



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:53 PM BST

PDB ID : 6EBN  
Title : Crystal structure of Psilocybe cubensis noncanonical aromatic amino acid decarboxylase  
Authors : Torrens-Spence, M.P.; Chun-Ting, L.; Pluskal, T.; Chung, Y.K.; Weng, J.K.  
Deposited on : 2018-08-06  
Resolution : 1.97 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 : 2.13.1  
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) : 2.13.1

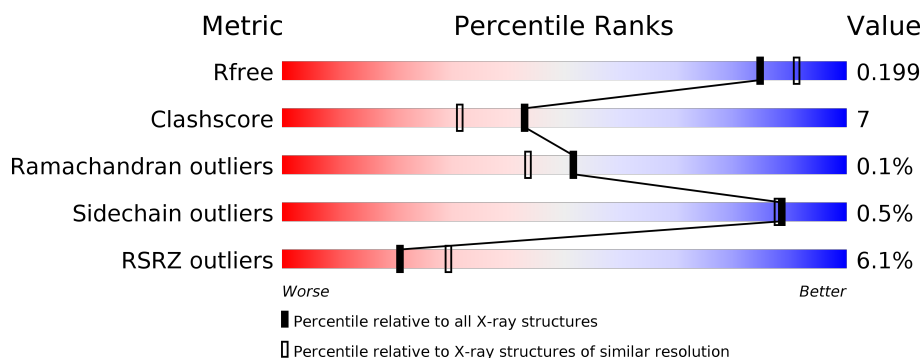
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	1013	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
1	B	1013	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>5%</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
3	FMT	A	1107	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16366 atoms, of which 64 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 non canonical aromatic amino acid decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	961	Total	C	N	O	P	S	0	13	0
			7680	4863	1310	1474	1	32			
1	B	958	Total	C	N	O	P	S	0	5	0
			7581	4802	1288	1458	1	32			

- Molecule 2 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
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			5	1	2	2		
3	B	1	Total	C	H	O	0	0
			5	1	2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		
4	A	2	Total	Na	0	0
			2	2		

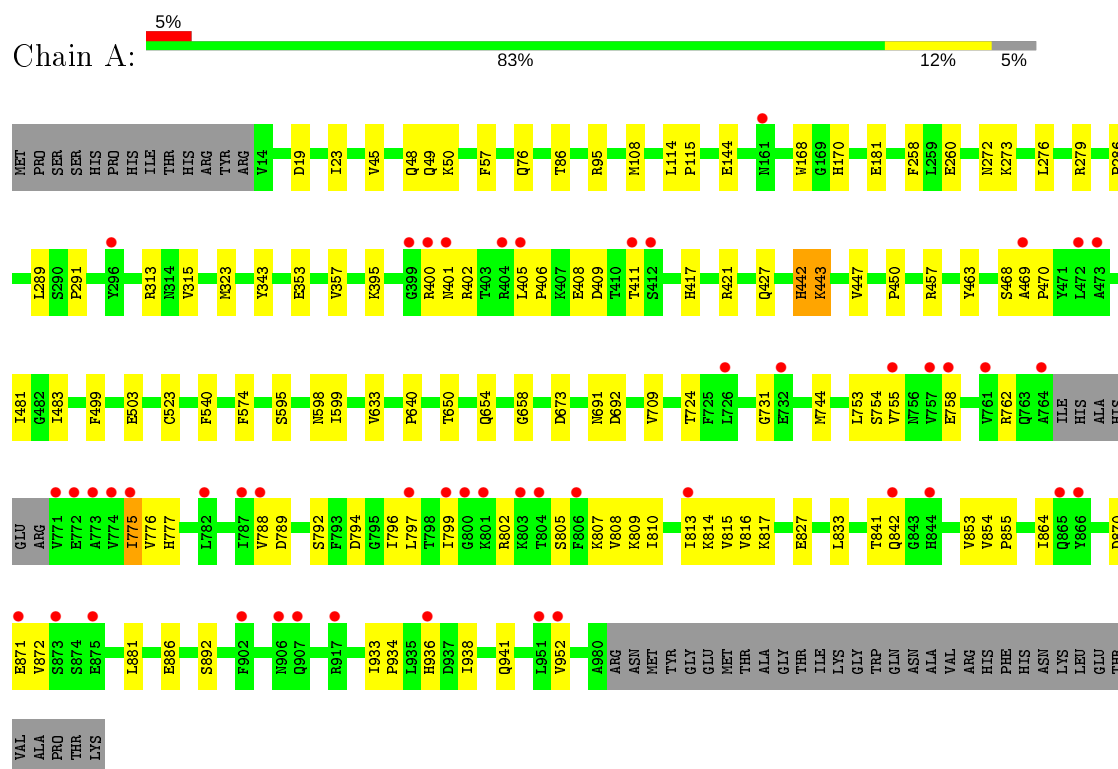
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	503	Total	O	0	0
			503	503		
5	B	468	Total	O	0	0
			468	468		

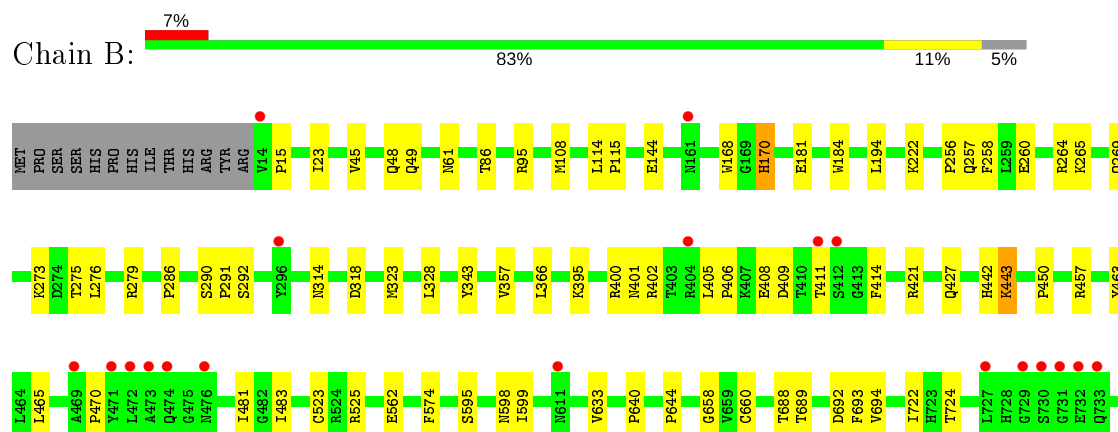
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: non canonical aromatic amino acid decarboxylase



- Molecule 1: non canonical aromatic amino acid decarboxylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	238.72Å 143.57Å 71.41Å 90.00° 92.78° 90.00°	Depositor
Resolution (Å)	71.78 – 1.97 119.22 – 1.97	Depositor EDS
% Data completeness (in resolution range)	89.7 (71.78-1.97) 89.5 (119.22-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.170 , 0.197 0.174 , 0.199	Depositor DCC
$R_{free}$ test set	2001 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, FMT, LLP, NA

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	0.52	0/7829	0.61	0/10642
1	B	0.50	0/7727	0.60	0/10505
All	All	0.51	0/15556	0.61	0/21147

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	7680	0	7516	105	0
1	B	7581	0	7422	110	0
2	A	18	24	23	3	0
