



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:36 am BST

PDB ID : 3LOY  
Title : Crystal structure of a Copper-containing benzylamine oxidase from Hansenula Polymorpha  
Authors : Klema, V.J.; Johnson, B.J.; Wilmot, C.M.  
Deposited on : 2010-02-04  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

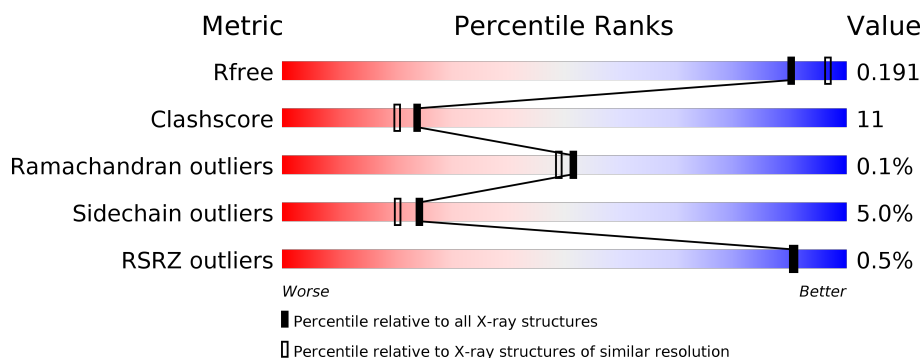
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	633	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>83%</span> <span>14%</span> <span>..</span> </div> </div>
1	B	633	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>77%</span> <span>19%</span> <span>..</span> </div> </div>
1	C	633	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>15%</span> <span>..</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
3	GOL	A	637	-	X	-	-
3	GOL	B	639	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18610 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 copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	6	0
			5115	3275	870	944	26			
1	B	633	Total	C	N	O	S	0	6	0
			5120	3276	874	943	27			
1	C	633	Total	C	N	O	S	0	1	0
			5086	3255	867	939	25			

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

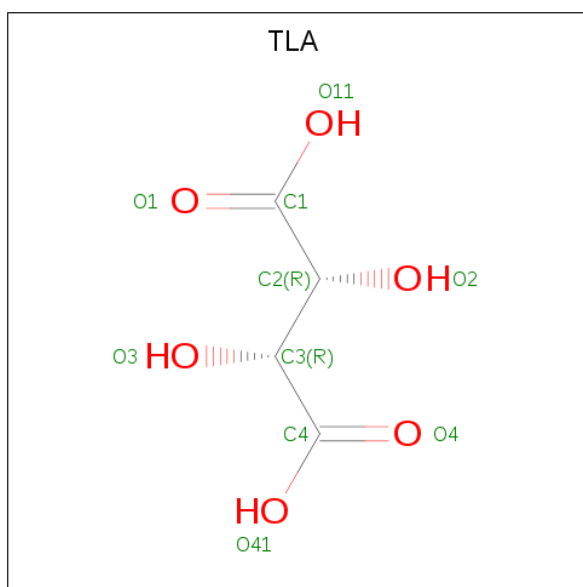
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



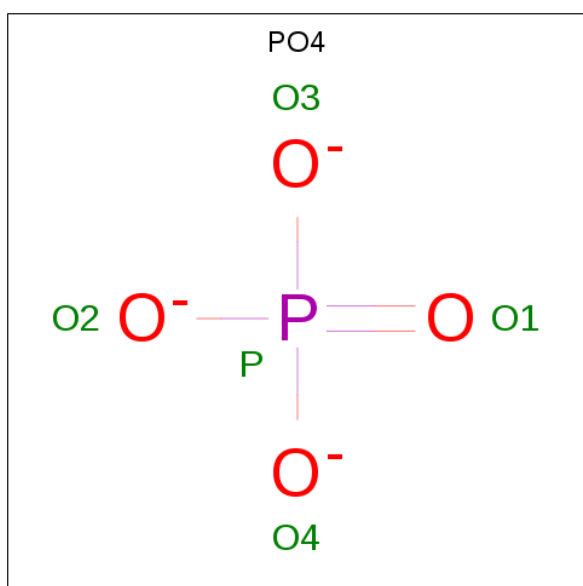
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

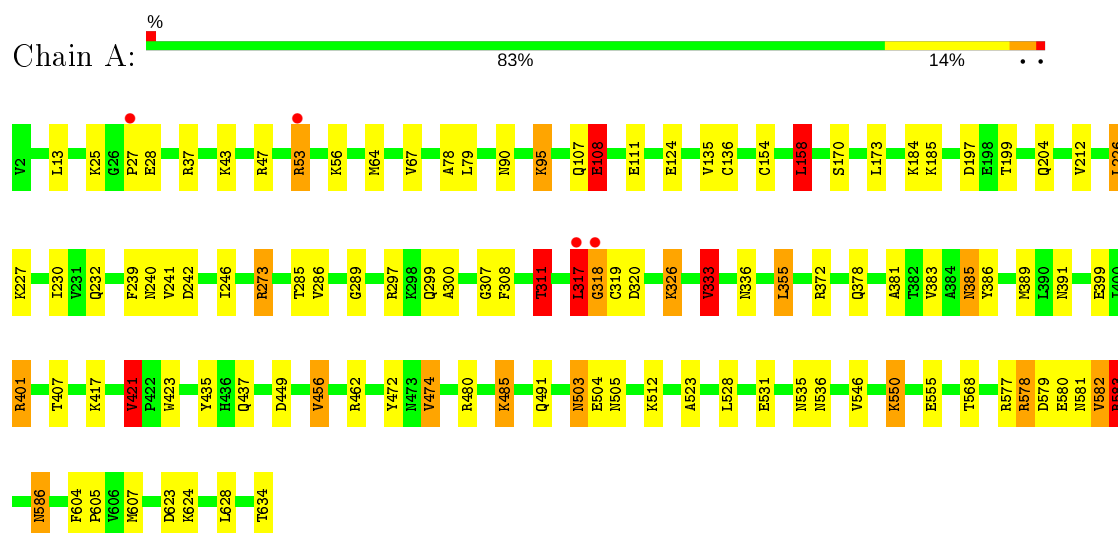
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1028	Total 1028	O 1028	0	0
6	B	1051	Total 1051	O 1051	0	0
6	C	1116	Total 1116	O 1116	0	0

