



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:44 AM GMT

PDB ID : 2Y74  
Title : THE CRYSTAL STRUCTURE OF HUMAN SOLUBLE PRIMARY AMINE  
OXIDASE AOC3 IN THE OFF-COPPER CONFORMATION  
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Smith, D.J.; Pihlavisto, M.; Salmi, M.; Jalkanen, S.; Salminen, T.A.  
Deposited on : 2011-01-28  
Resolution : 2.95 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

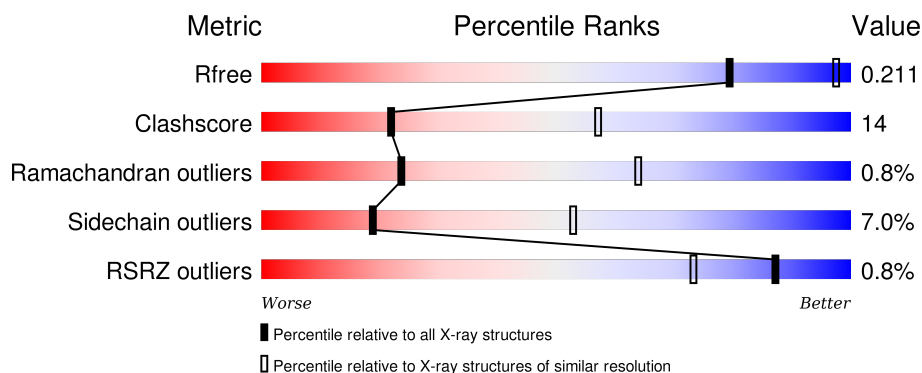
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	763	<div> <div></div> <div>67% 21% • 9%</div> </div>
1	B	763	<div> <div></div> <div>66% 22% • 8%</div> </div>

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
4	IMD	A	1766	-	-	-	X
4	IMD	B	1766	-	-	-	X
4	IMD	B	1767	-	-	-	X
6	NAG	A	1771	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11371 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 MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	0	0
			5490	3532	942	997	19			
1	B	699	Total	C	N	O	S	0	0	0
			5526	3551	950	1005	20			

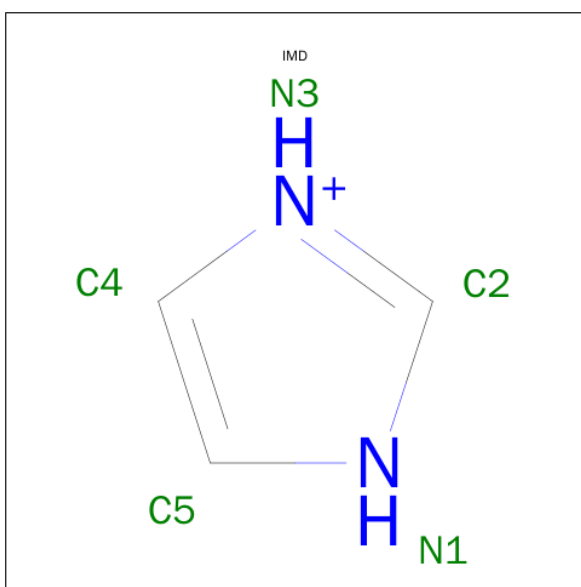
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

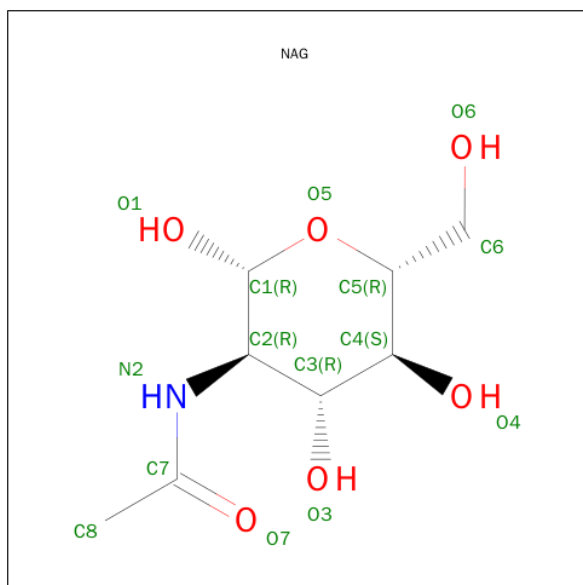
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

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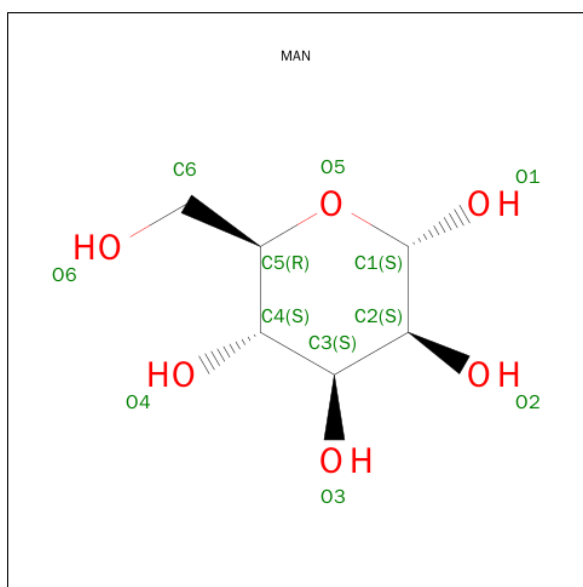
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			11	6	5		

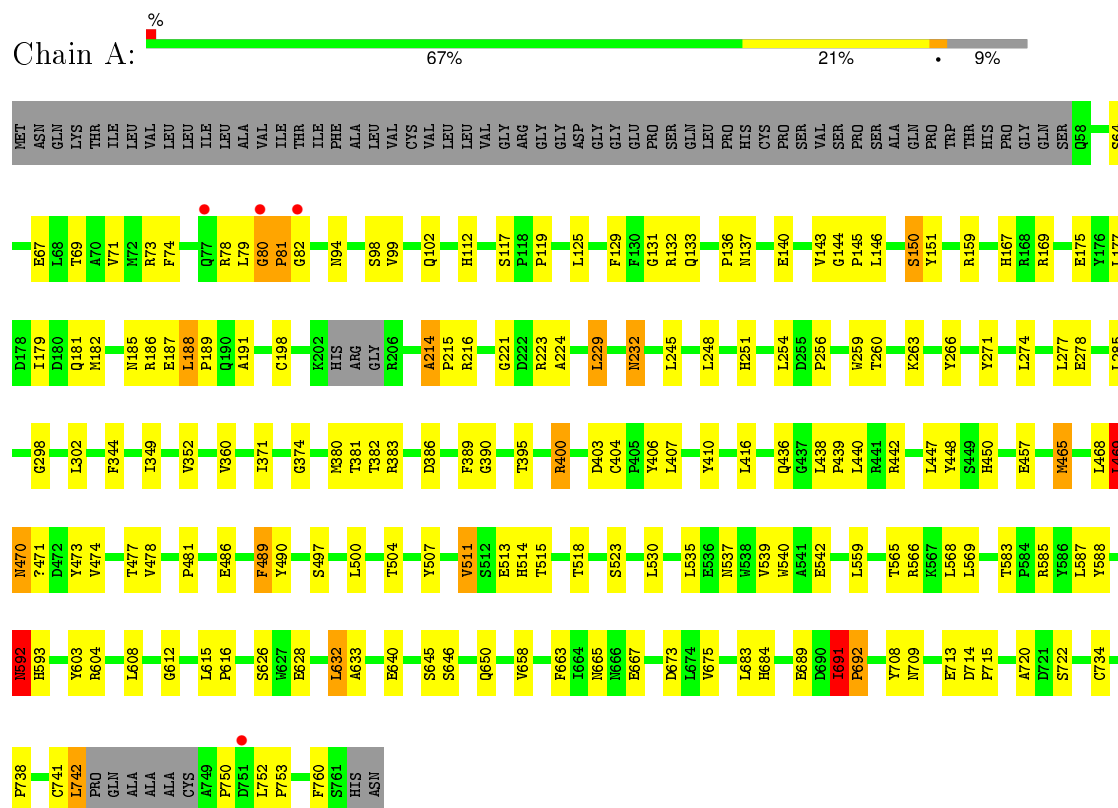
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	60	Total	O	0	0
			60	60		
9	B	69	Total	O	0	0
			69	69		

