

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

#### May 25, 2020 – 09:29 pm BST

PDB ID	:	2WVZ
$\operatorname{Title}$	:	Structure of the Family GH92 Inverting Mannosidase BT3990 from Bacteroides
		thetaiotaomicron VPI-5482
Authors	:	Suits, M.D.L.; Zhu, Y.; Thompson, A.; Gilbert, H.J.; Davies, G.J.
Deposited on	:	2009-10-21
Resolution	:	2.40  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The 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 as 541 be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398(2.40-2.40)
Ramachandran outliers	138981	4318(2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	А	744	79%	18%	••
1	В	744	74%	24%	•
1	С	744	75%	22%	••
1	D	744	71%	26%	••



#### 2WVZ

## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24878 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		A	toms			ZeroOcc	AltConf	Trace
1	Λ	738	Total	С	Ν	Ο	S	0	0	0
	I A (30	150	5994	3847	986	1127	34	0	2	U
1	В	749	Total	С	Ν	Ο	S	0	3	Ο
	D	142	6037	3870	997	1135	35	0	່ <u>ບໍ່</u>	0
1	C	727	Total	С	Ν	Ο	S	0	2	0
		191	5987	3839	984	1130	34	0	3	0
1	р	736	Total	С	Ν	Ο	S	0	1	0
			5970	3828	983	1125	34			U

• Molecule 1 is a protein called PUTATIVE ALPHA-1,2-MANNOSIDASE.

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Ca 1 1	0	0
2	А	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	С	1	Total Ca 1 1	0	0

• Molecule 3 is KIFUNENSINE (three-letter code: KIF) (formula:  $C_8H_{12}N_2O_6$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	Λ	1	Total	С	Ν	Ο	0	0
0	л	L	16	8	2	6	0	0
3	В	1	Total	С	Ν	Ο	0	0
0	D	L	16	8	2	6	0	0
3	С	1	Total	С	Ν	Ο	0	0
0	U	L	16	8	2	6	0	0
3	р	1	Total	С	Ν	0	0	0
0			16	8	2	6		U

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C O 6 3 3	0	0
4	В	1	Total         C         O           6         3         3	0	0
4	В	1	$\begin{array}{c c} \hline & & & \\ \hline \hline & & \\ \hline & & \\ \hline & & \\ \hline & & \\ \hline \hline & & \\ \hline & & \\ \hline & & \\ \hline & & \\ \hline \hline & & \\ \hline \hline \\ \hline & & \\ \hline \hline \\ & & \\ \hline \hline \hline \hline \hline \\ \hline \hline \hline \hline \hline \hline \hline \hline \\ \hline \hline$	0	0
4	С	1	TotalCO633	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	244	Total O 244 244	0	0
5	В	179	Total O 179 179	0	0
5	С	203	Total         O           203         203	0	0
5	D	166	Total O 166 166	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: PUTATIVE ALPHA-1,2-MANNOSIDASE





#### P5 71 P5 73 P5 73 P5 74 P5 87 P5

#### 

• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE





# F664 Y666 X677 X67 X68 X68 X68 X68 X68 X70 F701 X702 X703 F773 X736 X735 X735 X736 X735 X736 X736 X736 X736 X736 X736 X749 X744 X744 X744 X744 X754 X754 X755 X756 X756 X756 X756



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	68.90Å $150.19$ Å $382.29$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Baselution (Å)	191.14 - 2.40	Depositor
Resolution (A)	59.05 - 2.40	EDS
$\% { m Data \ completeness}$	88.1(191.14-2.40)	Depositor
(in resolution range)	88.1(59.05-2.40)	EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.08 (at $2.40$ Å)	Xtriage
Refinement program	REFMAC $5.4.0077$	Depositor
R R.	0.201 , $0.257$	Depositor
II, II, <i>free</i>	0.201 , $0.257$	DCC
$R_{free}$ test set	6859 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor ( $Å^2$ )	33.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 35.3	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24878	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, KIF

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		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.59	0/6183	0.66	0/8389	
1	В	0.55	0/6231	0.65	0/8452	
1	С	0.55	0/6177	0.64	0/8379	
1	D	0.53	0/6154	0.64	0/8348	
All	All	0.55	0/24745	0.65	0/33568	

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	<b>#Planarity outliers</b>
1	В	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	756	LEU	Peptide

#### 5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5994	0	5664	133	0
1	В	6037	0	5699	164	0
1	С	5987	0	5655	152	0
1	D	5970	0	5640	201	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	А	16	0	10	0	0
3	В	16	0	10	1	0
3	С	16	0	10	1	0
3	D	16	0	10	1	0
4	А	6	0	8	0	0
4	В	12	0	16	0	0
4	С	6	0	8	0	0
4	D	6	0	8	0	0
5	А	244	0	0	12	0
5	В	179	0	0	19	0
5	С	203	0	0	9	0
5	D	166	0	0	12	0
All	All	24878	0	22738	648	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 14.

All (648) 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:C:507:LYS:CD	1:C:559:MET:HE3	1.25	1.56
1:C:507:LYS:HE3	1:C:559:MET:CE	1.32	1.55
1:C:507:LYS:CE	1:C:559:MET:CE	1.88	1.49
1:C:507:LYS:CD	1:C:559:MET:CE	1.94	1.46
1:C:507:LYS:CE	1:C:559:MET:HE2	1.44	1.34
1:D:554:MET:CE	1:D:560:PHE:HD2	1.43	1.29
1:D:554:MET:CE	1:D:560:PHE:CD2	2.16	1.28
1:D:566:SER:O	1:D:570:VAL:HG22	1.15	1.28
1:D:566:SER:O	1:D:570:VAL:CG2	1.84	1.23
1:C:496:MET:CE	1:C:499:LYS:HE3	1.67	1.23
1:B:254:ILE:HB	5:B:2047:HOH:O	1.51	1.10
1:C:507:LYS:HD3	1:C:559:MET:CE	1.66	1.10
1:B:258:GLN:CB	5:B:2047:HOH:O	2.00	1.09
1:D:554:MET:HE3	1:D:560:PHE:HD2	1.19	1.08



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:554:MET:HE1	1:D:560:PHE:CD2	1.89	1.02
1:C:592[B]:MET:CE	1:C:631:MET:SD	2.49	1.00
1:A:755:GLU:C	1:A:756:LEU:HG	1.82	1.00
1:B:258:GLN:HG2	5:B:2047:HOH:O	1.62	0.99
1:C:507:LYS:CE	1:C:559:MET:HE3	1.65	0.99
1:C:496:MET:HE3	1:C:499:LYS:HE3	1.45	0.98
1:D:485:LYS:HD2	1:D:485:LYS:N	1.79	0.97
1:D:685:ASN:C	1:D:685:ASN:HD22	1.67	0.97
1:D:408:MET:HA	1:D:408:MET:CE	1.95	0.97
1:C:496:MET:CE	1:C:499:LYS:CE	2.43	0.96
1:C:496:MET:HE2	1:C:499:LYS:CE	1.97	0.94
1:C:257[A]:GLU:CD	1:C:257[A]:GLU:H	1.64	0.93
1:A:554:MET:O	1:A:559[B]:MET:HE3	1.67	0.93
1:C:592[B]:MET:HE3	1:C:631:MET:SD	2.09	0.93
1:D:564:MET:HE3	1:D:607:MET:HE3	1.49	0.93
1:C:592[B]:MET:HE2	1:C:631:MET:SD	2.09	0.92
1:D:685:ASN:HD22	1:D:686:GLY:N	1.67	0.92
1:B:175:ILE:O	1:B:175:ILE:HG22	1.68	0.92
1:A:705:SER:OG	1:A:732:ASP:OD2	1.86	0.92
1:D:592[A]:MET:SD	1:D:631:MET:CE	2.58	0.91
1:D:494:ARG:HA	1:D:497:ASN:ND2	1.84	0.91
1:B:431:HIS:CD2	1:B:432:PRO:HD2	2.05	0.91
1:C:496:MET:HE2	1:C:499:LYS:HE3	1.47	0.91
1:D:407:TYR:HD1	1:D:408:MET:HE3	1.35	0.91
1:D:685:ASN:ND2	1:D:687:ASN:H	1.69	0.91
1:B:758:HIS:HB3	1:B:760:HIS:CE1	2.06	0.90
1:A:188:ASN:HD22	1:A:190:GLY:H	1.20	0.90
1:D:408:MET:HA	1:D:408:MET:HE2	1.51	0.89
1:C:459:GLU:HG2	1:C:531:PHE:O	1.73	0.88
1:C:358:ASN:HD21	1:C:365:ASN:HD22	1.19	0.88
1:C:407:TYR:HD1	1:C:408:MET:HE2	1.39	0.87
1:B:758:HIS:HB3	1:B:760:HIS:HE1	1.39	0.87
1:A:754:LYS:O	1:A:755:GLU:HB3	1.75	0.86
1:A:755:GLU:O	1:A:756:LEU:HD12	1.76	0.86
1:B:496:MET:CE	1:B:499:LYS:HE2	2.05	0.86
1:A:736:ARG:HD2	5:A:2237:HOH:O	1.77	0.85
1:A:496:MET:CE	1:A:499:LYS:HE3	2.07	0.84
1:C:22:TRP:H	1:C:283:ASN:ND2	1.74	0.84
1:A:407:TYR:HD1	1:A:408:MET:CE	1.90	0.84
1:D:431:HIS:HD2	1:D:433:GLU:H	1.26	0.84
1:C:496:MET:HE2	1:C:499:LYS:NZ	1.93	0.84



