B:182:PRO:O	2.13	0.47
1:B:356:ASN:HA	1:B:376:ALA:O	2.14	0.47
1:A:70:GLU:HB3	1:A:72:TYR:HE1	1.80	0.47
1:A:93:LEU:HD21	1:A:95:ASN:C	2.35	0.47
1:A:113:PHE:O	1:A:115:PRO:HD3	2.15	0.47
1:B:98:ILE:HB	1:B:122:LEU:CD2	2.42	0.47
1:A:182:PRO:O	1:A:183:LEU:HB3	2.14	0.47
1:A:316:LEU:HB2	1:A:360:THR:HB	1.96	0.47
1:B:165:GLU:HB2	1:B:167:LEU:HG	1.97	0.47
1:B:313:LEU:HG	1:B:361:LEU:HD11	1.96	0.47
1:B:328:ILE:HG12	1:B:348:LEU:HD12	1.97	0.47
1:A:212:LEU:HD23	1:A:212:LEU:N	2.19	0.46
1:A:290:LEU:HD23	1:A:374:ILE:CG2	2.40	0.46
2:E:44:ILE:O	2:E:45:ASN:C	2.53	0.46
2:E:95:LYS:HG3	2:E:96:GLN:HG2	1.97	0.46
1:A:152:CYS:HA	1:A:156:LEU:HD12	1.97	0.46
2:F:39:LEU:HD23	2:F:90:LEU:C	2.36	0.46
1:A:99:VAL:CG2	1:A:124:PHE:HB2	2.45	0.46
1:B:68:LEU:N	1:B:68:LEU:HD23	2.31	0.46
1:B:270:ASP:OD2	1:B:271:VAL:HG12	2.15	0.46
1:A:75:ASN:O	1:A:76:GLN:HG3	2.16	0.46
1:A:84:LEU:CD1	1:A:112:HIS:HB3	2.44	0.46
1:A:53:ASP:HA	1:A:76:GLN:HG2	1.97	0.46
1:A:281:ASN:ND2	5:G:1:NAG:C7	2.73	0.46
1:A:365:ASN:ND2	1:A:367:PHE:HD1	2.11	0.46
1:A:183:LEU:HD21	1:A:185:HIS:ND1	2.30	0.46
1:A:349:ASN:O	2:F:103:ARG:NH2	2.49	0.46
1:A:37:PRO:O	1:A:38:ASP:HB2	2.16	0.46