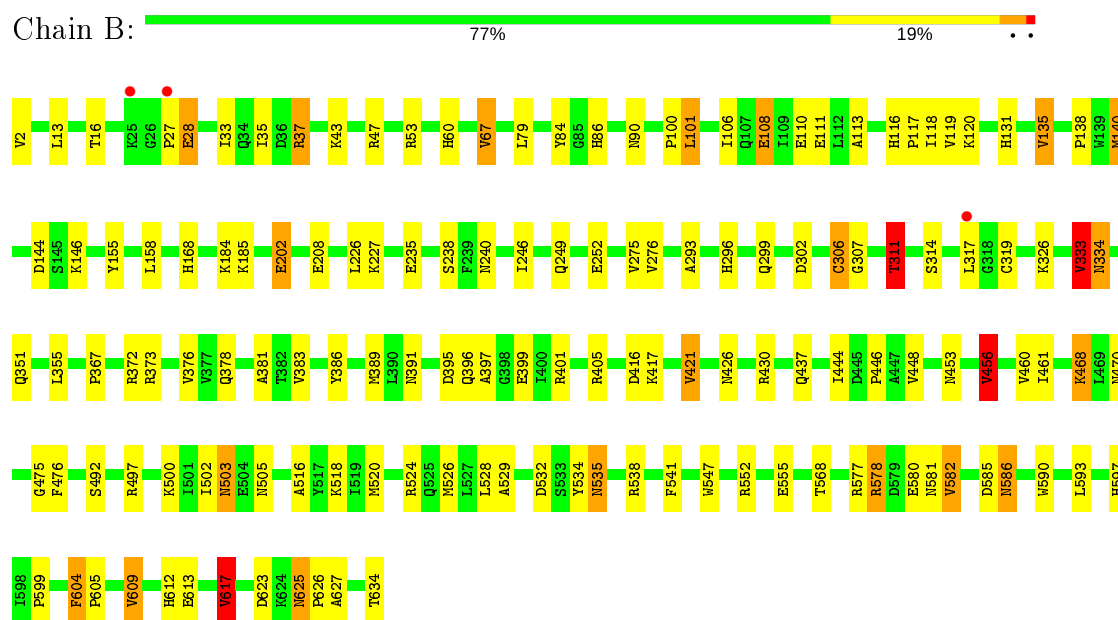
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: copper amine oxidase




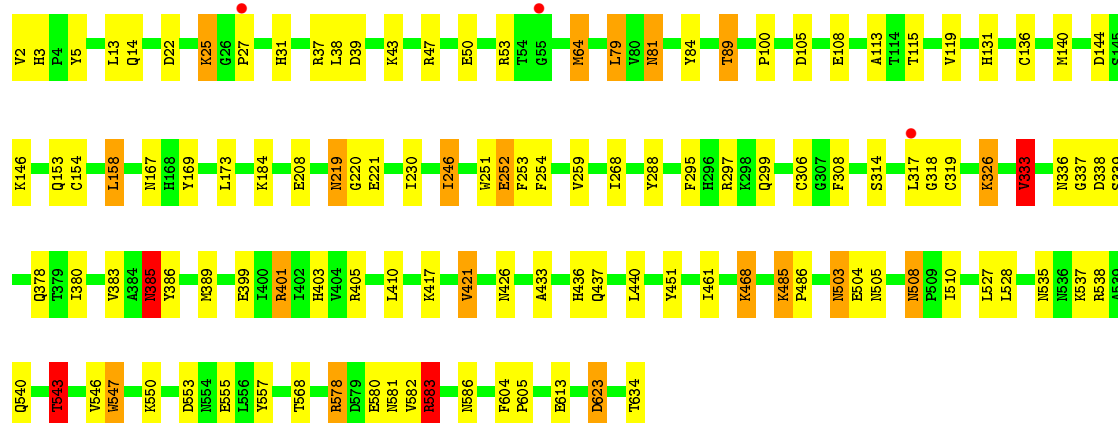
- Molecule 1: copper amine oxidase



- Molecule 1: copper amine oxidase



Chain C:  81% 15% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	288.51Å 91.06Å 151.10Å 90.00° 117.23° 90.00°	Depositor
Resolution (Å)	37.42 – 2.00 37.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.4 (37.42-2.00) 90.4 (37.42-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.145 , 0.191 0.146 , 0.191	Depositor DCC
$R_{free}$ test set	10514 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18610	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: GOL, PO4, CU, TLA, TPQ

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	1.17	3/5253 (0.1%)	1.08	22/7149 (0.3%)
1	B	1.22	13/5255 (0.2%)	1.05	16/7151 (0.2%)
1	C	1.25	7/5212 (0.1%)	1.06	21/7096 (0.3%)
All	All	1.21	23/15720 (0.1%)	1.06	59/21396 (0.3%)

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	2
1	C	0	1
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CB-CG	-8.01	1.36	1.52
1	C	295	PHE	CE1-CZ	7.79	1.52	1.37
1	B	202	GLU	CG-CD	7.31	1.62	1.51
1	C	546	VAL	CB-CG2	-7.24	1.37	1.52
1	C	254	PHE	CE1-CZ	6.72	1.50	1.37
1	B	306[A]	CYS	CB-SG	-6.52	1.71	1.82
1	B	306[B]	CYS	CB-SG	-6.52	1.71	1.82
1	B	541	PHE	CE1-CZ	6.41	1.49	1.37
1	C	451	TYR	CD1-CE1	6.29	1.48	1.39
1	B	613	GLU	CB-CG	-6.11	1.40	1.52
1	B	155	TYR	CD1-CE1	5.61	1.47	1.39
1	A	555	GLU	CB-CG	-5.59	1.41	1.52
1	C	547	TRP	CE3-CZ3	5.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	557	TYR	CD2-CE2	5.43	1.47	1.39
1	B	604	PHE	CE2-CZ	5.34	1.47	1.37
1	C	306	CYS	CB-SG	5.23	1.91	1.82
1	B	520	MET	CG-SD	-5.16	1.67	1.81
1	B	421	VAL	CB-CG1	-5.16	1.42	1.52
1	B	319	CYS	CB-SG	5.14	1.91	1.82
1	B	397	ALA	CA-CB	5.12	1.63	1.52
1	B	460	VAL	CB-CG2	5.12	1.63	1.52
1	B	37	ARG	CG-CD	-5.09	1.39	1.51
1	A	135	VAL	CB-CG2	5.04	1.63	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	ARG	NE-CZ-NH1	15.74	128.17	120.30
1	A	578	ARG	NE-CZ-NH2	-14.90	112.85	120.30
1	B	578	ARG	NE-CZ-NH2	-13.37	113.61	120.30
1	C	583	ARG	NE-CZ-NH1	12.97	126.78	120.30
1	A	583	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	C	578	ARG	NE-CZ-NH2	-12.07	114.27	120.30
1	C	401	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	A	578	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	A	64	MET	CG-SD-CE	-10.22	83.84	100.20
1	A	297	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	583	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	333	VAL	CB-CA-C	-8.86	94.58	111.40
1	B	456	VAL	CG1-CB-CG2	8.53	124.55	110.90
1	C	333	VAL	CB-CA-C	-8.50	95.25	111.40
1	A	582	VAL	CG1-CB-CG2	8.49	124.49	110.90
1	B	333	VAL	CB-CA-C	-8.35	95.54	111.40
1	B	609	VAL	CG1-CB-CG2	8.28	124.15	110.90
1	B	578	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	C	421	VAL	CG1-CB-CG2	7.72	123.26	110.90
1	A	333	VAL	CG1-CB-CG2	7.59	123.04	110.90
1	B	617	VAL	CG1-CB-CG2	-7.58	98.77	110.90
1	B	395	ASP	CB-CG-OD1	7.43	124.99	118.30
1	B	67	VAL	CB-CA-C	-7.22	97.69	111.40
1	C	333	VAL	CG1-CB-CG2	7.18	122.38	110.90
1	A	474	VAL	CG1-CB-CG2	7.12	122.30	110.90
1	A	456	VAL	CG1-CB-CG2	7.01	122.11	110.90
1	A	421	VAL	CG1-CB-CG2	6.84	121.85	110.90
1	B	582	VAL	CG1-CB-CG2	6.71	121.63	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	311	THR	N-CA-CB	-6.56	97.83	110.30
1	C	578	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	197	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	395	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	B	333	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	C	64	MET	CG-SD-CE	-6.16	90.34	100.20
1	C	22	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	623	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	79	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	135	VAL	CG1-CB-CG2	5.82	120.22	110.90
1	A	546	VAL	CG1-CB-CG2	-5.71	101.76	110.90
1	A	311	THR	CA-CB-CG2	5.52	120.13	112.40
1	C	246	ILE	CG1-CB-CG2	-5.44	99.44	111.40
1	B	416	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	449	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	543	THR	N-CA-CB	-5.25	100.33	110.30
1	A	480	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	C	333	VAL	CA-CB-CG2	5.24	118.75	110.90
1	A	158	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	38	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	C	39	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	C	543	THR	CA-CB-CG2	5.12	119.57	112.40
1	C	421	VAL	N-CA-CB	-5.11	100.27	111.50
1	C	538	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	319	CYS	N-CA-C	-5.09	97.25	111.00
1	B	421	VAL	CG1-CB-CG2	5.09	119.04	110.90
1	C	553	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	37	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	623	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	550	LYS	CD-CE-NZ	-5.01	100.17	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	LEU	Peptide
1	A	318	GLY	Peptide
1	C	385	ASN	Mainchain

