



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 03:23 PM EDT

PDB ID : 4XGS  
Title : Crystal structure analysis of novel iron uptake mechanism of Gram-negative bacterial ferritin  
Authors : Kim, S.  
Deposited on : 2015-01-02  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

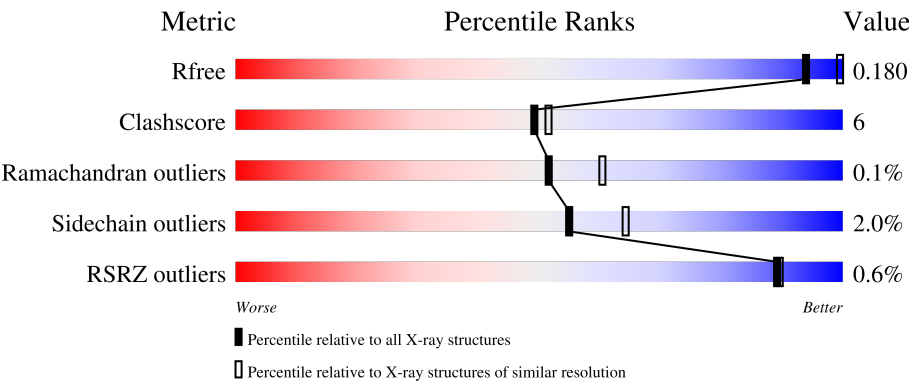
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	<div><div></div><div>84%13%...</div></div>
1	B	165	<div><div>%</div><div>84%13%..</div></div>
1	C	165	<div><div>2%</div><div>80%18%..</div></div>
1	D	165	<div><div></div><div>87%12%..</div></div>
1	E	165	<div><div>%</div><div>91%7%..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	165	 86% 12% ..

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	205	-	X	-	-
4	GOL	B	203	-	-	X	-
4	GOL	E	205	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9052 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.

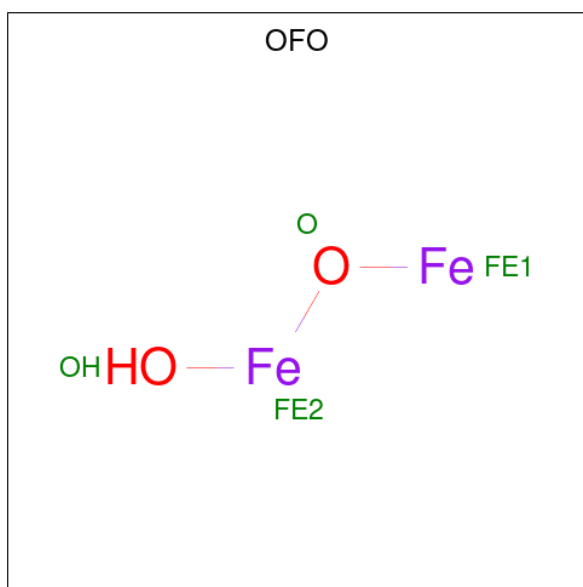
- Molecule 1 is a protein called Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	3	0
			1376	877	222	268	9			
1	B	164	Total	C	N	O	S	0	3	0
			1379	879	221	270	9			
1	C	164	Total	C	N	O	S	0	3	0
			1384	881	223	272	8			
1	D	163	Total	C	N	O	S	0	3	0
			1375	877	221	269	8			
1	E	163	Total	C	N	O	S	0	1	0
			1357	866	217	266	8			
1	F	163	Total	C	N	O	S	0	3	0
			1374	876	220	269	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P0A998
A	93	LEU	HIS	engineered mutation	UNP P0A998
B	1	HIS	-	expression tag	UNP P0A998
B	93	LEU	HIS	engineered mutation	UNP P0A998
C	1	HIS	-	expression tag	UNP P0A998
C	93	LEU	HIS	engineered mutation	UNP P0A998
D	1	HIS	-	expression tag	UNP P0A998
D	93	LEU	HIS	engineered mutation	UNP P0A998
E	1	HIS	-	expression tag	UNP P0A998
E	93	LEU	HIS	engineered mutation	UNP P0A998
F	1	HIS	-	expression tag	UNP P0A998
F	93	LEU	HIS	engineered mutation	UNP P0A998

- Molecule 2 is HYDROXY DIIRON-OXO MOIETY (three-letter code: OFO) (formula:  $\text{Fe}_2\text{HO}_2$ ).