		Interatomic	Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:A:281:ASN:HD22	5:G:1:NAG:C8	2.27	0.46
1:A:136:GLN:HE21	1:A:136:GLN:C	2.18	0.46
1:A:193:VAL:CG1	1:A:194:PRO:HD2	2.34	0.46
1:B:87:LEU:HD12	1:B:87:LEU:N	2.30	0.46
1:B:104:ARG:HG3	1:B:126:ALA:O	2.16	0.46
1:A:68:LEU:N	1:A:68:LEU:HD23	2.30	0.46
1:A:256:SER:O	1:A:258:LEU:N	2.47	0.46
1:B:85:ARG:HD2	1:B:85:ARG:C	2.37	0.46
2:F:37:MET:HB2	2:F:92:MET:HB2	1.98	0.46
1:A:244:LEU:N	1:A:245:PRO:HD2	2.30	0.46
1:A:260:ARG:HG2	1:A:338:ASN:N	2.31	0.46
1:B:247:LEU:HD12	1:B:247:LEU:N	2.31	0.46
2:E:39:LEU:N	2:E:39:LEU:HD22	2.31	0.46
2:F:57:LYS:HA	2:F:82:THR:HG23	1.97	0.46
1:A:103:LEU:HB3	1:A:125:ASN:HD21	1.81	0.45
1:A:213:LEU:N	1:A:213:LEU:HD23	2.31	0.45
1:A:239:MET:HB3	1:A:249:LEU:HD23	1.98	0.45
1:A:241:SER:HB3	1:A:248:GLY:HA3	1.98	0.45
1:A:271:VAL:O	1:A:271:VAL:HG22	2.15	0.45
1:B:183:LEU:CG	1:B:184:ALA:N	2.69	0.45
1:B:234:GLN:O	1:B:235:SER:HB2	2.16	0.45
1:A:183:LEU:O	1:A:185:HIS:N	2.37	0.45
1:B:316:LEU:HD23	1:B:321:VAL:HA	1.98	0.45
1:A:102:GLY:O	1:A:103:LEU:C	2.54	0.45
1:A:110:ALA:C	1:A:112:HIS:H	2.20	0.45
1:B:249:LEU:HD13	1:B:249:LEU:C	2.37	0.45
2:F:59:ARG:O	2:F:60:ASP:C	2.54	0.45
1:A:353:HIS:CD2	1:A:381:ASN:HB2	2.52	0.45
1:B:148:ASN:HB2	1:B:150:LEU:HG	1.98	0.45
1:B:283:SER:HA	1:B:308:GLN:O	2.17	0.45
2:F:95:LYS:H	2:F:95:LYS:HD2	1.77	0.45
1:A:98:ILE:HG21	1:A:103:LEU:HD22	1.99	0.45
1:A:120:LEU:HD11	1:A:122:LEU:HG	1.99	0.45
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.82	0.45
2:E:90:LEU:HB2	2:E:99:TRP:HZ3	1.81	0.45
3:C:1:NAG:H5	3:C:2:NDG:O7	2.16	0.45
1:A:227:TRP:CE3	1:A:265:CYS:HB3	2.51	0.45
1:A:345:CYS:SG	2:E:6:ILE:HG13	2.56	0.45
1:A:127:LEU:HB2	1:A:148:ASN:OD1	2.17	0.45
1:B:51:THR:HG23	1:B:74:GLU:OE1	2.16	0.45
1:B:73:ILE:O	1:B:75:ASN:N	2.43	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:68:LEU:HD12	1:B:71:LEU:HG	1.99	0.45
2:F:39:LEU:N	2:F:39:LEU:HD22	2.32	0.45
1:B:100:LYS:N	1:B:124:PHE:O	2.50	0.44
1:B:108:PRO:HB3	1:B:133:LYS:HB3	1.98	0.44
1:A:87:LEU:N	1:A:87:LEU:HD12	2.32	0.44
1:A:207:VAL:HG22	1:A:208:GLY:N	2.32	0.44
1:B:136:GLN:C	1:B:136:GLN:HE21	2.19	0.44
1:A:125:ASN:OD1	1:A:126:ALA:N	2.45	0.44
1:A:353:HIS:HB3	1:A:380:ASP:O	2.16	0.44
1:B:51:THR:O	1:B:52:ARG:HB2	2.17	0.44
1:B:163:GLU:OE2	1:B:184:ALA:CB	2.66	0.44
2:F:87:VAL:CG2	2:F:104:ILE:HD11	2.47	0.44
1:A:100:LYS:N	1:A:124:PHE:O	2.48	0.44
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.76	0.44
2:E:9:ARG:HG2	2:E:9:ARG:NH1	2.32	0.44
4:L:1:NAG:O3	4:L:2:NDG:H2	2.18	0.44
1:A:68:LEU:HD12	1:A:71:LEU:HG	1.99	0.44
1:A:78:HIS:O	1:A:79:LEU:HB3	2.17	0.44
1:A:145:LEU:O	1:A:175:LEU:CD2	2.62	0.44
1:A:314:ARG:HH21	1:A:362:LEU:HG	1.83	0.44
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.73	0.44
1:B:52:ARG:CG	1:B:53:ASP:H	2.23	0.44
1:B:177:CYS:H	1:B:182:PRO:C	2.21	0.44
1:A:212:LEU:H	1:A:212:LEU:CD2	2.23	0.44
1:A:271:VAL:O	1:A:271:VAL:HG13	2.18	0.44
1:A:229:LEU:HD23	1:A:232:LEU:HD12	1.99	0.44
1:B:288:VAL:HG21	1:B:363:ALA:HB2	1.98	0.44
1:A:99:VAL:HG22	1:A:100:LYS:N	2.33	0.43
1:B:183:LEU:C	1:B:185:HIS:N	2.72	0.43
2:E:99:TRP:C	2:E:100:ARG:HG2	2.37	0.43
2:F:59:ARG:O	2:F:59:ARG:CG	2.66	0.43
1:A:183:LEU:C	1:A:185:HIS:N	2.72	0.43
1:A:36:CYS:HA	1:A:37:PRO:HA	1.83	0.43
1:A:100:LYS:O	1:A:101:SER:OG	2.33	0.43
1:A:288:VAL:HG23	1:A:370:ALA:CB	2.45	0.43
1:B:53:ASP:HA	1:B:76:GLN:HA	2.00	0.43
1:B:163:GLU:OE2	1:B:184:ALA:HB1	2.17	0.43
1:A:114:THR:O	1:A:114:THR:HG23	2.18	0.43
1:B:343:HIS:CD2	2:F:5:PRO:HG2	2.53	0.43
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.84	0.43
1:A:221:GLY:O	1:A:222:LEU:HB2	2.19	0.43



