



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:44 AM GMT

PDB ID : 3FU7  
Title : Melanocarpus albomyces laccase crystal soaked (4 sec) with 2,6-dimethoxyphenol  
Authors : Kallio, J.P.; Hakulinen, N.; Rouvinen, J.  
Deposited on : 2009-01-14  
Resolution : 1.67 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



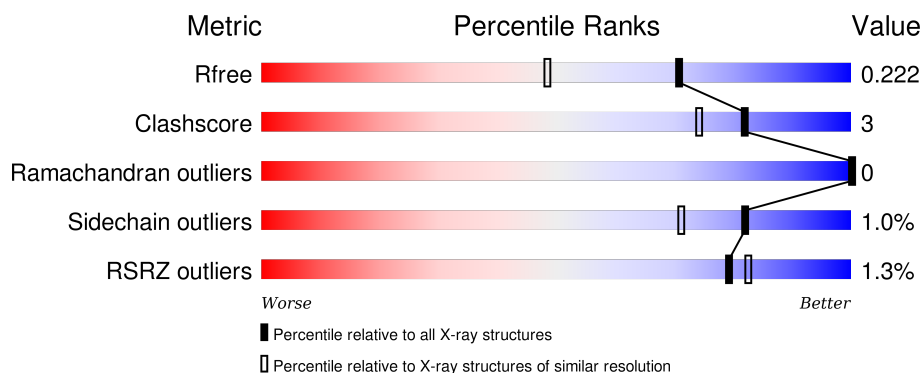
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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	559	<div> <div></div> <div>94%</div> <div>6%</div> </div>
2	B	559	<div> <div>2%</div> <div>96%</div> <div>.</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
11	3DM	A	3900[B]	-	-	-	X
12	D2M	B	2100[A]	-	-	X	X
4	CL	B	610	-	-	-	X
5	OXY	A	1620	-	-	-	X
5	OXY	B	1620	-	-	-	X
6	NAG	A	700	-	-	-	X
6	NAG	A	750	-	-	-	X
6	NAG	B	2760	-	-	-	X
6	NAG	B	700	-	-	-	X
7	MAN	A	712	X	-	-	-
7	MAN	B	712	X	-	-	-
8	NAG	A	760	-	-	-	X
9	MAN	A	732	X	-	-	-
9	MAN	B	732	X	-	-	-



## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 10365 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 Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	13	0
			4478	2823	785	853	17			

- Molecule 2 is a protein called Laccase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	559	Total	C	N	O	S	0	13	0
			4472	2822	782	851	17			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

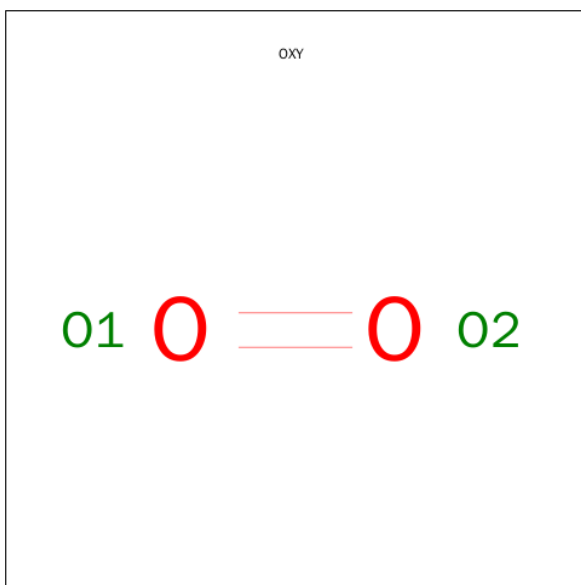
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cu	0	0
			4	4		
3	A	4	Total	Cu	0	0
			4	4		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

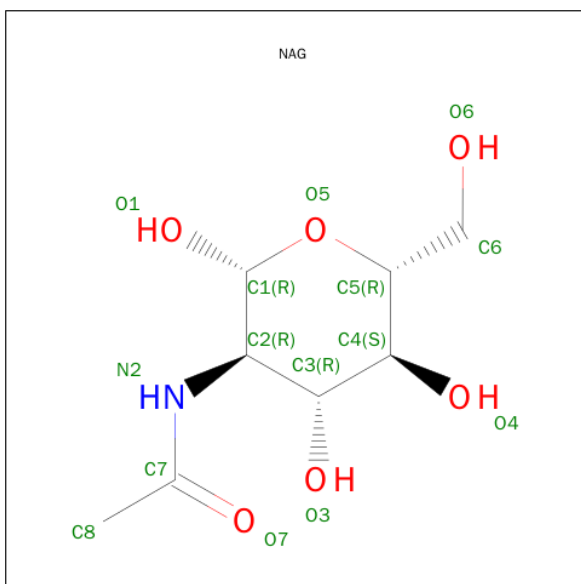
- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).