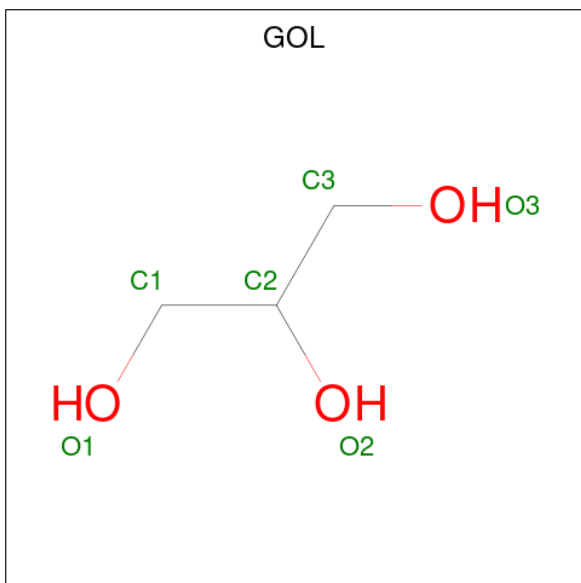
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	O	0	0
			4	2	2		
2	B	1	Total	Fe	O	0	0
			4	2	2		
2	C	1	Total	Fe	O	0	0
			4	2	2		
2	D	1	Total	Fe	O	0	0
			4	2	2		
2	E	1	Total	Fe	O	0	0
			4	2	2		
2	F	1	Total	Fe	O	0	0
			4	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total 110	O 110	0	0
5	B	115	Total 115	O 115	0	0
5	C	104	Total 104	O 104	0	0
5	D	104	Total 104	O 104	0	0
5	E	104	Total 104	O 104	0	0
5	F	94	Total 94	O 94	0	0



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


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

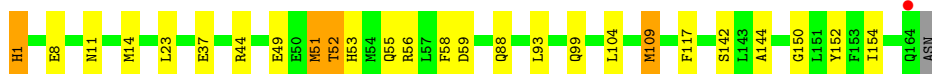
- Molecule 1: Ferritin

Chain A: 




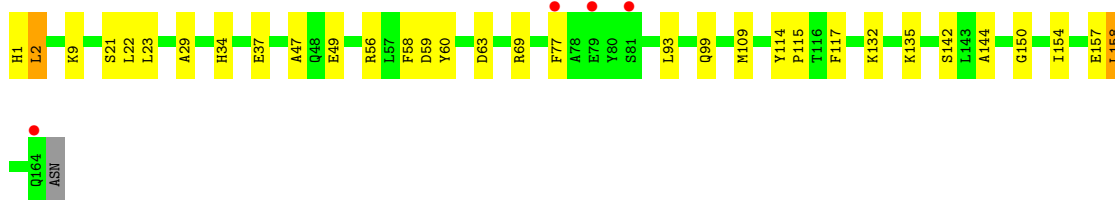
- Molecule 1: Ferritin

Chain B: 




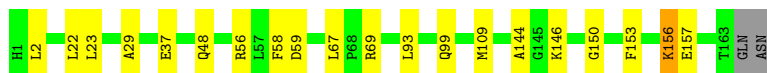
- Molecule 1: Ferritin

Chain C: 




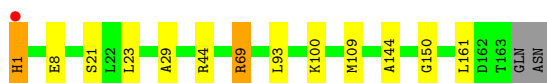
- Molecule 1: Ferritin

Chain D: 

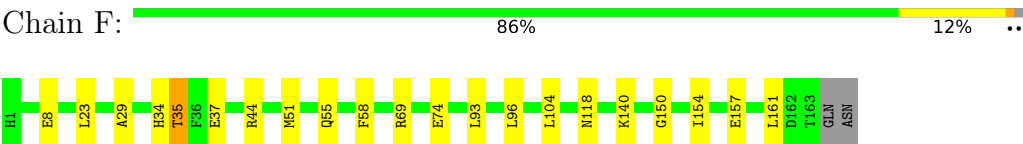


- Molecule 1: Ferritin

Chain E: 



● Molecule 1: Ferritin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.03Å 129.03Å 172.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.62 – 2.25 45.62 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.62-2.25) 100.0 (45.62-2.25)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.86 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.145 , 0.183 0.148 , 0.180	Depositor DCC
$R_{free}$ test set	3380 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, OFO

