



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 10:51 pm BST

PDB ID : 4DAS
Title : Crystal structure of Bullfrog M ferritin
Authors : Bertini, I.; Lalli, D.; Mangani, S.; Pozzi, C.; Rosa, C.; Turano, P.
Deposited on : 2012-01-13
Resolution : 2.56 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 ⓘ symbol.

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

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

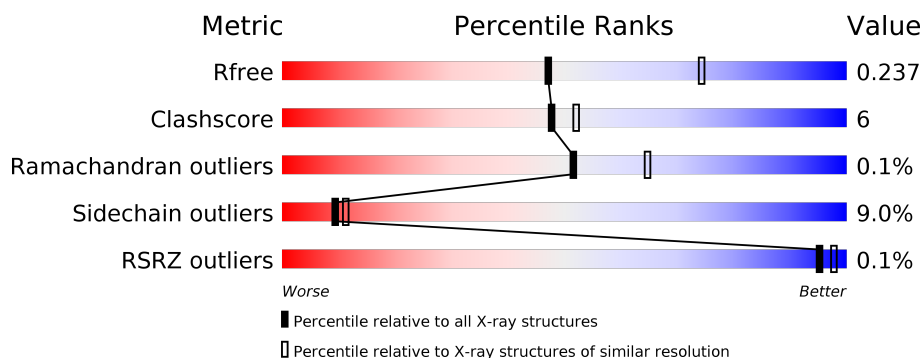
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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.




















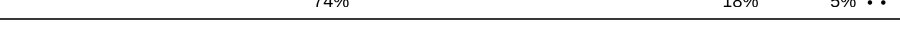
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	176	<div> <div>77%</div> <div>19%</div> <div>...</div> </div>
1	B	176	<div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	C	176	<div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	D	176	<div> <div>%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	E	176	<div> <div>%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	F	176	<div> <div>76%</div> <div>19%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	176	 80% 15% ...
1	H	176	 82% 15% ..
1	I	176	 % 79% 15% ...
1	J	176	 82% 13% ..
1	K	176	 84% 14% ..
1	L	176	 76% 20% ..
1	M	176	 % 79% 17% ..
1	N	176	 76% 18% ...
1	O	176	 79% 15% ..
1	P	176	 82% 14% ..
1	Q	176	 80% 17% ..
1	R	176	 73% 23% ..
1	S	176	 77% 18% ..
1	T	176	 % 85% 13% ..
1	U	176	 81% 13% ..
1	V	176	 77% 17% ...
1	W	176	 74% 18% 5% ..
1	X	176	 78% 16% ..

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	PGE	R	202	-	-	X	-
3	EDO	U	203	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35835 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.

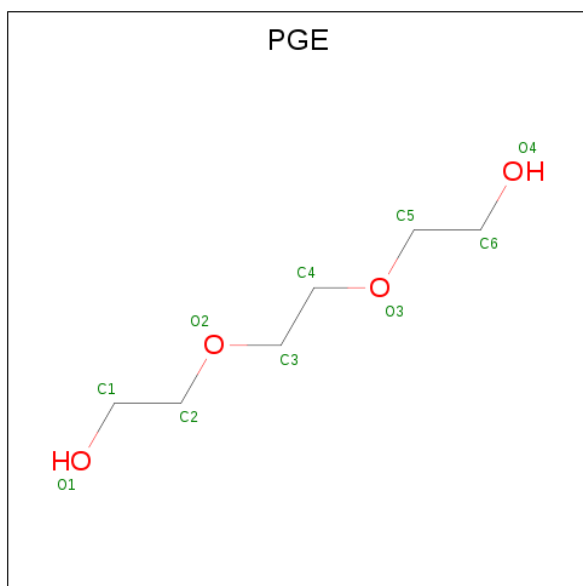
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	B	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	C	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	D	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	E	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	F	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	G	172	Total	C	N	O	S	0	0	0
			1415	891	246	271	7			
1	H	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	I	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	J	172	Total	C	N	O	S	0	0	0
			1415	890	246	272	7			
1	K	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	L	172	Total	C	N	O	S	0	0	0
			1415	891	247	270	7			
1	M	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	N	172	Total	C	N	O	S	0	0	0
			1415	891	247	270	7			
1	O	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	P	172	Total	C	N	O	S	0	0	0
			1414	890	246	271	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	R	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	S	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	T	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	U	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	V	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	X	172	Total	C	N	O	S	0	0	0
			1415	891	247	270	7			
1	W	173	Total	C	N	O	S	0	0	0
			1423	896	247	272	8			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			10	6	4		
2	E	1	Total	C	O	0	0
			10	6	4		
2	F	1	Total	C	O	0	0
			10	6	4		
2	G	1	Total	C	O	0	0
			10	6	4		
2	G	1	Total	C	O	0	0
			10	6	4		
2	H	1	Total	C	O	0	0
			10	6	4		
2	H	1	Total	C	O	0	0
			10	6	4		
2	I	1	Total	C	O	0	0
			10	6	4		
2	P	1	Total	C	O	0	0
			10	6	4		
2	Q	1	Total	C	O	0	0
			10	6	4		
2	Q	1	Total	C	O	0	0
			10	6	4		
2	R	1	Total	C	O	0	0
			10	6	4		
2	R	1	Total	C	O	0	0
			10	6	4		
2	R	1	Total	C	O	0	0
			10	6	4		
2	S	1	Total	C	O	0	0
			10	6	4		
2	U	1	Total	C	O	0	0
			10	6	4		
2	X	1	Total	C	O	0	0
			10	6	4		
2	W	1	Total	C	O	0	0
			10	6	4		
2	W	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	L	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	O	1	Total	C	O	0	0
			4	2	2		
3	P	1	Total	C	O	0	0
			4	2	2		
3	T	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0
4	B	46	Total O 46 46	0	0
4	C	68	Total O 68 68	0	0
4	D	68	Total O 68 68	0	0
4	E	49	Total O 49 49	0	0
4	F	52	Total O 52 52	0	0
4	G	69	Total O 69 69	0	0
4	H	70	Total O 70 70	0	0
4	I	51	Total O 51 51	0	0
4	J	78	Total O 78 78	0	0
4	K	85	Total O 85 85	0	0
4	L	48	Total O 48 48	0	0
4	M	52	Total O 52 52	0	0
4	N	72	Total O 72 72	0	0
4	O	82	Total O 82 82	0	0
4	P	62	Total O 62 62	0	0
4	Q	71	Total O 71 71	0	0
4	R	73	Total O 73 73	0	0
4	S	60	Total O 60 60	0	0
4	T	36	Total O 36 36	0	0
4	U	63	Total O 63 63	0	0
4	V	38	Total O 38 38	0	0