## 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	5115	0	5032	87	0
1	B	5120	0	5034	145	1
1	C	5086	0	4991	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	24	0	32	2	0
3	B	24	0	31	9	0
3	C	18	0	24	3	0
4	A	10	0	4	0	0
4	C	10	0	4	1	0
5	B	5	0	0	0	0
6	A	1028	0	0	36	0
6	B	1051	0	0	44	1
6	C	1116	0	0	46	0
All	All	18610	0	15152	340	2

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 11.

All (340) 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:623:ASP:HB3	6:A:3187:HOH:O	1.15	1.32
1:C:623:ASP:HB3	6:C:2705:HOH:O	1.20	1.30
1:B:623:ASP:HB3	6:B:1917:HOH:O	1.28	1.28
1:B:43:LYS:HB2	6:B:1590:HOH:O	1.27	1.27
1:C:634:THR:HA	6:C:2441:HOH:O	1.49	1.11
1:B:378:GLN:NE2	1:B:389[B]:MET:CG	2.13	1.11
1:B:351:GLN:HE22	3:B:639:GOL:H11	1.13	1.10
1:B:108:GLU:HG2	1:B:184:LYS:HE2	1.31	1.10
1:B:468:LYS:HE3	1:B:468:LYS:H	1.16	1.08
1:C:468:LYS:H	1:C:468:LYS:CD	1.66	1.08
1:B:378:GLN:HE21	1:B:389[B]:MET:CG	1.67	1.07
1:B:586:ASN:HB2	6:B:812:HOH:O	1.57	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PRO:HD2	6:A:2499:HOH:O	1.56	1.03
1:C:468:LYS:N	1:C:468:LYS:HD2	1.71	1.02
1:C:314:SER:HB3	6:C:1988:HOH:O	1.58	1.02
1:A:124:GLU:HG3	6:A:1791:HOH:O	1.59	1.02
1:C:468:LYS:H	1:C:468:LYS:HD2	0.86	1.01
1:C:64:MET:HE1	6:C:2721:HOH:O	1.61	0.98
1:B:378:GLN:NE2	1:B:389[B]:MET:HG3	1.79	0.94
1:B:202:GLU:HG3	6:B:3257:HOH:O	1.66	0.93
1:B:378:GLN:HE21	1:B:389[B]:MET:HG2	1.32	0.93
1:C:403:HIS:HE1	1:C:405:ARG:HE	1.05	0.93
1:A:25:LYS:HE2	6:A:2315:HOH:O	1.68	0.93
1:A:581:ASN:OD1	6:A:3260:HOH:O	1.86	0.93
1:B:140:MET:CE	6:B:1901:HOH:O	2.16	0.91
1:B:2:VAL:HG12	6:B:1378:HOH:O	1.69	0.91
1:B:252:GLU:HG2	6:B:2468:HOH:O	1.70	0.90
1:C:79:LEU:HB2	1:C:89:THR:HG22	1.51	0.90
1:B:448:VAL:H	1:B:453:ASN:HD21	1.10	0.89
1:C:64:MET:SD	6:C:2721:HOH:O	2.31	0.88
1:B:378:GLN:NE2	1:B:389[B]:MET:SD	2.45	0.86
1:A:43[A]:LYS:HD3	6:A:2602:HOH:O	1.76	0.85
1:A:550:LYS:HE3	6:A:2363:HOH:O	1.73	0.85
1:C:79:LEU:HD13	6:C:896:HOH:O	1.77	0.85
1:B:468:LYS:HE3	1:B:468:LYS:N	1.91	0.84
1:A:318:GLY:HA2	6:A:2462:HOH:O	1.77	0.84
1:B:468:LYS:CE	1:B:468:LYS:H	1.92	0.83
1:C:14:GLN:HE21	1:C:339:SER:H	1.26	0.83
1:C:64:MET:CE	6:C:2721:HOH:O	2.22	0.82
1:A:184:LYS:HE3	6:A:1318:HOH:O	1.80	0.82
1:B:202:GLU:CD	1:B:202:GLU:H	1.84	0.81
1:B:468:LYS:HD3	6:B:1087:HOH:O	1.80	0.81
1:C:113:ALA:O	1:C:119:VAL:HG11	1.81	0.81
1:A:240:ASN:HB2	6:A:1862:HOH:O	1.81	0.80
1:A:299:GLN:HE22	1:A:535:ASN:HA	1.47	0.79
1:B:28:GLU:HB3	6:B:1372:HOH:O	1.82	0.79
1:C:437:GLN:HE22	1:C:528:LEU:H	1.30	0.79
1:A:437:GLN:HE22	1:A:528:LEU:H	1.31	0.78
1:B:351:GLN:NE2	3:B:639:GOL:H11	1.96	0.78
1:C:144:ASP:OD1	3:C:639:GOL:H31	1.82	0.78
1:B:372:ARG:NH1	1:B:401[B]:ARG:NH1	2.31	0.78
1:C:634:THR:HB	6:C:1080:HOH:O	1.84	0.78
1:B:27:PRO:HD2	6:B:2485:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:LEU:HD21	1:B:333:VAL:HG13	1.65	0.77
1:C:540:GLN:O	1:C:543:THR:HB	1.83	0.77
1:A:108:GLU:HG2	1:A:184:LYS:HE2	1.65	0.77
1:A:13:LEU:HD21	1:A:333:VAL:HG13	1.66	0.77
1:A:378:GLN:OE1	1:A:389[B]:MET:HG3	1.84	0.77
1:C:403:HIS:CE1	1:C:405:ARG:HE	1.97	0.76
1:C:153:GLN:HE21	1:C:297:ARG:HH22	1.34	0.75
1:C:317:LEU:HD23	6:C:2524:HOH:O	1.85	0.75
3:B:639:GOL:H12	6:B:2035:HOH:O	1.85	0.75
1:B:116:HIS:HD2	1:B:118:ILE:H	1.32	0.74
1:C:140:MET:SD	6:C:2290:HOH:O	2.46	0.73
1:C:317:LEU:HD21	6:C:2087:HOH:O	1.89	0.73
1:A:378:GLN:OE1	1:A:389[B]:MET:CG	2.36	0.72
1:C:468:LYS:HG3	6:C:2091:HOH:O	1.87	0.72
1:B:334:ASN:C	1:B:334:ASN:HD22	1.93	0.72
3:B:639:GOL:H2	6:B:2313:HOH:O	1.88	0.72
3:C:638:GOL:H32	6:C:981:HOH:O	1.89	0.72
1:B:2:VAL:CG1	6:B:1378:HOH:O	2.32	0.71
1:B:577:ARG:HD3	6:B:2040:HOH:O	1.88	0.71
1:B:518:LYS:HE3	1:B:617:VAL:HG11	1.72	0.70
1:B:140:MET:HE1	6:B:1901:HOH:O	1.81	0.70
1:B:108:GLU:HG2	1:B:184:LYS:CE	2.17	0.70
1:B:208:GLU:OE1	1:B:417:LYS:HE3	1.92	0.70
1:A:311:THR:HG23	1:A:381:ALA:HB1	1.73	0.70
1:B:35:ILE:HG12	1:B:67:VAL:HG13	1.72	0.70
1:B:389[B]:MET:HE1	1:B:405:ARG:HD2	1.71	0.70
1:B:111[A]:GLU:HG3	6:B:2658:HOH:O	1.92	0.69
1:A:25:LYS:CE	6:A:2315:HOH:O	2.31	0.69
1:B:311:THR:HG23	1:B:381:ALA:HB1	1.75	0.68
1:C:3:HIS:HD2	1:C:5:TYR:H	1.40	0.68
1:B:311:THR:CG2	1:B:381:ALA:HB1	2.22	0.68
1:A:107[B]:GLN:HG3	6:A:3167:HOH:O	1.93	0.68
1:B:437:GLN:HE22	1:B:528:LEU:H	1.41	0.68
1:C:89:THR:HG23	6:C:640:HOH:O	1.94	0.67
1:B:389[B]:MET:HE1	1:B:405:ARG:CD	2.23	0.67
1:B:581:ASN:OD1	6:B:3224:HOH:O	2.11	0.67
1:A:437:GLN:NE2	1:A:528:LEU:H	1.92	0.66
1:C:153:GLN:NE2	1:C:297:ARG:HH12	1.94	0.66
1:C:27:PRO:HD2	6:C:2376:HOH:O	1.96	0.65
1:B:625:ASN:ND2	1:B:627:ALA:H	1.93	0.65
1:A:336[B]:ASN:OD1	6:A:2397:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:HIS:CD2	1:B:118:ILE:H	2.15	0.65
1:C:13:LEU:HD21	1:C:333:VAL:HG13	1.78	0.65
1:B:401[B]:ARG:HD3	6:B:2531:HOH:O	1.97	0.64
1:C:437:GLN:NE2	1:C:528:LEU:H	1.94	0.64
1:C:319:CYS:O	6:C:3253:HOH:O	2.14	0.64
1:A:311:THR:CG2	1:A:381:ALA:HB1	2.28	0.64
1:C:336:ASN:HB2	6:C:3272:HOH:O	1.97	0.64
1:C:485:LYS:HB2	1:C:486:PRO:HD2	1.80	0.63
1:C:153:GLN:HE22	1:C:297:ARG:HH12	1.44	0.63
1:B:524:ARG:HH12	1:B:612:HIS:CD2	2.16	0.63
1:B:468:LYS:HE2	6:B:2451:HOH:O	1.99	0.63
1:B:399:GLU:OE1	6:B:2531:HOH:O	2.15	0.63
