



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 08:01 am BST

PDB ID : 5BSE  
Title : Crystal structure of Medicago truncatula (delta)1-Pyrroline-5-Carboxylate Reductase (MtP5CR)  
Authors : Ruszkowski, M.; Nocek, B.; Forlani, G.; Dauter, Z.  
Deposited on : 2015-06-02  
Resolution : 1.70 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](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.

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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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

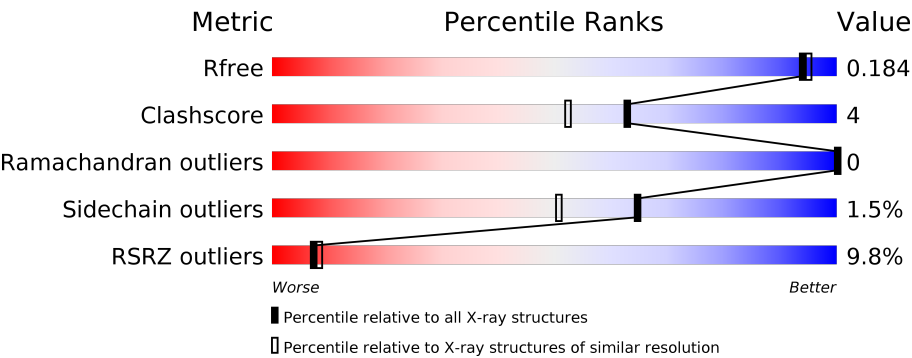
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	277	<div><div>4%</div><div>91%</div><div>6%</div><div>.</div></div>
1	B	277	<div><div>5%</div><div>92%</div><div>5%</div><div>..</div></div>
1	C	277	<div><div>5%</div><div>92%</div><div>6%</div><div>.</div></div>
1	D	277	<div><div>20%</div><div>87%</div><div>10%</div><div>.</div></div>
1	E	277	<div><div>5%</div><div>90%</div><div>8%</div><div>..</div></div>
1	F	277	<div><div>4%</div><div>90%</div><div>8%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	277	<div><div></div><div>30%</div><div></div><div>84%</div><div></div><div>11%</div><div></div><div></div></div>
1	H	277	<div><div></div><div>5%</div><div></div><div>90%</div><div></div><div>8%</div><div></div><div></div></div>
1	I	277	<div><div></div><div>7%</div><div></div><div>90%</div><div></div><div>9%</div><div></div><div></div></div>
1	J	277	<div><div></div><div>10%</div><div></div><div>89%</div><div></div><div>8%</div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21823 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 Pyrroline-5-carboxylate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	7	0
			2038	1285	354	392	7			
1	B	272	Total	C	N	O	S	0	5	0
			2024	1275	351	391	7			
1	C	272	Total	C	N	O	S	0	7	0
			2038	1283	354	394	7			
1	D	270	Total	C	N	O	S	0	6	0
			2014	1269	350	388	7			
1	E	272	Total	C	N	O	S	0	6	0
			2031	1281	352	391	7			
1	F	272	Total	C	N	O	S	0	6	0
			2030	1281	352	390	7			
1	G	268	Total	C	N	O	S	0	3	0
			1981	1246	346	383	6			
1	H	272	Total	C	N	O	S	0	11	0
			2068	1303	359	399	7			
1	I	272	Total	C	N	O	S	0	6	0
			2035	1283	354	391	7			
1	J	272	Total	C	N	O	S	0	4	0
			2018	1272	351	389	6			

There are 30 discrepancies between the modelled and reference sequences:

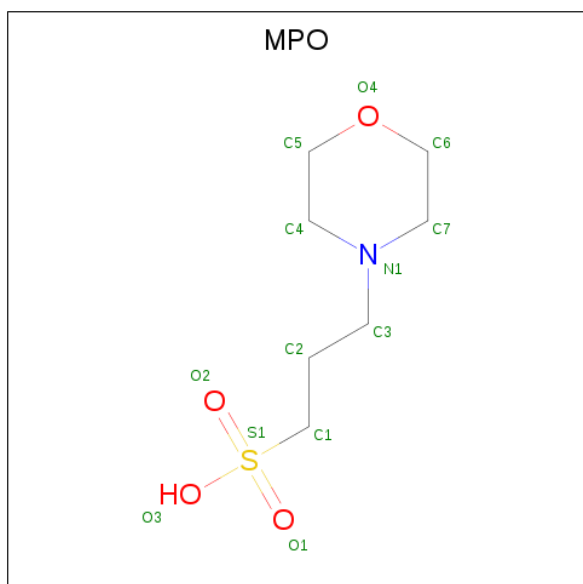
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7KRM5
A	-1	ASN	-	expression tag	UNP G7KRM5
A	0	ALA	-	expression tag	UNP G7KRM5
B	-2	SER	-	expression tag	UNP G7KRM5
B	-1	ASN	-	expression tag	UNP G7KRM5
B	0	ALA	-	expression tag	UNP G7KRM5
C	-2	SER	-	expression tag	UNP G7KRM5
C	-1	ASN	-	expression tag	UNP G7KRM5
C	0	ALA	-	expression tag	UNP G7KRM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP G7KRM5
D	-1	ASN	-	expression tag	UNP G7KRM5
D	0	ALA	-	expression tag	UNP G7KRM5
E	-2	SER	-	expression tag	UNP G7KRM5
E	-1	ASN	-	expression tag	UNP G7KRM5
E	0	ALA	-	expression tag	UNP G7KRM5
F	-2	SER	-	expression tag	UNP G7KRM5
F	-1	ASN	-	expression tag	UNP G7KRM5
F	0	ALA	-	expression tag	UNP G7KRM5
G	-2	SER	-	expression tag	UNP G7KRM5
G	-1	ASN	-	expression tag	UNP G7KRM5
G	0	ALA	-	expression tag	UNP G7KRM5
H	-2	SER	-	expression tag	UNP G7KRM5
H	-1	ASN	-	expression tag	UNP G7KRM5
H	0	ALA	-	expression tag	UNP G7KRM5
I	-2	SER	-	expression tag	UNP G7KRM5
I	-1	ASN	-	expression tag	UNP G7KRM5
I	0	ALA	-	expression tag	UNP G7KRM5
J	-2	SER	-	expression tag	UNP G7KRM5
J	-1	ASN	-	expression tag	UNP G7KRM5
J	0	ALA	-	expression tag	UNP G7KRM5

- Molecule 2 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	I	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	J	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	205	Total	O	0	2
			207	207		
4	B	160	Total	O	0	1
			161	161		
4	C	139	Total	O	0	1
			140	140		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	98	Total 98	O 98	0	0
4	E	182	Total 182	O 182	0	0
4	F	168	Total 168	O 168	0	0
4	G	95	Total 95	O 95	0	0
4	H	147	Total 147	O 147	0	0
4	I	146	Total 147	O 147	0	1
4	J	126	Total 126	O 126	0	0

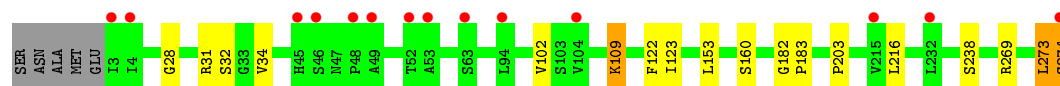
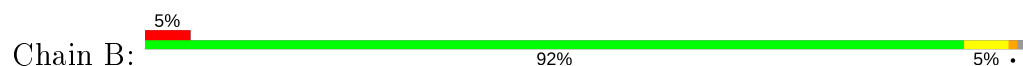
### 3 Residue-property plots [i](#)

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

- Molecule 1: Pyrroline-5-carboxylate reductase



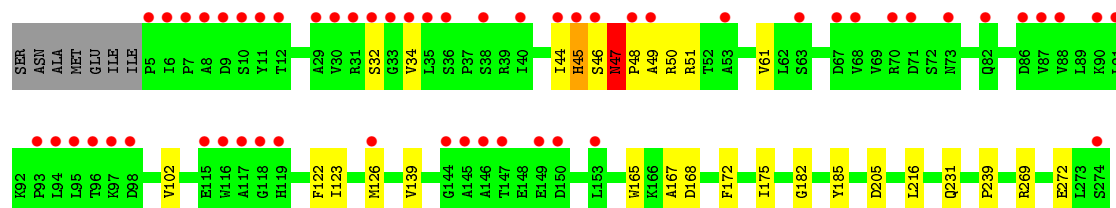
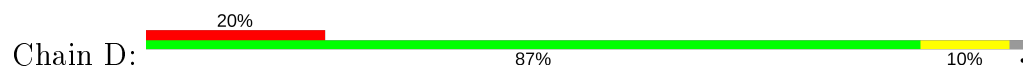
- Molecule 1: Pyrroline-5-carboxylate reductase



