



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:54 pm GMT

PDB ID : 3OZM  
Title : Crystal structure of enolase superfamily member from Bordetella bronchiseptica complexed with Mg, m-Xylarate and L-Lyxarate  
Authors : Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.  
Deposited on : 2010-09-25  
Resolution : 1.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : trunk28620

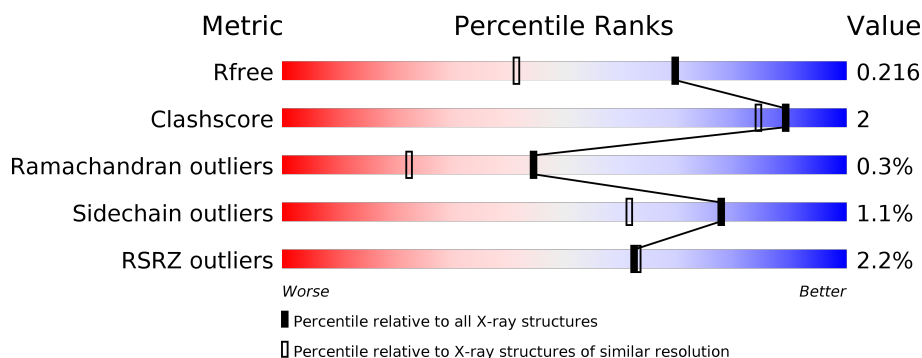
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	389	<div> <div>94%</div> <div>5% •</div> </div>
1	B	389	<div> <div>2%</div> <div>96%</div> <div>• •</div> </div>
1	C	389	<div> <div>2%</div> <div>94%</div> <div>5% •</div> </div>
1	D	389	<div> <div>2%</div> <div>89%</div> <div>9% •</div> </div>
1	E	389	<div> <div>2%</div> <div>93%</div> <div>6% ••</div> </div>
1	F	389	<div> <div>3%</div> <div>95%</div> <div>5% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	389	
1	H	389	

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
4	GOL	A	392	-	-	-	X
4	GOL	B	392	-	-	-	X
4	GOL	B	393	-	-	-	X
4	GOL	C	392	-	-	-	X
4	GOL	C	393	-	-	-	X
4	GOL	C	394	-	-	-	X
4	GOL	D	392	-	-	-	X
4	GOL	E	392	-	-	-	X
4	GOL	G	392	-	-	-	X
4	GOL	H	392	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26586 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 Putative mandelate racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	4	0
			2990	1884	539	556	11			
1	B	386	Total	C	N	O	S	0	10	0
			3037	1914	548	564	11			
1	C	386	Total	C	N	O	S	0	9	0
			3026	1908	544	563	11			
1	D	381	Total	C	N	O	S	0	10	0
			3011	1899	544	558	10			
1	E	386	Total	C	N	O	S	0	10	0
			3042	1917	551	563	11			
1	F	386	Total	C	N	O	S	0	9	0
			3031	1911	547	562	11			
1	G	386	Total	C	N	O	S	0	10	0
			3037	1913	548	564	12			
1	H	380	Total	C	N	O	S	0	0	0
			2926	1846	527	544	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	EXPRESSION TAG	UNP Q7WEE8
A	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8
B	2	SER	-	EXPRESSION TAG	UNP Q7WEE8
B	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8
C	2	SER	-	EXPRESSION TAG	UNP Q7WEE8
C	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8
D	2	SER	-	EXPRESSION TAG	UNP Q7WEE8
D	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8
E	2	SER	-	EXPRESSION TAG	UNP Q7WEE8
E	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8
F	2	SER	-	EXPRESSION TAG	UNP Q7WEE8
F	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8
G	2	SER	-	EXPRESSION TAG	UNP Q7WEE8