1:B:372:ARG:NH1	1:B:401[B]:ARG:HH12	1.95	0.63
1:C:252:GLU:HG3	6:C:733:HOH:O	1.99	0.63
1:A:95:LYS:HE2	6:A:1863:HOH:O	1.99	0.62
1:B:43:LYS:HE3	1:B:47:ARG:HH12	1.64	0.62
1:A:185:LYS:HE3	6:A:1062:HOH:O	1.99	0.62
1:C:385:ASN:HD22	1:C:385:ASN:H	1.47	0.62
1:C:14:GLN:NE2	1:C:339:SER:H	1.94	0.62
1:A:389[A]:MET:HE2	1:B:355:LEU:HD12	1.80	0.62
1:C:79:LEU:HB3	6:C:896:HOH:O	1.99	0.62
1:C:385:ASN:H	1:C:385:ASN:ND2	1.97	0.62
1:C:508:ASN:ND2	1:C:510:ILE:H	1.98	0.62
1:C:89:THR:HG21	6:C:2488:HOH:O	1.99	0.62
1:B:351:GLN:HE22	3:B:639:GOL:C1	2.01	0.61
1:B:116:HIS:HE1	4:C:637:TLA:O41	1.83	0.61
1:B:293:ALA:HA	1:B:296:HIS:HD2	1.64	0.61
1:B:144:ASP:OD2	1:B:296:HIS:HE1	1.83	0.61
6:A:2578:HOH:O	1:B:235:GLU:HG2	2.01	0.61
1:B:60:HIS:HB2	6:B:1656:HOH:O	1.99	0.61
1:C:634:THR:HG21	6:C:1895:HOH:O	2.01	0.61
1:C:399:GLU:OE2	6:C:2160:HOH:O	2.16	0.61
1:B:518:LYS:HG3	1:B:617:VAL:HG12	1.81	0.61
1:C:81:ASN:ND2	1:C:84:TYR:H	2.00	0.60
1:B:518:LYS:HE3	1:B:617:VAL:CG1	2.31	0.60
1:A:47:ARG:HD2	6:A:2321:HOH:O	1.99	0.60
1:C:508:ASN:HD22	1:C:510:ILE:H	1.50	0.60
1:B:503:ASN:HD22	1:B:505:ASN:H	1.50	0.60
1:A:586:ASN:HB2	6:A:921:HOH:O	2.01	0.59
1:C:403:HIS:HD2	1:C:613:GLU:OE2	1.85	0.59
1:A:385:ASN:H	1:A:385:ASN:ND2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ASN:C	1:B:503:ASN:HD22	2.05	0.59
1:A:199:THR:HG22	6:A:2444:HOH:O	2.03	0.59
1:A:241:VAL:HG22	1:A:246:ILE:HD12	1.84	0.59
1:A:378:GLN:OE1	1:A:389[B]:MET:SD	2.61	0.59
1:B:249:GLN:HE21	1:B:396:GLN:HE21	1.50	0.59
1:C:136:CYS:SG	1:C:154:CYS:HB3	2.42	0.59
1:C:503:ASN:HD22	1:C:505:ASN:H	1.51	0.58
1:A:504:GLU:OE2	1:A:583:ARG:HD2	2.03	0.58
1:C:43:LYS:HD3	6:C:1474:HOH:O	2.03	0.58
1:C:184:LYS:HE2	6:C:2476:HOH:O	2.03	0.58
1:C:3:HIS:CD2	1:C:5:TYR:H	2.21	0.58
1:A:43[B]:LYS:HE2	6:A:2322:HOH:O	2.04	0.57
1:B:552[A]:ARG:HD3	6:B:1498:HOH:O	2.04	0.57
1:B:518:LYS:CG	1:B:617:VAL:HG12	2.34	0.57
1:A:503:ASN:HD22	1:A:505:ASN:H	1.50	0.57
1:B:86:HIS:CE1	6:B:3111:HOH:O	2.58	0.57
1:C:468:LYS:HD3	6:C:992:HOH:O	2.04	0.57
1:B:113:ALA:O	1:B:119:VAL:HG11	2.04	0.57
1:B:378:GLN:HE21	1:B:389[B]:MET:HG3	1.50	0.57
1:C:417:LYS:HD3	6:C:2560:HOH:O	2.06	0.56
1:C:485:LYS:HA	1:C:582:VAL:HG22	1.87	0.56
1:B:625:ASN:HD22	1:B:627:ALA:H	1.54	0.55
1:B:526:MET:H	3:B:640:GOL:C1	2.18	0.55
1:A:184:LYS:HD3	6:A:2311:HOH:O	2.06	0.55
1:C:485:LYS:HB2	1:C:486:PRO:CD	2.36	0.55
1:C:504:GLU:OE2	1:C:583:ARG:HD2	2.07	0.55
1:C:581[A]:ASN:ND2	1:C:583:ARG:H	2.05	0.55
1:A:230:ILE:CG2	6:B:2064:HOH:O	2.55	0.55
1:C:115:THR:HG22	6:C:1410:HOH:O	2.07	0.55
1:B:249:GLN:NE2	1:B:396:GLN:HE21	2.06	0.54
1:B:437:GLN:NE2	1:B:528:LEU:H	2.04	0.54
1:B:534:TYR:O	1:B:538:ARG:HG3	2.07	0.54
1:C:399:GLU:OE1	1:C:401:ARG:HD2	2.06	0.54
1:A:578:ARG:HD2	1:A:580:GLU:OE2	2.07	0.54
1:B:383:VAL:O	1:B:386:TPQ:H6	2.07	0.53
1:A:399:GLU:OE1	1:A:401:ARG:HD2	2.08	0.53
1:B:597:HIS:O	1:B:599:PRO:HD3	2.08	0.53
1:B:275:VAL:HG12	1:B:276:VAL:HG23	1.90	0.53
1:C:47:ARG:HD2	6:C:2310:HOH:O	2.09	0.53
1:B:293:ALA:HA	1:B:296:HIS:CD2	2.45	0.52
1:B:526:MET:H	3:B:640:GOL:H12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:GLU:HB3	6:C:2643:HOH:O	2.09	0.52
1:A:421:VAL:HG22	1:A:423:TRP:CZ2	2.44	0.52
1:C:383:VAL:O	1:C:386:TPQ:H6	2.10	0.52
1:A:385:ASN:H	1:A:385:ASN:HD22	1.57	0.52
1:B:108:GLU:CG	1:B:184:LYS:HE2	2.22	0.52
1:B:389[B]:MET:HE1	1:B:405:ARG:CG	2.40	0.52
1:C:604:PHE:CG	1:C:605:PRO:HA	2.45	0.52
1:C:31:HIS:HD2	6:C:1564:HOH:O	1.93	0.51
3:A:639:GOL:H11	6:A:2301:HOH:O	2.11	0.51
1:B:184:LYS:HD2	6:B:2433:HOH:O	2.10	0.51
1:B:399:GLU:CD	1:B:401[B]:ARG:HH11	2.12	0.51
1:B:240:ASN:HB2	6:B:1111:HOH:O	2.11	0.51
1:A:226:LEU:HD22	1:B:373:ARG:NH1	2.26	0.51
1:B:578:ARG:HD2	1:B:580:GLU:OE2	2.11	0.51
1:B:524:ARG:HH12	1:B:612:HIS:HD2	1.56	0.50
1:C:568:THR:HG22	6:C:2535:HOH:O	2.09	0.50
1:C:219:ASN:C	1:C:219:ASN:HD22	2.15	0.50
1:A:504:GLU:OE2	1:A:583:ARG:CD	2.59	0.50
1:A:230:ILE:HG21	6:B:2064:HOH:O	2.12	0.50
1:C:144:ASP:OD1	3:C:639:GOL:C3	2.58	0.50
1:B:101:LEU:HG	1:B:106:ILE:HD11	1.94	0.49
1:C:578:ARG:HD2	1:C:580:GLU:OE2	2.10	0.49
1:A:307:GLY:O	1:A:311:THR:HB	2.12	0.49
1:C:31:HIS:HE1	1:C:105:ASP:OD2	1.94	0.49
1:A:230:ILE:HB	6:B:2064:HOH:O	2.11	0.49
1:C:219:ASN:HD22	1:C:221:GLU:H	1.60	0.49
1:C:403:HIS:HE1	1:C:405:ARG:NE	1.89	0.49
1:C:219:ASN:ND2	1:C:221:GLU:H	2.11	0.49
1:C:399:GLU:OE1	1:C:401:ARG:CD	2.61	0.49
1:A:435:TYR:HB3	1:B:476:PHE:CE2	2.48	0.48
1:B:405:ARG:HB3	1:B:609:VAL:HG22	1.96	0.48
1:C:503:ASN:HD21	1:C:505:ASN:HD22	1.62	0.48
1:A:185:LYS:HB3	1:A:185:LYS:HE2	1.57	0.48
1:B:625:ASN:HD22	1:B:626:PRO:N	2.11	0.48
1:C:437:GLN:HE22	1:C:528:LEU:N	2.04	0.48
1:A:239:PHE:CE1	1:A:326:LYS:HG3	2.49	0.48
1:B:16:THR:CG2	1:B:67:VAL:HG22	2.44	0.48
1:C:338:ASP:OD1	6:C:3025:HOH:O	2.20	0.48
1:B:524:ARG:HH22	1:B:612:HIS:HD2	1.63	0.47
1:C:380:ILE:HG12	1:C:389:MET:HG2	1.96	0.47
1:B:307:GLY:O	1:B:311:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:ASN:HD22	1:B:625:ASN:C	2.18	0.47
1:C:318:GLY:HA3	6:C:2293:HOH:O	2.13	0.47
1:C:326:LYS:HE3	6:C:2477:HOH:O	2.13	0.47
1:A:503:ASN:HD22	1:A:503:ASN:C	2.18	0.47
1:B:185:LYS:NZ	6:B:1462:HOH:O	2.47	0.47
1:C:426:ASN:ND2	6:C:962:HOH:O	2.47	0.47
1:B:417:LYS:HE2	6:B:1082:HOH:O	2.14	0.47