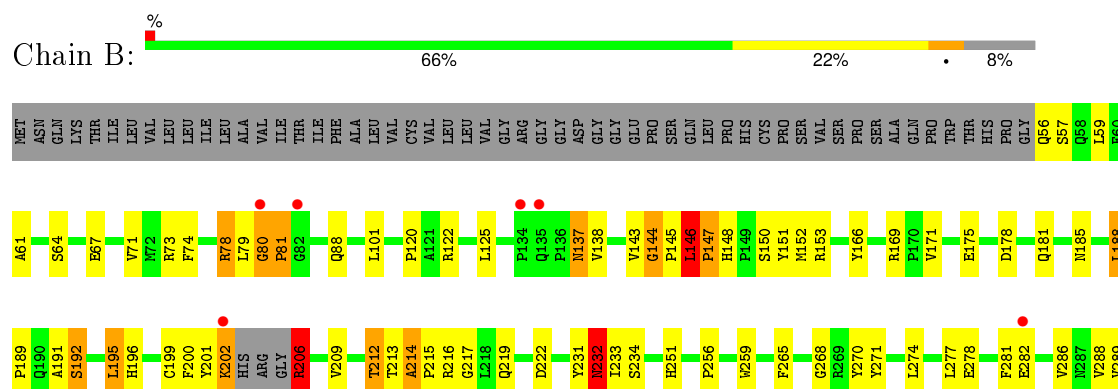
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: MEMBRANE PRIMARY AMINE OXIDASE



#### • Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.80 Å   225.80 Å   218.70 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	38.21 – 2.95 38.50 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.21-2.95) 99.9 (38.50-2.95)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.09 (at 2.95 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.179   ,   0.214 0.174   ,   0.211	Depositor DCC
$R_{free}$ test set	3500 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 69215 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: IMD, CA, T0I, MAN, CU, 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	0.60	5/5644 (0.1%)	0.55	3/7694 (0.0%)
1	B	0.59	3/5681 (0.1%)	0.55	4/7744 (0.1%)
All	All	0.59	8/11325 (0.1%)	0.55	7/15438 (0.0%)

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	3
1	B	0	3
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	LEU	C-N	11.74	1.61	1.34
1	B	137	ASN	CG-ND2	6.99	1.50	1.32
1	B	232	ASN	CG-ND2	5.89	1.47	1.32
1	A	266	TYR	CD2-CE2	-5.41	1.31	1.39
1	A	232	ASN	CG-ND2	5.40	1.46	1.32
1	A	266	TYR	CD1-CE1	-5.21	1.31	1.39
1	A	266	TYR	CE2-CZ	-5.19	1.31	1.38
1	B	592	ASN	CG-ND2	5.16	1.45	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	LEU	C-N-CA	-9.68	97.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	691	ILE	C-N-CD	-7.93	103.16	120.60
1	B	743	PRO	CB-CA-C	-6.88	94.80	112.00
1	A	592	ASN	N-CA-CB	6.36	122.04	110.60
1	B	592	ASN	CA-CB-CG	6.23	127.10	113.40
1	B	743	PRO	N-CA-C	5.11	125.38	112.10
1	B	206	ARG	NE-CZ-NH1	-5.07	117.76	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	LEU	Peptide
1	A	592	ASN	Sidechain
1	A	691	ILE	Peptide
1	B	137	ASN	Sidechain
1	B	146	LEU	Peptide
1	B	666	ASN	Sidechain