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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	4	Total	C	N	O	0	0
			50	28	2	20		
7	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

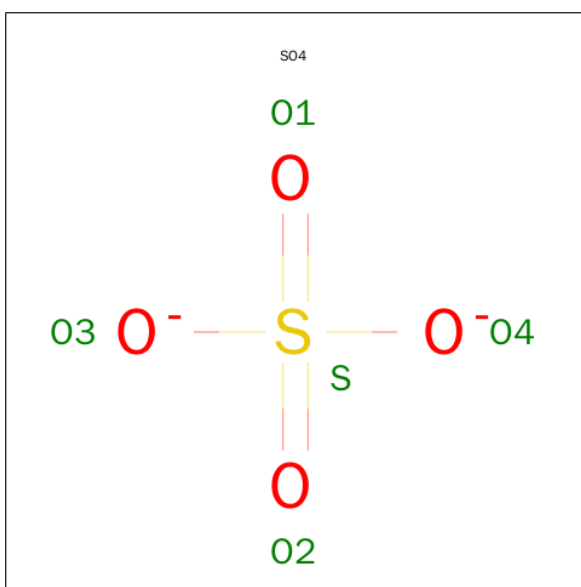
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	2	Total	C	N	O	0	0
			28	16	2	10		
8	A	2	Total	C	N	O	0	0
			28	16	2	10		
8	A	2	Total	C	N	O	0	0
			28	16	2	10		
8	B	2	Total	C	N	O	0	0
			28	16	2	10		
8	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

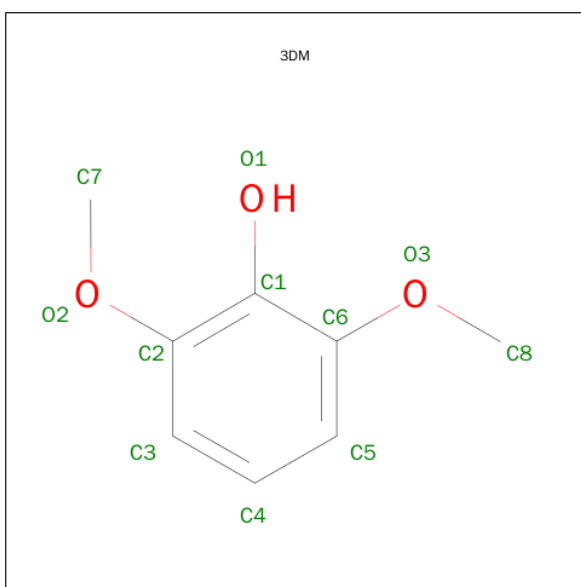
- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		

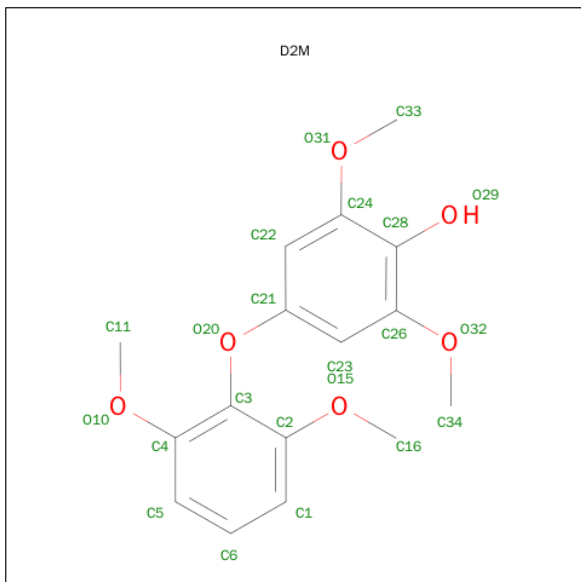
- Molecule 11 is 2,6-DIMETHOXYPHENOL (three-letter code: 3DM) (formula: C<sub>8</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	1
			11	8	3		

