



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:34 PM UTC

PDB ID : 1NMT / pdb\_00001nmt  
Title : N-MYRISTOYL TRANSFERASE FROM CANDIDA ALBICANS AT 2.45 Å  
Authors : Weston, S.A.; Pauptit, R.A.  
Deposited on : 1997-12-11  
Resolution : 2.45 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

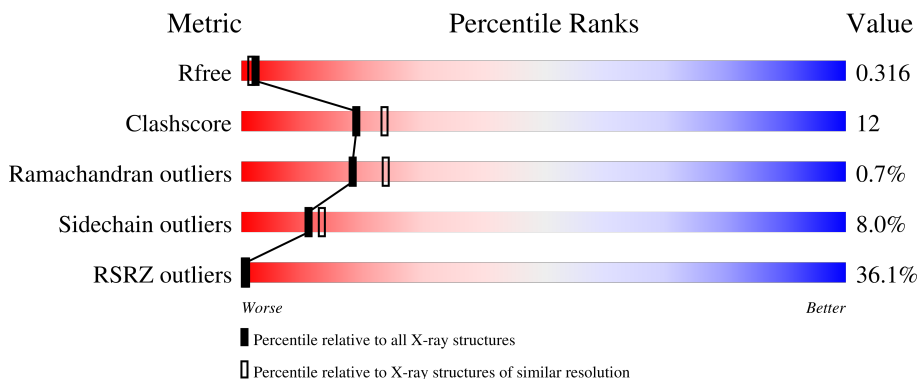
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 of 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	392	 14% 70% 27% 5% 2%
1	B	392	 45% 71% 23% 5% 2%
1	C	392	 49% 69% 27% 5% 2%

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
2	GOL	B	12	-	-	X	-

## 2 Entry composition [i](#)

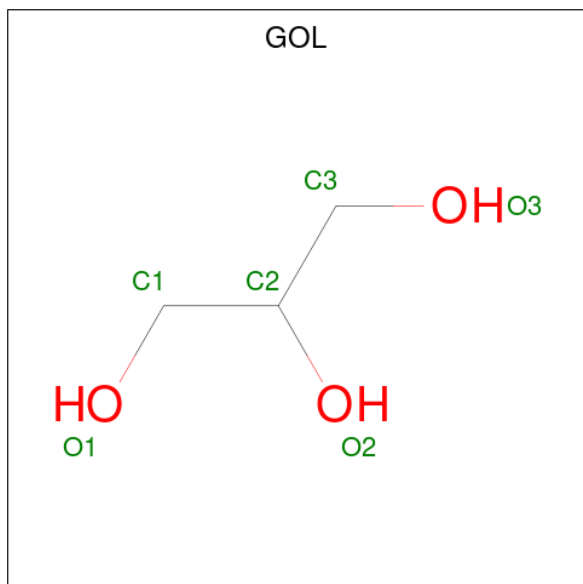
There are 3 unique types of molecules in this entry. The entry contains 10001 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-MYRISTOYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	Total 3210	C 2079	N 524	O 598	S 9	0	0	0
1	B	392	Total 3207	C 2078	N 524	O 596	S 9	0	0	0
1	C	389	Total 3185	C 2064	N 521	O 591	S 9	0	0	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

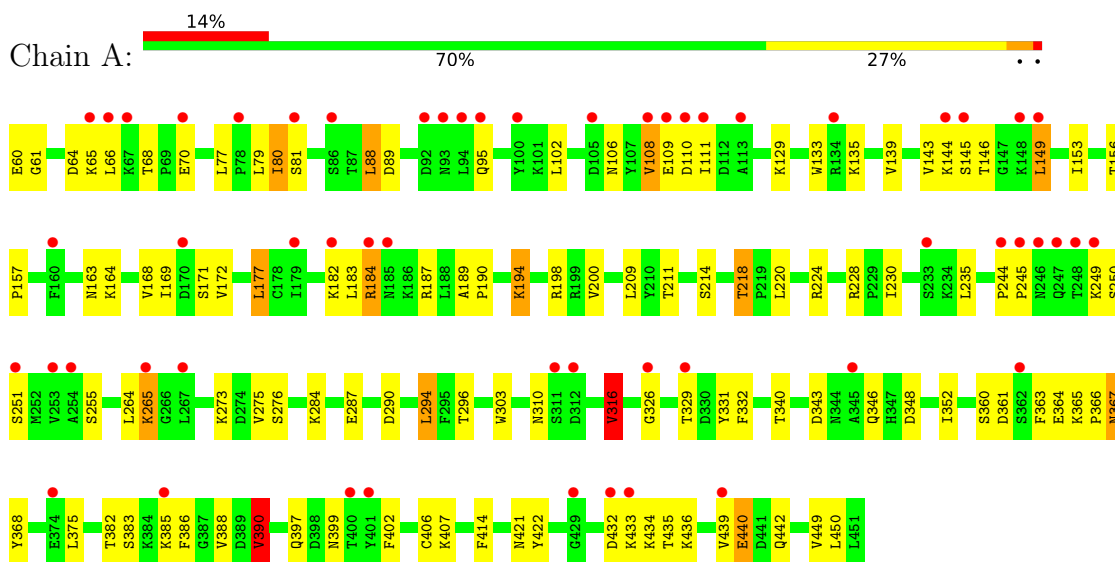
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	105	Total O 105 105	0	0
3	B	150	Total O 150 150	0	0
3	C	36	Total O 36 36	0	0

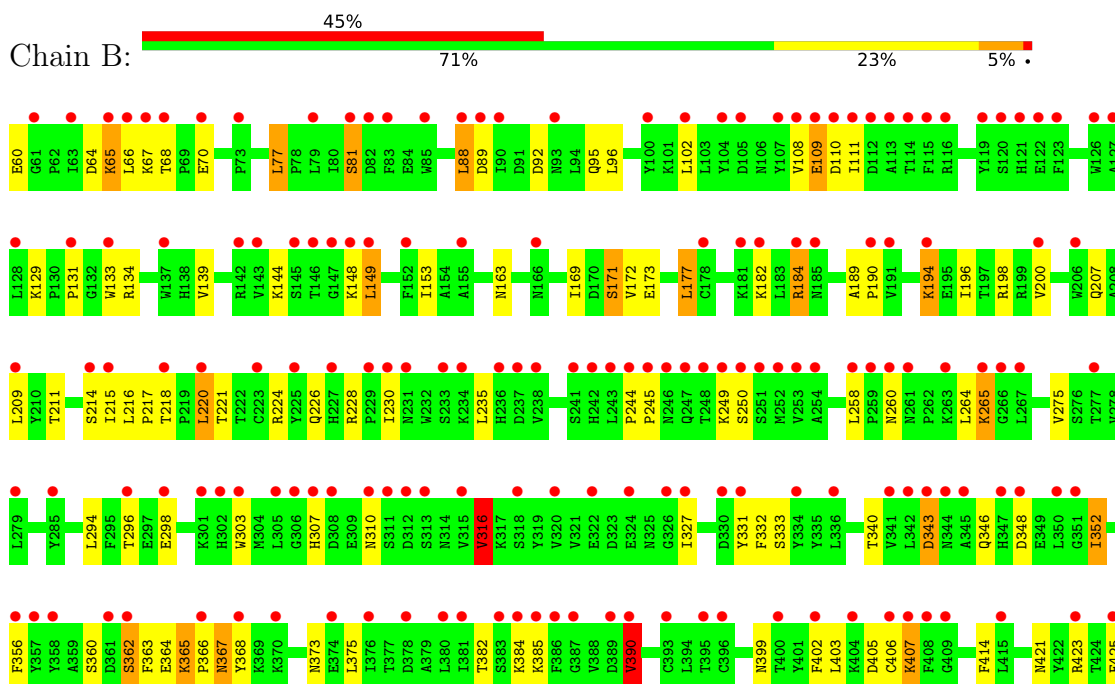
### 3 Residue-property plots

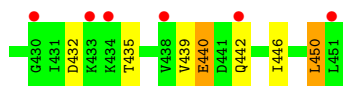
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: N-MYRISTOYL TRANSFERASE

