



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 PM GMT

PDB ID : 4LNV  
Title : Crystal Structure of TEP1s  
Authors : Le, B.V.; Williams, M.; Logarajah, S.; Baxter, R.H.G.  
Deposited on : 2013-07-12  
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



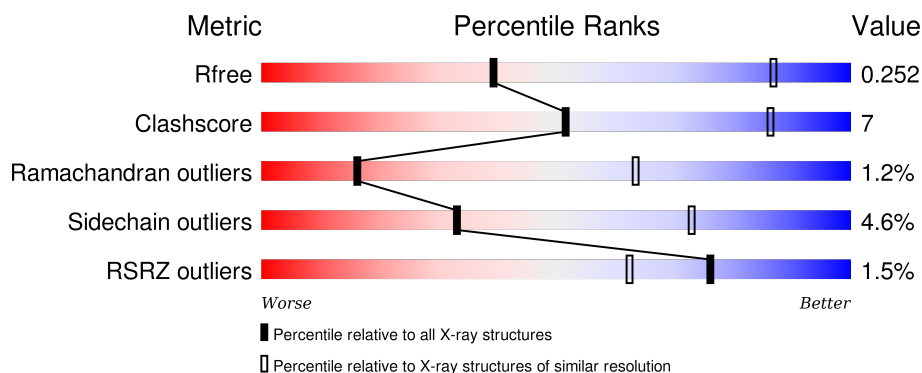
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	A	1323	 2% 79% 16% . .
1	B	1323	 % 64% 15% . 20%
1	C	1323	 % 79% 16% . .



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27034 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 Thioester-containing protein I.

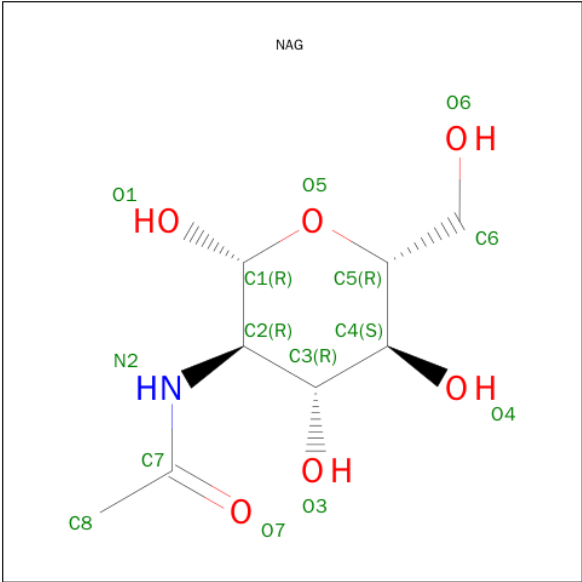
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1276	Total	C	N	O	S	0	0	0
			9704	6210	1583	1866	45			
1	B	1063	Total	C	N	O	S	0	0	0
			7461	4750	1225	1454	32			
1	C	1276	Total	C	N	O	S	0	0	0
			9631	6163	1573	1850	45			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1339	HIS	-	EXPRESSION TAG	UNP Q9GYW4
A	1340	HIS	-	EXPRESSION TAG	UNP Q9GYW4
A	1341	HIS	-	EXPRESSION TAG	UNP Q9GYW4
A	1342	HIS	-	EXPRESSION TAG	UNP Q9GYW4
A	1343	HIS	-	EXPRESSION TAG	UNP Q9GYW4
A	1344	HIS	-	EXPRESSION TAG	UNP Q9GYW4
B	1339	HIS	-	EXPRESSION TAG	UNP Q9GYW4
B	1340	HIS	-	EXPRESSION TAG	UNP Q9GYW4
B	1341	HIS	-	EXPRESSION TAG	UNP Q9GYW4
B	1342	HIS	-	EXPRESSION TAG	UNP Q9GYW4
B	1343	HIS	-	EXPRESSION TAG	UNP Q9GYW4
B	1344	HIS	-	EXPRESSION TAG	UNP Q9GYW4
C	1339	HIS	-	EXPRESSION TAG	UNP Q9GYW4
C	1340	HIS	-	EXPRESSION TAG	UNP Q9GYW4
C	1341	HIS	-	EXPRESSION TAG	UNP Q9GYW4
C	1342	HIS	-	EXPRESSION TAG	UNP Q9GYW4
C	1343	HIS	-	EXPRESSION TAG	UNP Q9GYW4
C	1344	HIS	-	EXPRESSION TAG	UNP Q9GYW4

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
			Total	C	N	O		
			14	8	1	5		
			Total	C	N	O		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

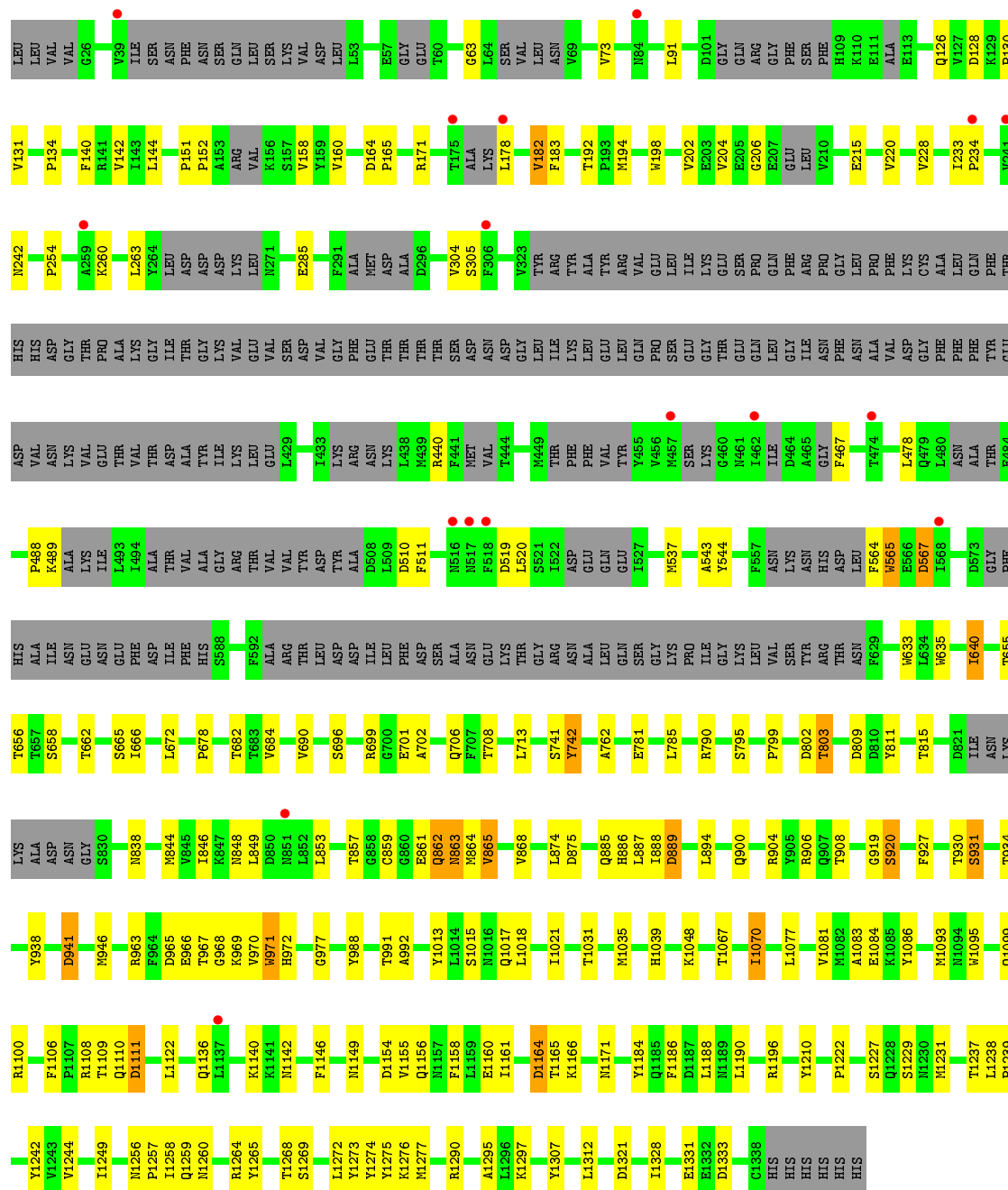
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