## 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	5490	0	5243	142	0
1	B	5526	0	5280	167	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	15	0	15	0	0
4	B	15	0	15	0	0
5	A	39	0	34	4	0
6	A	28	0	25	3	0
6	B	56	0	47	4	0
7	A	28	0	26	2	0
7	B	28	0	26	2	0
8	B	11	0	10	0	0
9	A	60	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	69	0	0	3	0
All	All	11371	0	10721	304	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 (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:HD21	5:A:1768:NAG:C1	1.25	1.45
1:B:214:ALA:HB1	1:B:215:PRO:CD	1.61	1.30
1:B:206:ARG:HH11	1:B:206:ARG:HG2	0.95	1.09
1:B:214:ALA:HB1	1:B:215:PRO:HD2	1.31	1.07
1:B:214:ALA:CB	1:B:215:PRO:CD	2.29	1.03
1:B:214:ALA:CB	1:B:215:PRO:HD2	1.88	1.00
1:B:206:ARG:CG	1:B:206:ARG:HH11	1.69	0.99
1:A:214:ALA:HB1	1:A:215:PRO:HD2	1.44	0.98
1:B:78:ARG:HH11	1:B:78:ARG:HG3	1.30	0.96
1:B:383:ARG:HD3	1:B:383:ARG:N	1.81	0.95
1:B:214:ALA:HB1	1:B:215:PRO:HD3	1.48	0.94
1:A:214:ALA:CB	1:A:383:ARG:H	1.81	0.94
1:A:125:LEU:HD11	1:A:159:ARG:HH12	1.34	0.93
1:A:214:ALA:HB1	1:A:215:PRO:CD	2.01	0.90
1:B:206:ARG:HG2	1:B:206:ARG:NH1	1.76	0.90
1:A:214:ALA:CB	1:A:215:PRO:HD2	2.06	0.85
1:B:511:VAL:CG1	1:B:691:ILE:HD11	2.07	0.84
1:A:214:ALA:HB1	1:A:383:ARG:H	1.40	0.84
1:A:741:CYS:O	1:A:742:LEU:HB2	1.75	0.84
1:B:214:ALA:HB2	1:B:382:THR:HA	1.61	0.82
1:B:469:LEU:HD12	1:B:471:TOL:H15	1.63	0.81
1:A:145:PRO:HD3	1:A:151:TYR:CE2	2.16	0.81
1:B:214:ALA:CB	1:B:382:THR:HA	2.13	0.78
1:B:511:VAL:HG11	1:B:691:ILE:HD11	1.65	0.78
1:B:59:LEU:HD11	1:B:120:PRO:HD2	1.66	0.78
1:A:436:GLN:HG3	1:A:457:GLU:HG2	1.66	0.78
1:B:403:ASP:HB3	1:B:465:MET:CE	2.14	0.77
1:B:145:PRO:HD3	1:B:151:TYR:CD2	2.20	0.76
1:B:465:MET:SD	1:B:474:VAL:HG22	2.26	0.75
6:A:1771:NAG:O3	6:A:1772:NAG:O5	2.03	0.75
1:B:383:ARG:CD	1:B:383:ARG:N	2.49	0.75
1:B:145:PRO:HD3	1:B:151:TYR:CE2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:HH11	1:B:78:ARG:CG	2.00	0.73
1:A:298:GLY:CA	1:A:692:PRO:HD3	2.19	0.73
1:B:206:ARG:CG	1:B:206:ARG:NH1	2.32	0.73
1:A:145:PRO:HD3	1:A:151:TYR:CD2	2.24	0.72
1:B:214:ALA:CB	1:B:383:ARG:H	2.02	0.72
1:A:539:VAL:HG22	1:A:569:LEU:HB2	1.70	0.72
1:B:214:ALA:HB1	1:B:383:ARG:H	1.54	0.72
1:A:144:GLY:HA2	1:A:151:TYR:CE1	2.25	0.71
1:B:403:ASP:HB3	1:B:465:MET:HE3	1.72	0.71
1:B:500:LEU:HD12	1:B:516:LEU:HB2	1.73	0.71
1:B:265:PHE:HD2	1:B:270:TYR:CE1	2.08	0.70
1:A:214:ALA:CB	1:A:215:PRO:CD	2.66	0.70
1:B:192:SER:O	1:B:196:HIS:HB2	1.92	0.70
1:B:344:PHE:HA	1:B:390:GLY:HA2	1.74	0.70
1:A:691:ILE:HG22	1:A:692:PRO:CD	2.22	0.69
1:B:214:ALA:HB2	1:B:382:THR:CA	2.22	0.69
1:A:738:PRO:HA	1:A:741:CYS:SG	2.33	0.69
1:A:214:ALA:CB	1:A:383:ARG:N	2.56	0.69
1:A:214:ALA:CB	1:A:382:THR:HA	2.25	0.67
1:A:298:GLY:HA3	1:A:692:PRO:HD3	1.77	0.67
1:B:233:ILE:HG22	1:B:234:SER:N	2.09	0.67
1:A:214:ALA:HB2	1:A:382:THR:HG23	1.77	0.66
1:B:511:VAL:HG13	1:B:691:ILE:HD11	1.76	0.66
1:B:214:ALA:HB2	1:B:382:THR:HG23	1.78	0.65
1:A:438:LEU:HD12	1:A:439:PRO:HD2	1.78	0.65
1:B:232:ASN:ND2	6:B:1771:NAG:O7	2.30	0.65
1:B:144:GLY:HA2	1:B:151:TYR:CZ	2.30	0.65
1:A:145:PRO:HD2	1:A:150:SER:H	1.60	0.65
1:B:122:ARG:O	1:B:146:LEU:HB2	1.95	0.65
1:B:438:LEU:HD12	1:B:439:PRO:HD2	1.78	0.65
1:B:212:THR:OG1	1:B:213:THR:N	2.30	0.64
1:B:559:LEU:O	1:B:559:LEU:HD23	1.98	0.64
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.62	0.64
1:A:450:HIS:H	6:B:1772:NAG:H81	1.64	0.63
1:A:102:GLN:OE1	1:A:125:LEU:HD12	1.97	0.63
1:B:608:LEU:HD21	1:B:704:PHE:CE2	2.32	0.63
1:A:675:VAL:O	1:A:675:VAL:HG13	1.98	0.63
1:A:440:LEU:HD22	1:A:481:PRO:HG2	1.79	0.63
1:B:147:PRO:HD2	1:B:148:HIS:H	1.63	0.63
1:B:145:PRO:HD2	1:B:150:SER:H	1.63	0.63
1:B:294:ASN:HA	1:B:300:TRP:CZ3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:VAL:HG22	1:B:569:LEU:HB2	1.81	0.62
1:B:144:GLY:HA2	1:B:151:TYR:CE1	2.34	0.62
1:A:615:LEU:HD12	1:A:616:PRO:HD2	1.81	0.61
1:B:511:VAL:HG13	1:B:691:ILE:CD1	2.30	0.61
1:B:214:ALA:CB	1:B:383:ARG:N	2.63	0.61
1:A:403:ASP:HB3	1:A:465:MET:HE3	1.83	0.60
1:B:374:GLY:HA2	1:B:507:TYR:HB3	1.82	0.60
1:A:741:CYS:O	1:A:742:LEU:CB	2.49	0.60
1:B:214:ALA:HB3	1:B:215:PRO:HD2	1.77	0.60
1:A:73:ARG:HH11	1:A:73:ARG:HG2	1.67	0.60
1:A:131:GLY:HA2	1:A:136:PRO:HB3	1.83	0.59
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.84	0.59
1:A:298:GLY:HA3	1:A:692:PRO:CD	2.32	0.59
1:B:476:ASP:HB2	1:B:488:ARG:HB2	1.85	0.58
1:A:298:GLY:C	1:A:692:PRO:HD3	2.22	0.58
1:A:760:PHE:CE2	1:B:727:GLY:HA2	2.38	0.58
1:B:317:TYR:HE2	1:B:433:GLU:HB2	1.68	0.57
1:A:214:ALA:HB2	1:A:382:THR:HA	1.85	0.57
1:A:263:LYS:HD3	1:A:271:TYR:O	2.05	0.57
1:A:271:TYR:CE1	1:A:277:LEU:HD13	2.38	0.57
1:B:214:ALA:HB2	1:B:383:ARG:N	2.19	0.56
1:B:436:GLN:HG3	1:B:457:GLU:HG2	1.88	0.56
1:B:286:VAL:HG23	1:B:288:VAL:HG23	1.87	0.56
1:A:125:LEU:HD11	1:A:159:ARG:NH1	2.13	0.56
1:A:80:GLY:O	1:A:81:PRO:O	2.24	0.56
1:A:468:LEU:O	1:A:470:ASN:N	2.39	0.55
1:A:82:GLY:HA3	1:A:132:ARG:NH1	2.21	0.55
1:B:539:VAL:CG2	1:B:569:LEU:HB2	2.36	0.55
1:B:739:LEU:O	1:B:742:LEU:HB2	2.06	0.55
1:A:112:HIS:CD2	1:A:112:HIS:C	2.81	0.55
1:A:99:VAL:HB	1:A:416:LEU:HD23	1.89	0.55
1:B:742:LEU:CB	1:B:743:PRO:HD3	2.37	0.55
1:A:232:ASN:CG	1:A:232:ASN:O	2.43	0.55
1:B:231:TYR:O	1:B:233:ILE:N	2.40	0.54
1:A:214:ALA:HB2	1:A:383:ARG:N	2.22	0.54
1:A:665:ASN:OD1	1:A:667:GLU:HG3	2.08	0.54
1:B:64:SER:OG	1:B:67:GLU:HG3	2.08	0.53
1:B:232:ASN:ND2	6:B:1771:NAG:C7	2.70	0.53
1:B:147:PRO:CD	1:B:148:HIS:H	2.20	0.53
1:B:80:GLY:O	1:B:81:PRO:O	2.26	0.53
1:B:360:VAL:HG12	1:B:530:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:HIS:HA	1:B:259:TRP:CD1	2.44	0.53
1:B:233:ILE:HG22	1:B:234:SER:H	1.72	0.53
1:A:82:GLY:HA3	1:A:132:ARG:HH12	1.73	0.53
1:A:144:GLY:HA2	1:A:151:TYR:CD1	2.42	0.53
1:A:750:PRO:HD2	1:B:749:ALA:HB2	1.91	0.53
1:B:680:ALA:HB1	1:B:701:VAL:HB	1.91	0.53
1:B:214:ALA:HB2	1:B:382:THR:CG2	2.39	0.53
1:B:592:ASN:ND2	7:B:1773:NAG:H83	2.24	0.53
1:A:760:PHE:HE2	1:B:727:GLY:HA2	1.74	0.52
1:B:377:PRO:O	1:B:381:THR:OG1	2.27	0.52
1:A:407:LEU:HD21	1:A:752:LEU:HD23	1.91	0.52
1:A:349:ILE:HG13	1:A:477:THR:HG21	1.92	0.52
1:B:382:THR:C	1:B:383:ARG:HD3	2.27	0.52
1:B:742:LEU:HB2	1:B:743:PRO:HD3	1.91	0.52
1:B:369:LEU:HD12	1:B:384:TYR:O	2.10	0.52
1:A:675:VAL:O	1:A:675:VAL:CG1	2.57	0.52
1:B:61:ALA:O	1:B:101:LEU:HD22	2.10	0.52
1:A:214:ALA:HB3	1:A:382:THR:HA	1.92	0.52
1:A:223:ARG:NH1	1:A:223:ARG:HG3	2.26	0.51
1:A:381:THR:HG22	1:B:559:LEU:HD12	1.92	0.51
1:A:447:LEU:HG	1:A:448:TYR:CD2	2.45	0.51
1:A:632:LEU:HG	1:A:633:ALA:N	2.25	0.51
1:A:133:GLN:HE22	5:A:1768:NAG:H61	1.75	0.51
1:B:542:GLU:HA	1:B:565:THR:O	2.11	0.51
1:A:403:ASP:HB3	1:A:465:MET:CE	2.40	0.51
1:B:281:PHE:HA	1:B:286:VAL:HG22	1.92	0.51
1:B:594:SER:HB3	1:B:598:GLY:HA2	1.92	0.51
1:A:593:HIS:NE2	7:A:1773:NAG:O3	2.43	0.51
1:A:468:LEU:HD12	1:A:473:TYR:CE2	2.46	0.51
1:B:380:MET:O	1:B:380:MET:HG2	2.10	0.51
1:B:213:THR:O	1:B:214:ALA:O	2.29	0.50
1:B:440:LEU:HD23	1:B:455:LEU:HD23	1.92	0.50
1:B:478:VAL:HB	1:B:486:GLU:HB3	1.93	0.50
1:B:430:CYS:SG	1:B:463:ARG:HB3	2.51	0.50
1:B:389:PHE:HE1	1:B:650:GLN:HE21	1.59	0.50
6:A:1771:NAG:HO3	6:A:1772:NAG:C1	2.24	0.50
1:A:374:GLY:HA2	1:A:507:TYR:HB3	1.94	0.50
