Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:57 am BST

PDB ID	:	3RAM
Title	:	Crystal structure of HmrA
Authors	:	Botelho, T.; Guevara, T.; Marrero, A.; Gomis-Ruth, F.X.
Deposited on	:	2011-03-28
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/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:

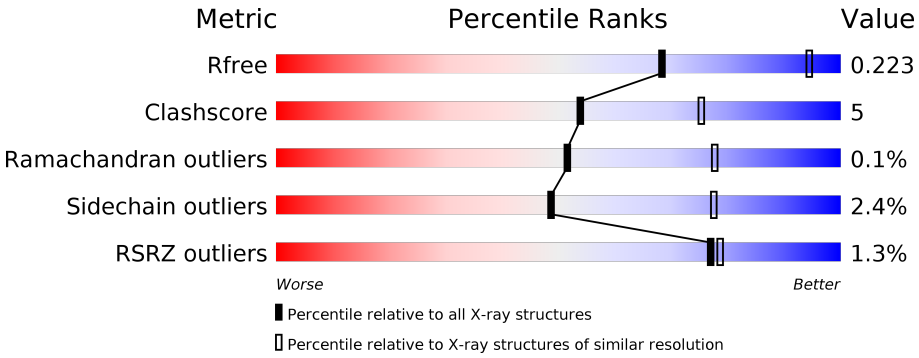
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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 <=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	394	% 87% 11% ··
1	B	394	% 86% 12% ··
1	C	394	4% 90% 9% ··
1	D	394	88% 10% ··

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12547 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 HmrA protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	Se	0	0	0
			2999	1888	518	584	3	6			
1	B	389	Total	C	N	O	S	Se	0	0	0
			2987	1881	516	582	3	5			
1	C	390	Total	C	N	O	S	Se	0	0	0
			2995	1886	517	583	3	6			
1	D	391	Total	C	N	O	S	Se	0	0	0
			2999	1888	518	584	3	6			

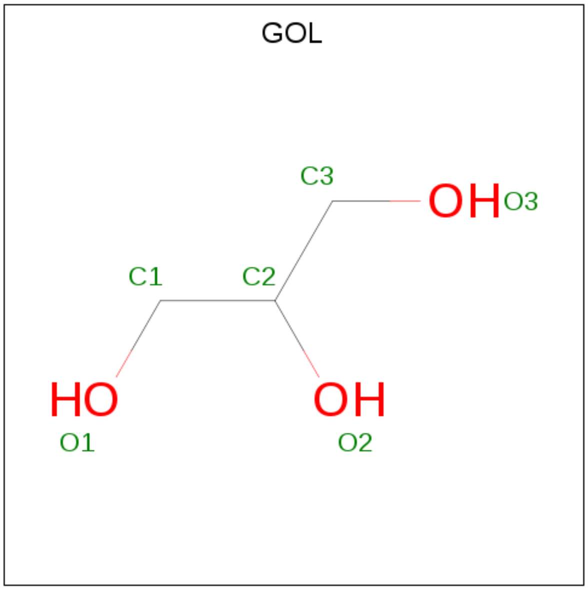
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	SER	CLONING ARTIFACT	UNP Q99Q45
B	2	GLY	SER	CLONING ARTIFACT	UNP Q99Q45
C	2	GLY	SER	CLONING ARTIFACT	UNP Q99Q45
D	2	GLY	SER	CLONING ARTIFACT	UNP Q99Q45

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	109	Total O 109 109	0	0

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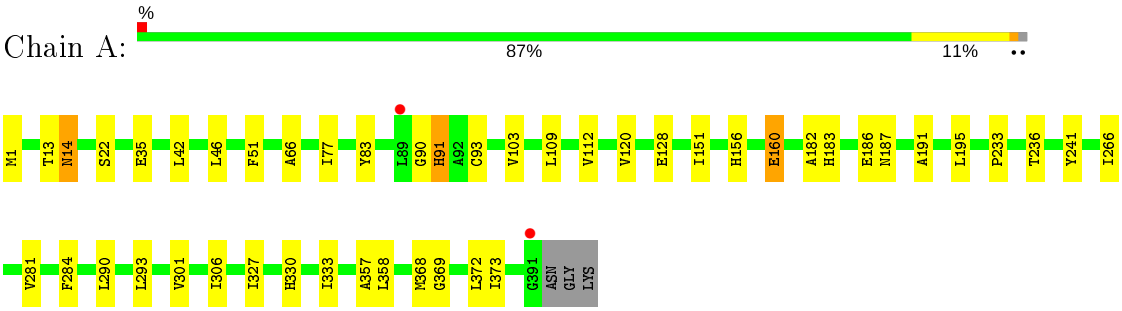
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	71	Total O 71 71	0	0
4	C	75	Total O 75 75	0	0
4	D	111	Total O 111 111	0	0