- Molecule 1: Pyrroline-5-carboxylate reductase



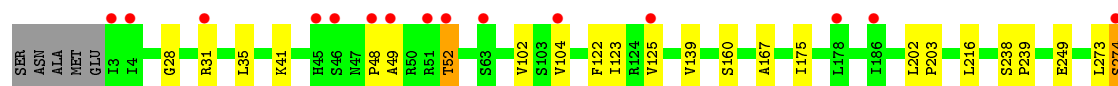
- Molecule 1: Pyrroline-5-carboxylate reductase



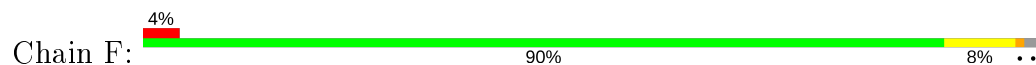
- Molecule 1: Pyrroline-5-carboxylate reductase



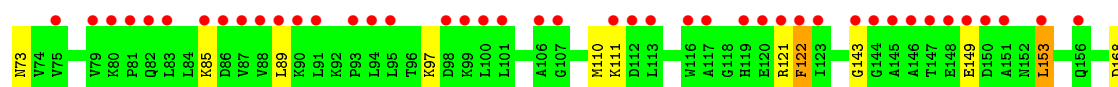
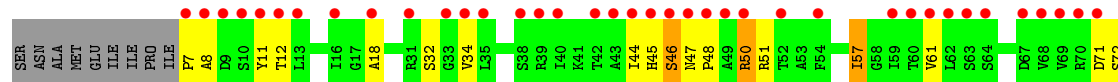
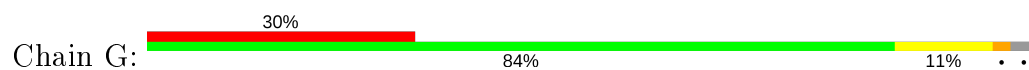




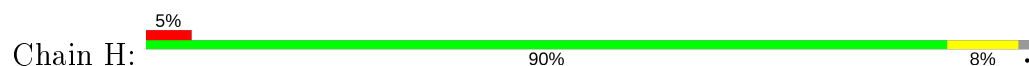
- Molecule 1: Pyrroline-5-carboxylate reductase



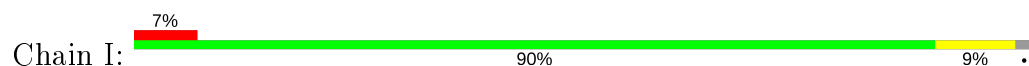
- Molecule 1: Pyrroline-5-carboxylate reductase



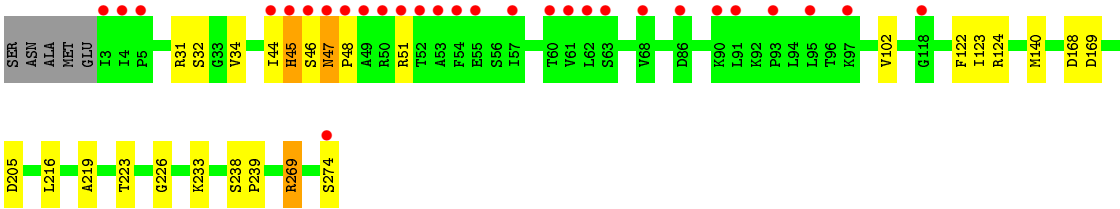
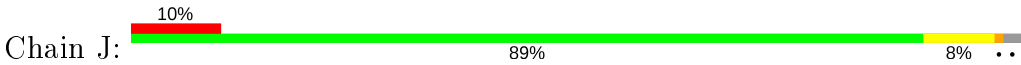
- Molecule 1: Pyrroline-5-carboxylate reductase



- Molecule 1: Pyrroline-5-carboxylate reductase



- Molecule 1: Pyrroline-5-carboxylate reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.80Å 100.60Å 101.20Å 67.90° 85.30° 89.30°	Depositor
Resolution (Å)	38.93 – 1.70 38.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.93-1.70) 97.3 (38.93-1.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.160 , 0.180 0.169 , 0.184	Depositor DCC
$R_{free}$ test set	2709 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	21823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.02	0/2070	0.92	2/2800 (0.1%)
1	B	0.98	1/2052 (0.0%)	0.92	2/2773 (0.1%)
1	C	0.97	2/2067 (0.1%)	0.89	2/2796 (0.1%)
1	D	0.87	1/2046 (0.0%)	0.86	3/2768 (0.1%)
1	E	1.05	2/2062 (0.1%)	0.95	1/2787 (0.0%)
1	F	0.99	3/2062 (0.1%)	0.90	3/2791 (0.1%)
1	G	0.87	2/2009 (0.1%)	0.85	0/2715
1	H	0.95	0/2099	0.92	1/2835 (0.0%)
1	I	0.92	0/2064	0.86	3/2792 (0.1%)
1	J	0.93	1/2047 (0.0%)	0.88	5/2770 (0.2%)
All	All	0.96	12/20578 (0.1%)	0.90	22/27827 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	H	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	272	GLU	CD-OE1	5.87	1.32	1.25
1	C	191	GLU	CD-OE2	5.67	1.31	1.25
1	B	238	SER	CB-OG	-5.53	1.35	1.42
1	C	155	SER	CB-OG	-5.46	1.35	1.42
1	F	173	ASP	N-CA	5.37	1.57	1.46

