wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2023 – 03:06 PM EDT

PDB ID	:	4P18
Title	:	Crystal Structure of frog M ferritin mutant D80K
Authors	:	Pozzi, C.; Di Pisa, F.; Mangani, S.; Bernacchioni, C.; Ghini, V.; Turano, P.
Deposited on	:	2014-02-25
Resolution	:	1.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

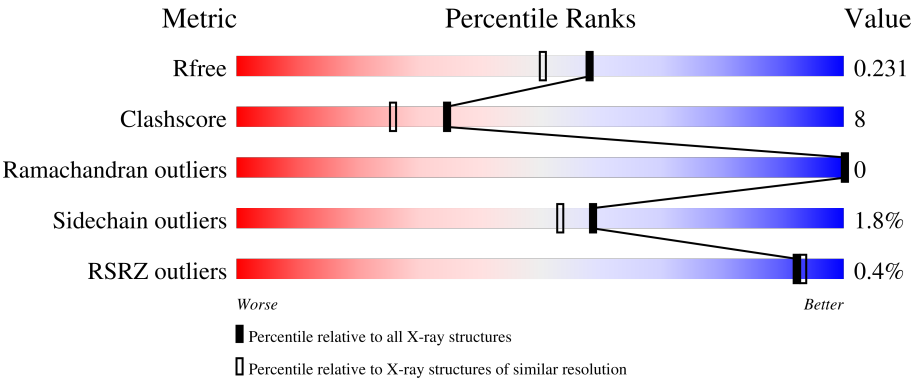
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 >=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	176	79% 19% .
1	B	176	84% 14% .
1	C	176	84% 14% ..
1	D	176	% 89% 9% ..
1	E	176	89% 9% .

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Mol	Chain	Length	Quality of chain
1	F	176	84% 13%
1	G	176	81% 16%
1	H	176	82% 15%
1	I	176	86% 11%
1	J	176	86% 12%
1	K	176	78% 18%
1	L	176	85% 13%
1	M	176	90% 7%
1	N	176	85% 13%
1	O	176	87% 11%
1	P	176	82% 15%
1	Q	176	78% 19%
1	R	176	82% 15%
1	S	176	87% 10%
1	T	176	85% 13%
1	U	176	83% 14%
1	V	176	86% 11%
1	W	176	83% 14%
1	X	176	90% 7%

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	SO4	D	201	-	-	X	-
2	SO4	J	201	-	-	X	-
2	SO4	L	201	-	-	X	-
2	SO4	R	201	-	-	X	-
2	SO4	W	201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	E	204	-	-	X	-
3	EDO	G	207	-	-	X	-
3	EDO	G	211	-	-	X	-
3	EDO	J	205	-	-	X	-
3	EDO	N	203	-	-	X	-
3	EDO	Q	202	-	-	X	-
3	EDO	R	206	-	-	X	-
3	EDO	S	202	-	-	X	-
3	EDO	W	204	-	-	X	-
4	ACT	A	203	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 40182 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, middle subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	9	0
			1460	922	251	280	7			
1	B	172	Total	C	N	O	S	0	6	0
			1452	915	250	280	7			
1	C	172	Total	C	N	O	S	0	8	0
			1460	922	251	280	7			
1	D	172	Total	C	N	O	S	0	6	0
			1446	912	250	277	7			
1	M	172	Total	C	N	O	S	0	2	0
			1426	899	249	271	7			
1	N	172	Total	C	N	O	S	0	8	0
			1457	919	251	280	7			
1	O	172	Total	C	N	O	S	0	5	0
			1432	903	249	273	7			
1	P	172	Total	C	N	O	S	0	5	0
			1441	908	250	276	7			
1	S	172	Total	C	N	O	S	0	8	0
			1459	922	252	278	7			
1	T	172	Total	C	N	O	S	0	5	0
			1444	912	251	274	7			
1	E	172	Total	C	N	O	S	0	4	0
			1436	904	251	274	7			
1	F	172	Total	C	N	O	S	0	8	0
			1461	923	252	279	7			
1	G	172	Total	C	N	O	S	0	5	0
			1451	913	253	278	7			
1	H	172	Total	C	N	O	S	0	6	0
			1447	913	250	277	7			
1	I	172	Total	C	N	O	S	0	8	0
			1461	923	252	279	7			
1	J	172	Total	C	N	O	S	0	6	0
			1445	912	250	276	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	172	Total	C	N	O	S	0	8	0
			1464	923	254	280	7			
1	L	172	Total	C	N	O	S	0	6	0
			1441	909	252	273	7			
1	Q	172	Total	C	N	O	S	0	7	0
			1452	917	252	276	7			
1	R	172	Total	C	N	O	S	0	5	0
			1447	914	252	274	7			
1	U	172	Total	C	N	O	S	0	4	0
			1437	907	250	273	7			
1	V	172	Total	C	N	O	S	0	8	0
			1457	919	252	279	7			
1	W	172	Total	C	N	O	S	0	7	0
			1453	917	253	276	7			
1	X	172	Total	C	N	O	S	0	3	0
			1431	902	249	273	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	LYS	ASP	engineered mutation	UNP P07798
B	80	LYS	ASP	engineered mutation	UNP P07798
C	80	LYS	ASP	engineered mutation	UNP P07798
D	80	LYS	ASP	engineered mutation	UNP P07798
M	80	LYS	ASP	engineered mutation	UNP P07798
N	80	LYS	ASP	engineered mutation	UNP P07798
O	80	LYS	ASP	engineered mutation	UNP P07798
P	80	LYS	ASP	engineered mutation	UNP P07798
S	80	LYS	ASP	engineered mutation	UNP P07798
T	80	LYS	ASP	engineered mutation	UNP P07798
E	80	LYS	ASP	engineered mutation	UNP P07798
F	80	LYS	ASP	engineered mutation	UNP P07798
G	80	LYS	ASP	engineered mutation	UNP P07798
H	80	LYS	ASP	engineered mutation	UNP P07798
I	80	LYS	ASP	engineered mutation	UNP P07798
J	80	LYS	ASP	engineered mutation	UNP P07798
K	80	LYS	ASP	engineered mutation	UNP P07798
L	80	LYS	ASP	engineered mutation	UNP P07798
Q	80	LYS	ASP	engineered mutation	UNP P07798
R	80	LYS	ASP	engineered mutation	UNP P07798
U	80	LYS	ASP	engineered mutation	UNP P07798
V	80	LYS	ASP	engineered mutation	UNP P07798
W	80	LYS	ASP	engineered mutation	UNP P07798

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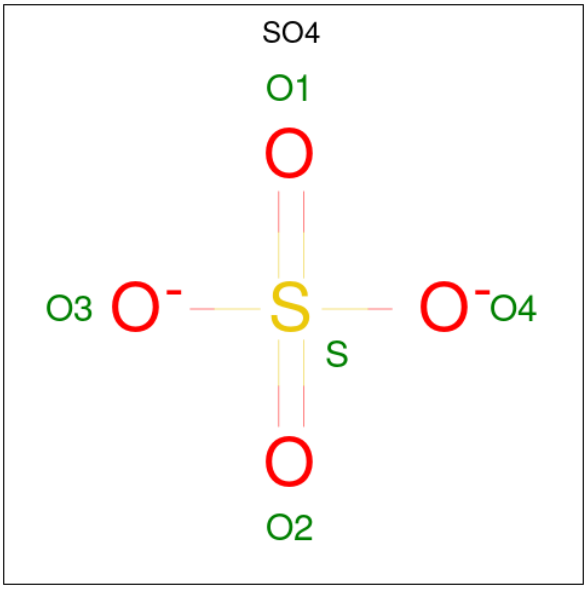
Chain	Residue	Modelled	Actual	Comment	Reference
X	80	LYS	ASP	engineered mutation	UNP P07798