3 Residue-property plots (i)

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

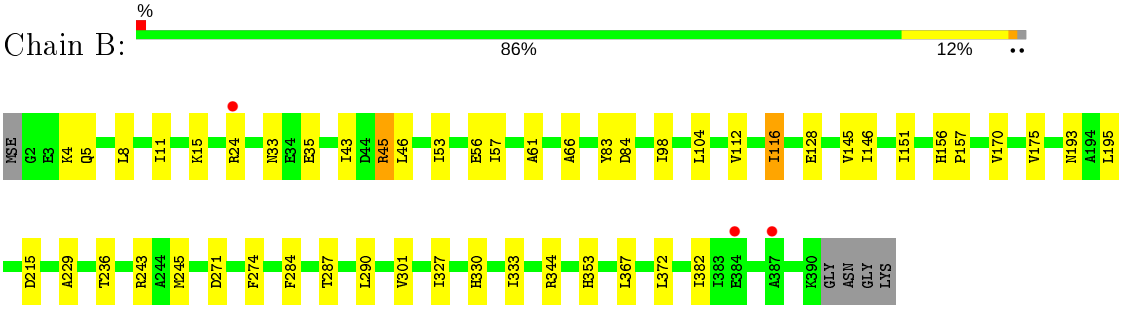
- Molecule 1: HmrA protein

Chain A:



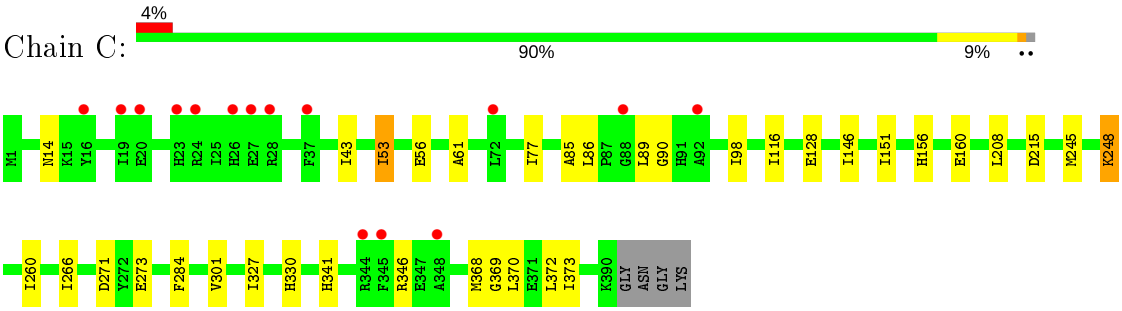
- Molecule 1: HmrA protein

Chain B:



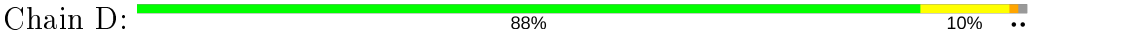
- Molecule 1: HmrA protein

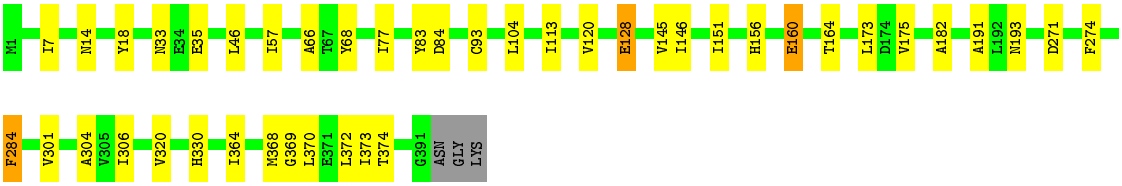
Chain C:



- Molecule 1: HmrA protein

Chain D:




M1
I7
N14
Y18
N33
E34
E35
L46
I57
A66
T67
Y68
I77
Y83
D84
C93
L104
I113
V120
E128
V145
I146
I151
H156
E160
T164
L173
D174
V175
A182
A191
L192
N193
D271
F274
F284
V301
A304
V305
I306
V320
H330
I364
M368
G369
L370
E371
L372
I373
T374
G391
ASN
GLY
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.73Å 132.73Å 336.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 2.70 48.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.52-2.70) 99.5 (48.52-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.191 , 0.218 0.196 , 0.223	Depositor DCC
R_{free} test set	1396 reflections (1.68%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12547	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/3049	0.60	0/4116
1	B	0.51	0/3037	0.58	0/4101
1	C	0.53	0/3045	0.59	0/4111
1	D	0.54	0/3049	0.60	0/4116
All	All	0.53	0/12180	0.59	0/16444