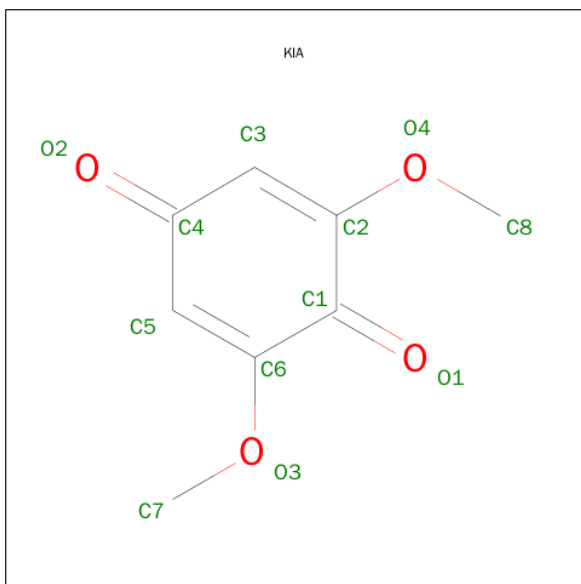


- Molecule 12 is 4-(2,6-DIMETHOXYPHENOXY)-2,6-DIMETHOXYPHENOL (three-letter code: D2M) (formula: C<sub>16</sub>H<sub>18</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	1
			22	16	6		

- Molecule 13 is 2,6-DIMETHOXYCYCLOHEXA-2,5-DIENE-1,4-DIONE (three-letter code: KIA) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	1
			12	8	4		



- Molecule 14 is water.

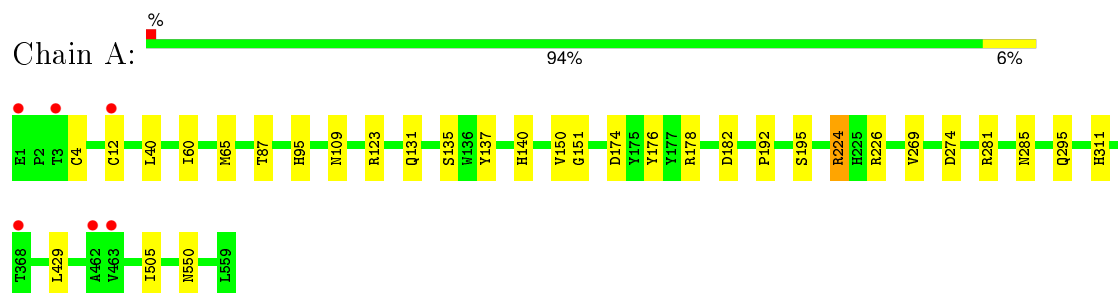
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	506	Total 506	O 506	0	0
14	B	447	Total 447	O 447	0	0



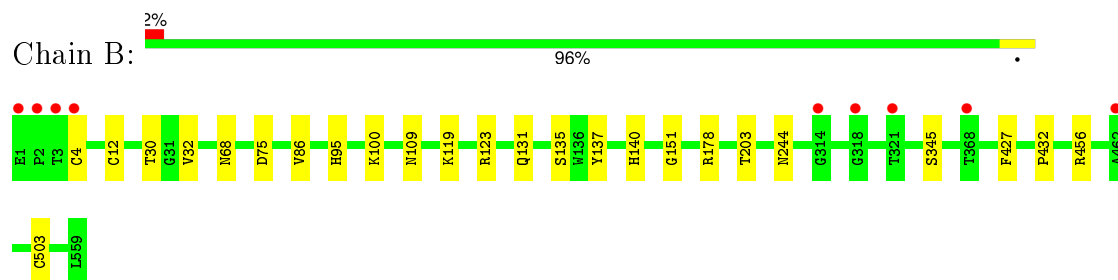
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: Laccase-1



#### • Molecule 2: Laccase-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.12Å 62.10Å 124.63Å 90.00° 96.36° 90.00°	Depositor
Resolution (Å)	19.61 – 1.67 19.60 – 1.67	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.61-1.67) 97.5 (19.60-1.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.189 , 0.220 0.190 , 0.222	Depositor DCC
$R_{free}$ test set	7468 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 149347 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: OHI, CL, OXY, D2M, SO4, 3DM, KIA, 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	0.55	0/4603	0.69	2/6316 (0.0%)
2	B	0.54	0/4610	0.67	0/6329
All	All	0.54	0/9213	0.68	2/12645 (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
7	A	1	0
7	B	1	0
9	A	1	0
9	B	1	0
All	All	4	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	174	ASP	CB-CG-OD1	5.10	122.89	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	712	MAN	C1
9	A	732	MAN	C1
7	B	712	MAN	C1
9	B	732	MAN	C1



There are no planarity outliers.

