



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:09 PM GMT

PDB ID : 1NMT
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

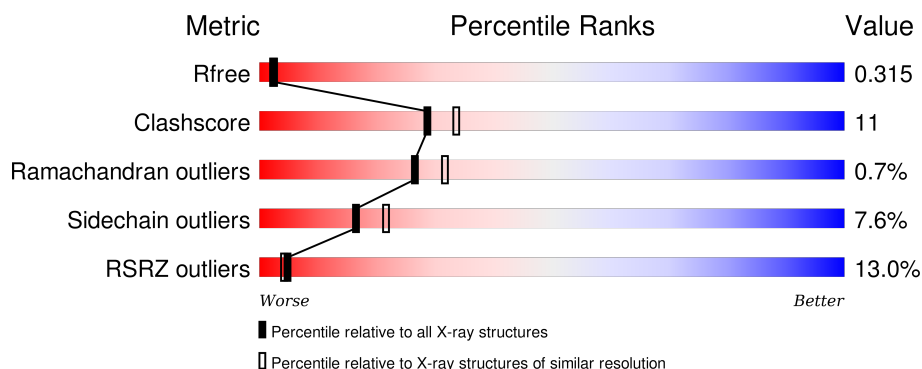
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	<div> <div>4%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	B	392	<div> <div>14%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>
1	C	392	<div> <div>21%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	13	-	-	-	X
2	GOL	A	16	-	-	-	X
2	GOL	A	3	-	-	-	X
2	GOL	A	4	-	-	-	X
2	GOL	A	7	-	-	-	X
2	GOL	A	8	-	-	-	X
2	GOL	A	9	-	-	-	X
2	GOL	B	12	-	-	X	X
2	GOL	B	17	-	-	-	X
2	GOL	C	10	-	-	-	X
2	GOL	C	14	-	-	-	X
2	GOL	C	6	-	-	-	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
1	A	392	Total	C	N	O	S	0	0	0
			3210	2079	524	598	9			
1	B	392	Total	C	N	O	S	0	0	0
			3207	2078	524	596	9			
1	C	389	Total	C	N	O	S	0	0	0
			3185	2064	521	591	9			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

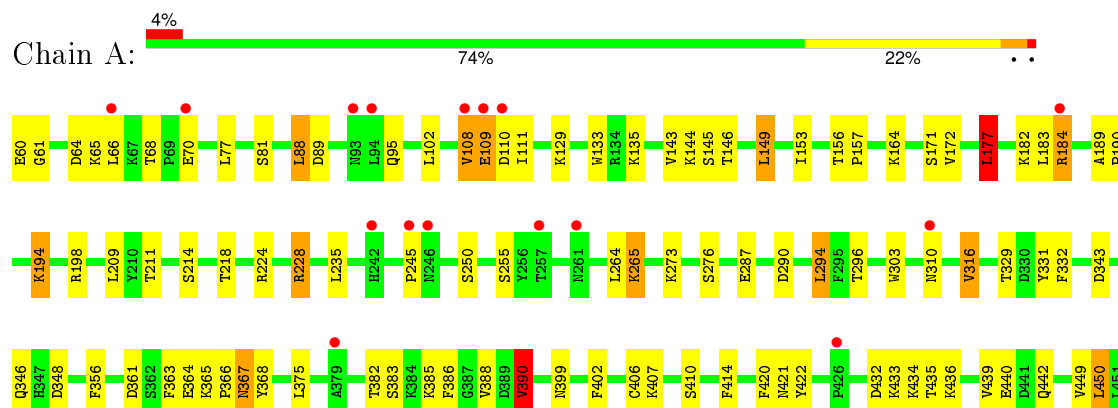
- Molecule 3 is water.