			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:288:VAL:CG2	1:A:363:ALA:CB	2.97	0.43
1:A:102:GLY:O	1:A:126:ALA:HB3	2.18	0.43
1:A:118:SER:C	1:A:140:LEU:HD12	2.39	0.43
1:A:254:VAL:HG12	1:A:255:THR:O	2.19	0.43
1:A:258:LEU:HD21	1:A:280:VAL:HG21	2.01	0.43
1:B:104:ARG:HA	1:B:127:LEU:CA	2.32	0.43
1:B:120:LEU:N	1:B:140:LEU:HD11	2.33	0.43
1:B:146:SER:O	1:B:148:ASN:N	2.49	0.43
1:B:221:GLY:HA3	1:B:269:ASN:HB2	2.01	0.43
2:F:94:GLY:C	2:F:96:GLN:H	2.22	0.43
1:B:243:GLY:C	1:B:244:LEU:HD22	2.38	0.43
2:F:42:VAL:CG1	2:F:44:ILE:HD11	2.48	0.43
1:A:298:HIS:ND1	1:A:347:ARG:NH2	2.66	0.43
2:E:14:VAL:HB	2:F:112:LEU:CD1	2.48	0.43
1:A:75:ASN:O	1:A:76:GLN:CG	2.67	0.42
1:B:114:THR:HG21	1:B:117:LEU:HD12	2.01	0.42
2:F:87:VAL:HG21	2:F:104:ILE:HD11	2.00	0.42
1:A:138:LEU:O	1:A:139:SER:HB2	2.19	0.42
1:A:316:LEU:HG	1:A:362:LEU:CD2	2.47	0.42
1:B:99:VAL:HB	1:B:123:SER:OG	2.19	0.42
1:A:301:ILE:HB	1:A:346:LEU:HB3	2.00	0.42
1:A:84:LEU:HB2	1:A:109:ASP:CG	2.39	0.42
1:A:291:HIS:HB2	1:A:302:PRO:HB2	2.01	0.42
1:B:172:GLU:CD	1:B:172:GLU:H	2.23	0.42
1:B:205:VAL:HG12	1:B:206:ASP:N	2.34	0.42
1:A:374:ILE:HD12	1:A:375:MET:N	2.34	0.42
1:A:308:GLN:HA	1:A:308:GLN:HE21	1.85	0.42
1:B:41:CYS:N	1:B:42:PRO:CD	2.83	0.42
1:B:109:ASP:OD2	1:B:112:HIS:HB2	2.19	0.42
1:B:146:SER:O	1:B:147:GLY:C	2.55	0.42
1:B:176:GLN:HA	1:B:183:LEU:CB	2.50	0.42
2:F:79:TYR:CE1	2:F:111:VAL:HB	2.55	0.42
1:B:74:GLU:O	1:B:100:LYS:HB2	2.20	0.42
1:B:123:SER:O	1:B:124:PHE:C	2.58	0.42
1:B:288:VAL:CG2	1:B:363:ALA:CB	2.95	0.42
1:A:234:GLN:O	1:A:235:SER:HB2	2.20	0.42
1:B:114:THR:HG23	1:B:114:THR:O	2.20	0.42
2:E:22:VAL:CG2	2:E:55:GLU:HG3	2.49	0.42
2:E:74:LYS:C	2:E:75:HIS:HD2	2.23	0.42
2:E:84:HIS:ND1	2:E:103:ARG:NH1	2.67	0.42
2:F:99:TRP:HA	2:F:99:TRP:CE3	2.54	0.42



			Clash
Atom-1	Atom-1 Atom-2		overlap (Å)
1:A:39:ALA:O	1:A:40:CYS:HB2	2.17	0.41
1:A:82:LEU:HD11	1:A:87:LEU:CD1	2.47	0.41
1:A:295:GLU:HB2	1:A:299:TRP:CZ2	2.54	0.41
1:B:54:GLY:N	1:B:76:GLN:HG2	2.34	0.41
1:B:99:VAL:HG23	1:B:123:SER:O	2.19	0.41
1:B:162:TRP:HB3	1:B:170:VAL:HG21	2.02	0.41
2:F:88:LYS:HD2	2:F:88:LYS:HA	1.88	0.41
1:B:43:HIS:CD2	1:B:49:ARG:NE	2.88	0.41
1:B:111:PHE:O	1:B:112:HIS:C	2.58	0.41
2:F:76:TRP:CZ3	2:F:114:ARG:HG3	2.55	0.41
2:F:90:LEU:HB2	2:F:99:TRP:HZ3	1.84	0.41
1:A:288:VAL:HG12	1:A:289:GLN:N	2.35	0.41
1:A:300:CYS:O	1:A:302:PRO:HD3	2.21	0.41
1:B:183:LEU:HD21	1:B:185:HIS:ND1	2.35	0.41
1:B:269:ASN:ND2	1:B:271:VAL:CG1	2.84	0.41
1:B:288:VAL:HG23	1:B:370:ALA:HB3	2.01	0.41
1:A:87:LEU:O	1:A:89:GLY:N	2.54	0.41
1:A:311:PRO:HA	1:A:364:ALA:O	2.21	0.41
1:A:335:PRO:HB3	1:A:342:ARG:NH1	2.36	0.41
1:A:247:LEU:HD12	1:A:247:LEU:N	2.35	0.41
1:A:92:GLU:O	1:A:92:GLU:HG3	2.21	0.41
1:B:335:PRO:HD3	1:B:342:ARG:NH1	2.26	0.41
1:A:74:GLU:H	1:A:74:GLU:HG3	1.65	0.41
1:A:104:ARG:HA	1:A:126:ALA:O	2.21	0.41
1:A:244:LEU:HD22	1:A:244:LEU:N	2.35	0.41
1:A:289:GLN:HG2	1:A:304:SER:HB2	2.03	0.41
1:B:258:LEU:HD23	1:B:280:VAL:HG11	2.02	0.41
2:E:18:VAL:O	2:E:18:VAL:HG13	2.20	0.41
2:E:45:ASN:O	2:E:46:ASN:CG	2.59	0.41
2:E:99:TRP:CE3	2:E:99:TRP:HA	2.55	0.41
2:F:95:LYS:CD	2:F:96:GLN:HE21	2.33	0.41
1:A:172:GLU:CD	1:A:172:GLU:H	2.25	0.41
1:A:333:LEU:HB3	2:E:9:ARG:HH21	1.85	0.41
1:B:87:LEU:O	1:B:89:GLY:N	2.54	0.41
1:B:109:ASP:O	1:B:110:ALA:C	2.59	0.41
1:B:110:ALA:C	1:B:112:HIS:N	2.75	0.41
1:B:287:SER:C	1:B:288:VAL:HG23	2.42	0.41
2:F:45:ASN:HD22	2:F:45:ASN:HA	1.62	0.41
2:F:115:LYS:O	2:F:116:ALA:CB	2.69	0.41
1:A:196:LEU:HB3	1:A:276:VAL:HG11	2.03	0.40
1:A:308:GLN:NE2	1:A:309:PRO:HA	2.36	0.40



