



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2017 – 10:56 AM EDT

PDB ID : 2Y73  
Title : THE NATIVE STRUCTURES OF SOLUBLE HUMAN PRIMARY AMINE  
OXIDASE AOC3  
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Deposited on : unknown  
Resolution : 2.60 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

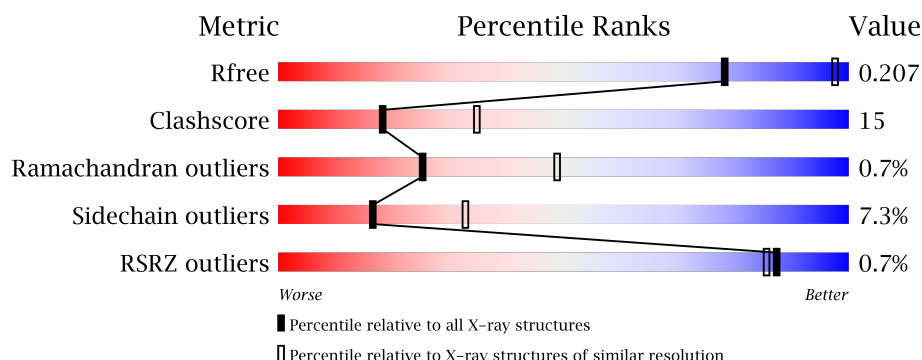
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 23%, green 66%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>1%</span> <span>66%</span> <span>23%</span> <span>8%</span> </div> </div>
1	B	763	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 22%, green 66%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>1%</span> <span>66%</span> <span>22%</span> <span>8%</span> </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	804	-	-	X	-
4	IMD	A	814	-	-	-	X
4	IMD	B	805	-	-	-	X
5	NAG	A	810	-	-	-	X
5	NAG	A	811	-	-	-	X
5	NAG	B	810	-	-	-	X
5	NAG	B	811	-	-	-	X
7	FMT	A	815	-	-	X	-
7	FMT	A	816	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11675 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	705	Total	C	N	O	S	0	0	0
			5560	3570	957	1013	20			
1	B	701	Total	C	N	O	S	0	0	0
			5527	3551	950	1007	19			

- 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	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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



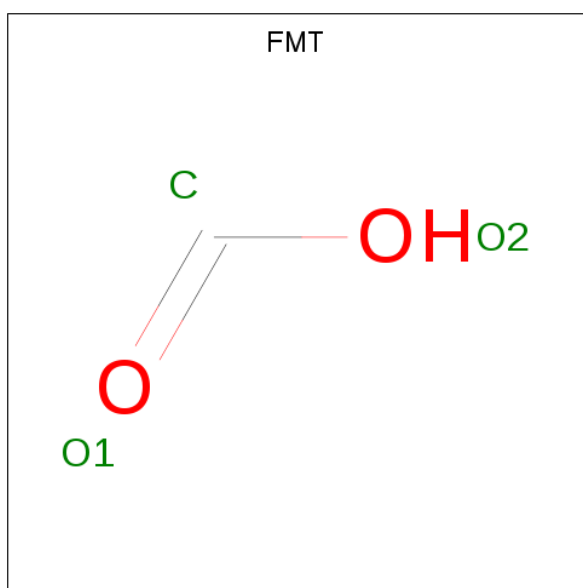
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1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

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is water.

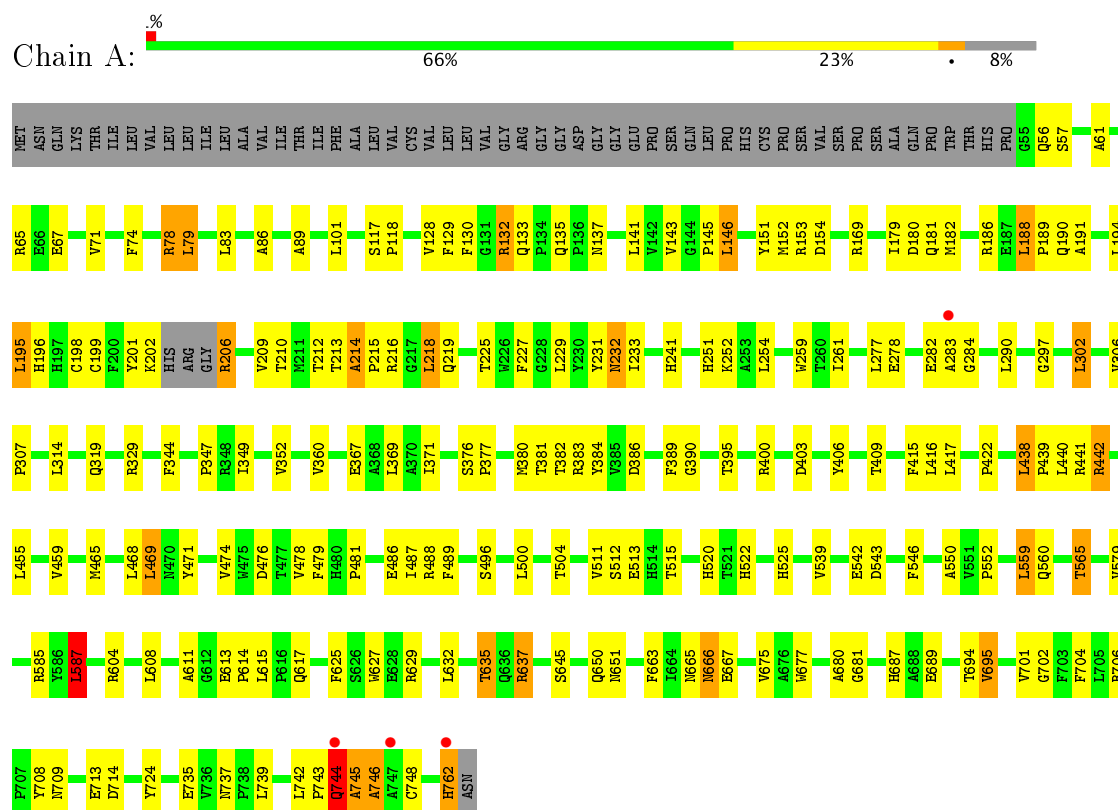
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	191	Total 191	O 191	0	0
8	B	155	Total 155	O 155	0	0