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	41	LYS	CD-CE-NZ	6.00	125.50	111.70
1	D	47	ASN	C-N-CD	5.87	140.72	128.40
1	B	269[A]	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	269[B]	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	269[A]	ARG	NE-CZ-NH2	-5.69	117.45	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	273	LEU	Peptide
1	C	226[B]	GLY	Peptide
1	H	226[B]	GLY	Peptide

## 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	2038	0	2106	14	0
1	B	2024	0	2085	12	0
1	C	2038	0	2092	12	0
1	D	2014	0	2076	31	0
1	E	2031	0	2097	20	0
1	F	2030	0	2097	17	0
1	G	1981	0	2035	41	0
1	H	2068	0	2134	14	0
1	I	2035	0	2101	19	0
1	J	2018	0	2079	20	0
2	A	13	0	14	0	0
2	C	13	0	15	1	0
2	H	13	0	15	0	0
2	I	13	0	15	1	0
2	J	13	0	15	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	207	0	0	4	0
4	B	161	0	0	1	0
4	C	140	0	0	1	0
4	D	98	0	0	3	0
4	E	182	0	0	2	0
4	F	168	0	0	3	0
4	G	95	0	0	5	0
4	H	147	0	0	3	0
4	I	147	0	0	3	0
4	J	126	0	0	6	0
All	All	21823	0	20976	177	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 4.

The worst 5 of 177 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:126[B]:MET:CE	4:A:531:HOH:O	1.64	1.28
1:G:110:MET:HE2	1:G:143:GLY:CA	1.68	1.24
1:A:126[B]:MET:HE1	4:A:531:HOH:O	1.21	1.22
1:G:110:MET:CE	1:G:143:GLY:CA	2.28	1.10
1:G:18:ALA:O	1:G:50:ARG:HD3	1.53	1.09

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	277/277 (100%)	276 (100%)	1 (0%)	0	100	100
1	B	274/277 (99%)	271 (99%)	3 (1%)	0	100	100
1	C	277/277 (100%)	276 (100%)	1 (0%)	0	100	100
1	D	274/277 (99%)	270 (98%)	4 (2%)	0	100	100
1	E	275/277 (99%)	272 (99%)	3 (1%)	0	100	100
1	F	276/277 (100%)	275 (100%)	1 (0%)	0	100	100
1	G	269/277 (97%)	265 (98%)	4 (2%)	0	100	100
1	H	280/277 (101%)	278 (99%)	2 (1%)	0	100	100
1	I	276/277 (100%)	274 (99%)	2 (1%)	0	100	100
1	J	274/277 (99%)	273 (100%)	1 (0%)	0	100	100
All	All	2752/2770 (99%)	2730 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	215/212 (101%)	213 (99%)	2 (1%)	78	70
1	B	213/212 (100%)	208 (98%)	5 (2%)	50	33
1	C	214/212 (101%)	213 (100%)	1 (0%)	88	83
1	D	212/212 (100%)	209 (99%)	3 (1%)	67	53
1	E	214/212 (101%)	209 (98%)	5 (2%)	50	33
1	F	214/212 (101%)	212 (99%)	2 (1%)	78	70
1	G	207/212 (98%)	200 (97%)	7 (3%)	37	18
1	H	218/212 (103%)	215 (99%)	3 (1%)	67	53
1	I	214/212 (101%)	212 (99%)	2 (1%)	78	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	212/212 (100%)	208 (98%)	4 (2%)	57 41
All	All	2133/2120 (101%)	2099 (98%)	34 (2%)	65 48