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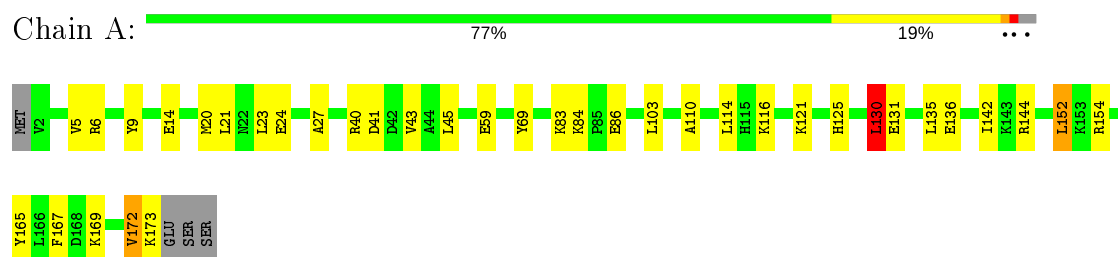
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	87	Total	O	0	0
			87	87		
4	W	71	Total	O	0	0
			71	71		

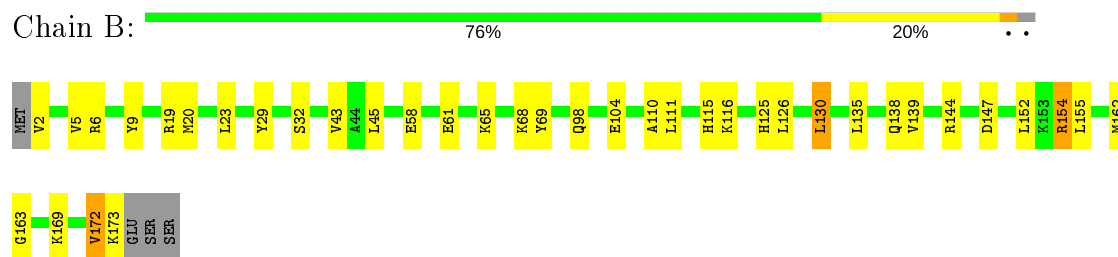
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

