



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:37 am BST

PDB ID : 5XIX  
Title : The canonical domain of human asparaginyl-tRNA synthetase  
Authors : Park, J.S.; Han, B.W.  
Deposited on : 2017-04-28  
Resolution : 2.25 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

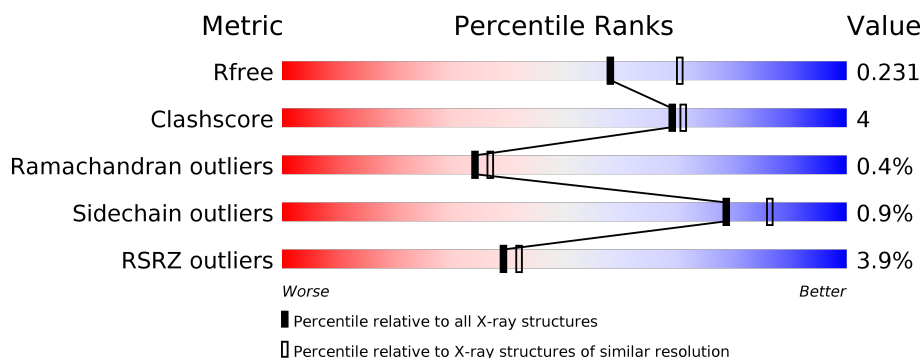
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	472	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	472	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>10%</div> </div> </div>
1	C	472	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	D	472	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>10%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	608	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14958 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 Asparagine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3413	2178	581	628	26			
1	B	423	Total	C	N	O	S	0	0	0
			3422	2183	582	631	26			
1	C	423	Total	C	N	O	S	0	0	0
			3422	2183	582	631	26			
1	D	424	Total	C	N	O	S	0	0	0
			3433	2189	586	632	26			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP O43776
A	78	GLY	-	expression tag	UNP O43776
A	79	SER	-	expression tag	UNP O43776
A	80	SER	-	expression tag	UNP O43776
A	81	HIS	-	expression tag	UNP O43776
A	82	HIS	-	expression tag	UNP O43776
A	83	HIS	-	expression tag	UNP O43776
A	84	HIS	-	expression tag	UNP O43776
A	85	HIS	-	expression tag	UNP O43776
A	86	HIS	-	expression tag	UNP O43776
A	87	SER	-	expression tag	UNP O43776
A	88	SER	-	expression tag	UNP O43776
A	89	GLY	-	expression tag	UNP O43776
A	90	LEU	-	expression tag	UNP O43776
A	91	VAL	-	expression tag	UNP O43776
A	92	PRO	-	expression tag	UNP O43776
A	93	ARG	-	expression tag	UNP O43776
A	94	GLY	-	expression tag	UNP O43776
A	95	SER	-	expression tag	UNP O43776
A	96	HIS	-	expression tag	UNP O43776
A	97	MET	-	expression tag	UNP O43776