2	B	12	16	15	5	0
3	A	18	12	6	3	0
3	B	18	12	6	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	503	0	0	4	0
5	B	468	0	0	11	0
All	All	16302	64	14988	207	0

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

All (207) 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:724:THR:HG23	1:A:775:ILE:HD13	1.53	0.90
1:B:797:LEU:HD13	1:B:808:VAL:HG21	1.53	0.89
1:A:797:LEU:HD13	1:A:808:VAL:HG11	1.55	0.89
1:A:48:GLN:HE22	1:B:86:THR:HG23	1.36	0.86
1:A:799:ILE:O	1:A:802:ARG:HG2	1.79	0.82
1:B:799:ILE:CG2	1:B:802:ARG:HD2	2.09	0.81
1:A:724:THR:HG23	1:A:775:ILE:CD1	2.15	0.75
1:B:256:PRO:O	1:B:260:GLU:HG2	1.86	0.75
1:A:400:ARG:HD3	1:A:402:ARG:H	1.52	0.75
1:B:400:ARG:HD3	1:B:402:ARG:H	1.51	0.75
1:B:400:ARG:NH1	1:B:402:ARG:HG3	2.03	0.74
1:A:754:SER:OG	1:A:814:LYS:HB2	1.89	0.73
1:A:483:ILE:HG13	1:A:483:ILE:O	1.88	0.73
1:A:48:GLN:NE2	1:B:86:THR:HG23	2.04	0.72
1:B:483:ILE:HG13	1:B:483:ILE:O	1.89	0.72
1:B:400:ARG:HH11	1:B:401:ASN:H	1.36	0.72
1:B:761:VAL:O	1:B:762:ARG:NH1	2.24	0.71
1:A:457:ARG:HH12	3:A:1107:FMT:H	1.54	0.71
1:B:799:ILE:HG22	1:B:802:ARG:HD2	1.72	0.71
1:A:499:PHE:O	1:A:503[A]:GLU:HG2	1.92	0.68
1:A:789:ASP:OD1	1:A:815:VAL:HG22	1.94	0.67
1:A:864:ILE:HA	1:A:952:VAL:HG23	1.76	0.67
1:A:934:PRO:HB2	2:A:1103:GOL:H31	1.76	0.67
1:B:144:GLU:HG2	1:B:481:ILE:HD12	1.76	0.67
1:A:400:ARG:HH11	1:A:401:ASN:H	1.41	0.67
1:A:463:TYR:CD1	1:A:470:PRO:HG3	2.30	0.66
1:B:409:ASP:OD1	1:B:411:THR:HG23	1.95	0.65
1:A:144:GLU:CG	1:A:481:ILE:HD12	2.26	0.65
1:A:409:ASP:OD2	1:A:411:THR:HG23	1.97	0.64
1:B:761:VAL:HG11	1:B:797:LEU:HD22	1.81	0.63
1:B:222:LYS:HE2	3:B:1104:FMT:O1	1.98	0.63
1:B:872:VAL:HG21	1:B:881:LEU:HD11	1.80	0.62
1:A:289:LEU:HD23	1:A:313:ARG:HB2	1.82	0.62
1:A:797:LEU:HD13	1:A:808:VAL:CG1	2.29	0.62
1:B:777[B]:HIS:ND1	1:B:778:ASN:O	2.33	0.61
1:B:938:ILE:HD12	1:B:941:GLN:HG3	1.82	0.61
1:B:108:MET:SD	1:B:443:LLP:HE3	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PRO:HB2	1:A:343:TYR:CZ	2.37	0.60
1:B:797:LEU:HD13	1:B:808:VAL:CG2	2.30	0.60
1:A:108:MET:SD	1:A:443:LLP:HE3	2.42	0.60
1:B:257:GLN:O	1:B:260:GLU:HG3	2.02	0.59
1:B:798:THR:HA	5:B:1208:HOH:O	2.02	0.59
1:A:353[B]:GLU:HG2	1:A:650:THR:HG21	1.83	0.59
1:B:523:CYS:SG	1:B:598:ASN:HA	2.43	0.59
1:A:19:ASP:OD2	1:A:417:HIS:HE1	1.86	0.58
1:B:275:THR:HG21	5:B:1421:HOH:O	2.02	0.58
1:B:757:VAL:HG13	1:B:808:VAL:HG11	1.86	0.58
1:A:144:GLU:HG2	1:A:481:ILE:HD12	1.83	0.58
1:A:315:VAL:CG2	1:A:323:MET:HE2	2.33	0.58