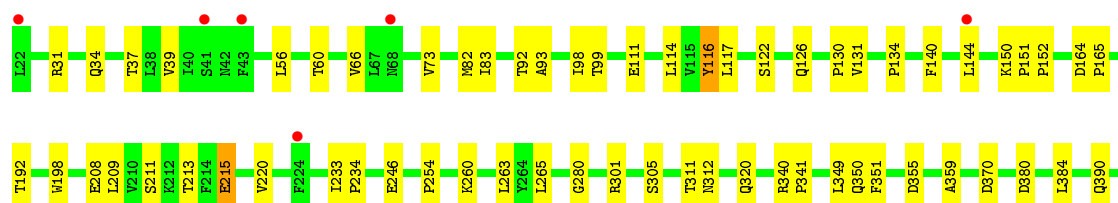
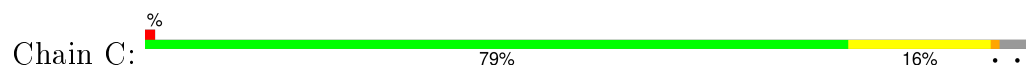




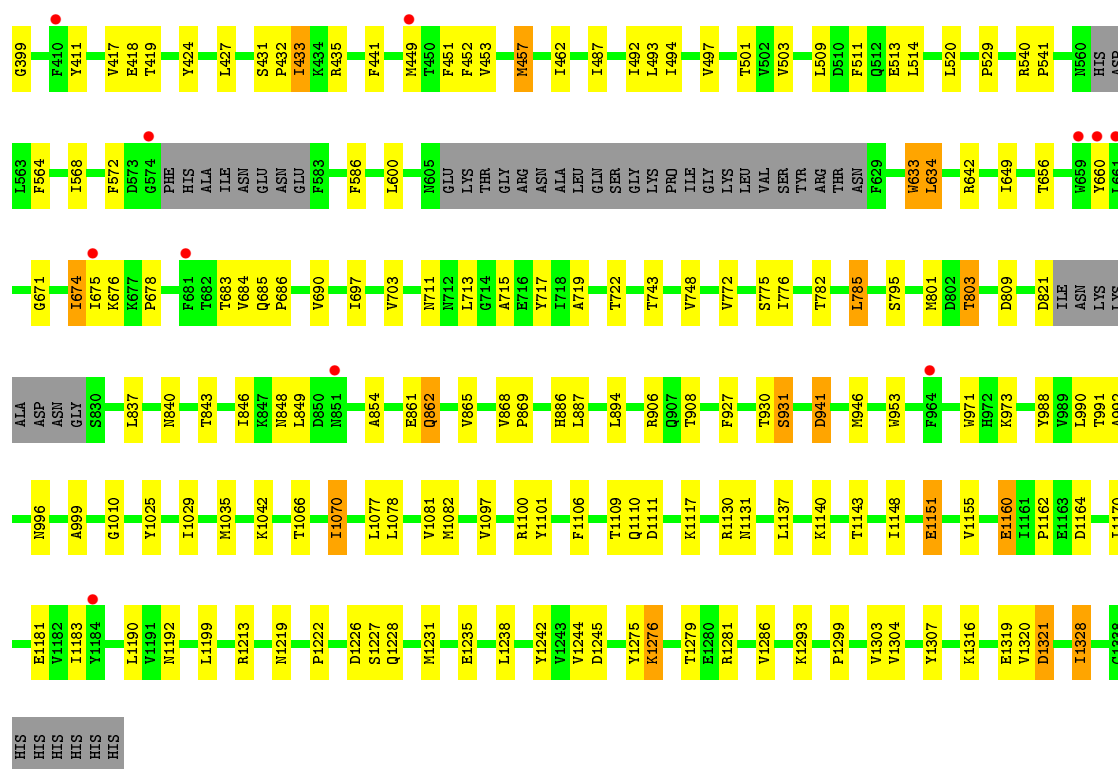




### • Molecule 1: Thioester-containing protein I









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.47Å 196.47Å 225.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 3.70 49.12 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.12-3.70) 99.7 (49.12-3.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.89	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, $R_{free}$	0.237 , 0.276 0.215 , 0.252	Depositor DCC
$R_{free}$ test set	4582 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	147.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 111.5	EDS
Estimated twinning fraction	0.504 for H, K, L 0.496 for K, H, -L 0.196 for h,-k,-l	Xtriage
Reported twinning fraction	0.504 for H, K, L 0.496 for K, H, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 90746 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.1834e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	6/9902 (0.1%)	0.53	0/13515
1	B	0.42	3/7592 (0.0%)	0.52	0/10410
1	C	0.40	2/9825 (0.0%)	0.52	0/13417
All	All	0.41	11/27319 (0.0%)	0.53	0/37342

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	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	TRP	CD2-CE2	5.30	1.47	1.41
1	A	198	TRP	CD2-CE2	5.27	1.47	1.41
1	A	971	TRP	CD2-CE2	5.24	1.47	1.41
1	B	971	TRP	CD2-CE2	5.24	1.47	1.41
1	C	953	TRP	CD2-CE2	5.08	1.47	1.41
1	A	953	TRP	CD2-CE2	5.07	1.47	1.41
1	A	635	TRP	CD2-CE2	5.06	1.47	1.41
1	A	565	TRP	CD2-CE2	5.04	1.47	1.41
1	A	633	TRP	CD2-CE2	5.03	1.47	1.41
1	B	565	TRP	CD2-CE2	5.03	1.47	1.41
1	C	198	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1064	TRP	Peptide