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	T	1	Total O S 5 4 1	0	0
2	T	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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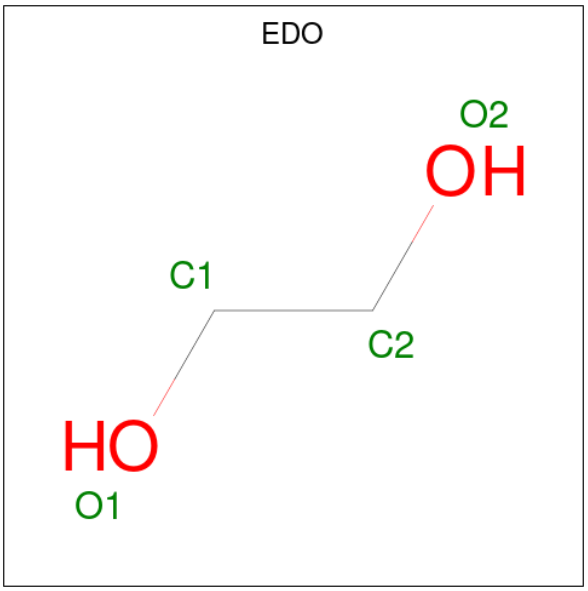
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	U	1	Total O S 5 4 1	0	0
2	W	1	Total O S 5 4 1	0	0
2	W	1	Total O S 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	M	1	Total	C	O	0	0
			4	2	2		
3	N	1	Total	C	O	0	0
			4	2	2		
3	N	1	Total	C	O	0	0
			4	2	2		
3	N	1	Total	C	O	0	0
			4	2	2		
3	O	1	Total	C	O	0	0
			4	2	2		
3	P	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total C O 4 2 2	0	0
3	P	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0

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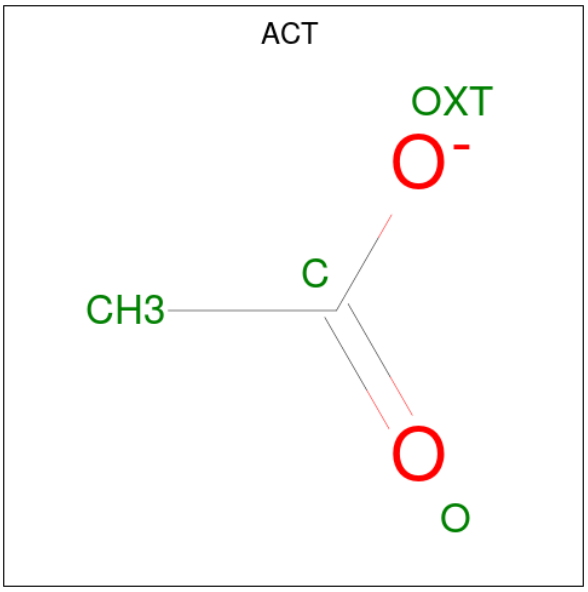
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	Q	1	Total	C	O	0	0
			4	2	2		
3	Q	1	Total	C	O	0	0
			4	2	2		
3	R	1	Total	C	O	0	0
			4	2	2		
3	R	1	Total	C	O	0	0
			4	2	2		
3	R	1	Total	C	O	0	0
			4	2	2		
3	R	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		
3	V	1	Total	C	O	0	0
			4	2	2		
3	V	1	Total	C	O	0	0
			4	2	2		
3	W	1	Total	C	O	0	0
			4	2	2		
3	X	1	Total	C	O	0	0
			4	2	2		
3	X	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	Q	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Cl 2 2	0	0
5	C	1	Total Cl 1 1	0	0
5	D	2	Total Cl 2 2	0	0
5	M	1	Total Cl 1 1	0	0
5	O	2	Total Cl 2 2	0	0
5	S	1	Total Cl 1 1	0	0
5	T	2	Total Cl 2 2	0	0
5	E	3	Total Cl 3 3	0	0
5	F	2	Total Cl 2 2	0	0
5	G	3	Total Cl 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Cl 1 1	0	0
5	I	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0
5	L	2	Total Cl 2 2	0	0
5	Q	1	Total Cl 1 1	0	0
5	U	2	Total Cl 2 2	0	0
5	W	1	Total Cl 1 1	0	0
5	X	3	Total Cl 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	214	Total O 214 214	0	0
6	B	211	Total O 211 211	0	0
6	C	203	Total O 203 203	0	0
6	D	193	Total O 193 193	0	0
6	M	208	Total O 208 208	0	0
6	N	194	Total O 194 194	0	0
6	O	210	Total O 210 210	0	0
6	P	191	Total O 191 191	0	0
6	S	226	Total O 226 226	0	0
6	T	207	Total O 207 207	0	0
6	E	205	Total O 205 205	0	0

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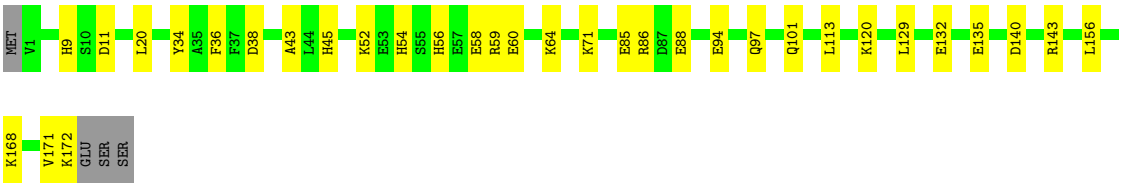
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	229	Total O 229 229	0	0
6	G	210	Total O 210 210	0	0
6	H	194	Total O 194 194	0	0
6	I	224	Total O 224 224	0	0
6	J	231	Total O 231 231	0	0
6	K	199	Total O 199 199	0	0
6	L	209	Total O 209 209	0	0
6	Q	203	Total O 203 203	0	0
6	R	207	Total O 207 207	0	0
6	U	204	Total O 204 204	0	0
6	V	245	Total O 245 245	0	0
6	W	227	Total O 227 227	0	0
6	X	210	Total O 210 210	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, middle subunit

Chain A:

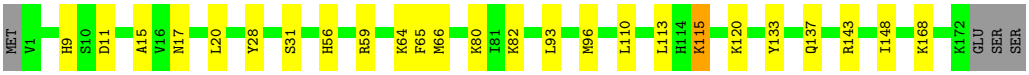


• Molecule 1: Ferritin, middle subunit

Chain B:

• Molecule 1: Ferritin, middle subunit

Chain C:



• Molecule 1: Ferritin, middle subunit

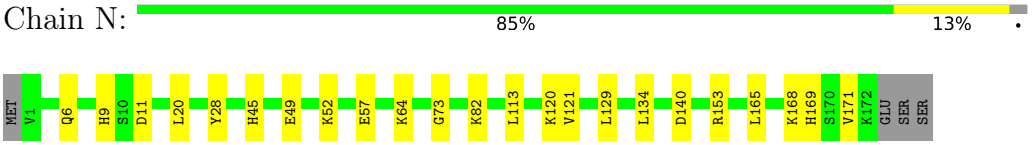
Chain D:

• Molecule 1: Ferritin, middle subunit

Chain M:

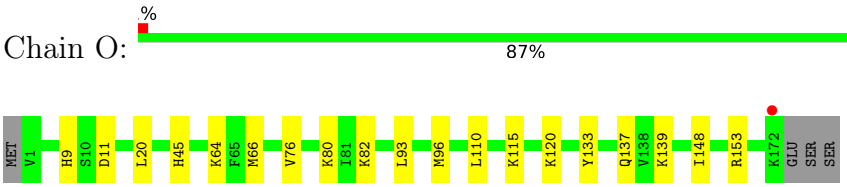
• Molecule 1: Ferritin, middle subunit

Chain N:



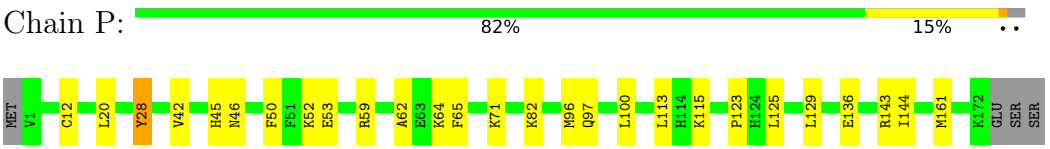
• Molecule 1: Ferritin, middle subunit

Chain O:



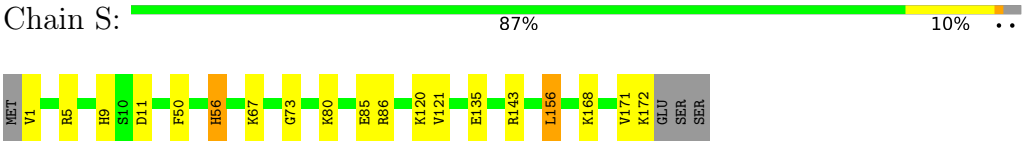
• Molecule 1: Ferritin, middle subunit

Chain P:



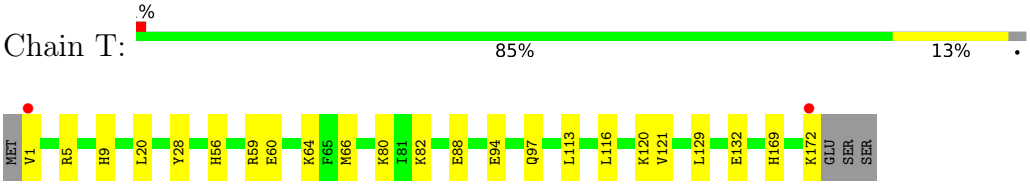
• Molecule 1: Ferritin, middle subunit

Chain S:



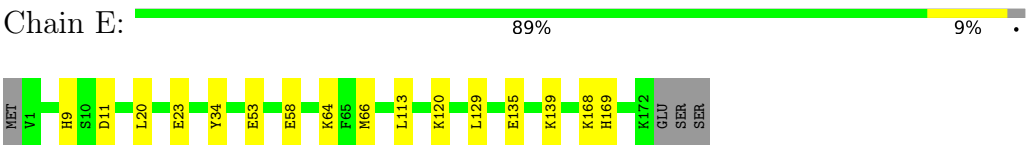
• Molecule 1: Ferritin, middle subunit

Chain T:



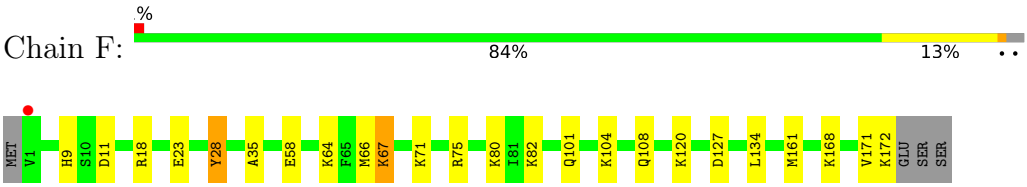
• Molecule 1: Ferritin, middle subunit

Chain E:



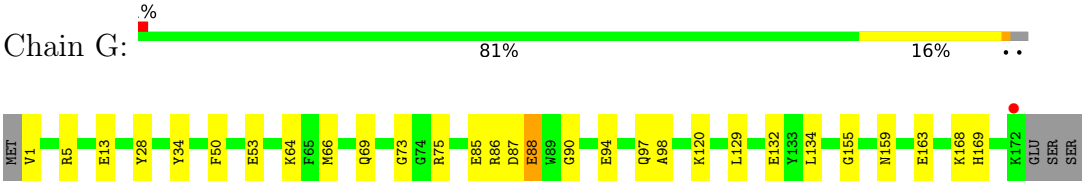
• Molecule 1: Ferritin, middle subunit

Chain F:



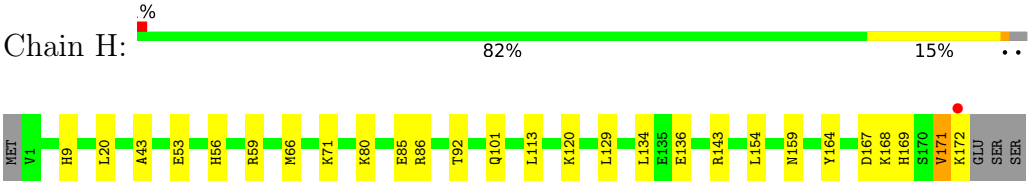
• Molecule 1: Ferritin, middle subunit

Chain G:



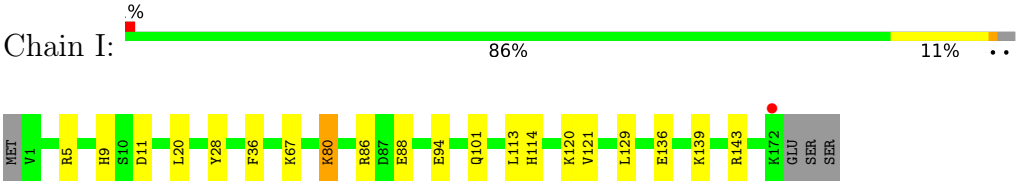
• Molecule 1: Ferritin, middle subunit

Chain H:



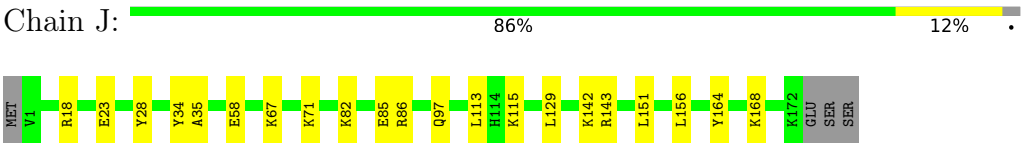
• Molecule 1: Ferritin, middle subunit

Chain I:



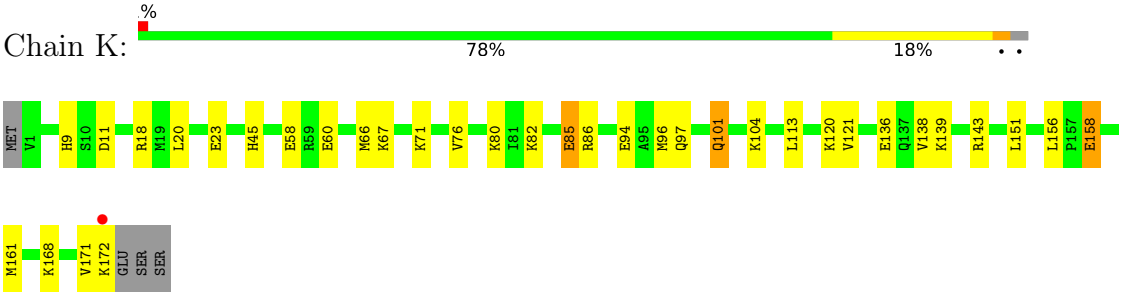
• Molecule 1: Ferritin, middle subunit

Chain J:



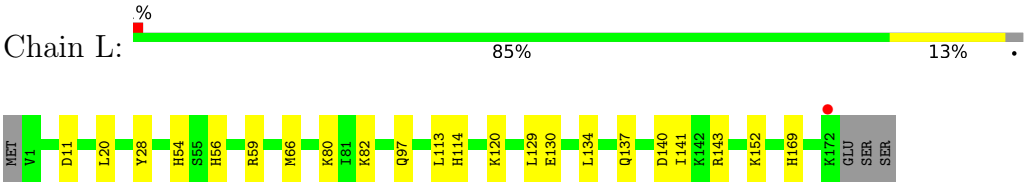
• Molecule 1: Ferritin, middle subunit

Chain K:



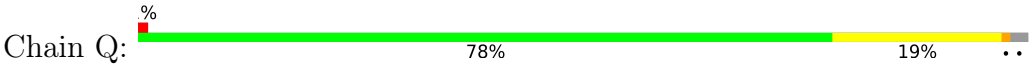
• Molecule 1: Ferritin, middle subunit

Chain L:

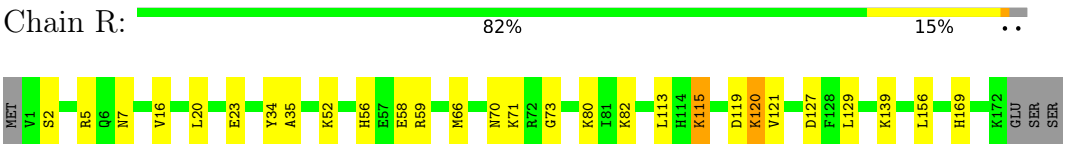


• Molecule 1: Ferritin, middle subunit

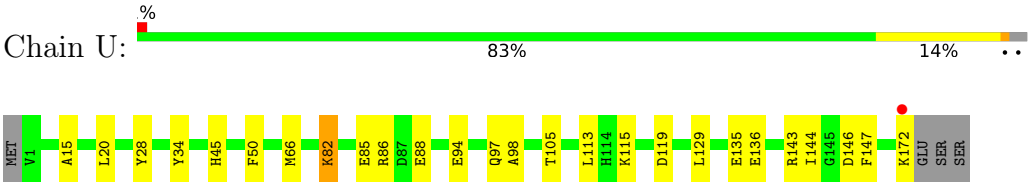
Chain Q:



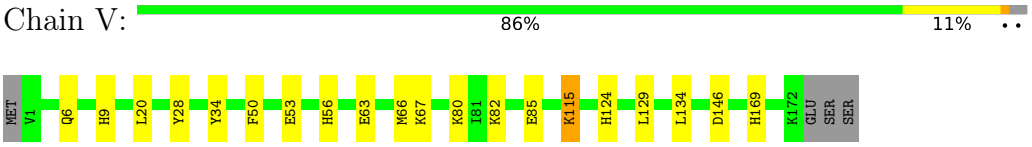
• Molecule 1: Ferritin, middle subunit



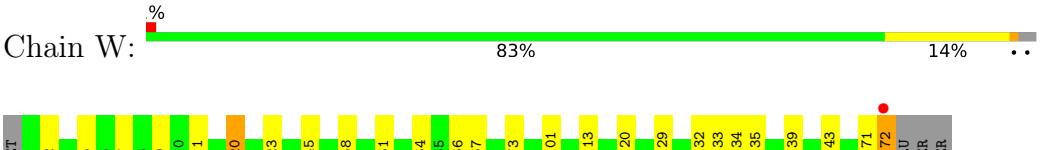
• Molecule 1: Ferritin, middle subunit



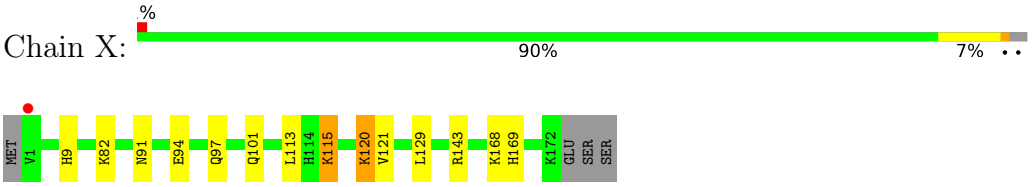
• Molecule 1: Ferritin, middle subunit



• Molecule 1: Ferritin, middle subunit



• Molecule 1: Ferritin, middle subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	238.93Å 238.43Å 119.69Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	75.35 – 1.91 75.35 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.7 (75.35-1.91) 96.7 (75.35-1.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.196 , 0.231 0.196 , 0.231	Depositor DCC
R_{free} test set	25123 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	9.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	40182	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.26% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, EDO, ACT

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	0.49	0/1513	0.65	1/2033 (0.0%)
1	B	0.51	0/1496	0.62	0/2011
1	C	0.53	0/1510	0.63	0/2030
1	D	0.51	0/1490	0.65	0/2003
1	E	0.51	0/1471	0.63	0/1978
1	F	0.51	0/1511	0.63	0/2029
1	G	0.51	0/1488	0.65	0/1998
1	H	0.50	0/1494	0.63	0/2007
1	I	0.51	0/1514	0.65	1/2033 (0.0%)
1	J	0.53	0/1492	0.66	0/2005
1	K	0.50	0/1511	0.60	0/2029
1	L	0.54	0/1488	0.64	0/2000
1	M	0.52	0/1461	0.62	1/1964 (0.1%)
1	N	0.49	0/1507	0.63	1/2025 (0.0%)
1	O	0.50	0/1476	0.63	1/1985 (0.1%)
1	P	0.51	0/1484	0.63	0/1994
1	Q	0.51	0/1502	0.63	0/2017
1	R	0.56	0/1485	0.66	0/1996
1	S	0.49	0/1510	0.62	1/2029 (0.0%)
1	T	0.51	0/1485	0.63	0/1996
1	U	0.52	0/1477	0.64	0/1983
1	V	0.54	0/1504	0.67	0/2021
1	W	0.50	0/1501	0.63	1/2017 (0.0%)
1	X	0.51	0/1469	0.62	0/1975
All	All	0.51	0/35839	0.63	7/48158 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	153	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	20	LEU	CA-CB-CG	5.64	128.28	115.30
1	W	20	LEU	CA-CB-CG	5.63	128.25	115.30
1	S	156	LEU	CA-CB-CG	-5.59	102.44	115.30
1	M	153	ARG	NE-CZ-NH2	-5.47	117.57	120.30