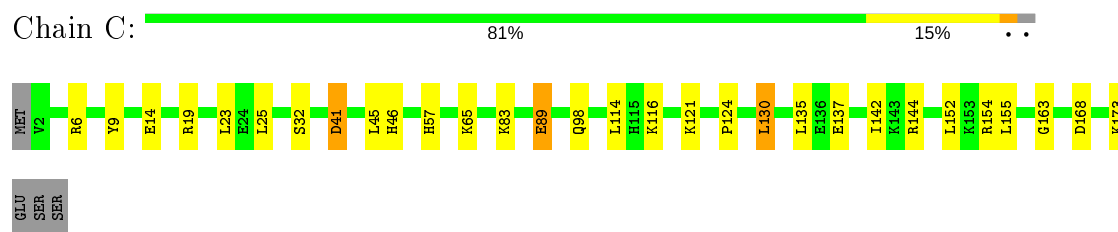
- Molecule 1: Ferritin, middle subunit



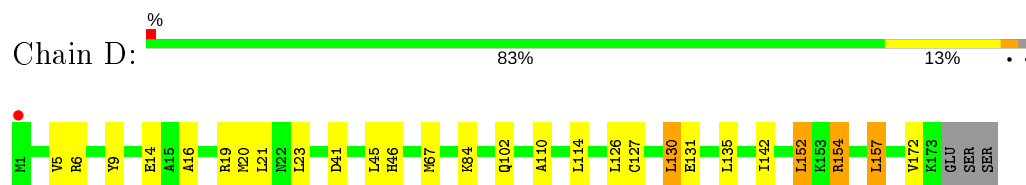
- Molecule 1: Ferritin, middle subunit



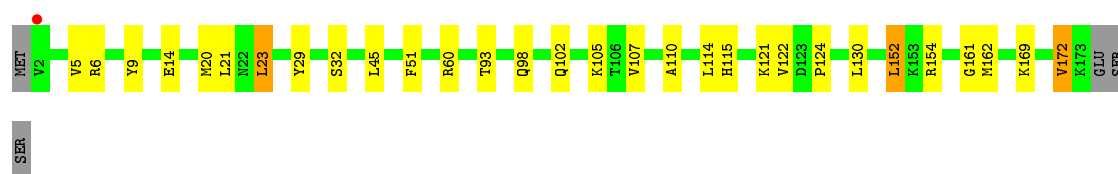
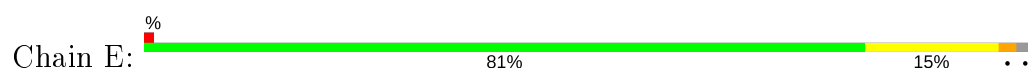
- Molecule 1: Ferritin, middle subunit



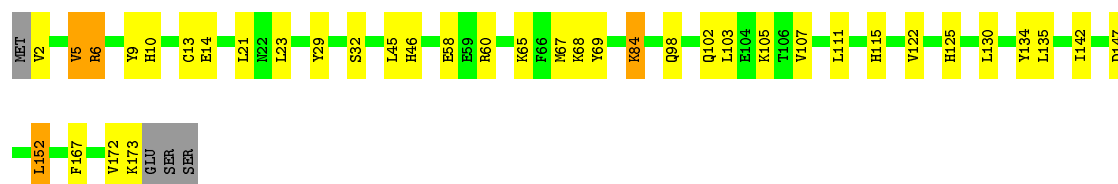
- Molecule 1: Ferritin, middle subunit



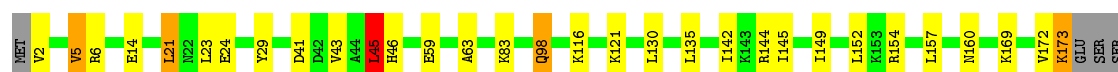
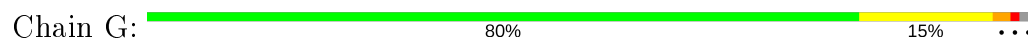
- Molecule 1: Ferritin, middle subunit



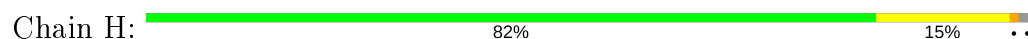
- Molecule 1: Ferritin, middle subunit



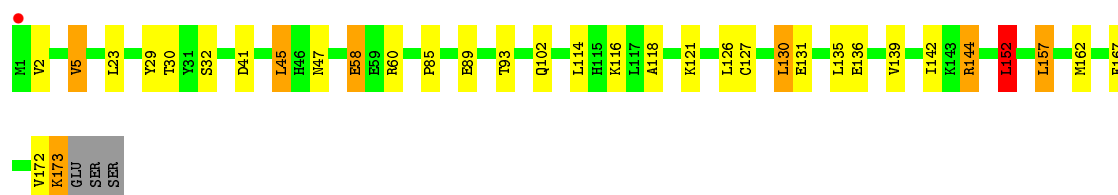
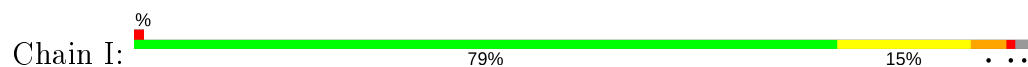
- Molecule 1: Ferritin, middle subunit



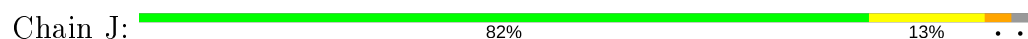
- Molecule 1: Ferritin, middle subunit




- Molecule 1: Ferritin, middle subunit

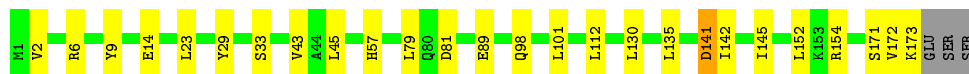


- Molecule 1: Ferritin, middle subunit



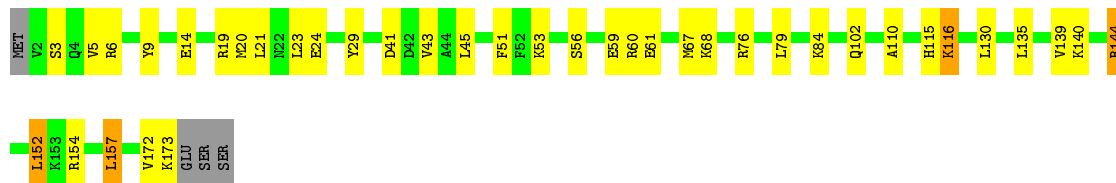
- Molecule 1: Ferritin, middle subunit

Chain K:  84% 14% ..




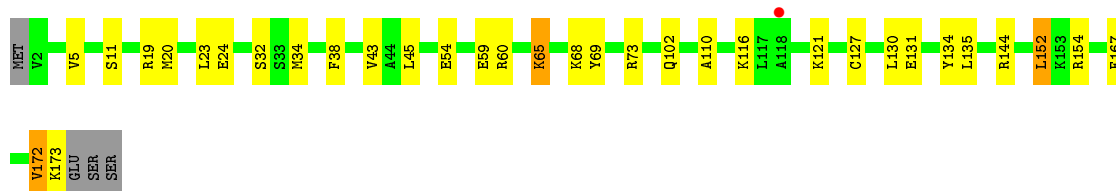
- Molecule 1: Ferritin, middle subunit

Chain L:  76% 20% ..