## 5.2 Too-close contacts

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	A	9704	0	9100	130	0
1	B	7461	0	6369	101	0
1	C	9631	0	8983	126	0
2	A	98	0	91	0	0
2	B	14	0	13	0	0
2	C	98	0	91	3	0
3	A	28	0	25	0	0
All	All	27034	0	24672	352	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1402:NAG:H4	2:C:1403:NAG:H5	1.59	0.84
1:A:62:ASN:HB3	1:B:970:VAL:HG23	1.63	0.79
1:C:862:GLN:HA	1:C:1109:THR:HG21	1.64	0.79
1:A:1100:ARG:HG2	1:A:1106:PHE:HE1	1.48	0.77
1:A:1100:ARG:HG2	1:A:1106:PHE:CE1	2.20	0.77
1:A:862:GLN:HA	1:A:1109:THR:HG21	1.66	0.76
1:C:1100:ARG:HG2	1:C:1106:PHE:CE1	2.23	0.74
1:C:1293:LYS:HB3	1:C:1328:ILE:HG12	1.69	0.74
1:A:568:ILE:HG12	1:A:674:ILE:HD11	1.69	0.74
1:C:1131:ASN:H	1:C:1151:GLU:HB3	1.52	0.74
1:A:1131:ASN:H	1:A:1151:GLU:HB3	1.53	0.73
1:A:1238:LEU:HD11	1:A:1244:VAL:HG13	1.68	0.73
1:A:971:TRP:HB2	1:A:1231:MET:HB2	1.71	0.73
1:A:1293:LYS:HB3	1:A:1328:ILE:HG12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:HE2	1:A:462:ILE:HG12	1.71	0.73
1:C:971:TRP:HB2	1:C:1231:MET:HB2	1.71	0.72
1:C:1238:LEU:HD11	1:C:1244:VAL:HG13	1.71	0.72
1:A:1070:ILE:H	1:A:1070:ILE:HD12	1.54	0.72
1:C:568:ILE:HG12	1:C:674:ILE:HD11	1.72	0.72
1:C:424:TYR:HA	1:C:503:VAL:HG11	1.72	0.72
1:C:1100:ARG:HG2	1:C:1106:PHE:HE1	1.53	0.71
1:C:131:VAL:HG12	1:C:215:GLU:HB3	1.72	0.71
1:C:457:MET:HE2	1:C:462:ILE:HG12	1.72	0.71
1:A:424:TYR:HA	1:A:503:VAL:HG11	1.72	0.70
1:B:1260:ASN:HB3	1:B:1273:TYR:HB2	1.71	0.70
1:A:131:VAL:HG12	1:A:215:GLU:HB3	1.75	0.69
1:A:927:PHE:O	1:A:931:SER:HB2	1.92	0.69
1:B:158:VAL:HG12	1:B:204:VAL:HG22	1.76	0.68
1:B:803:THR:HG21	1:B:1100:ARG:HH21	1.59	0.68
1:C:927:PHE:O	1:C:931:SER:HB2	1.93	0.67
1:B:853:LEU:HD11	1:B:865:VAL:HG11	1.75	0.67
1:C:1070:ILE:HD12	1:C:1070:ILE:H	1.61	0.66
1:A:435:ARG:HH11	1:A:514:LEU:HD11	1.61	0.66
1:C:435:ARG:HH11	1:C:514:LEU:HD11	1.61	0.66
1:A:351:PHE:HB3	1:A:359:ALA:HB3	1.76	0.65
1:A:795:SER:HA	1:A:1190:LEU:HD13	1.79	0.65
1:B:1210:TYR:HD1	1:B:1290:ARG:HD2	1.61	0.65
1:A:62:ASN:O	1:B:969:LYS:HA	1.96	0.65
1:A:930:THR:HG21	1:A:992:ALA:HB1	1.78	0.65
1:B:713:LEU:HD11	1:B:781:GLU:HG3	1.78	0.64
1:C:930:THR:HG21	1:C:992:ALA:HB1	1.78	0.64
1:B:171:ARG:HA	1:B:941:ASP:HB3	1.80	0.64
1:C:351:PHE:HB3	1:C:359:ALA:HB3	1.79	0.64
1:A:31:ARG:HB3	1:A:34:GLN:HB2	1.80	0.62
1:A:64:LEU:HD11	1:B:977:GLY:HA2	1.81	0.62
1:A:840:ASN:HB3	1:A:843:THR:HG23	1.80	0.62
1:A:553:ALA:O	1:A:556:LEU:HB2	2.00	0.62
1:B:857:THR:HG21	1:B:865:VAL:HG21	1.81	0.62
1:C:116:TYR:HD1	1:C:117:LEU:N	1.98	0.62
1:A:1035:MET:HB3	1:A:1082:MET:HG2	1.82	0.62
1:C:990:LEU:HD21	1:C:1010:GLY:HA3	1.82	0.62
1:B:128:ASP:HB3	1:B:635:TRP:CZ3	2.34	0.61
1:C:840:ASN:HB3	1:C:843:THR:HG23	1.81	0.61
1:C:31:ARG:HB3	1:C:34:GLN:HB2	1.81	0.60
1:B:838:ASN:ND2	1:B:844:MET:HG2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LEU:HD21	1:C:586:PHE:CE1	2.37	0.60
1:A:116:TYR:HD1	1:A:117:LEU:N	1.99	0.60
1:C:887:LEU:HD21	1:C:1155:VAL:HG23	1.84	0.60
1:A:990:LEU:HD21	1:A:1010:GLY:HA3	1.83	0.59
1:A:887:LEU:HD21	1:A:1155:VAL:HG23	1.84	0.59
1:B:861:GLU:OE2	1:B:1110:GLN:HG2	2.01	0.59
1:B:658:SER:HA	1:B:682:THR:HA	1.84	0.59
1:C:795:SER:HA	1:C:1190:LEU:HD13	1.83	0.59
1:A:862:GLN:HG2	1:A:1307:TYR:CZ	2.38	0.59
1:C:719:ALA:HB2	1:C:776:ILE:HG22	1.83	0.59
1:A:493:LEU:HD21	1:A:586:PHE:CE1	2.38	0.59
1:B:1070:ILE:HD12	1:B:1070:ILE:H	1.68	0.59
1:C:862:GLN:HG2	1:C:1307:TYR:CZ	2.37	0.59
1:C:837:LEU:HD21	1:C:1148:ILE:CD1	2.33	0.59
1:C:427:LEU:HD13	1:C:494:ILE:HD12	1.85	0.58
1:B:164:ASP:HB2	1:B:165:PRO:CD	2.32	0.58
1:C:1078:LEU:HD21	1:C:1117:LYS:HG2	1.86	0.57
1:C:1035:MET:HB3	1:C:1082:MET:HG2	1.86	0.57
1:B:1108:ARG:O	1:B:1111:ASP:HB2	2.04	0.57
1:B:846:ILE:HG21	1:B:887:LEU:HD22	1.85	0.57
1:C:399:GLY:HA2	1:C:411:TYR:HE1	1.69	0.57
1:B:142:VAL:HB	1:B:183:PHE:HB3	1.87	0.57
1:B:565:TRP:CD1	1:B:678:PRO:HG3	2.39	0.57
1:A:427:LEU:HD13	1:A:494:ILE:HD12	1.87	0.57
1:A:390:GLN:HE22	1:C:380:ASP:HA	1.69	0.57
1:B:164:ASP:HB2	1:B:165:PRO:HD2	1.87	0.57
1:A:837:LEU:HD21	1:A:1148:ILE:CD1	2.34	0.56
1:A:399:GLY:HA2	1:A:411:TYR:HE1	1.71	0.56
