wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 10:25 PM GMT

PDB ID	:	5BSG
Title	:	Crystal structure of Medicago truncatula (delta)1-Pyrroline-5-Carboxylate Reductase (MtP5CR) in complex with NADP+
Authors	:	Ruszkowski, M.; Nocek, B.; Forlani, G.; Dauter, Z.
Deposited on	:	2015-06-02
Resolution	:	1.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

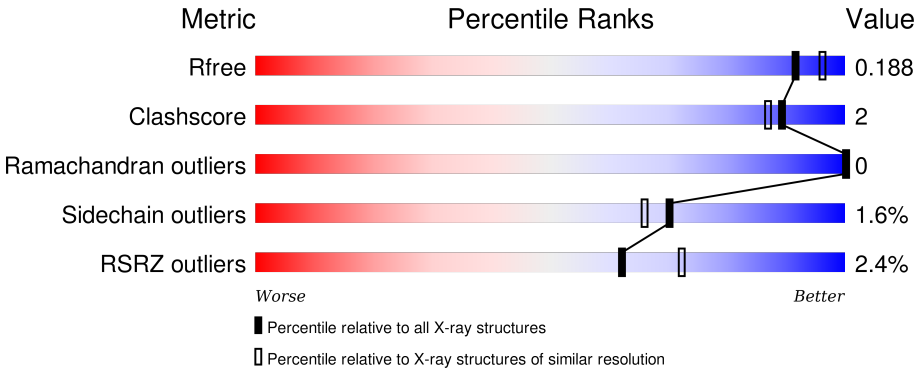
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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. 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	277	94%
1	B	277	2% 95%
1	C	277	% 93% 5%
1	D	277	4% 94%
1	E	277	2% 91% 6%

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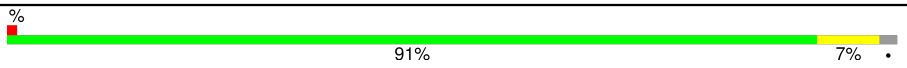
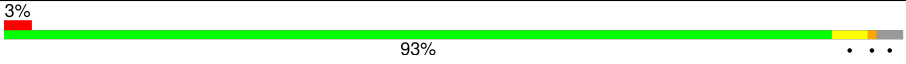
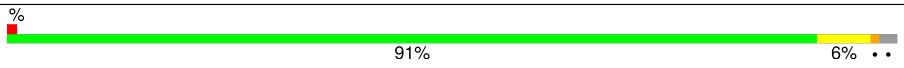
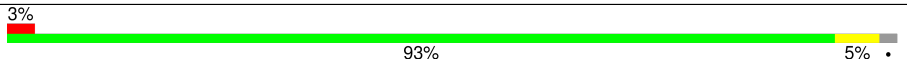
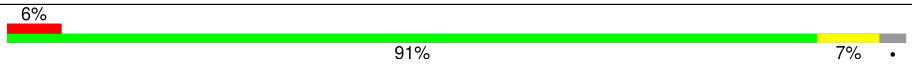
Mol	Chain	Length	Quality of chain
1	F	277	
1	G	277	
1	H	277	
1	I	277	
1	J	277	