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	1460	0	1425	28	0
1	B	1452	0	1407	18	0
1	C	1460	0	1424	37	0
1	D	1446	0	1403	17	0
1	E	1436	0	1389	17	0
1	F	1461	0	1432	31	0
1	G	1451	0	1415	28	0
1	H	1447	0	1416	34	0
1	I	1461	0	1436	19	0
1	J	1445	0	1411	22	0
1	K	1464	0	1433	44	0
1	L	1441	0	1408	23	0
1	M	1426	0	1385	14	0
1	N	1457	0	1421	16	0
1	O	1432	0	1393	13	0
1	P	1441	0	1406	33	0
1	Q	1452	0	1429	49	0
1	R	1447	0	1408	41	0
1	S	1459	0	1421	21	0
1	T	1444	0	1410	20	0
1	U	1437	0	1413	27	0
1	V	1457	0	1418	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1453	0	1418	24	0
1	X	1431	0	1389	13	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	2	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	I	5	0	0	0	0
2	J	10	0	0	2	0
2	K	10	0	0	1	0
2	L	5	0	0	2	0
2	N	10	0	0	2	0
2	O	5	0	0	0	0
2	P	5	0	0	1	0
2	R	10	0	0	3	0
2	T	10	0	0	1	0
2	U	5	0	0	0	0
2	W	10	0	0	3	0
3	A	4	0	6	2	0
3	B	12	0	18	4	0
3	C	12	0	18	0	0
3	D	4	0	6	1	0
3	E	8	0	12	4	0
3	F	8	0	12	3	0
3	G	28	0	42	12	0
3	I	8	0	12	4	0
3	J	8	0	12	5	0
3	K	8	0	12	2	0
3	L	8	0	12	1	0
3	M	4	0	6	0	0
3	N	12	0	18	7	0
3	O	4	0	6	0	0
3	P	12	0	18	5	0
3	Q	8	0	12	5	0
3	R	16	0	24	9	0
3	S	12	0	18	5	0
3	T	4	0	6	2	0
3	U	4	0	6	0	0
3	V	8	0	12	3	0
3	W	4	0	6	7	0
3	X	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	3	4	0
4	Q	4	0	3	1	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	F	2	0	0	0	0
5	G	3	0	0	1	0
5	H	1	0	0	1	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	L	2	0	0	0	0
5	M	1	0	0	0	0
5	O	2	0	0	0	0
5	Q	1	0	0	0	0
5	S	1	0	0	1	0
5	T	2	0	0	0	0
5	U	2	0	0	1	0
5	W	1	0	0	1	0
5	X	3	0	0	0	0
6	A	214	0	0	11	0
6	B	211	0	0	5	0
6	C	203	0	0	8	0
6	D	193	0	0	10	0
6	E	205	0	0	7	0
6	F	229	0	0	14	0
6	G	210	0	0	7	0
6	H	194	0	0	11	0
6	I	224	0	0	3	0
6	J	231	0	0	5	0
6	K	199	0	0	16	0
6	L	209	0	0	11	0
6	M	208	0	0	5	0
6	N	194	0	0	8	0
6	O	210	0	0	6	0
6	P	191	0	0	19	0
6	Q	203	0	0	23	0
6	R	207	0	0	3	0
6	S	226	0	0	8	0
6	T	207	0	0	3	0
6	U	204	0	0	11	0
6	V	245	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	W	227	0	0	3	0
6	X	210	0	0	6	0
All	All	40182	0	34222	573	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 8.

The worst 5 of 573 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:20[B]:LEU:CD2	1:C:65:PHE:HB3	1.78	1.11
1:F:171:VAL:HG11	6:F:524:HOH:O	1.50	1.09
1:C:148:ILE:HG12	6:C:451:HOH:O	1.52	1.07
1:J:115:LYS:HD2	6:J:525:HOH:O	1.52	1.07
1:R:80:LYS:HE3	1:R:82[A]:LYS:HE2	1.32	1.05

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	179/176 (102%)	176 (98%)	3 (2%)	0	100	100
1	B	176/176 (100%)	172 (98%)	4 (2%)	0	100	100
1	C	178/176 (101%)	175 (98%)	3 (2%)	0	100	100
1	D	176/176 (100%)	172 (98%)	4 (2%)	0	100	100
1	E	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
1	F	178/176 (101%)	175 (98%)	3 (2%)	0	100	100
1	G	175/176 (99%)	173 (99%)	2 (1%)	0	100	100
1	H	176/176 (100%)	172 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	178/176 (101%)	174 (98%)	4 (2%)	0	100	100
1	J	176/176 (100%)	172 (98%)	4 (2%)	0	100	100
1	K	178/176 (101%)	174 (98%)	4 (2%)	0	100	100
1	L	176/176 (100%)	173 (98%)	3 (2%)	0	100	100
1	M	172/176 (98%)	169 (98%)	3 (2%)	0	100	100
1	N	178/176 (101%)	175 (98%)	3 (2%)	0	100	100
1	O	175/176 (99%)	171 (98%)	4 (2%)	0	100	100
1	P	175/176 (99%)	171 (98%)	4 (2%)	0	100	100
1	Q	177/176 (101%)	175 (99%)	2 (1%)	0	100	100
1	R	175/176 (99%)	173 (99%)	2 (1%)	0	100	100
1	S	178/176 (101%)	175 (98%)	3 (2%)	0	100	100
1	T	175/176 (99%)	170 (97%)	5 (3%)	0	100	100
1	U	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
1	V	178/176 (101%)	174 (98%)	4 (2%)	0	100	100
1	W	177/176 (101%)	172 (97%)	5 (3%)	0	100	100
1	X	173/176 (98%)	169 (98%)	4 (2%)	0	100	100
All	All	4227/4224 (100%)	4143 (98%)	84 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	160/157 (102%)	160 (100%)	0	100	100
1	B	158/157 (101%)	156 (99%)	2 (1%)	69	66
1	C	160/157 (102%)	157 (98%)	3 (2%)	57	51
1	D	157/157 (100%)	153 (98%)	4 (2%)	47	39
1	E	155/157 (99%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	160/157 (102%)	157 (98%)	3 (2%)	57	51
1	G	158/157 (101%)	152 (96%)	6 (4%)	33	22
1	H	159/157 (101%)	156 (98%)	3 (2%)	57	51
1	I	161/157 (102%)	159 (99%)	2 (1%)	71	69
1	J	158/157 (101%)	155 (98%)	3 (2%)	57	51
1	K	161/157 (102%)	155 (96%)	6 (4%)	34	23
1	L	157/157 (100%)	155 (99%)	2 (1%)	69	66
1	M	154/157 (98%)	151 (98%)	3 (2%)	57	51
1	N	160/157 (102%)	157 (98%)	3 (2%)	57	51
1	O	156/157 (99%)	154 (99%)	2 (1%)	69	66
1	P	157/157 (100%)	155 (99%)	2 (1%)	69	66
1	Q	160/157 (102%)	156 (98%)	4 (2%)	47	39
1	R	156/157 (99%)	153 (98%)	3 (2%)	57	51
1	S	159/157 (101%)	155 (98%)	4 (2%)	47	39
1	T	157/157 (100%)	156 (99%)	1 (1%)	86	86
1	U	157/157 (100%)	153 (98%)	4 (2%)	47	39
1	V	159/157 (101%)	155 (98%)	4 (2%)	47	39
1	W	159/157 (101%)	156 (98%)	3 (2%)	57	51
1	X	155/157 (99%)	153 (99%)	2 (1%)	69	66
All	All	3793/3768 (101%)	3724 (98%)	69 (2%)	59	53

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	82	LYS
1	U	172	LYS
1	W	134	LEU
1	F	28	TYR
1	T	28	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	97	GLN

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Mol	Chain	Res	Type
1	L	45	HIS
1	H	159	ASN
1	J	97	GLN
1	Q	97	GLN

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)