## 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	4478	0	4201	27	0
2	B	4472	0	4199	29	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	28	0	26	0	0
6	B	42	0	39	0	0
7	A	50	0	43	0	0
7	B	50	0	43	3	0
8	A	84	0	75	1	0
8	B	56	0	50	0	0
9	A	39	0	34	0	0
9	B	39	0	34	0	0
10	A	10	0	0	0	0
10	B	5	0	0	0	0
11	A	11	0	3	3	0
12	B	22	0	13	9	0
13	B	12	0	8	5	0
14	A	506	0	0	6	0
14	B	447	0	0	6	0
All	All	10365	0	8768	58	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 3.

All (58) 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:B:68[A]:ASN:OD1	14:B:880:HOH:O	1.62	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:HH11	1:A:224:ARG:HG3	1.27	0.98
2:B:427[A]:PHE:CZ	12:B:2100[A]:D2M:O15	2.17	0.97
2:B:30[A]:THR:HG21	2:B:75:ASP:OD1	1.72	0.89
1:A:505:ILE:HA	14:A:986:HOH:O	1.73	0.88
2:B:427[B]:PHE:HE1	13:B:2910[B]:KIA:H8A	1.37	0.86
2:B:427[A]:PHE:CE2	12:B:2100[A]:D2M:O15	2.29	0.86
2:B:427[B]:PHE:CE1	13:B:2910[B]:KIA:H8A	2.12	0.85
1:A:295[A]:GLN:NE2	14:A:1039:HOH:O	2.11	0.83
2:B:427[A]:PHE:CZ	12:B:2100[A]:D2M:C2	2.61	0.83
2:B:178[A]:ARG:NH1	7:B:714:MAN:O2	2.12	0.82
1:A:224:ARG:CG	1:A:224:ARG:HH11	1.97	0.77
2:B:30[A]:THR:HG23	2:B:32:VAL:H	1.51	0.73
1:A:285:ASN:OD1	1:A:311:HIS:HD2	1.73	0.71
11:A:3900[B]:3DM:C4	13:B:2910[B]:KIA:O1	2.38	0.71
2:B:427[A]:PHE:CD2	12:B:2100[A]:D2M:O20	2.46	0.68
1:A:224:ARG:NH1	1:A:224:ARG:HG3	1.99	0.67
1:A:269:VAL:HG21	14:A:986:HOH:O	1.96	0.66
1:A:269:VAL:HG11	14:A:986:HOH:O	1.96	0.65
2:B:427[B]:PHE:CE1	13:B:2910[B]:KIA:C8	2.80	0.65
1:A:131:GLN:HG3	14:A:831:HOH:O	1.98	0.64
2:B:203:THR:OG1	14:B:974:HOH:O	2.16	0.63
1:A:178[A]:ARG:NH2	1:A:182[A]:ASP:OD1	2.27	0.62
1:A:40:LEU:CD2	1:A:60:ILE:HG12	2.30	0.61
2:B:427[B]:PHE:HA	2:B:456[B]:ARG:NH2	2.15	0.60
1:A:281:ARG:HB3	14:A:659:HOH:O	2.00	0.60
2:B:427[B]:PHE:HA	2:B:456[B]:ARG:HH22	1.66	0.59
2:B:4:CYS:SG	2:B:12[B]:CYS:HB3	2.42	0.58
1:A:192:PRO:HG2	11:A:3900[B]:3DM:H8B	1.88	0.56
1:A:40:LEU:HD21	1:A:60:ILE:HG12	1.89	0.54
1:A:311:HIS:HE1	8:A:721:NAG:O7	1.90	0.54
1:A:285:ASN:OD1	1:A:311:HIS:CD2	2.58	0.53
2:B:427[B]:PHE:CA	2:B:456[B]:ARG:HH22	2.23	0.51
1:A:4:CYS:SG	1:A:12:CYS:HB3	2.50	0.51
1:A:226:ARG:NH2	1:A:274:ASP:OD2	2.38	0.51
2:B:119:LYS:HE2	14:B:810:HOH:O	2.11	0.51
2:B:137:TYR:CZ	2:B:151:GLY:HA3	2.47	0.50
1:A:87:THR:HB	1:A:550:ASN:HD21	1.77	0.50
2:B:427[A]:PHE:CE2	12:B:2100[A]:D2M:C2	2.92	0.49
2:B:427[A]:PHE:CB	12:B:2100[A]:D2M:H11B	2.42	0.49
1:A:95:HIS:O	1:A:135:SER:HB3	2.12	0.49
1:A:137:TYR:CZ	1:A:151:GLY:HA3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:PRO:HD2	2:B:503:CYS:SG	2.54	0.47
2:B:178[A]:ARG:NH2	7:B:714:MAN:O2	2.47	0.46
2:B:131:GLN:HG3	14:B:746:HOH:O	2.16	0.45
1:A:176:TYR:CE2	1:A:195:SER:HA	2.52	0.45
1:A:192:PRO:CG	11:A:3900[B]:3DM:H8B	2.47	0.45
1:A:40:LEU:HD23	1:A:60:ILE:HG12	1.97	0.44
2:B:95:HIS:O	2:B:135:SER:HB3	2.18	0.44
2:B:427[A]:PHE:CE1	12:B:2100[A]:D2M:C2	3.01	0.43
2:B:178[A]:ARG:CZ	7:B:714:MAN:O2	2.65	0.43
1:A:429:LEU:HD11	12:B:2100[A]:D2M:O29	2.19	0.42
2:B:131:GLN:CD	14:B:813:HOH:O	2.57	0.42
1:A:65[B]:MET:HG2	1:A:150:VAL:HG13	2.02	0.42
2:B:427[B]:PHE:CZ	13:B:2910[B]:KIA:C3	3.04	0.41
1:A:65[B]:MET:HE2	1:A:150:VAL:HG22	2.03	0.41
2:B:86:VAL:HA	2:B:119:LYS:HE3	2.02	0.41
12:B:2100[A]:D2M:H33B	14:B:989:HOH:O	2.21	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	569/559 (102%)	555 (98%)	14 (2%)	0	100	100
2	B	570/559 (102%)	554 (97%)	16 (3%)	0	100	100
All	All	1139/1118 (102%)	1109 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.