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

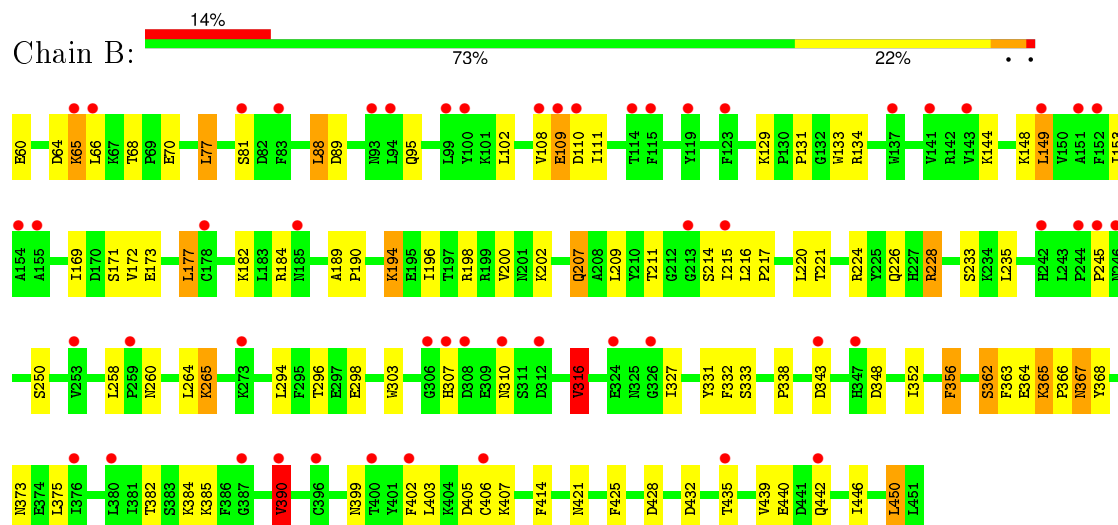
3 Residue-property plots

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

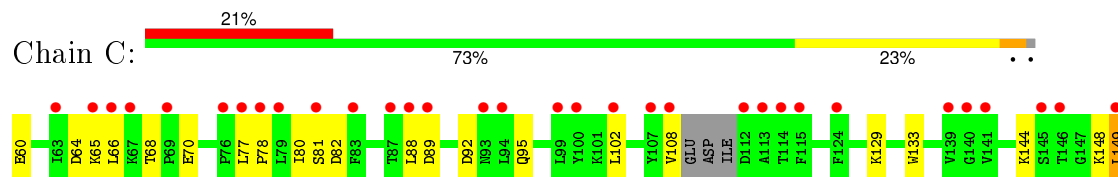
• Molecule 1: N-MYRISTOYL TRANSFERASE

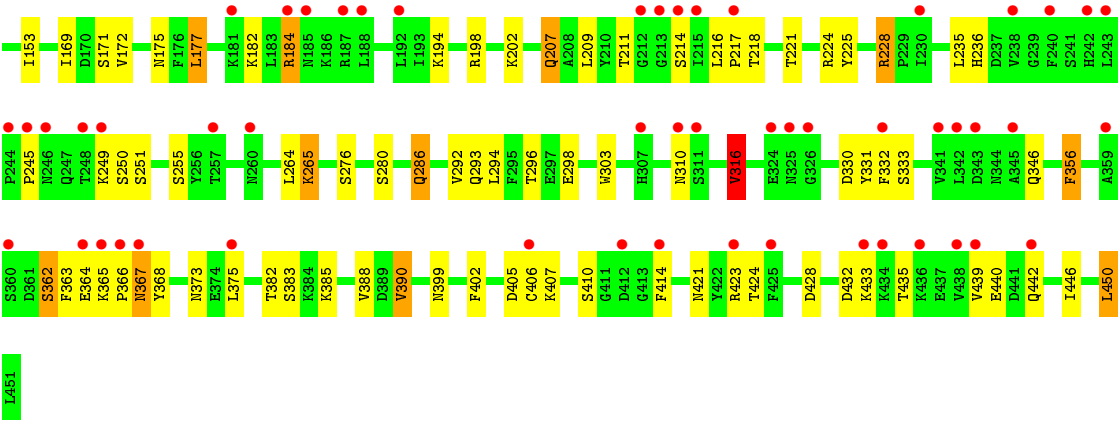


• Molecule 1: N-MYRISTOYL TRANSFERASE



• 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, α , β , γ	132.00 Å 166.50 Å 179.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.85 – 2.45 20.72 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.85-2.45) 97.5 (20.72-2.43)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.44 Å)	Xtriage
Refinement program	X-PLOR 3.98	Depositor
R, R_{free}	0.214 , 0.251 0.298 , 0.315	Depositor DCC
R_{free} test set	3660 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 72615 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10001	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	0/3296	0.74	4/4473 (0.1%)
1	B	0.58	0/3293	0.75	4/4469 (0.1%)
1	C	0.51	0/3270	0.71	3/4436 (0.1%)
All	All	0.55	0/9859	0.73	11/13378 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	LEU	CA-CB-CG	-6.44	100.48	115.30
1	B	450	LEU	CA-CB-CG	-6.19	101.06	115.30
1	B	390	VAL	CB-CA-C	-6.17	99.67	111.40
1	C	450	LEU	CA-CB-CG	-6.17	101.12	115.30
1	B	316	VAL	CB-CA-C	-5.78	100.43	111.40
1	A	296	THR	N-CA-C	-5.61	95.86	111.00
1	A	390	VAL	CB-CA-C	-5.39	101.16	111.40
1	C	296	THR	N-CA-C	-5.11	97.21	111.00
1	C	316	VAL	CB-CA-C	-5.10	101.71	111.40
1	A	177	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	296	THR	N-CA-C	-5.07	97.32	111.00

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	69	6
1	B	3207	0	3165	84	5
1	C	3185	0	3145	75	4
2	A	54	0	72	13	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	2	1
3	C	36	0	0	0	0
All	All	10001	0	9621	222	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 11.