1:A:758:GLU:HB2	1:A:809:LYS:HB3	1.86	0.58
1:A:797:LEU:CD1	1:A:808:VAL:HG21	2.33	0.58
1:A:279:ARG:NH2	5:A:1207:HOH:O	2.37	0.58
1:A:724:THR:CG2	1:A:775:ILE:HD13	2.32	0.57
1:B:400:ARG:HD3	1:B:401:ASN:N	2.18	0.57
1:B:291:PRO:HD3	1:B:323:MET:HE1	1.85	0.57
1:B:722:ILE:HG23	1:B:777[B]:HIS:HD1	1.69	0.57
1:B:265:LYS:HD2	5:B:1229:HOH:O	2.04	0.57
1:B:144:GLU:CG	1:B:481:ILE:HD12	2.35	0.57
1:A:744:MET:HE3	5:A:1475:HOH:O	2.05	0.56
1:A:400:ARG:NH1	1:A:402:ARG:HG3	2.19	0.56
1:A:276:LEU:HD23	1:A:276:LEU:C	2.25	0.56
1:A:279:ARG:HG3	5:A:1253:HOH:O	2.06	0.56
1:A:76[B]:GLN:OE1	1:B:405:LEU:HD11	2.05	0.56
1:A:753:LEU:CD2	1:A:815:VAL:HG12	2.36	0.56
1:B:421:ARG:HD2	2:B:1102:GOL:C1	2.36	0.56
1:A:400:ARG:HD3	1:A:401:ASN:N	2.21	0.56
1:B:286:PRO:HB2	1:B:343:TYR:CZ	2.41	0.56
1:B:463:TYR:CD1	1:B:470:PRO:HG3	2.40	0.55
1:B:525:ARG:HD2	5:B:1393:HOH:O	2.06	0.55
1:A:144:GLU:HG3	1:A:481:ILE:HD12	1.88	0.55
1:A:315:VAL:HB	1:A:323:MET:HE2	1.88	0.55
1:A:731:GLY:CA	1:A:762:ARG:HH12	2.20	0.55
1:A:291:PRO:HD3	1:A:323:MET:HE1	1.88	0.54
1:B:45:VAL:O	1:B:49:GLN:HG2	2.07	0.54
1:A:315:VAL:HG21	1:A:323:MET:HE2	1.89	0.54
1:A:807[A]:LYS:HD2	1:A:808:VAL:N	2.24	0.53
1:A:691:ASN:HB2	2:B:1101:GOL:H31	1.90	0.53
1:B:421:ARG:HD2	2:B:1102:GOL:H12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827[A]:GLU:O	1:A:853:VAL:HG22	2.09	0.53
1:B:260:GLU:O	1:B:264:ARG:HG3	2.09	0.53
1:A:95:ARG:HH11	1:A:95:ARG:HG2	1.73	0.52
1:A:933:ILE:O	1:A:933:ILE:HG13	2.09	0.52
1:B:788:VAL:HG12	5:B:1243:HOH:O	2.08	0.52
1:B:483:ILE:O	1:B:483:ILE:CG1	2.58	0.52
1:B:633:VAL:HG21	1:B:640:PRO:HB3	1.92	0.52
1:A:523:CYS:SG	1:A:598:ASN:HA	2.49	0.51
1:A:794:ASP:HB3	1:A:807[A]:LYS:HE2	1.93	0.51
1:A:775:ILE:HD12	1:A:776:VAL:N	2.25	0.51
1:B:276:LEU:HD23	1:B:276:LEU:C	2.31	0.51
1:B:757:VAL:HG13	1:B:808:VAL:CG1	2.40	0.51
1:A:833:LEU:HD13	1:A:886:GLU:HA	1.93	0.51
1:B:273:LYS:HE3	5:B:1382:HOH:O	2.11	0.51
1:B:724:THR:HG23	1:B:775:ILE:HG13	1.92	0.51
1:A:114:LEU:N	1:A:115:PRO:HD2	2.26	0.51
1:A:776:VAL:HG22	1:A:797:LEU:CD1	2.40	0.51
1:B:688:THR:HG22	1:B:694:VAL:HG22	1.92	0.51
1:A:405:LEU:HD23	1:A:405:LEU:H	1.76	0.50
1:A:421:ARG:HA	2:A:1102:GOL:H11	1.92	0.50
1:A:45:VAL:O	1:A:49:GLN:HG2	2.11	0.50
1:B:457:ARG:HH22	3:B:1105:FMT:H	1.75	0.50
1:A:315:VAL:CB	1:A:323:MET:HE2	2.41	0.50
1:A:815:VAL:HG23	1:A:815:VAL:O	2.11	0.50
1:B:802:ARG:HG2	1:B:802:ARG:HH21	1.75	0.50
1:A:633:VAL:HG21	1:A:640:PRO:HB3	1.92	0.50