### 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	490/477 (103%)	486 (99%)	4 (1%)	86	78
2	B	491/478 (103%)	484 (99%)	7 (1%)	74	57
All	All	981/955 (103%)	970 (99%)	11 (1%)	82	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	123	ARG
1	A	140	HIS
1	A	224	ARG
2	B	100	LYS
2	B	109	ASN
2	B	123	ARG
2	B	140	HIS
2	B	244	ASN
2	B	345[A]	SER
2	B	345[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	HIS
1	A	550	ASN
2	B	99	GLN
2	B	144	GLN
2	B	455	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

1 non-standard protein/DNA/RNA residue is 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	OHI	A	98	1	10,11,12	1.19	1 (10%)	4,14,16	2.52	2 (50%)

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	OHI	A	98	1	-	0/2/15/17	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	OHI	O12-CE1	2.91	1.28	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	OHI	O-C-CA	-3.62	116.07	125.49
1	A	98	OHI	CA-CB-CG	-3.47	107.20	114.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

24 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	$\# Z  > 2$
7	NAG	A	710	1,7	14,14,15	0.73	0	15,19,21	0.71	0
7	NAG	A	711	7	14,14,15	0.48	0	15,19,21	0.99	1 (6%)
7	MAN	A	712	7	11,11,12	0.50	0	14,15,17	1.39	2 (14%)
7	MAN	A	714	7	11,11,12	0.66	0	14,15,17	0.86	0
8	NAG	A	720	1,8	14,14,15	0.53	0	15,19,21	1.25	1 (6%)
8	NAG	A	721	8	14,14,15	0.50	0	15,19,21	0.90	0
9	NAG	A	730	1,9	14,14,15	0.70	1 (7%)	15,19,21	0.70	0
9	NAG	A	731	9	14,14,15	0.50	0	15,19,21	1.10	1 (6%)
9	MAN	A	732	9	11,11,12	0.64	0	14,15,17	1.56	3 (21%)
8	NAG	A	740	1,8	14,14,15	0.55	0	15,19,21	1.35	2 (13%)
8	NAG	A	741	8	14,14,15	0.52	0	15,19,21	0.86	1 (6%)
8	NAG	A	760	1,8	14,14,15	0.74	0	15,19,21	0.66	0
8	NAG	A	761	8	14,14,15	0.48	0	15,19,21	1.12	1 (6%)
7	NAG	B	710	2,7	14,14,15	0.45	0	15,19,21	0.84	0
7	NAG	B	711	7	14,14,15	0.60	0	15,19,21	0.85	0
7	MAN	B	712	7	11,11,12	0.58	0	14,15,17	0.96	0
7	MAN	B	714	7	11,11,12	0.57	0	14,15,17	1.59	2 (14%)
8	NAG	B	720	8,2	14,14,15	0.51	0	15,19,21	1.09	2 (13%)
8	NAG	B	721	8	14,14,15	0.52	0	15,19,21	1.03	1 (6%)
9	NAG	B	730	9,2	14,14,15	0.62	0	15,19,21	0.88	0
9	NAG	B	731	9	14,14,15	0.62	0	15,19,21	0.93	1 (6%)
9	MAN	B	732	9	11,11,12	0.57	0	14,15,17	1.08	1 (7%)
8	NAG	B	740	8,2	14,14,15	0.54	0	15,19,21	1.09	0
8	NAG	B	741	8	14,14,15	0.50	0	15,19,21	1.06	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