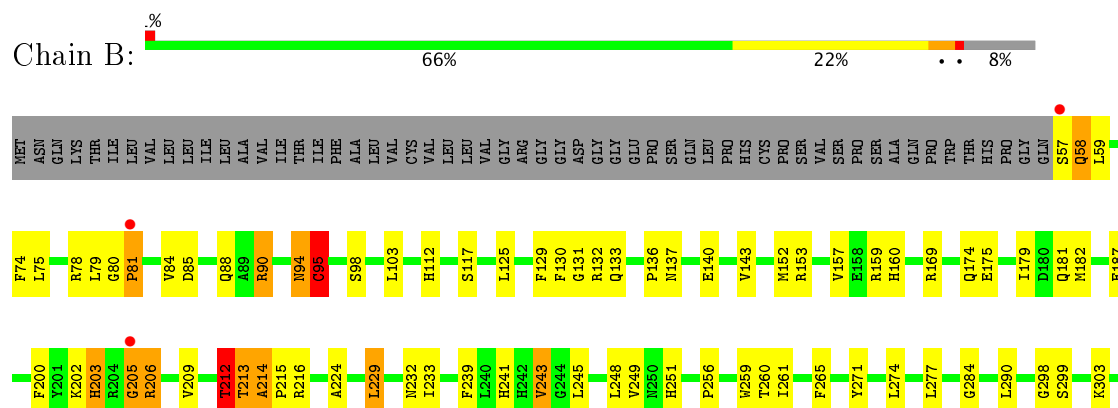
### 3 Residue-property plots

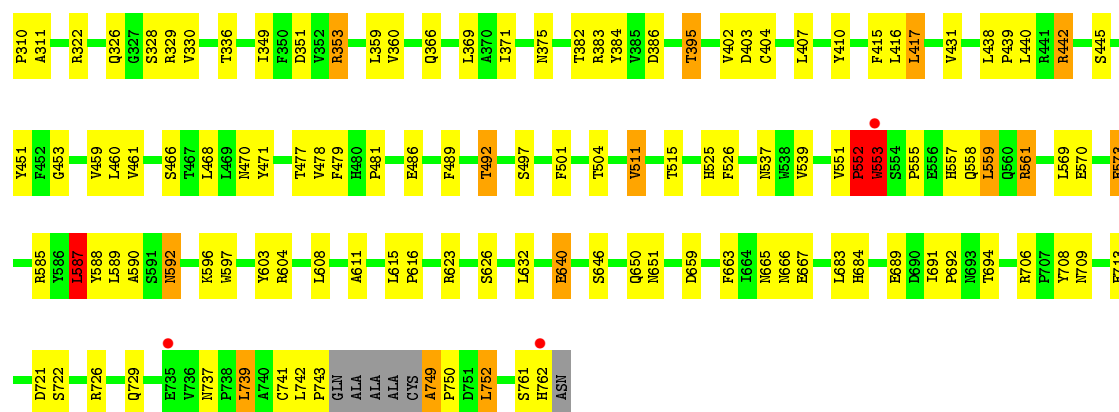
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 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, $\alpha$ , $\beta$ , $\gamma$	225.75Å 225.75Å 216.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-2.60) 100.0 (19.93-2.60)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.56 (at 2.59Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.175 , 0.213 0.165 , 0.207	Depositor DCC
$R_{free}$ test set	4977 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, IMD, CA, TPQ, FMT, CU, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	4/5721 (0.1%)	0.87	9/7800 (0.1%)
1	B	0.80	7/5688 (0.1%)	0.82	5/7757 (0.1%)
All	All	0.78	11/11409 (0.1%)	0.85	14/15557 (0.1%)

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
1	B	0	7
All	All	0	8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	552	PRO	C-N	-19.80	0.88	1.34
1	B	553	TRP	C-N	-11.17	1.08	1.34
1	B	741	CYS	CA-CB	-10.79	1.30	1.53
1	B	95	CYS	CB-SG	-7.89	1.68	1.82
1	A	137	ASN	CG-ND2	7.80	1.52	1.32
1	B	137	ASN	CG-ND2	7.35	1.51	1.32
1	B	232	ASN	CG-ND2	7.09	1.50	1.32
1	A	232	ASN	CG-ND2	6.91	1.50	1.32
1	A	666	ASN	CG-ND2	6.24	1.48	1.32
1	B	592	ASN	CG-ND2	5.96	1.47	1.32
1	A	748	CYS	CB-SG	5.48	1.91	1.82

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	SER	N-CA-CB	-14.32	89.03	110.50
1	A	329	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	B	229	LEU	CA-CB-CG	-9.35	93.80	115.30
1	A	56	GLN	N-CA-C	7.77	131.98	111.00
1	A	587	LEU	CA-CB-CG	-7.31	98.49	115.30
1	B	468	LEU	CA-CB-CG	-6.50	100.35	115.30
1	A	329	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	706	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	552	PRO	O-C-N	-6.21	112.77	122.70
1	B	212	THR	CB-CA-C	-5.94	95.56	111.60
1	A	56	GLN	CB-CA-C	-5.73	98.94	110.40
1	A	438	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	587	LEU	CA-CB-CG	-5.51	102.62	115.30
1	A	637	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	THR	Peptide
1	B	203	HIS	Peptide
1	B	205	GLY	Peptide
1	B	213	THR	Peptide
1	B	552	PRO	Mainchain
1	B	553	TRP	Mainchain
1	B	749	ALA	Peptide
1	B	94	ASN	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	A	5560	0	5307	179	0
1	B	5527	0	5264	174	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	20	6	0
4	B	20	0	20	5	0
5	A	84	0	74	6	0
5	B	84	0	75	4	0
6	A	11	0	10	0	0
6	B	11	0	10	0	0
7	A	6	0	2	4	0
8	A	191	0	0	5	0
8	B	155	0	0	2	0
All	All	11675	0	10782	331	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 15.