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
3	MPO	B	302	-	-	-	X
3	MPO	J	302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22670 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	5	0
			2020	1274	348	392	6			
1	B	272	Total	C	N	O	S	0	3	0
			2011	1268	349	388	6			
1	C	270	Total	C	N	O	S	0	5	0
			2008	1263	350	389	6			
1	D	271	Total	C	N	O	S	0	4	0
			2012	1267	350	389	6			
1	E	272	Total	C	N	O	S	0	6	0
			2032	1281	353	392	6			
1	F	272	Total	C	N	O	S	0	6	0
			2034	1283	354	391	6			
1	G	269	Total	C	N	O	S	0	4	0
			1990	1252	347	385	6			
1	H	272	Total	C	N	O	S	0	3	0
			2002	1265	346	385	6			
1	I	272	Total	C	N	O	S	0	2	0
			2001	1263	348	384	6			
1	J	270	Total	C	N	O	S	0	1	0
			1976	1246	342	382	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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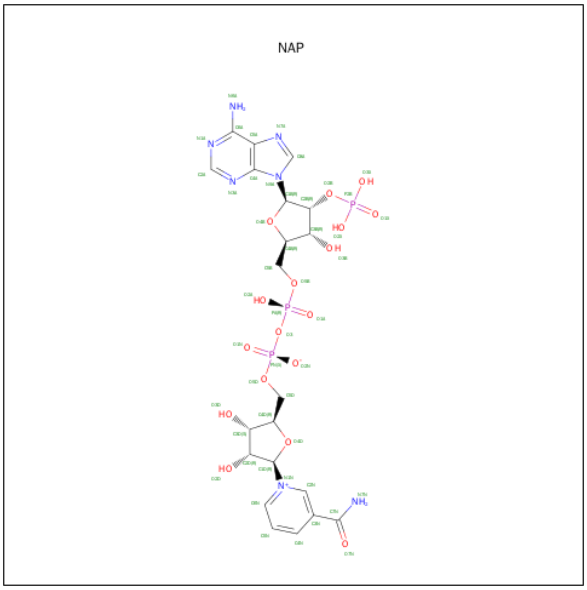
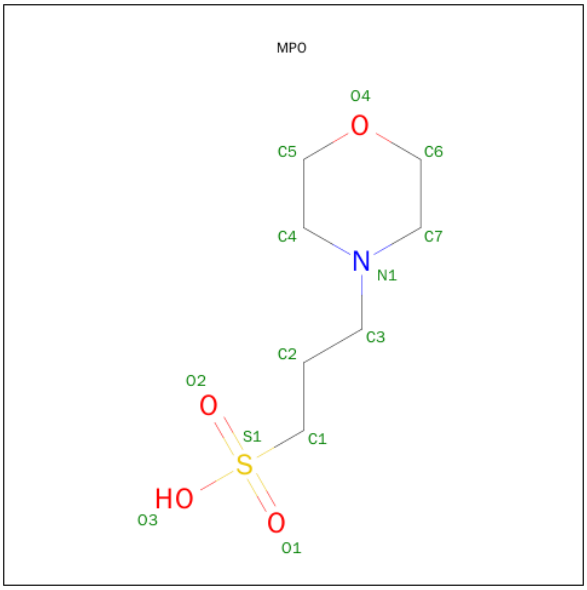
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP G7KRM5
D	-1	ASN	-	expression tag	UNP G7KRM5
D	0	ALA	-	expression tag	UNP G7KRM5
E	-2	SER	-	expression tag	UNP G7KRM5
E	-1	ASN	-	expression tag	UNP G7KRM5
E	0	ALA	-	expression tag	UNP G7KRM5
F	-2	SER	-	expression tag	UNP G7KRM5
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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	I	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	J	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

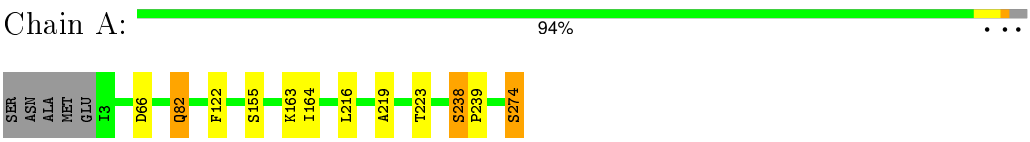
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	248	Total O 248 248	0	0
5	B	202	Total O 203 203	0	1
5	C	205	Total O 206 206	0	1
5	D	158	Total O 159 159	0	1
5	E	203	Total O 205 205	0	2
5	F	231	Total O 231 231	0	0
5	G	155	Total O 155 155	0	0
5	H	193	Total O 194 194	0	1
5	I	194	Total O 194 194	0	0
5	J	169	Total O 169 169	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 errors 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.