1:B:184:TRP:CD2	1:B:465:LEU:HD22	2.47	0.50
1:A:421:ARG:NE	2:A:1102:GOL:O1	2.23	0.50
1:A:258:PHE:CG	1:B:892:SER:HA	2.47	0.50
1:A:315:VAL:HB	1:A:323:MET:CE	2.42	0.50
1:A:775:ILE:HD11	1:A:777[B]:HIS:CE1	2.47	0.50
1:A:442:HIS:HA	1:A:447:VAL:O	2.12	0.49
1:A:50:LYS:HE2	5:B:1435:HOH:O	2.11	0.49
1:A:788:VAL:HG12	1:A:789:ASP:N	2.28	0.49
1:B:758:GLU:HB2	1:B:809:LYS:HB3	1.94	0.49
1:B:562:GLU:OE1	5:B:1201:HOH:O	2.20	0.49
1:A:841[A]:THR:HG22	1:A:842:GLN:N	2.28	0.49
1:B:933:ILE:O	1:B:933:ILE:HG13	2.12	0.49
1:A:775:ILE:HD11	1:A:777[B]:HIS:NE2	2.28	0.48
1:B:421:ARG:HA	2:B:1102:GOL:H31	1.93	0.48
1:B:170:HIS:HE1	1:B:181:GLU:OE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HH22	3:A:1107:FMT:C	2.26	0.48
1:A:574:PHE:HA	1:A:692:ASP:OD2	2.14	0.48
1:B:777[B]:HIS:CE1	1:B:778:ASN:O	2.67	0.48
1:B:799:ILE:CB	1:B:802:ARG:HD2	2.44	0.48
1:B:779:THR:CG2	1:B:796:ILE:HG13	2.44	0.47
1:B:722:ILE:CG2	1:B:777[B]:HIS:HD1	2.27	0.47
1:A:260:GLU:CG	1:A:469:ALA:H	2.27	0.47
1:B:61:ASN:HB2	2:B:1101:GOL:H11	1.95	0.47
1:A:406:PRO:HB2	1:A:408:GLU:HG2	1.97	0.46
1:B:95:ARG:HH21	1:B:95:ARG:HG2	1.80	0.46
1:A:872:VAL:HG21	1:A:881:LEU:HD11	1.96	0.46
1:B:689:THR:HA	1:B:694:VAL:HG23	1.97	0.46
1:A:731:GLY:HA3	1:A:762:ARG:HH12	1.80	0.46
1:B:799:ILE:HD12	1:B:799:ILE:N	2.29	0.46
1:A:170:HIS:HE1	1:A:181:GLU:OE1	1.99	0.46
1:B:23:ILE:HD12	1:B:23:ILE:C	2.35	0.46
1:B:595:SER:HB2	1:B:599:ILE:O	2.16	0.46
1:B:724:THR:HG23	1:B:775:ILE:HD11	1.96	0.46
1:B:481:ILE:HG23	1:B:481:ILE:O	2.14	0.46
1:B:763:GLN:HG2	1:B:763:GLN:O	2.16	0.46
1:A:286:PRO:HB2	1:A:343:TYR:CE2	2.51	0.46
1:B:753:LEU:CD2	1:B:815:VAL:HG22	2.46	0.46
1:B:775:ILE:HD11	1:B:777[A]:HIS:CE1	2.51	0.46
1:B:802:ARG:NH2	1:B:802:ARG:HG2	2.30	0.46
1:A:776:VAL:HG22	1:A:797:LEU:HD12	1.97	0.45
1:A:540:PHE:HB3	1:A:709:VAL:HG21	1.98	0.45
1:B:168:TRP:CH2	1:B:170:HIS:HB3	2.51	0.45
1:B:724:THR:HG23	1:B:775:ILE:CG1	2.47	0.45
1:A:273:LYS:HE3	5:A:1354:HOH:O	2.16	0.45
1:A:357:VAL:HG11	1:A:427:GLN:HB2	1.98	0.45
1:B:114:LEU:N	1:B:115:PRO:HD2	2.31	0.45
1:B:792:SER:HB2	1:B:809:LYS:HE2	1.98	0.45
1:B:357:VAL:HG11	1:B:427:GLN:HB2	1.99	0.45
1:B:194:LEU:HD12	1:B:194:LEU:N	2.32	0.45
1:B:292:SER:HA	1:B:314:ASN:HB3	1.99	0.45
1:B:279:ARG:HG3	5:B:1354:HOH:O	2.17	0.44
1:A:892:SER:HA	1:B:258:PHE:CG	2.53	0.44
1:B:794:ASP:OD2	1:B:809:LYS:HD3	2.17	0.44
1:A:400:ARG:CD	1:A:402:ARG:H	2.26	0.44
1:B:269:GLN:HG2	5:B:1557:HOH:O	2.18	0.44