All (331) 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:206:ARG:N	1:A:206:ARG:HD2	1.52	1.13
1:B:58:GLN:HG3	1:B:59:LEU:H	1.15	1.11
1:A:201:TYR:O	1:A:202:LYS:HG2	1.50	1.09
1:B:214:ALA:CB	1:B:215:PRO:HD2	1.90	1.01
1:B:212:THR:HG21	1:B:216:ARG:NH2	1.76	1.01
1:A:314:LEU:HD12	7:A:816:FMT:H	1.44	1.00
1:B:214:ALA:HB1	1:B:383:ARG:H	1.26	0.99
1:A:214:ALA:HB1	1:A:215:PRO:HD3	1.45	0.95
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.29	0.93
1:B:57:SER:O	1:B:58:GLN:HB3	1.67	0.93
1:A:206:ARG:N	1:A:206:ARG:CD	2.30	0.93
1:B:214:ALA:CB	1:B:215:PRO:CD	2.48	0.90
1:B:214:ALA:HB1	1:B:215:PRO:CD	2.02	0.90
1:B:214:ALA:HB2	1:B:382:THR:HA	1.50	0.90
1:B:214:ALA:HB3	1:B:215:PRO:HD2	1.55	0.87
1:B:214:ALA:CB	1:B:383:ARG:H	1.86	0.87
1:B:561:ARG:HH11	1:B:561:ARG:HG3	1.37	0.87
1:B:726:ARG:HB2	1:B:729:GLN:HE21	1.40	0.87
1:B:615:LEU:HD12	1:B:616:PRO:HD2	1.56	0.87
1:A:441:ARG:HA	1:B:492:THR:HG21	1.56	0.86
1:A:209:VAL:HG13	1:A:232:ASN:HB2	1.55	0.86
1:B:95:CYS:HB3	1:B:129:PHE:HB2	1.58	0.86
1:A:214:ALA:CB	1:A:215:PRO:CD	2.54	0.85
1:A:743:PRO:O	1:A:744:GLN:HB3	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HB1	1:B:215:PRO:HD2	1.59	0.84
1:B:58:GLN:HG3	1:B:59:LEU:N	1.94	0.83
1:A:201:TYR:O	1:A:202:LYS:CG	2.27	0.83
1:A:762:HIS:CD2	1:A:762:HIS:N	2.46	0.83
1:A:666:ASN:HD22	5:A:813:NAG:H83	1.43	0.83
1:B:57:SER:HB3	1:B:328:SER:H	1.44	0.82
1:B:212:THR:HG21	1:B:216:ARG:HH22	1.43	0.82
1:A:680:ALA:HB1	1:A:701:VAL:HG13	1.63	0.81
1:B:57:SER:HA	1:B:329:ARG:HG3	1.62	0.80
1:B:214:ALA:CB	1:B:382:THR:HA	2.11	0.80
1:B:212:THR:CG2	1:B:216:ARG:NH2	2.44	0.80
1:B:561:ARG:HH11	1:B:561:ARG:CG	1.95	0.79
1:B:57:SER:O	1:B:58:GLN:CB	2.30	0.79
1:A:214:ALA:CB	1:A:383:ARG:H	1.95	0.79
1:B:94:ASN:ND2	1:B:130:PHE:HA	1.98	0.79
1:A:214:ALA:CB	1:A:215:PRO:HD3	2.14	0.78
1:B:587:LEU:HD22	1:B:632:LEU:CD2	2.14	0.78
1:B:561:ARG:HG3	1:B:561:ARG:NH1	1.99	0.76
1:B:587:LEU:HD22	1:B:632:LEU:HD21	1.67	0.76
1:A:214:ALA:HB1	1:A:215:PRO:CD	2.13	0.75
1:A:214:ALA:CB	1:A:382:THR:HA	2.18	0.74
1:A:214:ALA:HB1	1:A:383:ARG:H	1.53	0.73
1:A:500:LEU:HD12	1:A:504:THR:HG21	1.68	0.73
1:A:319:GLN:NE2	1:B:311:ALA:H	1.88	0.72
1:B:552:PRO:HB2	1:B:553:TRP:HE3	1.55	0.72
1:A:319:GLN:HE21	1:B:311:ALA:H	1.37	0.71
1:A:762:HIS:CD2	1:A:762:HIS:H	2.09	0.71
1:A:415:PHE:CD2	1:A:417:LEU:HD12	2.28	0.69
1:B:216:ARG:HD2	1:B:651:ASN:OD1	1.93	0.69
1:B:739:LEU:O	1:B:742:LEU:HD12	1.93	0.69
1:B:573:GLU:OE2	1:B:666:ASN:N	2.27	0.68
1:B:88:GLN:HA	1:B:174:GLN:HE21	1.58	0.67
1:A:214:ALA:HB2	1:A:382:THR:HA	1.74	0.67
1:B:592:ASN:HD22	5:B:812:NAG:H83	1.59	0.67
1:A:442:ARG:HD3	1:B:403:ASP:OD1	1.95	0.67
1:A:180:ASP:OD1	1:A:210:THR:HG21	1.95	0.66
1:B:214:ALA:HB2	1:B:382:THR:HG23	1.76	0.66
1:A:383:ARG:HH21	7:A:815:FMT:H	1.61	0.66
1:B:214:ALA:HB2	1:B:382:THR:CA	2.22	0.66
1:A:214:ALA:HB2	1:A:382:THR:HG23	1.77	0.66
1:A:278:GLU:HA	1:A:278:GLU:OE1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:SER:HB3	1:A:515:THR:HB	1.76	0.66
1:B:726:ARG:H	1:B:729:GLN:HE21	1.42	0.66
1:B:140:GLU:OE2	1:B:160:HIS:NE2	2.28	0.66
1:B:749:ALA:N	1:B:750:PRO:O	2.29	0.66
1:B:131:GLY:HA2	1:B:136:PRO:HB3	1.78	0.65
1:A:744:GLN:O	1:A:744:GLN:HG3	1.96	0.65
1:B:551:VAL:CG1	1:B:553:TRP:CE2	2.80	0.65
1:A:438:LEU:HD22	1:A:439:PRO:HD2	1.77	0.65
1:B:706:ARG:HD2	8:B:955:HOH:O	1.96	0.65
1:B:588:TYR:HB3	1:B:604:ARG:HA	1.79	0.64
1:A:282:GLU:C	1:A:284:GLY:H	2.01	0.64
1:A:440:LEU:HD23	1:A:455:LEU:HD23	1.79	0.64
1:A:201:TYR:C	1:A:202:LYS:CG	2.66	0.64
1:A:78:ARG:CG	1:A:78:ARG:HH11	2.06	0.64
1:A:695:VAL:HG22	1:B:440:LEU:HG	1.80	0.64
1:B:407:LEU:HD21	1:B:752:LEU:HD12	1.80	0.64
1:B:726:ARG:H	1:B:729:GLN:NE2	1.96	0.63
1:A:666:ASN:HD22	5:A:813:NAG:C8	2.10	0.63
1:A:762:HIS:HD2	1:A:762:HIS:H	1.45	0.63
1:B:737:ASN:OD1	1:B:739:LEU:HB2	1.97	0.63
1:A:214:ALA:HB3	1:A:215:PRO:CD	2.27	0.63
1:A:744:GLN:CA	1:A:744:GLN:HE21	2.11	0.63
1:A:347:PRO:HB3	4:A:805:IMD:C4	2.28	0.63
1:A:744:GLN:C	1:A:744:GLN:HE21	2.02	0.63
1:A:214:ALA:CB	1:A:383:ARG:N	2.64	0.61
1:A:560:GLN:HG3	1:B:616:PRO:HG2	1.82	0.61
1:A:441:ARG:HA	1:B:492:THR:CG2	2.28	0.61
1:B:587:LEU:CD2	1:B:632:LEU:HD21	2.30	0.61
1:B:551:VAL:HG13	1:B:553:TRP:CZ2	2.36	0.60
1:B:551:VAL:CG1	1:B:553:TRP:CZ2	2.84	0.60
1:A:565:THR:HG22	1:A:565:THR:O	2.00	0.60
1:B:214:ALA:CB	1:B:383:ARG:N	2.63	0.60
1:A:302:LEU:HD13	1:B:453:GLY:HA3	1.82	0.60
1:B:552:PRO:HB2	1:B:553:TRP:CE3	2.36	0.60
1:A:476:ASP:HB2	1:A:488:ARG:HB2	1.84	0.60
1:A:216:ARG:HD2	1:A:651:ASN:OD1	2.02	0.59
1:B:125:LEU:CD1	1:B:159:ARG:HH12	2.15	0.59
1:B:129:PHE:CZ	1:B:169:ARG:HB2	2.37	0.59
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.68	0.59
1:B:440:LEU:HD22	1:B:481:PRO:HG2	1.84	0.59
1:B:95:CYS:CB	1:B:129:PHE:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLN:NE2	5:B:807:NAG:O6	2.35	0.58
1:A:194:LEU:CD2	1:A:277:LEU:HD21	2.33	0.58
1:A:306:VAL:HG13	1:A:307:PRO:HD2	1.85	0.58
1:A:403:ASP:OD1	1:B:442:ARG:HD3	2.03	0.58
1:A:201:TYR:C	1:A:202:LYS:HG2	2.23	0.58
1:A:78:ARG:NH1	1:A:78:ARG:HG3	2.07	0.58
1:B:214:ALA:HB1	1:B:383:ARG:N	2.09	0.58
1:A:744:GLN:O	1:A:745:ALA:CB	2.52	0.57
1:B:359:LEU:HD13	1:B:603:TYR:CZ	2.39	0.57
1:A:608:LEU:HD11	1:A:704:PHE:CE1	2.39	0.57
1:A:78:ARG:CG	1:A:78:ARG:NH1	2.66	0.57
1:A:442:ARG:H	1:B:492:THR:HG21	1.68	0.57
1:B:553:TRP:C	1:B:555:PRO:HD3	2.25	0.57
1:B:79:LEU:O	1:B:81:PRO:HD3	2.05	0.57
1:B:79:LEU:HD21	1:B:152:MET:HE1	1.87	0.57
1:A:252:LYS:HG3	1:A:252:LYS:O	2.05	0.57
1:A:471:TPQ:O2	4:A:804:IMD:N3	2.36	0.57
1:B:478:VAL:HB	1:B:486:GLU:HB3	1.86	0.56
1:B:80:GLY:O	1:B:81:PRO:C	2.43	0.56
1:B:125:LEU:HD11	1:B:159:ARG:NH1	2.20	0.56
5:B:807:NAG:H61	5:B:808:NAG:C1	2.36	0.56
1:B:739:LEU:HD12	1:B:742:LEU:HD11	1.87	0.56
1:A:665:ASN:OD1	1:A:667:GLU:HG3	2.07	0.55
1:A:145:PRO:HD3	1:A:151:TYR:CE2	2.41	0.54
1:A:478:VAL:HB	1:A:486:GLU:HB3	1.89	0.54
1:A:559:LEU:O	1:A:559:LEU:HD12	2.07	0.54
1:B:749:ALA:N	1:B:750:PRO:C	2.60	0.54
1:A:743:PRO:O	1:A:744:GLN:CB	2.52	0.54
1:A:383:ARG:HH21	7:A:815:FMT:C	2.20	0.54
1:A:233:ILE:HG13	1:A:241:HIS:CD2	2.42	0.54
1:A:214:ALA:HB3	1:A:382:THR:HA	1.88	0.54
1:B:349:ILE:HD11	4:B:804:IMD:H5	1.89	0.54
1:B:623:ARG:HD3	1:B:659:ASP:OD2	2.07	0.53
1:B:205:GLY:N	1:B:206:ARG:HA	2.22	0.53
1:A:352:VAL:HB	1:A:360:VAL:CG2	2.39	0.53
1:B:726:ARG:HB2	1:B:729:GLN:NE2	2.17	0.53
1:B:551:VAL:HG12	1:B:553:TRP:CE2	2.42	0.53
1:A:395:THR:HG23	8:A:923:HOH:O	2.08	0.53
1:B:552:PRO:HD2	1:B:553:TRP:CZ3	2.44	0.53
1:B:58:GLN:CG	1:B:59:LEU:H	1.99	0.52
1:B:251:HIS:HA	1:B:259:TRP:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:LEU:HD22	1:A:632:LEU:HD21	1.92	0.52
1:B:200:PHE:CZ	1:B:290:LEU:HD21	2.45	0.52
1:B:395:THR:HA	1:B:466:SER:HA	1.91	0.52
1:B:592:ASN:ND2	5:B:812:NAG:H83	2.24	0.52
1:A:500:LEU:CD1	1:A:504:THR:HG21	2.40	0.52
1:A:441:ARG:CA	1:B:492:THR:HG21	2.34	0.52
1:B:125:LEU:HD11	1:B:159:ARG:HH12	1.73	0.51
1:A:377:PRO:HA	1:A:380:MET:HE3	1.92	0.51
1:A:133:GLN:HE22	5:A:807:NAG:H61	1.75	0.51
1:B:726:ARG:N	1:B:729:GLN:HE21	2.07	0.51
1:B:94:ASN:HA	1:B:129:PHE:O	2.11	0.51
1:B:369:LEU:HD12	1:B:384:TYR:O	2.10	0.51
1:A:637:ARG:HD2	8:A:939:HOH:O	2.10	0.51
1:A:744:GLN:O	1:A:744:GLN:CG	2.58	0.51
1:A:739:LEU:HD11	1:B:402:VAL:HG23	1.93	0.51
1:B:182:MET:CE	1:B:261:ILE:HG12	2.40	0.51
1:A:61:ALA:O	1:A:101:LEU:HD22	2.11	0.51
1:B:438:LEU:HD12	1:B:439:PRO:HD2	1.93	0.51
1:A:465:MET:SD	1:B:442:ARG:HD3	2.52	0.50
1:A:195:LEU:HB3	1:A:201:TYR:HB2	1.93	0.50
1:A:635:THR:HG22	1:A:675:VAL:CG1	2.40	0.50
1:A:635:THR:CG2	1:A:677:TRP:HE1	2.24	0.50
1:B:415:PHE:CD2	1:B:417:LEU:HD12	2.46	0.50
1:A:71:VAL:HG13	1:A:143:VAL:HG11	1.94	0.50