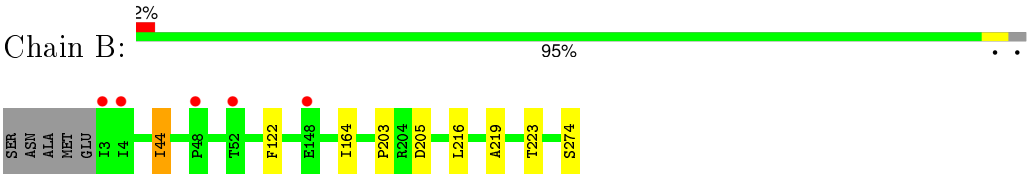
- Molecule 1: Pyrroline-5-carboxylate reductase

Chain A:



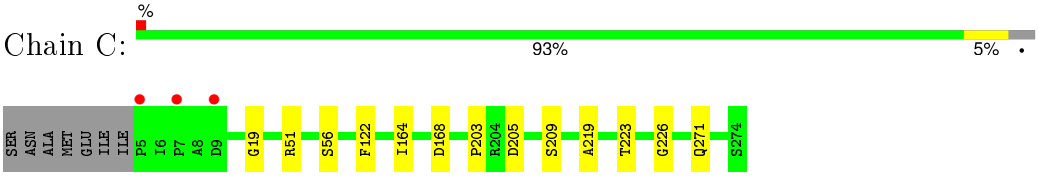
- Molecule 1: Pyrroline-5-carboxylate reductase

Chain B:



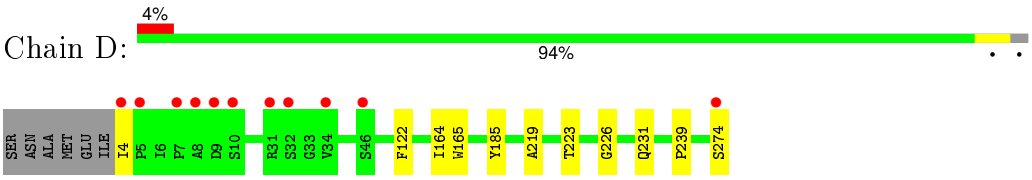
- Molecule 1: Pyrroline-5-carboxylate reductase

Chain C:



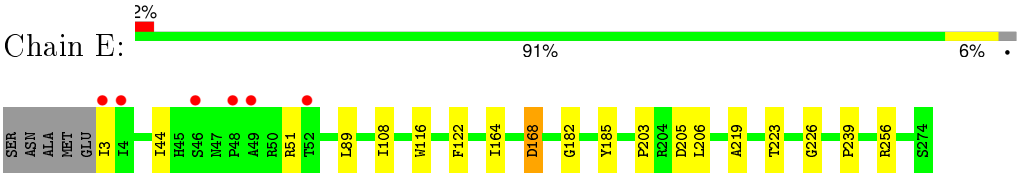
- Molecule 1: Pyrroline-5-carboxylate reductase

Chain D:



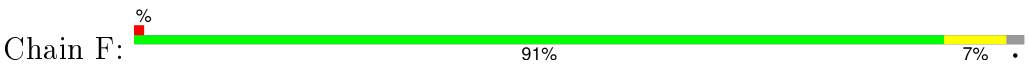
- Molecule 1: Pyrroline-5-carboxylate reductase

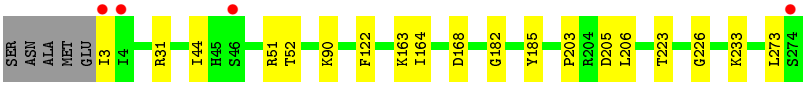
Chain E:



- Molecule 1: Pyrroline-5-carboxylate reductase

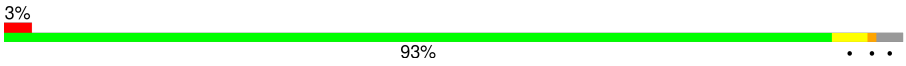
Chain F:

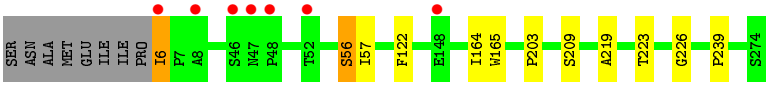




• Molecule 1: Pyrroline-5-carboxylate reductase

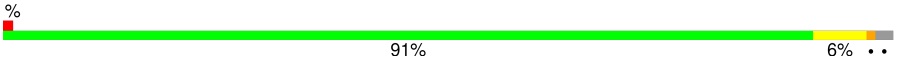
Chain G:





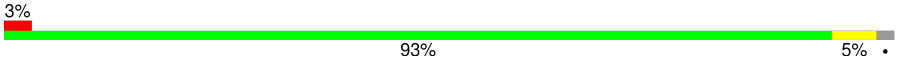
• Molecule 1: Pyrroline-5-carboxylate reductase

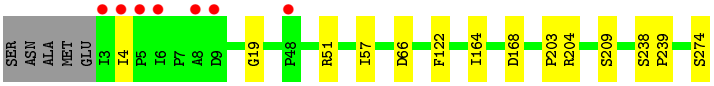
Chain H:



• Molecule 1: Pyrroline-5-carboxylate reductase

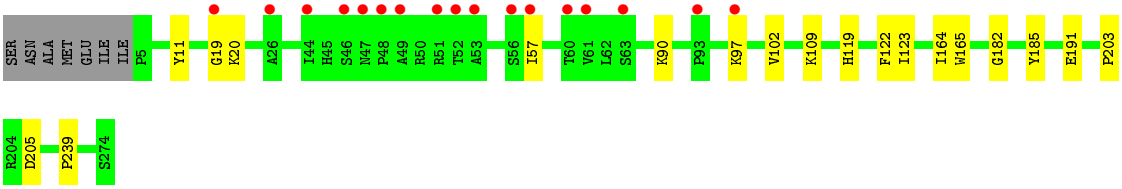
Chain I:





• Molecule 1: Pyrroline-5-carboxylate reductase

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	87.24Å 100.30Å 100.79Å 68.13° 85.76° 89.30°	Depositor
Resolution (Å)	39.39 – 1.95 39.39 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.39-1.95) 86.1 (39.39-1.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.155 , 0.178 0.167 , 0.188	Depositor DCC
R_{free} test set	2253 reflections (1.01%)	DCC
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.6	EDS
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 225657 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22670	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 3.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, NAP, 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	0.95	1/2049 (0.0%)	0.87	4/2774 (0.1%)
1	B	0.92	0/2040	0.89	3/2760 (0.1%)
1	C	0.90	0/2037	0.87	3/2754 (0.1%)
1	D	0.81	0/2041	0.86	1/2761 (0.0%)
1	E	0.90	0/2061	0.87	5/2788 (0.2%)
1	F	0.92	0/2065	0.88	4/2788 (0.1%)
1	G	0.87	0/2018	0.84	1/2728 (0.0%)
1	H	0.96	2/2034 (0.1%)	0.88	3/2751 (0.1%)
1	I	0.87	0/2030	0.88	2/2747 (0.1%)
1	J	0.95	2/2005 (0.1%)	0.86	1/2712 (0.0%)
All	All	0.91	5/20380 (0.0%)	0.87	27/27563 (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	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	191	GLU	CD-OE1	5.64	1.31	1.25
1	H	251	GLU	CD-OE1	5.29	1.31	1.25
1	J	11	TYR	CE1-CZ	5.25	1.45	1.38
1	A	155	SER	CB-OG	-5.10	1.35	1.42
1	H	11	TYR	CE1-CZ	5.07	1.45	1.38

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	274	SER	N-CA-CB	5.98	119.47	110.50
1	E	108	ILE	CG1-CB-CG2	-5.91	98.40	111.40
1	C	51	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	F	31	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	H	51	ARG	NE-CZ-NH1	5.76	123.18	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	273	LEU	Peptide