Atom-1	Atom-1 Atom-2		Clash
		distance (A)	overlap (A)
1:B:214:ARG:HG2	1:B:214:ARG:NH1	2.36	0.40
1:B:124:PHE:CD1	1:B:124:PHE:N	2.90	0.40
1:B:296:MET:HE1	2:F:6:ILE:HG23	2.02	0.40
2:F:4:HIS:HA	2:F:5:PRO:HD3	1.97	0.40
2:F:84:HIS:ND1	2:F:103:ARG:NH1	2.69	0.40
5:H:2:NDG:C1	5:H:2:NDG:O6	2.69	0.40
1:B:239:MET:O	1:B:240:LYS:HB2	2.22	0.40
2:E:93:ASP:OD1	2:E:93:ASP:O	2.39	0.40
1:B:213:LEU:HD23	1:B:213:LEU:N	2.37	0.40
1:A:196:LEU:HA	1:A:196:LEU:HD23	1.92	0.40
2:E:88:LYS:HE2	2:E:99:TRP:CD1	2.57	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	Pe	erce	entiles
1	А	345/347~(99%)	250 (72%)	57 (16%)	38 (11%)		0	3
1	В	345/347~(99%)	262~(76%)	47 (14%)	36 (10%)		0	3
2	Ε	104/120~(87%)	96~(92%)	4 (4%)	4 (4%)		3	19
2	F	105/120~(88%)	102 (97%)	3 (3%)	0	1	.00	100
All	All	899/934~(96%)	710 (79%)	111 (12%)	78 (9%)		1	5

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	38	ASP
1	А	78	HIS
1	А	90	LEU
1	А	103	LEU



Mol	Chain	Res	Type
1	А	110	ALA
1	А	111	PHE
1	А	182	PRO
1	А	186	MET
1	А	271	VAL
1	В	111	PHE
1	В	133	LYS
1	В	182	PRO
1	В	186	MET
2	Е	45	ASN
1	А	42	PRO
1	А	88	ARG
1	А	100	LYS
1	A	109	ASP
1	А	116	ARG
1	А	134	THR
1	А	137	GLY
1	А	235	SER
1	А	267	ALA
1	В	42	PRO
1	В	44	GLY
1	В	51	THR
1	В	53	ASP
1	В	75	ASN
1	В	79	LEU
1	В	88	ARG
1	В	100	LYS
1	В	101	SER
1	В	109	ASP
1	В	110	ALA
1	В	116	ARG
1	В	123	SER
1	В	184	ALA
1	В	204	SER
1	В	235	SER
2	Е	46	ASN
2	Е	93	ASP
1	A	69	THR
1	А	124	PHE
1	А	155	ALA
1	А	180	GLN
1	А	184	ALA



Mol	Chain	Res	Type
1	А	257	ASP
1	А	270	ASP
1	А	281	ASN
1	В	38	ASP
1	В	41	CYS
1	В	74	GLU
1	В	180	GLN
1	В	267	ALA
1	А	55	ALA
1	А	68	LEU
1	А	75	ASN
1	А	117	LEU
1	А	222	LEU
1	В	39	ALA
1	В	117	LEU
1	В	231	GLU
1	А	46	SER
1	А	77	GLN
1	А	131	SER
1	В	45	SER
1	В	113	PHE
1	В	171	PRO
1	В	338	ASN
1	A	171	PRO
1	В	102	GLY
1	В	108	PRO
1	В	155	ALA
2	Е	95	LYS
1	A	221	GLY
1	A	244	LEU
1	А	179	GLY
1	В	244	LEU

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5.3.2 Protein sidechains (i)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	P	erce	entiles
1	А	293/293~(100%)	274~(94%)	19 (6%)		17	46
1	В	293/293~(100%)	277~(94%)	16 (6%)		21	51
2	Ε	96/106~(91%)	86 (90%)	10 (10%)		7	25
2	F	96/106~(91%)	86~(90%)	10 (10%)		7	25
All	All	778/798~(98%)	723~(93%)	55 (7%)		14	44