1:A:868:VAL:HG21	1:A:927:PHE:HZ	1.72	0.55
1:B:1238:LEU:HD11	1:B:1244:VAL:HG13	1.88	0.55
1:C:492:ILE:HB	1:C:509:LEU:HD11	1.87	0.55
1:A:1078:LEU:HD21	1:A:1117:LYS:HG2	1.88	0.55
1:A:868:VAL:HG21	1:A:927:PHE:CZ	2.42	0.55
1:B:666:ILE:HG12	1:B:672:LEU:HD12	1.89	0.54
1:A:1111:ASP:N	1:A:1111:ASP:OD1	2.40	0.54
1:C:868:VAL:HG21	1:C:927:PHE:HZ	1.72	0.54
1:A:719:ALA:HB2	1:A:776:ILE:HG22	1.89	0.54
1:B:254:PRO:HD2	1:B:690:VAL:HG11	1.89	0.54
1:B:795:SER:HA	1:B:1190:LEU:HD13	1.89	0.54
1:B:1239:PRO:HG2	1:B:1242:TYR:CD1	2.42	0.54
1:C:1242:TYR:OH	1:C:1320:VAL:HG11	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:SER:HB2	1:C:432:PRO:HD2	1.90	0.54
1:A:656:THR:OG1	1:A:685:GLN:HG2	2.08	0.53
1:A:1242:TYR:OH	1:A:1320:VAL:HG11	2.07	0.53
1:C:656:THR:OG1	1:C:685:GLN:HG2	2.09	0.53
1:A:39:VAL:HG22	1:A:82:MET:HG2	1.90	0.53
1:C:846:ILE:HA	1:C:849:LEU:HG	1.89	0.53
1:C:868:VAL:HG21	1:C:927:PHE:CZ	2.43	0.53
1:A:431:SER:HB2	1:A:432:PRO:HD2	1.90	0.53
1:A:492:ILE:HB	1:A:509:LEU:HD11	1.88	0.53
1:A:803:THR:HB	1:A:1097:VAL:HG12	1.90	0.53
1:B:941:ASP:N	1:B:941:ASP:OD1	2.42	0.53
1:C:39:VAL:HG22	1:C:82:MET:HG2	1.90	0.53
1:A:93:ALA:HA	1:A:116:TYR:HD2	1.74	0.53
1:C:1100:ARG:HA	1:C:1106:PHE:HD1	1.74	0.53
1:A:1160:GLU:O	1:A:1162:PRO:HD3	2.10	0.52
1:C:98:ILE:CG1	1:C:114:LEU:HD11	2.39	0.52
1:A:98:ILE:CG1	1:A:114:LEU:HD11	2.40	0.52
1:C:803:THR:HB	1:C:1097:VAL:HG12	1.92	0.52
1:B:864:MET:HB3	1:B:868:VAL:HG23	1.91	0.52
1:C:93:ALA:HA	1:C:116:TYR:HD2	1.75	0.52
1:A:349:LEU:O	1:A:384:LEU:HA	2.10	0.52
1:B:1222:PRO:HB3	1:B:1227:SER:HA	1.91	0.52
1:A:390:GLN:NE2	1:C:380:ASP:HA	2.25	0.52
1:B:228:VAL:HG21	1:B:304:VAL:HG21	1.91	0.52
1:A:449:MET:CE	1:A:452:PHE:HB3	2.40	0.51
1:C:449:MET:CE	1:C:452:PHE:HB3	2.40	0.51
1:C:1111:ASP:N	1:C:1111:ASP:OD1	2.43	0.51
1:B:862:GLN:O	1:B:865:VAL:HG22	2.11	0.51
1:B:885:GLN:HA	1:B:888:ILE:HD12	1.93	0.51
1:B:696:SER:HA	1:B:790:ARG:O	2.10	0.51
1:C:1213:ARG:HA	1:C:1286:VAL:O	2.11	0.51
1:A:846:ILE:HA	1:A:849:LEU:HG	1.92	0.51
1:A:887:LEU:HD21	1:A:1155:VAL:CG2	2.41	0.51
1:B:182:VAL:HG22	1:B:666:ILE:HD12	1.93	0.51
1:A:1100:ARG:HA	1:A:1106:PHE:HD1	1.74	0.50
1:B:886:HIS:O	1:B:889:ASP:HB2	2.11	0.50
1:B:1265:TYR:O	1:B:1268:THR:HB	2.11	0.50
1:C:887:LEU:HD21	1:C:1155:VAL:CG2	2.42	0.50
1:C:1299:PRO:HB3	1:C:1319:GLU:HG2	1.94	0.50
1:C:1160:GLU:O	1:C:1162:PRO:HD3	2.11	0.50
1:B:1013:TYR:O	1:B:1017:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:GLN:HA	1:B:1109:THR:HG21	1.94	0.50
1:B:544:TYR:O	1:B:665:SER:HA	2.11	0.50
1:A:150:LYS:HA	1:A:671:GLY:HA2	1.94	0.50
1:A:1222:PRO:HB3	1:A:1227:SER:HA	1.93	0.50
1:B:702:ALA:HB3	1:B:1295:ALA:HB3	1.92	0.50
1:C:433:ILE:HG22	1:C:511:PHE:HE1	1.76	0.50
1:A:99:THR:HG23	1:A:111:GLU:HB3	1.94	0.50
2:C:1406:NAG:O7	2:C:1406:NAG:H3	2.11	0.50
1:B:701:GLU:HG2	1:B:1297:LYS:HA	1.94	0.50
1:A:451:PHE:HZ	1:A:497:VAL:HG23	1.77	0.49
1:A:433:ILE:HG22	1:A:511:PHE:HE1	1.77	0.49
1:B:919:GLY:O	1:B:920:SER:C	2.50	0.49
1:B:699:ARG:HA	1:B:762:ALA:HB3	1.95	0.49
1:A:1213:ARG:HA	1:A:1286:VAL:O	2.12	0.49
1:C:1199:LEU:HD22	1:C:1304:VAL:HG23	1.94	0.49
1:A:164:ASP:HB2	1:A:165:PRO:CD	2.42	0.49
1:B:489:LYS:HA	1:B:510:ASP:HA	1.93	0.49
1:C:164:ASP:HB2	1:C:165:PRO:CD	2.43	0.49
1:A:164:ASP:HB2	1:A:165:PRO:HD2	1.95	0.49
1:A:1299:PRO:HB3	1:A:1319:GLU:HG2	1.94	0.49
1:A:656:THR:HA	1:A:683:THR:O	2.13	0.49
1:C:1222:PRO:HB3	1:C:1227:SER:HA	1.95	0.49
1:B:126:GLN:O	1:B:140:PHE:HA	2.13	0.49
1:C:656:THR:HA	1:C:683:THR:O	2.13	0.49
1:A:854:ALA:HB2	1:A:1101:TYR:OH	2.13	0.49
1:C:99:THR:HG23	1:C:111:GLU:HB3	1.94	0.48
1:C:150:LYS:HA	1:C:671:GLY:HA2	1.95	0.48
1:C:37:THR:HA	1:C:83:ILE:O	2.13	0.48
1:C:501:THR:HG22	1:C:600:LEU:HB2	1.95	0.48
1:B:741:SER:O	1:B:742:TYR:HB2	2.13	0.48
1:C:775:SER:HB3	1:C:782:THR:HG22	1.95	0.48
1:A:501:THR:HG22	1:A:600:LEU:HB2	1.95	0.48
1:C:451:PHE:HZ	1:C:497:VAL:HG23	1.79	0.48
1:A:775:SER:HB3	1:A:782:THR:HG22	1.94	0.48
1:A:37:THR:HA	1:A:83:ILE:O	2.13	0.48
1:C:349:LEU:O	1:C:384:LEU:HA	2.14	0.48
1:B:966:GLU:HG3	1:B:968:GLY:O	2.12	0.48
1:B:144:LEU:HD12	1:B:178:LEU:HD11	1.96	0.48
1:B:543:ALA:HB3	1:B:640:ILE:HD12	1.96	0.48