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	1.04	2/1407 (0.1%)	1.08	6/1898 (0.3%)
1	B	1.05	3/1410 (0.2%)	0.97	7/1903 (0.4%)
1	C	0.92	1/1415 (0.1%)	0.89	2/1910 (0.1%)
1	D	0.93	0/1406	0.89	4/1897 (0.2%)
1	E	0.98	0/1388	0.93	2/1874 (0.1%)
1	F	1.00	0/1405	0.88	1/1896 (0.1%)
All	All	0.99	6/8431 (0.1%)	0.94	22/11378 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	GLU	CG-CD	7.40	1.63	1.51
1	B	142	SER	CB-OG	-5.63	1.34	1.42
1	B	37	GLU	CD-OE1	5.35	1.31	1.25
1	A	56[A]	ARG	CZ-NH1	5.08	1.39	1.33
1	A	56[B]	ARG	CZ-NH1	5.08	1.39	1.33
1	C	60	TYR	CE1-CZ	-5.00	1.32	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56[A]	ARG	NE-CZ-NH1	12.68	126.64	120.30
1	A	56[B]	ARG	NE-CZ-NH1	12.68	126.64	120.30
1	A	56[A]	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	A	56[B]	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	D	56	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	B	44	ARG	NE-CZ-NH1	-9.65	115.48	120.30
1	B	109	MET	CG-SD-CE	-9.57	84.88	100.20
1	B	44	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	B	56	ARG	NE-CZ-NH1	-7.84	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	MET	CG-SD-CE	-7.70	87.88	100.20
1	C	56	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	B	59	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	69	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	E	109	MET	CG-SD-CE	-6.49	89.82	100.20
1	E	69	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	F	44	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	59	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	B	51	MET	CG-SD-CE	-5.70	91.09	100.20
1	D	59	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	D	69	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	59	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	C	59	ASP	CB-CG-OD2	-5.20	113.62	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1376	0	1321	16	1
1	B	1379	0	1319	21	2
1	C	1384	0	1323	22	1
1	D	1375	0	1320	15	0
1	E	1357	0	1301	12	0
1	F	1374	0	1317	15	2
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
3	A	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	24	0	32	4	0
4	B	12	0	16	4	2
4	C	24	0	32	4	0
4	D	24	0	32	1	0
4	E	18	0	24	2	2
4	F	30	0	40	4	0
5	A	110	0	0	4	1
5	B	115	0	0	6	0
5	C	104	0	0	7	1
5	D	104	0	0	7	0
5	E	104	0	0	8	0
5	F	94	0	0	2	0
All	All	9052	0	8077	98	6

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 6.