7	NAG	A	710	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	711	7	-	0/6/23/26	0/1/1/1
7	MAN	A	712	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	A	714	7	-	0/2/19/22	0/1/1/1
8	NAG	A	720	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	721	8	-	0/6/23/26	0/1/1/1
9	NAG	A	730	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	731	9	-	0/6/23/26	0/1/1/1
9	MAN	A	732	9	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	A	740	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	741	8	-	0/6/23/26	0/1/1/1
8	NAG	A	760	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	761	8	-	0/6/23/26	0/1/1/1
7	NAG	B	710	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	711	7	-	0/6/23/26	0/1/1/1
7	MAN	B	712	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	B	714	7	-	0/2/19/22	0/1/1/1
8	NAG	B	720	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	721	8	-	0/6/23/26	0/1/1/1
9	NAG	B	730	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	731	9	-	0/6/23/26	0/1/1/1
9	MAN	B	732	9	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	B	740	8,2	-	0/6/23/26	0/1/1/1
8	NAG	B	741	8	-	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)
9	A	730	NAG	O5-C1	-2.09	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	741	NAG	C2-N2-C7	-2.67	119.61	123.04
8	B	720	NAG	O4-C4-C5	-2.48	102.67	109.24
8	B	721	NAG	O7-C7-C8	-2.21	118.01	122.06
8	A	740	NAG	O7-C7-C8	-2.07	118.27	122.06
8	A	741	NAG	C2-N2-C7	-2.02	120.45	123.04
8	A	761	NAG	C1-O5-C5	2.13	114.95	112.25
9	B	731	NAG	C4-C3-C2	2.21	114.66	111.23
8	B	741	NAG	C1-O5-C5	2.22	115.07	112.25
9	A	732	MAN	C1-C2-C3	2.30	112.26	109.54
8	B	720	NAG	C1-O5-C5	2.33	115.20	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	731	NAG	C4-C3-C2	2.46	115.05	111.23
7	A	712	MAN	C1-C2-C3	2.46	112.45	109.54
9	B	732	MAN	C1-C2-C3	2.52	112.53	109.54
7	A	711	NAG	C1-O5-C5	2.81	115.82	112.25
9	A	732	MAN	C2-C3-C4	2.82	115.83	111.04
7	B	714	MAN	C1-O5-C5	3.00	116.06	112.25
8	A	720	NAG	C1-O5-C5	3.09	116.17	112.25
7	B	714	MAN	C1-C2-C3	3.33	113.48	109.54
8	A	740	NAG	C1-O5-C5	3.65	116.88	112.25
9	A	732	MAN	C3-C4-C5	3.65	116.57	110.20
7	A	712	MAN	C1-O5-C5	4.26	117.66	112.25

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	712	MAN	C1
9	B	732	MAN	C1
9	A	732	MAN	C1
7	A	712	MAN	C1

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
8	A	721	NAG	1	0
7	B	714	MAN	3	0