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ( { m \AA} )$	overlap (Å)
1:A:755:GLU:O	1:A:756:LEU:CG	2.26	0.84
1:D:571:PRO:HB2	1:D:573:ILE:HD13	1.60	0.83
1:B:616:GLN:HG2	1:B:618:TRP:CZ2	2.13	0.83
1:A:407:TYR:HD1	1:A:408:MET:HE2	1.44	0.83
1:A:755:GLU:C	1:A:757:GLU:H	1.81	0.83
1:D:571:PRO:HB2	1:D:573:ILE:CD1	2.09	0.82
1:D:502:PHE:CG	1:D:553:LEU:HD13	2.14	0.81
1:C:505:GLU:HG2	5:C:2110:HOH:O	1.79	0.81
1:D:407:TYR:CD1	1:D:408:MET:HE3	2.16	0.79
1:B:284:GLN:HG2	5:B:2056:HOH:O	1.81	0.79
1:C:507:LYS:HD3	1:C:559:MET:HE3	0.79	0.79
1:D:506:SER:HB3	5:D:2136:HOH:O	1.83	0.79
1:A:559[A]:MET:CE	1:A:563:MET:HG2	2.14	0.78
1:D:188:ASN:HD22	1:D:190:GLY:H	1.27	0.78
1:C:504:LYS:CB	1:C:504:LYS:NZ	2.46	0.77
1:D:685:ASN:HD21	1:D:687:ASN:H	1.31	0.77
1:B:685:ASN:C	1:B:685:ASN:HD22	1.87	0.77
1:D:508:LEU:HB2	5:D:2137:HOH:O	1.83	0.77
1:A:507:LYS:HZ1	1:A:559[B]:MET:HE1	1.50	0.76
1:D:537:TRP:O	1:D:541:TRP:NE1	2.19	0.76
1:D:584:HIS:ND1	1:D:588:GLU:OE2	2.11	0.76
1:A:358:ASN:HD21	1:A:365:ASN:HD22	1.33	0.76
1:D:588:GLU:O	1:D:592[B]:MET:SD	2.45	0.75
1:D:313:PRO:HD2	1:D:368:MET:HE1	1.68	0.75
1:A:755:GLU:O	1:A:756:LEU:CD1	2.35	0.75
1:D:431:HIS:CD2	1:D:433:GLU:H	2.03	0.75
1:C:407:TYR:HD1	1:C:408:MET:CE	1.99	0.74
1:D:313:PRO:HG2	1:D:368:MET:HE2	1.70	0.74
1:A:134:HIS:HB3	1:A:136:ILE:HD12	1.69	0.74
1:C:507:LYS:HD2	1:C:559:MET:CE	2.13	0.74
1:D:86:SER:HB2	1:D:87:PRO:HD2	1.70	0.74
1:A:559[A]:MET:HE2	1:A:563:MET:HG2	1.69	0.73
1:C:22:TRP:H	1:C:283:ASN:HD21	1.35	0.73
1:A:754:LYS:O	1:A:755:GLU:CB	2.33	0.73
1:B:358:ASN:HD21	1:B:365:ASN:HD22	1.35	0.73
1:A:755:GLU:C	1:A:756:LEU:CG	2.55	0.73
1:C:188:ASN:HD22	1:C:190:GLY:H	1.34	0.73
1:D:526:LYS:HA	1:D:575:ASP:HB3	1.71	0.73
1:C:597:TYR:OH	1:C:599:HIS:HD2	1.72	0.72
1:A:358:ASN:ND2	1:A:365:ASN:HD22	1.87	0.72
1:A:685:ASN:ND2	1:A:687:ASN:H	1.87	0.72



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ( { m \AA} )$	overlap (Å)
1:B:188:ASN:HD22	1:B:190:GLY:H	1.37	0.72
1:B:554:MET:O	1:B:559[B]:MET:HE3	1.90	0.72
1:C:685:ASN:ND2	1:C:687:ASN:H	1.87	0.72
1:D:613:TYR:CE2	1:D:749:PRO:HG2	2.25	0.72
1:B:365:ASN:O	1:B:369:GLN:HG2	1.90	0.72
1:D:592[A]:MET:SD	1:D:631:MET:HE2	2.30	0.71
1:C:597:TYR:CE2	1:C:599:HIS:HB2	2.25	0.71
1:A:685:ASN:C	1:A:685:ASN:HD22	1.93	0.71
1:C:507:LYS:CD	1:C:559:MET:HE1	2.14	0.71
1:B:685:ASN:ND2	1:B:687:ASN:H	1.89	0.70
1:D:554:MET:HE2	1:D:560:PHE:CD2	2.24	0.70
1:A:753:SER:O	1:A:756:LEU:HD11	1.91	0.70
1:B:685:ASN:HD22	1:B:686:GLY:N	1.89	0.70
1:D:554:MET:HE1	1:D:560:PHE:CE2	2.26	0.70
1:C:504:LYS:CB	1:C:504:LYS:HZ2	2.04	0.70
1:B:547:PRO:HG2	1:B:613:TYR:CE2	2.26	0.70
1:B:258:GLN:CG	5:B:2047:HOH:O	2.13	0.70
1:C:692:ASP:OD1	5:C:2175:HOH:O	2.09	0.69
1:A:755:GLU:O	1:A:756:LEU:CB	2.39	0.69
1:B:153:PHE:HA	5:B:2027:HOH:O	1.91	0.69
1:A:295:ASN:OD1	1:A:297:ASP:HB2	1.92	0.69
1:A:407:TYR:CD1	1:A:408:MET:CE	2.75	0.68
1:D:554:MET:HE3	1:D:560:PHE:CD2	2.04	0.68
1:B:58:PRO:HG3	1:B:127:TYR:CZ	2.29	0.68
1:B:172:ILE:HG22	1:B:231:ALA:HB1	1.74	0.68
1:C:755:GLU:O	1:C:756:LEU:CB	2.43	0.67
1:D:494:ARG:HA	1:D:497:ASN:HD21	1.56	0.67
1:D:554:MET:CE	1:D:560:PHE:CE2	2.76	0.67
1:A:431:HIS:HD2	1:A:433:GLU:H	1.40	0.67
1:B:529:ASP:HB3	5:B:2117:HOH:O	1.95	0.67
1:A:755:GLU:HG2	1:A:756:LEU:H	1.59	0.67
1:D:564:MET:CE	1:D:607:MET:HE3	2.21	0.67
1:A:755:GLU:C	1:A:757:GLU:N	2.48	0.67
1:C:496:MET:CE	1:C:499:LYS:NZ	2.58	0.67
1:D:400:ALA:O	1:D:404:VAL:HG23	1.95	0.67
1:A:496:MET:HE3	1:A:499:LYS:HE3	1.75	0.66
1:A:188:ASN:ND2	1:A:190:GLY:H	1.90	0.66
1:A:709:ASN:HD21	1:A:728:THR:H	1.43	0.66
1:B:211:LYS:HZ2	1:B:222:ASN:HA	1.61	0.66
1:D:503:ASP:OD2	1:D:510:ARG:NH1	2.29	0.66
1:D:507:LYS:HB3	1:D:554:MET:HG2	1.76	0.66