1:C:131:HIS:CD2	1:C:131:HIS:H	2.33	0.47
1:A:462:ARG:NH1	1:B:529:ALA:O	2.48	0.47
1:A:437:GLN:HE22	1:A:528:LEU:N	2.06	0.47
1:C:81:ASN:HD22	1:C:81:ASN:C	2.19	0.47
1:A:389[B]:MET:HG2	1:A:391:ASN:HD21	1.79	0.46
1:A:485:LYS:HE3	1:A:579:ASP:OD2	2.16	0.46
1:A:531:GLU:HG2	6:B:2593:HOH:O	2.15	0.46
1:C:251:TRP:C	1:C:252:GLU:HG2	2.35	0.46
1:B:372:ARG:HH11	1:B:401[B]:ARG:HH12	1.61	0.46
1:B:401[A]:ARG:HD2	6:B:2531:HOH:O	2.15	0.46
1:A:568:THR:HG22	6:A:1048:HOH:O	2.15	0.46
1:B:399:GLU:CD	1:B:401[B]:ARG:NH1	2.69	0.46
1:A:273:ARG:HD3	6:A:1045:HOH:O	2.15	0.46
1:B:391:ASN:ND2	3:B:639:GOL:O3	2.49	0.46
1:B:503:ASN:ND2	1:B:505:ASN:H	2.13	0.46
1:B:634:THR:C	6:B:2011:HOH:O	2.53	0.46
1:C:31:HIS:CD2	6:C:1564:HOH:O	2.69	0.46
1:C:550:LYS:HE2	6:C:2960:HOH:O	2.17	0.45
1:B:426:ASN:ND2	6:B:1003:HOH:O	2.48	0.45
1:B:468:LYS:CD	1:B:468:LYS:H	2.28	0.45
1:A:417:LYS:CD	6:A:2257:HOH:O	2.64	0.45
1:B:314[A]:SER:OG	6:B:1311:HOH:O	2.20	0.45
1:C:503:ASN:C	1:C:503:ASN:HD22	2.19	0.45
1:A:299:GLN:NE2	1:A:535:ASN:HA	2.23	0.45
1:B:140:MET:H	1:B:140:MET:CE	2.30	0.45
1:B:552[B]:ARG:NH2	1:B:580:GLU:OE1	2.43	0.45
1:A:399:GLU:OE1	1:A:401:ARG:CD	2.65	0.45
1:B:140:MET:HE3	6:B:2089:HOH:O	2.16	0.45
1:B:456:VAL:HG12	1:B:500:LYS:HB2	1.99	0.45
1:B:417:LYS:HD2	1:B:430:ARG:HD3	1.99	0.44
1:C:253:PHE:HB3	1:C:268:ILE:HA	2.00	0.44
1:A:242:ASP:HB2	6:A:2572:HOH:O	2.16	0.44
1:B:302:ASP:O	1:B:306[B]:CYS:HB2	2.18	0.44
1:A:108:GLU:HG2	1:A:184:LYS:CE	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLN:HE22	1:C:527:LEU:HA	1.82	0.44
1:B:585:ASP:CB	6:B:1852:HOH:O	2.66	0.44
1:A:286:VAL:HA	1:A:437:GLN:O	2.18	0.44
1:B:110:GLU:HB2	1:B:138:PRO:HG2	2.00	0.44
1:B:503:ASN:HD21	1:B:505:ASN:HD22	1.64	0.44
1:B:111[A]:GLU:CG	6:B:2658:HOH:O	2.59	0.44
1:A:355:LEU:HD23	1:B:389[A]:MET:HE2	2.00	0.44
1:B:604:PHE:CG	1:B:605:PRO:HA	2.52	0.44
1:C:25:LYS:HA	6:C:3005:HOH:O	2.17	0.44
1:C:299:GLN:OE1	1:C:535:ASN:HA	2.18	0.43
1:C:543:THR:HG22	1:C:547:TRP:HZ2	1.82	0.43
1:C:555:GLU:OE2	1:C:578:ARG:NH2	2.39	0.43
1:A:53:ARG:HG3	6:A:1822:HOH:O	2.17	0.43
1:B:376:VAL:CG1	1:B:391:ASN:HD22	2.31	0.43
1:A:604:PHE:CG	1:A:605:PRO:HA	2.53	0.43
1:B:555:GLU:CD	1:B:578:ARG:HH22	2.21	0.43
1:C:543:THR:HG23	6:C:860:HOH:O	2.17	0.43
1:A:383:VAL:O	1:A:386:TPQ:H6	2.17	0.43
1:B:334:ASN:ND2	1:B:334:ASN:C	2.65	0.43
1:A:67:VAL:CG1	1:A:78:ALA:HB3	2.49	0.43
1:B:208:GLU:CD	1:B:417:LYS:HE3	2.38	0.43
1:A:158:LEU:HD22	1:A:173:LEU:HD21	2.01	0.43
1:A:389[A]:MET:HE2	1:B:355:LEU:CD1	2.49	0.42
1:C:537:LYS:HA	1:C:537:LYS:HD3	1.84	0.42
1:B:448:VAL:H	1:B:453:ASN:ND2	1.94	0.42
1:B:502:ILE:HG22	1:B:516:ALA:HB2	2.01	0.42
1:B:568:THR:HG22	6:B:1038:HOH:O	2.19	0.42
1:B:33:ILE:HG22	1:B:100:PRO:HG2	2.01	0.42
1:B:547:TRP:HB2	1:B:590:TRP:HB2	2.00	0.42
1:C:537:LYS:CE	6:C:2382:HOH:O	2.66	0.42
1:C:537:LYS:HE3	6:C:2382:HOH:O	2.19	0.42
1:A:232:GLN:HB2	1:A:232:GLN:HE21	1.58	0.42
1:B:389[B]:MET:CE	1:B:391:ASN:OD1	2.68	0.42
1:C:333:VAL:HG12	1:C:337:GLY:HA2	2.01	0.42
1:A:204:GLN:HG2	6:A:1713:HOH:O	2.19	0.42
1:A:491:GLN:OE1	1:A:523:ALA:HA	2.19	0.42
1:B:526:MET:N	3:B:640:GOL:H12	2.35	0.42
1:C:503:ASN:ND2	1:C:505:ASN:HD22	2.17	0.42
1:A:407:THR:HA	1:A:607:MET:HG3	2.01	0.42
1:B:140:MET:HB3	1:B:140:MET:HE2	1.79	0.42
1:A:472:TYR:CE2	1:B:144:ASP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LYS:CE	1:B:617:VAL:CG1	2.98	0.42
1:C:410:LEU:HD13	1:C:433:ALA:CB	2.50	0.42
1:A:136:CYS:SG	1:A:154:CYS:HB3	2.60	0.42
1:C:108:GLU:HG2	1:C:184:LYS:HD3	2.01	0.42
1:A:289:GLY:O	1:B:475:GLY:HA2	2.20	0.42
1:A:43[A]:LYS:HE2	6:A:2474:HOH:O	2.19	0.42
3:A:639:GOL:O3	6:A:2614:HOH:O	2.20	0.42
6:A:1826:HOH:O	1:B:227:LYS:HE3	2.18	0.41
1:C:158:LEU:HD13	1:C:173:LEU:HD11	2.02	0.41
1:A:285:THR:HA	1:A:300:ALA:O	2.20	0.41
1:A:56:LYS:HG3	6:A:2654:HOH:O	2.20	0.41
1:B:470:ASN:HD21	1:B:475:GLY:H	1.67	0.41
1:C:259:VAL:HG21	6:C:886:HOH:O	2.20	0.41
1:A:170:SER:CB	1:A:212:VAL:H	2.34	0.41
1:C:167:ASN:HD21	1:C:169:TYR:HB2	1.85	0.41
1:C:288:TYR:CD2	1:C:436:HIS:HB3	2.56	0.41
1:C:440:LEU:HD12	1:C:440:LEU:N	2.35	0.41
1:C:79:LEU:HB2	1:C:89:THR:CG2	2.37	0.41
1:A:407:THR:HA	1:A:607:MET:CG	2.50	0.41
1:B:117:PRO:HG3	6:C:1599:HOH:O	2.20	0.41
1:C:219:ASN:HD22	1:C:220:GLY:N	2.18	0.41
1:C:50:GLU:OE2	1:C:53:ARG:NH1	2.54	0.41
1:B:468:LYS:HG2	6:B:1395:HOH:O	2.21	0.41
1:B:299:GLN:OE1	1:B:535:ASN:HA	2.20	0.41
1:A:634:THR:C	6:A:930:HOH:O	2.59	0.41
1:B:131:HIS:HD2	6:B:2296:HOH:O	2.04	0.41
1:C:543:THR:CG2	6:C:860:HOH:O	2.69	0.41
1:B:492:SER:HB3	1:B:497:ARG:HB2	2.03	0.40
1:C:378:GLN:NE2	6:C:2679:HOH:O	2.46	0.40
1:A:204:GLN:CG	6:A:1713:HOH:O	2.69	0.40
1:A:308:PHE:HA	1:A:311:THR:HG22	2.03	0.40
1:A:372:ARG:NH2	6:A:1497:HOH:O	2.54	0.40
1:B:532:ASP:OD2	6:B:2724:HOH:O	2.22	0.40
1:B:135:VAL:HG22	1:B:168:HIS:CD2	2.56	0.40
1:B:444:ILE:O	1:B:446:PRO:HD3	2.21	0.40
1:C:2:VAL:HG21	6:C:2786:HOH:O	2.21	0.40
1:A:317:LEU:CD2	6:A:1061:HOH:O	2.70	0.40
1:B:367:PRO:HG3	6:B:2068:HOH:O	2.21	0.40
1:B:468:LYS:CG	6:B:1395:HOH:O	2.69	0.40
1:B:593:LEU:HD21	1:B:612:HIS:HB3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TYR:OH	1:B:86:HIS:NE2[2_556]	2.02	0.18
6:B:1986:HOH:O	6:B:2006:HOH:O[2_556]	2.17	0.03