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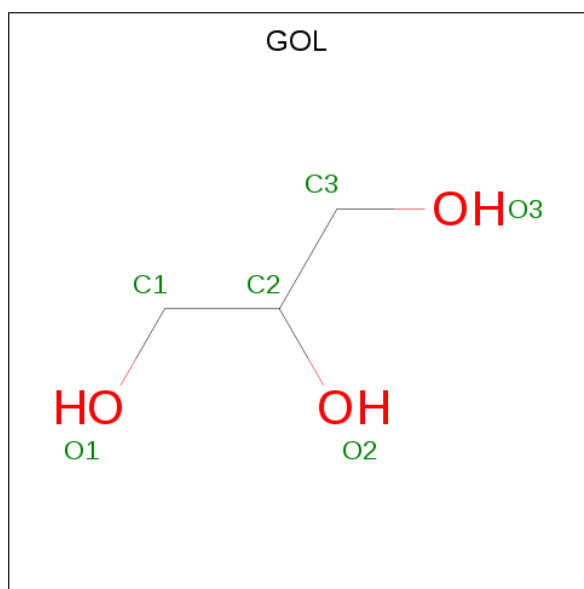
Chain	Residue	Modelled	Actual	Comment	Reference
B	77	MET	-	initiating methionine	UNP O43776
B	78	GLY	-	expression tag	UNP O43776
B	79	SER	-	expression tag	UNP O43776
B	80	SER	-	expression tag	UNP O43776
B	81	HIS	-	expression tag	UNP O43776
B	82	HIS	-	expression tag	UNP O43776
B	83	HIS	-	expression tag	UNP O43776
B	84	HIS	-	expression tag	UNP O43776
B	85	HIS	-	expression tag	UNP O43776
B	86	HIS	-	expression tag	UNP O43776
B	87	SER	-	expression tag	UNP O43776
B	88	SER	-	expression tag	UNP O43776
B	89	GLY	-	expression tag	UNP O43776
B	90	LEU	-	expression tag	UNP O43776
B	91	VAL	-	expression tag	UNP O43776
B	92	PRO	-	expression tag	UNP O43776
B	93	ARG	-	expression tag	UNP O43776
B	94	GLY	-	expression tag	UNP O43776
B	95	SER	-	expression tag	UNP O43776
B	96	HIS	-	expression tag	UNP O43776
B	97	MET	-	expression tag	UNP O43776
C	77	MET	-	initiating methionine	UNP O43776
C	78	GLY	-	expression tag	UNP O43776
C	79	SER	-	expression tag	UNP O43776
C	80	SER	-	expression tag	UNP O43776
C	81	HIS	-	expression tag	UNP O43776
C	82	HIS	-	expression tag	UNP O43776
C	83	HIS	-	expression tag	UNP O43776
C	84	HIS	-	expression tag	UNP O43776
C	85	HIS	-	expression tag	UNP O43776
C	86	HIS	-	expression tag	UNP O43776
C	87	SER	-	expression tag	UNP O43776
C	88	SER	-	expression tag	UNP O43776
C	89	GLY	-	expression tag	UNP O43776
C	90	LEU	-	expression tag	UNP O43776
C	91	VAL	-	expression tag	UNP O43776
C	92	PRO	-	expression tag	UNP O43776
C	93	ARG	-	expression tag	UNP O43776
C	94	GLY	-	expression tag	UNP O43776
C	95	SER	-	expression tag	UNP O43776
C	96	HIS	-	expression tag	UNP O43776
C	97	MET	-	expression tag	UNP O43776

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Chain	Residue	Modelled	Actual	Comment	Reference
D	77	MET	-	initiating methionine	UNP O43776
D	78	GLY	-	expression tag	UNP O43776
D	79	SER	-	expression tag	UNP O43776
D	80	SER	-	expression tag	UNP O43776
D	81	HIS	-	expression tag	UNP O43776
D	82	HIS	-	expression tag	UNP O43776
D	83	HIS	-	expression tag	UNP O43776
D	84	HIS	-	expression tag	UNP O43776
D	85	HIS	-	expression tag	UNP O43776
D	86	HIS	-	expression tag	UNP O43776
D	87	SER	-	expression tag	UNP O43776
D	88	SER	-	expression tag	UNP O43776
D	89	GLY	-	expression tag	UNP O43776
D	90	LEU	-	expression tag	UNP O43776
D	91	VAL	-	expression tag	UNP O43776
D	92	PRO	-	expression tag	UNP O43776
D	93	ARG	-	expression tag	UNP O43776
D	94	GLY	-	expression tag	UNP O43776
D	95	SER	-	expression tag	UNP O43776
D	96	HIS	-	expression tag	UNP O43776
D	97	MET	-	expression tag	UNP O43776

- 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	O	0	0
			6	3	3		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

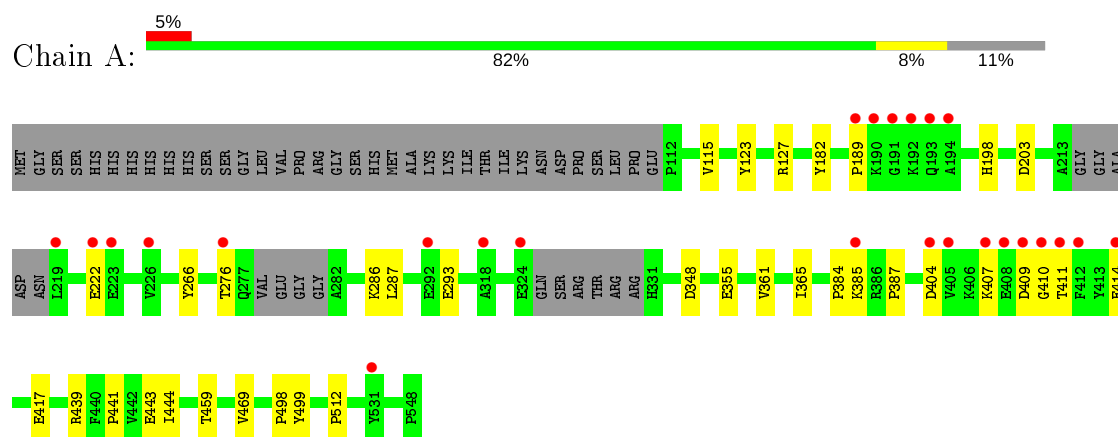
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	278	Total	O	0	0
			278	278		
3	B	234	Total	O	0	0
			234	234		
3	C	306	Total	O	0	0
			306	306		
3	D	288	Total	O	0	0
			288	288		