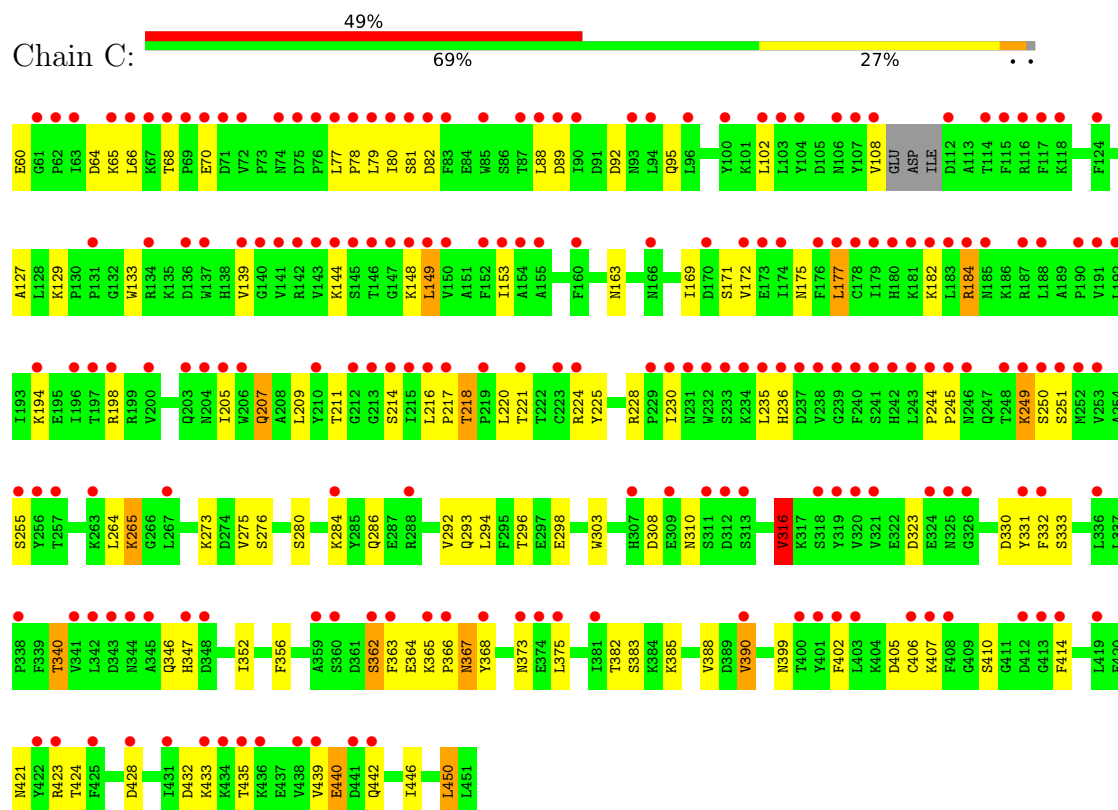


#### • Molecule 1: N-MYRISTOYL TRANSFERASE





• Molecule 1: N-MYRISTOYL TRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.00Å 166.50Å 179.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.85 – 2.45 20.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.85-2.45) 98.6 (20.85-2.45)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.44Å)	Xtrriage
Refinement program	X-PLOR 3.98	Depositor
R, $R_{free}$	0.214 , 0.251 0.299 , 0.316	Depositor DCC
$R_{free}$ test set	3703 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.218	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	10001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 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	0.63	0/3296	1.04	20/4473 (0.4%)
1	B	0.70	1/3293 (0.0%)	1.05	20/4469 (0.4%)
1	C	0.56	0/3270	1.01	16/4436 (0.4%)
All	All	0.63	1/9859 (0.0%)	1.03	56/13378 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	THR	CA-CB	7.34	1.57	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	THR	N-CA-C	-9.90	95.86	110.52
1	C	296	THR	N-CA-C	-9.22	97.21	110.59
1	B	296	THR	N-CA-C	-9.15	97.32	110.59
1	C	230	ILE	N-CA-C	-7.97	105.44	111.90
1	B	139	VAL	N-CA-C	7.91	120.08	107.73
1	B	275	VAL	N-CA-C	7.89	118.65	110.36
1	A	440	GLU	N-CA-C	7.34	119.78	110.24
1	C	139	VAL	N-CA-C	7.12	118.12	107.51
1	B	230	ILE	N-CA-C	-7.00	106.23	111.90
1	B	316	VAL	CB-CA-C	-6.98	100.43	110.83
1	B	218	THR	CA-C-N	-6.85	112.93	119.85
1	B	218	THR	C-N-CA	-6.85	112.93	119.85
1	B	244	PRO	CA-C-N	6.82	128.37	119.84
1	B	244	PRO	C-N-CA	6.82	128.37	119.84
1	A	230	ILE	N-CA-C	-6.80	105.71	111.56
1	A	80	ILE	N-CA-C	-6.77	99.82	109.51
1	C	275	VAL	N-CA-C	6.76	117.26	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	VAL	N-CA-C	6.71	117.21	110.23
1	A	340	THR	N-CA-C	-6.69	98.72	109.96
1	A	106	ASN	N-CA-C	6.64	122.20	113.30
1	A	139	VAL	N-CA-C	6.62	118.05	107.73
1	C	340	THR	N-CA-C	-6.55	99.85	110.20
1	C	220	LEU	N-CA-C	-6.38	104.25	111.07
1	B	390	VAL	CB-CA-C	-6.29	99.67	111.30
1	B	220	LEU	N-CA-C	-6.25	103.61	111.11
1	C	163	ASN	N-CA-C	6.20	118.04	111.28
1	B	340	THR	N-CA-C	-6.05	99.80	109.96
1	A	316	VAL	CB-CA-C	-5.99	101.91	110.83
1	C	316	VAL	CB-CA-C	-5.99	101.71	110.81
1	C	440	GLU	N-CA-C	5.64	117.58	110.24
1	A	163	ASN	N-CA-C	5.55	117.33	111.28
1	A	360	SER	CA-C-N	5.54	127.64	120.44
1	A	360	SER	C-N-CA	5.54	127.64	120.44
1	A	390	VAL	CB-CA-C	-5.52	101.16	110.71
1	A	218	THR	N-CA-C	5.48	124.28	112.23
1	A	244	PRO	CA-C-N	5.43	126.63	119.84
1	A	244	PRO	C-N-CA	5.43	126.63	119.84
1	B	343	ASP	N-CA-C	5.43	119.20	112.58
1	B	81	SER	N-CA-C	5.42	119.39	112.34
1	C	244	PRO	CA-C-N	5.36	126.54	119.84
1	C	244	PRO	C-N-CA	5.36	126.54	119.84
1	B	96	LEU	N-CA-C	-5.31	105.50	111.28
1	B	360	SER	CA-C-N	5.28	127.31	120.44
1	B	360	SER	C-N-CA	5.28	127.31	120.44
1	C	127	ALA	N-CA-C	5.22	117.87	111.82
1	C	205	ILE	N-CA-C	-5.21	100.97	108.53
1	B	440	GLU	N-CA-C	5.19	117.41	110.35
1	C	347	HIS	N-CA-C	5.18	117.84	109.40
1	A	326	GLY	CA-C-N	-5.15	115.93	122.37
1	A	326	GLY	C-N-CA	-5.15	115.93	122.37
1	A	220	LEU	N-CA-C	-5.12	105.70	111.28
1	A	397	GLN	CB-CA-C	-5.12	110.66	116.54
1	B	163	ASN	N-CA-C	5.07	116.80	111.28
1	C	323	ASP	N-CA-C	5.05	116.45	110.19
1	C	218	THR	N-CA-C	5.05	120.97	109.81
1	B	407	LYS	N-CA-C	5.00	118.62	111.92

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	3210	0	3167	70	6
1	B	3207	0	3165	87	5
1	C	3185	0	3145	77	4
2	A	54	0	72	12	0
2	B	30	0	40	8	0
2	C	24	0	32	6	0
3	A	105	0	0	3	0
3	B	150	0	0	3	1
3	C	36	0	0	0	0
All	All	10001	0	9621	228	10

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 12.