All (55) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	36	CYS
1	А	77	GLN
1	А	117	LEU
1	А	127	LEU
1	А	136	GLN
1	А	157	ARG
1	А	182	PRO
1	А	183	LEU
1	А	193	VAL
1	А	212	LEU
1	А	234	GLN
1	А	260	ARG
1	А	294	VAL
1	А	300	CYS
1	А	321	VAL
1	А	338	ASN
1	А	348	LEU
1	А	352	THR
1	А	381	ASN
1	В	50	CYS
1	В	68	LEU
1	В	74	GLU
1	В	77	GLN
1	В	136	GLN
1	В	157	ARG
1	В	182	PRO
1	В	183	LEU
1	В	193	VAL
1	В	234	GLN
1	В	260	ARG
1	В	294	VAL
1	В	300	CYS
1	В	308	GLN



Mol	Chain	Res	Type
1	В	338	ASN
1	В	381	ASN
2	Ε	6	ILE
2	Е	9	ARG
2	Е	45	ASN
2	Ε	51	GLN
2	Е	60	ASP
2	Е	77	ASN
2	Е	93	ASP
2	Ε	99	TRP
2	Е	100	ARG
2	Е	104	ILE
2	F	6	ILE
2	F	45	ASN
2	F	46	ASN
2	F	47	SER
2	F	51	GLN
2	F	60	ASP
2	F	68	CYS
2	F	93	ASP
2	F	95	LYS
2	F	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	76	GLN
1	А	136	GLN
1	А	176	GLN
1	А	180	GLN
1	А	234	GLN
1	А	253	ASN
1	А	308	GLN
1	А	369	GLN
1	А	381	ASN
1	В	136	GLN
1	В	148	ASN
1	В	176	GLN
1	В	180	GLN
1	В	234	GLN
1	В	253	ASN
1	В	297	HIS



RNA (i) 5.3.3

There are no RNA molecules in this entry.

Non-standard residues in protein, DNA, RNA chains (i) 5.4

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

Carbohydrates (i) 5.5

34 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	Bo	ond leng	ths	B	ond ang	gles
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	NAG	С	1	1,3	14,14,15	0.70	0	17,19,21	0.73	0
3	NDG	С	2	3	14,14,15	0.63	0	17,19,21	0.78	1 (5%)
4	NAG	D	1	4,1	14,14,15	0.66	0	17,19,21	0.79	0
4	NDG	D	2	4	14,14,15	0.66	0	17,19,21	0.71	0
4	MAN	D	3	4	11,11,12	0.56	0	15,15,17	0.42	0
5	NAG	G	1	1,5	14,14,15	0.58	0	17,19,21	0.69	0
5	NDG	G	2	5	14,14,15	0.55	0	17,19,21	0.76	0
5	BMA	G	3	5	11,11,12	0.44	0	15,15,17	0.22	0
5	NAG	Н	1	1,5	14,14,15	0.69	0	17,19,21	0.75	0
5	NDG	Н	2	5	14,14,15	0.63	0	17,19,21	0.80	0
5	BMA	Н	3	5	11,11,12	0.50	0	15,15,17	0.27	0



Chain Res Mol Type В GLN 1 308 В GLN 1 369 $\mathbf{2}$ Ε 75HIS F $\mathbf{2}$ ASN 452F ASN 462F 75HIS $\mathbf{2}$ F GLN 96