1:B:1186:PHE:HB3	1:B:1188:LEU:HD21	1.95	0.48
1:A:772:VAL:HB	1:A:785:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:HA	1:A:1106:PHE:CD1	2.50	0.47
1:C:803:THR:HG23	1:C:1181:GLU:HG2	1.95	0.47
1:C:164:ASP:HB2	1:C:165:PRO:HD2	1.97	0.47
1:A:1219:ASN:HB3	1:A:1281:ARG:HA	1.97	0.47
1:A:906:ARG:CZ	1:A:946:MET:HG2	2.45	0.47
1:B:260:LYS:HB2	1:B:305:SER:HB2	1.96	0.47
1:A:660:TYR:CZ	1:A:678:PRO:HG2	2.50	0.47
1:A:660:TYR:OH	1:A:678:PRO:HG2	2.15	0.47
1:B:874:LEU:HB3	1:B:938:TYR:CE1	2.50	0.47
1:C:772:VAL:HB	1:C:785:LEU:HD12	1.97	0.46
1:C:1100:ARG:HA	1:C:1106:PHE:CD1	2.50	0.46
1:C:837:LEU:HD21	1:C:1148:ILE:HD11	1.98	0.46
1:B:927:PHE:O	1:B:931:SER:HB2	2.14	0.46
1:C:854:ALA:HB2	1:C:1101:TYR:OH	2.14	0.46
1:B:1077:LEU:HD11	1:B:1122:LEU:HD22	1.96	0.46
1:A:380:ASP:HA	1:C:390:GLN:HE22	1.80	0.46
1:A:220:VAL:O	1:A:221:LEU:HB2	2.15	0.46
1:C:1192:ASN:OD1	1:C:1316:LYS:HA	2.15	0.46
1:A:457:MET:SD	1:A:457:MET:N	2.89	0.46
1:A:1070:ILE:H	1:A:1070:ILE:CD1	2.16	0.46
1:A:1199:LEU:HD22	1:A:1304:VAL:HG23	1.98	0.46
1:A:656:THR:HG23	1:A:684:VAL:HA	1.98	0.46
1:B:160:VAL:HG22	1:B:202:VAL:HG22	1.98	0.45
1:B:1095:TRP:O	1:B:1099:GLN:HG2	2.16	0.45
1:A:941:ASP:OD1	1:A:941:ASP:N	2.50	0.45
1:C:311:THR:O	1:C:312:ASN:HB2	2.16	0.45
1:A:801:MET:HG3	1:A:1183:ILE:HG12	1.99	0.45
1:C:846:ILE:C	1:C:848:ASN:H	2.20	0.45
1:A:520:LEU:HB3	1:A:675:ILE:HG21	1.99	0.45
1:B:131:VAL:HA	1:B:215:GLU:O	2.17	0.45
2:C:1402:NAG:O4	2:C:1403:NAG:N2	2.49	0.45
1:C:1137:LEU:HD12	1:C:1170:ILE:HG12	1.98	0.45
1:A:1192:ASN:OD1	1:A:1316:LYS:HA	2.16	0.45
1:C:208:GLU:OE2	1:C:211:SER:HB2	2.17	0.45
1:A:862:GLN:O	1:A:865:VAL:HG22	2.17	0.45
1:A:846:ILE:C	1:A:848:ASN:H	2.19	0.45
1:A:803:THR:HG23	1:A:1181:GLU:HG2	1.97	0.45
1:B:1258:ILE:HD13	1:B:1272:LEU:HD13	1.98	0.45
1:C:449:MET:HE2	1:C:452:PHE:HB3	1.99	0.45
1:C:801:MET:HG3	1:C:1183:ILE:HG12	1.99	0.45
1:A:837:LEU:HD21	1:A:1148:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:PRO:HB3	1:A:683:THR:HB	1.99	0.45
1:B:1013:TYR:O	1:B:1017:GLN:CG	2.65	0.45
1:C:417:VAL:O	1:C:419:THR:HG23	2.17	0.44
1:B:1106:PHE:HB3	1:B:1111:ASP:HB3	2.00	0.44
1:A:301:ARG:HD3	1:A:320:GLN:HE22	1.81	0.44
1:B:1231:MET:O	1:B:1307:TYR:HB2	2.17	0.44
1:C:846:ILE:HG21	1:C:887:LEU:HD22	1.99	0.44
1:A:449:MET:HE2	1:A:452:PHE:HB3	1.98	0.44
1:C:996:ASN:HB2	1:C:999:ALA:HB3	1.98	0.44
1:A:1077:LEU:O	1:A:1081:VAL:HG23	2.17	0.44
1:B:1015:SER:HB2	1:B:1039:HIS:CE1	2.53	0.44
1:A:1231:MET:O	1:A:1307:TYR:HB2	2.18	0.44
1:C:520:LEU:HB3	1:C:675:ILE:HG21	2.00	0.44
1:C:686:PRO:HB3	1:C:713:LEU:HD21	2.00	0.44
1:B:564:PHE:HA	1:B:567:ASP:OD2	2.18	0.44
1:C:427:LEU:HD11	1:C:441:PHE:CD2	2.53	0.44
1:C:350:GLN:HA	1:C:384:LEU:HD23	2.00	0.44
1:C:254:PRO:HD2	1:C:690:VAL:HG11	1.98	0.44
1:B:1196:ARG:HB2	1:B:1312:LEU:CD2	2.47	0.44
1:B:930:THR:HG21	1:B:992:ALA:HB1	2.00	0.44
1:A:846:ILE:HG21	1:A:887:LEU:HD22	1.99	0.44
1:A:433:ILE:HD13	1:A:509:LEU:HA	1.99	0.44
1:C:260:LYS:HB2	1:C:305:SER:HB2	2.00	0.44
1:C:1235:GLU:HB3	1:C:1303:VAL:HG12	2.00	0.44
1:A:427:LEU:HD11	1:A:441:PHE:CD2	2.53	0.44
1:B:1161:ILE:O	1:B:1161:ILE:HG23	2.17	0.44
1:B:233:ILE:HA	1:B:234:PRO:HD3	1.87	0.44
1:A:906:ARG:NH1	1:A:946:MET:HG2	2.33	0.43
1:B:988:TYR:O	1:B:991:THR:HB	2.18	0.43
1:B:1021:ILE:O	1:B:1048:LYS:NZ	2.47	0.43
1:A:973:LYS:NZ	1:A:1226:ASP:OD1	2.51	0.43
1:C:868:VAL:HB	1:C:869:PRO:HD3	2.00	0.43
1:A:260:LYS:HB2	1:A:305:SER:HB2	2.00	0.43
1:B:1264:ARG:HG3	1:B:1269:SER:HB3	2.00	0.43
1:C:1219:ASN:HB3	1:C:1281:ARG:HA	2.00	0.43
1:C:1077:LEU:O	1:C:1081:VAL:HG23	2.17	0.43
1:C:529:PRO:HB3	1:C:683:THR:HB	2.00	0.43
1:A:417:VAL:O	1:A:419:THR:HG23	2.18	0.43
1:C:862:GLN:O	1:C:865:VAL:HG22	2.18	0.43
1:A:487:ILE:HD13	1:A:511:PHE:CE2	2.53	0.43
1:B:656:THR:HG23	1:B:684:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:VAL:HB	1:A:869:PRO:HD3	2.00	0.43
1:C:92:THR:HA	1:C:116:TYR:HE2	1.83	0.43
1:C:719:ALA:HB2	1:C:776:ILE:CG2	2.48	0.43
1:A:686:PRO:HB3	1:A:713:LEU:HD21	2.00	0.43
1:B:1184:TYR:CD1	1:B:1184:TYR:N	2.86	0.43
1:C:656:THR:HG23	1:C:684:VAL:HA	1.99	0.43