All (98) 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:A:63:ASP:OD2	4:A:204:GOL:H31	1.60	1.01
1:B:51:MET:O	1:B:55[B]:GLN:HG3	1.72	0.90
1:D:37:GLU:OE1	5:D:301:HOH:O	1.90	0.88
1:F:51:MET:O	1:F:55[B]:GLN:HG3	1.74	0.88
1:A:63:ASP:OD2	4:A:204:GOL:C3	2.25	0.84
1:A:82:SER:HB2	4:A:205:GOL:H2	1.62	0.81
1:A:1:HIS:HA	5:A:312:HOH:O	1.81	0.80
1:A:74:GLU:OE1	5:A:301:HOH:O	1.99	0.79
1:F:34:HIS:O	1:F:35:THR:HB	1.83	0.78
1:D:99:GLN:NE2	5:D:303:HOH:O	2.19	0.74
1:E:1:HIS:HB2	5:E:301:HOH:O	1.90	0.71
1:B:99:GLN:NE2	5:B:302:HOH:O	2.24	0.69
1:C:9:LYS:NZ	5:C:303:HOH:O	2.26	0.69
1:D:48[A]:GLN:NE2	5:D:302:HOH:O	2.05	0.67
1:D:22:LEU:HD23	4:D:203:GOL:O1	1.95	0.67
1:E:1:HIS:ND1	5:E:301:HOH:O	2.27	0.67
1:C:37:GLU:OE1	5:C:301:HOH:O	2.14	0.66
1:F:37:GLU:OE1	5:F:301:HOH:O	2.12	0.66
1:B:14[B]:MET:HE1	1:B:58:PHE:HD2	1.61	0.66
1:C:1:HIS:CE1	5:C:337:HOH:O	2.50	0.65
1:D:156:LYS:NZ	5:D:305:HOH:O	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:SER:OG	4:C:203:GOL:H11	1.96	0.65
1:F:74:GLU:OE1	5:F:302:HOH:O	2.15	0.64
1:C:132:LYS:NZ	5:C:306:HOH:O	2.33	0.62
1:C:1:HIS:O	1:C:2:LEU:HB2	1.99	0.61
1:A:23:LEU:HD23	1:A:93:LEU:HD22	1.83	0.60
1:C:63:ASP:OD2	4:C:205:GOL:O3	2.16	0.60
1:B:1:HIS:N	5:B:307:HOH:O	2.35	0.60
1:B:55[A]:GLN:NE2	1:E:44:ARG:HD2	2.18	0.58
1:E:8:GLU:HG3	5:E:394:HOH:O	2.02	0.58
1:F:140:LYS:HB3	1:F:154:ILE:HD12	1.86	0.58
1:B:23:LEU:HD23	1:B:93:LEU:HD22	1.85	0.57
1:C:69:ARG:NH2	3:C:202:SO4:O3	2.37	0.57
1:E:23:LEU:HD23	1:E:93:LEU:HD22	1.87	0.57
1:D:146:LYS:CE	5:D:386:HOH:O	2.54	0.55
1:F:140:LYS:HE3	1:F:157:GLU:CD	2.27	0.55
1:F:23:LEU:HD23	1:F:93:LEU:HD22	1.87	0.54
1:A:29:ALA:HB2	1:F:58:PHE:CZ	2.42	0.54
1:E:144:ALA:O	1:E:150:GLY:HA3	2.07	0.54
1:E:1:HIS:CB	5:E:301:HOH:O	2.54	0.54
1:B:88:GLN:NE2	5:B:310:HOH:O	2.41	0.54
1:E:1:HIS:CG	5:E:301:HOH:O	2.61	0.53
1:F:118:ASN:O	4:F:205:GOL:H12	2.08	0.53
1:C:22:LEU:HD23	4:C:203:GOL:O1	2.10	0.52
1:B:14[B]:MET:HE1	1:B:58:PHE:CD2	2.44	0.51
1:E:69:ARG:NE	5:E:303:HOH:O	2.41	0.51
1:F:140:LYS:HE3	1:F:157:GLU:OE1	2.11	0.51
1:A:144:ALA:HB3	1:A:154:ILE:HD11	1.93	0.51
1:F:51:MET:HE2	4:F:202:GOL:H12	1.93	0.51
1:C:144:ALA:O	1:C:150:GLY:HA3	2.11	0.51
4:E:204:GOL:C1	5:E:341:HOH:O	2.59	0.50
4:B:203:GOL:O1	5:B:301:HOH:O	2.18	0.50
1:C:49:GLU:OE2	5:C:302:HOH:O	2.19	0.49
1:B:109:MET:CE	1:B:117:PHE:CG	2.95	0.49
1:D:23:LEU:HD23	1:D:93:LEU:HD22	1.94	0.49
4:B:203:GOL:C1	5:B:301:HOH:O	2.60	0.49
1:C:58:PHE:CZ	1:D:29:ALA:HB2	2.47	0.49
1:C:154:ILE:HG22	1:C:158:LEU:HD22	1.95	0.49
1:B:58:PHE:CZ	1:E:29:ALA:HB2	2.48	0.49
4:F:204:GOL:H31	4:F:205:GOL:O3	2.14	0.48
1:C:99:GLN:NE2	5:C:310:HOH:O	2.47	0.47
4:F:204:GOL:C3	4:F:205:GOL:O3	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLN:HG2	5:A:386:HOH:O	2.14	0.47
1:C:77:PHE:HE1	1:D:67:LEU:HD21	1.80	0.47
1:D:144:ALA:O	1:D:150:GLY:HA3	2.15	0.47
1:D:146:LYS:HE2	5:D:386:HOH:O	2.14	0.47
1:B:144:ALA:O	1:B:150:GLY:HA3	2.15	0.46
1:C:109:MET:HE2	1:C:117:PHE:CG	2.51	0.45
1:A:56[B]:ARG:NE	5:A:302:HOH:O	2.36	0.45
1:B:152:TYR:OH	1:D:157:GLU:OE1	2.25	0.45
1:B:14[B]:MET:HE1	1:B:58:PHE:HB2	1.99	0.44
1:A:22:LEU:HD12	1:A:73:VAL:HG11	2.00	0.44
1:C:23:LEU:HD23	1:C:93:LEU:HD22	1.99	0.44
1:A:58:PHE:CZ	1:F:29:ALA:HB2	2.53	0.44
1:E:21:SER:OG	4:E:203:GOL:O1	2.31	0.43
4:B:203:GOL:H11	5:B:301:HOH:O	2.19	0.43
1:D:37:GLU:OE2	5:D:304:HOH:O	2.21	0.43
1:C:114:TYR:N	1:C:115:PRO:CD	2.81	0.43
1:F:34:HIS:O	1:F:35:THR:CB	2.61	0.43
1:B:11:ASN:O	1:B:14[B]:MET:HG3	2.19	0.43
1:C:47:ALA:HB1	4:C:203:GOL:H12	2.01	0.43
1:B:14[B]:MET:HE2	1:B:14[B]:MET:HB2	1.68	0.42
1:B:144:ALA:HB3	1:B:154:ILE:HD11	2.00	0.42
1:B:109:MET:CE	1:B:117:PHE:CD1	3.02	0.42
1:A:153:PHE:CD2	1:D:153:PHE:HZ	2.37	0.42
1:A:24:TYR:HE1	1:A:90:THR:HG22	1.84	0.42
1:B:14[B]:MET:CE	1:B:58:PHE:HB2	2.49	0.42
1:B:49:GLU:O	1:B:52:THR:HB	2.19	0.42
1:C:29:ALA:HB2	1:D:58:PHE:CZ	2.54	0.42
1:A:144:ALA:O	1:A:150:GLY:HA3	2.20	0.41
1:F:150:GLY:O	1:F:154:ILE:HG12	2.21	0.41
1:C:34:HIS:HE1	5:C:389:HOH:O	2.04	0.41
1:C:144:ALA:HB3	1:C:154:ILE:HD11	2.03	0.41
1:A:60:TYR:HA	4:A:204:GOL:O3	2.22	0.40
1:B:51:MET:HE3	4:B:202:GOL:H12	2.02	0.40
1:B:52:THR:HG22	1:B:53:HIS:HD2	1.85	0.40
1:E:100:LYS:NZ	5:E:306:HOH:O	2.51	0.40
1:F:140:LYS:HE3	1:F:157:GLU:OE2	2.22	0.40