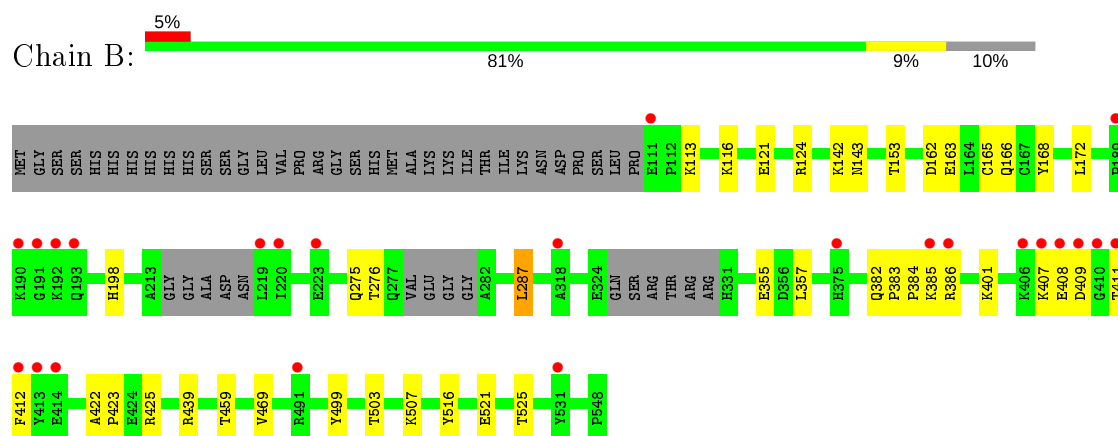
### 3 Residue-property plots [i](#)

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.

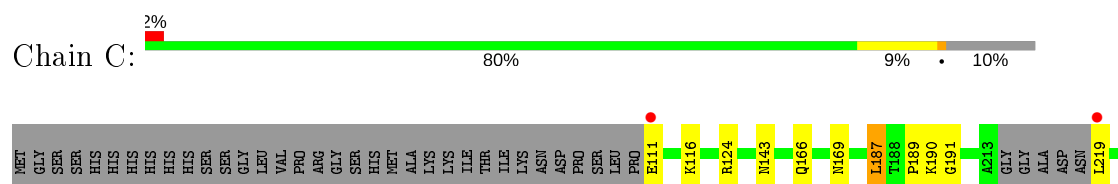
- Molecule 1: Asparagine–tRNA ligase, cytoplasmic



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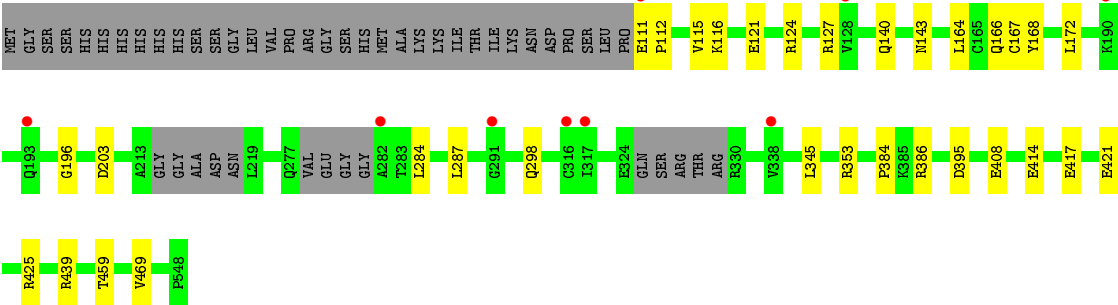
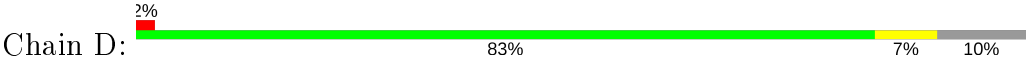