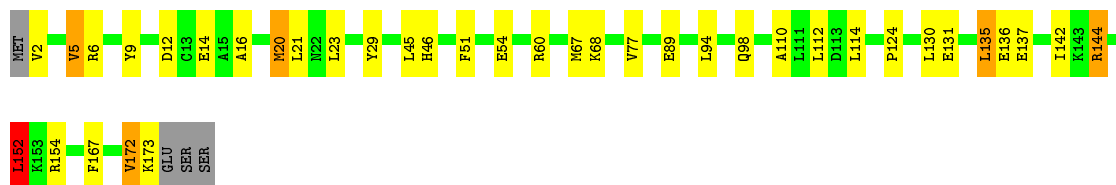
- Molecule 1: Ferritin, middle subunit

Chain M:  79% 17% ..




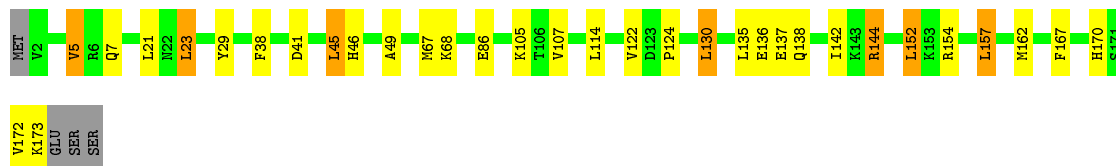
- Molecule 1: Ferritin, middle subunit

Chain N:  76% 18% ...




- Molecule 1: Ferritin, middle subunit

Chain O:  79% 15% ..




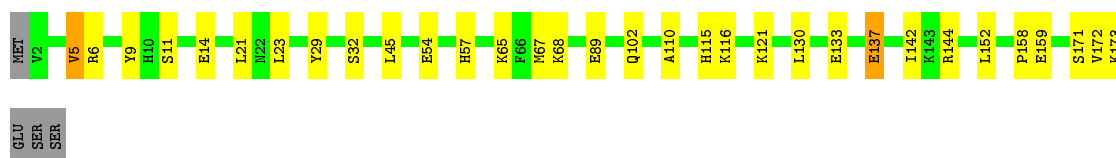
- Molecule 1: Ferritin, middle subunit

Chain P:  82% 14% ..



- Molecule 1: Ferritin, middle subunit

Chain Q:  80% 17% ..




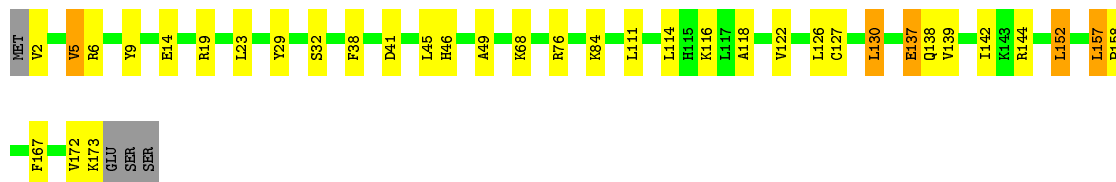
- Molecule 1: Ferritin, middle subunit

Chain R:  73% 23% ..




- Molecule 1: Ferritin, middle subunit

Chain S:  77% 18% ..




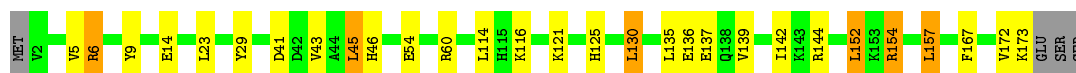
- Molecule 1: Ferritin, middle subunit

Chain T:  85% 13% ..




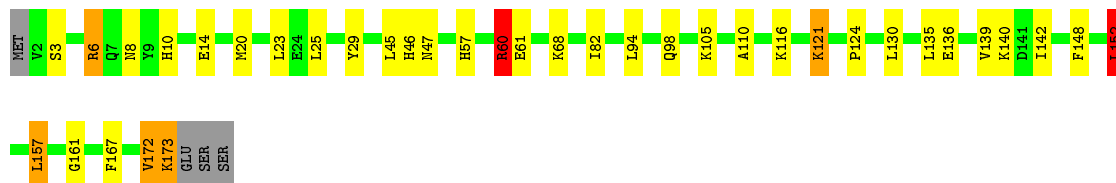
- Molecule 1: Ferritin, middle subunit

Chain U:  81% 13% ..




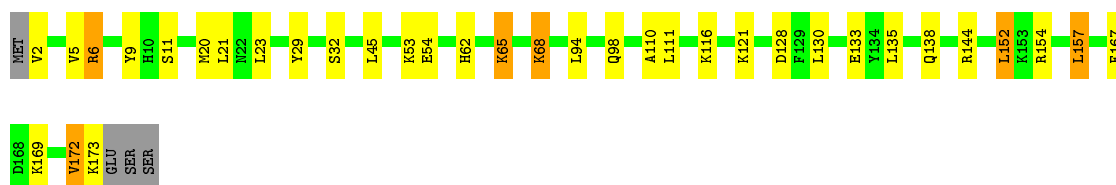
- Molecule 1: Ferritin, middle subunit

Chain V:  77% 17% ...