All (6) 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)
4:B:203:GOL:O1	4:E:205:GOL:O2[3_655]	1.37	0.83
1:B:8:GLU:OE1	1:F:8:GLU:OE1[6_554]	1.83	0.37
5:A:387:HOH:O	5:C:324:HOH:O[3_655]	1.99	0.21
1:B:8:GLU:OE1	1:F:69:ARG:NH1[6_554]	2.01	0.19
4:B:203:GOL:C1	4:E:205:GOL:O2[3_655]	2.04	0.16
1:A:152:TYR:OH	1:C:157:GLU:OE1[3_655]	2.19	0.01

## 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	164/165 (99%)	163 (99%)	1 (1%)	0	100	100
1	B	165/165 (100%)	164 (99%)	1 (1%)	0	100	100
1	C	165/165 (100%)	162 (98%)	2 (1%)	1 (1%)	25	25
1	D	164/165 (99%)	162 (99%)	2 (1%)	0	100	100
1	E	162/165 (98%)	161 (99%)	1 (1%)	0	100	100
1	F	164/165 (99%)	162 (99%)	2 (1%)	0	100	100
All	All	984/990 (99%)	974 (99%)	9 (1%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	LEU

### 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	151/150 (101%)	146 (97%)	5 (3%)	38	46
1	B	151/150 (101%)	148 (98%)	3 (2%)	55	64
1	C	152/150 (101%)	149 (98%)	3 (2%)	55	64
1	D	151/150 (101%)	149 (99%)	2 (1%)	69	79
1	E	149/150 (99%)	147 (99%)	2 (1%)	69	79
1	F	151/150 (101%)	147 (97%)	4 (3%)	46	55
All	All	905/900 (101%)	886 (98%)	19 (2%)	55	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	56[A]	ARG
1	A	56[B]	ARG
1	A	79	GLU
1	A	149	GLU
1	B	1	HIS
1	B	52	THR
1	B	104	LEU
1	C	135	LYS
1	C	142	SER
1	C	158	LEU
1	D	2	LEU
1	D	156	LYS
1	E	1	HIS
1	E	161	LEU
1	F	35	THR
1	F	96	LEU
1	F	104	LEU
1	F	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	127	GLN
1	B	127	GLN
1	C	127	GLN
1	D	55	GLN
1	D	99	GLN