- Molecule 1: Asparagine–tRNA ligase, cytoplasmic





● Molecule 1: Asparagine–tRNA ligase, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.35Å 127.10Å 163.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.25 43.73 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.62-2.25) 92.9 (43.73-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.78 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.177 , 0.229 0.180 , 0.231	Depositor DCC
$R_{free}$ test set	5547 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.907	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14958	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4423e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.41	0/3495	0.54	0/4728
1	B	0.40	0/3504	0.56	1/4741 (0.0%)
1	C	0.41	0/3504	0.55	0/4741
1	D	0.40	0/3515	0.54	0/4755
All	All	0.40	0/14018	0.55	1/18965 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	LEU	CA-CB-CG	6.28	129.74	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3413	0	3343	19	0
1	B	3422	0	3348	25	0
1	C	3422	0	3348	35	0
1	D	3433	0	3361	20	0
2	A	42	0	56	2	0
2	B	42	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	64	10	0
2	D	30	0	40	0	0
3	A	278	0	0	3	0
3	B	234	0	0	5	0
3	C	306	0	0	7	0
3	D	288	0	0	6	0
All	All	14958	0	13616	101	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 4.

All (101) 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:C:275:GLN:NE2	1:C:292:GLU:OE2	2.15	0.80
1:D:167:CYS:SG	3:D:982:HOH:O	2.42	0.78
1:C:322:ARG:NH2	1:C:332:LEU:O	2.18	0.77
1:D:384:PRO:O	3:D:701:HOH:O	2.01	0.77
1:B:143:ASN:OD1	3:B:701:HOH:O	2.01	0.76
1:C:264:GLY:O	2:C:608:GOL:H31	1.86	0.76
1:D:143:ASN:ND2	1:D:166:GLN:OE1	2.18	0.75
1:C:116:LYS:NZ	3:C:703:HOH:O	2.21	0.72
1:C:491:ARG:NH1	3:C:702:HOH:O	2.20	0.71
1:C:491:ARG:NH2	3:C:704:HOH:O	2.25	0.69
1:C:322:ARG:NH1	3:C:705:HOH:O	2.26	0.68
1:B:166:GLN:NE2	3:B:705:HOH:O	2.26	0.67
1:C:189:PRO:C	1:C:191:GLY:HA3	2.16	0.66
1:B:355:GLU:HB3	1:B:386:ARG:NH1	2.10	0.65
1:C:313:ASP:HB2	2:C:608:GOL:H32	1.78	0.65
1:C:124:ARG:HG2	1:C:187:LEU:HD13	1.78	0.64
1:A:222:GLU:OE2	3:A:702:HOH:O	2.16	0.63
1:C:169:ASN:ND2	2:C:601:GOL:O1	2.31	0.62
1:D:386:ARG:NH2	3:D:703:HOH:O	2.20	0.62
1:A:410:GLY:N	1:A:411:THR:HA	2.14	0.61
1:B:116:LYS:HE3	2:C:608:GOL:H12	1.82	0.61
1:B:276:THR:HG22	1:B:499:TYR:CZ	2.36	0.61
1:D:421:GLU:O	1:D:425:ARG:HG2	2.00	0.61
1:B:385:LYS:N	1:B:385:LYS:HD3	2.17	0.60
1:D:395:ASP:OD2	3:D:702:HOH:O	2.16	0.60
1:C:241:ASN:HA	1:C:244:LYS:HD2	1.81	0.60
1:A:407:LYS:HD3	1:A:410:GLY:HA3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ASN:OD1	1:C:166:GLN:NE2	2.36	0.58
1:B:153:THR:CG2	2:C:608:GOL:H2	2.34	0.58
1:C:313:ASP:H	2:C:608:GOL:H32	1.69	0.57
1:B:275:GLN:OE1	3:B:702:HOH:O	2.17	0.57
1:C:345:LEU:HB2	1:C:349:ASP:HB2	1.88	0.56
1:B:401:LYS:HG3	1:B:412:PHE:CD2	2.41	0.55
1:C:451:ARG:NH1	1:C:456:SER:O	2.39	0.55
1:B:142:LYS:N	3:B:701:HOH:O	2.38	0.55
1:A:407:LYS:HB2	1:A:410:GLY:H	1.72	0.54
1:D:284:LEU:HD22	1:D:298:GLN:HG3	1.91	0.53
1:A:384:PRO:O	3:A:703:HOH:O	2.19	0.53
1:B:409:ASP:O	1:B:411:THR:OG1	2.07	0.51