1:B:318:ASP:O	1:B:660:CYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ILE:O	1:A:483:ILE:CG1	2.62	0.44
1:B:788:VAL:HG22	1:B:789:ASP:N	2.33	0.44
1:B:799:ILE:HB	1:B:802:ARG:HD2	1.98	0.44
1:B:777[B]:HIS:NE2	1:B:796:ILE:HD12	2.32	0.44
1:A:938:ILE:HD12	1:A:941:GLN:HG3	2.00	0.44
1:B:265:LYS:CD	5:B:1229:HOH:O	2.63	0.44
1:B:481:ILE:HG12	1:B:481:ILE:O	2.18	0.44
1:B:724:THR:HG23	1:B:775:ILE:CD1	2.47	0.44
1:B:808:VAL:HG12	1:B:809:LYS:N	2.33	0.44
1:A:854:VAL:HA	1:A:855:PRO:C	2.38	0.43
1:A:86:THR:HG23	1:B:48:GLN:HE22	1.83	0.43
1:A:260:GLU:HG2	1:A:469:ALA:N	2.34	0.43
1:B:291:PRO:HD3	1:B:323:MET:CE	2.49	0.43
1:B:395:LYS:HA	1:B:395:LYS:HD3	1.89	0.43
1:B:574:PHE:HA	1:B:692:ASP:OD2	2.18	0.43
1:B:406:PRO:HB2	1:B:408:GLU:HG2	2.00	0.43
1:A:788:VAL:HG12	1:A:789:ASP:H	1.84	0.43
1:A:450:PRO:HG3	1:B:450:PRO:HG3	2.00	0.43
1:B:775:ILE:HG22	1:B:798:THR:O	2.18	0.43
1:A:395:LYS:HD3	1:A:395:LYS:HA	1.87	0.43
1:A:595:SER:HB2	1:A:599:ILE:O	2.18	0.43
1:A:799:ILE:HD12	1:A:799:ILE:N	2.33	0.42
1:B:328:LEU:HD23	1:B:366:LEU:HD12	2.01	0.42
1:B:400:ARG:CD	1:B:402:ARG:H	2.25	0.42
1:B:405:LEU:HD23	1:B:405:LEU:H	1.84	0.42
1:B:15:PRO:HB2	1:B:414:PHE:CE1	2.54	0.42
1:B:738:HIS:CE1	1:B:740:PRO:HA	2.55	0.42
1:A:755:VAL:HG12	1:A:813:ILE:HG12	2.01	0.42
1:B:839:TYR:CE2	1:B:846:HIS:HB2	2.54	0.42
1:A:827[A]:GLU:OE1	1:A:936:HIS:HE1	2.03	0.42
1:A:260:GLU:HG2	1:A:468:SER:HA	2.02	0.41
1:A:724:THR:H	3:A:1104:FMT:H	1.85	0.41
1:A:753:LEU:HD23	1:A:815:VAL:HA	2.03	0.41
1:B:925:TYR:OH	1:B:934:PRO:HD2	2.20	0.41
1:A:654:GLN:HG3	1:A:673:ASP:O	2.21	0.41
1:B:753:LEU:HD23	1:B:815:VAL:HA	2.02	0.41
1:A:23:ILE:C	1:A:23:ILE:HD12	2.41	0.41
1:A:792:SER:HB2	1:A:810:ILE:O	2.20	0.41
1:A:168:TRP:CH2	1:A:170:HIS:HB3	2.54	0.41
1:B:290:SER:O	1:B:314:ASN:HA	2.21	0.41
1:B:400:ARG:CZ	1:B:402:ARG:HG3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:854:VAL:HA	1:B:855:PRO:C	2.41	0.41
1:A:796:ILE:CG2	1:A:805:SER:HB2	2.51	0.41
1:B:688:THR:O	1:B:693:PHE:HB3	2.21	0.40
1:A:816:VAL:O	1:A:817:LYS:HD3	2.22	0.40
1:A:57:PHE:CZ	1:B:644:PRO:HB3	2.56	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	969/1013 (96%)	943 (97%)	25 (3%)	1 (0%)	51	43
1	B	958/1013 (95%)	932 (97%)	25 (3%)	1 (0%)	51	43
All	All	1927/2026 (95%)	1875 (97%)	50 (3%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	658	GLY
1	A	658	GLY

### 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	839/871 (96%)	834 (99%)	5 (1%)	86	85
1	B	829/871 (95%)	826 (100%)	3 (0%)	91	90