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Mol	Chain	Res	Type
1	D	127	GLN
1	E	55	GLN
1	E	127	GLN
1	F	66	ASN
1	F	127	GLN
1	F	128	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 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	$\# Z  > 2$
4	GOL	E	205	-	5,5,5	0.50	0	5,5,5	1.69	2 (40%)
4	GOL	D	205	-	5,5,5	0.89	0	5,5,5	0.71	0
4	GOL	C	203	-	5,5,5	0.67	0	5,5,5	0.86	0
4	GOL	C	205	-	5,5,5	1.07	1 (20%)	5,5,5	1.70	2 (40%)
2	OFO	B	201	1	0,3,3	-	-	-	-	-
4	GOL	A	205	-	5,5,5	0.97	0	5,5,5	1.72	2 (40%)
4	GOL	D	204	-	5,5,5	0.81	0	5,5,5	1.44	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	E	204	-	5,5,5	1.12	0	5,5,5	1.01	0
4	GOL	F	204	-	5,5,5	0.56	0	5,5,5	1.74	1 (20%)
4	GOL	B	202	-	5,5,5	0.59	0	5,5,5	1.08	0
4	GOL	B	203	-	5,5,5	0.36	0	5,5,5	0.34	0
4	GOL	F	202	-	5,5,5	0.42	0	5,5,5	0.80	0
4	GOL	D	203	-	5,5,5	0.63	0	5,5,5	0.51	0
2	OFO	F	201	1	0,3,3	-	-	-	-	-
3	SO4	C	202	-	4,4,4	0.31	0	6,6,6	0.50	0
4	GOL	C	206	-	5,5,5	0.62	0	5,5,5	1.11	0
2	OFO	C	201	1	0,3,3	-	-	-	-	-
2	OFO	A	201	1	0,3,3	-	-	-	-	-
3	SO4	D	202	-	4,4,4	0.44	0	6,6,6	0.42	0
4	GOL	D	206	-	5,5,5	0.48	0	5,5,5	1.34	1 (20%)
4	GOL	F	205	-	5,5,5	0.57	0	5,5,5	1.24	1 (20%)
2	OFO	E	201	1	0,3,3	-	-	-	-	-
2	OFO	D	201	1	0,3,3	-	-	-	-	-
4	GOL	A	206	-	5,5,5	0.46	0	5,5,5	0.81	0
3	SO4	A	202	-	4,4,4	0.16	0	6,6,6	1.23	1 (16%)
3	SO4	E	202	-	4,4,4	0.22	0	6,6,6	0.94	0
4	GOL	F	206	-	5,5,5	0.58	0	5,5,5	0.62	0
4	GOL	E	203	-	5,5,5	0.70	0	5,5,5	0.37	0
4	GOL	F	203	-	5,5,5	0.72	0	5,5,5	0.83	0
4	GOL	A	204	-	5,5,5	0.66	0	5,5,5	1.20	1 (20%)
4	GOL	C	204	-	5,5,5	0.69	0	5,5,5	0.56	0
4	GOL	A	203	-	5,5,5	0.30	0	5,5,5	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	205	-	-	3/4/4/4	-
4	GOL	A	203	-	-	2/4/4/4	-
4	GOL	D	205	-	-	4/4/4/4	-
4	GOL	C	203	-	-	2/4/4/4	-
4	GOL	C	205	-	-	0/4/4/4	-
4	GOL	A	205	-	-	4/4/4/4	-
4	GOL	D	204	-	-	2/4/4/4	-
4	GOL	E	204	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	F	204	-	-	2/4/4/4	-
4	GOL	B	202	-	-	3/4/4/4	-
4	GOL	B	203	-	-	2/4/4/4	-
4	GOL	F	202	-	-	0/4/4/4	-
4	GOL	D	203	-	-	4/4/4/4	-
4	GOL	C	206	-	-	4/4/4/4	-
4	GOL	D	206	-	-	2/4/4/4	-
4	GOL	F	205	-	-	3/4/4/4	-
4	GOL	A	206	-	-	2/4/4/4	-
4	GOL	F	206	-	-	4/4/4/4	-
4	GOL	E	203	-	-	2/4/4/4	-
4	GOL	A	204	-	-	3/4/4/4	-
4	GOL	C	204	-	-	4/4/4/4	-
4	GOL	F	203	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	205	GOL	O2-C2	2.05	1.49	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	204	GOL	O2-C2-C3	-3.23	94.90	109.12
4	E	205	GOL	O2-C2-C3	2.91	121.92	109.12
4	A	205	GOL	O2-C2-C1	2.87	121.77	109.12
4	C	205	GOL	C3-C2-C1	-2.82	100.73	111.70
4	D	204	GOL	C3-C2-C1	2.55	121.62	111.70
4	C	205	GOL	O2-C2-C1	2.31	119.30	109.12
4	E	205	GOL	O2-C2-C1	-2.28	99.07	109.12
4	A	204	GOL	O2-C2-C1	2.27	119.14	109.12
3	A	202	SO4	O4-S-O2	2.26	121.11	109.31
4	A	205	GOL	O1-C1-C2	2.20	120.75	110.20
4	D	206	GOL	O2-C2-C3	2.13	118.50	109.12
4	F	205	GOL	O1-C1-C2	-2.04	100.42	110.20