## 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	636/633 (100%)	618 (97%)	17 (3%)	1 (0%)	47	44
1	B	636/633 (100%)	619 (97%)	17 (3%)	0	100	100
1	C	631/633 (100%)	613 (97%)	18 (3%)	0	100	100
All	All	1903/1899 (100%)	1850 (97%)	52 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/558 (101%)	534 (95%)	29 (5%)	23	19
1	B	563/558 (101%)	534 (95%)	29 (5%)	23	19
1	C	558/558 (100%)	533 (96%)	25 (4%)	27	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1684/1674 (101%)	1601 (95%)	83 (5%)	24	21

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	37	ARG
1	A	53	ARG
1	A	90	ASN
1	A	95	LYS
1	A	108	GLU
1	A	158	LEU
1	A	226	LEU
1	A	227	LYS
1	A	273	ARG
1	A	311	THR
1	A	320	ASP
1	A	326	LYS
1	A	333	VAL
1	A	355	LEU
1	A	385	ASN
1	A	421	VAL
1	A	456	VAL
1	A	474	VAL
1	A	485	LYS
1	A	503	ASN
1	A	512	LYS
1	A	536	ASN
1	A	577	ARG
1	A	582	VAL
1	A	583	ARG
1	A	586	ASN
1	A	624	LYS
1	A	628	LEU
1	B	28	GLU
1	B	37	ARG
1	B	53	ARG
1	B	79	LEU
1	B	90	ASN
1	B	101	LEU
1	B	108	GLU
1	B	120	LYS