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2999	0	2942	34	0
1	B	2987	0	2927	40	0
1	C	2995	0	2939	24	0
1	D	2999	0	2942	31	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	54	0	72	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	60	0	80	3	0
3	C	42	0	56	2	0
3	D	36	0	48	2	0
4	A	109	0	0	1	0
4	B	71	0	0	1	0
4	C	75	0	0	1	0
4	D	111	0	0	0	0
All	All	12547	0	12006	127	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 5.

All (127) 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:43:ILE:HG23	1:C:53:ILE:HD12	1.47	0.94
1:D:160:GLU:HG2	1:D:306:ILE:HD13	1.52	0.92
1:B:43:ILE:HG23	1:B:53:ILE:HD12	1.62	0.82
1:C:215:ASP:HB2	1:C:245:MSE:HE3	1.66	0.75
1:A:281:VAL:HG21	3:A:516:GOL:O1	1.91	0.70
1:A:35:GLU:HG3	1:A:83:TYR:CD1	2.27	0.69
1:B:151:ILE:HD13	1:B:372:LEU:HD13	1.74	0.69
1:C:151:ILE:HD13	1:C:372:LEU:HD13	1.76	0.68
1:A:35:GLU:HG3	1:A:83:TYR:HD1	1.60	0.66
1:B:56:GLU:HG2	1:B:61:ALA:HA	1.75	0.66
1:A:13:THR:HG22	1:A:14:ASN:HD22	1.62	0.65
1:B:56:GLU:CG	1:B:61:ALA:HA	2.26	0.65
1:D:35:GLU:HG3	1:D:83:TYR:CD1	2.33	0.64
1:D:7:ILE:HD12	1:D:370:LEU:HD22	1.79	0.63
1:B:4:LYS:HG3	1:B:367:LEU:HD21	1.81	0.62
1:D:156:HIS:O	1:D:330:HIS:HA	2.00	0.61
1:D:193:ASN:HD21	3:D:510:GOL:H31	1.66	0.61
1:D:77:ILE:HD11	1:D:373:ILE:HG13	1.83	0.61
1:A:77:ILE:HD13	1:A:369:GLY:HA2	1.83	0.60
1:B:156:HIS:O	1:B:330:HIS:HA	2.02	0.60
1:B:35:GLU:HG3	1:B:83:TYR:CD1	2.37	0.60
1:D:113:ILE:HD13	1:D:120:VAL:HG23	1.83	0.59
1:D:128:GLU:OE1	3:D:504:GOL:H32	2.02	0.59
1:C:77:ILE:HD13	1:C:369:GLY:HA2	1.85	0.59
1:A:42:LEU:HD22	1:A:103:VAL:HG21	1.84	0.58
1:A:77:ILE:CD1	1:A:373:ILE:HG13	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLU:HG3	1:D:83:TYR:CE1	2.39	0.58
1:C:327:ILE:HD13	1:C:368:MSE:HE1	1.86	0.57
1:B:151:ILE:CD1	1:B:372:LEU:HD13	2.33	0.57
1:B:46:LEU:HD13	1:B:66:ALA:CB	2.35	0.56
1:D:146:ILE:HD13	1:D:320:VAL:HG13	1.88	0.56
1:A:195:LEU:HA	1:A:236:THR:HG21	1.88	0.56
1:C:56:GLU:HG2	1:C:61:ALA:HA	1.88	0.56
1:A:77:ILE:HD11	1:A:373:ILE:HG13	1.89	0.55
1:B:215:ASP:HB2	1:B:245:MSE:HE3	1.87	0.54
1:C:98:ILE:HD11	1:C:156:HIS:CD2	2.43	0.54
1:B:35:GLU:HG3	1:B:83:TYR:HD1	1.70	0.54
1:D:33:ASN:N	1:D:35:GLU:OE2	2.40	0.54
1:D:77:ILE:HD13	1:D:369:GLY:HA2	1.90	0.53
1:B:43:ILE:HG23	1:B:53:ILE:CD1	2.35	0.53
1:B:215:ASP:HB2	1:B:245:MSE:CE	2.38	0.53
1:D:151:ILE:CD1	1:D:372:LEU:HD22	2.39	0.52
1:A:233:PRO:HA	3:A:517:GOL:H32	1.92	0.52
1:C:215:ASP:HB2	1:C:245:MSE:CE	2.38	0.52
1:D:18:TYR:CD1	1:D:104:LEU:HD13	2.45	0.52
1:A:160:GLU:HG2	1:A:306:ILE:HD13	1.90	0.52
1:A:182:ALA:HB3	1:A:191:ALA:HB2	1.92	0.52
1:D:77:ILE:HD13	1:D:369:GLY:CA	2.40	0.51
1:C:301:VAL:O	1:C:301:VAL:CG1	2.59	0.51
1:A:281:VAL:HG21	3:A:516:GOL:HO1	1.76	0.51
1:A:156:HIS:O	1:A:330:HIS:HA	2.10	0.51
1:B:33:ASN:N	1:B:35:GLU:OE2	2.44	0.50
1:A:77:ILE:HD13	1:A:369:GLY:CA	2.42	0.50
1:B:146:ILE:HG22	1:B:146:ILE:O	2.11	0.50
1:B:45:ARG:NH1	4:B:783:HOH:O	2.45	0.50
1:A:301:VAL:O	1:A:301:VAL:HG12	2.12	0.49
1:C:56:GLU:CG	1:C:61:ALA:HA	2.42	0.49
1:B:57:ILE:CG2	1:B:145:VAL:HG21	2.43	0.49
1:A:46:LEU:HD13	1:A:66:ALA:CB	2.43	0.48
1:B:193:ASN:HD21	3:B:522:GOL:H31	1.78	0.48
1:B:193:ASN:HD21	3:B:522:GOL:C3	2.25	0.48
1:D:35:GLU:HG3	1:D:83:TYR:HD1	1.78	0.48