1:A:469:LEU:CD2	4:A:804:IMD:H5	2.42	0.50
1:A:611:ALA:O	1:B:585:ARG:NH1	2.44	0.50
1:B:202:LYS:O	1:B:203:HIS:C	2.51	0.49
1:A:251:HIS:HA	1:A:259:TRP:CD1	2.47	0.49
1:A:615:LEU:HD11	7:A:815:FMT:H	1.94	0.49
1:A:587:LEU:HD22	1:A:632:LEU:CD2	2.43	0.49
1:B:386:ASP:OD2	4:B:806:IMD:H2	2.12	0.49
1:B:526:PHE:HE1	4:B:814:IMD:H5	1.77	0.49
1:A:744:GLN:O	1:A:745:ALA:HB3	2.13	0.49
1:B:233:ILE:HG13	1:B:241:HIS:HD2	1.76	0.49
1:A:469:LEU:HD23	4:A:804:IMD:H5	1.95	0.49
1:A:349:ILE:HD12	1:A:352:VAL:CG2	2.42	0.49
1:B:349:ILE:HG13	1:B:477:THR:HG21	1.95	0.49
1:B:551:VAL:HG12	1:B:553:TRP:CD2	2.48	0.49
1:A:212:THR:OG1	1:A:216:ARG:NH2	2.46	0.48
1:A:214:ALA:HB2	1:A:382:THR:CA	2.43	0.48
1:A:133:GLN:HE22	5:A:807:NAG:C6	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:MET:HB2	1:A:186:ARG:NH2	2.29	0.48
1:A:585:ARG:NH1	1:B:611:ALA:O	2.47	0.48
1:A:542:GLU:HA	1:A:565:THR:O	2.13	0.48
1:A:742:LEU:HD23	1:A:742:LEU:HA	1.68	0.48
1:A:442:ARG:CD	1:B:403:ASP:OD1	2.61	0.48
1:A:382:THR:C	1:A:383:ARG:HD2	2.35	0.48
1:A:442:ARG:HG3	1:A:442:ARG:O	2.11	0.48
1:B:175:GLU:O	1:B:179:ILE:HG13	2.14	0.47
1:B:187:GLU:HB3	1:B:274:LEU:CD1	2.43	0.47
1:A:744:GLN:HA	1:A:744:GLN:HE21	1.78	0.47
1:B:371:ILE:HD13	1:B:615:LEU:HB2	1.96	0.47
1:B:588:TYR:CB	1:B:604:ARG:HA	2.45	0.47
1:A:714:ASP:HB2	1:B:689:GLU:O	2.15	0.47
1:A:129:PHE:CZ	1:A:169:ARG:HB2	2.50	0.47
1:A:560:GLN:CG	1:B:616:PRO:HG2	2.44	0.47
1:B:471:TPQ:O2	4:B:806:IMD:N1	2.39	0.47
1:A:319:GLN:NE2	1:B:310:PRO:HA	2.29	0.47
1:A:416:LEU:HD12	1:A:422:PRO:N	2.31	0.46
1:B:471:TPQ:H6	1:B:492:THR:O	2.16	0.46
1:B:665:ASN:OD1	1:B:667:GLU:HG3	2.15	0.46
1:B:239:PHE:CD1	1:B:470:ASN:HB3	2.50	0.46
1:A:381:THR:HG22	1:B:559:LEU:HD12	1.96	0.46
1:A:403:ASP:OD1	1:B:442:ARG:CD	2.63	0.46
1:A:694:THR:HG21	8:A:1089:HOH:O	2.14	0.46
1:A:386:ASP:OD2	4:A:804:IMD:H2	2.16	0.46
1:A:666:ASN:ND2	5:A:813:NAG:H83	2.22	0.46
1:B:214:ALA:HB2	1:B:382:THR:CG2	2.43	0.46
1:A:86:ALA:HA	1:A:89:ALA:HB2	1.98	0.46
1:B:386:ASP:OD1	4:B:806:IMD:H2	2.16	0.46
1:B:492:THR:HG23	1:B:694:THR:O	2.16	0.45
1:B:460:LEU:HB3	1:B:479:PHE:HB2	1.97	0.45
1:A:132:ARG:HH11	1:A:132:ARG:HG2	1.81	0.45
1:A:737:ASN:OD1	1:A:739:LEU:HB2	2.17	0.45
1:A:344:PHE:HA	1:A:390:GLY:HA2	1.99	0.45
1:B:551:VAL:HG13	1:B:553:TRP:CH2	2.51	0.45
1:A:608:LEU:HD11	1:A:704:PHE:HE1	1.78	0.45
1:A:680:ALA:CB	1:A:701:VAL:HG13	2.40	0.45
1:B:284:GLY:HA2	8:B:961:HOH:O	2.17	0.45
1:A:465:MET:HG2	1:A:474:VAL:HG22	1.98	0.45
1:A:218:LEU:HD13	1:B:557:HIS:ND1	2.32	0.45
1:A:349:ILE:HD13	1:A:479:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:THR:HG21	1:A:677:TRP:HE1	1.82	0.45
1:B:573:GLU:H	1:B:573:GLU:HG2	1.58	0.45
1:A:282:GLU:C	1:A:284:GLY:N	2.65	0.44
1:B:243:VAL:O	1:B:243:VAL:HG13	2.16	0.44
1:A:225:THR:HB	1:A:227:PHE:CE1	2.53	0.44
1:B:431:VAL:HA	1:B:461:VAL:O	2.17	0.44
1:B:322:ARG:NH1	1:B:721:ASP:OD2	2.46	0.44
1:A:117:SER:HB3	1:A:118:PRO:CD	2.48	0.44
1:A:188:LEU:HA	1:A:188:LEU:HD12	1.72	0.44
1:B:537:ASN:HA	1:B:590:ALA:O	2.17	0.44
1:B:663:PHE:N	1:B:663:PHE:CD1	2.85	0.44
1:B:683:LEU:HD12	1:B:684:HIS:H	1.82	0.44
1:A:141:LEU:HD23	1:A:154:ASP:HA	2.00	0.44
1:A:546:PHE:CD2	1:B:616:PRO:HD3	2.53	0.44
1:A:67:GLU:O	1:A:71:VAL:HG23	2.16	0.44
1:A:744:GLN:C	1:A:744:GLN:NE2	2.70	0.44
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.31	0.44
1:B:511:VAL:CG1	1:B:691:ILE:HD11	2.47	0.44
1:A:708:TYR:O	1:A:709:ASN:HB2	2.18	0.44
1:B:375:ASN:ND2	1:B:504:THR:HG22	2.33	0.44
1:A:635:THR:HG22	1:A:675:VAL:HG13	1.99	0.44
1:B:245:LEU:HD12	1:B:265:PHE:O	2.18	0.44
1:B:588:TYR:HB2	1:B:603:TYR:O	2.18	0.44
1:B:125:LEU:CD1	1:B:159:ARG:NH1	2.80	0.44
1:B:130:PHE:O	1:B:136:PRO:HA	2.18	0.44
1:A:65:ARG:HG3	8:A:1020:HOH:O	2.18	0.43
1:B:57:SER:HB3	1:B:328:SER:N	2.23	0.43
1:A:386:ASP:OD1	4:A:804:IMD:H2	2.18	0.43
1:A:74:PHE:HE1	1:A:152:MET:HB3	1.83	0.43
1:A:233:ILE:HG13	1:A:241:HIS:HD2	1.83	0.43
1:A:488:ARG:HD3	1:A:488:ARG:HA	1.57	0.43
1:B:351:ASP:OD2	1:B:353:ARG:NH1	2.52	0.43
1:A:179:ILE:HD11	1:A:251:HIS:CG	2.53	0.43
1:A:400:ARG:HG2	1:A:406:TYR:CD1	2.53	0.43
1:A:579:VAL:HG11	1:A:614:PRO:HD3	2.01	0.43
1:B:382:THR:C	1:B:383:ARG:HD2	2.39	0.43
1:B:366:GLN:HB2	1:B:525:HIS:HB3	1.99	0.43
1:A:145:PRO:HD3	1:A:151:TYR:HE2	1.83	0.43
1:B:375:ASN:ND2	1:B:501:PHE:O	2.51	0.43
1:A:282:GLU:O	1:A:284:GLY:N	2.51	0.43
1:A:386:ASP:HB3	1:A:468:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:HIS:HA	1:B:117:SER:O	2.19	0.43
1:B:179:ILE:HG23	1:B:249:VAL:HG11	2.00	0.43
1:A:471:TPQ:H6	1:A:471:TPQ:HA	1.85	0.43
1:B:256:PRO:HA	1:B:259:TRP:CE2	2.54	0.43
1:A:371:ILE:O	1:A:520:HIS:HA	2.19	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.53	0.42
1:A:383:ARG:HD2	1:A:383:ARG:N	2.33	0.42
1:A:525:HIS:HB2	1:A:627:TRP:CE3	2.54	0.42
1:B:351:ASP:CG	1:B:353:ARG:HH11	2.23	0.42
1:B:497:SER:HB2	1:B:515:THR:HG23	2.01	0.42
1:A:188:LEU:N	1:A:189:PRO:CD	2.83	0.42
1:B:75:LEU:HD21	1:B:143:VAL:HG21	2.01	0.42
1:A:487:ILE:O	1:A:702:GLY:HA3	2.19	0.42
1:B:404:CYS:HB2	1:B:410:TYR:OH	2.19	0.42
1:B:596:LYS:HD3	1:B:597:TRP:CH2	2.55	0.42
1:A:389:PHE:HE1	1:A:650:GLN:OE1	2.02	0.42
1:A:663:PHE:N	1:A:663:PHE:CD1	2.86	0.42
1:A:232:ASN:ND2	5:A:810:NAG:O7	2.52	0.42
1:B:132:ARG:O	1:B:133:GLN:HB3	2.20	0.42
1:B:98:SER:HB2	1:B:417:LEU:HD23	2.01	0.42
1:A:369:LEU:HD12	1:A:384:TYR:O	2.20	0.41
1:B:271:TYR:CE1	1:B:277:LEU:HD13	2.55	0.41
1:B:640:GLU:H	1:B:640:GLU:HG3	1.47	0.41
1:B:90:ARG:HD2	1:B:90:ARG:HA	1.81	0.41
1:A:189:PRO:C	1:A:191:ALA:H	2.23	0.41
1:A:231:TYR:O	1:A:233:ILE:HG12	2.20	0.41
1:A:352:VAL:HB	1:A:360:VAL:HG23	2.02	0.41
1:B:330:VAL:O	1:B:336:THR:HA	2.20	0.41
1:B:84:VAL:HG12	1:B:85:ASP:N	2.35	0.41
1:A:214:ALA:HB2	1:A:382:THR:CG2	2.47	0.41
1:A:559:LEU:C	1:A:559:LEU:HD12	2.40	0.41
1:B:74:PHE:HE1	1:B:152:MET:HB2	1.86	0.41
1:A:128:VAL:HG11	1:A:130:PHE:CZ	2.55	0.41
1:A:352:VAL:HB	1:A:360:VAL:HG22	2.03	0.41
1:A:687:HIS:HD2	1:A:689:GLU:OE1	2.03	0.41
1:A:744:GLN:NE2	1:A:744:GLN:CA	2.82	0.41
1:A:195:LEU:HB3	1:A:201:TYR:CB	2.50	0.41
1:B:762:HIS:CD2	1:B:762:HIS:N	2.89	0.41
1:A:67:GLU:HB3	1:A:146:LEU:HD22	2.02	0.41
1:A:522:HIS:O	1:A:681:GLY:HA3	2.21	0.41
1:B:742:LEU:HA	1:B:743:PRO:HA	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LEU:O	1:A:746:ALA:HB3	2.21	0.41
1:A:79:LEU:HA	1:A:79:LEU:HD12	1.52	0.41
1:A:481:PRO:HG3	8:A:1048:HOH:O	2.20	0.41
1:B:416:LEU:C	1:B:417:LEU:HG	2.41	0.41
1:A:194:LEU:HD23	1:A:277:LEU:HD21	2.01	0.40
1:B:94:ASN:HD22	1:B:130:PHE:HA	1.82	0.40
1:A:132:ARG:CG	1:A:132:ARG:HH11	2.35	0.40
1:A:543:ASP:O	1:A:565:THR:HB	2.22	0.40
1:A:550:ALA:O	1:A:552:PRO:HD3	2.21	0.40
1:A:724:TYR:C	1:A:724:TYR:CD1	2.94	0.40
1:B:212:THR:HG22	1:B:213:THR:N	2.35	0.40
1:B:224:ALA:HB1	1:B:248:LEU:HD11	2.03	0.40
1:B:182:MET:HE1	1:B:261:ILE:HG12	2.04	0.40
1:A:367:GLU:OE1	1:A:645:SER:OG	2.33	0.40
1:B:445:SER:CB	1:B:451:TYR:CE1	3.04	0.40
1:B:589:LEU:HD23	1:B:589:LEU:N	2.36	0.40
1:B:298:GLY:O	1:B:692:PRO:HB3	2.21	0.40
1:A:201:TYR:CG	1:A:202:LYS:N	2.90	0.40
1:B:539:VAL:HG22	1:B:569:LEU:HB2	2.02	0.40
1:B:708:TYR:O	1:B:709:ASN:HB2	2.20	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	Percentiles	
1	A	700/763 (92%)	656 (94%)	37 (5%)	7 (1%)	18	37
1	B	696/763 (91%)	653 (94%)	40 (6%)	3 (0%)	38	63
All	All	1396/1526 (92%)	1309 (94%)	77 (6%)	10 (1%)	25	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	744	GLN
1	A	745	ALA
1	A	746	ALA
1	B	58	GLN
1	B	214	ALA
1	A	190	GLN
1	A	283	ALA
1	A	297	GLY
1	B	81	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	585/634 (92%)	541 (92%)	44 (8%)	16	31
1	B	581/634 (92%)	540 (93%)	41 (7%)	17	34
All	All	1166/1268 (92%)	1081 (93%)	85 (7%)	16	33