All (222) 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:H	1:B:265:LYS:HE2	1.27	0.97
1:A:235:LEU:HD21	1:A:390:VAL:HG22	1.49	0.94
1:A:265:LYS:HE2	1:A:265:LYS:H	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:CE	1:B:265:LYS:H	1.83	0.92
1:B:64:ASP:H	1:B:421:ASN:HD21	1.23	0.86
1:C:265:LYS:CE	1:C:265:LYS:H	1.88	0.84
1:A:265:LYS:CE	1:A:265:LYS:H	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:HH11	1:A:184:ARG:HG3	1.45	0.82
1:B:184:ARG:HH11	1:B:184:ARG:HG3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:265:LYS:HE2	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:265:LYS:N	1:C:265:LYS:HE2	2.02	0.70
1:C:81:SER:O	1:C:144:LYS:HE3	1.91	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:439:VAL:CG1	1:A:442:GLN:HG3	2.29	0.62
1:A:367:ASN:H	1:A:367:ASN:HD22	1.48	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
1:B:362:SER:HA	1:B:365:LYS:HD3	1.83	0.61
1:A:198:ARG:HH22	2:A:13:GOL:H31	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ASN:H	1:C:367:ASN:HD22	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:C:264:LEU:HA	1:C:265:LYS:HE2	1.85	0.58
1:A:211:THR:HG21	1:A:450:LEU:CD1	2.32	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:B:169:ILE:CG2	1:B:207:GLN:HG3	2.30	0.57
1:A:68:THR:OG1	1:A:70:GLU:HB2	2.04	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:184:ARG:CG	1:A:184:ARG:HH11	2.17	0.56
1:A:89:ASP:H	1:A:95:GLN:NE2	2.03	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:N	1:B:367:ASN:HD22	2.04	0.55
1:B:77:LEU:HD11	1:B:194:LYS:HB3	1.89	0.54
1:B:211:THR:CG2	1:B:450:LEU:HD13	2.34	0.54
1:A:332:PHE:CD2	1:A:375:LEU:HD22	2.41	0.54
1:A:264:LEU:HA	1:A:265:LYS:HE2	1.88	0.54
1:C:373:ASN:ND2	1:C:405:ASP:HB2	2.23	0.54
1:A:273:LYS:HB2	3:A:533:HOH:O	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PHE:HD1	2:A:15:GOL:HO2	1.56	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:C:363:PHE:HA	1:C:368:TYR:CD1	2.47	0.50
1:B:68:THR:OG1	1:B:70:GLU:HB2	2.12	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:NH1	1:B:184:ARG:HG3	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:B:198:ARG:HH22	2:B:12:GOL:C2	2.23	0.49
1:A:108:VAL:HG13	1:A:111:ILE:HD11	1.95	0.49
1:A:184:ARG:NH1	1:A:184:ARG:HG3	2.23	0.49
1:C:184:ARG:HH11	1:C:184:ARG:CG	2.19	0.49
1:B:198:ARG:NH2	2:B:12:GOL:H2	2.24	0.49
1:A:135:LYS:HG2	3:A:454:HOH:O	2.12	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:A:440:GLU:O	1:A:442:GLN:HG2	2.13	0.48
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:NH1	1:C:184:ARG:HG3	2.24	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:102:LEU:HD22	1:B:149:LEU:HD13	1.97	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
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:C:406:CYS:O	1:C:407:LYS:HB2	2.16	0.46
1:A:109:GLU:O	1:A:110:ASP:HB2	2.14	0.46