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:216:ASN:HD22	1:D:216:ASN:N	1.94	0.66
1:B:158:HIS:HB3	1:B:160:TYR:HE1	1.62	0.65
1:D:350:PHE:HA	1:D:402:ILE:HD11	1.78	0.65
1:D:592[A]:MET:SD	1:D:631:MET:HE1	2.35	0.65
1:B:431:HIS:HD2	1:B:433:GLU:H	1.43	0.65
1:C:504:LYS:HZ2	1:C:504:LYS:HB2	1.61	0.65
1:B:559[B]:MET:HG3	5:B:2124:HOH:O	1.97	0.65
1:A:22[B]:TRP:CZ2	1:A:290:GLU:HG2	2.32	0.64
1:A:709:ASN:ND2	1:A:728:THR:H	1.95	0.64
1:D:452:PRO:HG2	1:D:455:VAL:HG21	1.79	0.64
1:B:175:ILE:CG2	1:B:175:ILE:O	2.42	0.64
1:C:358:ASN:ND2	1:C:365:ASN:HD22	1.93	0.64
1:C:685:ASN:HD22	1:C:685:ASN:C	1.99	0.64
1:D:685:ASN:ND2	1:D:685:ASN:C	2.41	0.64
1:A:365:ASN:O	1:A:369:GLN:HG2	1.98	0.64
1:C:496:MET:HE2	1:C:499:LYS:HZ2	1.63	0.63
1:D:503:ASP:C	1:D:503:ASP:OD1	2.34	0.63
1:D:313:PRO:HD2	1:D:368:MET:CE	2.27	0.63
1:A:477:LEU:HG	1:A:481:LEU:HD22	1.80	0.63
1:B:525:LEU:HD13	1:B:573:ILE:HG13	1.80	0.63
1:A:571:PRO:HB2	1:A:573:ILE:HD13	1.81	0.63
1:A:431:HIS:CD2	1:A:433:GLU:H	2.16	0.63
1:A:496:MET:CE	1:A:499:LYS:CE	2.76	0.63
1:C:358:ASN:HD21	1:C:365:ASN:ND2	1.95	0.63
1:B:407:TYR:HD1	1:B:408:MET:CE	2.12	0.62
1:A:615:GLY:O	1:A:743:THR:HG22	1.98	0.62
1:C:400:ALA:O	1:C:404:VAL:HG23	1.98	0.62
1:A:753:SER:O	1:A:756:LEU:CD1	2.48	0.62
1:D:358:ASN:HD21	1:D:365:ASN:HD22	1.48	0.62
1:A:526:LYS:HA	1:A:575:ASP:HB3	1.82	0.62
1:C:172:ILE:HG22	1:C:231:ALA:HB1	1.82	0.61
1:B:153:PHE:CD1	1:B:159:SER:HB3	2.35	0.61
1:C:547:PRO:HG2	1:C:613:TYR:CE2	2.35	0.61
1:D:408:MET:HA	1:D:408:MET:HE3	1.82	0.61
1:B:155:GLU:HB2	1:B:241:LYS:N	2.15	0.61
1:A:507:LYS:NZ	1:A:559[B]:MET:HE1	2.15	0.61
1:B:136:ILE:HG23	5:B:2027:HOH:O	1.99	0.61
1:C:407:TYR:CD1	1:C:408:MET:CE	2.81	0.61
1:B:555:GLY:HA3	1:B:559[B]:MET:HE2	1.82	0.61
1:D:496:MET:CE	1:D:752:PHE:CD2	2.84	0.61
1:A:331:TYR:CZ	1:A:375:THR:HG23	2.36	0.60



Atom 1	Atom 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:23:THR:HG23	1:B:283:ASN:ND2	2.16	0.60
1:D:494:ARG:CA	1:D:497:ASN:ND2	2.60	0.60
1:B:597:TYR:OH	1:B:599:HIS:HD2	1.85	0.60
1:D:352:CYS:HA	1:D:355:PRO:HG2	1.84	0.60
1:D:554:MET:HE2	1:D:560:PHE:HD2	1.56	0.60
1:D:613:TYR:CD2	1:D:749:PRO:HG2	2.35	0.60
1:D:548:GLN:NE2	1:D:552:ASP:OD1	2.35	0.59
1:D:754:LYS:O	1:D:755:GLU:C	2.39	0.59
1:B:104:PRO:HB2	1:B:219:LEU:HD21	1.83	0.59
1:C:365:ASN:O	1:C:369:GLN:HG2	2.02	0.59
1:B:496:MET:HE3	1:B:499:LYS:HE2	1.84	0.59
1:D:586:ILE:HB	5:D:2150:HOH:O	2.02	0.59
1:C:504:LYS:NZ	1:C:504:LYS:HB3	2.17	0.59
1:B:160:TYR:CD1	1:B:160:TYR:N	2.71	0.58
1:C:736:ARG:HD3	5:C:2190:HOH:O	2.02	0.58
1:B:700:ASN:HD22	1:B:735:ASN:HB3	1.67	0.58
1:A:685:ASN:HD22	1:A:686:GLY:N	2.00	0.58
1:C:431:HIS:HD2	1:C:433:GLU:H	1.49	0.58
1:D:496:MET:HE1	1:D:752:PHE:CD2	2.38	0.58
1:A:592:MET:O	1:A:593:ASN:HB3	2.03	0.58
1:D:523:SER:HB2	5:D:2140:HOH:O	2.03	0.58
1:C:175:ILE:O	1:C:175:ILE:HG22	2.02	0.58
1:D:327:HIS:ND1	1:D:338:GLY:O	2.33	0.57
1:C:58:PRO:HG3	1:C:127:TYR:CZ	2.40	0.57
1:D:354:PHE:N	1:D:355:PRO:CD	2.67	0.57
1:D:416:ILE:HD12	5:D:2124:HOH:O	2.04	0.57
1:D:615:GLY:O	1:D:743:THR:HG23	2.05	0.57
1:A:685:ASN:HD22	1:A:687:ASN:H	1.51	0.57
1:B:258:GLN:HB3	5:B:2047:HOH:O	1.82	0.57
1:B:415:ASP:OD2	1:B:418:THR:OG1	2.18	0.57
1:D:532:THR:HG22	1:D:532:THR:O	2.03	0.57
1:A:559[A]:MET:HE2	1:A:563:MET:CG	2.33	0.57
1:B:22:TRP:H	1:B:283:ASN:HD21	1.51	0.57
1:C:685:ASN:HD22	1:C:686:GLY:N	2.01	0.57
1:D:738:ASN:C	1:D:738:ASN:OD1	2.42	0.57
1:B:208:PHE:CD1	1:B:208:PHE:N	2.72	0.57
1:C:26:VAL:HG11	1:C:124:PRO:HG3	1.87	0.57
1:D:592[A]:MET:SD	1:D:631:MET:SD	3.02	0.57
1:D:358:ASN:ND2	1:D:365:ASN:HD22	2.02	0.56
1:B:419:LEU:C	1:B:419:LEU:HD12	2.24	0.56
1:B:533:GLU:OE2	3:B:801:KIF:O2	2.24	0.56



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:400:ALA:HA	1:C:423:LEU:HD21	1.87	0.56
1:A:721:GLU:HB3	5:A:2213:HOH:O	2.06	0.56
1:C:165:ALA:O	1:C:166:PHE:HB2	2.05	0.56
1:D:157:ASP:HA	1:D:238:LYS:HG2	1.87	0.56
1:C:407:TYR:HE2	1:C:416:ILE:HD13	1.70	0.56
1:B:685:ASN:HD21	1:B:687:ASN:HB2	1.69	0.56
1:A:263:MET:HG2	5:A:2080:HOH:O	2.04	0.56
1:A:559[A]:MET:HE3	1:A:563:MET:HG2	1.86	0.56
1:B:358:ASN:ND2	1:B:365:ASN:HD22	2.01	0.56
1:D:216:ASN:H	1:D:216:ASN:HD22	1.53	0.56
1:B:431:HIS:CD2	1:B:432:PRO:CD	2.86	0.56
1:C:564:MET:HE3	1:C:607:MET:HG2	1.88	0.56
1:A:43:THR:HB	1:A:308:ARG:NH1	2.20	0.56
1:A:602:GLN:N	1:A:603:PRO:CD	2.69	0.56
1:A:602:GLN:N	1:A:603:PRO:HD3	2.21	0.56
1:C:134:HIS:HB3	1:C:136:ILE:HD12	1.88	0.56
1:B:419:LEU:O	1:B:419:LEU:HD12	2.06	0.55
1:A:555:GLY:HA3	1:A:559[B]:MET:HE2	1.88	0.55
1:D:502:PHE:CD1	1:D:553:LEU:HD13	2.41	0.55
1:A:547:PRO:HG2	1:A:613:TYR:CE2	2.42	0.55
1:D:613:TYR:O	1:D:748:MET:SD	2.64	0.55
1:B:526:LYS:HA	1:B:575:ASP:HB3	1.89	0.55
1:D:571:PRO:HB2	1:D:573:ILE:HD11	1.87	0.55
1:C:709:ASN:HD21	1:C:727:GLY:HA3	1.71	0.55
1:A:673:THR:O	1:A:673:THR:HG23	2.06	0.55
1:C:270:ASN:OD1	1:C:273:GLN:HG3	2.07	0.55
1:A:194:GLU:HG3	5:A:2064:HOH:O	2.06	0.55
1:D:557:LYS:O	1:D:560:PHE:HB3	2.06	0.55
1:D:558:GLU:H	1:D:558:GLU:CD	2.09	0.55
1:B:139:GLU:OE2	5:B:2025:HOH:O	2.18	0.54
1:D:408:MET:CA	1:D:408:MET:CE	2.77	0.54
1:A:23:THR:H	1:A:283:ASN:HD21	1.55	0.54
1:C:199:TYR:O	1:C:251:SER:HA	2.06	0.54
1:B:293:GLY:HA3	1:B:677:LYS:HB2	1.89	0.54
1:C:685:ASN:HD22	1:C:687:ASN:H	1.54	0.54
1:D:103:GLN:HA	1:D:103:GLN:OE1	2.06	0.54
1:A:172:ILE:HG21	1:A:232:GLY:O	2.08	0.54
1:B:685:ASN:ND2	1:B:685:ASN:C	2.57	0.54
1:A:134:HIS:CB	1:A:136:ILE:HD12	2.37	0.54
1:D:199:TYR:O	1:D:251:SER:HA	2.08	0.54
1:D:546:ASP:N	1:D:547:PRO:HD3	2.23	0.54