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	2020	0	2077	9	0
1	B	2011	0	2070	5	0
1	C	2008	0	2058	13	0
1	D	2012	0	2066	7	0
1	E	2032	0	2089	14	0
1	F	2034	0	2104	10	0
1	G	1990	0	2044	11	0
1	H	2002	0	2070	14	0
1	I	2001	0	2069	11	0
1	J	1976	0	2034	15	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	0	0
2	H	48	0	25	1	0
2	I	48	0	25	1	0
2	J	48	0	25	2	0
3	A	13	0	14	0	0
3	B	13	0	14	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	13	0	15	0	0
3	D	13	0	14	0	0
3	E	13	0	15	0	0
3	F	13	0	14	1	0
3	G	13	0	14	1	0
3	H	13	0	15	0	0
3	I	13	0	14	0	0
3	J	13	0	15	2	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	1	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	1	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	248	0	0	1	0
5	B	203	0	0	1	0
5	C	206	0	0	7	0
5	D	159	0	0	5	0
5	E	205	0	0	8	0
5	F	231	0	0	6	0
5	G	155	0	0	5	0
5	H	194	0	0	4	0
5	I	194	0	0	3	0
5	J	169	0	0	2	0
All	All	22670	0	21075	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 100 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:168[B]:ASP:OD1	5:C:402:HOH:O	1.72	1.05
1:E:168[A]:ASP:OD1	5:E:402:HOH:O	1.90	0.89
1:E:89[A]:LEU:HD21	5:E:572:HOH:O	1.78	0.83
1:J:97:LYS:HE3	1:J:119:HIS:HB3	1.62	0.82
1:F:163[B]:LYS:HE2	5:F:401:HOH:O	1.83	0.78

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	275/277 (99%)	271 (98%)	4 (2%)	0	100	100
1	B	273/277 (99%)	268 (98%)	5 (2%)	0	100	100
1	C	273/277 (99%)	266 (97%)	7 (3%)	0	100	100
1	D	273/277 (99%)	267 (98%)	6 (2%)	0	100	100
1	E	276/277 (100%)	271 (98%)	5 (2%)	0	100	100
1	F	275/277 (99%)	270 (98%)	5 (2%)	0	100	100
1	G	271/277 (98%)	268 (99%)	3 (1%)	0	100	100
1	H	273/277 (99%)	268 (98%)	5 (2%)	0	100	100
1	I	272/277 (98%)	267 (98%)	5 (2%)	0	100	100
1	J	269/277 (97%)	266 (99%)	3 (1%)	0	100	100
All	All	2730/2770 (99%)	2682 (98%)	48 (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	213/212 (100%)	209 (98%)	4 (2%)	65	58
1	B	211/212 (100%)	208 (99%)	3 (1%)	74	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	210/212 (99%)	207 (99%)	3 (1%)	74	70
1	D	211/212 (100%)	208 (99%)	3 (1%)	74	70
1	E	213/212 (100%)	210 (99%)	3 (1%)	74	70
1	F	214/212 (101%)	210 (98%)	4 (2%)	65	58
1	G	208/212 (98%)	204 (98%)	4 (2%)	65	58
1	H	210/212 (99%)	206 (98%)	4 (2%)	65	58
1	I	210/212 (99%)	207 (99%)	3 (1%)	74	70
1	J	207/212 (98%)	205 (99%)	2 (1%)	82	80
All	All	2107/2120 (99%)	2074 (98%)	33 (2%)	70	66

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	122	PHE
1	F	164	ILE
1	I	164	ILE
1	E	164	ILE
1	F	44	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN

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 (i)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	NAP	A	301	-	45,52,52	1.45	9 (20%)	55,80,80	1.64	9 (16%)
3	MPO	A	302	-	13,13,13	2.41	4 (30%)	16,17,17	1.36	2 (12%)
2	NAP	B	301	-	45,52,52	1.52	9 (20%)	55,80,80	1.69	9 (16%)
3	MPO	B	302	-	13,13,13	2.47	3 (23%)	16,17,17	1.80	4 (25%)
2	NAP	C	301	-	45,52,52	1.45	8 (17%)	55,80,80	1.75	11 (20%)
3	MPO	C	302	-	13,13,13	2.30	4 (30%)	16,17,17	1.48	1 (6%)
2	NAP	D	301	-	45,52,52	1.25	6 (13%)	55,80,80	1.78	6 (10%)
3	MPO	D	302	-	13,13,13	2.22	4 (30%)	16,17,17	2.50	5 (31%)
2	NAP	E	301	-	45,52,52	1.47	10 (22%)	55,80,80	1.50	7 (12%)
3	MPO	E	302	-	13,13,13	2.42	3 (23%)	16,17,17	1.77	4 (25%)
2	NAP	F	301	-	45,52,52	1.37	9 (20%)	55,80,80	1.40	7 (12%)
3	MPO	F	302	-	13,13,13	2.22	4 (30%)	16,17,17	1.13	2 (12%)
2	NAP	G	301	-	45,52,52	1.23	5 (11%)	55,80,80	1.51	10 (18%)
3	MPO	G	302	-	13,13,13	2.61	4 (30%)	16,17,17	2.77	4 (25%)
2	NAP	H	301	-	45,52,52	1.47	8 (17%)	55,80,80	1.74	12 (21%)
3	MPO	H	302	-	13,13,13	2.00	3 (23%)	16,17,17	1.48	3 (18%)
2	NAP	I	301	-	45,52,52	1.41	8 (17%)	55,80,80	1.59	5 (9%)
3	MPO	I	302	-	13,13,13	2.48	4 (30%)	16,17,17	1.96	2 (12%)
2	NAP	J	301	-	45,52,52	1.29	7 (15%)	55,80,80	1.70	9 (16%)
3	MPO	J	302	-	13,13,13	2.54	4 (30%)	16,17,17	2.03	5 (31%)

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	NAP	A	301	-	-	0/27/67/67	0/5/5/5
3	MPO	A	302	-	-	0/7/15/15	0/1/1/1
2	NAP	B	301	-	-	0/27/67/67	0/5/5/5
3	MPO	B	302	-	-	0/7/15/15	0/1/1/1
2	NAP	C	301	-	-	0/27/67/67	0/5/5/5
3	MPO	C	302	-	-	0/7/15/15	0/1/1/1
2	NAP	D	301	-	-	0/27/67/67	0/5/5/5
3	MPO	D	302	-	-	0/7/15/15	0/1/1/1
2	NAP	E	301	-	-	0/27/67/67	0/5/5/5
3	MPO	E	302	-	-	0/7/15/15	0/1/1/1
2	NAP	F	301	-	-	0/27/67/67	0/5/5/5
3	MPO	F	302	-	-	0/7/15/15	0/1/1/1
2	NAP	G	301	-	-	0/27/67/67	0/5/5/5
3	MPO	G	302	-	-	0/7/15/15	0/1/1/1
2	NAP	H	301	-	-	0/27/67/67	0/5/5/5
3	MPO	H	302	-	-	0/7/15/15	0/1/1/1
2	NAP	I	301	-	-	0/27/67/67	0/5/5/5
3	MPO	I	302	-	-	0/7/15/15	0/1/1/1
2	NAP	J	301	-	-	0/27/67/67	0/5/5/5
3	MPO	J	302	-	-	0/7/15/15	0/1/1/1

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	302	MPO	C1-S1	-7.97	1.65	1.77
3	E	302	MPO	C1-S1	-7.34	1.66	1.77
3	G	302	MPO	C1-S1	-7.31	1.66	1.77
3	I	302	MPO	C1-S1	-7.24	1.66	1.77
3	B	302	MPO	C1-S1	-7.04	1.66	1.77