1:C:156:HIS:O	1:C:330:HIS:HA	2.13	0.48
1:D:113:ILE:HD13	1:D:120:VAL:CG2	2.43	0.48
1:D:173:LEU:HD13	1:D:274:PHE:CZ	2.47	0.48
1:B:112:VAL:HG12	1:B:116:ILE:HG12	1.95	0.48
1:D:68:TYR:CD2	1:D:113:ILE:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ILE:HD12	1:C:373:ILE:HG13	1.96	0.48
1:B:35:GLU:OE1	1:B:84:ASP:HB3	2.14	0.47
1:B:157:PRO:HB3	1:B:333:ILE:HG21	1.97	0.47
1:D:364:ILE:O	1:D:368:MSE:HG3	2.14	0.47
1:B:290:LEU:CD1	1:B:382:ILE:HD13	2.45	0.47
1:B:301:VAL:O	1:B:301:VAL:HG12	2.14	0.46
1:B:290:LEU:HD23	1:B:327:ILE:HG23	1.98	0.46
1:D:164:THR:HG21	1:D:284:PHE:CE2	2.51	0.46
1:B:56:GLU:HG3	1:B:61:ALA:HA	1.96	0.45
1:C:116:ILE:HD13	1:C:370:LEU:HD12	1.96	0.45
1:B:146:ILE:CG2	1:B:146:ILE:O	2.64	0.45
1:A:266:ILE:HD12	1:C:266:ILE:HD12	1.98	0.45
1:D:301:VAL:CG1	1:D:301:VAL:O	2.65	0.45
1:A:290:LEU:HG	1:A:327:ILE:HG23	1.99	0.45
1:B:112:VAL:HG12	1:B:112:VAL:O	2.16	0.45
1:D:46:LEU:HD13	1:D:66:ALA:CB	2.47	0.45
1:C:248:LYS:NZ	4:C:854:HOH:O	2.50	0.44
1:D:370:LEU:O	1:D:374:THR:HB	2.17	0.44
1:B:175:VAL:HG22	1:B:274:PHE:CD1	2.51	0.44
1:A:151:ILE:CD1	1:A:372:LEU:HD22	2.48	0.44
1:B:170:VAL:HG22	1:B:243:ARG:HG3	2.00	0.44
1:C:146:ILE:HG22	1:C:146:ILE:O	2.17	0.44
1:A:293:LEU:HB3	1:A:368:MSE:HE3	1.99	0.43
1:A:51:PHE:HE1	1:A:120:VAL:HG12	1.83	0.43
1:B:46:LEU:HD13	1:B:66:ALA:HB2	1.99	0.43
1:D:182:ALA:HB3	1:D:191:ALA:HB2	1.99	0.43
1:B:290:LEU:HD13	1:B:382:ILE:HD13	1.99	0.43
1:B:98:ILE:HD11	1:B:156:HIS:CD2	2.54	0.43
1:A:333:ILE:HG22	1:A:357:ALA:CB	2.48	0.43
1:A:77:ILE:HD12	1:A:373:ILE:HD11	2.00	0.43
1:D:304:ALA:O	1:D:306:ILE:HD12	2.19	0.43
1:A:241:TYR:CE1	1:B:229:ALA:HB3	2.54	0.43
1:B:287:THR:HG21	1:B:382:ILE:HG23	2.01	0.43
1:B:151:ILE:CD1	1:B:372:LEU:HD22	2.48	0.43
1:B:195:LEU:HA	1:B:236:THR:HG21	2.00	0.42
1:C:273:GLU:HA	3:C:526:GOL:C3	2.48	0.42
1:C:273:GLU:HA	3:C:526:GOL:H31	2.01	0.42
1:C:86:LEU:HD11	1:C:341:HIS:CE1	2.54	0.42
1:A:51:PHE:CE1	1:A:120:VAL:HG12	2.54	0.42
1:A:183:HIS:CD2	1:A:186:GLU:HG2	2.55	0.42
1:A:109:LEU:HD23	1:A:120:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:HIS:HD2	3:B:524:GOL:C1	2.31	0.42
1:A:90:GLY:O	1:A:91:HIS:HB2	2.18	0.42
1:C:43:ILE:HG23	1:C:53:ILE:CD1	2.35	0.42
1:B:8:LEU:HD21	1:B:367:LEU:HD11	2.02	0.42
1:D:35:GLU:OE1	1:D:84:ASP:HB3	2.19	0.42
1:D:175:VAL:HG22	1:D:274:PHE:CD1	2.55	0.42
1:C:208:LEU:HD22	1:C:260:ILE:CD1	2.50	0.42
1:C:85:ALA:HB1	1:C:90:GLY:HA2	2.02	0.41
1:D:18:TYR:CE1	1:D:104:LEU:HD13	2.55	0.41
1:A:109:LEU:HD23	1:A:120:VAL:CG2	2.50	0.41
1:A:35:GLU:HG3	1:A:83:TYR:CE1	2.56	0.41
1:D:7:ILE:CD1	1:D:370:LEU:HD22	2.46	0.41
1:A:183:HIS:HB2	4:A:738:HOH:O	2.20	0.41
1:C:89:LEU:O	1:C:346:ARG:HD3	2.21	0.41
1:A:22:SER:HB2	1:A:358:LEU:HD11	2.03	0.41
1:A:13:THR:CG2	1:A:14:ASN:HD22	2.32	0.40
1:D:57:ILE:CG2	1:D:145:VAL:HG21	2.51	0.40
1:B:11:ILE:HG23	1:B:104:LEU:HD21	2.04	0.40
1:C:151:ILE:CD1	1:C:372:LEU:HD22	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	389/394 (99%)	378 (97%)	10 (3%)	1 (0%)	41 66
1	B	387/394 (98%)	378 (98%)	9 (2%)	0	100 100
1	C	388/394 (98%)	376 (97%)	12 (3%)	0	100 100
1	D	389/394 (99%)	384 (99%)	5 (1%)	0	100 100
All	All	1553/1576 (98%)	1516 (98%)	36 (2%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	HIS