Of 109 ligands modelled in this entry, 31 are monoatomic - leaving 78 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	EDO	X	204	-	3,3,3	0.54	0	2,2,2	0.32	0
2	SO4	N	202	-	4,4,4	0.29	0	6,6,6	0.20	0
2	SO4	H	202	-	4,4,4	0.29	0	6,6,6	0.19	0
3	EDO	E	205	-	3,3,3	0.34	0	2,2,2	0.56	0
2	SO4	U	201	-	4,4,4	0.30	0	6,6,6	0.14	0
3	EDO	G	210	-	3,3,3	0.44	0	2,2,2	0.58	0
3	EDO	B	203	-	3,3,3	0.33	0	2,2,2	0.63	0
3	EDO	G	211	-	3,3,3	0.30	0	2,2,2	0.54	0
3	EDO	F	204	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	A	202	-	3,3,3	0.47	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	L	205	-	3,3,3	0.54	0	2,2,2	0.11	0
2	SO4	G	201	-	4,4,4	0.26	0	6,6,6	0.12	0
3	EDO	C	205	-	3,3,3	0.41	0	2,2,2	0.50	0
3	EDO	K	203	-	3,3,3	0.37	0	2,2,2	0.83	0
3	EDO	J	205	-	3,3,3	0.40	0	2,2,2	0.46	0
2	SO4	T	202	-	4,4,4	0.30	0	6,6,6	0.21	0
3	EDO	G	207	-	3,3,3	0.34	0	2,2,2	0.60	0
2	SO4	R	201	-	4,4,4	0.18	0	6,6,6	0.24	0
3	EDO	O	204	-	3,3,3	0.49	0	2,2,2	0.29	0
4	ACT	Q	204	-	3,3,3	0.85	0	3,3,3	0.75	0
3	EDO	T	205	-	3,3,3	0.37	0	2,2,2	0.60	0
3	EDO	G	209	-	3,3,3	0.48	0	2,2,2	0.18	0
2	SO4	W	201	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	P	201	-	4,4,4	0.32	0	6,6,6	0.17	0
3	EDO	U	204	-	3,3,3	0.44	0	2,2,2	0.55	0
2	SO4	L	201	-	4,4,4	0.18	0	6,6,6	0.37	0
3	EDO	P	203	-	3,3,3	0.52	0	2,2,2	0.25	0
3	EDO	I	204	-	3,3,3	0.47	0	2,2,2	0.56	0
3	EDO	Q	203	-	3,3,3	0.55	0	2,2,2	0.26	0
2	SO4	N	201	-	4,4,4	0.31	0	6,6,6	0.18	0
3	EDO	W	204	-	3,3,3	0.29	0	2,2,2	0.62	0
3	EDO	L	204	-	3,3,3	0.63	0	2,2,2	0.20	0
2	SO4	T	201	-	4,4,4	0.35	0	6,6,6	0.20	0
3	EDO	R	204	-	3,3,3	0.35	0	2,2,2	0.65	0
3	EDO	S	204	-	3,3,3	0.39	0	2,2,2	0.53	0
2	SO4	D	202	-	4,4,4	0.33	0	6,6,6	0.22	0
3	EDO	C	203	-	3,3,3	0.51	0	2,2,2	0.44	0
2	SO4	J	201	-	4,4,4	0.26	0	6,6,6	0.22	0
3	EDO	M	202	-	3,3,3	0.56	0	2,2,2	0.19	0
3	EDO	V	201	-	3,3,3	0.41	0	2,2,2	0.45	0
3	EDO	K	204	-	3,3,3	0.55	0	2,2,2	0.28	0
3	EDO	P	202	-	3,3,3	0.47	0	2,2,2	0.20	0
2	SO4	D	201	-	4,4,4	0.27	0	6,6,6	0.30	0
2	SO4	J	202	-	4,4,4	0.38	0	6,6,6	0.14	0
3	EDO	Q	202	-	3,3,3	0.38	0	2,2,2	0.55	0
3	EDO	E	204	-	3,3,3	0.53	0	2,2,2	0.06	0
3	EDO	X	205	-	3,3,3	0.43	0	2,2,2	0.43	0
2	SO4	R	202	-	4,4,4	0.32	0	6,6,6	0.11	0
3	EDO	J	204	-	3,3,3	0.34	0	2,2,2	0.65	0
3	EDO	D	205	-	3,3,3	0.43	0	2,2,2	0.29	0
2	SO4	C	201	-	4,4,4	0.37	0	6,6,6	0.23	0
3	EDO	N	203	-	3,3,3	0.29	0	2,2,2	0.35	0
2	SO4	K	202	-	4,4,4	0.39	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	F	205	-	3,3,3	0.50	0	2,2,2	0.43	0
3	EDO	S	202	-	3,3,3	0.40	0	2,2,2	0.39	0
2	SO4	W	202	-	4,4,4	0.33	0	6,6,6	0.14	0
3	EDO	P	204	-	3,3,3	0.48	0	2,2,2	0.27	0
3	EDO	B	204	-	3,3,3	0.38	0	2,2,2	0.16	0
2	SO4	I	201	-	4,4,4	0.35	0	6,6,6	0.12	0
3	EDO	G	208	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	B	205	-	3,3,3	0.36	0	2,2,2	0.51	0
3	EDO	N	204	-	3,3,3	0.58	0	2,2,2	0.17	0
3	EDO	N	205	-	3,3,3	0.41	0	2,2,2	0.36	0
3	EDO	R	206	-	3,3,3	0.36	0	2,2,2	0.51	0
2	SO4	F	201	-	4,4,4	0.38	0	6,6,6	0.20	0
3	EDO	I	203	-	3,3,3	0.26	0	2,2,2	0.88	0
3	EDO	G	206	-	3,3,3	0.40	0	2,2,2	0.49	0
3	EDO	C	204	-	3,3,3	0.56	0	2,2,2	0.10	0
3	EDO	R	205	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	V	202	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	R	203	-	3,3,3	0.54	0	2,2,2	0.22	0
4	ACT	A	203	-	3,3,3	0.61	0	3,3,3	1.22	0
3	EDO	S	203	-	3,3,3	0.40	0	2,2,2	0.62	0
2	SO4	K	201	-	4,4,4	0.20	0	6,6,6	0.20	0
2	SO4	H	201	-	4,4,4	0.34	0	6,6,6	0.13	0
3	EDO	G	205	-	3,3,3	0.51	0	2,2,2	0.74	0
2	SO4	O	201	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	A	201	-	4,4,4	0.34	0	6,6,6	0.15	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	EDO	X	204	-	-	0/1/1/1	-
3	EDO	P	202	-	-	0/1/1/1	-
3	EDO	B	204	-	-	1/1/1/1	-
3	EDO	T	205	-	-	0/1/1/1	-
3	EDO	G	209	-	-	1/1/1/1	-
3	EDO	E	205	-	-	1/1/1/1	-
3	EDO	Q	202	-	-	0/1/1/1	-
3	EDO	U	204	-	-	0/1/1/1	-
3	EDO	E	204	-	-	1/1/1/1	-
3	EDO	P	203	-	-	0/1/1/1	-
3	EDO	G	210	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	X	205	-	-	0/1/1/1	-
3	EDO	G	208	-	-	1/1/1/1	-
3	EDO	B	203	-	-	0/1/1/1	-
3	EDO	B	205	-	-	0/1/1/1	-
3	EDO	G	211	-	-	1/1/1/1	-
3	EDO	J	204	-	-	1/1/1/1	-
3	EDO	I	204	-	-	0/1/1/1	-
3	EDO	N	204	-	-	1/1/1/1	-
3	EDO	F	204	-	-	1/1/1/1	-
3	EDO	N	205	-	-	1/1/1/1	-
3	EDO	D	205	-	-	1/1/1/1	-
3	EDO	Q	203	-	-	1/1/1/1	-
3	EDO	R	206	-	-	1/1/1/1	-
3	EDO	I	203	-	-	0/1/1/1	-
3	EDO	A	202	-	-	1/1/1/1	-
3	EDO	G	206	-	-	0/1/1/1	-
3	EDO	C	204	-	-	0/1/1/1	-
3	EDO	W	204	-	-	1/1/1/1	-
3	EDO	L	205	-	-	1/1/1/1	-
3	EDO	N	203	-	-	1/1/1/1	-
3	EDO	C	205	-	-	0/1/1/1	-
3	EDO	R	205	-	-	1/1/1/1	-
3	EDO	L	204	-	-	0/1/1/1	-
3	EDO	K	203	-	-	0/1/1/1	-
3	EDO	V	202	-	-	1/1/1/1	-
3	EDO	J	205	-	-	1/1/1/1	-
3	EDO	R	204	-	-	1/1/1/1	-
3	EDO	G	207	-	-	1/1/1/1	-
3	EDO	R	203	-	-	0/1/1/1	-
3	EDO	F	205	-	-	1/1/1/1	-
3	EDO	P	204	-	-	1/1/1/1	-
3	EDO	S	202	-	-	1/1/1/1	-
3	EDO	S	203	-	-	1/1/1/1	-
3	EDO	S	204	-	-	0/1/1/1	-
3	EDO	C	203	-	-	0/1/1/1	-
3	EDO	G	205	-	-	0/1/1/1	-
3	EDO	O	204	-	-	0/1/1/1	-
3	EDO	M	202	-	-	0/1/1/1	-
3	EDO	V	201	-	-	0/1/1/1	-
3	EDO	K	204	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	206	EDO	O1-C1-C2-O2
3	V	202	EDO	O1-C1-C2-O2
3	A	202	EDO	O1-C1-C2-O2
3	D	205	EDO	O1-C1-C2-O2
3	F	205	EDO	O1-C1-C2-O2