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	205	GOL	O1-C1-C2-C3
4	A	206	GOL	C1-C2-C3-O3
4	B	203	GOL	O1-C1-C2-C3
4	C	203	GOL	C1-C2-C3-O3
4	C	204	GOL	O1-C1-C2-C3
4	C	204	GOL	C1-C2-C3-O3
4	C	206	GOL	O1-C1-C2-C3
4	C	206	GOL	C1-C2-C3-O3
4	D	203	GOL	C1-C2-C3-O3
4	D	204	GOL	C1-C2-C3-O3
4	E	203	GOL	C1-C2-C3-O3
4	E	204	GOL	C1-C2-C3-O3
4	E	205	GOL	C1-C2-C3-O3
4	F	203	GOL	O1-C1-C2-C3
4	F	203	GOL	C1-C2-C3-O3
4	F	203	GOL	O2-C2-C3-O3
4	F	204	GOL	C1-C2-C3-O3
4	F	205	GOL	C1-C2-C3-O3
4	F	206	GOL	C1-C2-C3-O3
4	F	206	GOL	O2-C2-C3-O3
4	A	204	GOL	O1-C1-C2-O2
4	C	204	GOL	O2-C2-C3-O3
4	E	205	GOL	O2-C2-C3-O3
4	A	203	GOL	O1-C1-C2-C3
4	A	204	GOL	O1-C1-C2-C3
4	A	205	GOL	C1-C2-C3-O3
4	B	202	GOL	O1-C1-C2-C3
4	D	203	GOL	O1-C1-C2-C3
4	D	205	GOL	O1-C1-C2-C3
4	D	205	GOL	C1-C2-C3-O3
4	F	206	GOL	O1-C1-C2-C3
4	A	205	GOL	O1-C1-C2-O2
4	A	205	GOL	O2-C2-C3-O3
4	B	203	GOL	O1-C1-C2-O2
4	C	203	GOL	O2-C2-C3-O3
4	C	204	GOL	O1-C1-C2-O2
4	D	203	GOL	O1-C1-C2-O2
4	D	205	GOL	O1-C1-C2-O2
4	E	203	GOL	O2-C2-C3-O3
4	F	203	GOL	O1-C1-C2-O2
4	F	204	GOL	O2-C2-C3-O3
4	F	205	GOL	O2-C2-C3-O3
4	C	206	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	203	GOL	O2-C2-C3-O3
4	F	206	GOL	O1-C1-C2-O2
4	D	205	GOL	O2-C2-C3-O3
4	D	206	GOL	O2-C2-C3-O3
4	A	206	GOL	O2-C2-C3-O3
4	B	202	GOL	O2-C2-C3-O3
4	D	204	GOL	O2-C2-C3-O3
4	E	205	GOL	O1-C1-C2-O2
4	D	206	GOL	C1-C2-C3-O3
4	A	203	GOL	O1-C1-C2-O2
4	F	205	GOL	O1-C1-C2-C3
4	A	204	GOL	O2-C2-C3-O3
4	B	202	GOL	O1-C1-C2-O2
4	C	206	GOL	O2-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	205	GOL	0	2
4	C	203	GOL	3	0
4	C	205	GOL	1	0
4	A	205	GOL	1	0
4	E	204	GOL	1	0
4	F	204	GOL	2	0
4	B	202	GOL	1	0
4	B	203	GOL	3	2
4	F	202	GOL	1	0
4	D	203	GOL	1	0
3	C	202	SO4	1	0
4	F	205	GOL	3	0
4	E	203	GOL	1	0
4	A	204	GOL	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	163/165 (98%)	-0.56	0 <span>100</span> <span>100</span>	24, 32, 50, 76	0
1	B	164/165 (99%)	-0.31	1 (0%) <span>89</span> <span>89</span>	23, 32, 51, 86	0
1	C	164/165 (99%)	-0.38	4 (2%) <span>59</span> <span>62</span>	25, 34, 53, 101	0
1	D	163/165 (98%)	-0.56	0 <span>100</span> <span>100</span>	25, 34, 52, 94	0
1	E	163/165 (98%)	-0.50	1 (0%) <span>89</span> <span>89</span>	24, 32, 48, 84	0
1	F	163/165 (98%)	-0.36	0 <span>100</span> <span>100</span>	23, 32, 47, 81	0
All	All	980/990 (98%)	-0.44	6 (0%) <span>89</span> <span>89</span>	23, 33, 53, 101	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	GLN	4.4
1	E	1	HIS	2.2
1	C	77	PHE	2.2
1	C	81	SER	2.2
1	C	79	GLU	2.1
1	B	164	GLN	2.1