## 5.6 Ligand geometry

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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
5	OXY	A	1620	3	1,1,1	1.02	0	0,0,0	0.00	-
10	SO4	A	3800	-	4,4,4	0.23	0	6,6,6	0.19	0
10	SO4	A	3801	-	4,4,4	0.22	0	6,6,6	0.11	0
11	3DM	A	3900[B]	-	11,11,11	3.03	2 (18%)	14,14,14	3.96	5 (35%)
6	NAG	A	700	1	14,14,15	0.68	0	15,19,21	0.97	1 (6%)
6	NAG	A	750	1	14,14,15	0.60	0	15,19,21	0.75	0
5	OXY	B	1620	3	1,1,1	1.01	0	0,0,0	0.00	-
6	NAG	B	1750	2	14,14,15	0.59	0	15,19,21	1.07	1 (6%)
12	D2M	B	2100[A]	-	23,23,23	0.55	0	31,31,31	2.29	13 (41%)
6	NAG	B	2760	2	14,14,15	0.59	0	15,19,21	0.94	0
13	KIA	B	2910[B]	-	12,12,12	1.08	2 (16%)	16,16,16	1.82	6 (37%)
10	SO4	B	4802	-	4,4,4	0.19	0	6,6,6	0.10	0
6	NAG	B	700	2	14,14,15	0.67	0	15,19,21	1.03	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
5	OXY	A	1620	3	-	0/0/0/0	0/0/0/0
10	SO4	A	3800	-	-	0/0/0/0	0/0/0/0
10	SO4	A	3801	-	-	0/0/0/0	0/0/0/0
11	3DM	A	3900[B]	-	-	0/4/4/4	0/1/1/1
6	NAG	A	700	1	-	0/6/23/26	0/1/1/1
6	NAG	A	750	1	-	0/6/23/26	0/1/1/1
5	OXY	B	1620	3	-	0/0/0/0	0/0/0/0
6	NAG	B	1750	2	-	0/6/23/26	0/1/1/1
12	D2M	B	2100[A]	-	-	0/12/12/12	0/2/2/2
6	NAG	B	2760	2	-	0/6/23/26	0/1/1/1
13	KIA	B	2910[B]	-	-	2/4/20/20	0/1/1/1
10	SO4	B	4802	-	-	0/0/0/0	0/0/0/0
6	NAG	B	700	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	2910[B]	KIA	C3-C4	-2.11	1.40	1.45
13	B	2910[B]	KIA	C5-C4	-2.02	1.40	1.45
11	A	3900[B]	3DM	C2-C1	6.55	1.49	1.40
11	A	3900[B]	3DM	C6-C1	7.44	1.50	1.40



All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	3900[B]	3DM	O3-C6-C5	-4.73	116.40	124.35
12	B	2100[A]	D2M	O31-C24-C22	-2.98	119.13	124.21
12	B	2100[A]	D2M	O10-C4-C5	-2.74	119.75	124.35
12	B	2100[A]	D2M	O15-C2-C1	-2.59	120.00	124.35
11	A	3900[B]	3DM	O2-C2-C3	-2.51	120.13	124.35
12	B	2100[A]	D2M	O32-C26-C23	-2.38	120.14	124.21
13	B	2910[B]	KIA	O4-C2-C3	-2.01	121.01	125.70
13	B	2910[B]	KIA	C5-C4-C3	2.10	121.75	117.17
12	B	2100[A]	D2M	C11-O10-C4	2.24	120.94	117.54
6	A	700	NAG	C1-O5-C5	2.30	115.17	112.25
12	B	2100[A]	D2M	C34-O32-C26	2.32	121.05	117.54
12	B	2100[A]	D2M	C16-O15-C2	2.35	121.11	117.54
13	B	2910[B]	KIA	C7-O3-C6	2.59	122.01	116.98
13	B	2910[B]	KIA	C8-O4-C2	2.60	122.03	116.98
12	B	2100[A]	D2M	O15-C2-C3	2.70	120.14	115.26
6	B	700	NAG	C1-O5-C5	2.72	115.70	112.25
6	B	1750	NAG	C1-O5-C5	2.81	115.81	112.25
12	B	2100[A]	D2M	O10-C4-C3	2.82	120.34	115.26
12	B	2100[A]	D2M	C21-O20-C3	2.92	123.54	118.46
13	B	2910[B]	KIA	O3-C6-C1	3.03	120.10	111.88
13	B	2910[B]	KIA	O4-C2-C1	3.16	120.44	111.88
12	B	2100[A]	D2M	C33-O31-C24	3.73	123.20	117.54
11	A	3900[B]	3DM	O2-C2-C1	5.24	119.74	114.47
12	B	2100[A]	D2M	O32-C26-C28	5.40	119.91	114.47
11	A	3900[B]	3DM	C8-O3-C6	5.97	126.60	117.54
12	B	2100[A]	D2M	O31-C24-C28	6.76	121.28	114.47
11	A	3900[B]	3DM	O3-C6-C1	10.70	125.23	114.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	2910[B]	KIA	C8-O4-C2-C1
13	B	2910[B]	KIA	C8-O4-C2-C3