There are no ring outliers.

45 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	204	EDO	1	0
2	N	202	SO4	1	0
3	G	210	EDO	3	0
3	B	203	EDO	3	0
3	G	211	EDO	5	0
3	F	204	EDO	1	0
3	A	202	EDO	2	0
3	L	205	EDO	1	0
3	K	203	EDO	2	0
3	J	205	EDO	5	0
3	G	207	EDO	4	0
2	R	201	SO4	2	0
4	Q	204	ACT	1	0
3	T	205	EDO	2	0
2	W	201	SO4	2	0
2	P	201	SO4	1	0
2	L	201	SO4	2	0
3	P	203	EDO	1	0
3	I	204	EDO	1	0
2	N	201	SO4	1	0
3	W	204	EDO	7	0
2	T	201	SO4	1	0
3	R	204	EDO	1	0
2	J	201	SO4	2	0
3	V	201	EDO	2	0
3	P	202	EDO	3	0
2	D	201	SO4	2	0
3	Q	202	EDO	5	0
3	E	204	EDO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	202	SO4	1	0
3	D	205	EDO	1	0
3	N	203	EDO	4	0
3	F	205	EDO	2	0
3	S	202	EDO	5	0
2	W	202	SO4	1	0
3	P	204	EDO	1	0
3	B	204	EDO	1	0
3	N	204	EDO	1	0
3	N	205	EDO	2	0
3	R	206	EDO	7	0
3	I	203	EDO	3	0
3	R	205	EDO	1	0
3	V	202	EDO	1	0
4	A	203	ACT	4	0
2	K	201	SO4	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	172/176 (97%)	-0.09	0 100 100	3, 6, 12, 29	7 (4%)
1	B	172/176 (97%)	-0.10	0 100 100	2, 6, 11, 27	3 (1%)
1	C	172/176 (97%)	-0.02	0 100 100	3, 6, 13, 23	8 (4%)
1	D	172/176 (97%)	0.03	1 (0%) 89 90	4, 7, 14, 28	6 (3%)
1	E	172/176 (97%)	-0.13	0 100 100	3, 5, 12, 22	6 (3%)
1	F	172/176 (97%)	-0.02	1 (0%) 89 90	5, 7, 13, 36	10 (5%)
1	G	172/176 (97%)	-0.04	1 (0%) 89 90	3, 6, 12, 31	7 (4%)
1	H	172/176 (97%)	-0.04	1 (0%) 89 90	4, 6, 14, 34	6 (3%)
1	I	172/176 (97%)	-0.02	1 (0%) 89 90	3, 6, 12, 31	5 (2%)
1	J	172/176 (97%)	-0.10	0 100 100	3, 6, 11, 22	6 (3%)
1	K	172/176 (97%)	-0.00	1 (0%) 89 90	4, 6, 15, 29	4 (2%)
1	L	172/176 (97%)	-0.07	1 (0%) 89 90	3, 6, 11, 23	5 (2%)
1	M	172/176 (97%)	-0.10	1 (0%) 89 90	2, 6, 12, 19	10 (5%)
1	N	172/176 (97%)	-0.06	0 100 100	5, 7, 14, 32	5 (2%)
1	O	172/176 (97%)	-0.07	1 (0%) 89 90	3, 6, 12, 26	7 (4%)
1	P	172/176 (97%)	0.04	0 100 100	4, 7, 16, 32	11 (6%)
1	Q	172/176 (97%)	-0.04	1 (0%) 89 90	4, 6, 13, 30	5 (2%)
1	R	172/176 (97%)	-0.02	0 100 100	3, 6, 11, 20	7 (4%)
1	S	172/176 (97%)	-0.08	0 100 100	3, 6, 12, 29	3 (1%)
1	T	172/176 (97%)	-0.07	2 (1%) 79 81	2, 5, 12, 24	6 (3%)
1	U	172/176 (97%)	-0.03	1 (0%) 89 90	4, 6, 13, 32	8 (4%)
1	V	172/176 (97%)	-0.06	0 100 100	3, 6, 11, 27	7 (4%)
1	W	172/176 (97%)	-0.12	1 (0%) 89 90	3, 6, 12, 29	7 (4%)
1	X	172/176 (97%)	-0.06	1 (0%) 89 90	3, 6, 12, 25	8 (4%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4128/4224 (97%)	-0.05	15 (0%)	92	93	2, 6, 13, 36	157 (3%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	1	VAL	3.4
1	L	172	LYS	3.3
1	H	172	LYS	3.1
1	T	172	LYS	3.0
1	O	172	LYS	2.7