All (228) 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:265:LYS:H	1:C:265:LYS:HE2	1.26	1.00
1:B:215:ILE:HD12	1:C:276:SER:HB2	1.44	0.98
1:B:265:LYS:HE2	1:B:265:LYS:H	1.27	0.97
1:A:235:LEU:HD21	1:A:390:VAL:HG22	1.49	0.94
1:A:265:LYS:H	1:A:265:LYS:HE2	1.30	0.94
1:A:64:ASP:H	1:A:421:ASN:HD21	1.17	0.93
1:C:235:LEU:HD21	1:C:390:VAL:HG22	1.51	0.93
1:B:169:ILE:HG21	1:B:207:GLN:HG3	1.51	0.92
1:B:265:LYS:H	1:B:265:LYS:CE	1.83	0.92
1:B:64:ASP:H	1:B:421:ASN:HD21	1.23	0.86
1:C:265:LYS:H	1:C:265:LYS:CE	1.88	0.84
1:A:265:LYS:H	1:A:265:LYS:CE	1.89	0.83
1:C:64:ASP:H	1:C:421:ASN:HD21	1.22	0.83
1:B:211:THR:HG21	1:B:450:LEU:HD13	1.60	0.82
1:A:184:ARG:HG3	1:A:184:ARG:HH11	1.45	0.82
1:B:184:ARG:HG3	1:B:184:ARG:HH11	1.47	0.79
1:C:184:ARG:HG3	1:C:184:ARG:HH11	1.46	0.79
1:C:77:LEU:HD12	1:C:78:PRO:HD2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:THR:HG21	1:C:450:LEU:HD13	1.64	0.78
1:B:439:VAL:HG12	1:B:442:GLN:HG3	1.65	0.78
1:B:153:ILE:HD12	1:B:177:LEU:HD22	1.64	0.78
1:B:332:PHE:HD2	1:B:375:LEU:HD22	1.49	0.77
1:A:439:VAL:HG12	1:A:442:GLN:HG3	1.66	0.77
1:B:215:ILE:CD1	1:C:276:SER:HB2	2.15	0.77
1:C:153:ILE:HD12	1:C:177:LEU:HD22	1.66	0.77
1:C:216:LEU:HB3	1:C:217:PRO:HD2	1.70	0.74
1:C:332:PHE:HD2	1:C:375:LEU:HD22	1.53	0.73
1:B:265:LYS:HE2	1:B:265:LYS:N	2.02	0.73
1:A:332:PHE:HD2	1:A:375:LEU:HD22	1.54	0.72
1:A:164:LYS:HG3	2:A:16:GOL:H12	1.72	0.72
1:A:64:ASP:H	1:A:421:ASN:ND2	1.87	0.72
1:B:235:LEU:HD21	1:B:390:VAL:HG22	1.71	0.72
1:C:169:ILE:HG21	1:C:207:GLN:HG3	1.71	0.72
1:B:215:ILE:HD12	1:C:276:SER:CB	2.21	0.71
1:A:265:LYS:HE2	1:A:265:LYS:N	2.05	0.71
1:A:65:LYS:O	1:A:66:LEU:HB3	1.88	0.71
1:A:153:ILE:HD12	1:A:177:LEU:HD22	1.72	0.70
1:A:211:THR:HG21	1:A:450:LEU:HD13	1.74	0.70
1:C:81:SER:O	1:C:144:LYS:HE3	1.91	0.70
1:C:265:LYS:HE2	1:C:265:LYS:N	2.02	0.70
1:B:215:ILE:HD13	1:C:280:SER:OG	1.92	0.69
1:B:439:VAL:CG1	1:B:442:GLN:HG3	2.21	0.69
1:C:64:ASP:H	1:C:421:ASN:ND2	1.90	0.69
1:A:434:LYS:HB3	1:B:327:ILE:HD13	1.74	0.69
1:B:198:ARG:HH22	2:B:12:GOL:H2	1.58	0.69
1:C:65:LYS:O	1:C:66:LEU:HB3	1.93	0.69
1:B:367:ASN:H	1:B:367:ASN:HD22	1.39	0.68
1:C:293:GLN:HE22	2:C:10:GOL:H12	1.58	0.68
1:B:64:ASP:H	1:B:421:ASN:ND2	1.91	0.68
1:B:65:LYS:O	1:B:66:LEU:HB3	1.93	0.67
1:B:365:LYS:HB3	1:B:366:PRO:HD2	1.78	0.66
1:B:216:LEU:HB3	1:B:217:PRO:HD2	1.78	0.65
1:A:365:LYS:HB3	1:A:366:PRO:HD2	1.77	0.65
1:B:307:HIS:HB3	3:B:574:HOH:O	1.96	0.64
1:A:399:ASN:HA	1:A:402:PHE:CE2	2.33	0.64
1:A:367:ASN:HD22	1:A:367:ASN:H	1.48	0.62
1:A:439:VAL:CG1	1:A:442:GLN:HG3	2.29	0.62
1:C:225:TYR:OH	2:C:6:GOL:H32	2.01	0.61
1:C:399:ASN:HA	1:C:402:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH22	2:A:13:GOL:H31	1.66	0.61
1:B:362:SER:HA	1:B:365:LYS:HD3	1.83	0.61
1:C:60:GLU:HG2	1:C:424:THR:HA	1.83	0.60
1:B:399:ASN:HA	1:B:402:PHE:CE2	2.36	0.60
1:C:367:ASN:HD22	1:C:367:ASN:H	1.50	0.59
1:B:211:THR:HG21	1:B:450:LEU:CD1	2.32	0.59
1:C:365:LYS:HB3	1:C:366:PRO:HD2	1.84	0.59
1:B:81:SER:O	1:B:144:LYS:HE3	2.02	0.59
1:C:129:LYS:HD2	1:C:133:TRP:CZ2	2.38	0.59
1:B:439:VAL:HG12	1:B:442:GLN:CG	2.31	0.58
1:A:211:THR:HG21	1:A:450:LEU:CD1	2.32	0.58
1:C:264:LEU:HA	1:C:265:LYS:HE2	1.85	0.58
1:B:363:PHE:HA	1:B:368:TYR:CD1	2.39	0.58
1:B:332:PHE:CD2	1:B:375:LEU:HD22	2.35	0.58
2:A:8:GOL:H12	3:A:525:HOH:O	2.04	0.58
1:B:264:LEU:HA	1:B:265:LYS:HE2	1.85	0.57
1:A:68:THR:OG1	1:A:70:GLU:HB2	2.04	0.57
1:B:169:ILE:CG2	1:B:207:GLN:HG3	2.30	0.57
1:B:109:GLU:HG3	1:B:110:ASP:H	1.68	0.57
1:A:211:THR:CG2	1:A:450:LEU:HD13	2.35	0.56