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	3900[B]	3DM	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	2100[A]	D2M	9	0
13	B	2910[B]	KIA	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	558/559 (99%)	-0.09	6 (1%) 82 85	7, 14, 24, 36	0
2	B	559/559 (100%)	-0.01	9 (1%) 74 78	8, 15, 26, 36	0
All	All	1117/1118 (99%)	-0.05	15 (1%) 79 82	7, 14, 25, 36	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	462	ALA	4.9
2	B	1	GLU	4.0
1	A	368	THR	3.7
1	A	463	VAL	3.4
1	A	462	ALA	3.2
1	A	1	GLU	3.2
2	B	314	GLY	3.1
2	B	3	THR	3.0
2	B	318	GLY	2.8
1	A	12	CYS	2.6
1	A	3	THR	2.6
2	B	2	PRO	2.3
2	B	321	THR	2.1
2	B	368	THR	2.1
2	B	4	CYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
1	OHI	A	98	11/12	0.90	0.12	-	14,18,24,25	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( $\text{\AA}^2$ )	Q<0.9
8	NAG	A	760	14/15	0.87	0.16	4.14	21,24,31,32	0
8	NAG	A	720	14/15	0.84	0.15	1.73	22,25,28,32	0
8	NAG	A	740	14/15	0.88	0.11	1.56	15,18,26,28	0
9	NAG	A	731	14/15	0.90	0.13	1.45	19,23,29,32	0
8	NAG	B	740	14/15	0.90	0.10	1.20	18,21,25,27	0
9	NAG	B	731	14/15	0.89	0.15	1.06	22,27,30,32	0
8	NAG	B	721	14/15	0.85	0.20	1.04	28,33,36,36	0
8	NAG	A	721	14/15	0.89	0.15	1.03	24,28,30,31	0
8	NAG	B	720	14/15	0.85	0.13	0.07	25,28,29,31	0
9	NAG	A	730	14/15	0.93	0.09	-0.20	14,16,20,21	0
7	NAG	A	711	14/15	0.94	0.10	-0.31	15,19,25,29	0
7	NAG	A	710	14/15	0.97	0.08	-0.98	9,10,14,14	0
9	NAG	B	730	14/15	0.97	0.07	-1.08	16,19,22,22	0
7	NAG	B	711	14/15	0.96	0.06	-1.51	16,19,26,29	0
7	NAG	B	710	14/15	0.97	0.06	-1.75	10,13,15,15	0
7	MAN	B	712	11/12	0.72	0.23	-	31,35,38,40	0
7	MAN	A	714	11/12	0.74	0.24	-	35,36,37,37	0
8	NAG	A	741	14/15	0.83	0.26	-	30,33,38,39	0
8	NAG	B	741	14/15	0.79	0.29	-	32,36,39,39	0
9	MAN	B	732	11/12	0.79	0.36	-	37,40,41,41	0
9	MAN	A	732	11/12	0.74	0.29	-	36,39,42,43	0
7	MAN	A	712	11/12	0.71	0.27	-	29,34,35,36	0
8	NAG	A	761	14/15	0.78	0.40	-	37,41,43,44	0
7	MAN	B	714	11/12	0.65	0.27	-	43,44,45,46	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
5	OXY	A	1620	2/2	0.98	0.30	29.53	22,22,22,24	0
5	OXY	B	1620	2/2	0.98	0.24	20.29	20,20,20,21	0
6	NAG	A	700	14/15	0.88	0.16	8.90	19,22,26,28	0
6	NAG	B	2760	14/15	0.85	0.15	6.44	22,25,29,31	0
11	3DM	A	3900[B]	11/11	0.55	0.26	6.06	24,26,28,28	11
4	CL	B	610	1/1	0.99	0.15	6.04	22,22,22,22	0
12	D2M	B	2100[A]	22/22	0.83	0.23	4.43	62,62,62,62	22
6	NAG	B	700	14/15	0.90	0.15	3.29	21,24,27,31	0
6	NAG	A	750	14/15	0.84	0.20	2.84	28,33,36,36	0
13	KIA	B	2910[B]	12/12	0.80	0.16	1.43	28,29,29,29	12
6	NAG	B	1750	14/15	0.93	0.09	0.72	14,18,21,23	0
4	CL	A	610	1/1	1.00	0.07	-0.01	20,20,20,20	0
10	SO4	A	3801	5/5	0.95	0.10	-0.42	45,46,46,46	0
3	CU	B	602	1/1	1.00	0.06	-1.21	17,17,17,17	0
3	CU	A	601	1/1	1.00	0.02	-3.06	13,13,13,13	0
3	CU	B	604	1/1	1.00	0.04	-3.95	18,18,18,18	0
3	CU	A	602	1/1	1.00	0.04	-4.03	16,16,16,16	0
3	CU	B	601	1/1	1.00	0.02	-4.47	14,14,14,14	0
3	CU	A	603	1/1	1.00	0.02	-6.10	13,13,13,13	0
3	CU	A	604	1/1	1.00	0.03	-6.27	16,16,16,16	0
3	CU	B	603	1/1	1.00	0.02	-6.85	15,15,15,15	0
10	SO4	A	3800	5/5	0.93	0.09	-	58,59,59,59	0
10	SO4	B	4802	5/5	0.91	0.13	-	62,62,62,62	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.