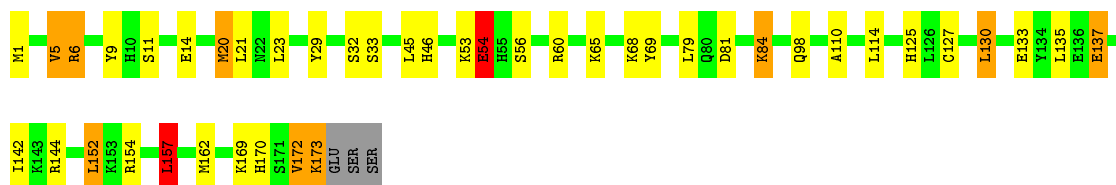
- Molecule 1: Ferritin, middle subunit

Chain X:  78% 16% ..



- Molecule 1: Ferritin, middle subunit

Chain W:  74% 18% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.95Å 210.95Å 323.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.51 – 2.56 79.51 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.5 (79.51-2.56) 97.5 (79.51-2.56)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.239 0.187 , 0.237	Depositor DCC
R_{free} test set	13045 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35835	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.89	1/1442 (0.1%)	0.85	3/1939 (0.2%)
1	B	0.84	1/1446 (0.1%)	0.85	1/1944 (0.1%)
1	C	0.86	0/1446	0.84	0/1944
1	D	0.96	0/1454	0.89	1/1954 (0.1%)
1	E	0.81	0/1442	0.80	0/1939
1	F	0.85	0/1442	0.78	0/1939
1	G	0.83	0/1443	0.82	1/1940 (0.1%)
1	H	0.84	0/1454	0.83	0/1954
1	I	0.84	2/1454 (0.1%)	0.83	3/1954 (0.2%)
1	J	0.92	2/1443 (0.1%)	0.86	1/1941 (0.1%)
1	K	0.90	0/1454	0.85	1/1954 (0.1%)
1	L	0.80	0/1443	0.79	0/1940
1	M	0.79	0/1446	0.81	0/1944
1	N	0.87	1/1443 (0.1%)	0.82	2/1940 (0.1%)
1	O	0.85	0/1446	0.81	1/1944 (0.1%)
1	P	0.85	0/1442	0.84	2/1939 (0.1%)
1	Q	0.88	1/1446 (0.1%)	0.82	0/1944
1	R	0.92	1/1446 (0.1%)	0.91	3/1944 (0.2%)
1	S	0.82	1/1442 (0.1%)	0.75	0/1939
1	T	0.86	0/1454	0.81	0/1954
1	U	0.89	2/1446 (0.1%)	0.89	3/1944 (0.2%)
1	V	0.86	1/1446 (0.1%)	0.89	3/1944 (0.2%)
1	W	0.94	3/1451 (0.2%)	0.86	5/1950 (0.3%)
1	X	0.90	1/1443 (0.1%)	0.84	1/1940 (0.1%)
All	All	0.87	17/34714 (0.0%)	0.84	31/46668 (0.1%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	86	GLU	CG-CD	5.91	1.60	1.51
1	I	136	GLU	CG-CD	5.75	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	GLU	CG-CD	5.70	1.60	1.51
1	U	136	GLU	CG-CD	5.65	1.60	1.51
1	B	58	GLU	CG-CD	5.64	1.60	1.51

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	154	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	V	60	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	154	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	N	152	LEU	CA-CB-CG	5.76	128.54	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1414	0	1366	24	0
1	B	1418	0	1370	22	0
1	C	1418	0	1370	17	0
1	D	1426	0	1382	19	0
1	E	1414	0	1366	16	0
1	F	1414	0	1366	25	0
1	G	1415	0	1366	18	0
1	H	1426	0	1382	15	0
1	I	1426	0	1382	19	0
1	J	1415	0	1361	16	0
1	K	1426	0	1382	14	0
1	L	1415	0	1368	20	0
1	M	1418	0	1370	14	0
1	N	1415	0	1368	25	0
1	O	1418	0	1370	25	0
1	P	1414	0	1364	13	0
1	Q	1418	0	1370	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1418	0	1370	25	0
1	S	1414	0	1366	18	0
1	T	1426	0	1382	12	0
1	U	1418	0	1370	19	0
1	V	1418	0	1370	28	0
1	W	1423	0	1378	30	0
1	X	1415	0	1368	19	0
2	B	10	0	14	1	0
2	C	20	0	28	1	0
2	D	10	0	14	1	0
2	E	10	0	14	0	0
2	F	10	0	14	0	0
2	G	20	0	28	1	0
2	H	20	0	28	3	0
2	I	10	0	14	0	0
2	P	10	0	14	1	0
2	Q	20	0	28	1	0
2	R	30	0	42	8	0
2	S	10	0	14	1	0
2	U	10	0	14	0	0
2	W	20	0	28	0	0
2	X	10	0	14	0	0
3	B	4	0	6	0	0
3	D	4	0	6	1	0
3	J	4	0	6	0	0
3	L	4	0	6	1	0
3	M	4	0	6	1	0
3	N	8	0	12	1	0
3	O	4	0	6	1	0
3	P	4	0	6	1	0
3	T	4	0	6	0	0
3	U	8	0	12	9	0
4	A	74	0	0	3	0
4	B	46	0	0	4	0
4	C	68	0	0	6	0
4	D	68	0	0	2	0
4	E	49	0	0	1	0
4	F	52	0	0	2	0
4	G	69	0	0	3	0
4	H	70	0	0	3	0
4	I	51	0	0	6	0
4	J	78	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	85	0	0	3	0
4	L	48	0	0	2	0
4	M	52	0	0	1	0
4	N	72	0	0	5	0
4	O	82	0	0	4	0
4	P	62	0	0	4	0
4	Q	71	0	0	5	0
4	R	73	0	0	6	0
4	S	60	0	0	4	0
4	T	36	0	0	1	0
4	U	63	0	0	1	0
4	V	38	0	0	2	0
4	W	71	0	0	3	0
4	X	87	0	0	5	0
All	All	35835	0	33287	413	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 6.