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	311/307 (101%)	303 (97%)	8 (3%)	46	75
1	B	310/307 (101%)	301 (97%)	9 (3%)	42	71
1	C	311/307 (101%)	304 (98%)	7 (2%)	50	78
1	D	311/307 (101%)	305 (98%)	6 (2%)	57	82
All	All	1243/1228 (101%)	1213 (98%)	30 (2%)	49	77

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	14	ASN
1	A	93	CYS
1	A	112	VAL
1	A	128	GLU
1	A	160	GLU
1	A	187	ASN
1	A	284	PHE
1	B	5	GLN
1	B	15	LYS
1	B	24	ARG
1	B	45	ARG
1	B	116	ILE
1	B	128	GLU
1	B	271	ASP
1	B	284	PHE
1	B	344	ARG
1	C	14	ASN
1	C	53	ILE

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Mol	Chain	Res	Type
1	C	128	GLU
1	C	160	GLU
1	C	248	LYS
1	C	271	ASP
1	C	284	PHE
1	D	14	ASN
1	D	93	CYS
1	D	128	GLU
1	D	160	GLU
1	D	271	ASP
1	D	284	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	187	ASN
1	A	210	GLN
1	A	328	HIS
1	B	207	GLN
1	B	278	GLN
1	B	328	HIS
1	B	353	HIS
1	B	380	GLN
1	C	187	ASN
1	C	210	GLN
1	C	279	ASN
1	C	337	ASN
1	D	14	ASN
1	D	210	GLN
1	D	328	HIS

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)