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	274[B]	SER
1	G	47	ASN
1	J	46	SER
1	F	274	SER
1	B	274[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	C	65	ASN
1	D	47	ASN
1	G	45	HIS
1	G	152	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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
2	MPO	J	301	-	13,13,13	1.18	1 (7%)	17,17,17	1.90	6 (35%)
2	MPO	I	301	-	13,13,13	1.31	2 (15%)	17,17,17	2.35	7 (41%)
2	MPO	C	301	-	13,13,13	1.48	3 (23%)	17,17,17	2.73	8 (47%)
2	MPO	H	301	-	13,13,13	1.47	2 (15%)	17,17,17	2.26	7 (41%)
2	MPO	A	301	-	13,13,13	1.61	3 (23%)	17,17,17	1.62	4 (23%)

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	MPO	J	301	-	-	4/7/15/15	0/1/1/1
2	MPO	I	301	-	-	6/7/15/15	0/1/1/1
2	MPO	C	301	-	-	0/7/15/15	0/1/1/1
2	MPO	H	301	-	-	0/7/15/15	0/1/1/1
2	MPO	A	301	-	-	4/7/15/15	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	MPO	C1-S1	3.52	1.82	1.77
2	H	301	MPO	O2-S1	3.45	1.55	1.45
2	J	301	MPO	O2-S1	3.21	1.54	1.45
2	H	301	MPO	O1-S1	2.79	1.53	1.45
2	A	301	MPO	O1-S1	2.73	1.53	1.45

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	MPO	O2-S1-C1	6.18	114.36	106.92
2	I	301	MPO	O2-S1-C1	-4.66	101.31	106.92
2	C	301	MPO	O3-S1-O2	-4.52	100.24	111.27
2	H	301	MPO	O4-C5-C4	-4.26	102.42	111.80
2	I	301	MPO	O3-S1-C1	4.13	112.45	105.77

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	301	MPO	C2-C1-S1-O2
2	I	301	MPO	C2-C1-S1-O3
2	I	301	MPO	C1-C2-C3-N1
2	A	301	MPO	C2-C1-S1-O1
2	A	301	MPO	C2-C1-S1-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	301	MPO	1	0
2	C	301	MPO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	272/277 (98%)	-0.00	11 (4%) 38 42	29, 39, 61, 88	0
1	B	272/277 (98%)	0.35	14 (5%) 28 31	28, 45, 78, 112	0
1	C	272/277 (98%)	0.36	14 (5%) 28 31	28, 46, 79, 120	0
1	D	270/277 (97%)	1.02	56 (20%) 1 0	28, 63, 122, 137	0
1	E	272/277 (98%)	0.33	15 (5%) 25 27	29, 42, 71, 102	0
1	F	272/277 (98%)	0.05	10 (3%) 41 46	28, 42, 69, 106	0
1	G	268/277 (96%)	1.55	83 (30%) 0 0	30, 65, 140, 167	0
1	H	272/277 (98%)	0.23	14 (5%) 28 31	29, 44, 76, 109	0
1	I	272/277 (98%)	0.31	19 (6%) 16 18	30, 46, 83, 119	0
1	J	272/277 (98%)	0.50	29 (10%) 6 7	29, 53, 97, 129	0
All	All	2714/2770 (97%)	0.47	265 (9%) 7 8	28, 45, 104, 167	0

The worst 5 of 265 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	8	ALA	17.9
1	C	4	ILE	12.9
1	H	3	ILE	10.1
1	D	35	LEU	10.0
1	J	3	ILE	9.9

### 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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
2	MPO	I	301	13/13	0.84	0.21	46,52,68,70	13
2	MPO	H	301	13/13	0.88	0.14	43,51,66,69	13
2	MPO	C	301	13/13	0.89	0.18	51,61,72,74	13
2	MPO	J	301	13/13	0.91	0.16	47,52,70,72	13
2	MPO	A	301	13/13	0.93	0.12	42,48,65,75	13
3	CL	H	302	1/1	0.97	0.06	47,47,47,47	1
3	CL	C	302	1/1	0.98	0.07	45,45,45,45	1
3	CL	J	302	1/1	0.98	0.10	43,43,43,43	1
3	CL	D	301	1/1	0.98	0.06	42,42,42,42	1
3	CL	I	302	1/1	0.98	0.10	41,41,41,41	1
3	CL	F	301	1/1	0.98	0.08	43,43,43,43	1
3	CL	A	302	1/1	0.99	0.04	42,42,42,42	1
3	CL	G	301	1/1	0.99	0.04	40,40,40,40	1
3	CL	B	301	1/1	0.99	0.06	38,38,38,38	1
3	CL	E	301	1/1	0.99	0.06	39,39,39,39	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.