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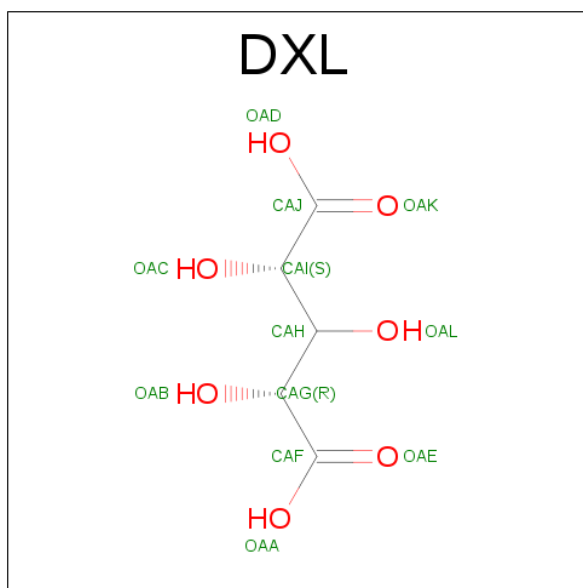
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Chain	Residue	Modelled	Actual	Comment	Reference
G	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8
H	2	SER	-	EXPRESSION TAG	UNP Q7WEE8
H	3	LEU	-	EXPRESSION TAG	UNP Q7WEE8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

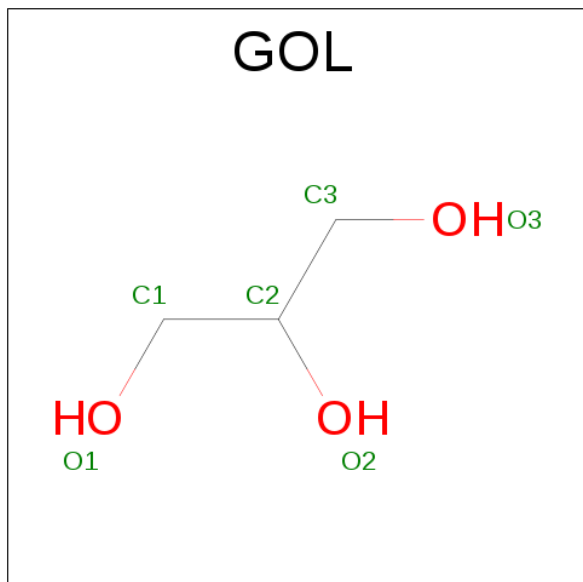
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is D-XYLARIC ACID (three-letter code: DXL) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	5	7		
3	B	1	Total	C	O	0	0
			12	5	7		
3	C	1	Total	C	O	0	0
			12	5	7		
3	E	1	Total	C	O	0	0
			12	5	7		
3	F	1	Total	C	O	0	0
			12	5	7		
3	G	1	Total	C	O	0	0
			12	5	7		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



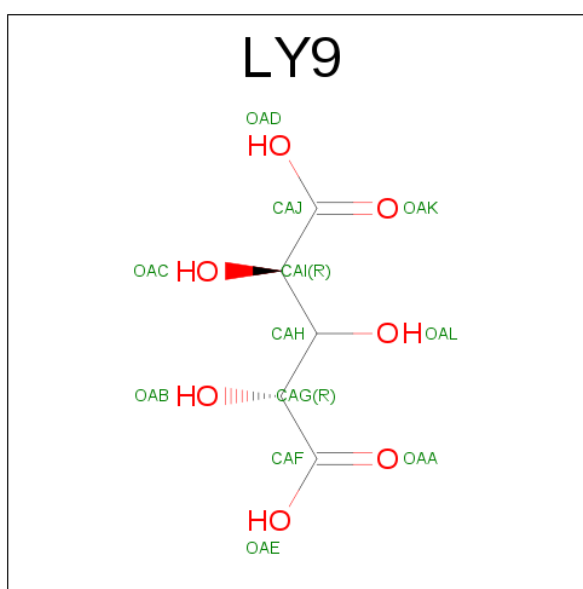
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is L-ARABINARIC ACID (three-letter code: LY9) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			12	5	7		
5	H	1	Total	C	O	0	0
			12	5	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	318	Total	O		0	0
			318	318			
6	B	306	Total	O		0	0
			306	306			
6	C	288	Total	O		0	0
			288	288			

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	306	Total 306	O 306	0	0
6	E	269	Total 269	O 269	0	0
6	F	313	Total 313	O 313	0	0
6	G	277	Total 277	O 277	0	0
6	H	245	Total 245	O 245	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.