Atom-1	Atom-2	Interatomic	Clash
	1100m 2	distance (Å)	overlap (Å)
1:B:212:ALA:HB2	1:B:221:GLU:HA	1.90	0.54
1:C:700:ASN:HD22	1:C:735:ASN:HB3	1.72	0.53
1:D:331:TYR:CE2	1:D:375:THR:HG23	2.43	0.53
1:A:248:ARG:NH1	5:A:2080:HOH:O	2.36	0.53
1:C:188:ASN:ND2	1:C:190:GLY:H	2.04	0.53
1:B:329:SER:HB2	1:B:378:GLU:OE1	2.09	0.53
1:B:507:LYS:HE3	1:B:559[A]:MET:SD	2.49	0.53
1:A:130:TYR:HE2	1:C:590:THR:O	1.91	0.53
1:A:361:TYR:N	1:A:362:PRO:HD3	2.23	0.53
1:D:485:LYS:H	1:D:485:LYS:HD2	1.71	0.53
1:D:22:TRP:H	1:D:283:ASN:ND2	2.05	0.53
1:B:107:ASP:O	1:B:111:ARG:HG2	2.09	0.53
1:C:293:GLY:HA3	1:C:677:LYS:HB2	1.91	0.53
1:A:752:PHE:O	1:A:754:LYS:O	2.26	0.53
1:C:611:TYR:HB2	1:C:620:ALA:HB2	1.90	0.53
1:A:756:LEU:O	1:A:757:GLU:O	2.27	0.53
1:B:459:GLU:HG2	1:B:531:PHE:O	2.08	0.52
1:B:40:THR:O	1:B:639:TYR:HB2	2.09	0.52
1:B:58:PRO:HG3	1:B:127:TYR:CE1	2.45	0.52
1:D:564:MET:CE	1:D:607:MET:CE	2.87	0.52
1:B:153:PHE:HB3	1:B:154:PRO:HD2	1.91	0.52
1:B:451:VAL:O	1:B:460:ASN:HB2	2.10	0.52
1:D:407:TYR:HE2	1:D:416:ILE:HD13	1.74	0.52
1:B:685:ASN:HD22	1:B:687:ASN:H	1.56	0.52
1:B:756:LEU:O	1:B:756:LEU:HG	2.08	0.52
1:D:527:TRP:CZ2	1:D:538:HIS:HE1	2.27	0.52
1:A:483:ARG:HB3	1:A:484:PRO:CD	2.40	0.52
1:B:506:SER:O	1:B:507:LYS:HB2	2.09	0.52
1:C:348:ASP:OD2	3:C:801:KIF:O3	2.28	0.52
1:A:507:LYS:HZ1	1:A:559[B]:MET:CE	2.23	0.52
1:A:555:GLY:HA3	1:A:559[B]:MET:CE	2.40	0.52
1:B:155:GLU:H	1:B:241:LYS:HA	1.75	0.52
1:B:153:PHE:CE1	1:B:159:SER:HB3	2.44	0.52
1:B:705:SER:OG	1:B:732[A]:ASP:OD2	2.27	0.52
1:D:557:LYS:O	1:D:561:VAL:HG23	2.09	0.52
1:A:21:ASP:OD1	1:A:279:LYS:HE3	2.10	0.51
1:B:459:GLU:CG	1:B:531:PHE:O	2.59	0.51
1:A:101:VAL:HG13	1:A:136:ILE:HD11	1.92	0.51
1:B:407:TYR:CD1	1:B:408:MET:CE	2.92	0.51
1:D:502:PHE:CD1	1:D:553:LEU:CD1	2.94	0.51
1:A:134:HIS:HB3	1:A:136:ILE:CD1	2.38	0.51



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:677:LYS:HE2	5:A:2085:HOH:O	2.10	0.51
1:C:506:SER:O	1:C:507:LYS:HB2	2.10	0.51
1:D:602:GLN:N	1:D:603:PRO:CD	2.74	0.51
1:B:597:TYR:CD1	1:B:604:ILE:HD13	2.46	0.51
1:C:504:LYS:HZ3	1:C:504:LYS:HB3	1.75	0.51
1:C:507:LYS:HD2	1:C:559:MET:HE1	1.87	0.51
1:D:293:GLY:HA3	1:D:677:LYS:HB2	1.92	0.51
1:D:616:GLN:HG2	1:D:618:TRP:CZ2	2.45	0.51
1:C:504:LYS:HZ3	1:C:504:LYS:CB	2.24	0.51
1:D:397:ASN:HB3	1:D:470:ASP:OD2	2.11	0.51
1:A:90:ASN:HB3	1:A:189:SER:OG	2.11	0.51
1:D:559:MET:O	1:D:559:MET:SD	2.69	0.51
1:D:527:TRP:CD2	1:D:586:ILE:HG12	2.46	0.51
1:A:507:LYS:NZ	1:A:559[B]:MET:CE	2.74	0.51
1:D:547:PRO:HG2	1:D:613:TYR:CE2	2.46	0.51
1:A:485:LYS:HE2	1:A:488:ILE:HD12	1.93	0.50
1:B:172:ILE:CG2	1:B:231:ALA:HB1	2.39	0.50
1:C:212:ALA:HB2	1:C:221:GLU:HA	1.93	0.50
1:D:415:ASP:OD2	1:D:418:THR:OG1	2.20	0.50
1:A:755:GLU:O	1:A:756:LEU:HG	1.95	0.50
1:D:167:ASP:O	1:D:168:LYS:HB2	2.10	0.50
1:D:708:PHE:HD1	1:D:708:PHE:C	2.14	0.50
1:B:270:ASN:OD1	1:B:270:ASN:C	2.49	0.50
1:B:443:GLU:CD	1:B:443:GLU:H	2.13	0.50
1:C:408:MET:CE	1:C:480:GLU:HG2	2.42	0.50
1:A:266:LEU:HD22	1:A:274:LEU:HD11	1.91	0.50
1:C:547:PRO:HB2	1:C:613:TYR:CD2	2.46	0.50
1:A:496:MET:HE2	1:A:499:LYS:NZ	2.27	0.50
1:D:562:THR:O	1:D:566:SER:OG	2.30	0.50
1:B:209:THR:O	1:B:209:THR:CG2	2.58	0.50
1:C:162:VAL:HG22	1:C:234:ILE:HG12	1.93	0.50
1:B:559[A]:MET:HE2	1:B:563:MET:HG2	1.94	0.50
1:B:194:GLU:HB3	5:B:2037:HOH:O	2.11	0.50
1:B:498:TYR:OH	1:B:546:ASP:OD2	2.23	0.50
1:D:162:VAL:HG22	1:D:234:ILE:HG12	1.94	0.50
1:D:508:LEU:CB	5:D:2137:HOH:O	2.51	0.50
1:D:708:PHE:C	1:D:708:PHE:CD1	2.86	0.50
1:B:158:HIS:HB3	1:B:160:TYR:CE1	2.44	0.49
1:C:134:HIS:CB	1:C:136:ILE:HD12	2.41	0.49
1:D:443:GLU:H	1:D:443:GLU:CD	2.14	0.49
1:B:709:ASN:HD21	1:B:727:GLY:HA3	1.77	0.49



Atom 1	A 4 D	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:B:85:PRO:HG2	1:B:89:ILE:HG21	1.93	0.49
1:D:452:PRO:HG2	1:D:455:VAL:CG2	2.42	0.49
1:B:171:TYR:HD1	1:B:227:THR:HG1	1.60	0.49
1:D:528:GLY:HA3	1:D:578:TYR:CD2	2.47	0.49
1:B:155:GLU:HB2	1:B:241:LYS:H	1.77	0.49
1:D:352:CYS:C	1:D:355:PRO:HD2	2.33	0.49
1:A:709:ASN:HD21	1:A:727:GLY:HA3	1.78	0.49
1:C:362:PRO:HD2	1:C:684:GLU:CD	2.31	0.49
1:A:756:LEU:C	1:A:757:GLU:O	2.51	0.49
1:B:134:HIS:O	1:B:136:ILE:HG13	2.12	0.49
1:D:540:THR:HG22	1:D:540:THR:O	2.12	0.49
1:A:216:ASN:ND2	1:A:230:HIS:H	2.10	0.49
1:C:212:ALA:CB	1:C:221:GLU:HA	2.43	0.49
1:C:496:MET:HE1	5:C:2126:HOH:O	2.13	0.49
1:B:258:GLN:HB2	5:B:2047:HOH:O	1.89	0.49
1:D:331:TYR:CZ	1:D:375:THR:HG23	2.48	0.49
1:D:408:MET:HE1	1:D:480:GLU:HG2	1.94	0.49
1:A:443:GLU:H	1:A:443:GLU:CD	2.15	0.49
1:B:26:VAL:HG11	1:B:124:PRO:HG3	1.95	0.49
1:C:507:LYS:HE3	1:C:559:MET:HE2	0.54	0.49
1:D:520:SER:HA	1:D:521:PRO:C	2.34	0.49
1:D:72:THR:O	1:D:72:THR:CG2	2.61	0.49
1:A:755:GLU:HG2	1:A:756:LEU:N	2.27	0.48
1:D:201:ILE:O	1:D:249:ILE:HA	2.13	0.48
1:D:32:SER:HB3	5:D:2002:HOH:O	2.12	0.48
1:D:350:PHE:HA	1:D:402:ILE:CD1	2.42	0.48
1:B:330:PRO:HB3	1:B:388:PRO:HB2	1.95	0.48
1:B:408:MET:HE3	1:B:480:GLU:HG2	1.96	0.48
1:B:616:GLN:HG2	1:B:618:TRP:CH2	2.47	0.48
1:C:167:ASP:HA	1:C:229:ASP:O	2.14	0.48
1:D:129:VAL:HG22	1:D:130:TYR:N	2.28	0.48
1:D:609:TYR:CE1	1:D:624:LEU:HD21	2.49	0.48
1:B:63:MET:HE1	1:B:167:ASP:CG	2.33	0.48
1:B:385:TRP:CD1	1:B:393:CYS:HB3	2.49	0.48
1:C:730:LYS:HB3	5:C:2189:HOH:O	2.12	0.48
1:D:407:TYR:CD1	1:D:408:MET:CE	2.91	0.48
1:D:618:TRP:CE2	1:D:739:LEU:HD12	2.48	0.48
1:A:143:THR:HB	5:A:2054:HOH:O	2.14	0.48
1:C:588:GLU:O	1:C:592[B]:MET:HG3	2.14	0.48
1:D:570:VAL:O	1:D:595:GLY:HA2	2.14	0.48
1:B:547:PRO:HB2	1:B:613:TYR:CD2	2.49	0.48