1:C:80:ILE:HG22	1:C:82:ASP:H	1.71	0.56
1:C:211:THR:CG2	1:C:450:LEU:HD13	2.34	0.56
1:A:89:ASP:H	1:A:95:GLN:NE2	2.03	0.56
1:A:184:ARG:HH11	1:A:184:ARG:CG	2.17	0.56
1:C:77:LEU:HD12	1:C:78:PRO:CD	2.33	0.56
1:B:198:ARG:HH22	2:B:12:GOL:H31	1.71	0.56
1:A:386:PHE:HA	2:A:18:GOL:H31	1.87	0.56
1:C:224:ARG:HD2	1:C:414:PHE:CE2	2.41	0.55
1:C:303:TRP:CE2	2:C:10:GOL:H11	2.42	0.55
1:A:287:GLU:O	2:A:16:GOL:H32	2.05	0.55
1:B:131:PRO:HG2	1:B:298:GLU:HG2	1.89	0.55
1:B:367:ASN:HD22	1:B:367:ASN:N	2.04	0.55
1:B:77:LEU:HD11	1:B:194:LYS:HB3	1.89	0.54
1:A:332:PHE:CD2	1:A:375:LEU:HD22	2.41	0.54
1:B:211:THR:CG2	1:B:450:LEU:HD13	2.34	0.54
1:A:264:LEU:HA	1:A:265:LYS:HE2	1.88	0.54
1:A:273:LYS:HB2	3:A:533:HOH:O	2.08	0.54
1:C:373:ASN:ND2	1:C:405:ASP:HB2	2.23	0.54
1:A:224:ARG:HD2	1:A:414:PHE:CE2	2.43	0.54
1:A:449:VAL:O	2:A:8:GOL:H32	2.08	0.53
1:C:432:ASP:OD2	1:C:435:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ARG:HD3	1:B:406:CYS:O	2.09	0.53
1:A:209:LEU:HD21	1:A:450:LEU:HD11	1.90	0.53
1:C:382:THR:O	1:C:385:LYS:HG2	2.08	0.53
1:B:198:ARG:HH22	2:B:12:GOL:C3	2.22	0.52
1:C:332:PHE:CD2	1:C:375:LEU:HD22	2.41	0.51
1:A:290:ASP:OD1	2:A:16:GOL:H11	2.09	0.51
1:C:198:ARG:HH22	2:C:14:GOL:H2	1.74	0.51
1:A:434:LYS:HB3	1:B:327:ILE:CD1	2.41	0.50
1:B:68:THR:OG1	1:B:70:GLU:HB2	2.12	0.50
1:C:363:PHE:HA	1:C:368:TYR:CD1	2.47	0.50
1:A:102:LEU:HD22	1:A:149:LEU:HD13	1.92	0.50
1:A:382:THR:O	1:A:385:LYS:HG2	2.12	0.50
1:A:439:VAL:HG12	1:A:442:GLN:CG	2.39	0.49
1:B:209:LEU:HD23	1:B:450:LEU:HD22	1.94	0.49
1:B:171:SER:HB3	1:B:207:GLN:O	2.13	0.49
1:B:184:ARG:HG3	1:B:184:ARG:NH1	2.24	0.49
1:B:221:THR:HG22	1:B:446:ILE:HD11	1.93	0.49
1:B:209:LEU:HD23	1:B:450:LEU:CD2	2.42	0.49
1:C:228:ARG:HD3	1:C:406:CYS:O	2.12	0.49
1:A:108:VAL:HG13	1:A:111:ILE:HD11	1.95	0.49
1:B:198:ARG:HH22	2:B:12:GOL:C2	2.23	0.49
1:A:135:LYS:HG2	3:A:454:HOH:O	2.12	0.49
1:A:184:ARG:HG3	1:A:184:ARG:NH1	2.23	0.49
1:B:198:ARG:NH2	2:B:12:GOL:H2	2.24	0.49
1:C:184:ARG:HH11	1:C:184:ARG:CG	2.19	0.49
1:A:218:THR:OG1	2:A:15:GOL:H31	2.12	0.49
1:A:329:THR:HG22	1:A:361:ASP:OD2	2.13	0.48
1:C:211:THR:HG21	1:C:450:LEU:CD1	2.37	0.48
1:B:440:GLU:O	1:B:442:GLN:HG2	2.13	0.48
1:B:215:ILE:HD12	1:C:276:SER:C	2.39	0.48
1:A:440:GLU:O	1:A:442:GLN:HG2	2.13	0.48
1:C:92:ASP:C	1:C:92:ASP:OD1	2.57	0.47
1:B:129:LYS:HD2	1:B:133:TRP:CZ2	2.50	0.47
1:C:89:ASP:H	1:C:95:GLN:NE2	2.13	0.47
1:C:184:ARG:HG3	1:C:184:ARG:NH1	2.24	0.47
1:B:102:LEU:HD22	1:B:149:LEU:HD13	1.97	0.47
1:B:216:LEU:HB3	1:B:217:PRO:CD	2.45	0.47
1:C:383:SER:HB2	1:C:388:VAL:HG21	1.95	0.47
1:B:224:ARG:HD2	1:B:414:PHE:CE1	2.50	0.46
1:A:228:ARG:HD3	1:A:406:CYS:O	2.15	0.46
1:A:88:LEU:HD22	1:A:95:GLN:HE21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ALA:HB3	1:A:190:PRO:HD3	1.98	0.46
1:C:333:SER:OG	1:C:356:PHE:HB3	2.15	0.46
1:A:77:LEU:CD1	1:A:194:LYS:HB3	2.45	0.46
1:A:109:GLU:O	1:A:110:ASP:HB2	2.14	0.46
2:A:4:GOL:O2	2:A:9:GOL:H32	2.14	0.46
1:B:373:ASN:OD1	1:B:405:ASP:HB2	2.15	0.46
1:C:406:CYS:O	1:C:407:LYS:HB2	2.16	0.46
1:C:439:VAL:HG12	1:C:442:GLN:HG3	1.98	0.46
1:A:156:THR:CG2	1:A:157:PRO:HD2	2.45	0.46
1:B:399:ASN:O	1:B:403:LEU:HG	2.16	0.46
1:A:383:SER:HB2	1:A:388:VAL:HG21	1.98	0.46
1:C:439:VAL:HG12	1:C:442:GLN:CG	2.46	0.46
1:B:196:ILE:O	1:B:200:VAL:HG13	2.17	0.45
1:C:439:VAL:CG1	1:C:442:GLN:HG3	2.46	0.45
1:A:108:VAL:CG1	1:A:111:ILE:HD11	2.47	0.45
1:A:363:PHE:HA	1:A:368:TYR:CD1	2.50	0.45
1:B:131:PRO:CG	1:B:298:GLU:HG2	2.46	0.45
1:C:236:HIS:CE1	1:C:249:LYS:HD3	2.52	0.45
1:C:236:HIS:ND1	1:C:249:LYS:HD3	2.31	0.45