All	All	1668/1742 (96%)	1660 (100%)	8 (0%)	88	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	ASN
1	A	442	HIS
1	A	775	ILE
1	A	870	ASP
1	A	871	GLU
1	B	170	HIS
1	B	442	HIS
1	B	762	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	170	HIS
1	B	48	GLN
1	B	170	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	LLP	A	443	1	23,24,25	2.70	7 (30%)	25,32,34	1.64	6 (24%)
1	LLP	B	443	1	23,24,25	2.56	7 (30%)	25,32,34	1.48	6 (24%)

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	LLP	A	443	1	-	4/16/17/19	0/1/1/1
1	LLP	B	443	1	-	4/16/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	LLP	C4-C4'	8.02	1.61	1.46
1	B	443	LLP	C4-C4'	7.98	1.61	1.46
1	A	443	LLP	C4'-NZ	5.49	1.45	1.27
1	B	443	LLP	C4'-NZ	5.17	1.44	1.27
1	A	443	LLP	C6-N1	3.68	1.42	1.34
1	B	443	LLP	C4-C5	-3.65	1.37	1.42
1	A	443	LLP	C4-C5	-3.47	1.37	1.42
1	B	443	LLP	C2'-C2	3.45	1.56	1.50
1	A	443	LLP	C2'-C2	3.20	1.55	1.50
1	A	443	LLP	C5'-C5	3.10	1.59	1.50
1	B	443	LLP	C5'-C5	2.46	1.57	1.50
1	B	443	LLP	P-OP2	-2.35	1.45	1.54
1	A	443	LLP	P-OP2	-2.34	1.45	1.54
1	B	443	LLP	C6-N1	2.19	1.39	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	LLP	C4-C4'-NZ	-4.35	104.33	124.31
1	B	443	LLP	C4-C4'-NZ	-3.87	106.55	124.31
1	A	443	LLP	C3-C4-C5	2.98	120.55	118.26
1	B	443	LLP	C3-C4-C5	2.81	120.42	118.26
1	A	443	LLP	OP3-P-OP2	2.35	116.61	107.64
1	A	443	LLP	C5-C6-N1	-2.31	119.97	123.82
1	A	443	LLP	C3-C4-C4'	-2.26	116.21	120.41
1	B	443	LLP	OP4-P-OP1	2.14	112.47	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	LLP	C5-C6-N1	-2.12	120.29	123.82
1	B	443	LLP	O3-C3-C2	2.09	122.05	117.49
1	A	443	LLP	C2'-C2-N1	2.06	121.69	117.67
1	B	443	LLP	CE-NZ-C4'	-2.06	112.59	118.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	443	LLP	C3-C4-C4'-NZ
1	A	443	LLP	C4-C4'-NZ-CE
1	A	443	LLP	O-C-CA-CB
1	B	443	LLP	C3-C4-C4'-NZ
1	B	443	LLP	C4-C4'-NZ-CE
1	B	443	LLP	O-C-CA-CB
1	A	443	LLP	CG-CD-CE-NZ
1	B	443	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	443	LLP	1	0
1	B	443	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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
2	GOL	B	1101	-	5,5,5	0.69	0	5,5,5	1.01	0
3	FMT	A	1108	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1106	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	A	1103	-	5,5,5	1.15	1 (20%)	5,5,5	0.77	0