The worst 5 of 413 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:G:169:LYS:HE3	4:G:361:HOH:O	1.42	1.17
1:I:102:GLN:HG3	4:I:348:HOH:O	1.48	1.11
1:C:98:GLN:HG2	4:C:362:HOH:O	1.49	1.09
1:I:144:ARG:HD2	4:I:308:HOH:O	1.55	1.06
1:R:46:HIS:HB3	4:R:310:HOH:O	1.58	1.02

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	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	B	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	C	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
1	D	171/176 (97%)	166 (97%)	4 (2%)	1 (1%)	25	33
1	E	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	F	170/176 (97%)	167 (98%)	3 (2%)	0	100	100
1	G	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	H	171/176 (97%)	169 (99%)	1 (1%)	1 (1%)	25	33
1	I	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
1	J	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	K	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
1	L	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	M	170/176 (97%)	166 (98%)	3 (2%)	1 (1%)	25	33
1	N	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	O	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	P	170/176 (97%)	168 (99%)	2 (1%)	0	100	100
1	Q	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
1	R	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	S	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	T	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
1	U	170/176 (97%)	167 (98%)	3 (2%)	0	100	100
1	V	170/176 (97%)	164 (96%)	5 (3%)	1 (1%)	25	33
1	W	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
1	X	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
All	All	4086/4224 (97%)	3974 (97%)	108 (3%)	4 (0%)	51	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	11	SER
1	V	3	SER
1	D	172	VAL
1	H	91	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	152/157 (97%)	140 (92%)	12 (8%)	12	15
1	B	153/157 (98%)	140 (92%)	13 (8%)	10	13
1	C	153/157 (98%)	139 (91%)	14 (9%)	9	11
1	D	154/157 (98%)	146 (95%)	8 (5%)	23	31
1	E	152/157 (97%)	139 (91%)	13 (9%)	10	13
1	F	152/157 (97%)	138 (91%)	14 (9%)	9	11
1	G	152/157 (97%)	137 (90%)	15 (10%)	8	9
1	H	154/157 (98%)	142 (92%)	12 (8%)	12	16
1	I	154/157 (98%)	137 (89%)	17 (11%)	6	6
1	J	152/157 (97%)	142 (93%)	10 (7%)	16	21
1	K	154/157 (98%)	143 (93%)	11 (7%)	14	19
1	L	152/157 (97%)	134 (88%)	18 (12%)	5	5
1	M	153/157 (98%)	138 (90%)	15 (10%)	8	9
1	N	152/157 (97%)	139 (91%)	13 (9%)	10	13
1	O	153/157 (98%)	141 (92%)	12 (8%)	12	16
1	P	152/157 (97%)	139 (91%)	13 (9%)	10	13
1	Q	153/157 (98%)	137 (90%)	16 (10%)	7	7
1	R	153/157 (98%)	140 (92%)	13 (8%)	10	13
1	S	152/157 (97%)	136 (90%)	16 (10%)	7	7
1	T	154/157 (98%)	143 (93%)	11 (7%)	14	19
1	U	153/157 (98%)	139 (91%)	14 (9%)	9	11
1	V	153/157 (98%)	140 (92%)	13 (8%)	10	13
1	W	153/157 (98%)	134 (88%)	19 (12%)	4	5
1	X	152/157 (97%)	135 (89%)	17 (11%)	6	6
All	All	3667/3768 (97%)	3338 (91%)	329 (9%)	9	11