1:C:390:ARG:HD2	3:C:706:HOH:O	2.10	0.51
1:C:190:LYS:N	1:C:191:GLY:HA3	2.24	0.51
1:A:276:THR:HG22	1:A:499:TYR:CZ	2.46	0.51
1:A:355:GLU:OE2	1:A:387:PRO:HA	2.11	0.50
1:C:313:ASP:CB	2:C:608:GOL:H32	2.42	0.50
1:A:348:ASP:OD2	3:A:704:HOH:O	2.20	0.49
1:A:414:GLU:HG3	1:A:417:GLU:HG3	1.95	0.49
1:C:331:HIS:CD2	1:C:331:HIS:N	2.79	0.49
1:C:124:ARG:HG2	1:C:187:LEU:CD1	2.42	0.49
1:D:414:GLU:O	1:D:417:GLU:HG2	2.11	0.49
1:C:439:ARG:HA	1:C:459:THR:O	2.12	0.49
1:D:111:GLU:HB2	1:D:112:PRO:HD2	1.95	0.49
1:C:313:ASP:N	2:C:608:GOL:H32	2.28	0.48
1:D:112:PRO:HD3	1:D:127:ARG:HH11	1.78	0.48
1:D:115:VAL:HG12	1:D:116:LYS:O	2.13	0.47
1:D:345:LEU:HD21	1:D:353:ARG:CZ	2.45	0.47
1:D:124:ARG:NH1	1:D:196:GLY:O	2.45	0.47
1:B:422:ALA:HB3	1:B:423:PRO:HD3	1.97	0.46
1:A:266:TYR:CE1	2:A:606:GOL:H32	2.51	0.46
1:B:407:LYS:HD2	1:B:408:GLU:N	2.30	0.45
1:B:124:ARG:HH21	1:B:198:HIS:HB3	1.81	0.45
1:C:382:GLN:HA	1:C:383:PRO:HD2	1.77	0.45
1:B:121:GLU:HG3	1:B:124:ARG:HH11	1.81	0.45
1:D:439:ARG:HA	1:D:459:THR:O	2.17	0.45
1:D:408:GLU:HG2	3:D:940:HOH:O	2.16	0.45
1:B:168:TYR:CZ	1:B:172:LEU:HD11	2.52	0.44
1:A:441:PRO:HD2	1:A:444:ILE:HD11	1.99	0.44
1:B:425:ARG:NH2	3:B:715:HOH:O	2.50	0.44
1:B:503:THR:HG22	1:B:507:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:GOL:H12	1:C:254:ARG:HH22	1.83	0.44
1:D:127:ARG:NH2	1:D:203:ASP:OD1	2.50	0.44
1:D:121:GLU:HG3	1:D:124:ARG:NH2	2.32	0.44
1:B:162:ASP:HB3	1:B:163:GLU:OE1	2.18	0.43
1:A:385:LYS:H	1:A:385:LYS:HG2	1.68	0.43
1:C:451:ARG:HH21	1:C:491:ARG:HH22	1.66	0.43
1:C:244:LYS:HG3	1:C:373:ILE:HG23	2.00	0.43
1:A:361:VAL:O	1:A:365:ILE:HG13	2.19	0.43
1:C:538:LEU:HG	1:C:539:TYR:CD2	2.54	0.43
1:A:127:ARG:HD2	1:A:203:ASP:OD2	2.19	0.43
1:B:113:LYS:HD2	1:B:113:LYS:HA	1.86	0.43
1:C:521:GLU:O	1:C:525:THR:HG23	2.19	0.43
1:B:439:ARG:HA	1:B:459:THR:O	2.19	0.42
1:A:276:THR:HG21	1:A:498:PRO:HB2	2.01	0.42
1:A:439:ARG:HA	1:A:459:THR:O	2.20	0.42
1:C:338:VAL:HB	1:C:518:LEU:HG	2.00	0.42
2:C:602:GOL:H11	3:C:843:HOH:O	2.19	0.42
1:C:445:LYS:HB3	1:C:449:MET:SD	2.59	0.42
2:B:605:GOL:H12	1:C:254:ARG:NH2	2.35	0.42
1:D:164:LEU:HD12	3:D:721:HOH:O	2.19	0.42
1:A:512:PRO:HG2	2:A:604:GOL:H2	2.01	0.41
1:D:168:TYR:CZ	1:D:172:LEU:HD11	2.55	0.41
1:A:286:LYS:HD2	1:A:293:GLU:HB2	2.02	0.41
2:B:605:GOL:C1	1:C:254:ARG:HH22	2.34	0.41
1:C:469:VAL:O	1:C:522:ARG:NH2	2.53	0.41
1:D:425:ARG:HH21	1:D:425:ARG:HB3	1.86	0.41
1:B:357:LEU:HD22	1:B:516:TYR:CE1	2.56	0.41
1:A:115:VAL:HG11	1:A:123:TYR:CZ	2.56	0.41
1:B:382:GLN:HA	1:B:383:PRO:HD2	1.92	0.41
2:C:608:GOL:O2	3:C:701:HOH:O	2.12	0.41
1:B:383:PRO:HA	1:B:384:PRO:HD3	1.88	0.40
1:C:391:MET:HE1	1:C:431:ILE:HD13	2.03	0.40
1:B:521:GLU:O	1:B:525:THR:HG23	2.22	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	414/472 (88%)	401 (97%)	9 (2%)	4 (1%)	15	13
1	B	415/472 (88%)	397 (96%)	17 (4%)	1 (0%)	47	55
1	C	415/472 (88%)	406 (98%)	8 (2%)	1 (0%)	47	55
1	D	416/472 (88%)	406 (98%)	9 (2%)	1 (0%)	47	55
All	All	1660/1888 (88%)	1610 (97%)	43 (3%)	7 (0%)	34	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	ASP
1	A	409	ASP
1	C	469	VAL
1	A	189	PRO
1	B	469	VAL
1	D	469	VAL
1	A	469	VAL