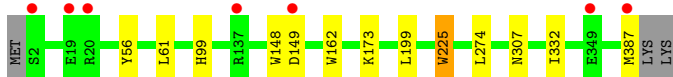
- Molecule 1: Putative mandelate racemase

Chain A: 



- Molecule 1: Putative mandelate racemase

Chain B: 

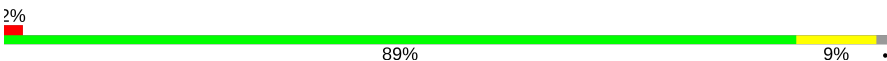


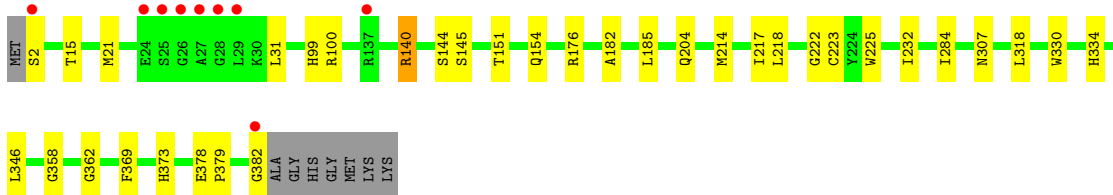
- Molecule 1: Putative mandelate racemase

Chain C: 



- Molecule 1: Putative mandelate racemase

Chain D: 



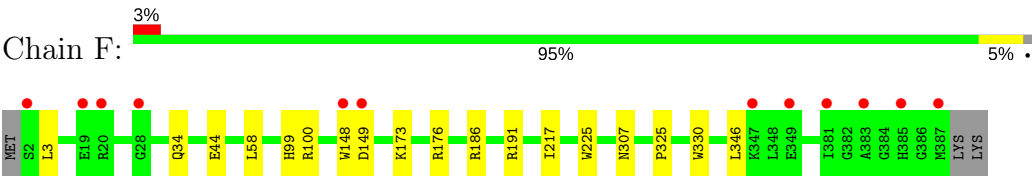
- Molecule 1: Putative mandelate racemase

Chain E: 

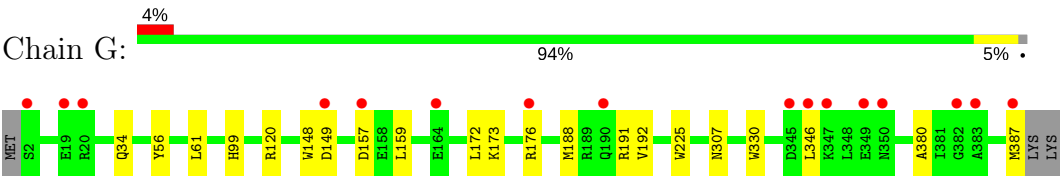


LYS  
LYS

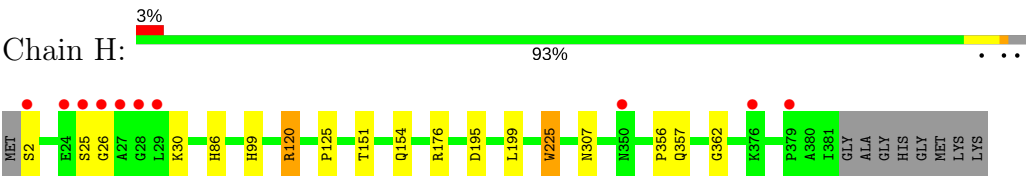
• Molecule 1: Putative mandelate racemase



• Molecule 1: Putative mandelate racemase



• Molecule 1: Putative mandelate racemase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.17Å 134.34Å 146.75Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	39.00 – 1.60 39.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (39.00-1.60) 95.5 (39.00-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.191 , 0.222 0.184 , 0.216	Depositor DCC
$R_{free}$ test set	22039 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	26586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.41 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6397e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, DXL, LY9

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	0.36	0/3057	0.54	0/4156
1	B	0.33	0/3104	0.52	0/4220
1	C	0.34	0/3093	0.52	0/4206
1	D	0.33	0/3077	0.53	0/4184
1	E	0.33	0/3109	0.53	0/4226
1	F	0.34	0/3098	0.53	0/4212
1	G	0.33	0/3104	0.53	0/4219
1	H	0.32	0/2992	0.51	0/4071
All	All	0.34	0/24634	0.53	0/33494

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2990	0	2941	10	0
1	B	3037	0	2992	9	0
1	C	3026	0	2980	15	0
1	D	3011	0	2973	21	0
1	E	3042	0	3000	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3031	0	2988	12	0
1	G	3037	0	2990	13	0
1	H	2926	0	2880	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	5	2	0
3	B	12	0	5	2	0
3	C	12	0	5	3	0
3	E	12	0	5	4	0
3	F	12	0	6	3	0
3	G	12	0	5	3	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	18	0	24	1	0
4	D	6	0	8	2	0
4	E	6	0	8	2	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	D	12	0	5	0	0
5	H	12	0	5	0	0
6	A	318	0	0	0	0
6	B	306	0	0	0	0
6	C	288	0	0	0	0
6	D	306	0	0	3	0
6	E	269	0	0	4	0
6	F	313	0	0	2	0
6	G	277	0	0	1	0
6	H	245	0	0	2	0
All	All	26586	0	23865	106	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 2.