5 of 329 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	102	GLN
1	N	173	LYS
1	X	121	LYS
1	L	140	LYS
1	M	130	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	98	GLN
1	O	62	HIS
1	X	80	GLN
1	M	98	GLN
1	O	80	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PGE	G	202	-	9,9,9	0.62	0	8,8,8	0.36	0
2	PGE	C	201	-	9,9,9	0.97	0	8,8,8	1.03	0
3	EDO	O	201	-	3,3,3	0.83	0	2,2,2	0.39	0
2	PGE	R	201	-	9,9,9	0.85	0	8,8,8	0.69	0
3	EDO	D	202	-	3,3,3	0.88	0	2,2,2	0.43	0
3	EDO	U	202	-	3,3,3	0.88	0	2,2,2	0.49	0
3	EDO	U	203	-	3,3,3	1.31	0	2,2,2	1.05	0
2	PGE	Q	202	-	9,9,9	0.45	0	8,8,8	0.58	0
2	PGE	E	201	-	9,9,9	0.84	0	8,8,8	0.88	0
3	EDO	L	201	-	3,3,3	0.55	0	2,2,2	0.41	0
2	PGE	R	203	-	9,9,9	0.48	0	8,8,8	0.46	0
2	PGE	I	201	-	9,9,9	0.65	0	8,8,8	0.48	0
2	PGE	C	202	-	9,9,9	0.49	0	8,8,8	0.53	0
3	EDO	M	201	-	3,3,3	0.58	0	2,2,2	0.25	0
3	EDO	T	201	-	3,3,3	0.73	0	2,2,2	0.26	0
3	EDO	N	202	-	3,3,3	0.95	0	2,2,2	0.65	0
3	EDO	B	202	-	3,3,3	0.81	0	2,2,2	0.39	0
2	PGE	B	201	-	9,9,9	0.51	0	8,8,8	0.54	0
2	PGE	H	202	-	9,9,9	0.59	0	8,8,8	0.44	0
2	PGE	W	202	-	9,9,9	0.55	0	8,8,8	0.33	0
2	PGE	S	201	-	9,9,9	0.54	0	8,8,8	0.54	0
3	EDO	P	202	-	3,3,3	0.41	0	2,2,2	0.53	0
2	PGE	F	201	-	9,9,9	0.53	0	8,8,8	0.25	0
3	EDO	N	201	-	3,3,3	0.68	0	2,2,2	0.30	0
2	PGE	G	201	-	9,9,9	0.80	0	8,8,8	0.86	0
2	PGE	R	202	-	9,9,9	0.97	0	8,8,8	1.37	1 (12%)
2	PGE	H	201	-	9,9,9	0.71	0	8,8,8	0.80	0
2	PGE	U	201	-	9,9,9	0.56	0	8,8,8	0.72	0
2	PGE	Q	201	-	9,9,9	0.91	0	8,8,8	0.97	0
2	PGE	P	201	-	9,9,9	0.72	0	8,8,8	0.60	0
2	PGE	W	201	-	9,9,9	0.99	0	8,8,8	1.02	0
3	EDO	J	201	-	3,3,3	0.72	0	2,2,2	0.37	0
2	PGE	X	201	-	9,9,9	0.55	0	8,8,8	0.71	0
2	PGE	D	201	-	9,9,9	0.48	0	8,8,8	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	G	202	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	C	201	-	-	6/7/7/7	-
3	EDO	O	201	-	-	0/1/1/1	-
2	PGE	R	201	-	-	7/7/7/7	-
3	EDO	D	202	-	-	1/1/1/1	-
3	EDO	U	202	-	-	0/1/1/1	-
3	EDO	U	203	-	-	1/1/1/1	-
2	PGE	Q	202	-	-	3/7/7/7	-
2	PGE	E	201	-	-	5/7/7/7	-
3	EDO	L	201	-	-	1/1/1/1	-
2	PGE	R	203	-	-	3/7/7/7	-
2	PGE	I	201	-	-	3/7/7/7	-
2	PGE	C	202	-	-	6/7/7/7	-
3	EDO	M	201	-	-	1/1/1/1	-
3	EDO	T	201	-	-	1/1/1/1	-
3	EDO	N	202	-	-	1/1/1/1	-
3	EDO	B	202	-	-	1/1/1/1	-
2	PGE	B	201	-	-	5/7/7/7	-
2	PGE	H	202	-	-	5/7/7/7	-
2	PGE	W	202	-	-	3/7/7/7	-
2	PGE	S	201	-	-	3/7/7/7	-
3	EDO	P	202	-	-	0/1/1/1	-
2	PGE	F	201	-	-	2/7/7/7	-
3	EDO	N	201	-	-	1/1/1/1	-
2	PGE	G	201	-	-	2/7/7/7	-
2	PGE	R	202	-	-	4/7/7/7	-
2	PGE	H	201	-	-	5/7/7/7	-
2	PGE	U	201	-	-	3/7/7/7	-
2	PGE	Q	201	-	-	4/7/7/7	-
2	PGE	P	201	-	-	3/7/7/7	-
2	PGE	W	201	-	-	6/7/7/7	-
3	EDO	J	201	-	-	1/1/1/1	-
2	PGE	X	201	-	-	4/7/7/7	-
2	PGE	D	201	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	R	202	PGE	O2-C2-C1	2.44	120.77	110.07

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	201	PGE	C1-C2-O2-C3
2	E	201	PGE	C6-C5-O3-C4
2	C	201	PGE	C4-C3-O2-C2
2	G	202	PGE	O2-C3-C4-O3
2	P	201	PGE	O2-C3-C4-O3

There are no ring outliers.