1:B:209:VAL:HG13	1:B:232:ASN:HB2	1.93	0.49
1:A:720:ALA:O	1:B:308:PRO:HA	2.12	0.49
1:B:389:PHE:HE1	1:B:650:GLN:NE2	2.09	0.49
1:B:382:THR:C	1:B:383:ARG:CD	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:LEU:HD12	1:B:473:TYR:CE2	2.47	0.49
1:B:511:VAL:CG1	1:B:691:ILE:CD1	2.83	0.49
1:B:400:ARG:HD3	1:B:406:TYR:O	2.13	0.49
1:B:349:ILE:HG13	1:B:477:THR:HG21	1.93	0.49
1:B:265:PHE:CD2	1:B:270:TYR:CE1	2.96	0.49
1:A:125:LEU:HD21	1:A:140:GLU:HB3	1.95	0.49
1:A:473:TYR:CD1	1:A:489:PHE:HE1	2.31	0.49
1:A:298:GLY:O	1:A:692:PRO:HD3	2.13	0.49
1:B:642:PRO:HD2	9:B:2056:HOH:O	2.11	0.49
1:B:398:LEU:HD22	1:B:465:MET:HE3	1.94	0.49
1:A:588:TYR:HB3	1:A:604:ARG:HA	1.95	0.49
6:A:1771:NAG:O6	6:A:1771:NAG:O4	2.30	0.48
1:A:251:HIS:HA	1:A:259:TRP:CD1	2.48	0.48
1:A:64:SER:OG	1:A:67:GLU:HG3	2.13	0.48
1:A:214:ALA:HB2	1:A:382:THR:CA	2.44	0.48
1:B:78:ARG:NH1	1:B:78:ARG:CG	2.63	0.48
1:A:79:LEU:O	1:A:80:GLY:C	2.51	0.48
1:B:663:PHE:N	1:B:663:PHE:CD1	2.81	0.48
1:B:489:PHE:C	1:B:489:PHE:CD1	2.87	0.48
1:B:201:TYR:CD1	1:B:202:LYS:N	2.82	0.48
1:B:352:VAL:HB	1:B:360:VAL:HG22	1.94	0.48
1:B:577:PHE:CD2	1:B:632:LEU:HD23	2.49	0.48
1:A:474:VAL:HB	1:A:490:TYR:HB2	1.94	0.48
1:A:478:VAL:HB	1:A:486:GLU:HB3	1.94	0.48
1:A:129:PHE:CZ	1:A:169:ARG:HB2	2.49	0.48
1:A:137:ASN:ND2	5:A:1768:NAG:O5	2.30	0.48
1:B:278:GLU:HA	1:B:278:GLU:OE1	2.14	0.48
1:B:468:LEU:HD12	1:B:473:TYR:HE2	1.78	0.47
1:A:500:LEU:HD12	1:A:504:THR:HG21	1.96	0.47
1:A:407:LEU:HD21	1:A:752:LEU:CD2	2.44	0.47
1:A:125:LEU:CD1	1:A:159:ARG:HH12	2.14	0.47
1:A:440:LEU:HB2	1:A:457:GLU:HB2	1.96	0.47
1:A:389:PHE:HE1	1:A:650:GLN:HE21	1.62	0.47
1:A:511:VAL:HG13	1:A:691:ILE:HD11	1.97	0.47
1:B:233:ILE:CG2	1:B:234:SER:N	2.78	0.47
1:A:112:HIS:ND1	1:A:119:PRO:HA	2.30	0.46
1:B:500:LEU:HD22	1:B:510:GLN:HG3	1.97	0.46
1:A:592:ASN:OD1	1:A:592:ASN:N	2.34	0.46
1:A:224:ALA:HB1	1:A:248:LEU:HD11	1.97	0.46
1:B:217:GLY:HA3	1:B:222:ASP:CB	2.45	0.46
1:B:271:TYR:CE1	1:B:277:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:VAL:HG12	1:A:530:LEU:HD23	1.96	0.46
1:B:499:PHE:CE2	1:B:501:PHE:HB2	2.51	0.46
1:A:513:GLU:O	1:A:514:HIS:HB2	2.14	0.46
1:B:495:ILE:HG23	9:B:2060:HOH:O	2.15	0.46
1:B:742:LEU:CB	1:B:743:PRO:CD	2.93	0.46
1:A:593:HIS:CD2	7:A:1773:NAG:O3	2.69	0.46
1:A:214:ALA:HB1	1:A:383:ARG:N	2.21	0.45
1:A:136:PRO:HG2	1:A:254:LEU:HD21	1.98	0.45
1:B:359:LEU:HD22	1:B:603:TYR:CE1	2.51	0.45
1:A:382:THR:C	1:A:383:ARG:HD2	2.37	0.45
1:A:144:GLY:HA2	1:A:151:TYR:CZ	2.50	0.45
1:B:533:ALA:HA	9:B:2042:HOH:O	2.17	0.45
1:A:386:ASP:OD1	1:A:471:T0I:N11	2.50	0.45
1:B:403:ASP:CB	1:B:465:MET:CE	2.90	0.45
1:B:403:ASP:CB	1:B:465:MET:HE3	2.45	0.45
1:B:640:GLU:C	1:B:642:PRO:HD3	2.37	0.45
1:A:400:ARG:HD3	1:A:406:TYR:O	2.17	0.45
1:A:389:PHE:HE1	1:A:650:GLN:NE2	2.15	0.45
1:B:214:ALA:HB3	1:B:382:THR:HA	1.97	0.45
6:B:1772:NAG:O5	6:B:1771:NAG:O3	2.30	0.45
1:B:166:TYR:O	1:B:169:ARG:HD3	2.17	0.45
1:B:540:TRP:CZ2	1:B:568:LEU:HD13	2.51	0.45
1:A:73:ARG:NH1	1:A:73:ARG:HG2	2.31	0.45
1:B:587:LEU:CD2	1:B:632:LEU:HD21	2.47	0.45
1:A:380:MET:HG3	1:A:381:THR:HG23	1.99	0.44
1:B:440:LEU:HB2	1:B:457:GLU:HB2	1.98	0.44
1:B:80:GLY:HA2	1:B:81:PRO:HD2	1.82	0.44
1:B:251:HIS:H	1:B:251:HIS:CD2	2.36	0.44
1:B:274:LEU:H	1:B:274:LEU:HD12	1.82	0.44
1:A:497:SER:HB2	1:A:515:THR:HG23	1.99	0.44
1:B:74:PHE:HE1	1:B:152:MET:HB2	1.81	0.44
1:B:360:VAL:HG21	1:B:363:ILE:HG13	1.99	0.44
1:B:202:LYS:HE3	1:B:202:LYS:HB3	1.20	0.44
1:B:188:LEU:HA	1:B:188:LEU:HD12	1.79	0.44
1:B:708:TYR:O	1:B:709:ASN:HB2	2.16	0.44
1:A:112:HIS:HA	1:A:117:SER:O	2.18	0.44
1:A:468:LEU:CD1	1:A:473:TYR:CE2	3.00	0.44
1:B:577:PHE:HD2	1:B:632:LEU:HD23	1.83	0.44
1:A:734:CYS:O	1:A:734:CYS:SG	2.75	0.44
1:A:187:GLU:O	1:A:274:LEU:HD13	2.18	0.44
1:A:133:GLN:HE22	5:A:1768:NAG:C6	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HD13	1:A:245:LEU:HD23	2.00	0.43
1:B:588:TYR:HB3	1:B:604:ARG:HB3	1.98	0.43
1:A:683:LEU:HG	1:A:684:HIS:N	2.33	0.43
1:B:440:LEU:HD22	1:B:481:PRO:HG2	1.99	0.43
1:B:200:PHE:CD1	1:B:200:PHE:N	2.86	0.43
1:A:74:PHE:CE1	1:A:78:ARG:HG3	2.52	0.43
1:A:71:VAL:HG13	1:A:143:VAL:HG11	2.00	0.43
1:A:540:TRP:CE2	1:A:568:LEU:HD13	2.53	0.43
1:B:405:PRO:HG2	1:B:432:PHE:CD2	2.53	0.43
1:A:188:LEU:N	1:A:189:PRO:CD	2.81	0.43
1:B:79:LEU:O	1:B:80:GLY:C	2.56	0.43
1:A:628:GLU:O	1:A:628:GLU:HG2	2.19	0.43
1:A:714:ASP:HA	1:A:715:PRO:HD2	1.88	0.43
1:A:94:ASN:HA	1:A:129:PHE:O	2.17	0.43
1:A:404:CYS:HB2	1:A:410:TYR:OH	2.19	0.43
1:B:470:ASN:OD1	1:B:471:T0I:H14	2.18	0.43
1:B:181:GLN:O	1:B:185:ASN:HB2	2.19	0.43
1:A:175:GLU:O	1:A:179:ILE:HG13	2.18	0.43
1:B:189:PRO:C	1:B:191:ALA:H	2.21	0.43
1:B:265:PHE:CD2	1:B:377:PRO:HD3	2.54	0.43
1:A:167:HIS:CD2	1:A:221:GLY:HA2	2.54	0.43
1:A:371:ILE:HD13	1:A:615:LEU:HB2	2.01	0.42
1:A:403:ASP:CB	1:A:465:MET:HE3	2.49	0.42
1:B:646:SER:HB2	1:B:658:VAL:CG1	2.49	0.42
1:B:337:PHE:CE2	1:B:462:VAL:HG21	2.54	0.42
1:B:195:LEU:HB3	1:B:201:TYR:CG	2.55	0.42
1:B:316:PHE:CD2	1:B:750:PRO:HD3	2.54	0.42
1:A:689:GLU:O	1:B:714:ASP:HB2	2.19	0.42
1:B:347:PRO:HG2	1:B:475:TRP:CG	2.55	0.42
1:A:542:GLU:HA	1:A:565:THR:O	2.19	0.42
1:A:181:GLN:O	1:A:185:ASN:HB2	2.20	0.42
1:B:138:VAL:HG11	1:B:648:PHE:CZ	2.55	0.42
1:B:251:HIS:N	1:B:251:HIS:CD2	2.87	0.42
1:B:71:VAL:HG13	1:B:143:VAL:HG11	2.01	0.42
1:A:186:ARG:HH11	1:A:186:ARG:HG3	1.85	0.42
1:A:256:PRO:HA	1:A:259:TRP:CE2	2.54	0.42
1:A:468:LEU:O	1:A:469:LEU:HB2	2.19	0.42
1:B:271:TYR:CZ	1:B:277:LEU:HD13	2.55	0.42
1:A:752:LEU:HA	1:A:753:PRO:HD2	1.86	0.41
1:A:182:MET:HA	1:A:186:ARG:NH2	2.35	0.41
1:A:535:LEU:O	1:A:673:ASP:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:PHE:N	1:A:663:PHE:CD1	2.85	0.41
1:B:171:VAL:HG13	1:B:175:GLU:HB3	2.01	0.41
1:B:632:LEU:HG	1:B:633:ALA:N	2.33	0.41
1:B:178:ASP:O	1:B:181:GLN:HB2	2.20	0.41
1:A:537:ASN:ND2	9:A:2042:HOH:O	2.53	0.41
1:A:585:ARG:NH1	1:B:611:ALA:O	2.53	0.41
1:A:360:VAL:HG12	1:A:530:LEU:CD2	2.50	0.41
1:B:268:GLY:HA3	1:B:501:PHE:CE1	2.54	0.41
1:B:733:ALA:HB3	1:B:736:VAL:CG1	2.50	0.41
1:A:352:VAL:HB	1:A:360:VAL:HG22	2.02	0.41
1:A:708:TYR:O	1:A:709:ASN:HB2	2.20	0.41
1:B:217:GLY:HA3	1:B:222:ASP:HB3	2.03	0.41
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.88	0.41
1:B:578:LEU:HD23	1:B:578:LEU:HA	1.79	0.41
1:B:488:ARG:HD3	1:B:488:ARG:HA	1.74	0.41
1:B:256:PRO:HA	1:B:259:TRP:CD2	2.56	0.41
1:B:447:LEU:HG	1:B:448:TYR:CD2	2.56	0.41
1:A:191:ALA:HA	1:A:278:GLU:HB2	2.04	0.41
1:B:231:TYR:O	1:B:233:ILE:HG12	2.22	0.40
1:A:403:ASP:OD1	1:B:442:ARG:HD3	2.21	0.40
1:B:592:ASN:HD22	7:B:1773:NAG:H83	1.86	0.40
1:B:587:LEU:HD22	1:B:632:LEU:CD2	2.52	0.40
1:A:214:ALA:HB2	1:A:382:THR:CG2	2.48	0.40
1:A:468:LEU:HD12	1:A:473:TYR:CD2	2.56	0.40
1:A:187:GLU:HB3	1:A:274:LEU:HD12	2.04	0.40
1:A:612:GLY:HA2	1:B:585:ARG:NH1	2.37	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	688/763 (90%)	645 (94%)	38 (6%)	5 (1%)	26	67
1	B	692/763 (91%)	650 (94%)	36 (5%)	6 (1%)	21	61
All	All	1380/1526 (90%)	1295 (94%)	74 (5%)	11 (1%)	24	64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	214	ALA
1	A	692	PRO
1	B	81	PRO
1	B	147	PRO
1	B	214	ALA
1	A	80	GLY
1	B	144	GLY
1	A	469	LEU
1	B	80	GLY
1	B	232	ASN