1:B:373:ASN:OD1	1:B:405:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:CD1	1:A:194:LYS:HB3	2.45	0.46
2:A:4:GOL:O2	2:A:9:GOL:H32	2.14	0.46
1:C:439:VAL:HG12	1:C:442:GLN:HG3	1.98	0.46
1:B:399:ASN:O	1:B:403:LEU:HG	2.16	0.46
1:A:156:THR:CG2	1:A:157:PRO:HD2	2.45	0.46
1:C:439:VAL:HG12	1:C:442:GLN:CG	2.46	0.46
1:A:383:SER:HB2	1:A:388:VAL:HG21	1.98	0.46
1:C:439:VAL:CG1	1:C:442:GLN:HG3	2.46	0.45
1:B:196:ILE:O	1:B:200:VAL:HG13	2.17	0.45
1:A:108:VAL:CG1	1:A:111:ILE:HD11	2.47	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:A:363:PHE:HA	1:A:368:TYR:CD1	2.50	0.45
1:C:236:HIS:ND1	1:C:249:LYS:HD3	2.31	0.45
1:B:134:ARG:HA	2:B:11:GOL:H2	1.98	0.45
1:A:294:LEU:HD11	2:A:7:GOL:H31	1.99	0.45
1:C:303:TRP:O	1:C:316:VAL:HG11	2.16	0.45
1:B:432:ASP:HB3	1:B:435:THR:OG1	2.16	0.45
1:B:382:THR:O	1:B:385:LYS:HG2	2.17	0.45
1:B:356:PHE:HE1	2:B:17:GOL:O1	1.99	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:C:362:SER:HA	1:C:365:LYS:HG3	1.99	0.44
1:A:433:LYS:O	1:A:433:LYS:HG3	2.17	0.44
1:B:303:TRP:O	1:B:316:VAL:HG11	2.16	0.44
1:A:367:ASN:N	1:A:367:ASN:HD22	2.13	0.44
1:A:303:TRP:O	1:A:316:VAL:HG11	2.18	0.44
1:A:61:GLY:HA2	1:A:422:TYR:CZ	2.53	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:352:ILE:HD13	1:B:390:VAL:HG23	2.00	0.43
1:B:226:GLN:NE2	3:B:522:HOH:O	2.49	0.43
1:B:215:ILE:HD12	1:C:276:SER:C	2.39	0.43
1:B:402:PHE:O	1:B:406:CYS:HB2	2.19	0.43
1:B:215:ILE:HD12	1:C:276:SER:CA	2.48	0.43
1:B:385:LYS:HE2	1:B:385:LYS:HB3	1.86	0.43
1:B:333:SER:OG	1:B:356:PHE:HB3	2.18	0.43
1:C:367:ASN:N	1:C:367:ASN:HD22	2.14	0.43
1:B:70:GLU:HA	1:B:70:GLU:OE1	2.19	0.43
1:C:228:ARG:HH11	1:C:407:LYS:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ASP:C	1:C:92:ASP:OD1	2.57	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: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:A:189:ALA:HB3	1:A:190:PRO:CD	2.50	0.42
1:C:375:LEU:HA	1:C:375:LEU:HD23	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:C:235:LEU:HD21	1:C:390:VAL:CG2	2.36	0.42
1:B:184:ARG:CG	1:B:184:ARG:HH11	2.23	0.42
1:C:286:GLN:HG3	1:C:292:VAL:HG11	2.01	0.42
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:143:VAL:O	1:A:143:VAL:HG13	2.20	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:A:228:ARG:HH11	1:A:407:LYS:HB2	1.86	0.41
1:A:156:THR:HG23	1:A:157:PRO:HD2	2.02	0.41
1:B:173:GLU:OE1	2:B:17:GOL:H32	2.20	0.41
1:C:198:ARG:HH22	2:C:14:GOL:H31	1.86	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: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:A:434:LYS:CD	1:B:327:ILE:HD13	2.51	0.40
1:A:198:ARG:HH22	2:A:13:GOL:C3	2.33	0.40
1:A:182:LYS:O	1:A:183:LEU:HD23	2.22	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%)	46	57
1	B	390/392 (100%)	368 (94%)	18 (5%)	4 (1%)	19	21
1	C	385/392 (98%)	364 (94%)	18 (5%)	3 (1%)	24	28
All	All	1165/1176 (99%)	1099 (94%)	58 (5%)	8 (1%)	26	32