19 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	202	PGE	1	0
3	O	201	EDO	1	0
3	D	202	EDO	1	0
3	U	202	EDO	3	0
3	U	203	EDO	6	0
2	Q	202	PGE	1	0
3	L	201	EDO	1	0
2	R	203	PGE	1	0
2	C	202	PGE	1	0
3	M	201	EDO	1	0
3	N	202	EDO	1	0
2	B	201	PGE	1	0
2	H	202	PGE	1	0
2	S	201	PGE	1	0
3	P	202	EDO	1	0
2	R	202	PGE	7	0
2	H	201	PGE	2	0
2	P	201	PGE	1	0
2	D	201	PGE	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	172/176 (97%)	-0.12	0 100 100	18, 27, 37, 45	0
1	B	172/176 (97%)	-0.02	0 100 100	26, 34, 44, 51	0
1	C	172/176 (97%)	-0.16	0 100 100	21, 29, 40, 52	0
1	D	173/176 (98%)	-0.08	1 (0%) 89 93	17, 27, 38, 59	0
1	E	172/176 (97%)	0.00	1 (0%) 89 93	26, 35, 44, 50	0
1	F	172/176 (97%)	-0.11	0 100 100	22, 32, 42, 55	0
1	G	172/176 (97%)	-0.08	0 100 100	21, 29, 40, 55	0
1	H	173/176 (98%)	-0.08	0 100 100	19, 29, 39, 50	0
1	I	173/176 (98%)	-0.02	1 (0%) 89 93	24, 32, 42, 59	0
1	J	172/176 (97%)	-0.18	0 100 100	19, 25, 36, 48	0
1	K	173/176 (98%)	-0.07	0 100 100	19, 26, 37, 49	0
1	L	172/176 (97%)	-0.06	0 100 100	27, 36, 44, 52	0
1	M	172/176 (97%)	0.06	1 (0%) 89 93	27, 36, 45, 52	0
1	N	172/176 (97%)	-0.07	0 100 100	17, 27, 39, 50	0
1	O	172/176 (97%)	-0.11	0 100 100	20, 27, 37, 50	0
1	P	172/176 (97%)	-0.10	0 100 100	22, 30, 40, 47	0
1	Q	172/176 (97%)	-0.13	0 100 100	17, 27, 37, 43	0
1	R	172/176 (97%)	-0.15	0 100 100	18, 27, 38, 48	0
1	S	172/176 (97%)	-0.08	0 100 100	24, 33, 41, 51	0
1	T	173/176 (98%)	0.04	1 (0%) 89 93	22, 34, 45, 62	0
1	U	172/176 (97%)	-0.08	0 100 100	19, 28, 38, 51	0
1	V	172/176 (97%)	-0.07	0 100 100	26, 36, 45, 52	0
1	W	173/176 (98%)	-0.13	0 100 100	20, 28, 39, 56	0
1	X	172/176 (97%)	-0.17	0 100 100	18, 26, 36, 47	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4134/4224 (97%)	-0.08	5 (0%) 95 98	17, 30, 42, 62	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.8
1	T	1	MET	2.8
1	I	1	MET	2.4
1	M	118	ALA	2.3
1	E	2	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 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	N	201	4/4	0.79	0.23	50,51,52,53	0
3	EDO	N	202	4/4	0.83	0.32	48,48,50,50	0
3	EDO	U	203	4/4	0.83	0.28	28,33,34,34	0
2	PGE	R	202	10/10	0.83	0.31	38,46,47,48	0
3	EDO	B	202	4/4	0.85	0.17	45,45,46,47	0
3	EDO	D	202	4/4	0.85	0.30	42,47,49,50	0
3	EDO	U	202	4/4	0.85	0.32	42,43,43,46	0
3	EDO	M	201	4/4	0.86	0.14	50,51,52,53	0
3	EDO	T	201	4/4	0.86	0.16	38,40,40,41	0
3	EDO	O	201	4/4	0.88	0.32	50,52,53,54	0
2	PGE	G	202	10/10	0.88	0.21	52,55,59,59	0
2	PGE	I	201	10/10	0.88	0.23	48,51,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PGE	P	201	10/10	0.88	0.18	53,55,63,64	0
2	PGE	Q	201	10/10	0.89	0.18	41,44,46,48	0
2	PGE	X	201	10/10	0.89	0.17	42,47,51,53	0
3	EDO	J	201	4/4	0.90	0.16	30,33,35,36	0
2	PGE	C	201	10/10	0.90	0.18	37,46,49,50	0
2	PGE	D	201	10/10	0.90	0.19	56,58,59,60	0
2	PGE	U	201	10/10	0.91	0.19	40,44,52,53	0
2	PGE	S	201	10/10	0.91	0.17	42,47,55,56	0
2	PGE	H	202	10/10	0.92	0.18	40,47,53,55	0
2	PGE	W	202	10/10	0.92	0.18	43,45,48,50	0
3	EDO	L	201	4/4	0.92	0.15	33,34,36,37	0
2	PGE	W	201	10/10	0.92	0.19	40,43,44,44	0
2	PGE	C	202	10/10	0.92	0.23	56,59,60,60	0
2	PGE	G	201	10/10	0.92	0.19	39,40,46,49	0
2	PGE	B	201	10/10	0.92	0.18	54,56,59,59	0
2	PGE	R	203	10/10	0.93	0.23	55,57,62,63	0
2	PGE	E	201	10/10	0.93	0.17	51,53,57,58	0
2	PGE	Q	202	10/10	0.93	0.27	54,56,62,64	0
2	PGE	R	201	10/10	0.94	0.15	41,42,44,44	0
2	PGE	F	201	10/10	0.94	0.23	45,56,66,67	0
2	PGE	H	201	10/10	0.96	0.17	35,39,42,45	0
3	EDO	P	202	4/4	0.96	0.25	48,48,49,49	0

6.5 Other polymers

There are no such residues in this entry.