### 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	577/634 (91%)	543 (94%)	34 (6%)	24	61
1	B	583/634 (92%)	536 (92%)	47 (8%)	15	44
All	All	1160/1268 (92%)	1079 (93%)	81 (7%)	19	53

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	98	SER
1	A	150	SER
1	A	177	LEU
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	198	CYS
1	A	216	ARG
1	A	229	LEU
1	A	260	THR
1	A	285	LEU
1	A	395	THR
1	A	400	ARG
1	A	442	ARG
1	A	465	MET
1	A	470	ASN
1	A	489	PHE
1	A	511	VAL
1	A	518	THR
1	A	523	SER
1	A	559	LEU
1	A	566	ARG
1	A	583	THR
1	A	587	LEU
1	A	603	TYR
1	A	608	LEU
1	A	626	SER
1	A	632	LEU
1	A	640	GLU
1	A	645	SER
1	A	646	SER
1	A	658	VAL
1	A	713	GLU
1	A	722	SER
1	A	742	LEU
1	B	56	GLN
1	B	57	SER
1	B	73	ARG
1	B	78	ARG
1	B	88	GLN
1	B	125	LEU
1	B	146	LEU
1	B	153	ARG
1	B	188	LEU
1	B	192	SER
1	B	195	LEU
1	B	199	CYS
1	B	202	LYS