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 ⓘ

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%)	334 (93%)	26 (7%)	18	24
1	B	359/360 (100%)	332 (92%)	27 (8%)	17	22
1	C	357/360 (99%)	328 (92%)	29 (8%)	15	19
All	All	1076/1080 (100%)	994 (92%)	82 (8%)	16	21

All (82) 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	109	GLU
1	A	149	LEU
1	A	171	SER
1	A	172	VAL
1	A	177	LEU
1	A	184	ARG
1	A	194	LYS
1	A	214	SER
1	A	228	ARG
1	A	250	SER
1	A	255	SER
1	A	265	LYS
1	A	294	LEU
1	A	310	ASN
1	A	316	VAL
1	A	331	TYR
1	A	346	GLN
1	A	356	PHE
1	A	364	GLU
1	A	367	ASN
1	A	390	VAL
1	A	410	SER
1	A	436	LYS

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Mol	Chain	Res	Type
1	B	77	LEU
1	B	88	LEU
1	B	108	VAL
1	B	111	ILE
1	B	149	LEU
1	B	172	VAL
1	B	177	LEU
1	B	194	LYS
1	B	202	LYS
1	B	207	GLN
1	B	214	SER
1	B	220	LEU
1	B	228	ARG
1	B	233	SER
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	338	PRO
1	B	356	PHE
1	B	364	GLU
1	B	365	LYS
1	B	367	ASN
1	B	390	VAL
1	B	428	ASP
1	C	88	LEU
1	C	108	VAL
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	202	LYS
1	C	207	GLN
1	C	214	SER
1	C	228	ARG
1	C	250	SER
1	C	251	SER
1	C	255	SER

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Mol	Chain	Res	Type
1	C	265	LYS
1	C	286	GLN
1	C	294	LEU
1	C	310	ASN
1	C	316	VAL
1	C	331	TYR
1	C	356	PHE
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	163	ASN
1	A	201	ASN
1	A	260	ASN
1	A	286	GLN
1	A	310	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	367	ASN
1	B	397	GLN
1	B	421	ASN
1	C	95	GLN
1	C	163	ASN
1	C	201	ASN
1	C	260	ASN
1	C	286	GLN
1	C	293	GLN
1	C	310	ASN