Of 41 ligands modelled in this entry, 9 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	517	-	5,5,5	0.59	0	5,5,5	1.07	0
3	GOL	B	515	-	5,5,5	0.31	0	5,5,5	0.61	0
3	GOL	B	506	-	5,5,5	0.40	0	5,5,5	0.26	0
3	GOL	B	532	-	5,5,5	0.40	0	5,5,5	0.18	0
3	GOL	D	504	2	5,5,5	0.56	0	5,5,5	0.78	0
3	GOL	A	520	-	5,5,5	0.45	0	5,5,5	0.47	0
3	GOL	D	502	-	5,5,5	0.43	0	5,5,5	0.46	0
3	GOL	C	531	2	5,5,5	0.41	0	5,5,5	0.25	0
3	GOL	C	526	-	5,5,5	0.32	0	5,5,5	0.47	0
3	GOL	A	501	-	5,5,5	0.60	0	5,5,5	0.66	0
3	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	C	509	-	5,5,5	0.50	0	5,5,5	0.50	0
3	GOL	D	529	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	B	507	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	B	523	-	5,5,5	0.47	0	5,5,5	0.29	0
3	GOL	B	524	-	5,5,5	0.33	0	5,5,5	0.42	0
3	GOL	D	511	-	5,5,5	0.47	0	5,5,5	0.64	0
3	GOL	B	528	-	5,5,5	0.43	0	5,5,5	0.21	0
3	GOL	A	513	-	5,5,5	0.42	0	5,5,5	0.43	0
3	GOL	C	518	-	5,5,5	0.30	0	5,5,5	0.49	0
3	GOL	C	525	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	C	527	-	5,5,5	0.38	0	5,5,5	0.15	0
3	GOL	A	514	-	5,5,5	0.38	0	5,5,5	0.33	0
3	GOL	A	519	-	5,5,5	0.42	0	5,5,5	0.59	0
3	GOL	C	508	-	5,5,5	0.47	0	5,5,5	0.28	0
3	GOL	B	522	-	5,5,5	0.45	0	5,5,5	0.42	0
3	GOL	A	516	-	5,5,5	0.41	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	512	-	5,5,5	0.48	0	5,5,5	0.71	0
3	GOL	D	521	-	5,5,5	0.41	0	5,5,5	0.38	0
3	GOL	D	510	-	5,5,5	0.49	0	5,5,5	0.40	0
3	GOL	B	503	-	5,5,5	0.40	0	5,5,5	0.66	0
3	GOL	B	530	2	5,5,5	0.42	0	5,5,5	0.51	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
3	GOL	A	517	-	-	4/4/4/4	-
3	GOL	B	515	-	-	3/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-
3	GOL	B	532	-	-	3/4/4/4	-
3	GOL	D	504	2	-	4/4/4/4	-
3	GOL	A	520	-	-	2/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	C	531	2	-	4/4/4/4	-
3	GOL	C	526	-	-	2/4/4/4	-
3	GOL	A	501	-	-	4/4/4/4	-
3	GOL	A	505	-	-	1/4/4/4	-
3	GOL	C	509	-	-	2/4/4/4	-
3	GOL	D	529	-	-	2/4/4/4	-
3	GOL	B	507	-	-	1/4/4/4	-
3	GOL	B	523	-	-	0/4/4/4	-
3	GOL	B	524	-	-	4/4/4/4	-
3	GOL	D	511	-	-	2/4/4/4	-
3	GOL	B	528	-	-	4/4/4/4	-
3	GOL	A	513	-	-	4/4/4/4	-
3	GOL	C	518	-	-	2/4/4/4	-
3	GOL	C	525	-	-	2/4/4/4	-
3	GOL	C	527	-	-	2/4/4/4	-
3	GOL	A	514	-	-	4/4/4/4	-
3	GOL	A	519	-	-	2/4/4/4	-
3	GOL	C	508	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	522	-	-	3/4/4/4	-
3	GOL	A	516	-	-	2/4/4/4	-
3	GOL	A	512	-	-	2/4/4/4	-
3	GOL	D	521	-	-	2/4/4/4	-