1:A:1222:PRO:CB	1:A:1227:SER:HA	2.48	0.43
1:A:254:PRO:HD2	1:A:690:VAL:HG11	2.00	0.43
1:A:988:TYR:O	1:A:991:THR:HB	2.17	0.43
1:A:92:THR:HA	1:A:116:TYR:HE2	1.82	0.43
1:B:488:PRO:HA	1:B:511:PHE:HB2	2.01	0.43
1:B:1257:PRO:HB2	1:B:1259:GLN:HE21	1.82	0.43
1:C:722:THR:HG23	1:C:743:THR:OG1	2.19	0.43
1:B:969:LYS:H	1:B:969:LYS:HD2	1.84	0.43
1:C:697:ILE:HG21	1:C:703:VAL:HG21	2.01	0.43
1:A:311:THR:O	1:A:312:ASN:HB2	2.19	0.43
1:C:60:THR:HG23	1:C:66:VAL:CG2	2.49	0.43
1:A:1235:GLU:HB3	1:A:1303:VAL:HG12	2.00	0.43
1:B:848:ASN:O	1:B:849:LEU:C	2.58	0.43
1:A:263:LEU:HD21	1:A:265:LEU:HG	2.00	0.43
1:C:973:LYS:NZ	1:C:1226:ASP:OD1	2.51	0.43
1:C:1231:MET:O	1:C:1307:TYR:HB2	2.19	0.42
1:B:862:GLN:O	1:B:864:MET:N	2.52	0.42
1:C:116:TYR:CD1	1:C:117:LEU:N	2.83	0.42
1:A:116:TYR:CD1	1:A:117:LEU:N	2.83	0.42
1:B:1259:GLN:HG3	1:B:1275:TYR:CD2	2.54	0.42
1:A:1137:LEU:HD12	1:A:1170:ILE:HG12	2.01	0.42
1:B:242:ASN:OD1	1:B:285:GLU:HG3	2.19	0.42
1:C:233:ILE:HA	1:C:234:PRO:HD3	1.85	0.42
1:C:660:TYR:CZ	1:C:678:PRO:HG2	2.54	0.42
1:C:660:TYR:OH	1:C:678:PRO:HG2	2.20	0.42
1:B:1154:ASP:O	1:B:1156:GLN:N	2.47	0.42
1:A:122:SER:HA	1:A:209:LEU:HD11	2.01	0.42
1:B:862:GLN:HB3	1:B:1109:THR:HG21	2.02	0.42
1:C:122:SER:HA	1:C:209:LEU:HD11	2.02	0.42
1:C:301:ARG:HD3	1:C:320:GLN:HE22	1.84	0.42
1:A:151:PRO:HA	1:A:152:PRO:HD3	1.92	0.42
1:C:1320:VAL:CG1	1:C:1321:ASP:N	2.81	0.42
1:C:906:ARG:CZ	1:C:946:MET:HG2	2.49	0.42
1:C:711:ASN:HB3	1:C:748:VAL:HG12	2.01	0.42
1:C:433:ILE:HD13	1:C:509:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:906:ARG:NH1	1:C:946:MET:HG2	2.35	0.42
1:C:1025:TYR:CE1	1:C:1029:ILE:HD11	2.55	0.41
1:B:1295:ALA:HB2	1:B:1328:ILE:HG13	2.01	0.41
1:C:1222:PRO:CB	1:C:1227:SER:HA	2.50	0.41
1:C:941:ASP:OD1	1:C:941:ASP:N	2.51	0.41
1:C:457:MET:N	1:C:457:MET:SD	2.93	0.41
1:A:1228:GLN:HE22	1:B:63:GLY:C	2.23	0.41
1:B:1229:SER:OG	1:B:1277:MET:N	2.54	0.41
1:A:1127:SER:HA	1:A:1128:PRO:HD3	1.91	0.41
1:C:340:ARG:HA	1:C:341:PRO:HD3	1.89	0.41
1:A:841:LEU:HA	1:A:1179:LEU:HD11	2.02	0.41
1:A:158:VAL:HG12	1:A:204:VAL:HG22	2.01	0.41
1:A:1025:TYR:CE1	1:A:1029:ILE:HD11	2.55	0.41
1:B:1031:THR:O	1:B:1035:MET:HG2	2.21	0.41
1:A:1320:VAL:CG1	1:A:1321:ASP:N	2.83	0.41
1:A:60:THR:HG23	1:A:66:VAL:CG2	2.50	0.41
1:C:540:ARG:HA	1:C:541:PRO:HD2	1.93	0.41
1:B:862:GLN:HG2	1:B:1307:TYR:CZ	2.55	0.41
1:B:1258:ILE:HG12	1:B:1274:TYR:CZ	2.55	0.41
1:C:151:PRO:HA	1:C:152:PRO:HD3	1.91	0.41
1:C:263:LEU:HD21	1:C:265:LEU:HG	2.02	0.41
1:A:697:ILE:HG21	1:A:703:VAL:HG21	2.02	0.41
1:C:246:GLU:HA	1:C:280:GLY:O	2.20	0.41
1:C:861:GLU:OE2	1:C:1110:GLN:HG2	2.21	0.41
1:B:971:TRP:HB2	1:B:1231:MET:HB2	2.02	0.41
1:B:151:PRO:HA	1:B:152:PRO:HD3	1.92	0.41
1:C:988:TYR:O	1:C:991:THR:HB	2.20	0.41
1:A:208:GLU:OE2	1:A:211:SER:HB2	2.21	0.41
1:A:455:TYR:HB3	1:A:457:MET:HE3	2.02	0.41
1:A:1070:ILE:N	1:A:1070:ILE:HD12	2.30	0.41
1:B:440:ARG:HA	1:B:478:LEU:O	2.20	0.41
1:B:1146:PHE:CE2	1:B:1158:PHE:HB3	2.56	0.41
1:A:1100:ARG:CG	1:A:1106:PHE:HE1	2.24	0.41
1:A:1131:ASN:N	1:A:1151:GLU:HB3	2.30	0.41
1:A:1095:TRP:O	1:A:1099:GLN:HG2	2.20	0.41
1:B:1256:ASN:HA	1:B:1257:PRO:HD3	1.84	0.40
1:B:194:MET:HE3	1:B:904:ARG:HA	2.03	0.40
1:C:633:TRP:CD1	1:C:634:LEU:N	2.89	0.40
1:C:1228:GLN:CD	1:C:1276:LYS:HD3	2.42	0.40
1:A:711:ASN:HB3	1:A:748:VAL:HG12	2.02	0.40
1:B:1136:GLN:HB3	1:B:1171:ASN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:THR:HG22	1:B:678:PRO:HB3	2.03	0.40
1:C:126:GLN:O	1:C:140:PHE:HA	2.22	0.40
1:B:1093:MET:HB2	1:B:1122:LEU:HD23	2.02	0.40
1:B:1083:ALA:O	1:B:1084:GLU:HB2	2.21	0.40
1:C:715:ALA:HB3	1:C:717:TYR:CZ	2.57	0.40
1:B:906:ARG:NH1	1:B:946:MET:HG2	2.37	0.40
1:A:380:ASP:HA	1:C:390:GLN:NE2	2.36	0.40
1:A:1234:ILE:HD12	1:A:1274:TYR:HE2	1.86	0.40
1:B:520:LEU:HA	1:B:537:MET:HA	2.04	0.40
1:B:1081:VAL:HG13	1:B:1086:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	Percentiles	
1	A	1266/1323 (96%)	1154 (91%)	101 (8%)	11 (1%)	21	68
1	B	1011/1323 (76%)	898 (89%)	94 (9%)	19 (2%)	10	55
1	C	1266/1323 (96%)	1157 (91%)	97 (8%)	12 (1%)	21	68
All	All	3543/3969 (89%)	3209 (91%)	292 (8%)	42 (1%)	16	63