1:A:294:LEU:HD11	2:A:7:GOL:H31	1.99	0.45
1:B:134:ARG:HA	2:B:11:GOL:H2	1.98	0.45
1:B:432:ASP:HB3	1:B:435:THR:OG1	2.16	0.45
1:C:303:TRP:O	1:C:316:VAL:HG11	2.16	0.45
1:B:356:PHE:HE1	2:B:17:GOL:O1	1.99	0.45
1:B:382:THR:O	1:B:385:LYS:HG2	2.17	0.45
1:C:68:THR:OG1	1:C:70:GLU:HB2	2.17	0.45
1:C:209:LEU:HD23	1:C:450:LEU:CD2	2.47	0.44
1:C:102:LEU:HD22	1:C:149:LEU:HD13	1.99	0.44
1:A:433:LYS:HG3	1:A:433:LYS:O	2.17	0.44
1:C:362:SER:HA	1:C:365:LYS:HG3	1.99	0.44
1:B:67:LYS:NZ	3:B:591:HOH:O	2.49	0.44
1:B:303:TRP:O	1:B:316:VAL:HG11	2.16	0.44
1:A:168:VAL:C	1:A:169:ILE:HG13	2.42	0.44
1:A:367:ASN:HD22	1:A:367:ASN:N	2.13	0.44
1:A:61:GLY:HA2	1:A:422:TYR:CZ	2.53	0.44
1:A:303:TRP:O	1:A:316:VAL:HG11	2.18	0.44
1:C:298:GLU:H	1:C:298:GLU:HG2	1.62	0.44
1:B:109:GLU:CG	1:B:110:ASP:H	2.31	0.44
1:B:226:GLN:NE2	3:B:522:HOH:O	2.49	0.43
1:B:352:ILE:HD13	1:B:390:VAL:HG23	2.00	0.43
1:B:402:PHE:O	1:B:406:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ILE:HD12	1:C:276:SER:CA	2.48	0.43
1:B:333:SER:OG	1:B:356:PHE:HB3	2.18	0.43
1:B:385:LYS:HE2	1:B:385:LYS:HB3	1.86	0.43
1:C:367:ASN:HD22	1:C:367:ASN:N	2.14	0.43
1:B:70:GLU:OE1	1:B:70:GLU:HA	2.19	0.43
1:C:228:ARG:HH11	1:C:407:LYS:HB2	1.84	0.43
1:B:92:ASP:OD1	1:B:92:ASP:C	2.61	0.43
1:C:175:ASN:HB2	2:C:5:GOL:O1	2.19	0.43
1:C:221:THR:HG22	1:C:446:ILE:HD11	2.01	0.42
1:B:189:ALA:HB3	1:B:190:PRO:HD3	2.01	0.42
1:B:260:ASN:ND2	1:B:384:LYS:NZ	2.67	0.42
1:A:79:LEU:O	1:A:80:ILE:C	2.61	0.42
1:A:189:ALA:HB3	1:A:190:PRO:CD	2.50	0.42
1:C:216:LEU:HB3	1:C:217:PRO:CD	2.44	0.42
1:C:330:ASP:HB3	1:C:375:LEU:HD11	2.01	0.42
1:C:432:ASP:HB3	1:C:435:THR:OG1	2.20	0.42
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.91	0.42
1:C:440:GLU:O	1:C:442:GLN:HG2	2.20	0.42
1:A:81:SER:O	1:A:144:LYS:HE3	2.20	0.42
1:B:184:ARG:HH11	1:B:184:ARG:CG	2.23	0.42
1:C:235:LEU:HD21	1:C:390:VAL:CG2	2.36	0.42
1:C:286:GLN:HG3	1:C:292:VAL:HG11	2.01	0.42
1:A:143:VAL:O	1:A:143:VAL:HG13	2.20	0.41
1:B:406:CYS:O	1:B:407:LYS:HB2	2.20	0.41
1:B:432:ASP:OD2	1:B:435:THR:HG23	2.18	0.41
1:A:156:THR:HG23	1:A:157:PRO:HD2	2.02	0.41
1:A:228:ARG:HH11	1:A:407:LYS:HB2	1.86	0.41
1:C:216:LEU:CB	1:C:217:PRO:HD2	2.47	0.41
1:C:365:LYS:HB3	1:C:366:PRO:CD	2.51	0.41
1:B:173:GLU:OE1	2:B:17:GOL:H32	2.20	0.41
1:C:79:LEU:O	1:C:80:ILE:C	2.64	0.41
2:A:4:GOL:C2	2:A:9:GOL:H32	2.51	0.41
1:B:89:ASP:H	1:B:95:GLN:NE2	2.19	0.41
1:C:198:ARG:HH22	2:C:14:GOL:H31	1.86	0.41
1:C:308:ASP:OD1	1:C:308:ASP:C	2.63	0.41
1:B:88:LEU:HD22	1:B:95:GLN:HE21	1.86	0.41
1:C:224:ARG:HD2	1:C:414:PHE:CZ	2.57	0.40
1:B:60:GLU:HG3	1:B:425:PHE:CE2	2.56	0.40
1:A:129:LYS:HD2	1:A:133:TRP:CZ2	2.56	0.40
1:A:432:ASP:OD2	1:A:435:THR:HG23	2.22	0.40
1:B:177:LEU:HD12	1:B:177:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:O	1:A:183:LEU:HD23	2.22	0.40
1:A:198:ARG:HH22	2:A:13:GOL:C3	2.33	0.40
1:A:434:LYS:CD	1:B:327:ILE:HD13	2.51	0.40
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.95	0.40
1:B:365:LYS:HB3	1:B:366:PRO:CD	2.48	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LYS:NZ	1:B:348:ASP:OD1[3_655]	1.35	0.85
1:A:145:SER:OG	1:C:346:GLN:OE1[7_555]	1.76	0.44
3:B:455:HOH:O	3:B:556:HOH:O[3_655]	1.78	0.42
1:B:148:LYS:CE	1:B:348:ASP:OD1[3_655]	1.94	0.26
1:A:348:ASP:OD1	1:C:148:LYS:NZ[7_555]	2.04	0.16
1:A:146:THR:OG1	1:C:346:GLN:O[7_555]	2.12	0.08
1:A:276:SER:OG	1:B:258:LEU:O[8_455]	2.12	0.08
1:A:343:ASP:O	1:C:182:LYS:CE[7_555]	2.15	0.05
1:A:273:LYS:NZ	1:B:407:LYS:NZ[8_455]	2.18	0.02
1:B:182:LYS:CG	1:B:343:ASP:O[3_655]	2.18	0.02