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Mol	Chain	Res	Type
1	C	367	ASN
1	C	373	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	A	13	-	5,5,5	0.48	0	5,5,5	1.05	0
2	GOL	A	15	-	5,5,5	0.34	0	5,5,5	0.85	0
2	GOL	A	16	-	5,5,5	0.43	0	5,5,5	0.91	0
2	GOL	A	18	-	5,5,5	0.39	0	5,5,5	0.95	0
2	GOL	A	3	-	5,5,5	0.42	0	5,5,5	0.94	0
2	GOL	A	4	-	5,5,5	0.12	0	5,5,5	0.85	0
2	GOL	A	7	-	5,5,5	0.41	0	5,5,5	0.86	0
2	GOL	A	8	-	5,5,5	0.48	0	5,5,5	0.89	0
2	GOL	A	9	-	5,5,5	0.70	0	5,5,5	0.99	0
2	GOL	B	1	-	5,5,5	0.33	0	5,5,5	0.84	0
2	GOL	B	11	-	5,5,5	0.53	0	5,5,5	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	12	-	5,5,5	0.63	0	5,5,5	1.10	0
2	GOL	B	17	-	5,5,5	0.40	0	5,5,5	0.93	0
2	GOL	B	2	-	5,5,5	0.37	0	5,5,5	0.89	0
2	GOL	C	10	-	5,5,5	0.52	0	5,5,5	0.95	0
2	GOL	C	14	-	5,5,5	0.59	0	5,5,5	1.05	0
2	GOL	C	5	-	5,5,5	0.41	0	5,5,5	0.84	0
2	GOL	C	6	-	5,5,5	0.59	0	5,5,5	1.01	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	A	13	-	-	0/4/4/4	0/0/0/0
2	GOL	A	15	-	-	0/4/4/4	0/0/0/0
2	GOL	A	16	-	-	0/4/4/4	0/0/0/0
2	GOL	A	18	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3	-	-	0/4/4/4	0/0/0/0
2	GOL	A	4	-	-	0/4/4/4	0/0/0/0
2	GOL	A	7	-	-	0/4/4/4	0/0/0/0
2	GOL	A	8	-	-	0/4/4/4	0/0/0/0
2	GOL	A	9	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1	-	-	0/4/4/4	0/0/0/0
2	GOL	B	11	-	-	0/4/4/4	0/0/0/0
2	GOL	B	12	-	-	0/4/4/4	0/0/0/0
2	GOL	B	17	-	-	0/4/4/4	0/0/0/0
2	GOL	B	2	-	-	0/4/4/4	0/0/0/0
2	GOL	C	10	-	-	0/4/4/4	0/0/0/0
2	GOL	C	14	-	-	0/4/4/4	0/0/0/0
2	GOL	C	5	-	-	0/4/4/4	0/0/0/0
2	GOL	C	6	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	13	GOL	2	0
2	A	15	GOL	2	0
2	A	16	GOL	3	0
2	A	18	GOL	1	0
2	A	4	GOL	2	0
2	A	7	GOL	1	0
2	A	8	GOL	2	0
2	A	9	GOL	2	0
2	B	11	GOL	1	0
2	B	12	GOL	5	0
2	B	17	GOL	2	0
2	C	10	GOL	2	0
2	C	14	GOL	2	0
2	C	5	GOL	1	0
2	C	6	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, 95th 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 ²)	Q<0.9
1	A	392/392 (100%)	0.52	16 (4%) 41 44	20, 34, 59, 88	0
1	B	392/392 (100%)	1.12	53 (13%) 4 4	15, 28, 55, 90	0
1	C	389/392 (99%)	1.33	84 (21%) 1 1	27, 44, 69, 89	0
All	All	1173/1176 (99%)	0.99	153 (13%) 5 4	15, 35, 64, 90	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	PRO	6.3
1	A	245	PRO	5.6
1	A	310	ASN	4.9
1	C	213	GLY	4.8
1	B	244	PRO	4.7
1	C	243	LEU	4.4
1	C	249	LYS	4.4
1	C	423	ARG	4.2
1	C	245	PRO	4.2
1	C	66	LEU	4.1
1	A	246	ASN	4.1
1	C	434	LYS	4.1
1	B	310	ASN	4.1
1	B	66	LEU	3.9
1	A	110	ASP	3.9
1	C	67	LYS	3.9
1	A	66	LEU	3.9
1	C	141	VAL	3.9
1	C	325	ASN	3.8
1	C	81	SER	3.8
1	C	65	LYS	3.8
1	C	425	PHE	3.8
1	C	406	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	326	GLY	3.7
1	C	242	HIS	3.5
1	C	76	PRO	3.5
1	A	261	ASN	3.4
1	C	248	THR	3.4
1	C	214	SER	3.4
1	C	311	SER	3.4
1	C	345	ALA	3.3
1	C	439	VAL	3.3
1	C	63	ILE	3.3
1	C	112	ASP	3.3
1	C	246	ASN	3.2
1	A	94	LEU	3.2
1	C	94	LEU	3.2
1	B	110	ASP	3.2
1	C	187	ARG	3.2
1	A	70	GLU	3.1