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 (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, 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	B-factors(Å^2)	Q<0.9
3	EDO	Q	203	4/4	0.69	0.31	23,24,24,25	0
3	EDO	G	208	4/4	0.72	0.24	29,32,32,34	0
3	EDO	K	204	4/4	0.75	0.24	23,24,24,24	0
3	EDO	R	204	4/4	0.76	0.18	28,29,29,30	0
3	EDO	A	202	4/4	0.77	0.17	27,27,28,28	0
3	EDO	C	205	4/4	0.77	0.20	23,24,24,27	0
3	EDO	E	204	4/4	0.78	0.21	25,28,28,29	0
3	EDO	Q	202	4/4	0.78	0.23	22,22,24,26	0
3	EDO	X	204	4/4	0.78	0.18	19,20,20,21	0
3	EDO	P	202	4/4	0.79	0.20	17,17,18,21	0
3	EDO	N	205	4/4	0.80	0.24	26,28,28,30	0
2	SO4	T	201	5/5	0.80	0.22	58,59,61,62	0
3	EDO	V	202	4/4	0.80	0.19	20,20,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	N	204	4/4	0.80	0.13	21,21,21,21	0
4	ACT	A	203	4/4	0.80	0.19	17,18,19,20	0
5	CL	G	204	1/1	0.82	0.12	46,46,46,46	0
3	EDO	P	203	4/4	0.84	0.14	22,22,23,24	0
3	EDO	R	205	4/4	0.84	0.16	29,29,30,30	0
3	EDO	F	205	4/4	0.85	0.14	24,25,25,25	0
3	EDO	B	205	4/4	0.85	0.19	23,25,26,26	0
3	EDO	K	203	4/4	0.85	0.28	25,25,26,26	0
3	EDO	X	205	4/4	0.86	0.17	29,30,31,31	0
3	EDO	B	204	4/4	0.86	0.19	20,20,20,23	0
3	EDO	I	203	4/4	0.86	0.28	20,22,25,27	0
3	EDO	I	204	4/4	0.87	0.24	20,20,20,21	0
3	EDO	G	206	4/4	0.87	0.10	31,33,34,35	0
3	EDO	S	204	4/4	0.87	0.19	30,32,34,39	0
3	EDO	T	205	4/4	0.87	0.26	23,24,24,25	0
3	EDO	S	203	4/4	0.88	0.26	18,21,22,25	0
3	EDO	J	205	4/4	0.88	0.20	26,26,27,27	0
3	EDO	U	204	4/4	0.88	0.21	25,26,26,26	0
3	EDO	C	204	4/4	0.88	0.17	14,14,15,15	0
3	EDO	B	203	4/4	0.88	0.16	27,28,28,32	0
3	EDO	L	205	4/4	0.88	0.18	17,17,18,20	0
3	EDO	G	209	4/4	0.88	0.13	28,30,30,31	0
3	EDO	P	204	4/4	0.88	0.20	25,25,26,27	0
3	EDO	N	203	4/4	0.89	0.23	17,19,20,21	0
2	SO4	T	202	5/5	0.89	0.18	31,34,34,35	0
3	EDO	S	202	4/4	0.89	0.25	16,19,19,23	0
3	EDO	L	204	4/4	0.89	0.17	11,12,12,12	0
5	CL	D	203	1/1	0.89	0.07	36,36,36,36	0
3	EDO	G	207	4/4	0.89	0.18	27,27,27,27	0
5	CL	X	201	1/1	0.89	0.11	45,45,45,45	0
3	EDO	G	210	4/4	0.91	0.14	14,14,14,15	0
5	CL	M	201	1/1	0.91	0.09	32,32,32,32	0
3	EDO	D	205	4/4	0.91	0.21	22,22,23,25	0
3	EDO	W	204	4/4	0.91	0.24	21,23,24,25	0
3	EDO	R	203	4/4	0.92	0.13	12,13,13,13	0
5	CL	F	202	1/1	0.92	0.07	35,35,35,35	0
2	SO4	K	202	5/5	0.92	0.14	38,39,40,40	0
3	EDO	V	201	4/4	0.92	0.20	17,18,19,19	0
2	SO4	J	202	5/5	0.93	0.15	35,36,38,38	0
2	SO4	N	202	5/5	0.93	0.18	45,45,47,48	0
2	SO4	F	201	5/5	0.93	0.18	30,31,32,32	0
4	ACT	Q	204	4/4	0.93	0.12	24,24,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	R	206	4/4	0.93	0.27	16,17,18,19	0
2	SO4	G	201	5/5	0.93	0.22	40,40,41,41	0
3	EDO	G	211	4/4	0.93	0.40	24,25,25,26	0
3	EDO	M	202	4/4	0.93	0.12	9,10,10,11	0
5	CL	Q	201	1/1	0.93	0.11	34,34,34,34	0
2	SO4	I	201	5/5	0.93	0.17	42,42,43,44	0
5	CL	X	203	1/1	0.93	0.14	37,37,37,37	0
2	SO4	A	201	5/5	0.94	0.16	45,45,47,47	0
3	EDO	J	204	4/4	0.94	0.25	14,15,15,15	0
5	CL	O	202	1/1	0.94	0.06	36,36,36,36	0
2	SO4	L	201	5/5	0.94	0.24	14,15,16,16	5
5	CL	F	203	1/1	0.94	0.12	40,40,40,40	0
3	EDO	F	204	4/4	0.94	0.13	24,25,25,25	0
2	SO4	W	202	5/5	0.94	0.21	34,34,36,37	0
3	EDO	G	205	4/4	0.94	0.12	7,7,7,8	0
5	CL	X	202	1/1	0.94	0.12	32,32,32,32	0
2	SO4	K	201	5/5	0.94	0.25	13,14,14,14	5
3	EDO	C	203	4/4	0.95	0.12	10,11,11,12	0
3	EDO	E	205	4/4	0.95	0.14	25,26,27,27	0
2	SO4	C	201	5/5	0.95	0.17	36,37,39,39	0
5	CL	L	203	1/1	0.95	0.18	38,38,38,38	0
2	SO4	P	201	5/5	0.95	0.11	38,41,41,42	0
2	SO4	R	201	5/5	0.95	0.28	15,16,17,17	5
2	SO4	H	201	5/5	0.95	0.12	39,39,41,41	0
5	CL	T	204	1/1	0.95	0.12	40,40,40,40	0
2	SO4	U	201	5/5	0.96	0.17	30,32,32,32	0
5	CL	D	204	1/1	0.96	0.12	38,38,38,38	0
5	CL	L	202	1/1	0.96	0.14	32,32,32,32	0
2	SO4	W	201	5/5	0.96	0.22	22,25,26,26	0
2	SO4	J	201	5/5	0.96	0.17	22,24,25,26	0
2	SO4	H	202	5/5	0.96	0.18	32,33,34,35	0
5	CL	E	203	1/1	0.96	0.10	31,31,31,31	0
2	SO4	R	202	5/5	0.96	0.12	39,40,41,42	0
2	SO4	N	201	5/5	0.97	0.16	31,31,31,31	0
5	CL	I	202	1/1	0.97	0.10	31,31,31,31	0
5	CL	O	203	1/1	0.97	0.11	38,38,38,38	0
5	CL	B	201	1/1	0.97	0.12	29,29,29,29	0
5	CL	E	202	1/1	0.97	0.08	39,39,39,39	0
5	CL	U	202	1/1	0.97	0.08	27,27,27,27	0
2	SO4	D	201	5/5	0.97	0.21	16,18,19,19	5
2	SO4	O	201	5/5	0.97	0.14	38,38,40,40	0
2	SO4	D	202	5/5	0.97	0.14	32,32,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	C	202	1/1	0.98	0.10	31,31,31,31	0
5	CL	G	202	1/1	0.98	0.14	36,36,36,36	0
3	EDO	O	204	4/4	0.98	0.08	11,11,11,11	0
5	CL	U	203	1/1	0.98	0.10	38,38,38,38	0
5	CL	W	203	1/1	0.98	0.11	24,24,24,24	0
5	CL	H	203	1/1	0.98	0.05	38,38,38,38	0
5	CL	B	202	1/1	0.98	0.12	23,23,23,23	0
5	CL	S	201	1/1	0.98	0.11	25,25,25,25	0
5	CL	T	203	1/1	0.99	0.13	23,23,23,23	0
5	CL	G	203	1/1	0.99	0.09	24,24,24,24	0
5	CL	J	203	1/1	0.99	0.18	30,30,30,30	0
5	CL	E	201	1/1	0.99	0.10	29,29,29,29	1

6.5 Other polymers (i)

There are no such residues in this entry.