All (106) 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:D:15:THR:HG22	1:D:373:HIS:CD2	2.18	0.78
1:C:173:LYS:NZ	3:C:391:DXL:HAI	2.01	0.76
1:B:173:LYS:NZ	3:B:391:DXL:HAI	2.02	0.74
4:E:392:GOL:H31	6:E:2125:HOH:O	1.90	0.71
1:E:173:LYS:NZ	3:E:391:DXL:HAI	2.06	0.71
1:A:173:LYS:NZ	3:A:391:DXL:HAI	2.06	0.70
1:B:173:LYS:HZ1	3:B:391:DXL:HAI	1.55	0.69
1:H:25:SER:OG	1:H:30:LYS:HG3	1.94	0.67
1:G:173:LYS:NZ	3:G:391:DXL:HAI	2.09	0.66
1:A:148:TRP:O	1:A:149:ASP:HB2	1.97	0.65
1:A:173:LYS:HZ1	3:A:391:DXL:HAI	1.61	0.64
1:D:151:THR:OG1	1:D:154:GLN:HG3	1.98	0.63
1:B:387:MET:HE3	1:H:86:HIS:HB2	1.79	0.62
1:C:173:LYS:HZ1	3:C:391:DXL:HAI	1.66	0.60
1:E:173:LYS:HZ1	3:E:391:DXL:HAI	1.66	0.59
1:F:173:LYS:NZ	3:F:391:DXL:HAI	2.18	0.59
1:D:185[B]:LEU:HD21	1:D:223:CYS:SG	2.44	0.58
1:F:330:TRP:CZ2	1:F:346:LEU:HB2	2.39	0.57
1:C:173:LYS:HZ2	3:C:391:DXL:HAI	1.68	0.57
1:G:149:ASP:OD1	1:G:176:ARG:NH2	2.37	0.57
1:C:149:ASP:CG	1:C:176:ARG:HH22	2.08	0.56
1:D:223:CYS:O	4:D:392:GOL:H11	2.06	0.56
1:G:173:LYS:HZ1	3:G:391:DXL:HAI	1.69	0.55
1:B:148:TRP:O	1:B:149:ASP:HB2	2.07	0.54
4:C:394:GOL:H32	6:E:2216:HOH:O	2.05	0.54
1:F:149:ASP:CG	1:F:176:ARG:HH22	2.11	0.54
1:E:159:LEU:HG	1:E:192:VAL:HG11	1.90	0.52
1:F:148:TRP:O	1:F:149:ASP:HB2	2.09	0.52
1:C:149:ASP:OD1	1:C:176:ARG:NH2	2.41	0.52
1:D:222:GLY:O	4:D:392:GOL:H12	2.09	0.52
1:D:217[B]:ILE:HD12	6:D:1492:HOH:O	2.09	0.52
1:E:149:ASP:OD1	1:E:176:ARG:NH2	2.37	0.52
1:E:173:LYS:HZ2	3:E:391:DXL:HAI	1.75	0.52
1:E:199:LEU:HD23	1:E:225:TRP:CZ2	2.45	0.51
1:D:2:SER:HB3	6:D:2390:HOH:O	2.09	0.51
1:A:175:GLY:HA3	1:A:205[B]:SER:OG	2.10	0.51
1:B:162:TRP:CZ2	1:B:332:ILE:HD13	2.46	0.51
1:C:148:TRP:O	1:C:149:ASP:HB2	2.11	0.50
1:H:125:PRO:HG3	1:H:357:GLN:O	2.12	0.50
4:E:392:GOL:H12	6:E:2125:HOH:O	2.12	0.50
1:G:159:LEU:HG	1:G:192:VAL:HG11	1.94	0.50
1:D:330:TRP:CE2	1:D:346:LEU:HD23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:THR:HG21	1:D:369:PHE:HZ	1.76	0.49
1:D:182:ALA:HB2	1:D:217[B]:ILE:HD13	1.95	0.49
1:A:149:ASP:OD1	1:A:176:ARG:NH2	2.35	0.48
1:B:199:LEU:HD23	1:B:225:TRP:CZ2	2.49	0.48
1:C:162:TRP:CZ2	1:C:332:ILE:HD13	2.48	0.48
1:F:325:PRO:HD2	6:F:1786:HOH:O	2.13	0.48
1:C:186:ARG:NH2	1:C:217[A]:ILE:HD12	2.30	0.47
1:C:387:MET:HE3	1:E:86:HIS:HB2	1.96	0.47
1:H:199:LEU:HD23	1:H:225:TRP:CE2	2.50	0.47
1:D:15:THR:HG21	1:D:369:PHE:CZ	2.50	0.47
1:F:173:LYS:HZ2	3:F:391:DXL:HAI	1.80	0.46
1:D:284:ILE:HG23	1:D:318:LEU:HD11	1.97	0.46
1:D:140:ARG:NH2	6:D:2005:HOH:O	2.48	0.46
1:F:186:ARG:NH2	1:F:217[A]:ILE:HD12	2.31	0.45
1:B:56:TYR:HB2	1:B:61:LEU:HD11	1.97	0.45
1:D:31:LEU:HD11	1:D:382:GLY:HA2	1.96	0.45
1:F:34:GLN:HB3	1:F:58:LEU:HD11	1.98	0.45
1:C:90:HIS:HB2	1:E:387:MET:HG3	1.98	0.45