3	FMT	B	1108	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1104	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1107	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1106	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1105	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1107	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1103	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1104	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1109	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1105	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	A	1102	-	5,5,5	1.54	1 (20%)	5,5,5	1.13	0
2	GOL	B	1102	-	5,5,5	1.51	1 (20%)	5,5,5	0.81	0
2	GOL	A	1101	-	5,5,5	1.29	0	5,5,5	0.90	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
2	GOL	B	1101	-	-	0/4/4/4	-
2	GOL	A	1103	-	-	0/4/4/4	-
2	GOL	A	1102	-	-	0/4/4/4	-
2	GOL	B	1102	-	-	3/4/4/4	-
2	GOL	A	1101	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1102	GOL	O2-C2	-3.10	1.34	1.43
2	B	1102	GOL	O2-C2	-2.97	1.34	1.43
2	A	1103	GOL	O2-C2	-2.05	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1102	GOL	C1-C2-C3-O3
2	B	1102	GOL	O2-C2-C3-O3
2	A	1101	GOL	C1-C2-C3-O3
2	A	1101	GOL	O2-C2-C3-O3
2	B	1102	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	GOL	2	0
2	A	1103	GOL	1	0
3	B	1104	FMT	1	0
3	A	1107	FMT	2	0
3	A	1104	FMT	1	0
3	B	1105	FMT	1	0
2	A	1102	GOL	2	0
2	B	1102	GOL	3	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	960/1013 (94%)	0.29	49 (5%)	28 37	24, 40, 82, 132	0
1	B	957/1013 (94%)	0.37	68 (7%)	16 24	22, 43, 84, 130	0
All	All	1917/2026 (94%)	0.33	117 (6%)	21 29	22, 41, 84, 132	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	764	ALA	7.9
1	B	799	ILE	6.9
1	B	802	ARG	5.5
1	B	473	ALA	5.2
1	A	757	VAL	5.0
1	B	875	GLU	4.9
1	B	472	LEU	4.9
1	B	774	VAL	4.9
1	B	761	VAL	4.8
1	A	800	GLY	4.6
1	B	977	VAL	4.5
1	B	803	LYS	4.5
1	B	800	GLY	4.5
1	A	771	VAL	4.4
1	B	771	VAL	4.4
1	A	761	VAL	4.4
1	B	903	LYS	4.3
1	B	904	ILE	4.2
1	A	161	ASN	4.1
1	B	775	ILE	4.1
1	B	14	VAL	4.0
1	B	780	VAL	3.9
1	B	801	LYS	3.8
1	A	405	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	763	GLN	3.7
1	B	412	SER	3.7
1	B	806	PHE	3.7
1	A	472	LEU	3.6
1	A	788	VAL	3.6
1	B	872	VAL	3.6
1	A	404	ARG	3.5
1	B	797	LEU	3.5
1	B	815	VAL	3.3
1	B	732	GLU	3.3
1	B	871	GLU	3.3
1	B	404	ARG	3.3
1	A	758	GLU	3.2
1	A	806	PHE	3.2
1	B	727	LEU	3.2
1	B	840	GLY	3.2
1	B	469	ALA	3.1
1	A	902	PHE	3.1
1	B	841	THR	3.1
1	A	775	ILE	3.1
1	B	729	GLY	3.1
1	A	866	TYR	3.1
1	A	774	VAL	3.1
1	B	758	GLU	3.1
1	A	803	LYS	3.0