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Mol	Chain	Res	Type
1	B	140	MET
1	B	146	LYS
1	B	158	LEU
1	B	226	LEU
1	B	238	SER
1	B	246	ILE
1	B	311	THR
1	B	317	LEU
1	B	326	LYS
1	B	333	VAL
1	B	334	ASN
1	B	421	VAL
1	B	456	VAL
1	B	461	ILE
1	B	468	LYS
1	B	503	ASN
1	B	535	ASN
1	B	582	VAL
1	B	586	ASN
1	B	617	VAL
1	B	625	ASN
1	C	25	LYS
1	C	37	ARG
1	C	79	LEU
1	C	81	ASN
1	C	89	THR
1	C	100	PRO
1	C	146	LYS
1	C	158	LEU
1	C	219	ASN
1	C	230	ILE
1	C	246	ILE
1	C	252	GLU
1	C	308	PHE
1	C	326	LYS
1	C	333	VAL
1	C	385	ASN
1	C	421	VAL
1	C	461	ILE
1	C	468	LYS
1	C	485	LYS
1	C	503	ASN

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Mol	Chain	Res	Type
1	C	508	ASN
1	C	543	THR
1	C	583	ARG
1	C	586	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	232	GLN
1	A	249	GLN
1	A	299	GLN
1	A	344	ASN
1	A	385	ASN
1	A	396	GLN
1	A	437	GLN
1	A	503	ASN
1	A	505	ASN
1	A	525	GLN
1	A	536	ASN
1	A	540	GLN
1	A	581	ASN
1	A	584	ASN
1	B	90	ASN
1	B	116	HIS
1	B	167	ASN
1	B	204	GLN
1	B	249	GLN
1	B	296	HIS
1	B	334	ASN
1	B	351	GLN
1	B	378	GLN
1	B	391	ASN
1	B	426	ASN
1	B	437	GLN
1	B	453	ASN
1	B	466	ASN
1	B	470	ASN
1	B	503	ASN
1	B	612	HIS
1	B	625	ASN
1	C	3	HIS