1:H:199:LEU:HD23	1:H:225:TRP:CZ2	2.51	0.45
1:E:199:LEU:HD23	1:E:225:TRP:CE2	2.51	0.45
1:G:173:LYS:HZ2	3:G:391:DXL:HAI	1.80	0.45
1:A:56:TYR:HB2	1:A:61:LEU:HD11	1.98	0.45
1:D:204:GLN:OE1	1:D:232[B]:ILE:HG23	2.17	0.45
1:D:214[B]:MET:O	1:D:218:LEU:HG	2.17	0.44
1:G:172:LEU:HD22	1:G:188:MET:SD	2.58	0.44
1:E:120:ARG:CZ	6:E:2125:HOH:O	2.66	0.44
1:G:148:TRP:O	1:G:149:ASP:HB2	2.18	0.44
1:G:56:TYR:HB2	1:G:61:LEU:HD11	1.99	0.44
1:E:184:ASN:O	1:E:188:MET:HG3	2.18	0.43
1:A:87:LYS:HA	1:G:387:MET:SD	2.58	0.43
1:H:25:SER:CB	1:H:30:LYS:HE3	2.47	0.43
1:G:157:ASP:OD1	1:G:191[A]:ARG:NH1	2.46	0.43
1:C:199:LEU:HD23	1:C:225:TRP:CZ2	2.54	0.43
1:B:199:LEU:HD23	1:B:225:TRP:CE2	2.53	0.43
1:D:378:GLU:HA	1:D:379:PRO:HD3	1.86	0.42
1:A:199:LEU:HD23	1:A:225:TRP:CZ2	2.54	0.42
1:D:144:SER:HA	1:D:145:SER:HA	1.83	0.42
1:F:191[A]:ARG:NH2	6:F:1904:HOH:O	2.52	0.42
1:C:214[B]:MET:O	1:C:218:LEU:HG	2.19	0.42
1:G:34:GLN:OE1	1:G:380:ALA:HB2	2.20	0.42
1:H:195:ASP:HB2	6:H:1730:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TRP:O	1:A:149:ASP:CB	2.67	0.42
1:D:21:MET:HE2	1:D:334:HIS:HB2	2.02	0.42
1:E:358:GLY:C	1:E:362:GLY:HA2	2.40	0.42
1:H:120:ARG:NH1	6:H:1524:HOH:O	2.53	0.42
1:C:284:ILE:HG23	1:C:318:LEU:HD11	2.01	0.41
1:E:162:TRP:CZ2	1:E:332:ILE:HD13	2.55	0.41
1:E:329:GLU:OE2	3:E:391:DXL:OAD	2.38	0.41
1:D:100:ARG:HB2	1:F:100:ARG:HB2	2.03	0.41
1:F:173:LYS:HZ1	3:F:391:DXL:HAI	1.84	0.41
1:A:185:LEU:HD21	1:A:223:CYS:SG	2.61	0.41
1:B:274:LEU:HD12	1:B:274:LEU:N	2.36	0.41
1:G:120:ARG:NH1	6:G:2394:HOH:O	2.53	0.41
1:G:330:TRP:CE2	1:G:346:LEU:HD13	2.56	0.41
1:E:116:ASP:CG	1:E:120:ARG:HE	2.24	0.40
1:F:3:LEU:HD22	1:F:44:GLU:HB2	2.01	0.40
1:D:358:GLY:C	1:D:362:GLY:HA2	2.42	0.40
1:E:15:THR:HA	1:E:16:PRO:HD3	1.94	0.40
1:H:356:PRO:HB2	1:H:362:GLY:HA3	2.02	0.40
1:C:175:GLY:HA3	1:C:205[B]:SER:OG	2.22	0.40
1:C:185[B]:LEU:HD21	1:C:223:CYS:SG	2.61	0.40
1:E:3:LEU:HD22	1:E:44:GLU:HB2	2.03	0.40
1:E:56:TYR:HB2	1:E:61:LEU:HD11	2.03	0.40
1:H:151:THR:OG1	1:H:154:GLN:HG3	2.22	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	388/389 (100%)	373 (96%)	14 (4%)	1 (0%)	44	22
1	B	394/389 (101%)	382 (97%)	11 (3%)	1 (0%)	44	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	393/389 (101%)	380 (97%)	12 (3%)	1 (0%)	44	22
1	D	389/389 (100%)	378 (97%)	10 (3%)	1 (0%)	44	22
1	E	394/389 (101%)	382 (97%)	11 (3%)	1 (0%)	44	22
1	F	393/389 (101%)	379 (96%)	13 (3%)	1 (0%)	44	22
1	G	394/389 (101%)	379 (96%)	14 (4%)	1 (0%)	44	22
1	H	378/389 (97%)	365 (97%)	11 (3%)	2 (0%)	32	12
All	All	3123/3112 (100%)	3018 (97%)	96 (3%)	9 (0%)	44	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	307	ASN
1	C	307	ASN
1	D	307	ASN
1	E	307	ASN
1	F	307	ASN
1	G	307	ASN
1	H	307	ASN
1	H	26	GLY