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Mol	Chain	Res	Type
1	B	206	ARG
1	B	212	THR
1	B	216	ARG
1	B	219	GLN
1	B	282	GLU
1	B	289	VAL
1	B	294	ASN
1	B	329	ARG
1	B	381	THR
1	B	383	ARG
1	B	395	THR
1	B	400	ARG
1	B	442	ARG
1	B	459	VAL
1	B	465	MET
1	B	489	PHE
1	B	511	VAL
1	B	523	SER
1	B	539	VAL
1	B	556	GLU
1	B	559	LEU
1	B	587	LEU
1	B	608	LEU
1	B	625	PHE
1	B	632	LEU
1	B	637	ARG
1	B	658	VAL
1	B	694	THR
1	B	713	GLU
1	B	722	SER
1	B	734	CYS
1	B	736	VAL
1	B	742	LEU
1	B	748	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	267	GLN
1	A	470	ASN
1	A	537	ASN

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Mol	Chain	Res	Type
1	A	650	GLN
1	A	699	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	T0I	A	471	1	17,19,20	1.31	1 (5%)	20,26,28	1.08	2 (10%)
1	T0I	B	471	1	17,19,20	1.31	1 (5%)	20,26,28	1.19	2 (10%)

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
1	T0I	A	471	1	-	0/8/10/12	0/2/2/2
1	T0I	B	471	1	-	0/8/10/12	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	T0I	C14-N13	-3.33	1.34	1.39
1	B	471	T0I	C14-N13	-3.29	1.34	1.39

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	T0I	C4-C5-N13	2.09	120.92	118.43
1	A	471	T0I	C6-C1-C2	2.12	120.29	118.33
1	B	471	T0I	C6-C5-N13	2.26	119.96	117.44
1	B	471	T0I	C6-C1-C2	2.42	120.57	118.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	471	T0I	1	0
1	B	471	T0I	2	0