3	GOL	D	510	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	B	530	2	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	517	GOL	C1-C2-C3-O3
3	A	517	GOL	O2-C2-C3-O3
3	B	506	GOL	C1-C2-C3-O3
3	B	532	GOL	O1-C1-C2-C3
3	D	504	GOL	C1-C2-C3-O3
3	A	520	GOL	C1-C2-C3-O3
3	A	513	GOL	C1-C2-C3-O3
3	A	513	GOL	O2-C2-C3-O3
3	C	531	GOL	O1-C1-C2-C3
3	A	501	GOL	O1-C1-C2-O2
3	A	501	GOL	O1-C1-C2-C3
3	A	501	GOL	C1-C2-C3-O3
3	D	511	GOL	C1-C2-C3-O3
3	D	511	GOL	O2-C2-C3-O3
3	B	528	GOL	O1-C1-C2-C3
3	C	527	GOL	O1-C1-C2-C3
3	A	514	GOL	C1-C2-C3-O3
3	A	519	GOL	C1-C2-C3-O3
3	A	519	GOL	O2-C2-C3-O3
3	C	508	GOL	O1-C1-C2-C3
3	C	508	GOL	C1-C2-C3-O3
3	A	512	GOL	O1-C1-C2-O2
3	A	512	GOL	O1-C1-C2-C3
3	D	521	GOL	O1-C1-C2-O2
3	D	521	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	510	GOL	C1-C2-C3-O3
3	B	503	GOL	O1-C1-C2-C3
3	B	530	GOL	O1-C1-C2-C3
3	B	506	GOL	O2-C2-C3-O3
3	B	532	GOL	O1-C1-C2-O2
3	A	513	GOL	O1-C1-C2-O2
3	B	528	GOL	O1-C1-C2-O2
3	C	525	GOL	O2-C2-C3-O3
3	C	527	GOL	O1-C1-C2-O2
3	D	510	GOL	O2-C2-C3-O3
3	A	517	GOL	O1-C1-C2-C3
3	D	504	GOL	O1-C1-C2-C3
3	A	513	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-C3
3	C	531	GOL	C1-C2-C3-O3
3	C	526	GOL	C1-C2-C3-O3
3	C	509	GOL	O1-C1-C2-C3
3	B	524	GOL	O1-C1-C2-C3
3	C	525	GOL	C1-C2-C3-O3
3	A	514	GOL	O1-C1-C2-C3
3	D	529	GOL	C1-C2-C3-O3
3	B	522	GOL	C1-C2-C3-O3
3	A	516	GOL	O1-C1-C2-C3
3	B	530	GOL	C1-C2-C3-O3
3	D	504	GOL	O2-C2-C3-O3
3	A	520	GOL	O2-C2-C3-O3
3	C	531	GOL	O2-C2-C3-O3
3	A	501	GOL	O2-C2-C3-O3
3	C	509	GOL	O1-C1-C2-O2
3	B	524	GOL	O1-C1-C2-O2
3	A	514	GOL	O2-C2-C3-O3
3	D	529	GOL	O2-C2-C3-O3
3	C	508	GOL	O1-C1-C2-O2
3	C	508	GOL	O2-C2-C3-O3
3	A	516	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-O2
3	B	530	GOL	O1-C1-C2-O2
3	B	515	GOL	O2-C2-C3-O3
3	B	522	GOL	O1-C1-C2-O2
3	B	530	GOL	O2-C2-C3-O3
3	B	528	GOL	C1-C2-C3-O3
3	B	522	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	517	GOL	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-O2
3	C	531	GOL	O1-C1-C2-O2
3	A	505	GOL	O1-C1-C2-O2
3	C	518	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-O2
3	B	532	GOL	C1-C2-C3-O3
3	B	507	GOL	C1-C2-C3-O3
3	B	524	GOL	C1-C2-C3-O3
3	C	526	GOL	O2-C2-C3-O3
3	B	528	GOL	O2-C2-C3-O3
3	A	514	GOL	O1-C1-C2-O2
3	B	524	GOL	O2-C2-C3-O3
3	C	518	GOL	O1-C1-C2-O2
3	B	515	GOL	O1-C1-C2-C3
3	B	515	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	517	GOL	1	0
3	D	504	GOL	1	0
3	C	526	GOL	2	0
3	B	524	GOL	1	0
3	B	522	GOL	2	0
3	A	516	GOL	2	0
3	D	510	GOL	1	0