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	NAP	N3A-C2A-N1A	-7.46	123.01	128.87
2	I	301	NAP	N3A-C2A-N1A	-7.13	123.27	128.87
2	C	301	NAP	N3A-C2A-N1A	-6.21	124.00	128.87
2	E	301	NAP	N3A-C2A-N1A	-6.02	124.14	128.87
2	B	301	NAP	N3A-C2A-N1A	-5.76	124.35	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	1	0
3	B	302	MPO	3	0
2	C	301	NAP	1	0
3	F	302	MPO	1	0
3	G	302	MPO	1	0
2	H	301	NAP	1	0
2	I	301	NAP	1	0
2	J	301	NAP	2	0
3	J	302	MPO	2	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	272/277 (98%)	-0.57	0 100 100	14, 22, 40, 62	0
1	B	272/277 (98%)	-0.20	5 (1%) 71 80	14, 26, 58, 86	0
1	C	270/277 (97%)	-0.37	3 (1%) 82 88	14, 25, 47, 77	0
1	D	271/277 (97%)	-0.09	11 (4%) 41 52	14, 33, 66, 96	0
1	E	272/277 (98%)	-0.22	6 (2%) 65 74	14, 25, 51, 74	0
1	F	272/277 (98%)	-0.46	4 (1%) 76 84	14, 23, 48, 69	0
1	G	269/277 (97%)	-0.01	7 (2%) 59 69	14, 35, 73, 89	0
1	H	272/277 (98%)	-0.27	4 (1%) 76 84	14, 27, 59, 85	0
1	I	272/277 (98%)	-0.31	7 (2%) 59 69	14, 28, 57, 82	0
1	J	270/277 (97%)	0.01	17 (6%) 23 33	14, 34, 67, 89	0
All	All	2712/2770 (97%)	-0.25	64 (2%) 62 72	14, 27, 60, 96	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	4	ILE	6.9
1	H	3	ILE	6.8
1	D	4	ILE	6.4
1	J	57	ILE	6.3
1	D	8	ALA	5.0

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MPO	B	302	13/13	0.88	0.16	3.52	36,45,65,65	0
3	MPO	J	302	13/13	0.91	0.14	2.11	36,49,61,62	0
3	MPO	F	302	13/13	0.95	0.11	1.93	22,25,33,34	0
3	MPO	I	302	13/13	0.96	0.10	1.30	27,29,41,42	0
3	MPO	H	302	13/13	0.95	0.10	1.24	22,24,33,35	0
3	MPO	A	302	13/13	0.96	0.10	0.82	20,24,27,28	0
3	MPO	G	302	13/13	0.95	0.11	0.75	32,43,51,56	0
2	NAP	G	301	48/48	0.94	0.14	0.38	26,39,65,79	0
3	MPO	D	302	13/13	0.94	0.10	0.30	26,30,48,51	0
3	MPO	C	302	13/13	0.96	0.08	0.29	24,28,36,36	0
2	NAP	A	301	48/48	0.97	0.08	0.28	16,21,34,38	0
2	NAP	H	301	48/48	0.96	0.10	0.25	17,32,52,74	0
2	NAP	J	301	48/48	0.93	0.15	0.23	23,37,60,78	0
2	NAP	D	301	48/48	0.95	0.10	0.05	27,35,56,64	0
2	NAP	F	301	48/48	0.97	0.07	-0.31	20,29,50,55	0
2	NAP	I	301	48/48	0.96	0.08	-0.34	18,27,48,60	0
3	MPO	E	302	13/13	0.96	0.09	-0.44	23,27,36,38	0
2	NAP	E	301	48/48	0.96	0.08	-0.45	21,33,54,67	0
2	NAP	C	301	48/48	0.96	0.07	-0.54	22,27,43,51	0
2	NAP	B	301	48/48	0.97	0.08	-0.64	20,32,44,64	0
4	CL	A	303	1/1	0.98	0.07	-1.04	31,31,31,31	0
4	CL	H	303	1/1	0.97	0.06	-1.18	29,29,29,29	0
4	CL	F	303	1/1	1.00	0.05	-2.03	24,24,24,24	0
4	CL	I	303	1/1	0.99	0.04	-2.16	30,30,30,30	0
4	CL	C	303	1/1	0.99	0.05	-2.21	25,25,25,25	0
4	CL	B	303	1/1	0.99	0.04	-2.40	22,22,22,22	0
4	CL	G	303	1/1	0.99	0.03	-2.49	23,23,23,23	0
4	CL	E	303	1/1	0.99	0.04	-2.59	22,22,22,22	0
4	CL	D	303	1/1	1.00	0.04	-3.13	23,23,23,23	0
4	CL	J	303	1/1	0.98	0.05	-4.16	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.