### 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	304/303 (100%)	298 (98%)	6 (2%)	60	34
1	B	310/303 (102%)	308 (99%)	2 (1%)	89	80
1	C	309/303 (102%)	307 (99%)	2 (1%)	89	80
1	D	308/303 (102%)	304 (99%)	4 (1%)	73	55
1	E	310/303 (102%)	307 (99%)	3 (1%)	80	65
1	F	309/303 (102%)	307 (99%)	2 (1%)	89	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	310/303 (102%)	308 (99%)	2 (1%)	89	80
1	H	297/303 (98%)	292 (98%)	5 (2%)	66	42
All	All	2457/2424 (101%)	2431 (99%)	26 (1%)	78	61

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	99	HIS
1	A	153	ASP
1	A	225	TRP
1	A	226	PHE
1	A	387	MET
1	B	99	HIS
1	B	225	TRP
1	C	99	HIS
1	C	225	TRP
1	D	99	HIS
1	D	140	ARG
1	D	176	ARG
1	D	225	TRP
1	E	99	HIS
1	E	225	TRP
1	E	387	MET
1	F	99	HIS
1	F	225	TRP
1	G	99	HIS
1	G	225	TRP
1	H	2	SER
1	H	99	HIS
1	H	120	ARG
1	H	176	ARG
1	H	225	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	DXL	A	391	2	5,11,11	0.60	0	6,15,15	1.40	2 (33%)
4	GOL	A	392	-	5,5,5	0.31	0	5,5,5	0.22	0
3	DXL	B	391	2	5,11,11	0.70	0	6,15,15	1.23	1 (16%)
4	GOL	B	392	-	5,5,5	0.35	0	5,5,5	0.35	0
4	GOL	B	393	-	5,5,5	0.34	0	5,5,5	0.33	0
3	DXL	C	391	2	5,11,11	0.62	0	6,15,15	1.37	1 (16%)
4	GOL	C	392	-	5,5,5	0.26	0	5,5,5	0.88	0
4	GOL	C	393	-	5,5,5	0.28	0	5,5,5	0.47	0
4	GOL	C	394	-	5,5,5	0.39	0	5,5,5	0.36	0
5	LY9	D	391	2	5,11,11	0.57	0	6,15,15	0.57	0
4	GOL	D	392	-	5,5,5	0.28	0	5,5,5	0.58	0
3	DXL	E	391	2	5,11,11	0.67	0	6,15,15	1.06	0
4	GOL	E	392	-	5,5,5	0.36	0	5,5,5	0.16	0
3	DXL	F	391	2	5,11,11	0.65	0	6,15,15	1.26	1 (16%)
3	DXL	G	391	2	5,11,11	0.67	0	6,15,15	1.33	1 (16%)
4	GOL	G	392	-	5,5,5	0.40	0	5,5,5	0.28	0
5	LY9	H	391	2	5,11,11	0.57	0	6,15,15	0.46	0
4	GOL	H	392	-	5,5,5	0.23	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	DXL	A	391	2	-	0/8/16/16	0/0/0/0
4	GOL	A	392	-	-	0/4/4/4	0/0/0/0
3	DXL	B	391	2	-	0/8/16/16	0/0/0/0
4	GOL	B	392	-	-	0/4/4/4	0/0/0/0
4	GOL	B	393	-	-	0/4/4/4	0/0/0/0
3	DXL	C	391	2	-	0/8/16/16	0/0/0/0
4	GOL	C	392	-	-	0/4/4/4	0/0/0/0
4	GOL	C	393	-	-	0/4/4/4	0/0/0/0