## 5.5 Carbohydrates ⓘ

9 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$
5	NAG	A	1768	1,5	14,14,15	2.55	6 (42%)	15,19,21	1.39	3 (20%)
5	NAG	A	1769	5	14,14,15	2.07	4 (28%)	15,19,21	1.27	1 (6%)
5	MAN	A	1770	5	11,11,12	2.03	4 (36%)	14,15,17	1.16	1 (7%)
6	NAG	A	1771	1,6	14,14,15	2.21	6 (42%)	15,19,21	1.71	3 (20%)
6	NAG	A	1772	6	14,14,15	2.21	6 (42%)	15,19,21	1.71	3 (20%)
6	NAG	B	1768	1,6	14,14,15	2.57	6 (42%)	15,19,21	2.07	6 (40%)
6	NAG	B	1769	8,6	14,14,15	2.59	8 (57%)	15,19,21	2.16	6 (40%)
6	NAG	B	1771	1,6	14,14,15	2.43	6 (42%)	15,19,21	1.83	4 (26%)
6	NAG	B	1772	6	14,14,15	2.14	8 (57%)	15,19,21	1.49	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1768	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1769	5	-	0/6/23/26	0/1/1/1
5	MAN	A	1770	5	-	0/2/19/22	1/1/1/1
6	NAG	A	1771	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1772	6	-	0/6/23/26	0/1/1/1
6	NAG	B	1768	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1769	8,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1771	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1772	6	-	0/6/23/26	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1771	NAG	C3-C2	-5.18	1.40	1.52
5	A	1768	NAG	C3-C2	-5.14	1.40	1.52
6	B	1768	NAG	C3-C2	-5.02	1.40	1.52
5	A	1768	NAG	C1-C2	-4.95	1.45	1.52
6	B	1771	NAG	C1-C2	-4.39	1.46	1.52
6	A	1771	NAG	C4-C5	-4.32	1.43	1.53
6	A	1772	NAG	C4-C5	-4.31	1.43	1.53
6	B	1768	NAG	C4-C3	-4.19	1.41	1.52
5	A	1770	MAN	C4-C3	-4.05	1.41	1.52
6	B	1769	NAG	C1-C2	-4.03	1.46	1.52
6	B	1769	NAG	C4-C5	-3.96	1.44	1.53
6	B	1772	NAG	C4-C5	-3.81	1.45	1.53
6	B	1768	NAG	C1-C2	-3.78	1.47	1.52
6	B	1768	NAG	C4-C5	-3.59	1.45	1.53
6	B	1771	NAG	C4-C3	-3.55	1.43	1.52
6	B	1769	NAG	C4-C3	-3.22	1.43	1.52
6	A	1771	NAG	C4-C3	-3.22	1.43	1.52
6	A	1772	NAG	C4-C3	-3.21	1.44	1.52
6	B	1769	NAG	O5-C1	-3.03	1.38	1.43
6	B	1769	NAG	C3-C2	-2.82	1.45	1.52
6	B	1772	NAG	C4-C3	-2.80	1.45	1.52
6	B	1769	NAG	C6-C5	-2.79	1.42	1.51
5	A	1769	NAG	C4-C5	-2.73	1.47	1.53
5	A	1770	MAN	C2-C3	-2.49	1.49	1.52
5	A	1769	NAG	C1-C2	-2.46	1.49	1.52
6	A	1772	NAG	C6-C5	-2.32	1.43	1.51
6	A	1771	NAG	C6-C5	-2.32	1.43	1.51
5	A	1768	NAG	O5-C1	-2.32	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1772	NAG	C1-C2	-2.30	1.49	1.52
5	A	1770	MAN	C4-C5	-2.26	1.48	1.53
6	B	1771	NAG	O5-C5	-2.16	1.38	1.43
6	B	1771	NAG	C4-C5	-2.14	1.48	1.53
6	B	1772	NAG	C6-C5	-2.12	1.44	1.51
6	A	1772	NAG	C3-C2	-2.11	1.47	1.52
6	A	1771	NAG	C3-C2	-2.09	1.47	1.52
6	B	1772	NAG	O5-C1	-2.03	1.40	1.43
6	B	1768	NAG	O5-C5	-2.02	1.39	1.43
6	B	1772	NAG	C3-C2	-2.01	1.47	1.52
6	A	1771	NAG	C7-N2	2.14	1.42	1.34
5	A	1768	NAG	O4-C4	2.14	1.48	1.43
6	A	1772	NAG	C7-N2	2.15	1.42	1.34
6	B	1769	NAG	C7-N2	2.25	1.43	1.34
6	B	1768	NAG	C7-N2	2.35	1.43	1.34
5	A	1768	NAG	C7-N2	2.51	1.44	1.34
6	B	1772	NAG	C7-N2	2.69	1.44	1.34
6	B	1771	NAG	C7-N2	2.74	1.44	1.34
5	A	1769	NAG	C7-N2	2.79	1.45	1.34
5	A	1770	MAN	O5-C5	3.09	1.50	1.43
6	B	1769	NAG	O5-C5	3.49	1.51	1.43
6	B	1772	NAG	O5-C5	3.53	1.51	1.43
6	A	1771	NAG	O5-C5	3.73	1.51	1.43
6	A	1772	NAG	O5-C5	3.75	1.51	1.43
5	A	1768	NAG	C2-N2	4.03	1.53	1.46
5	A	1769	NAG	O5-C5	4.61	1.53	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1769	NAG	C2-N2-C7	-4.70	117.00	123.04
6	A	1772	NAG	C3-C2-N2	-4.45	99.91	110.56
6	A	1771	NAG	C3-C2-N2	-4.44	99.92	110.56
6	B	1768	NAG	C3-C2-N2	-4.00	100.98	110.56
6	B	1771	NAG	O4-C4-C3	-3.60	102.23	110.34
5	A	1769	NAG	C2-N2-C7	-3.13	119.02	123.04
6	B	1772	NAG	C1-O5-C5	-3.09	108.33	112.25
6	B	1768	NAG	O4-C4-C3	-2.98	103.63	110.34
6	B	1771	NAG	C3-C2-N2	-2.96	103.47	110.56
6	B	1769	NAG	O5-C5-C6	-2.84	101.21	107.35
6	B	1769	NAG	O3-C3-C4	-2.78	104.08	110.34
6	B	1769	NAG	C6-C5-C4	-2.74	106.26	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1768	NAG	C2-N2-C7	-2.72	119.54	123.04
6	A	1772	NAG	C3-C4-C5	-2.53	105.78	110.20
6	A	1771	NAG	C3-C4-C5	-2.53	105.79	110.20
6	B	1768	NAG	C6-C5-C4	-2.52	106.79	113.02
6	B	1768	NAG	C3-C4-C5	-2.38	106.04	110.20
6	B	1768	NAG	O7-C7-N2	-2.36	117.04	121.86
6	B	1768	NAG	C2-N2-C7	-2.30	120.08	123.04
6	B	1771	NAG	C6-C5-C4	-2.22	107.55	113.02
6	B	1769	NAG	O4-C4-C3	-2.17	105.46	110.34
6	A	1771	NAG	C6-C5-C4	-2.09	107.86	113.02
6	A	1772	NAG	C6-C5-C4	-2.09	107.86	113.02
6	B	1771	NAG	C2-N2-C7	-2.04	120.42	123.04
6	B	1772	NAG	C2-N2-C7	-2.01	120.46	123.04
5	A	1768	NAG	O6-C6-C5	2.03	118.03	111.33
5	A	1770	MAN	O5-C5-C6	2.15	112.00	107.35
6	B	1769	NAG	C8-C7-N2	2.59	121.06	116.11
5	A	1768	NAG	C3-C4-C5	2.90	115.25	110.20