### 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 monosaccharides in this entry.



## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	E	205	6/6	0.76	0.60	81,109,131,142	0
4	GOL	E	204	6/6	0.79	0.27	44,56,69,70	0
4	GOL	C	204	6/6	0.79	0.24	61,69,72,76	0
4	GOL	F	205	6/6	0.79	0.23	51,70,74,84	0
4	GOL	D	204	6/6	0.84	0.18	59,65,71,71	0
4	GOL	A	205	6/6	0.88	0.33	44,52,63,64	0
4	GOL	F	203	6/6	0.88	0.20	59,64,71,75	0
3	SO4	C	202	5/5	0.88	0.29	75,82,87,95	0
4	GOL	D	206	6/6	0.90	0.22	44,53,58,84	0
4	GOL	D	205	6/6	0.91	0.16	45,50,62,62	0
4	GOL	F	204	6/6	0.92	0.18	37,54,65,68	0
4	GOL	B	203	6/6	0.92	0.34	47,71,86,100	0
4	GOL	F	206	6/6	0.92	0.15	47,58,61,64	0
4	GOL	C	203	6/6	0.93	0.20	41,47,57,60	0
3	SO4	D	202	5/5	0.93	0.30	82,91,105,108	0
4	GOL	C	206	6/6	0.93	0.18	43,46,49,60	0
4	GOL	A	204	6/6	0.94	0.18	53,58,60,66	0
4	GOL	C	205	6/6	0.94	0.14	51,53,60,61	0
4	GOL	D	203	6/6	0.95	0.22	45,48,53,62	0
4	GOL	B	202	6/6	0.96	0.16	35,39,41,44	0
4	GOL	E	203	6/6	0.96	0.18	44,52,53,61	0
4	GOL	A	203	6/6	0.96	0.19	49,52,59,59	0
4	GOL	A	206	6/6	0.96	0.17	42,51,63,66	0
4	GOL	F	202	6/6	0.97	0.12	37,41,42,42	0
3	SO4	E	202	5/5	0.98	0.12	47,49,50,61	0
2	OFO	D	201	4/4	0.99	0.09	27,28,33,41	0
2	OFO	F	201	4/4	0.99	0.11	25,26,30,36	0
3	SO4	A	202	5/5	0.99	0.10	41,42,46,48	0
2	OFO	B	201	4/4	0.99	0.10	24,25,31,37	0
2	OFO	C	201	4/4	1.00	0.09	23,26,31,39	0
2	OFO	A	201	4/4	1.00	0.07	24,27,30,42	0
2	OFO	E	201	4/4	1.00	0.08	23,26,31,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.