5.7 Other polymers

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^{th} 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	385/394 (97%)	-0.29	2 (0%) 91 92	19, 35, 60, 90	0
1	B	384/394 (97%)	-0.15	3 (0%) 86 87	21, 43, 87, 116	0
1	C	384/394 (97%)	-0.09	15 (3%) 39 38	20, 45, 82, 104	0
1	D	385/394 (97%)	-0.35	0 100 100	19, 32, 53, 88	0
All	All	1538/1576 (97%)	-0.22	20 (1%) 77 78	19, 38, 76, 116	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	GLY	4.9
1	C	19	ILE	3.1
1	C	28	ARG	2.9
1	C	26	HIS	2.9
1	C	72	LEU	2.8
1	B	387	ALA	2.7
1	C	23	HIS	2.6
1	C	344	ARG	2.4
1	B	384	GLU	2.4
1	C	348	ALA	2.3
1	C	20	GLU	2.3
1	C	92	ALA	2.3
1	B	24	ARG	2.3
1	C	16	TYR	2.3
1	C	24	ARG	2.3
1	C	88	GLY	2.2
1	C	37	PHE	2.2
1	C	345	PHE	2.2
1	A	89	LEU	2.0
1	C	27	GLU	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^{th} 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^2)	Q<0.9
3	GOL	A	501	6/6	0.77	0.28	67,67,68,68	0
3	GOL	C	508	6/6	0.80	0.23	70,71,72,73	0
3	GOL	A	517	6/6	0.81	0.25	54,55,56,56	0
3	GOL	A	505	6/6	0.82	0.23	72,73,74,74	0
3	GOL	D	529	6/6	0.82	0.41	69,69,70,70	0
3	GOL	B	532	6/6	0.82	0.29	63,64,64,65	0
3	GOL	A	520	6/6	0.83	0.25	62,63,63,63	0
3	GOL	B	524	6/6	0.84	0.39	65,66,66,68	0
3	GOL	D	502	6/6	0.85	0.34	72,73,73,74	0
3	GOL	C	527	6/6	0.86	0.33	81,81,81,81	0
3	GOL	A	514	6/6	0.86	0.29	67,68,68,68	0
3	GOL	A	513	6/6	0.87	0.21	51,53,53,53	0
3	GOL	B	503	6/6	0.87	0.22	68,69,70,71	0
3	GOL	D	511	6/6	0.88	0.24	66,67,68,69	0
3	GOL	A	519	6/6	0.90	0.25	56,58,58,59	0
3	GOL	B	515	6/6	0.90	0.21	61,62,62,63	0
3	GOL	B	528	6/6	0.91	0.22	60,61,62,62	0
3	GOL	A	512	6/6	0.91	0.25	49,53,54,54	0
3	GOL	C	518	6/6	0.91	0.19	67,67,68,68	0
3	GOL	C	525	6/6	0.92	0.20	73,74,74,74	0
3	GOL	C	509	6/6	0.92	0.21	40,43,44,46	0
3	GOL	B	523	6/6	0.92	0.24	53,54,55,55	0
3	GOL	D	510	6/6	0.92	0.21	53,54,55,56	0
3	GOL	B	506	6/6	0.92	0.28	63,63,63,63	0
3	GOL	C	526	6/6	0.93	0.23	66,66,67,67	0
3	GOL	B	530	6/6	0.93	0.27	52,54,57,57	0
3	GOL	D	521	6/6	0.94	0.22	47,47,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	516	6/6	0.95	0.22	48,49,49,50	0
3	GOL	C	531	6/6	0.95	0.23	74,75,76,76	0
3	GOL	D	504	6/6	0.96	0.22	41,43,44,45	0
3	GOL	B	522	6/6	0.96	0.27	48,49,49,51	0
3	GOL	B	507	6/6	0.97	0.20	44,45,45,46	0
2	ZN	B	533	1/1	0.97	0.06	81,81,81,81	1
2	ZN	A	998	1/1	0.99	0.10	33,33,33,33	0
2	ZN	C	999	1/1	0.99	0.14	47,47,47,47	0
2	ZN	D	998	1/1	0.99	0.11	31,31,31,31	0
2	ZN	B	999	1/1	0.99	0.14	36,36,36,36	0
2	ZN	C	998	1/1	0.99	0.10	54,54,54,54	0
2	ZN	D	999	1/1	0.99	0.16	26,26,26,26	0
2	ZN	B	998	1/1	0.99	0.10	37,37,37,37	0
2	ZN	A	999	1/1	1.00	0.13	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.