### 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	374/415 (90%)	370 (99%)	4 (1%)	73	82
1	B	375/415 (90%)	373 (100%)	2 (0%)	88	92
1	C	375/415 (90%)	369 (98%)	6 (2%)	62	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	376/415 (91%)	374 (100%)	2 (0%)	88	92
All	All	1500/1660 (90%)	1486 (99%)	14 (1%)	78	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	TYR
1	A	198	HIS
1	A	287	LEU
1	A	443	GLU
1	B	165	CYS
1	B	287	LEU
1	C	111	GLU
1	C	187	LEU
1	C	219	LEU
1	C	331	HIS
1	C	345	LEU
1	C	418	ASP
1	D	140	GLN
1	D	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	319	GLN
1	C	143	ASN
1	C	166	GLN
1	C	169	ASN
1	C	331	HIS
1	D	143	ASN
1	D	166	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

27 ligands 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	$\# Z  > 2$
2	GOL	C	602	-	5,5,5	0.52	0	5,5,5	0.82	0
2	GOL	A	602	-	5,5,5	0.35	0	5,5,5	0.26	0
2	GOL	B	607	-	5,5,5	0.39	0	5,5,5	0.25	0
2	GOL	C	607	-	5,5,5	0.33	0	5,5,5	0.65	0
2	GOL	D	602	-	5,5,5	0.37	0	5,5,5	0.68	0
2	GOL	B	605	-	5,5,5	0.31	0	5,5,5	0.53	0
2	GOL	A	605	-	5,5,5	0.35	0	5,5,5	0.20	0
2	GOL	C	605	-	5,5,5	0.41	0	5,5,5	0.41	0
2	GOL	A	601	-	5,5,5	0.31	0	5,5,5	0.54	0
2	GOL	D	604	-	5,5,5	0.37	0	5,5,5	0.45	0
2	GOL	C	608	-	5,5,5	0.45	0	5,5,5	0.69	0
2	GOL	A	607	-	5,5,5	0.41	0	5,5,5	0.38	0
2	GOL	A	604	-	5,5,5	0.34	0	5,5,5	0.49	0
2	GOL	A	603	-	5,5,5	0.39	0	5,5,5	0.67	0
2	GOL	D	601	-	5,5,5	0.28	0	5,5,5	0.61	0
2	GOL	D	605	-	5,5,5	0.29	0	5,5,5	0.55	0
2	GOL	A	606	-	5,5,5	0.31	0	5,5,5	0.38	0
2	GOL	D	603	-	5,5,5	0.35	0	5,5,5	0.82	0
2	GOL	B	603	-	5,5,5	0.36	0	5,5,5	0.23	0
2	GOL	C	603	-	5,5,5	0.28	0	5,5,5	0.46	0
2	GOL	B	606	-	5,5,5	0.42	0	5,5,5	0.29	0
2	GOL	B	601	-	5,5,5	0.49	0	5,5,5	0.65	0
2	GOL	C	606	-	5,5,5	0.29	0	5,5,5	0.35	0
2	GOL	C	601	-	5,5,5	0.38	0	5,5,5	0.35	0
2	GOL	B	604	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	C	604	-	5,5,5	0.33	0	5,5,5	0.48	0
2	GOL	B	602	-	5,5,5	0.39	0	5,5,5	0.44	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	C	602	-	-	4/4/4/4	-
2	GOL	A	602	-	-	0/4/4/4	-
2	GOL	B	607	-	-	4/4/4/4	-
2	GOL	C	607	-	-	2/4/4/4	-
2	GOL	D	602	-	-	0/4/4/4	-
2	GOL	B	605	-	-	2/4/4/4	-
2	GOL	A	605	-	-	2/4/4/4	-
2	GOL	C	605	-	-	2/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	D	604	-	-	4/4/4/4	-
2	GOL	C	608	-	-	3/4/4/4	-
2	GOL	A	607	-	-	4/4/4/4	-
2	GOL	A	604	-	-	2/4/4/4	-
2	GOL	A	603	-	-	2/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