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	79	LEU
1	A	83	LEU
1	A	132	ARG
1	A	135	GLN
1	A	146	LEU
1	A	153	ARG
1	A	181	GLN
1	A	188	LEU
1	A	195	LEU
1	A	196	HIS
1	A	198	CYS
1	A	199	CYS
1	A	206	ARG

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Mol	Chain	Res	Type
1	A	218	LEU
1	A	219	GLN
1	A	229	LEU
1	A	261	ILE
1	A	290	LEU
1	A	302	LEU
1	A	376	SER
1	A	409	THR
1	A	442	ARG
1	A	459	VAL
1	A	469	LEU
1	A	489	PHE
1	A	496	SER
1	A	511	VAL
1	A	513	GLU
1	A	539	VAL
1	A	559	LEU
1	A	565	THR
1	A	587	LEU
1	A	604	ARG
1	A	613	GLU
1	A	617	GLN
1	A	625	PHE
1	A	629	ARG
1	A	635	THR
1	A	695	VAL
1	A	713	GLU
1	A	735	GLU
1	A	744	GLN
1	A	762	HIS
1	B	78	ARG
1	B	90	ARG
1	B	95	CYS
1	B	103	LEU
1	B	153	ARG
1	B	157	VAL
1	B	181	GLN
1	B	206	ARG
1	B	209	VAL
1	B	212	THR
1	B	229	LEU
1	B	243	VAL