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:168:LYS:HD3	5:D:2077:HOH:O	2.14	0.48
1:D:478:ALA:HA	1:D:483:ARG:HG2	1.96	0.48
1:A:342:THR:O	1:A:343:ASP:HB2	2.14	0.48
1:D:216:ASN:HD21	1:D:230:HIS:H	1.62	0.48
1:B:407:TYR:HD1	1:B:408:MET:HE1	1.78	0.47
1:B:702:TYR:CE2	1:B:737:PRO:HD3	2.49	0.47
1:D:564:MET:HE3	1:D:607:MET:CE	2.33	0.47
1:A:685:ASN:ND2	1:A:685:ASN:C	2.63	0.47
1:B:758:HIS:N	1:B:758:HIS:ND1	2.61	0.47
1:C:177:GLU:OE2	1:C:177:GLU:N	2.26	0.47
1:D:44:TYR:CD1	5:D:2009:HOH:O	2.65	0.47
1:D:496:MET:HE2	1:D:752:PHE:CD2	2.50	0.47
1:D:143:THR:HB	5:D:2044:HOH:O	2.14	0.47
1:D:219:LEU:HA	1:D:219:LEU:HD12	1.77	0.47
1:D:90:ASN:OD1	1:D:91:ASP:N	2.45	0.47
1:A:216:ASN:HD21	1:A:230:HIS:H	1.61	0.47
1:D:354:PHE:N	1:D:355:PRO:HD2	2.29	0.47
1:A:26:VAL:HG11	1:A:124:PRO:HG3	1.97	0.47
1:B:417:LYS:HE2	1:B:421:GLU:OE2	2.14	0.47
1:C:573:ILE:HG22	1:C:574:PHE:N	2.29	0.47
1:A:496:MET:HE2	1:A:499:LYS:CE	2.45	0.47
1:A:630:ARG:HD3	5:A:2200:HOH:O	2.15	0.47
1:A:755:GLU:CG	1:A:756:LEU:H	2.28	0.47
1:D:745:GLU:OE1	1:D:745:GLU:C	2.53	0.47
1:A:525:LEU:HD13	1:A:573:ILE:HG13	1.97	0.47
1:A:22[B]:TRP:H	1:A:283:ASN:ND2	2.13	0.47
1:A:22[A]:TRP:H	1:A:283:ASN:ND2	2.13	0.47
1:A:345:GLY:HA3	1:A:385:TRP:CE2	2.49	0.47
1:B:559[A]:MET:CE	1:B:563:MET:HG2	2.44	0.47
1:C:22:TRP:N	1:C:283:ASN:HD21	2.06	0.47
1:D:494:ARG:O	1:D:497:ASN:ND2	2.45	0.47
1:A:23:THR:HG23	1:A:283:ASN:ND2	2.30	0.46
1:B:136:ILE:HG12	5:B:2027:HOH:O	2.15	0.46
1:B:68:GLN:OE1	1:B:80:LYS:HE3	2.15	0.46
1:C:145:ARG:HD2	1:C:265:GLU:OE2	2.16	0.46
1:B:214:VAL:HG12	5:B:2042:HOH:O	2.16	0.46
1:D:533:GLU:OE2	3:D:801:KIF:O2	2.33	0.46
1:A:354:PHE:N	1:A:355:PRO:CD	2.79	0.46
1:B:721:GLU:HB3	5:B:2150:HOH:O	2.15	0.46
1:C:472:TRP:HB2	1:C:545:HIS:CD2	2.51	0.46
1:D:494:ARG:CA	1:D:497:ASN:HD22	2.29	0.46



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:D:630:ARG:HD3	5:D:2156:HOH:O	2.14	0.46
1:A:449:GLY:HA2	5:A:2159:HOH:O	2.14	0.46
1:B:700:ASN:ND2	1:B:735:ASN:HB3	2.30	0.46
1:D:383:PRO:HA	1:D:390:HIS:CE1	2.50	0.46
1:D:419:LEU:HD12	1:D:419:LEU:O	2.15	0.46
1:B:566:SER:O	1:B:570:VAL:HG22	2.16	0.46
1:D:84:GLN:HA	1:D:85:PRO:HD3	1.78	0.46
1:B:73:ALA:HB1	5:B:2013:HOH:O	2.16	0.46
1:C:602:GLN:N	1:C:603:PRO:CD	2.78	0.46
1:D:702:TYR:CE2	1:D:737:PRO:HD3	2.50	0.46
1:B:167:ASP:HA	1:B:229:ASP:O	2.15	0.46
1:B:22:TRP:H	1:B:283:ASN:ND2	2.13	0.46
1:B:588:GLU:O	1:B:592[B]:MET:HG3	2.15	0.46
1:D:188:ASN:ND2	1:D:190:GLY:H	2.03	0.46
1:A:731:VAL:HG12	1:A:733:MET:SD	2.56	0.46
1:B:99:PRO:HG3	1:B:151:PHE:CD2	2.51	0.46
1:C:395:VAL:HB	1:C:463:ARG:HG2	1.96	0.46
1:A:597:TYR:OH	1:A:599:HIS:HD2	1.98	0.45
1:C:172:ILE:HG12	1:C:233:ALA:HB2	1.98	0.45
1:C:219:LEU:HA	1:C:219:LEU:HD12	1.75	0.45
1:D:585:GLU:HG2	1:D:601:ASN:ND2	2.31	0.45
1:A:750:TYR:C	1:A:750:TYR:CD2	2.89	0.45
1:B:155:GLU:HA	1:B:239:THR:O	2.17	0.45
1:A:34:SER:HB3	1:A:42:ASN:OD1	2.17	0.45
1:C:99:PRO:HG3	1:C:151:PHE:CD2	2.51	0.45
1:D:540:THR:CG2	1:D:540:THR:O	2.64	0.45
1:B:184:TYR:HA	1:B:198:ASN:O	2.17	0.45
1:B:219:LEU:HD11	1:B:234:ILE:HD12	1.99	0.45
1:B:751:SER:HB2	5:B:2172:HOH:O	2.16	0.45
1:B:754:LYS:HD2	5:B:2171:HOH:O	2.16	0.45
1:C:528:GLY:HA3	1:C:578:TYR:CD2	2.51	0.45
1:D:470:ASP:O	1:D:473:CYS:HB2	2.17	0.45
1:A:496:MET:CE	1:A:499:LYS:NZ	2.79	0.45
1:A:527:TRP:HA	1:A:534:GLY:O	2.17	0.45
1:B:157:ASP:CB	1:B:158:HIS:CD2	3.00	0.45
1:B:523:SER:HA	1:B:524:PRO:HD2	1.46	0.45
1:B:709:ASN:ND2	1:B:728:THR:H	2.15	0.45
1:B:154:PRO:O	1:B:154:PRO:CD	2.65	0.45
1:D:459:GLU:HG2	1:D:532:THR:OG1	2.17	0.45
1:D:750:TYR:C	1:D:750:TYR:CD2	2.90	0.45
1:D:329:SER:HB2	1:D:378:GLU:OE1	2.17	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:D:622:TYR:HA	1:D:701:PHE:CE1	2.51	0.45
1:D:618:TRP:CZ3	1:D:739:LEU:HA	2.52	0.45
1:A:293:GLY:HA3	1:A:677:LYS:HB2	1.99	0.44
1:B:162:VAL:HG22	1:B:234:ILE:HG12	1.98	0.44
1:B:175:ILE:HA	1:B:176:PRO:HD2	1.60	0.44
1:B:25:TYR:HB3	1:B:300:ARG:HA	1.99	0.44
1:B:84:GLN:OE1	1:B:90:ASN:HA	2.16	0.44
1:C:685:ASN:ND2	1:C:685:ASN:C	2.70	0.44
1:A:349:THR:HG21	5:A:2100:HOH:O	2.17	0.44
1:A:408:MET:HE3	1:A:480:GLU:HG2	1.99	0.44
1:C:235:ILE:C	1:C:235:ILE:HD12	2.38	0.44
1:C:408:MET:HE3	1:C:480:GLU:HG2	1.99	0.44
1:C:548:GLN:HG2	1:C:754:LYS:HE3	1.98	0.44
1:D:529:ASP:HB3	1:D:530:ALA:H	1.55	0.44
1:D:56:TRP:CE2	1:D:147:VAL:HG11	2.53	0.44
1:A:575:ASP:OD1	1:A:577:SER:OG	2.29	0.44
1:C:592[A]:MET:HE2	5:C:2154:HOH:O	2.17	0.44
1:D:358:ASN:ND2	1:D:411:VAL:HG21	2.32	0.44
1:C:342:THR:OG1	1:C:343:ASP:N	2.50	0.44
1:C:628:MET:CE	1:C:655:SER:HB3	2.47	0.44
1:D:86:SER:CB	1:D:87:PRO:HD2	2.44	0.44
1:B:305:CYS:O	1:B:649:SER:HB3	2.18	0.44
1:B:599:HIS:HE1	1:B:632:TYR:OH	2.00	0.44
1:D:383:PRO:HA	1:D:390:HIS:HE1	1.82	0.44
1:D:538:HIS:O	1:D:541:TRP:HD1	2.00	0.44
1:A:609:TYR:CZ	1:A:660:TYR:HB2	2.53	0.44
1:B:208:PHE:HD1	1:B:208:PHE:N	2.16	0.44
1:C:305:CYS:O	1:C:649:SER:HB3	2.18	0.44
1:C:29:LEU:HD23	1:C:45:PRO:HG3	1.99	0.44
1:D:185:THR:CG2	1:D:198:ASN:HB3	2.48	0.44
1:D:72:THR:O	1:D:72:THR:HG22	2.17	0.44
1:C:520:SER:HA	1:C:521:PRO:C	2.38	0.44
1:C:709:ASN:ND2	1:C:728:THR:H	2.15	0.44
1:D:506:SER:O	1:D:507:LYS:HB2	2.17	0.44
1:C:312:PHE:HA	1:C:313:PRO:C	2.38	0.44
1:C:416:ILE:HD12	5:C:2085:HOH:O	2.18	0.44
1:D:451:VAL:HA	1:D:452:PRO:HD2	1.77	0.44
1:B:408:MET:CE	1:B:480:GLU:HG2	2.48	0.44
1:D:216:ASN:ND2	1:D:230:HIS:H	2.16	0.44
1:A:212:ALA:HB2	1:A:221:GLU:HA	2.00	0.43
1:A:503:ASP:OD1	1:A:503:ASP:C	2.56	0.43