4	GOL	C	394	-	-	0/4/4/4	0/0/0/0
5	LY9	D	391	2	-	0/8/16/16	0/0/0/0
4	GOL	D	392	-	-	0/4/4/4	0/0/0/0
3	DXL	E	391	2	-	0/8/16/16	0/0/0/0
4	GOL	E	392	-	-	0/4/4/4	0/0/0/0
3	DXL	F	391	2	-	0/8/16/16	0/0/0/0
3	DXL	G	391	2	-	0/8/16/16	0/0/0/0
4	GOL	G	392	-	-	0/4/4/4	0/0/0/0
5	LY9	H	391	2	-	0/8/16/16	0/0/0/0
4	GOL	H	392	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	391	DXL	OAC-CAI-CAH	2.19	112.38	107.52
3	A	391	DXL	OAL-CAH-CAI	2.20	113.75	108.92
3	A	391	DXL	OAC-CAI-CAH	2.30	112.63	107.52
3	F	391	DXL	OAC-CAI-CAH	2.31	112.64	107.52
3	C	391	DXL	OAC-CAI-CAH	2.59	113.28	107.52
3	G	391	DXL	OAC-CAI-CAH	2.60	113.28	107.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	391	DXL	2	0
3	B	391	DXL	2	0
3	C	391	DXL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	394	GOL	1	0
4	D	392	GOL	2	0
3	E	391	DXL	4	0
4	E	392	GOL	2	0
3	F	391	DXL	3	0
3	G	391	DXL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	386/389 (99%)	-0.45	1 (0%) 93 93	12, 18, 35, 49	0
1	B	386/389 (99%)	-0.33	7 (1%) 69 69	12, 20, 37, 51	0
1	C	386/389 (99%)	-0.28	7 (1%) 69 69	14, 20, 38, 51	0
1	D	381/389 (97%)	-0.31	9 (2%) 59 59	14, 20, 40, 80	0
1	E	386/389 (99%)	-0.30	7 (1%) 69 69	14, 20, 42, 58	0
1	F	386/389 (99%)	-0.26	12 (3%) 49 48	13, 19, 38, 52	0
1	G	386/389 (99%)	-0.10	16 (4%) 38 36	13, 20, 40, 57	0
1	H	380/389 (97%)	-0.11	10 (2%) 56 55	15, 22, 46, 88	0
All	All	3077/3112 (98%)	-0.27	69 (2%) 62 63	12, 20, 40, 88	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	27	ALA	12.1
1	H	25	SER	7.9
1	D	27	ALA	7.7
1	H	26	GLY	7.7
1	D	26	GLY	4.9
1	G	19	GLU	4.8
1	B	387	MET	4.7
1	H	28	GLY	4.4
1	G	149	ASP	4.1
1	F	387	MET	4.0
1	F	148	TRP	3.9
1	D	382	GLY	3.9
1	G	387	MET	3.8
1	D	28	GLY	3.7
1	H	29	LEU	3.5
1	C	387	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	24	GLU	3.4
1	E	190	GLN	3.3
1	D	25	SER	3.3
1	F	19	GLU	3.3
1	G	349	GLU	3.2
1	F	383	ALA	3.2
1	F	149	ASP	3.1
1	B	349	GLU	3.0
1	A	2	SER	3.0
1	D	2	SER	2.9
1	E	2	SER	2.9
1	B	20	ARG	2.8
1	H	376	LYS	2.7
1	C	20	ARG	2.7