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	642	ARG
1	A	1160	GLU
1	C	642	ARG
1	C	1160	GLU
1	A	418	GLU
1	A	676	LYS
1	A	1140	LYS

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Mol	Chain	Res	Type
1	A	1164	ASP
1	A	1321	ASP
1	B	73	VAL
1	B	91	LEU
1	B	742	TYR
1	B	811	TYR
1	B	863	ASN
1	B	920	SER
1	B	1140	LYS
1	B	1160	GLU
1	B	1164	ASP
1	B	1321	ASP
1	B	1331	GLU
1	C	418	GLU
1	C	676	LYS
1	C	1140	LYS
1	C	1164	ASP
1	C	1321	ASP
1	B	1155	VAL
1	A	355	ASP
1	B	220	VAL
1	B	1018	LEU
1	B	1166	LYS
1	C	355	ASP
1	B	134	PRO
1	C	1245	ASP
1	B	206	GLY
1	C	134	PRO
1	A	130	PRO
1	A	220	VAL
1	C	220	VAL
1	A	134	PRO
1	C	130	PRO
1	B	799	PRO
1	B	130	PRO

### 5.3.2 Protein sidechains ⓘ

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	A	997/1177 (85%)	957 (96%)	40 (4%)	38	76
1	B	670/1177 (57%)	627 (94%)	43 (6%)	22	64
1	C	979/1177 (83%)	940 (96%)	39 (4%)	38	76
All	All	2646/3531 (75%)	2524 (95%)	122 (5%)	33	73

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	73	VAL
1	A	116	TYR
1	A	192	THR
1	A	213	THR
1	A	215	GLU
1	A	221	LEU
1	A	370	ASP
1	A	433	ILE
1	A	450	THR
1	A	453	VAL
1	A	457	MET
1	A	513	GLU
1	A	557	PHE
1	A	564	PHE
1	A	570	GLN
1	A	572	PHE
1	A	633	TRP
1	A	634	LEU
1	A	649	ILE
1	A	674	ILE
1	A	785	LEU
1	A	803	THR
1	A	809	ASP
1	A	821	ASP
1	A	862	GLN
1	A	886	HIS
1	A	894	LEU
1	A	908	THR
1	A	941	ASP
1	A	1042	LYS
1	A	1066	THR

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Mol	Chain	Res	Type
1	A	1070	ILE
1	A	1130	ARG
1	A	1143	THR
1	A	1151	GLU
1	A	1275	TYR
1	A	1276	LYS
1	A	1279	THR
1	A	1328	ILE
1	B	182	VAL
1	B	192	THR
1	B	263	LEU
1	B	467	PHE
1	B	519	ASP
1	B	567	ASP
1	B	633	TRP
1	B	640	ILE
1	B	655	THR
1	B	706	GLN
1	B	708	THR
1	B	785	LEU
1	B	802	ASP
1	B	803	THR
1	B	809	ASP
1	B	815	THR
1	B	859	CYS
1	B	862	GLN
1	B	863	ASN
1	B	865	VAL
1	B	875	ASP
1	B	889	ASP
1	B	894	LEU
1	B	900	GLN
1	B	908	THR
1	B	931	SER
1	B	934	THR
1	B	941	ASP
1	B	963	ARG
1	B	965	ASP
1	B	967	THR
1	B	972	HIS
1	B	1067	THR
1	B	1070	ILE

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Mol	Chain	Res	Type
1	B	1111	ASP
1	B	1142	ASN
1	B	1149	ASN
1	B	1164	ASP
1	B	1165	THR
1	B	1237	THR
1	B	1249	ILE
1	B	1276	LYS
1	B	1333	ASP
1	C	56	LEU
1	C	73	VAL
1	C	116	TYR
1	C	144	LEU
1	C	192	THR
1	C	213	THR
1	C	215	GLU
1	C	370	ASP
1	C	433	ILE
1	C	453	VAL
1	C	457	MET
1	C	487	ILE
1	C	513	GLU
1	C	564	PHE
1	C	572	PHE
1	C	633	TRP
1	C	634	LEU
1	C	649	ILE
1	C	674	ILE
1	C	785	LEU
1	C	803	THR
1	C	809	ASP
1	C	821	ASP
1	C	862	GLN
1	C	886	HIS
1	C	894	LEU
1	C	908	THR
1	C	931	SER
1	C	941	ASP
1	C	1042	LYS
1	C	1066	THR
1	C	1070	ILE
1	C	1130	ARG

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Mol	Chain	Res	Type
1	C	1143	THR
1	C	1151	GLU
1	C	1275	TYR
1	C	1276	LYS
1	C	1279	THR
1	C	1328	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	283	GLN
1	A	320	GLN
1	A	390	GLN
1	A	1136	GLN
1	A	1171	ASN
1	A	1228	GLN
1	A	1324	ASN
1	B	1039	HIS
1	B	1098	ASN
1	B	1256	ASN
1	B	1259	GLN
1	C	271	ASN
1	C	283	GLN
1	C	320	GLN
1	C	1136	GLN
1	C	1171	ASN
1	C	1324	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	2006	1,3	14,14,15	0.67	0	15,19,21	1.76	3 (20%)
3	NAG	A	2007	3	14,14,15	0.43	0	15,19,21	0.97	1 (6%)