## 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	390/392 (100%)	367 (94%)	22 (6%)	1 (0%)	36 45
1	B	390/392 (100%)	368 (94%)	18 (5%)	4 (1%)	12 14
1	C	385/392 (98%)	364 (94%)	18 (5%)	3 (1%)	16 20
All	All	1165/1176 (99%)	1099 (94%)	58 (5%)	8 (1%)	18 24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	GLU
1	A	245	PRO
1	C	362	SER
1	B	65	LYS
1	B	245	PRO
1	C	245	PRO
1	B	362	SER
1	C	218	THR

### 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	360/360 (100%)	332 (92%)	28 (8%)	11	14
1	B	359/360 (100%)	332 (92%)	27 (8%)	12	16
1	C	357/360 (99%)	326 (91%)	31 (9%)	9	11
All	All	1076/1080 (100%)	990 (92%)	86 (8%)	11	13

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	88	LEU
1	A	108	VAL
1	A	149	LEU
1	A	171	SER
1	A	172	VAL
1	A	177	LEU
1	A	184	ARG
1	A	187	ARG
1	A	194	LYS
1	A	200	VAL
1	A	214	SER
1	A	249	LYS
1	A	250	SER
1	A	251	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	255	SER
1	A	265	LYS
1	A	284	LYS
1	A	294	LEU
1	A	310	ASN
1	A	316	VAL
1	A	331	TYR
1	A	346	GLN
1	A	352	ILE
1	A	364	GLU
1	A	367	ASN
1	A	390	VAL
1	A	436	LYS
1	B	77	LEU
1	B	88	LEU
1	B	108	VAL
1	B	111	ILE
1	B	149	LEU
1	B	171	SER
1	B	172	VAL
1	B	177	LEU
1	B	184	ARG
1	B	194	LYS
1	B	214	SER
1	B	220	LEU
1	B	249	LYS
1	B	250	SER
1	B	265	LYS
1	B	294	LEU
1	B	310	ASN
1	B	316	VAL
1	B	331	TYR
1	B	346	GLN
1	B	352	ILE
1	B	364	GLU
1	B	365	LYS
1	B	367	ASN
1	B	390	VAL
1	B	423	ARG
1	B	450	LEU
1	C	88	LEU
1	C	108	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	149	LEU
1	C	171	SER
1	C	172	VAL
1	C	177	LEU
1	C	184	ARG
1	C	194	LYS
1	C	207	GLN
1	C	214	SER
1	C	249	LYS
1	C	250	SER
1	C	251	SER
1	C	255	SER
1	C	265	LYS
1	C	273	LYS
1	C	284	LYS
1	C	294	LEU
1	C	310	ASN
1	C	316	VAL
1	C	331	TYR
1	C	340	THR
1	C	352	ILE
1	C	364	GLU
1	C	367	ASN
1	C	390	VAL
1	C	410	SER
1	C	423	ARG
1	C	428	ASP
1	C	433	LYS
1	C	450	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	93	ASN
1	A	95	GLN
1	A	163	ASN
1	A	166	ASN
1	A	201	ASN
1	A	226	GLN
1	A	260	ASN
1	A	286	GLN
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	314	ASN
1	A	367	ASN
1	A	421	ASN
1	B	95	GLN
1	B	163	ASN
1	B	201	ASN
1	B	226	GLN
1	B	260	ASN
1	B	286	GLN
1	B	307	HIS
1	B	310	ASN
1	B	347	HIS
1	B	367	ASN
1	B	397	GLN
1	B	421	ASN
1	C	95	GLN
1	C	163	ASN
1	C	201	ASN
1	C	226	GLN
1	C	260	ASN
1	C	286	GLN
1	C	293	GLN
1	C	310	ASN
1	C	367	ASN
1	C	373	ASN
1	C	397	GLN
1	C	421	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

18 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	B	17	-	5,5,5	0.49	0	5,5,5	0.93	0
2	GOL	C	6	-	5,5,5	0.67	0	5,5,5	1.01	0
2	GOL	C	10	-	5,5,5	0.61	0	5,5,5	0.95	0
2	GOL	B	12	-	5,5,5	0.71	0	5,5,5	1.11	0
2	GOL	A	9	-	5,5,5	0.79	0	5,5,5	1.00	0
2	GOL	A	16	-	5,5,5	0.51	0	5,5,5	0.91	0
2	GOL	B	2	-	5,5,5	0.44	0	5,5,5	0.89	0
2	GOL	B	11	-	5,5,5	0.61	0	5,5,5	0.96	0
2	GOL	A	15	-	5,5,5	0.42	0	5,5,5	0.84	0
2	GOL	C	14	-	5,5,5	0.67	0	5,5,5	1.05	0
2	GOL	A	8	-	5,5,5	0.55	0	5,5,5	0.91	0
2	GOL	B	1	-	5,5,5	0.40	0	5,5,5	0.83	0
2	GOL	A	3	-	5,5,5	0.49	0	5,5,5	0.95	0
2	GOL	A	4	-	5,5,5	0.19	0	5,5,5	0.84	0
2	GOL	A	18	-	5,5,5	0.47	0	5,5,5	0.95	0
2	GOL	C	5	-	5,5,5	0.50	0	5,5,5	0.83	0
2	GOL	A	7	-	5,5,5	0.48	0	5,5,5	0.85	0
2	GOL	A	13	-	5,5,5	0.56	0	5,5,5	1.06	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	17	-	-	4/4/4/4	-
2	GOL	C	6	-	-	0/4/4/4	-
2	GOL	C	10	-	-	2/4/4/4	-
2	GOL	B	12	-	-	2/4/4/4	-
2	GOL	A	9	-	-	2/4/4/4	-
2	GOL	A	16	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	2	-	-	0/4/4/4	-
2	GOL	B	11	-	-	2/4/4/4	-
2	GOL	A	15	-	-	1/4/4/4	-
2	GOL	C	14	-	-	4/4/4/4	-
2	GOL	A	8	-	-	2/4/4/4	-
2	GOL	B	1	-	-	3/4/4/4	-
2	GOL	A	3	-	-	4/4/4/4	-
2	GOL	A	4	-	-	2/4/4/4	-
2	GOL	A	18	-	-	2/4/4/4	-
2	GOL	C	5	-	-	2/4/4/4	-
2	GOL	A	7	-	-	2/4/4/4	-
2	GOL	A	13	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3	GOL	O1-C1-C2-C3
2	A	3	GOL	C1-C2-C3-O3
2	A	4	GOL	C1-C2-C3-O3
2	A	7	GOL	O1-C1-C2-C3
2	A	8	GOL	C1-C2-C3-O3
2	B	17	GOL	O1-C1-C2-O2
2	B	17	GOL	O1-C1-C2-C3
2	A	8	GOL	O2-C2-C3-O3
2	A	9	GOL	O1-C1-C2-C3
2	A	15	GOL	C1-C2-C3-O3
2	A	16	GOL	C1-C2-C3-O3
2	A	18	GOL	C1-C2-C3-O3
2	B	1	GOL	C1-C2-C3-O3
2	B	11	GOL	C1-C2-C3-O3
2	B	12	GOL	O1-C1-C2-C3
2	B	17	GOL	C1-C2-C3-O3
2	C	10	GOL	C1-C2-C3-O3
2	C	14	GOL	O1-C1-C2-C3
2	C	14	GOL	C1-C2-C3-O3
2	A	3	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	7	GOL	O1-C1-C2-O2
2	B	11	GOL	O2-C2-C3-O3
2	A	4	GOL	O2-C2-C3-O3
2	B	1	GOL	O1-C1-C2-O2
2	B	12	GOL	O1-C1-C2-O2
2	B	17	GOL	O2-C2-C3-O3
2	C	5	GOL	O1-C1-C2-O2
2	C	5	GOL	O2-C2-C3-O3
2	C	10	GOL	O2-C2-C3-O3
2	A	9	GOL	O1-C1-C2-O2
2	A	18	GOL	O2-C2-C3-O3
2	B	1	GOL	O2-C2-C3-O3
2	C	14	GOL	O2-C2-C3-O3
2	C	14	GOL	O1-C1-C2-O2
2	A	3	GOL	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	17	GOL	2	0
2	C	6	GOL	1	0
2	C	10	GOL	2	0
2	B	12	GOL	5	0
2	A	9	GOL	2	0
2	A	16	GOL	3	0
2	B	11	GOL	1	0
2	A	15	GOL	1	0
2	C	14	GOL	2	0
2	A	8	GOL	2	0
2	A	4	GOL	2	0
2	A	18	GOL	1	0
2	C	5	GOL	1	0
2	A	7	GOL	1	0
2	A	13	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	392/392 (100%)	1.11	55 (14%) <b>6</b> <b>5</b>	20, 34, 59, 88	0
1	B	392/392 (100%)	1.97	175 (44%) <b>0</b> <b>0</b>	15, 28, 55, 90	0
1	C	389/392 (99%)	2.15	194 (49%) <b>0</b> <b>0</b>	27, 44, 69, 89	0
All	All	1173/1176 (99%)	1.74	424 (36%) <b>1</b> <b>0</b>	15, 35, 64, 90	0