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:168:LYS:HA	1:B:168:LYS:HD3	1.81	0.43
1:D:202:ILE:HG12	1:D:249:ILE:HG12	1.99	0.43
1:C:354:PHE:CD2	1:C:402:ILE:HD12	2.53	0.43
1:A:212:ALA:CB	1:A:221:GLU:HA	2.48	0.43
1:B:597:TYR:HD1	1:B:604:ILE:HD13	1.83	0.43
1:B:602:GLN:N	1:B:603:PRO:CD	2.81	0.43
1:C:99:PRO:HG3	1:C:151:PHE:CE2	2.54	0.43
1:D:588:GLU:HG2	1:D:640:CYS:O	2.19	0.43
1:D:496:MET:HE2	1:D:752:PHE:CE2	2.52	0.43
1:C:527:TRP:CZ2	1:C:538:HIS:HE1	2.37	0.43
1:A:483:ARG:HB3	1:A:484:PRO:HD2	2.01	0.43
1:A:755:GLU:O	1:A:756:LEU:HB2	2.16	0.43
1:B:283:ASN:HD22	1:B:283:ASN:HA	1.56	0.43
1:D:420:TYR:O	1:D:424:ILE:HG12	2.19	0.43
1:A:725:LYS:HE2	5:A:2234:HOH:O	2.18	0.43
1:C:353:LEU:HD13	1:C:353:LEU:C	2.38	0.43
1:C:477:LEU:HG	1:C:481:LEU:HD22	1.99	0.43
1:D:40:THR:HG21	1:D:637:ASP:HB2	2.00	0.43
1:A:459:GLU:O	1:A:463:ARG:HG3	2.19	0.43
1:D:153:PHE:CD1	1:D:159:SER:HB3	2.54	0.43
1:D:167:ASP:O	1:D:187:ARG:HB2	2.18	0.43
1:D:346:PHE:O	1:D:350:PHE:HD1	2.02	0.43
1:D:358:ASN:HD22	1:D:411:VAL:HG21	1.83	0.43
1:C:362:PRO:HD2	1:C:684:GLU:OE1	2.19	0.43
1:D:383:PRO:CA	1:D:390:HIS:HE1	2.32	0.43
1:C:576:ASP:O	1:C:579:TYR:N	2.45	0.43
1:A:329:SER:OG	1:A:378:GLU:OE1	2.31	0.42
1:B:331:TYR:CZ	1:B:375:THR:HG23	2.54	0.42
1:C:21:ASP:OD1	1:C:279:LYS:HE3	2.19	0.42
1:C:503:ASP:OD1	1:C:503:ASP:C	2.58	0.42
1:D:431:HIS:HD2	1:D:433:GLU:N	2.04	0.42
1:A:335:VAL:HG12	1:D:334:GLN:HG2	2.00	0.42
1:A:50:PRO:HD3	1:A:282:TRP:CE2	2.55	0.42
1:C:248:ARG:NH2	1:C:267:GLY:O	2.50	0.42
1:D:405:ASP:OD1	1:D:409:LYS:HD2	2.19	0.42
1:D:586:ILE:HD12	5:D:2150:HOH:O	2.18	0.42
1:D:685:ASN:ND2	1:D:687:ASN:N	2.52	0.42
1:A:219:LEU:HA	1:A:219:LEU:HD12	1.73	0.42
1:B:79:PHE:N	1:B:79:PHE:CD1	2.87	0.42
1:C:756:LEU:HA	5:C:2202:HOH:O	2.19	0.42
1:D:329:SER:CB	1:D:378:GLU:OE1	2.67	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:206:LYS:HA	1:B:207:PRO:HD3	1.71	0.42
1:B:212:ALA:CB	1:B:221:GLU:HA	2.49	0.42
1:B:361:TYR:N	1:B:362:PRO:HD3	2.35	0.42
1:D:512:ARG:NE	1:D:516:GLY:O	2.52	0.42
1:B:387:SER:HA	1:B:388:PRO:HA	1.91	0.42
1:B:84:GLN:HA	1:B:85:PRO:HD3	1.83	0.42
1:C:201:ILE:O	1:C:249:ILE:HA	2.20	0.42
1:D:609:TYR:CZ	1:D:660:TYR:HB2	2.54	0.42
1:A:27:ASN:HB2	5:A:2001:HOH:O	2.18	0.42
1:B:56:TRP:CE2	1:B:147:VAL:HG11	2.55	0.42
1:C:553:LEU:HD23	1:C:553:LEU:HA	1.73	0.42
1:C:86:SER:HB2	1:C:87:PRO:HD2	2.01	0.42
1:B:179:ASN:OD1	1:B:207:PRO:HA	2.19	0.42
1:B:342:THR:OG1	1:B:343:ASP:N	2.50	0.42
1:B:40:THR:HG21	1:B:637:ASP:HB2	2.00	0.42
1:B:575:ASP:OD1	1:B:577:SER:OG	2.35	0.42
1:C:592[A]:MET:CE	5:C:2154:HOH:O	2.68	0.42
1:D:477:LEU:HG	1:D:481:LEU:HD22	2.01	0.42
1:C:274:LEU:HA	1:C:274:LEU:HD23	1.90	0.42
1:C:407:TYR:CD1	1:C:408:MET:HE2	2.31	0.42
1:A:155:GLU:O	1:A:156:ASN:HB2	2.19	0.42
1:B:178:GLU:O	1:B:179:ASN:HB2	2.20	0.42
1:C:42:ASN:ND2	1:C:642:ASP:OD1	2.47	0.42
1:C:101:VAL:HG13	1:C:136:ILE:HD11	2.01	0.42
1:C:345:GLY:HA3	1:C:385:TRP:CE2	2.55	0.42
1:D:23:THR:HG23	1:D:283:ASN:ND2	2.34	0.42
1:B:203:GLU:OE1	1:B:248:ARG:NH1	2.52	0.41
1:C:546:ASP:N	1:C:547:PRO:HD3	2.35	0.41
1:A:558:GLU:H	1:A:558:GLU:CD	2.22	0.41
1:A:570:VAL:O	1:A:595:GLY:HA2	2.19	0.41
1:A:86:SER:HB2	1:A:87:PRO:HD2	2.01	0.41
1:B:173:LYS:HE3	1:B:175:ILE:HD11	2.01	0.41
1:C:597:TYR:HE2	1:C:599:HIS:HB2	1.76	0.41
1:D:391:ARG:HA	1:D:391:ARG:HD2	1.82	0.41
1:B:159:SER:OG	1:B:239:THR:OG1	2.28	0.41
1:B:155:GLU:N	1:B:241:LYS:HA	2.35	0.41
1:B:239:THR:HA	1:B:243:GLU:OE1	2.21	0.41
1:C:419:LEU:C	1:C:419:LEU:HD12	2.40	0.41
1:C:592[B]:MET:HE3	1:C:631:MET:CG	2.49	0.41
1:D:107:ASP:HB3	1:D:110:LYS:HB2	2.02	0.41
1:D:22:TRP:H	1:D:283:ASN:HD21	1.66	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:527:TRP:CZ2	1:D:538:HIS:CE1	3.08	0.41
1:C:388:PRO:HD2	1:C:389:GLY:H	1.85	0.41
1:D:462:ALA:O	1:D:466:GLU:HG3	2.20	0.41
1:B:219:LEU:CD1	1:B:234:ILE:HD12	2.50	0.41
1:C:58:PRO:HG3	1:C:127:TYR:CE1	2.54	0.41
1:D:618:TRP:CZ2	1:D:739:LEU:HD12	2.56	0.41
1:D:90:ASN:HB3	1:D:189:SER:OG	2.20	0.41
1:B:77:ARG:CZ	1:B:77:ARG:HB3	2.50	0.41
1:C:361:TYR:N	1:C:362:PRO:HD3	2.35	0.41
1:D:138:THR:HG23	1:D:151:PHE:CE2	2.56	0.41
1:D:419:LEU:C	1:D:419:LEU:HD12	2.40	0.41
1:A:452:PRO:HB2	1:A:455:VAL:HG22	2.01	0.41
1:A:554:MET:O	1:A:559[B]:MET:CE	2.55	0.41
1:C:523:SER:HA	1:C:524:PRO:HD2	1.69	0.41
1:B:171:TYR:HD1	1:B:227:THR:OG1	2.03	0.41
1:B:312:PHE:HA	1:B:313:PRO:C	2.40	0.41
1:B:571:PRO:HB2	1:B:573:ILE:HD13	2.02	0.41
1:C:206:LYS:HA	1:C:207:PRO:HD3	1.95	0.41
1:C:657:LEU:HA	1:C:657:LEU:HD23	1.95	0.41
1:D:465:LEU:HA	1:D:465:LEU:HD23	1.87	0.41
1:B:188:ASN:HD22	1:B:190:GLY:N	2.12	0.41
1:B:451:VAL:HA	1:B:452:PRO:HD3	1.83	0.41
1:C:193:PRO:HD3	1:C:330:PRO:O	2.21	0.41
1:C:415:ASP:OD2	1:C:418:THR:OG1	2.31	0.41
1:C:748:MET:HA	1:C:749:PRO:HD3	1.86	0.41
1:A:80:LYS:HD2	1:A:82:THR:HB	2.03	0.41
1:C:107:ASP:O	1:C:111:ARG:HG2	2.20	0.41
1:D:533:GLU:HB3	1:D:601:ASN:ND2	2.35	0.41
1:D:610:LEU:HA	1:D:613:TYR:CD1	2.56	0.41
1:B:153:PHE:HB3	1:B:154:PRO:CD	2.50	0.41
1:C:483:ARG:HB3	1:C:484:PRO:HD2	2.03	0.41
1:C:615:GLY:O	1:C:743:THR:HG22	2.20	0.41
1:D:346:PHE:CD1	1:D:402:ILE:HG13	2.56	0.41
1:A:449:GLY:O	1:A:450:TYR:HB3	2.21	0.40
1:B:609:TYR:CZ	1:B:660:TYR:HB2	2.54	0.40
1:C:134:HIS:HB3	1:C:136:ILE:CD1	2.51	0.40
1:D:216:ASN:ND2	1:D:216:ASN:N	2.65	0.40
1:D:160:TYR:CD2	1:D:236:GLY:HA3	2.56	0.40
1:D:350:PHE:CA	1:D:402:ILE:HD11	2.49	0.40
1:D:494:ARG:C	1:D:497:ASN:HD22	2.24	0.40
1:B:209:THR:HG23	1:B:209:THR:O	2.22	0.40