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Mol	Chain	Res	Type
1	C	14	GLN
1	C	31	HIS
1	C	81	ASN
1	C	131	HIS
1	C	153	GLN
1	C	167	ASN
1	C	168	HIS
1	C	219	ASN
1	C	232	GLN
1	C	244	HIS
1	C	351	GLN
1	C	378	GLN
1	C	385	ASN
1	C	403	HIS
1	C	426	ASN
1	C	437	GLN
1	C	503	ASN
1	C	508	ASN
1	C	525	GLN
1	C	545	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	C	386	1	13,14,15	1.54	4 (30%)	15,19,21	1.61	3 (20%)
1	TPQ	B	386	1	13,14,15	1.89	6 (46%)	15,19,21	1.63	4 (26%)
1	TPQ	A	386	1	13,14,15	2.44	6 (46%)	15,19,21	1.98	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
1	TPQ	C	386	1	-	0/5/22/24	0/1/1/1
1	TPQ	B	386	1	-	0/5/22/24	0/1/1/1
1	TPQ	A	386	1	-	0/5/22/24	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	TPQ	O2-C2	4.18	1.35	1.24
1	A	386	TPQ	O5-C5	4.04	1.35	1.24
1	A	386	TPQ	C3-C4	3.97	1.41	1.35
1	B	386	TPQ	O5-C5	3.08	1.32	1.24
1	C	386	TPQ	O5-C5	2.90	1.32	1.24
1	B	386	TPQ	C6-C5	-2.88	1.36	1.44
1	A	386	TPQ	CB-CA	-2.86	1.47	1.53
1	A	386	TPQ	C3-C2	-2.70	1.37	1.44
1	B	386	TPQ	O2-C2	2.39	1.31	1.24
1	B	386	TPQ	C3-C2	-2.37	1.38	1.44
1	A	386	TPQ	C6-C1	2.27	1.40	1.34
1	B	386	TPQ	CB-CA	-2.24	1.48	1.53
1	B	386	TPQ	C1-C2	-2.21	1.45	1.49
1	C	386	TPQ	O2-C2	2.17	1.30	1.24
1	C	386	TPQ	C6-C5	-2.10	1.39	1.44
1	C	386	TPQ	C3-C2	-2.08	1.39	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	TPQ	CB-CA-C	-5.86	100.48	111.47
1	B	386	TPQ	CB-CA-C	-3.87	104.21	111.47
1	C	386	TPQ	CB-CA-C	-3.44	105.01	111.47
1	A	386	TPQ	C6-C1-C2	3.29	121.16	118.64
1	C	386	TPQ	C6-C5-C4	2.69	121.59	117.03
1	C	386	TPQ	C3-C4-C5	-2.44	118.74	121.26
1	B	386	TPQ	C3-C4-C5	-2.35	118.83	121.26
1	B	386	TPQ	O2-C2-C1	-2.25	115.74	120.90
1	B	386	TPQ	C6-C5-C4	2.05	120.52	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	386	TPQ	1	0
1	B	386	TPQ	1	0
1	A	386	TPQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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
3	GOL	A	638	-	5,5,5	1.04	0	5,5,5	1.05	1 (20%)
3	GOL	C	638	-	5,5,5	0.57	0	5,5,5	1.03	0
3	GOL	B	640	-	5,5,5	0.34	0	5,5,5	0.99	0
3	GOL	B	637	-	5,5,5	0.42	0	5,5,5	0.73	0
5	PO4	B	638	-	4,4,4	0.90	0	6,6,6	0.61	0
4	TLA	C	637	-	3,9,9	0.50	0	6,12,12	1.97	2 (33%)
4	TLA	A	640	-	3,9,9	1.76	1 (33%)	6,12,12	1.32	1 (16%)
3	GOL	B	639	-	5,5,5	0.66	0	5,5,5	1.11	0
3	GOL	A	639	-	5,5,5	0.48	0	5,5,5	0.96	1 (20%)
3	GOL	C	636	-	5,5,5	0.97	0	5,5,5	0.93	0
3	GOL	C	639	-	5,5,5	0.39	0	5,5,5	0.79	0
3	GOL	A	636	-	5,5,5	0.46	0	5,5,5	1.30	1 (20%)
3	GOL	B	636	-	5,5,5	1.05	0	5,5,5	0.85	0
3	GOL	A	637	-	5,5,5	0.36	0	5,5,5	1.95	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	638	-	-	0/4/4/4	-
3	GOL	C	638	-	-	4/4/4/4	-
3	GOL	B	640	-	-	3/4/4/4	-
3	GOL	B	637	-	-	0/4/4/4	-
4	TLA	C	637	-	-	0/4/12/12	-
4	TLA	A	640	-	-	0/4/12/12	-
3	GOL	B	639	-	-	2/4/4/4	-
3	GOL	A	639	-	-	0/4/4/4	-
3	GOL	C	636	-	-	2/4/4/4	-
3	GOL	C	639	-	-	0/4/4/4	-
3	GOL	A	636	-	-	2/4/4/4	-
3	GOL	B	636	-	-	2/4/4/4	-
3	GOL	A	637	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	640	TLA	O2-C2	2.23	1.47	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	637	TLA	C1-C2-C3	-3.30	106.01	113.11
4	C	637	TLA	O3-C3-C4	-2.98	103.92	111.10
3	A	637	GOL	O3-C3-C2	-2.93	96.17	110.20
3	A	637	GOL	O2-C2-C1	2.82	121.55	109.12
4	A	640	TLA	C4-C3-C2	-2.45	107.83	113.11
3	A	636	GOL	C3-C2-C1	-2.42	102.31	111.70
3	A	639	GOL	C3-C2-C1	-2.03	103.82	111.70
3	A	638	GOL	O3-C3-C2	2.01	119.84	110.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	640	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	638	GOL	O1-C1-C2-C3
3	C	638	GOL	C1-C2-C3-O3
3	C	636	GOL	O1-C1-C2-C3
3	A	636	GOL	C1-C2-C3-O3
3	A	637	GOL	O1-C1-C2-C3
3	A	637	GOL	C1-C2-C3-O3
3	A	637	GOL	O1-C1-C2-O2
3	B	640	GOL	O1-C1-C2-C3
3	B	639	GOL	O1-C1-C2-C3
3	C	638	GOL	O2-C2-C3-O3
3	A	636	GOL	O2-C2-C3-O3
3	A	637	GOL	O2-C2-C3-O3
3	C	636	GOL	O1-C1-C2-O2
3	B	640	GOL	O2-C2-C3-O3
3	C	638	GOL	O1-C1-C2-O2
3	B	639	GOL	O1-C1-C2-O2
3	B	636	GOL	O2-C2-C3-O3
3	B	636	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	638	GOL	1	0
3	B	640	GOL	3	0
4	C	637	TLA	1	0
3	B	639	GOL	6	0
3	A	639	GOL	2	0
3	C	639	GOL	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	632/633 (99%)	-0.78	4 (0%) 89 88	17, 24, 39, 59	0
1	B	632/633 (99%)	-0.79	3 (0%) 91 90	16, 25, 40, 62	0
1	C	632/633 (99%)	-0.86	3 (0%) 91 90	15, 22, 36, 57	0
All	All	1896/1899 (99%)	-0.81	10 (0%) 91 90	15, 24, 39, 62	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	LEU	7.0
1	A	317	LEU	3.9
1	C	317	LEU	3.4
1	A	53	ARG	2.6
1	A	27	PRO	2.4
1	C	55	GLY	2.4
1	C	27	PRO	2.3
1	B	27	PRO	2.1
1	B	25	LYS	2.1
1	A	318	GLY	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPQ	B	386	14/15	0.96	0.10	18,24,27,28	1
1	TPQ	C	386	14/15	0.97	0.13	16,22,29,29	1
1	TPQ	A	386	14/15	0.98	0.14	18,26,29,29	1



### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	B	638	5/5	0.82	0.34	125,125,126,126	0
3	GOL	B	640	6/6	0.87	0.14	40,52,54,60	0
3	GOL	B	639	6/6	0.91	0.13	48,56,57,57	0
3	GOL	C	639	6/6	0.91	0.13	53,54,57,58	0
3	GOL	A	637	6/6	0.92	0.13	35,41,44,45	0
3	GOL	A	639	6/6	0.93	0.11	39,43,46,51	0
3	GOL	B	636	6/6	0.95	0.09	20,26,31,31	0
3	GOL	B	637	6/6	0.95	0.13	41,42,45,47	0
3	GOL	A	638	6/6	0.96	0.08	21,27,29,30	0
3	GOL	A	636	6/6	0.96	0.18	49,53,56,56	0
3	GOL	C	638	6/6	0.96	0.12	41,51,57,58	0
3	GOL	C	636	6/6	0.96	0.08	21,30,31,31	0
4	TLA	A	640	10/10	0.98	0.06	21,25,28,28	0
4	TLA	C	637	10/10	0.99	0.05	24,27,30,30	0
2	CU	B	635	1/1	1.00	0.07	24,24,24,24	0
2	CU	C	635	1/1	1.00	0.07	21,21,21,21	0
2	CU	A	635	1/1	1.00	0.07	22,22,22,22	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.