All (424) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	LEU	7.0
1	B	244	PRO	6.1
1	C	108	VAL	5.9
1	C	345	ALA	5.9
1	A	66	LEU	5.4
1	B	66	LEU	5.3
1	C	68	THR	4.8
1	C	245	PRO	4.7
1	C	67	LYS	4.7
1	B	307	HIS	4.7
1	A	109	GLU	4.7
1	C	192	LEU	4.6
1	C	342	LEU	4.6
1	B	253	VAL	4.6
1	C	244	PRO	4.6
1	C	76	PRO	4.5
1	C	62	PRO	4.3
1	C	246	ASN	4.2
1	B	306	GLY	4.2
1	B	143	VAL	4.2
1	B	343	ASP	4.2
1	B	109	GLU	4.1
1	C	238	VAL	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	240	PHE	4.1
1	C	311	SER	4.1
1	C	115	PHE	4.1
1	B	247	GLN	4.0
1	C	83	PHE	4.0
1	C	442	GLN	4.0
1	C	326	GLY	4.0
1	B	347	HIS	4.0
1	C	185	ASN	3.9
1	A	108	VAL	3.9
1	B	110	ASP	3.8
1	B	83	PHE	3.8
1	B	108	VAL	3.8
1	B	65	LYS	3.8
1	A	70	GLU	3.7
1	C	140	GLY	3.7
1	C	112	ASP	3.7
1	C	343	ASP	3.7
1	A	93	ASN	3.7
1	A	170	ASP	3.7
1	B	105	ASP	3.7
1	B	259	PRO	3.7
1	C	188	LEU	3.7
1	C	65	LYS	3.6
1	C	439	VAL	3.6
1	C	344	ASN	3.6
1	C	221	THR	3.6
1	B	245	PRO	3.6
1	C	100	TYR	3.6
1	B	81	SER	3.6
1	C	93	ASN	3.5
1	C	249	LYS	3.5
1	C	70	GLU	3.5
1	C	107	TYR	3.5
1	B	243	LEU	3.5
1	A	245	PRO	3.5
1	C	196	ILE	3.5
1	C	172	VAL	3.5
1	B	113	ALA	3.5
1	C	124	PHE	3.5
1	B	116	ARG	3.5
1	C	88	LEU	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	381	ILE	3.5
1	B	312	ASP	3.4
1	C	243	LEU	3.4
1	C	213	GLY	3.4
1	C	181	LYS	3.4
1	C	80	ILE	3.4
1	C	233	SER	3.4
1	C	248	THR	3.4
1	C	433	LYS	3.4
1	B	121	HIS	3.4
1	B	236	HIS	3.4
1	C	414	PHE	3.4
1	C	184	ARG	3.4
1	B	246	ASN	3.4
1	B	115	PHE	3.4
1	B	344	ASN	3.4
1	B	111	ILE	3.4
1	C	69	PRO	3.3
1	C	102	LEU	3.3
1	A	311	SER	3.3
1	B	67	LYS	3.3
1	C	255	SER	3.3
1	C	235	LEU	3.3
1	C	139	VAL	3.3
1	C	182	LYS	3.3
1	B	123	PHE	3.2
1	B	184	ARG	3.2
1	C	204	ASN	3.2
1	C	242	HIS	3.2
1	C	359	ALA	3.2
1	B	361	ASP	3.2
1	C	406	CYS	3.2
1	C	141	VAL	3.2
1	C	200	VAL	3.2
1	C	341	VAL	3.2
1	C	438	VAL	3.2
1	C	114	THR	3.2
1	B	442	GLN	3.2
1	C	423	ARG	3.2
1	B	89	ASP	3.2
1	B	406	CYS	3.2
1	C	206	TRP	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	110	ASP	3.1
1	C	368	TYR	3.1
1	B	185	ASN	3.1
1	B	251	SER	3.1
1	B	348	ASP	3.1
1	C	237	ASP	3.1
1	B	423	ARG	3.1
1	B	100	TYR	3.1
1	B	178	CYS	3.1
1	A	244	PRO	3.1
1	B	308	ASP	3.1
1	B	402	PHE	3.1
1	C	232	TRP	3.1
1	C	146	THR	3.0
1	B	233	SER	3.0
1	C	81	SER	3.0
1	B	260	ASN	3.0
1	C	104	TYR	3.0
1	C	324	GLU	3.0
1	C	77	LEU	3.0
1	C	360	SER	3.0
1	B	182	LYS	3.0
1	C	143	VAL	3.0
1	B	119	TYR	3.0
1	B	322	GLU	3.0
1	C	116	ARG	3.0
1	C	375	LEU	3.0
1	B	181	LYS	3.0
1	B	378	ASP	3.0
1	A	81	SER	3.0
1	C	251	SER	3.0
1	B	70	GLU	2.9
1	B	400	THR	2.9
1	C	203	GLN	2.9
1	C	257	THR	2.9
1	A	184	ARG	2.9
1	C	402	PHE	2.9
1	B	231	ASN	2.9
1	B	430	GLY	2.9
1	C	191	VAL	2.9
1	B	263	LYS	2.9
1	C	320	VAL	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	407	LYS	2.9
1	B	215	ILE	2.8
1	C	390	VAL	2.8
1	A	65	LYS	2.8
1	A	362	SER	2.8
1	C	87	THR	2.8
1	C	89	ASP	2.8
1	A	67	LYS	2.8
1	A	249	LYS	2.8
1	C	187	ARG	2.8
1	C	331	TYR	2.8
1	A	86	SER	2.8
1	B	310	ASN	2.8
1	B	313	SER	2.8
1	B	73	PRO	2.8
1	B	104	TYR	2.8
1	C	401	TYR	2.8
1	A	345	ALA	2.8
1	C	177	LEU	2.8
1	C	183	LEU	2.8
1	B	234	LYS	2.8
1	C	434	LYS	2.8
1	B	146	THR	2.7
1	B	389	ASP	2.7
1	C	170	ASP	2.7
1	C	307	HIS	2.7
1	B	61	GLY	2.7
1	C	215	ILE	2.7
1	C	313	SER	2.7
1	C	319	TYR	2.7
1	C	309	GLU	2.7
1	B	237	ASP	2.7
1	C	145	SER	2.7
1	B	302	HIS	2.7
1	B	266	GLY	2.7
1	C	160	PHE	2.7
1	C	408	PHE	2.7
1	A	233	SER	2.7
1	A	251	SER	2.7
1	B	200	VAL	2.7
1	B	209	LEU	2.7
1	C	230	ILE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	383	SER	2.6
1	C	250	SER	2.6
1	B	114	THR	2.6
1	B	387	GLY	2.6
1	C	263	LYS	2.6
1	B	451	LEU	2.6
1	C	106	ASN	2.6
1	C	131	PRO	2.6
1	C	142	ARG	2.6
1	B	152	PHE	2.6
1	C	332	PHE	2.6
1	C	149	LEU	2.6
1	B	238	VAL	2.6
1	C	214	SER	2.6
1	B	68	THR	2.6
1	C	256	TYR	2.6
1	C	407	LYS	2.6
1	B	126	TRP	2.6
1	C	217	PRO	2.6
1	B	408	PHE	2.6
1	B	425	PHE	2.6
1	C	176	PHE	2.6
1	A	149	LEU	2.6
1	B	242	HIS	2.6
1	C	347	HIS	2.6
1	A	182	LYS	2.6
1	C	234	LYS	2.6
1	B	368	TYR	2.6
1	C	338	PRO	2.5
1	C	431	ILE	2.5
1	C	425	PHE	2.5
1	B	380	LEU	2.5
1	A	113	ALA	2.5
1	C	241	SER	2.5
1	B	107	TYR	2.5
1	C	412	ASP	2.5
1	A	179	ILE	2.5
1	B	303	TRP	2.5
1	A	385	LYS	2.5
1	C	194	LYS	2.5
1	B	318	SER	2.5
1	A	326	GLY	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	312	ASP	2.5