1	B	878	ALA	3.0
1	B	471	TYR	3.0
1	B	730	SER	3.0
1	B	813	ILE	2.9
1	A	473	ALA	2.9
1	B	476	ASN	2.9
1	B	798	THR	2.8
1	B	814	LYS	2.8
1	A	844	HIS	2.8
1	A	813	ILE	2.8
1	A	296[A]	TYR	2.7
1	B	804	THR	2.7
1	A	804	THR	2.7
1	B	816	VAL	2.7
1	A	797	LEU	2.7
1	A	799	ILE	2.7
1	A	865	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	760	GLN	2.7
1	B	762	ARG	2.7
1	A	907	GLN	2.6
1	A	412	SER	2.6
1	B	731	GLY	2.6
1	B	790	GLY	2.6
1	A	906	ASN	2.6
1	B	777[A]	HIS	2.6
1	A	732	GLU	2.6
1	A	772	GLU	2.5
1	B	796	ILE	2.5
1	B	753	LEU	2.5
1	B	812	ASN	2.4
1	A	411	THR	2.4
1	A	871	GLU	2.4
1	A	951	LEU	2.4
1	B	782	LEU	2.4
1	B	877	LEU	2.4
1	B	296	TYR	2.4
1	B	776	VAL	2.4
1	A	726	LEU	2.3
1	A	782	LEU	2.3
1	B	611	ASN	2.3
1	A	469	ALA	2.3
1	B	976	HIS	2.3
1	B	792	SER	2.3
1	A	873	SER	2.3
1	A	773	ALA	2.3
1	B	882	ILE	2.3
1	A	399	GLY	2.2
1	B	906	ASN	2.2
1	A	917	ARG	2.2
1	A	952	VAL	2.2
1	A	842	GLN	2.2
1	B	793	PHE	2.2
1	A	936	HIS	2.2
1	B	161	ASN	2.2
1	A	400	ARG	2.1
1	B	411	THR	2.1
1	A	801	LYS	2.1
1	B	902	PHE	2.1
1	A	755	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	875	GLU	2.1
1	A	787	ILE	2.1
1	B	879	LYS	2.1
1	B	866	TYR	2.0
1	B	474	GLN	2.0
1	B	733	GLN	2.0
1	B	927	ALA	2.0
1	A	401	ASN	2.0
1	A	764	ALA	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. 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	LLP	A	443	24/25	0.96	0.11	25,32,41,48	0
1	LLP	B	443	24/25	0.98	0.13	23,34,43,49	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	FMT	B	1105	3/3	0.69	0.18	76,77,92,94	0
3	FMT	A	1107	3/3	0.73	0.19	69,70,83,85	0
3	FMT	A	1109	3/3	0.78	0.15	70,71,84,85	0
3	FMT	B	1107	3/3	0.79	0.19	66,67,80,80	0
3	FMT	B	1103	3/3	0.83	0.11	68,69,81,84	0
2	GOL	A	1101	6/6	0.84	0.16	53,63,67,71	0
3	FMT	A	1104	3/3	0.85	0.10	70,71,84,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	1102	6/6	0.86	0.19	66,79,89,99	0
2	GOL	A	1103	6/6	0.86	0.24	65,78,81,84	0
3	FMT	A	1108	3/3	0.87	0.14	53,57,69,71	0
4	NA	B	1110	1/1	0.88	0.15	40,40,40,40	0
3	FMT	B	1108	3/3	0.89	0.16	75,75,91,93	0
2	GOL	B	1101	6/6	0.89	0.16	55,66,69,73	0
2	GOL	B	1102	6/6	0.90	0.17	59,70,79,85	0
3	FMT	B	1106	3/3	0.94	0.12	64,64,77,77	0
3	FMT	A	1106	3/3	0.95	0.11	37,45,48,57	0
3	FMT	A	1105	3/3	0.95	0.16	56,58,67,70	0
4	NA	A	1111	1/1	0.95	0.08	38,38,38,38	0
3	FMT	B	1104	3/3	0.95	0.14	50,52,60,63	0
4	NA	A	1110	1/1	0.97	0.20	17,17,17,17	0
4	NA	B	1109	1/1	0.99	0.12	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.