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Mol	Chain	Res	Type
1	B	260	THR
1	B	299	SER
1	B	303	LYS
1	B	326	GLN
1	B	353	ARG
1	B	360	VAL
1	B	395	THR
1	B	417	LEU
1	B	442	ARG
1	B	459	VAL
1	B	489	PHE
1	B	492	THR
1	B	511	VAL
1	B	558	GLN
1	B	559	LEU
1	B	561	ARG
1	B	570	GLU
1	B	573	GLU
1	B	587	LEU
1	B	608	LEU
1	B	626	SER
1	B	640	GLU
1	B	646	SER
1	B	650	GLN
1	B	713	GLU
1	B	722	SER
1	B	739	LEU
1	B	752	LEU
1	B	761	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	135	GLN
1	A	174	GLN
1	A	197	HIS
1	A	276	GLN
1	A	319	GLN
1	A	355	GLN
1	A	450	HIS
1	A	618	ASN

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Mol	Chain	Res	Type
1	A	744	GLN
1	A	762	HIS
1	B	58	GLN
1	B	77	GLN
1	B	94	ASN
1	B	112	HIS
1	B	174	GLN
1	B	185	ASN
1	B	241	HIS
1	B	262	GLN
1	B	267	GLN
1	B	276	GLN
1	B	287	ASN
1	B	650	GLN
1	B	693	ASN
1	B	699	ASN
1	B	729	GLN
1	B	762	HIS