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Mal	Tuno	Chain	Dec	Tink	Bond lengths		Bond angles		les	
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Ι	1	4,1	14,14,15	0.60	0	17,19,21	0.76	0
4	NDG	Ι	2	4	14,14,15	0.56	0	17,19,21	0.72	0
4	MAN	Ι	3	4	11,11,12	0.54	0	$15,\!15,\!17$	0.43	0
5	NAG	J	1	1,5	14,14,15	0.62	0	17,19,21	0.87	1 (5%)
5	NDG	J	2	5	14,14,15	0.60	0	17,19,21	0.77	1 (5%)
5	BMA	J	3	5	11,11,12	0.49	0	15,15,17	0.24	0
3	NAG	K	1	1,3	14,14,15	0.47	0	17,19,21	0.67	0
3	NDG	K	2	3	14,14,15	0.53	0	17,19,21	0.73	0
4	NAG	L	1	4,1	14,14,15	0.61	0	17,19,21	0.74	0
4	NDG	L	2	4	14,14,15	0.61	0	17,19,21	0.71	1 (5%)
4	MAN	L	3	4	11,11,12	0.55	0	$15,\!15,\!17$	0.44	0
5	NAG	М	1	1,5	14,14,15	0.60	0	17,19,21	0.67	1 (5%)
5	NDG	М	2	5	14,14,15	0.58	0	17,19,21	0.77	1 (5%)
5	BMA	М	3	5	11,11,12	0.48	0	$15,\!15,\!17$	0.28	0
5	NAG	N	1	1,5	14,14,15	0.53	0	17,19,21	0.68	0
5	NDG	N	2	5	14,14,15	0.61	0	17,19,21	0.85	0
5	BMA	Ν	3	5	11,11,12	0.49	0	$15,\!15,\!17$	0.25	0
4	NAG	0	1	4,1	14,14,15	0.64	0	17,19,21	0.66	0
4	NDG	0	2	4	14,14,15	0.69	0	17,19,21	0.68	0
4	MAN	0	3	4	11,11,12	0.55	0	$15,\!15,\!17$	0.40	0
5	NAG	Р	1	1,5	14,14,15	0.61	0	17,19,21	0.70	1(5%)
5	NDG	Р	2	5	14,14,15	0.61	0	17,19,21	0.73	0
5	BMA	Р	3	5	11,11,12	0.47	0	15,15,17	0.22	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	С	1	1,3	-	4/6/23/26	0/1/1/1
3	NDG	С	2	3	-	5/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NDG	D	2	4	-	4/6/23/26	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	3/6/23/26	0/1/1/1
5	NDG	G	2	5	-	3/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Н	1	1,5	1/1/5/7	6/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NDG	Н	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Н	3	5	-	1/2/19/22	0/1/1/1
4	NAG	Ι	1	4,1	1/1/5/7	3/6/23/26	0/1/1/1
4	NDG	Ι	2	4	-	3/6/23/26	0/1/1/1
4	MAN	Ι	3	4	-	0/2/19/22	0/1/1/1
5	NAG	J	1	1,5	1/1/5/7	4/6/23/26	0/1/1/1
5	NDG	J	2	5	-	5/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	5/6/23/26	0/1/1/1
3	NDG	K	2	3	-	5/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	5/6/23/26	0/1/1/1
4	NDG	L	2	4	-	2/6/23/26	0/1/1/1
4	MAN	L	3	4	-	2/2/19/22	0/1/1/1
5	NAG	М	1	1,5	-	4/6/23/26	0/1/1/1
5	NDG	М	2	5	-	4/6/23/26	0/1/1/1
5	BMA	М	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Ν	1	1,5	-	5/6/23/26	0/1/1/1
5	NDG	Ν	2	5	-	5/6/23/26	0/1/1/1
5	BMA	Ν	3	5	-	0/2/19/22	0/1/1/1
4	NAG	0	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1
4	NDG	0	2	4	-	3/6/23/26	0/1/1/1
4	MAN	Ο	3	4	-	2/2/19/22	0/1/1/1
5	NAG	Р	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NDG	Р	2	5	-	4/6/23/26	0/1/1/1
5	BMA	Р	3	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	J	1	NAG	C2-N2-C7	-2.19	119.78	122.90
3	С	2	NDG	C2-N2-C7	-2.16	119.83	122.90
5	J	2	NDG	C2-N2-C7	-2.10	119.92	122.90
4	L	2	NDG	C2-N2-C7	-2.05	119.98	122.90
5	Р	1	NAG	C2-N2-C7	-2.04	120.00	122.90
5	М	1	NAG	C2-N2-C7	-2.02	120.03	122.90
5	М	2	NDG	C2-N2-C7	-2.01	120.03	122.90



2IFG

All (5) chirality outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atom
4	Ι	1	NAG	C1
4	0	1	NAG	C1
5	Н	1	NAG	C1
5	J	1	NAG	C1
5	Р	1	NAG	C1

All (99) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type Atoms	
3	С	1	NAG	C8-C7-N2-C2
3	С	1	NAG	O7-C7-N2-C2
3	С	2	NDG	C8-C7-N2-C2
3	С	2	NDG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	Κ	1	NAG	O7-C7-N2-C2
3	К	2	NDG	C8-C7-N2-C2
3	K	2	NDG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NDG	C8-C7-N2-C2
4	D	2	NDG	O7-C7-N2-C2
4	Ι	1	NAG	C8-C7-N2-C2
4	Ι	1	NAG	O7-C7-N2-C2
4	Ι	2	NDG	C8-C7-N2-C2
4	Ι	2	NDG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	L	2	NDG	C8-C7-N2-C2
4	L	2	NDG	O7-C7-N2-C2
4	0	1	NAG	C8-C7-N2-C2
4	0	1	NAG	O7-C7-N2-C2
4	0	2	NDG	C8-C7-N2-C2
4	0	2	NDG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NDG	C8-C7-N2-C2
5	G	2	NDG	O7-C7-N2-C2
5	Н	1	NAG	C1-C2-N2-C7
5	Н	1	NAG	C8-C7-N2-C2
5	Н	1	NAG	O7-C7-N2-C2
5	Н	2	NDG	C8-C7-N2-C2
5	Н	2	NDG	O7-C7-N2-C2



Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	2	NDG	C8-C7-N2-C2
5	J	2	NDG	O7-C7-N2-C2
5	М	1	NAG	C8-C7-N2-C2
5	М	1	NAG	O7-C7-N2-C2
5	М	2	NDG	C8-C7-N2-C2
5	М	2	NDG	O7-C7-N2-C2
5	Ν	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	N	2	NDG	C8-C7-N2-C2
5	N	2	NDG	O7-C7-N2-C2
5	Р	1	NAG	C8-C7-N2-C2
5	Р	1	NAG	O7-C7-N2-C2
5	Р	2	NDG	C8-C7-N2-C2
5	Р	2	NDG	O7-C7-N2-C2
4	0	3	MAN	O5-C5-C6-O6
4	L	1	NAG	C1-C2-N2-C7
3	С	1	NAG	O5-C5-C6-O6
5	Ν	1	NAG	O5-C5-C6-O6
5	Н	1	NAG	C4-C5-C6-O6
5	Н	1	NAG	O5-C5-C6-O6
5	Ν	2	NDG	O5-C5-C6-O6
5	Р	2	NDG	O5-C5-C6-O6
5	J	2	NDG	C4-C5-C6-O6
3	С	2	NDG	O5-C5-C6-O6
4	0	3	MAN	C4-C5-C6-O6
5	J	2	NDG	O5-C5-C6-O6
5	М	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	3	MAN	C4-C5-C6-O6
3	K	2	NDG	C4-C5-C6-O6
4	D	2	NDG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	М	1	NAG	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	М	2	NDG	O5-C5-C6-O6
5	N	2	NDG	C4-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
3	C	2	NDG	C4-C5-C6-O6
4	D	2	NDG	O5-C5-C6-O6



Mol	Chain	Res	Type	Atoms
3	Κ	2	NDG	O5-C5-C6-O6
5	Р	2	NDG	C4-C5-C6-O6
4	Ι	1	NAG	O5-C5-C6-O6
5	G	2	NDG	O5-C5-C6-O6
3	Κ	1	NAG	O5-C5-C6-O6
4	Ι	2	NDG	O5-C5-C6-O6
5	N	1	NAG	C1-C2-N2-C7
5	Н	3	BMA	O5-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7
4	0	2	NDG	O5-C5-C6-O6
4	L	3	MAN	C4-C5-C6-O6
4	L	3	MAN	O5-C5-C6-O6
5	М	2	NDG	C4-C5-C6-O6
5	Р	3	BMA	C4-C5-C6-O6
5	J	2	NDG	C1-C2-N2-C7
4	L	1	NAG	C3-C2-N2-C7
5	Н	1	NAG	C3-C2-N2-C7
3	Κ	1	NAG	C1-C2-N2-C7
3	С	2	NDG	C1-C2-N2-C7
3	K	2	NDG	C1-C2-N2-C7
5	Р	3	BMA	O5-C5-C6-O6
5	N	2	NDG	C1-C2-N2-C7
4	L	1	NAG	C4-C5-C6-O6
3	К	1	NAG	C3-C2-N2-C7

Continued from previous page...

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	1	NAG	4	0
5	Н	1	NAG	1	0
5	G	2	NDG	1	0
4	L	1	NAG	2	0
4	L	2	NDG	1	0
4	D	1	NAG	1	0
5	Н	2	NDG	1	0
5	G	1	NAG	6	0
3	С	2	NDG	5	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.







































5.6 Ligand geometry (i)

There are no ligands in this entry.

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	347/347~(100%)	-0.13	18 (5%) 27 27	4, 70, 182, 200	0
1	В	347/347~(100%)	0.60	62 (17%) 1 1	15, 122, 195, 200	0
2	Ε	108/120~(90%)	0.21	12 (11%) 5 6	15, 69, 184, 200	0
2	F	109/120~(90%)	-0.06	4 (3%) 41 40	8, 65, 153, 200	0
All	All	911/934~(97%)	0.20	96 (10%) 6 7	4, 81, 191, 200	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Е	46	ASN	8.0
1	В	53	ASP	7.5
1	А	58	SER	7.5
1	В	50	CYS	7.4
1	В	60	HIS	7.2
1	В	61	HIS	7.0
2	Е	2	SER	6.6
1	В	90	LEU	6.2
2	Е	49	PHE	5.9
1	В	51	THR	5.6
1	В	57	ASP	5.6
1	В	54	GLY	5.4
1	В	41	CYS	5.2
1	А	78	HIS	5.1
1	В	63	PRO	4.7
2	Е	45	ASN	4.7
1	В	234	GLN	4.7
1	А	61	HIS	4.5
1	В	52	ARG	4.5
1	А	62	LEU	4.4
1	В	178	HIS	4.2