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1770	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1768	NAG	4	0
6	A	1771	NAG	3	0
6	A	1772	NAG	2	0
6	B	1771	NAG	3	0
6	B	1772	NAG	2	0

## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	IMD	A	1765	-	3,5,5	0.53	0	4,5,5	0.55	0
4	IMD	A	1766	-	3,5,5	1.07	0	4,5,5	1.08	0
4	IMD	A	1767	-	3,5,5	1.01	0	4,5,5	1.02	0
7	NAG	A	1773	1	14,14,15	0.97	1 (7%)	15,19,21	1.29	1 (6%)
7	NAG	A	1774	1	14,14,15	0.49	0	15,19,21	0.86	1 (6%)
4	IMD	B	1765	-	3,5,5	0.78	0	4,5,5	0.72	0
4	IMD	B	1766	-	3,5,5	1.53	0	4,5,5	0.83	0
4	IMD	B	1767	-	3,5,5	1.00	0	4,5,5	1.10	0
8	MAN	B	1770	6	11,11,12	2.03	4 (36%)	14,15,17	1.15	1 (7%)
7	NAG	B	1773	1	14,14,15	2.04	4 (28%)	15,19,21	2.06	7 (46%)
7	NAG	B	1774	1	14,14,15	0.66	0	15,19,21	0.92	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
4	IMD	A	1765	-	-	0/0/0/0	0/1/1/1
4	IMD	A	1766	-	-	0/0/0/0	0/1/1/1
4	IMD	A	1767	-	-	0/0/0/0	0/1/1/1
7	NAG	A	1773	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1774	1	-	0/6/23/26	0/1/1/1
4	IMD	B	1765	-	-	0/0/0/0	0/1/1/1
4	IMD	B	1766	-	-	0/0/0/0	0/1/1/1
4	IMD	B	1767	-	-	0/0/0/0	0/1/1/1
8	MAN	B	1770	6	-	0/2/19/22	1/1/1/1
7	NAG	B	1773	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1774	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1773	NAG	C4-C3	-4.39	1.40	1.52
8	B	1770	MAN	C4-C3	-4.06	1.41	1.52
7	B	1773	NAG	C3-C2	-3.45	1.44	1.52
7	A	1773	NAG	O5-C1	-2.61	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1770	MAN	C2-C3	-2.46	1.49	1.52
7	B	1773	NAG	O5-C1	-2.42	1.39	1.43
8	B	1770	MAN	C4-C5	-2.24	1.48	1.53
7	B	1773	NAG	C7-N2	3.07	1.46	1.34
8	B	1770	MAN	O5-C5	3.07	1.50	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1773	NAG	C1-O5-C5	-3.56	107.72	112.25
7	B	1773	NAG	C2-N2-C7	-2.97	119.23	123.04
7	B	1773	NAG	O3-C3-C4	-2.56	104.58	110.34
7	B	1773	NAG	C4-C3-C2	-2.47	107.39	111.23
7	B	1773	NAG	C6-C5-C4	-2.41	107.06	113.02
7	A	1774	NAG	C2-N2-C7	-2.07	120.38	123.04
8	B	1770	MAN	O5-C5-C6	2.15	112.01	107.35
7	B	1773	NAG	O4-C4-C5	2.64	116.23	109.24
7	B	1773	NAG	O5-C5-C6	3.08	114.02	107.35
7	B	1773	NAG	O6-C6-C5	3.27	122.12	111.33

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1770	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1773	NAG	2	0
7	B	1773	NAG	2	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	694/763 (90%)	-0.49	4 (0%) 90 78	17, 31, 55, 87	0
1	B	698/763 (91%)	-0.55	7 (1%) 84 67	12, 30, 54, 90	0
All	All	1392/1526 (91%)	-0.52	11 (0%) 87 73	12, 31, 54, 90	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	PRO	3.0
1	B	135	GLN	2.8
1	B	80	GLY	2.7
1	A	80	GLY	2.6
1	B	82	GLY	2.4
1	B	282	GLU	2.3
1	B	202	LYS	2.1
1	A	77	GLN	2.0
1	A	82	GLY	2.0
1	B	735	GLU	2.0
1	A	751	ASP	2.0

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

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
1	T0I	A	471	18/19	0.96	0.17	-	24,43,54,54	0
1	T0I	B	471	18/19	0.94	0.20	-	23,47,61,63	0

## 6.3 Carbohydrates ⓘ

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
6	NAG	A	1771	14/15	0.74	0.29	6.13	70,99,111,112	0
6	NAG	B	1768	14/15	0.97	0.18	0.22	24,43,54,59	0
6	NAG	B	1771	14/15	0.92	0.17	0.17	44,68,83,94	0
5	NAG	A	1768	14/15	0.97	0.15	-0.96	28,36,46,50	0
5	MAN	A	1770	11/12	0.71	0.34	-	59,84,96,98	0
6	NAG	B	1769	14/15	0.95	0.21	-	37,55,72,86	0
5	NAG	A	1769	14/15	0.89	0.27	-	46,55,78,83	0
6	NAG	B	1772	14/15	0.86	0.31	-	63,94,105,111	0
6	NAG	A	1772	14/15	0.77	0.48	-	70,99,111,112	0

## 6.4 Ligands ⓘ

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
4	IMD	B	1766	5/5	0.93	0.30	15.03	41,46,48,49	0
4	IMD	B	1767	5/5	0.97	0.24	5.02	41,46,48,49	0
4	IMD	A	1766	5/5	0.98	0.24	4.40	41,46,48,49	0
4	IMD	A	1767	5/5	0.97	0.23	1.94	41,46,48,49	0
4	IMD	A	1765	5/5	0.97	0.14	-0.54	41,46,48,49	0
4	IMD	B	1765	5/5	0.97	0.14	-0.73	44,48,54,59	0
3	CA	B	1764	1/1	0.81	0.10	-1.80	33,33,33,33	0
3	CA	A	1764	1/1	0.92	0.07	-2.08	22,22,22,22	0
3	CA	A	1763	1/1	0.97	0.07	-2.26	30,30,30,30	0
3	CA	B	1763	1/1	0.99	0.09	-2.42	23,23,23,23	0
8	MAN	B	1770	11/12	0.65	0.48	-	59,84,96,98	0
7	NAG	B	1773	14/15	0.75	0.37	-	44,75,101,104	0
7	NAG	A	1773	14/15	0.79	0.41	-	44,75,101,104	0
7	NAG	B	1774	14/15	0.87	0.51	-	0,4,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	A	1774	14/15	0.76	0.50	-	0,4,9,9	0
2	CU	B	1762	1/1	0.98	0.14	-	31,31,31,31	0
2	CU	A	1762	1/1	0.98	0.05	-	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.