### 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	TPQ	A	471	1,2	14,14,15	3.53	7 (50%)	17,19,21	1.36	3 (17%)
1	TPQ	B	471	1,2	14,14,15	3.42	7 (50%)	17,19,21	1.34	3 (17%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	A	471	1,2	-	0/4/22/24	0/1/1/1
1	TPQ	B	471	1,2	-	0/4/22/24	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	C1-C2	-7.57	1.37	1.49
1	B	471	TPQ	C1-C2	-6.59	1.39	1.49
1	A	471	TPQ	C4-C5	-2.36	1.40	1.47
1	B	471	TPQ	C4-C5	-2.29	1.40	1.47
1	A	471	TPQ	O4-C4	3.03	1.42	1.33
1	B	471	TPQ	O4-C4	3.24	1.42	1.33
1	B	471	TPQ	C6-C1	3.70	1.44	1.34
1	A	471	TPQ	C6-C1	3.75	1.44	1.34
1	A	471	TPQ	C3-C4	4.47	1.42	1.35
1	B	471	TPQ	C3-C4	4.65	1.43	1.35
1	A	471	TPQ	O2-C2	5.45	1.39	1.24
1	B	471	TPQ	O2-C2	5.63	1.39	1.24
1	B	471	TPQ	O5-C5	5.66	1.39	1.24
1	A	471	TPQ	O5-C5	5.73	1.40	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	TPQ	CB-C1-C6	-2.56	117.47	122.41
1	A	471	TPQ	CB-C1-C6	-2.51	117.57	122.41
1	B	471	TPQ	C3-C4-C5	-2.33	118.79	121.24
1	B	471	TPQ	CB-C1-C2	2.40	122.86	118.57
1	A	471	TPQ	CB-CA-C	2.44	116.11	111.41
1	A	471	TPQ	CB-C1-C2	2.54	123.12	118.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 6 are monoatomic - leaving 24 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	804	-	3,5,5	0.58	0	4,5,5	0.54	0
4	IMD	A	805	-	3,5,5	0.57	0	4,5,5	0.64	0
4	IMD	A	806	-	3,5,5	0.56	0	4,5,5	0.70	0
5	NAG	A	807	1,5	14,14,15	1.96	4 (28%)	15,19,21	1.70	4 (26%)
5	NAG	A	808	5,6	14,14,15	2.25	4 (28%)	15,19,21	1.68	4 (26%)
6	MAN	A	809	5	11,11,12	1.86	3 (27%)	13,15,17	2.02	5 (38%)
5	NAG	A	810	1,5	14,14,15	2.16	5 (35%)	15,19,21	1.61	4 (26%)
5	NAG	A	811	5	14,14,15	2.02	4 (28%)	15,19,21	1.40	3 (20%)
5	NAG	A	812	1	14,14,15	0.90	1 (7%)	15,19,21	2.97	4 (26%)
5	NAG	A	813	1	14,14,15	2.06	5 (35%)	15,19,21	2.77	4 (26%)
4	IMD	A	814	-	3,5,5	0.62	0	4,5,5	0.52	0
7	FMT	A	815	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	816	-	0,2,2	0.00	-	0,1,1	0.00	-
4	IMD	B	804	-	3,5,5	0.62	0	4,5,5	0.45	0
4	IMD	B	805	-	3,5,5	0.68	0	4,5,5	0.29	0
4	IMD	B	806	-	3,5,5	0.66	0	4,5,5	0.44	0
5	NAG	B	807	1,5	14,14,15	1.99	5 (35%)	15,19,21	1.52	3 (20%)
5	NAG	B	808	5,6	14,14,15	2.01	5 (35%)	15,19,21	2.38	3 (20%)
6	MAN	B	809	5	11,11,12	1.73	3 (27%)	13,15,17	2.33	4 (30%)
5	NAG	B	810	1,5	14,14,15	1.96	4 (28%)	15,19,21	2.16	5 (33%)
5	NAG	B	811	5	14,14,15	2.11	5 (35%)	15,19,21	2.29	5 (33%)
5	NAG	B	812	1	14,14,15	2.03	5 (35%)	15,19,21	2.68	7 (46%)
5	NAG	B	813	1	14,14,15	0.87	0	15,19,21	2.26	3 (20%)
4	IMD	B	814	-	3,5,5	0.63	0	4,5,5	0.78	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	804	-	-	0/0/0/0	0/1/1/1
4	IMD	A	805	-	-	0/0/0/0	0/1/1/1
4	IMD	A	806	-	-	0/0/0/0	0/1/1/1
5	NAG	A	807	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	808	5,6	-	0/6/23/26	0/1/1/1
6	MAN	A	809	5	-	0/2/19/22	1/1/1/1
5	NAG	A	810	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	811	5	-	0/6/23/26	0/1/1/1
5	NAG	A	812	1	-	0/6/23/26	0/1/1/1
5	NAG	A	813	1	-	0/6/23/26	0/1/1/1
4	IMD	A	814	-	-	0/0/0/0	0/1/1/1
7	FMT	A	815	-	-	0/0/0/0	0/0/0/0
7	FMT	A	816	-	-	0/0/0/0	0/0/0/0
4	IMD	B	804	-	-	0/0/0/0	0/1/1/1
4	IMD	B	805	-	-	0/0/0/0	0/1/1/1
4	IMD	B	806	-	-	0/0/0/0	0/1/1/1
5	NAG	B	807	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	808	5,6	-	0/6/23/26	0/1/1/1
6	MAN	B	809	5	-	0/2/19/22	1/1/1/1
5	NAG	B	810	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	811	5	-	0/6/23/26	0/1/1/1
5	NAG	B	812	1	-	0/6/23/26	0/1/1/1
5	NAG	B	813	1	-	0/6/23/26	0/1/1/1
4	IMD	B	814	-	-	0/0/0/0	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807	NAG	C3-C2	-4.49	1.42	1.52
5	A	807	NAG	C3-C2	-4.01	1.43	1.52
5	A	810	NAG	C3-C2	-3.73	1.44	1.52
5	B	810	NAG	C3-C2	-3.58	1.44	1.52
6	B	809	MAN	C4-C3	-3.48	1.43	1.52
6	A	809	MAN	C4-C3	-3.28	1.44	1.52
5	A	813	NAG	C4-C3	-2.95	1.44	1.52
5	B	808	NAG	C4-C5	-2.93	1.46	1.53
5	B	807	NAG	C1-C2	-2.92	1.48	1.52
5	A	808	NAG	C1-C2	-2.84	1.48	1.52
5	A	810	NAG	C1-C2	-2.82	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	809	MAN	C2-C3	-2.67	1.48	1.52
5	B	812	NAG	C3-C2	-2.61	1.46	1.52
5	B	811	NAG	C4-C5	-2.56	1.47	1.53
5	B	812	NAG	C4-C3	-2.48	1.46	1.52
5	A	807	NAG	C4-C3	-2.47	1.46	1.52
5	A	811	NAG	C4-C5	-2.47	1.47	1.53
5	A	808	NAG	C3-C2	-2.46	1.47	1.52
5	B	807	NAG	C4-C3	-2.44	1.46	1.52
5	A	813	NAG	C3-C2	-2.39	1.47	1.52
5	A	812	NAG	O5-C1	-2.14	1.40	1.43
5	B	808	NAG	C6-C5	-2.09	1.44	1.51
5	B	808	NAG	O5-C1	-2.08	1.40	1.43
6	B	809	MAN	C2-C3	-2.06	1.49	1.52
5	A	811	NAG	C8-C7	2.00	1.54	1.50
5	B	812	NAG	C1-C2	2.02	1.55	1.52
5	B	811	NAG	C2-N2	2.08	1.50	1.46
5	B	807	NAG	O5-C1	2.20	1.47	1.43
5	B	810	NAG	O4-C4	2.31	1.48	1.43
5	A	813	NAG	C1-C2	2.32	1.55	1.52
5	B	811	NAG	C8-C7	2.37	1.55	1.50
5	A	810	NAG	O5-C1	2.52	1.47	1.43
5	A	807	NAG	C7-N2	2.80	1.44	1.34
5	A	807	NAG	O5-C1	2.85	1.48	1.43
5	B	808	NAG	C7-N2	2.86	1.44	1.34
5	B	807	NAG	C7-N2	2.98	1.45	1.34
5	B	810	NAG	C2-N2	2.99	1.51	1.46
5	A	808	NAG	C7-N2	3.20	1.46	1.34
6	B	809	MAN	O5-C5	3.35	1.50	1.43
5	B	812	NAG	O5-C5	3.39	1.50	1.43
5	A	810	NAG	C2-N2	3.48	1.52	1.46
6	A	809	MAN	O5-C5	3.56	1.50	1.43
5	B	810	NAG	C7-N2	3.58	1.47	1.34
5	A	810	NAG	C7-N2	3.69	1.47	1.34
5	A	811	NAG	C7-N2	3.82	1.48	1.34
5	A	813	NAG	O5-C5	3.93	1.51	1.43
5	B	811	NAG	C7-N2	4.07	1.49	1.34
5	B	808	NAG	O5-C5	4.30	1.52	1.43
5	A	813	NAG	C7-N2	4.44	1.50	1.34
5	A	811	NAG	O5-C5	4.45	1.52	1.43
5	B	811	NAG	O5-C5	4.47	1.52	1.43
5	B	812	NAG	C7-N2	4.64	1.51	1.34
5	A	808	NAG	O5-C5	5.20	1.54	1.43