1	A	426	PRO	3.1
1	C	310	ASN	3.1
1	C	185	ASN	3.1
1	C	341	VAL	3.1
1	C	240	PHE	3.0
1	C	442	GLN	3.0
1	C	215	ILE	3.0
1	B	109	GLU	3.0
1	B	143	VAL	3.0
1	B	259	PRO	3.0
1	A	93	ASN	2.9
1	C	149	LEU	2.9
1	B	93	ASN	2.8
1	B	94	LEU	2.8
1	C	324	GLU	2.8
1	B	307	HIS	2.8
1	C	342	LEU	2.8
1	C	102	LEU	2.8
1	B	152	PHE	2.8
1	B	123	PHE	2.7
1	B	114	THR	2.7
1	B	308	ASP	2.6
1	C	114	THR	2.6
1	C	140	GLY	2.6
1	B	65	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	307	HIS	2.6
1	C	414	PHE	2.6
1	B	185	ASN	2.6
1	B	324	GLU	2.5
1	A	257	THR	2.5
1	C	115	PHE	2.5
1	B	253	VAL	2.5
1	A	109	GLU	2.5
1	B	242	HIS	2.5
1	A	108	VAL	2.5
1	B	213	GLY	2.5
1	C	139	VAL	2.5
1	B	347	HIS	2.5
1	C	113	ALA	2.5
1	C	238	VAL	2.5
1	C	100	TYR	2.5
1	C	69	PRO	2.5
1	C	433	LYS	2.5
1	C	88	LEU	2.5
1	C	260	ASN	2.5
1	C	124	PHE	2.4
1	C	146	THR	2.4
1	C	343	ASP	2.4
1	B	246	ASN	2.4
1	C	87	THR	2.4
1	B	400	THR	2.4
1	B	178	CYS	2.4
1	B	99	LEU	2.4
1	B	312	ASP	2.4
1	C	412	ASP	2.4
1	B	151	ALA	2.4
1	C	192	LEU	2.3
1	B	81	SER	2.3
1	B	100	TYR	2.3
1	C	77	LEU	2.3
1	B	387	GLY	2.3
1	C	108	VAL	2.3
1	C	83	PHE	2.3
1	B	215	ILE	2.3
1	B	442	GLN	2.3
1	C	375	LEU	2.3
1	B	435	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	359	ALA	2.2
1	B	245	PRO	2.2
1	B	406	CYS	2.2
1	B	108	VAL	2.2
1	C	78	PRO	2.2
1	A	184	ARG	2.2
1	B	115	PHE	2.2
1	B	149	LEU	2.2
1	C	438	VAL	2.2
1	C	364	GLU	2.2
1	C	360	SER	2.2
1	B	306	GLY	2.2
1	C	365	LYS	2.2
1	B	402	PHE	2.2
1	C	436	LYS	2.2
1	C	332	PHE	2.2
1	C	79	LEU	2.2
1	B	273	LYS	2.2
1	C	93	ASN	2.2
1	B	83	PHE	2.2
1	B	343	ASP	2.1
1	B	380	LEU	2.1
1	C	188	LEU	2.1
1	C	257	THR	2.1
1	B	154	ALA	2.1
1	C	145	SER	2.1
1	C	99	LEU	2.1
1	A	242	HIS	2.1
1	C	181	LYS	2.1
1	B	326	GLY	2.1
1	B	396	CYS	2.1
1	B	376	ILE	2.1
1	C	107	TYR	2.1
1	B	155	ALA	2.1
1	C	89	ASP	2.1
1	C	367	ASN	2.1
1	C	217	PRO	2.1
1	C	366	PRO	2.1
1	A	379	ALA	2.1
1	B	141	VAL	2.1
1	B	390	VAL	2.0
1	C	212	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	119	TYR	2.0
1	C	230	ILE	2.0
1	C	184	ARG	2.0
1	B	137	TRP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	B	12	6/6	0.65	0.37	10.48	61,69,71,74	0
2	GOL	A	16	6/6	0.61	0.40	7.73	78,79,80,80	0
2	GOL	B	17	6/6	0.80	0.43	7.28	75,80,82,83	0
2	GOL	C	14	6/6	0.56	0.58	6.40	79,81,83,84	0
2	GOL	A	7	6/6	0.76	0.23	5.31	45,46,50,59	0
2	GOL	C	10	6/6	0.83	0.29	4.97	41,51,55,56	0
2	GOL	A	9	6/6	0.71	0.26	4.74	36,49,55,59	0
2	GOL	A	13	6/6	0.78	0.30	4.04	61,67,67,70	0
2	GOL	A	4	6/6	0.91	0.20	3.08	32,36,45,46	0
2	GOL	A	3	6/6	0.82	0.23	2.91	39,46,50,52	0
2	GOL	A	8	6/6	0.84	0.22	2.85	32,43,46,50	0
2	GOL	C	6	6/6	0.87	0.23	2.32	61,63,71,73	0
2	GOL	A	15	6/6	0.78	0.24	1.52	63,72,75,86	0
2	GOL	C	5	6/6	0.86	0.24	0.96	52,55,57,61	0
2	GOL	A	18	6/6	0.86	0.19	0.66	32,46,47,59	0
2	GOL	B	1	6/6	0.85	0.23	-0.20	32,34,38,42	0
2	GOL	B	2	6/6	0.91	0.16	-1.31	40,49,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	B	11	6/6	0.74	0.48	-	52,55,59,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.