Mol	Chain	Res	Type	RSRZ
1	В	36	CYS	4.2
1	В	139	SER	4.1
1	В	336	ALA	4.0
1	В	39	ALA	4.0
1	А	44	GLY	4.0
1	В	55	ALA	3.9
1	В	40	CYS	3.8
1	В	94	ARG	3.7
1	А	37	PRO	3.7
1	В	56	LEU	3.6
1	В	117	LEU	3.6
2	Е	47	SER	3.6
1	В	37	PRO	3.5
1	В	89	GLY	3.5
1	В	102	GLY	3.5
1	А	60	HIS	3.4
1	В	199	GLN	3.4
1	В	78	HIS	3.4
1	А	36	CYS	3.3
2	F	46	ASN	3.1
1	В	65	ALA	3.1
2	Е	94	GLY	3.1
1	А	234	GLN	3.0
1	В	38	ASP	3.0
1	В	241	SER	3.0
2	F	45	ASN	3.0
1	В	112	HIS	3.0
2	F	95	LYS	3.0
2	Е	43	ASN	2.9
1	В	80	GLN	2.9
1	А	51	THR	2.9
1	А	90	LEU	2.9
1	В	73	ILE	2.9
1	В	124	PHE	2.9
1	В	71	LEU	2.8
1	В	75	ASN	2.8
1	В	85	ARG	2.8
2	E	95	LYS	2.8
1	A	52	ARG	2.7
1	А	41	CYS	2.7
1	В	49	ARG	2.7
2	Е	44	ILE	2.7



Continued from previous page					
Mol	Chain	Res	Type	RSRZ	

2	F	2	SER	2.6
2	Е	60	ASP	2.6
2	Е	96	GLN	2.6
1	В	43	HIS	2.6
1	А	214	ARG	2.5
1	А	178	HIS	2.5
1	В	266	TRP	2.5
1	В	177	CYS	2.5
1	В	67	ASN	2.5
1	В	172	GLU	2.4
1	А	55	ALA	2.4
1	А	57	ASP	2.4
1	В	62	LEU	2.3
2	Е	48	VAL	2.3
1	В	44	GLY	2.3
1	В	84	LEU	2.3
1	В	81	HIS	2.3
1	В	74	GLU	2.2
1	В	69	THR	2.2
1	В	225	ALA	2.2
1	В	79	LEU	2.2
1	А	248	GLY	2.2
1	В	83	GLU	2.2
1	В	337	ALA	2.1
1	В	115	PRO	2.1
1	В	214	ARG	2.1
1	В	59	LEU	2.1
1	В	100	LYS	2.1
1	В	58	SER	2.1
1	В	105	PHE	2.1
1	В	248	GLY	2.1
1	В	66	GLU	2.0
1	В	119	ARG	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	$B-factors(Å^2)$	Q<0.9
4	MAN	D	3	11/12	-0.02	0.64	200,200,200,200	0
4	MAN	Ι	3	11/12	0.28	0.84	200,200,200,200	0
5	BMA	J	3	11/12	0.31	0.87	200,200,200,200	0
5	BMA	Ν	3	11/12	0.34	0.55	200,200,200,200	0
5	BMA	Р	3	11/12	0.34	0.64	200,200,200,200	0
5	BMA	Н	3	11/12	0.41	0.42	194,194,194,194	0
4	NDG	0	2	14/15	0.44	0.58	197,197,197,197	0
4	NDG	D	2	14/15	0.46	0.58	198,198,198,198	0
5	BMA	G	3	11/12	0.54	0.66	197,197,197,197	0
4	NDG	Ι	2	14/15	0.56	0.55	188,188,188,188	0
4	MAN	L	3	11/12	0.56	0.54	193,193,193,193	0
3	NDG	K	2	14/15	0.63	0.42	191,191,191,191	0
5	NDG	J	2	14/15	0.67	0.43	191,191,191,191	0
3	NAG	K	1	14/15	0.67	0.27	170,170,170,170	0
4	NAG	0	1	14/15	0.68	0.43	200,200,200,200	0
4	NDG	L	2	14/15	0.70	0.35	166,166,166,166	0
4	MAN	0	3	11/12	0.70	0.41	166,166,166,166	0
5	BMA	М	3	11/12	0.71	0.58	180,180,180,180	0
5	NAG	Р	1	14/15	0.72	0.42	200,200,200,200	0
5	NDG	Н	2	14/15	0.78	0.26	184,185,185,185	0
5	NDG	Р	2	14/15	0.79	0.62	200,200,200,200	0
5	NDG	G	2	14/15	0.82	0.33	116,121,126,137	0
4	NAG	Ι	1	14/15	0.83	0.27	177,177,177,177	0
4	NAG	D	1	14/15	0.84	0.33	116,116,116,116	0
3	NDG	С	2	14/15	0.84	0.39	165,170,175,186	0
5	NAG	Н	1	14/15	0.85	0.23	89,93,98,105	0
5	NDG	N	2	14/15	0.85	0.24	131,132,132,132	0
5	NAG	J	1	14/15	0.85	0.27	107,111,115,122	0
4	NAG	L	1	14/15	0.87	0.27	116,116,116,116	0
3	NAG	С	1	14/15	0.87	0.18	81,85,90,97	0
5	NAG	М	1	14/15	0.87	0.24	116,120,123,123	0
5	NAG	N	1	14/15	0.89	0.20	75,79,83,85	0
5	NDG	M	2	14/15	0.89	0.24	146,146,146,146	0
5	NAG	G	1	14/15	0.94	0.22	65,69,74,81	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-





charide. Each fit is shown from different orientation to approximate a three-dimensional view.

























6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