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	812	NAG	O5-C1-C2	-7.75	100.68	111.47
5	B	808	NAG	C2-N2-C7	-6.59	113.33	122.94
5	B	813	NAG	C6-C5-C4	-5.01	101.27	113.00
6	B	809	MAN	C1-C2-C3	-4.45	104.01	109.65
5	A	812	NAG	C6-C5-C4	-4.06	103.51	113.00
5	A	808	NAG	O4-C4-C3	-4.02	101.62	110.36
5	B	811	NAG	C1-O5-C5	-3.88	106.81	112.17
5	A	807	NAG	C6-C5-C4	-3.61	104.55	113.00
5	B	813	NAG	C4-C3-C2	-3.27	106.22	111.02
6	A	809	MAN	O5-C1-C2	-3.22	105.75	110.79
5	B	807	NAG	C2-N2-C7	-3.19	118.28	122.94
6	A	809	MAN	C1-C2-C3	-3.16	105.65	109.65
5	B	811	NAG	O7-C7-C8	-3.16	116.31	122.06
5	B	812	NAG	O7-C7-C8	-3.10	116.42	122.06
6	A	809	MAN	C1-O5-C5	-2.90	108.17	112.17
5	B	812	NAG	O7-C7-N2	-2.85	116.42	121.92
5	A	812	NAG	C4-C3-C2	-2.85	106.84	111.02
5	B	808	NAG	O4-C4-C3	-2.64	104.60	110.36
5	B	810	NAG	C1-O5-C5	-2.53	108.68	112.17
5	B	810	NAG	C2-N2-C7	-2.52	119.27	122.94
5	B	807	NAG	C1-C2-N2	-2.48	106.26	110.49
5	A	813	NAG	O7-C7-C8	-2.44	117.61	122.06
5	A	808	NAG	O5-C1-C2	-2.31	108.26	111.47
5	A	810	NAG	C1-O5-C5	-2.28	109.02	112.17
5	A	808	NAG	C2-N2-C7	-2.25	119.67	122.94
5	A	807	NAG	O7-C7-N2	-2.21	117.67	121.92
5	A	811	NAG	C8-C7-N2	2.09	119.89	116.11
5	A	808	NAG	C4-C3-C2	2.13	114.14	111.02
5	A	811	NAG	O6-C6-C5	2.24	118.87	111.34
5	A	810	NAG	O5-C1-C2	2.28	114.64	111.47
5	B	812	NAG	C1-C2-N2	2.30	114.41	110.49
6	A	809	MAN	O6-C6-C5	2.30	119.08	111.34
5	A	811	NAG	C4-C3-C2	2.38	114.50	111.02
5	A	810	NAG	C3-C4-C5	2.41	114.46	110.22
5	A	807	NAG	C3-C4-C5	2.41	114.47	110.22
6	B	809	MAN	O6-C6-C5	2.53	119.87	111.34
5	B	807	NAG	C3-C4-C5	2.64	114.87	110.22
5	B	810	NAG	O5-C1-C2	2.65	115.16	111.47
6	A	809	MAN	O2-C2-C1	2.67	114.60	109.18
5	B	812	NAG	C3-C4-C5	2.69	114.96	110.22
6	B	809	MAN	O2-C2-C3	3.05	116.17	110.17
5	B	811	NAG	C8-C7-N2	3.37	122.19	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	812	NAG	O6-C6-C5	3.38	122.73	111.34
5	A	807	NAG	C1-O5-C5	3.47	116.95	112.17
5	B	811	NAG	C2-N2-C7	3.51	128.06	122.94
5	B	811	NAG	C1-C2-N2	3.58	116.59	110.49
5	A	813	NAG	O6-C6-C5	3.59	123.44	111.34
5	A	813	NAG	C8-C7-N2	3.77	122.92	116.11
5	A	810	NAG	C4-C3-C2	3.84	116.64	111.02
5	B	810	NAG	C3-C4-C5	4.00	117.27	110.22
6	B	809	MAN	O2-C2-C1	4.33	117.98	109.18
5	B	808	NAG	C4-C3-C2	4.36	117.40	111.02
5	B	812	NAG	C1-O5-C5	4.69	118.63	112.17
5	B	810	NAG	C4-C3-C2	4.92	118.23	111.02
5	B	813	NAG	C1-O5-C5	5.82	120.19	112.17
5	B	812	NAG	C8-C7-N2	5.88	126.72	116.11
5	A	812	NAG	C1-O5-C5	5.96	120.38	112.17
5	A	813	NAG	C1-O5-C5	8.25	123.53	112.17

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	809	MAN	C1-C2-C3-C4-C5-O5
6	B	809	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	IMD	5	0
4	A	805	IMD	1	0
5	A	807	NAG	2	0
5	A	810	NAG	1	0
5	A	813	NAG	3	0
7	A	815	FMT	3	0
7	A	816	FMT	1	0
4	B	804	IMD	1	0
4	B	806	IMD	3	0
5	B	807	NAG	2	0
5	B	808	NAG	1	0
5	B	812	NAG	2	0
4	B	814	IMD	1	0



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	553:TRP	C	554:SER	N	1.08
1	A	470:ASN	C	471:TPQ	N	1.04
1	B	552:PRO	C	553:TRP	N	0.88

## 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	704/763 (92%)	-0.90	4 (0%) 89 88	18, 33, 56, 101	0
1	B	700/763 (91%)	-0.86	6 (0%) 84 81	17, 35, 60, 104	0
All	All	1404/1526 (92%)	-0.88	10 (0%) 87 85	17, 34, 58, 104	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	762	HIS	4.0
1	B	57	SER	4.0
1	B	762	HIS	3.1
1	B	205	GLY	3.0
1	B	735	GLU	2.6
1	A	744	GLN	2.6
1	A	283	ALA	2.2
1	A	747	ALA	2.2
1	B	81	PRO	2.1
1	B	553	TRP	2.1

### 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	TPQ	B	471	14/15	0.98	0.09	-	27,35,43,45	0
1	TPQ	A	471	14/15	0.97	0.09	-	26,39,44,46	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 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	A	814	5/5	0.97	0.18	11.55	58,60,66,69	0
4	IMD	B	805	5/5	0.94	0.23	11.00	49,55,60,66	0
5	NAG	B	811	14/15	0.86	0.43	5.35	66,96,105,105	0
5	NAG	A	811	14/15	0.86	0.40	4.66	67,92,102,109	0
7	FMT	A	816	3/3	0.96	0.13	2.51	38,38,43,50	0
5	NAG	B	810	14/15	0.93	0.23	2.41	57,68,81,92	0
5	NAG	A	810	14/15	0.93	0.22	2.25	59,74,83,87	0
5	NAG	A	808	14/15	0.92	0.17	1.70	48,65,76,93	0
4	IMD	A	804	5/5	0.97	0.10	0.73	49,52,55,58	0
4	IMD	A	805	5/5	1.00	0.13	0.51	20,22,26,26	0
4	IMD	B	804	5/5	0.99	0.11	0.20	24,24,28,28	0
4	IMD	A	806	5/5	0.98	0.10	-0.14	23,27,32,33	0
3	CA	A	802	1/1	1.00	0.09	-0.52	24,24,24,24	0
3	CA	B	802	1/1	0.99	0.10	-0.56	29,29,29,29	0
5	NAG	A	807	14/15	0.96	0.11	-0.77	32,38,47,53	0
5	NAG	B	807	14/15	0.96	0.08	-1.27	35,44,56,61	0
4	IMD	B	814	5/5	0.99	0.07	-1.51	30,32,32,34	0
4	IMD	B	806	5/5	0.99	0.08	-1.61	43,43,48,48	0
3	CA	A	803	1/1	1.00	0.05	-2.12	29,29,29,29	0
7	FMT	A	815	3/3	0.99	0.07	-2.28	34,34,35,39	0
3	CA	B	803	1/1	0.99	0.06	-3.44	32,32,32,32	0
5	NAG	A	813	14/15	0.79	0.42	-	72,88,95,98	0
2	CU	A	801	1/1	1.00	0.06	-	32,32,32,32	0
5	NAG	B	808	14/15	0.88	0.20	-	48,72,82,88	0
5	NAG	B	812	14/15	0.78	0.33	-	52,85,100,105	0
5	NAG	A	812	14/15	0.86	0.32	-	77,78,78,79	0
2	CU	B	801	1/1	1.00	0.07	-	29,29,29,29	0
6	MAN	A	809	11/12	0.83	0.33	-	80,96,105,111	0
5	NAG	B	813	14/15	0.75	0.44	-	77,78,78,79	0
6	MAN	B	809	11/12	0.75	0.33	-	59,84,97,102	0

## 6.5 Other polymers

There are no such residues in this entry.