2	GOL	D	605	-	-	2/4/4/4	-
2	GOL	A	606	-	-	2/4/4/4	-
2	GOL	D	603	-	-	3/4/4/4	-
2	GOL	B	603	-	-	4/4/4/4	-
2	GOL	C	603	-	-	4/4/4/4	-
2	GOL	B	606	-	-	0/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	C	606	-	-	2/4/4/4	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	B	604	-	-	0/4/4/4	-
2	GOL	C	604	-	-	2/4/4/4	-
2	GOL	B	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	602	GOL	O1-C1-C2-O2
2	C	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	B	607	GOL	C1-C2-C3-O3
2	C	607	GOL	O1-C1-C2-C3
2	B	605	GOL	O1-C1-C2-O2
2	B	605	GOL	O1-C1-C2-C3
2	A	605	GOL	O1-C1-C2-C3
2	C	605	GOL	O1-C1-C2-C3
2	D	604	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2
2	A	607	GOL	C1-C2-C3-O3
2	A	607	GOL	O2-C2-C3-O3
2	D	605	GOL	C1-C2-C3-O3
2	A	606	GOL	O1-C1-C2-C3
2	B	603	GOL	O1-C1-C2-C3
2	B	603	GOL	C1-C2-C3-O3
2	B	603	GOL	O2-C2-C3-O3
2	C	603	GOL	O1-C1-C2-C3
2	C	603	GOL	C1-C2-C3-O3
2	C	604	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-C3
2	A	603	GOL	O1-C1-C2-O2
2	B	607	GOL	O1-C1-C2-C3
2	D	604	GOL	O1-C1-C2-C3
2	D	604	GOL	C1-C2-C3-O3
2	B	601	GOL	O1-C1-C2-C3
2	A	607	GOL	O1-C1-C2-C3
2	A	604	GOL	C1-C2-C3-O3
2	A	603	GOL	O1-C1-C2-C3
2	D	603	GOL	C1-C2-C3-O3
2	C	608	GOL	O1-C1-C2-C3
2	C	606	GOL	O1-C1-C2-C3
2	C	602	GOL	O2-C2-C3-O3
2	B	607	GOL	O1-C1-C2-O2
2	C	607	GOL	O1-C1-C2-O2
2	C	605	GOL	O1-C1-C2-O2
2	A	606	GOL	O1-C1-C2-O2
2	C	603	GOL	O2-C2-C3-O3
2	C	608	GOL	O1-C1-C2-O2
2	B	607	GOL	O2-C2-C3-O3
2	B	603	GOL	O1-C1-C2-O2
2	C	603	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	604	GOL	O1-C1-C2-O2
2	B	602	GOL	O1-C1-C2-O2
2	A	605	GOL	O1-C1-C2-O2
2	A	607	GOL	O1-C1-C2-O2
2	D	601	GOL	O2-C2-C3-O3
2	C	606	GOL	O1-C1-C2-O2
2	A	604	GOL	O2-C2-C3-O3
2	D	605	GOL	O2-C2-C3-O3
2	D	601	GOL	C1-C2-C3-O3
2	D	603	GOL	O1-C1-C2-C3
2	C	608	GOL	C1-C2-C3-O3
2	D	604	GOL	O2-C2-C3-O3
2	D	603	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	1	0
2	B	605	GOL	3	0
2	C	608	GOL	8	0
2	A	604	GOL	1	0
2	A	606	GOL	1	0
2	C	601	GOL	1	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	422/472 (89%)	-0.02	25 (5%) 22 24	20, 31, 64, 96	0
1	B	423/472 (89%)	0.04	24 (5%) 23 25	20, 33, 62, 100	0
1	C	423/472 (89%)	-0.23	8 (1%) 66 69	21, 30, 52, 70	0
1	D	424/472 (89%)	-0.04	9 (2%) 63 66	20, 31, 53, 78	0
All	All	1692/1888 (89%)	-0.06	66 (3%) 39 42	20, 31, 57, 100	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	LYS	8.2
1	B	410	GLY	6.6
1	B	409	ASP	5.5
1	A	411	THR	5.5