Atom 1	Atom 2	Interatomic	$\mathbf{Clash}$
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:158:HIS:HB3	1:C:160:TYR:CE1	2.57	0.40
1:C:39:SER:HB2	1:C:42:ASN:ND2	2.35	0.40
1:D:186:THR:O	1:D:187:ARG:C	2.59	0.40
1:D:504:LYS:HE3	1:D:504:LYS:HB2	1.67	0.40
1:A:216:ASN:N	1:A:216:ASN:HD22	2.20	0.40
1:C:331:TYR:CZ	1:C:375:THR:HG23	2.56	0.40
1:C:431:HIS:CD2	1:C:433:GLU:H	2.35	0.40
1:D:498:TYR:OH	1:D:546:ASP:OD2	2.40	0.40
1:B:459:GLU:HG2	1:B:532:THR:OG1	2.22	0.40
1:B:483:ARG:HB3	1:B:484:PRO:HD2	2.03	0.40
1:B:613:TYR:CZ	1:B:749:PRO:HG2	2.56	0.40
1:C:209:THR:HB	1:C:237:PHE:HA	2.04	0.40
1:A:506:SER:O	1:A:507:LYS:HB2	2.22	0.40
1:B:343:ASP:HA	1:B:386:ALA:O	2.20	0.40
1:D:546:ASP:N	1:D:547:PRO:CD	2.85	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	738/744~(99%)	707~(96%)	30~(4%)	1 (0%)	51	68
1	В	743/744~(100%)	700~(94%)	39~(5%)	4 (0%)	29	41
1	С	738/744~(99%)	695~(94%)	43~(6%)	0	100	100
1	D	735/744~(99%)	692~(94%)	42~(6%)	1 (0%)	51	68
All	All	2954/2976~(99%)	2794 (95%)	154~(5%)	6 (0%)	47	62

All (6) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	757	GLU
1	А	755	GLU
1	В	755	GLU
1	В	758	HIS
1	В	529	ASP
1	D	572	PRO

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	637/643~(99%)	616~(97%)	21 (3%)	38 57
1	В	643/643~(100%)	610~(95%)	33~(5%)	24 39
1	С	637/643~(99%)	609~(96%)	28 (4%)	28 45
1	D	635/643~(99%)	597 (94%)	38~(6%)	19 31
All	All	2552/2572~(99%)	2432 (95%)	120 (5%)	26 42

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	72	THR
1	А	77	ARG
1	А	80	LYS
1	А	209	THR
1	А	215	GLU
1	А	237	PHE
1	А	319	LEU
1	А	385	TRP
1	А	416	ILE
1	А	433	GLU
1	А	460	ASN
1	А	481	LEU
1	А	539	TYR
1	А	573	ILE
1	A	577	SER
1	A	596	ASN



Mol	Chain	Res	Type
1	А	685	ASN
1	А	708	PHE
1	А	721	GLU
1	А	734	SER
1	А	756	LEU
1	В	72	THR
1	В	77	ARG
1	В	105	VAL
1	В	160	TYR
1	В	170	SER
1	В	174	ILE
1	В	185	THR
1	В	189	SER
1	В	208	PHE
1	В	209	THR
1	В	237	PHE
1	В	307	TYR
1	В	385	TRP
1	В	419	LEU
1	В	433	GLU
1	В	460	ASN
1	В	475	TYR
1	В	481	LEU
1	В	482	LYS
1	В	539	TYR
1	В	566	SER
1	В	573	ILE
1	В	577	SER
1	В	593	ASN
1	В	685	ASN
1	В	698	THR
1	В	708	PHE
1	В	721	GLU
1	В	734	SER
1	В	736	ARG
1	В	739	LEU
1	В	751	SER
1	В	758	HIS
1	С	72	THR
1	С	77	ARG
1	С	105	VAL
1	С	172	ILE



Mol	Chain	Res	Type
1	С	185	THR
1	С	219	LEU
1	С	237	PHE
1	С	257[A]	GLU
1	С	257[B]	GLU
1	С	292	GLU
1	С	307	TYR
1	С	385	TRP
1	С	416	ILE
1	С	419	LEU
1	С	460	ASN
1	С	481	LEU
1	С	482	LYS
1	С	504	LYS
1	С	520	SER
1	С	539	TYR
1	С	681	LEU
1	С	685	ASN
1	С	708	PHE
1	С	721	GLU
1	С	734	SER
1	С	736	ARG
1	С	746	GLU
1	С	753	SER
1	D	77	ARG
1	D	80	LYS
1	D	209	THR
1	D	216	ASN
1	D	237	PHE
1	D	268	LYS
1	D	319	LEU
1	D	385	TRP
1	D	408	MET
1	D	416	ILE
1	D	433	GLU
1	D	460	ASN
1	D	475	TYR
1	D	481	LEU
1	D	482	LYS
1	D	485	LYS
1	D	529	ASP
1	D	532	THR