1	E	153	ASP	2.7
1	F	349	GLU	2.7
1	B	2	SER	2.7
1	F	381	ILE	2.7
1	G	190	GLN	2.7
1	G	20	ARG	2.6
1	C	19	GLU	2.6
1	E	387	MET	2.6
1	F	2	SER	2.6
1	H	2	SER	2.6
1	H	350	ASN	2.6
1	G	350	ASN	2.6
1	G	164	GLU	2.5
1	F	20	ARG	2.5
1	G	2	SER	2.5
1	D	137	ARG	2.5
1	B	137	ARG	2.4
1	G	383	ALA	2.4
1	G	157	ASP	2.4
1	B	19	GLU	2.4
1	C	148	TRP	2.4
1	C	349	GLU	2.3
1	G	347	LYS	2.3
1	E	164	GLU	2.2
1	C	2	SER	2.2
1	H	379	PRO	2.2
1	G	176	ARG	2.2
1	G	346	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	ASP	2.2
1	E	149	ASP	2.1
1	D	24	GLU	2.1
1	G	345	ASP	2.1
1	D	29	LEU	2.1
1	F	28	GLY	2.1
1	E	345	ASP	2.1
1	G	382	GLY	2.0
1	F	385	HIS	2.0
1	F	347	LYS	2.0
1	C	149	ASP	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	C	394	6/6	0.89	0.31	18.10	29,44,45,52	0
4	GOL	C	392	6/6	0.90	0.19	14.29	21,32,36,39	0
4	GOL	D	392	6/6	0.93	0.15	10.06	18,35,37,38	0
4	GOL	G	392	6/6	0.88	0.14	9.11	30,34,35,40	0
4	GOL	H	392	6/6	0.91	0.13	8.88	19,29,31,37	0
4	GOL	B	393	6/6	0.87	0.27	7.31	28,40,45,48	0
4	GOL	B	392	6/6	0.87	0.15	4.87	30,33,39,40	0
4	GOL	C	393	6/6	0.91	0.13	3.68	28,42,45,45	0
4	GOL	A	392	6/6	0.81	0.19	3.16	35,36,42,46	0
4	GOL	E	392	6/6	0.88	0.20	2.46	38,40,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	390	1/1	1.00	0.09	1.63	16,16,16,16	0
3	DXL	F	391	12/12	0.92	0.13	1.46	18,33,36,36	0
2	MG	F	390	1/1	0.99	0.10	1.06	19,19,19,19	0
3	DXL	E	391	12/12	0.94	0.09	0.74	17,28,34,38	0
3	DXL	B	391	12/12	0.94	0.10	0.57	17,27,31,36	0
3	DXL	A	391	12/12	0.94	0.08	0.51	18,24,28,34	0
5	LY9	D	391	12/12	0.94	0.10	0.37	15,24,47,58	0
2	MG	B	390	1/1	0.99	0.08	0.31	19,19,19,19	0
5	LY9	H	391	12/12	0.92	0.11	-0.04	18,31,57,66	0
2	MG	H	390	1/1	0.99	0.07	-0.26	20,20,20,20	0
3	DXL	G	391	12/12	0.95	0.08	-0.50	19,28,39,41	0
2	MG	G	390	1/1	0.99	0.07	-0.75	19,19,19,19	0
2	MG	A	390	1/1	0.99	0.07	-0.77	21,21,21,21	0
3	DXL	C	391	12/12	0.96	0.07	-0.84	17,26,35,35	0
2	MG	E	390	1/1	0.99	0.05	-1.10	22,22,22,22	0
2	MG	C	390	1/1	0.98	0.05	-1.38	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.