1	A	191	GLY	5.2
1	A	410	GLY	4.9
1	B	408	GLU	4.7
1	B	190	LYS	4.7
1	B	412	PHE	4.6
1	B	191	GLY	4.6
1	A	531	TYR	4.5
1	A	219	LEU	4.3
1	B	223	GLU	4.1
1	A	223	GLU	4.0
1	A	193	GLN	4.0
1	A	409	ASP	3.8
1	B	411	THR	3.7
1	A	276	THR	3.7
1	B	193	GLN	3.7
1	B	192	LYS	3.5
1	B	189	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	414	GLU	3.3
1	B	219	LEU	3.2
1	A	412	PHE	3.2
1	B	385	LYS	3.1
1	B	413	TYR	3.1
1	A	408	GLU	3.0
1	C	282	ALA	2.9
1	B	407	LYS	2.9
1	D	317	ILE	2.8
1	B	111	GLU	2.8
1	A	414	GLU	2.8
1	B	531	TYR	2.8
1	C	219	LEU	2.8
1	A	222	GLU	2.8
1	A	407	LYS	2.6
1	D	282	ALA	2.6
1	D	291	GLY	2.5
1	B	318	ALA	2.5
1	C	491	ARG	2.5
1	A	189	PRO	2.5
1	A	405	VAL	2.4
1	D	111	GLU	2.4
1	D	316	CYS	2.3
1	A	292	GLU	2.3
1	B	406	LYS	2.3
1	A	385	LYS	2.3
1	C	493	GLY	2.3
1	D	128	VAL	2.3
1	A	192	LYS	2.3
1	B	491	ARG	2.2
1	C	331	HIS	2.2
1	A	324	GLU	2.2
1	B	375	HIS	2.2
1	B	386	ARG	2.2
1	D	338	VAL	2.2
1	A	194	ALA	2.2
1	B	220	ILE	2.2
1	D	190	LYS	2.2
1	C	276	THR	2.2
1	C	277	GLN	2.1
1	D	193	GLN	2.1
1	C	111	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	226	VAL	2.1
1	A	404	ASP	2.1
1	A	318	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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
2	GOL	B	607	6/6	0.79	0.24	35,39,43,43	0
2	GOL	C	602	6/6	0.80	0.23	30,31,32,37	0
2	GOL	A	607	6/6	0.81	0.25	31,39,42,45	0
2	GOL	C	606	6/6	0.81	0.20	38,42,44,47	0
2	GOL	A	606	6/6	0.85	0.15	30,39,41,41	0
2	GOL	C	608	6/6	0.85	0.24	25,33,38,40	0
2	GOL	D	605	6/6	0.85	0.22	32,37,39,43	0
2	GOL	A	604	6/6	0.87	0.21	43,50,51,55	0
2	GOL	B	606	6/6	0.87	0.22	38,44,47,48	0
2	GOL	C	607	6/6	0.88	0.19	36,39,42,55	0
2	GOL	B	603	6/6	0.89	0.15	34,39,41,51	0
2	GOL	A	603	6/6	0.89	0.16	26,27,31,34	0
2	GOL	B	602	6/6	0.90	0.13	35,37,38,45	0
2	GOL	D	603	6/6	0.91	0.15	28,31,32,36	0
2	GOL	C	603	6/6	0.91	0.23	35,37,41,43	0
2	GOL	B	605	6/6	0.92	0.19	34,42,45,50	0
2	GOL	B	601	6/6	0.92	0.15	24,27,30,34	0
2	GOL	D	601	6/6	0.92	0.19	34,37,45,47	0
2	GOL	B	604	6/6	0.92	0.32	38,40,46,54	0
2	GOL	A	602	6/6	0.92	0.13	32,38,41,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	D	602	6/6	0.94	0.16	29,33,36,38	0
2	GOL	C	601	6/6	0.94	0.11	39,44,45,45	0
2	GOL	C	605	6/6	0.94	0.36	42,44,47,55	0
2	GOL	D	604	6/6	0.94	0.23	32,37,43,46	0
2	GOL	C	604	6/6	0.96	0.12	29,31,33,35	0
2	GOL	A	601	6/6	0.96	0.10	35,36,39,42	0
2	GOL	A	605	6/6	0.98	0.09	36,38,40,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.