Mol	Chain	Res	Type
1	D	539	TYR
1	D	559	MET
1	D	570	VAL
1	D	573	ILE
1	D	577	SER
1	D	593	ASN
1	D	596	ASN
1	D	612	ASP
1	D	654	PHE
1	D	685	ASN
1	D	692	ASP
1	D	708	PHE
1	D	709	ASN
1	D	721	GLU
1	D	734	SER
1	D	736	ARG
1	D	739	LEU
1	D	743	THR
1	D	746	GLU
1	D	750	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	188	ASN
1	А	216	ASN
1	А	226	GLN
1	А	264	ASN
1	А	283	ASN
1	А	358	ASN
1	А	374	ASN
1	А	431	HIS
1	А	446	ASN
1	А	593	ASN
1	А	599	HIS
1	А	685	ASN
1	А	700	ASN
1	А	709	ASN
1	А	716	ASN
1	В	188	ASN
1	В	216	ASN
1	В	226	GLN



Mol	Chain	Res	Type
1	В	283	ASN
1	В	358	ASN
1	В	374	ASN
1	В	425	HIS
1	В	431	HIS
1	В	446	ASN
1	В	460	ASN
1	В	593	ASN
1	В	599	HIS
1	В	685	ASN
1	В	700	ASN
1	В	709	ASN
1	В	713	HIS
1	В	716	ASN
1	В	761	HIS
1	С	188	ASN
1	С	216	ASN
1	С	226	GLN
1	С	264	ASN
1	С	283	ASN
1	С	358	ASN
1	С	374	ASN
1	С	398	ASN
1	С	431	HIS
1	С	446	ASN
1	С	460	ASN
1	С	593	ASN
1	С	599	HIS
1	С	685	ASN
1	С	700	ASN
1	С	709	ASN
1	С	716	ASN
1	D	188	ASN
1	D	216	ASN
1	D	226	GLN
1	D	264	ASN
_1	D	283	ASN
1	D	358	ASN
1	D	374	ASN
1	D	431	HIS
1			
T	D	446	ASN



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Mol	Chain	Res	Type
1	D	538	HIS
1	D	593	ASN
1	D	599	HIS
1	D	685	ASN
1	D	700	ASN
1	D	709	ASN
1	D	716	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

#### 5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tune	Chain	nin Ros I		Dog	Tink	Bond lengths			Bond angles		
MOI	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
3	KIF	А	801	2	$16,\!17,\!17$	2.11	2 (12%)	$15,\!26,\!26$	2.05	3 (20%)		
3	KIF	В	801	2	$16,\!17,\!17$	2.02	2 (12%)	$15,\!26,\!26$	2.04	4 (26%)		
4	GOL	D	802	-	$5,\!5,\!5$	0.39	0	5, 5, 5	0.46	0		
4	GOL	В	802	-	$5,\!5,\!5$	0.28	0	5, 5, 5	0.52	0		
4	GOL	A	802	-	$5,\!5,\!5$	0.31	0	5, 5, 5	0.27	0		
4	GOL	С	802	-	$5,\!5,\!5$	0.35	0	5, 5, 5	0.66	0		



Mol Turne	Chain	Dog	Tink	Link Bond lengths			Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	GOL	В	803	-	$5,\!5,\!5$	0.38	0	5, 5, 5	0.23	0
3	KIF	С	801	2	$16,\!17,\!17$	1.74	2 (12%)	15,26,26	1.91	3 (20%)
3	KIF	D	801	2	$16,\!17,\!17$	1.86	2 (12%)	15,26,26	2.00	3 (20%)

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	KIF	А	801	2	-	0/2/38/38	0/2/2/2
3	KIF	В	801	2	-	2/2/38/38	0/2/2/2
4	GOL	D	802	-	-	0/4/4/4	-
4	GOL	В	802	-	-	2/4/4/4	-
4	GOL	А	802	-	-	2/4/4/4	-
4	GOL	С	802	-	-	2/4/4/4	-
4	GOL	В	803	-	-	4/4/4/4	-
3	KIF	С	801	2	-	1/2/38/38	0/2/2/2
3	KIF	D	801	2	-	2/2/38/38	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	В	801	KIF	C7-C8	-6.79	1.38	1.53
3	D	801	KIF	C7-C8	-6.23	1.39	1.53
3	А	801	KIF	C7-C8	-5.85	1.40	1.53
3	С	801	KIF	C7-C8	-5.82	1.40	1.53
3	А	801	KIF	C1-N9	5.28	1.50	1.44
3	В	801	KIF	C1-N9	3.12	1.48	1.44
3	С	801	KIF	C1-N9	2.89	1.48	1.44
3	D	801	KIF	C1-N9	2.73	1.47	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	801	KIF	C8-C7-N	5.35	110.50	106.20
3	С	801	KIF	C7-C8-N9	5.34	110.46	105.42
3	D	801	KIF	C7-C8-N9	4.98	110.12	105.42
3	В	801	KIF	C7-C8-N9	4.73	109.89	105.42
3	А	801	KIF	C7-C8-N9	4.66	109.82	105.42



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	801	KIF	C8-C7-N	4.10	109.49	106.20
3	В	801	KIF	C8-C7-N	4.04	109.45	106.20
3	С	801	KIF	C8-C7-N	3.01	108.61	106.20
3	В	801	KIF	C3-C4-C5	2.36	115.36	111.37
3	С	801	KIF	C3-C4-C5	2.28	115.22	111.37
3	D	801	KIF	C3-C2-C1	-2.23	108.03	111.47
3	А	801	KIF	O6-C6-C5	-2.21	106.69	111.42
3	В	801	KIF	O4-C4-C5	-2.04	106.13	109.77

There are no chirality outliers.

Mol	Chain	$\mathbf{Res}$	Type	Atoms
3	В	801	KIF	C4-C5-C6-O6
4	В	803	GOL	O1-C1-C2-C3
4	В	803	GOL	C1-C2-C3-O3
4	В	803	GOL	O2-C2-C3-O3
4	В	802	GOL	C1-C2-C3-O3
4	А	802	GOL	O1-C1-C2-C3
4	С	802	GOL	C1-C2-C3-O3
3	D	801	KIF	C4-C5-C6-O6
3	С	801	KIF	C4-C5-C6-O6
4	В	803	GOL	O1-C1-C2-O2
4	В	802	GOL	O2-C2-C3-O3
4	А	802	GOL	O1-C1-C2-O2
3	В	801	KIF	N-C5-C6-O6
3	D	801	KIF	N-C5-C6-O6
4	С	802	GOL	O2-C2-C3-O3

All (15) torsion outliers are listed below:

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	801	KIF	1	0
3	С	801	KIF	1	0
3	D	801	KIF	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	$<$ RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	738/744~(99%)	-0.56	1 (0%) 95 95	15, 26, 40, 62	0
1	В	742/744~(99%)	-0.43	1 (0%) 95 95	20,  33,  51,  60	0
1	С	737/744~(99%)	-0.57	0 100 100	17, 30, 43, 50	0
1	D	736/744~(98%)	-0.37	5 (0%) 87 86	17, 35, 63, 76	0
All	All	2953/2976~(99%)	-0.48	7 (0%) 95 94	15, 31, 54, 76	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	745	GLU	2.8
1	D	755	GLU	2.8
1	А	756	LEU	2.6
1	D	613	TYR	2.5
1	D	743	THR	2.3
1	В	268	LYS	2.3
1	D	740	ASN	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)

There are no carbohydrates in this entry.



#### 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	${f B}$ -factors(Å <sup>2</sup> )	Q<0.9
4	GOL	В	802	6/6	0.77	0.16	$55,\!55,\!56,\!56$	0
4	GOL	В	803	6/6	0.84	0.22	$59,\!60,\!61,\!61$	0
4	GOL	А	802	6/6	0.88	0.20	$54,\!57,\!57,\!57$	0
4	GOL	D	802	6/6	0.91	0.15	44,45,45,45	0
4	GOL	С	802	6/6	0.91	0.16	$44,\!46,\!46,\!48$	0
3	KIF	В	801	16/16	0.94	0.14	$31,\!36,\!37,\!38$	0
3	KIF	А	801	16/16	0.94	0.12	$21,\!26,\!30,\!30$	0
3	KIF	D	801	16/16	0.94	0.13	$33,\!38,\!40,\!40$	0
3	KIF	С	801	16/16	0.94	0.11	$32,\!35,\!37,\!38$	0
2	CA	В	800	1/1	0.98	0.08	$30,\!30,\!30,\!30$	0
2	CA	А	800	1/1	0.98	0.11	32,32,32,32	0
2	CA	D	800	1/1	0.98	0.11	45,45,45,45	0
2	CA	С	800	1/1	0.99	0.08	26, 26, 26, 26	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