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	A	2006	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2007	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2006	NAG	C3-C4-C5	2.52	114.59	110.20
3	A	2007	NAG	C1-O5-C5	2.55	115.48	112.25
3	A	2006	NAG	C4-C3-C2	2.72	115.46	111.23
3	A	2006	NAG	C2-N2-C7	4.92	129.35	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	2001	1	14,14,15	0.52	0	15,19,21	0.96	1 (6%)
2	NAG	A	2002	1	14,14,15	0.48	0	15,19,21	0.84	0
2	NAG	A	2003	1	14,14,15	0.47	0	15,19,21	0.84	0
2	NAG	A	2004	-	14,14,15	0.43	0	15,19,21	0.97	1 (6%)
2	NAG	A	2005	1	14,14,15	0.61	0	15,19,21	2.32	2 (13%)
2	NAG	A	2008	1	14,14,15	0.42	0	15,19,21	2.76	2 (13%)
2	NAG	A	2009	1	14,14,15	0.79	1 (7%)	15,19,21	1.66	3 (20%)
2	NAG	B	1401	1	14,14,15	0.43	0	15,19,21	0.95	1 (6%)
2	NAG	C	1401	1	14,14,15	0.50	0	15,19,21	1.21	1 (6%)
2	NAG	C	1402	1	14,14,15	0.47	0	15,19,21	0.68	0
2	NAG	C	1403	-	14,14,15	0.46	0	15,19,21	1.63	3 (20%)
2	NAG	C	1404	1	14,14,15	0.47	0	15,19,21	0.96	1 (6%)
2	NAG	C	1405	1	14,14,15	0.49	0	15,19,21	1.12	1 (6%)
2	NAG	C	1406	1	14,14,15	0.27	0	15,19,21	0.53	0
2	NAG	C	1407	1	14,14,15	0.56	0	15,19,21	1.38	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
2	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2004	-	-	0/6/23/26	0/1/1/1
2	NAG	A	2005	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2009	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1403	-	-	0/6/23/26	0/1/1/1
2	NAG	C	1404	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1407	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2009	NAG	C1-C2	2.28	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2008	NAG	C4-C3-C2	-2.34	107.59	111.23
2	C	1407	NAG	C3-C4-C5	2.09	113.84	110.20
2	A	2009	NAG	C2-N2-C7	2.15	125.80	123.04
2	C	1403	NAG	C4-C3-C2	2.31	114.83	111.23
2	A	2001	NAG	O5-C5-C6	2.36	112.46	107.35
2	C	1404	NAG	C1-O5-C5	2.51	115.44	112.25
2	C	1407	NAG	C1-O5-C5	2.54	115.47	112.25
2	C	1403	NAG	C3-C4-C5	2.79	115.07	110.20
2	A	2004	NAG	C1-O5-C5	2.80	115.81	112.25
2	B	1401	NAG	C1-O5-C5	2.86	115.87	112.25
2	A	2009	NAG	C1-O5-C5	2.89	115.91	112.25
2	C	1407	NAG	C4-C3-C2	3.11	116.06	111.23
2	C	1401	NAG	C1-O5-C5	3.43	116.60	112.25
2	C	1405	NAG	C1-O5-C5	3.64	116.87	112.25
2	A	2009	NAG	C4-C3-C2	4.16	117.70	111.23
2	C	1403	NAG	C1-O5-C5	4.35	117.77	112.25
2	A	2005	NAG	C2-N2-C7	4.85	129.27	123.04
2	A	2005	NAG	C1-O5-C5	6.58	120.61	112.25
2	A	2008	NAG	C1-O5-C5	10.21	125.20	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1402	NAG	2	0
2	C	1403	NAG	2	0
2	C	1406	NAG	1	0



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1276/1323 (96%)	0.10	20 (1%) 74 60	113, 151, 175, 200	0
1	B	1063/1323 (80%)	0.06	17 (1%) 74 60	125, 165, 200, 200	0
1	C	1276/1323 (96%)	0.04	17 (1%) 79 66	123, 160, 191, 200	0
All	All	3615/3969 (91%)	0.07	54 (1%) 76 62	113, 157, 194, 200	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	PRO	3.0
1	C	660	TYR	3.0
1	A	410	PHE	2.9
1	B	84	ASN	2.9
1	B	241	VAL	2.8
1	A	144	LEU	2.7
1	B	259	ALA	2.7
1	B	39	VAL	2.7
1	B	457	MET	2.7
1	A	851	ASN	2.7
1	A	834	GLU	2.6
1	C	144	LEU	2.6
1	B	516	ASN	2.5
1	B	474	THR	2.5
1	A	1139	TYR	2.5
1	C	22	LEU	2.4
1	B	178	LEU	2.4
1	C	410	PHE	2.4
1	B	462	ILE	2.3
1	C	851	ASN	2.3
1	A	449	MET	2.3
1	A	835	PHE	2.3
1	A	22	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	661	LEU	2.3
1	C	41	SER	2.3
1	B	306	PHE	2.2
1	C	964	PHE	2.2
1	A	400	ILE	2.2
1	A	568	ILE	2.2
1	C	681	PHE	2.2
1	B	517	ASN	2.2
1	C	68	ASN	2.2
1	A	200	ILE	2.2
1	B	568	ILE	2.1
1	B	851	ASN	2.1
1	A	709	LEU	2.1
1	A	391	PRO	2.1
1	C	659	TRP	2.1
1	C	224	PHE	2.1
1	A	402	PHE	2.1
1	B	1137	LEU	2.1
1	B	518	PHE	2.1
1	A	1204	GLN	2.1
1	A	1137	LEU	2.1
1	C	1184	TYR	2.1
1	A	327	ALA	2.1
1	C	43	PHE	2.1
1	A	1168	LEU	2.0
1	A	1218	ALA	2.0
1	C	574	GLY	2.0
1	B	175	THR	2.0
1	A	664	PHE	2.0
1	C	675	ILE	2.0
1	C	449	MET	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.



The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	2006	14/15	0.87	0.28	-1.02	167,168,169,170	0
3	NAG	A	2007	14/15	0.92	0.12	-	169,171,172,173	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	2001	14/15	0.85	0.19	-0.35	165,168,168,169	0
2	NAG	C	1406	14/15	0.82	0.22	-0.85	174,175,176,176	0
2	NAG	C	1402	14/15	0.91	0.14	-1.30	166,166,167,168	0
2	NAG	A	2003	14/15	0.86	0.15	-1.32	160,160,161,162	0
2	NAG	B	1401	14/15	0.81	0.14	-1.43	175,176,176,176	0
2	NAG	A	2004	14/15	0.88	0.13	-	177,177,178,178	0
2	NAG	A	2002	14/15	0.84	0.20	-	156,157,158,158	0
2	NAG	C	1403	14/15	0.90	0.13	-	183,185,185,185	0
2	NAG	A	2005	14/15	0.81	0.22	-	170,172,173,173	0
2	NAG	C	1401	14/15	0.76	0.25	-	166,167,168,168	0
2	NAG	C	1405	14/15	0.84	0.16	-	162,163,163,164	0
2	NAG	C	1404	14/15	0.85	0.17	-	173,174,175,175	0
2	NAG	C	1407	14/15	0.79	0.25	-	168,169,169,169	0
2	NAG	A	2009	14/15	0.81	0.22	-	166,168,168,168	0
2	NAG	A	2008	14/15	0.78	0.27	-	152,152,152,153	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.