1	B	330	ASP	2.5
1	C	216	LEU	2.5
1	A	265	LYS	2.5
1	C	365	LYS	2.5
1	B	191	VAL	2.5
1	C	180	HIS	2.5
1	B	261	ASN	2.5
1	C	74	ASN	2.5
1	C	321	VAL	2.5
1	B	241	SER	2.5
1	A	105	ASP	2.5
1	B	358	TYR	2.5
1	C	428	ASP	2.5
1	B	350	LEU	2.5
1	B	415	LEU	2.5
1	B	206	TRP	2.5
1	B	395	THR	2.5
1	C	400	THR	2.5
1	C	219	PRO	2.4
1	C	147	GLY	2.4
1	A	432	ASP	2.4
1	B	370	LYS	2.4
1	B	433	LYS	2.4
1	C	75	ASP	2.4
1	C	312	ASP	2.4
1	B	93	ASN	2.4
1	B	145	SER	2.4
1	C	318	SER	2.4
1	B	384	LYS	2.4
1	C	284	LYS	2.4
1	C	198	ARG	2.4
1	B	315	VAL	2.4
1	B	252	MET	2.4
1	B	254	ALA	2.4
1	C	155	ALA	2.4
1	C	197	THR	2.4
1	A	148	LYS	2.4
1	B	249	LYS	2.4
1	B	385	LYS	2.4
1	A	92	ASP	2.4
1	B	267	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	390	VAL	2.4
1	C	231	ASN	2.4
1	B	311	SER	2.4
1	B	326	GLY	2.4
1	C	94	LEU	2.4
1	C	403	LEU	2.4
1	A	253	VAL	2.4
1	A	400	THR	2.3
1	B	366	PRO	2.3
1	C	413	GLY	2.3
1	B	149	LEU	2.3
1	B	227	HIS	2.3
1	B	336	LEU	2.3
1	C	178	CYS	2.3
1	B	265	LYS	2.3
1	C	150	VAL	2.3
1	A	78	PRO	2.3
1	C	190	PRO	2.3
1	A	248	THR	2.3
1	B	137	TRP	2.3
1	B	362	SER	2.3
1	C	96	LEU	2.3
1	C	174	ILE	2.3
1	B	148	LYS	2.3
1	B	194	LYS	2.3
1	B	356	PHE	2.3
1	B	404	LYS	2.3
1	C	253	VAL	2.3
1	A	246	ASN	2.3
1	C	166	ASN	2.3
1	B	127	ALA	2.3
1	B	142	ARG	2.3
1	C	137	TRP	2.3
1	A	247	GLN	2.3
1	B	386	PHE	2.3
1	B	223	CYS	2.3
1	A	100	TYR	2.3
1	C	210	TYR	2.3
1	C	239	GLY	2.3
1	B	133	TRP	2.3
1	B	376	ILE	2.3
1	C	152	PHE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	72	VAL	2.3
1	B	334	TYR	2.3
1	C	325	ASN	2.2
1	B	102	LEU	2.2
1	B	120	SER	2.2
1	B	250	SER	2.2
1	B	327	ILE	2.2
1	B	342	LEU	2.2
1	C	85	TRP	2.2
1	B	131	PRO	2.2
1	B	438	VAL	2.2
1	B	166	ASN	2.2
1	B	225	TYR	2.2
1	B	277	THR	2.2
1	B	351	GLY	2.2
1	C	61	GLY	2.2
1	C	212	GLY	2.2
1	A	94	LEU	2.2
1	B	79	LEU	2.2
1	C	79	LEU	2.2
1	C	103	LEU	2.2
1	C	336	LEU	2.2
1	C	63	ILE	2.2
1	C	134	ARG	2.2
1	A	160	PHE	2.2
1	B	296	THR	2.2
1	C	435	THR	2.2
1	A	429	GLY	2.2
1	B	90	ILE	2.2
1	B	230	ILE	2.2
1	A	145	SER	2.2
1	B	82	ASP	2.2
1	C	71	ASP	2.2
1	B	122	GLU	2.2
1	C	229	PRO	2.2
1	B	341	VAL	2.2
1	A	185	ASN	2.2
1	A	254	ALA	2.2
1	C	252	MET	2.2
1	A	329	THR	2.2
1	B	248	THR	2.2
1	B	88	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	128	LEU	2.2
1	B	331	TYR	2.2
1	B	396	CYS	2.2
1	C	179	ILE	2.2
1	C	381	ILE	2.2
1	C	136	ASP	2.2
1	C	288	ARG	2.2
1	B	434	LYS	2.2
1	A	95	GLN	2.1
1	B	147	GLY	2.1
1	B	409	GLY	2.1
1	C	422	TYR	2.1
1	C	118	LYS	2.1
1	C	144	LYS	2.1
1	C	117	PHE	2.1
1	C	363	PHE	2.1
1	A	439	VAL	2.1
1	A	267	LEU	2.1
1	C	90	ILE	2.1
1	C	153	ILE	2.1
1	A	134	ARG	2.1
1	A	374	GLU	2.1
1	C	173	GLU	2.1
1	C	224	ARG	2.1
1	C	441	ASP	2.1
1	C	236	HIS	2.1
1	B	85	TRP	2.1
1	B	345	ALA	2.1
1	B	220	LEU	2.1
1	B	258	LEU	2.1
1	B	305	LEU	2.1
1	B	218	THR	2.1
1	B	298	GLU	2.1
1	B	374	GLU	2.1
1	B	393	CYS	2.1
1	B	155	ALA	2.1
1	B	279	LEU	2.1
1	C	373	ASN	2.1
1	A	144	LYS	2.1
1	A	433	LYS	2.1
1	B	301	LYS	2.1
1	C	148	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	436	LYS	2.1
1	A	401	TYR	2.1
1	B	112	ASP	2.1
1	C	82	ASP	2.1
1	B	214	SER	2.1
1	C	362	SER	2.1
1	B	190	PRO	2.1
1	C	223	CYS	2.1
1	C	154	ALA	2.0
1	C	267	LEU	2.0
1	A	111	ILE	2.0
1	B	63	ILE	2.0
1	C	205	ILE	2.0
1	B	357	TYR	2.0
1	C	348	ASP	2.0
1	C	78	PRO	2.0
1	C	366	PRO	2.0
1	B	320	VAL	2.0
1	B	324	GLU	2.0
1	C	374	GLU	2.0
1	C	419	LEU	2.0
1	B	229	PRO	2.0
1	B	285	TYR	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 oligosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	C	14	6/6	0.57	0.34	79,81,83,84	0
2	GOL	B	11	6/6	0.65	0.24	52,55,59,66	0
2	GOL	B	12	6/6	0.66	0.29	61,69,71,74	0
2	GOL	A	16	6/6	0.67	0.22	78,79,80,80	0
2	GOL	A	9	6/6	0.70	0.20	36,49,55,59	0
2	GOL	C	6	6/6	0.71	0.21	61,63,71,73	0
2	GOL	B	17	6/6	0.72	0.35	75,80,82,83	0
2	GOL	A	15	6/6	0.73	0.24	63,72,75,86	0
2	GOL	A	13	6/6	0.74	0.24	61,67,67,70	0
2	GOL	C	10	6/6	0.75	0.18	41,51,55,56	0
2	GOL	A	7	6/6	0.75	0.19	45,46,50,59	0
2	GOL	B	1	6/6	0.80	0.15	32,34,38,42	0
2	GOL	C	5	6/6	0.81	0.19	52,55,57,61	0
2	GOL	A	8	6/6	0.81	0.16	32,43,46,50	0
2	GOL	B	2	6/6	0.82	0.13	40,49,54,56	0
2	GOL	A	3	6/6	0.84	0.17	39,46,50,52	0
2	GOL	A	18	6/6	0.88	0.13	32,46,47,59	0
2	GOL	A	4	6/6	0.89	0.14	32,36,45,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.