Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:10 PM GMT

PDB ID : 4UXA

Title : Improved variant of (R)-selective manganese-dependent hydroxynitrile lyase from bacteria

Authors : Pavkov-Keller, T.; Wiedner, R.; Kothbauer, B.; Gruber-Khadjawi, M.; Schwab, H.; Steiner, K.; Gruber, K.

Deposited on : 2014-08-21

Resolution : 2.10 Å(reported)

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

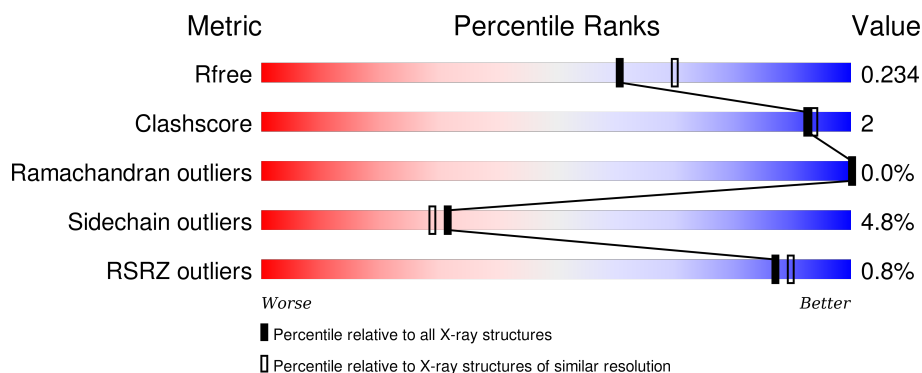|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		2
Ramachandran outliers		0.0%
Sidechain outliers		4.8%
RSRZ outliers		0.8%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	131	2% 94% 6%
1	B	131	% 88% 11% •
1	C	131	94% 6%
1	D	131	90% 10%
1	E	131	% 89% 10% •

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Mol	Chain	Length	Quality of chain
1	F	131	94% 5%
1	G	131	2% 95% 5%
1	H	131	92% 8%
1	I	131	2% 91% 9%
1	J	131	90% 10%
1	K	131	90% 8%
1	L	131	89% 10%
1	M	131	2% 94% 6%
1	N	131	% 85% 15%
1	O	131	96%
1	P	131	95%
1	Q	131	3% 92% 8%
1	R	131	% 93% 7%
1	S	131	2% 92% 8%
1	T	131	92% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21980 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 CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	B	131	Total	C	N	O	S	0	2	0
			1036	653	190	189	4			
1	C	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	D	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	E	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	F	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	G	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	H	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	I	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	J	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	K	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	L	131	Total	C	N	O	S	0	1	0
			1024	644	189	187	4			
1	M	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	N	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	O	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			
1	P	131	Total	C	N	O	S	0	0	0
			1013	638	185	186	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	131	Total 1013	C 638	N 185	O 186	S 4	0	0	0
1	R	131	Total 1013	C 638	N 185	O 186	S 4	0	0	0
1	S	131	Total 1013	C 638	N 185	O 186	S 4	0	0	0
1	T	131	Total 1013	C 638	N 185	O 186	S 4	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
A	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
A	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
B	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
B	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
B	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
C	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
C	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
C	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
D	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
D	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
D	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
E	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
E	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
E	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
F	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
F	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
F	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
G	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
G	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
G	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
H	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
H	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
H	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
I	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
I	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
I	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
J	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
J	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
J	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
K	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
K	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
L	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
L	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
L	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
M	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
M	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
M	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
N	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
N	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
N	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
O	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
O	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
O	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
P	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
P	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
P	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
Q	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
Q	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
Q	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
R	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
R	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
R	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
S	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
S	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
S	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5
T	40	HIS	ALA	ENGINEERED MUTATION	UNP E8WYN5
T	42	THR	VAL	ENGINEERED MUTATION	UNP E8WYN5
T	110	HIS	GLN	ENGINEERED MUTATION	UNP E8WYN5

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Mn	0	0
			1	1		
2	G	1	Total	Mn	0	0
			1	1		
2	J	1	Total	Mn	0	0
			1	1		
2	Q	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	T	1	Total 1	Mn 1	0	0
2	N	1	Total 1	Mn 1	0	0
2	O	1	Total 1	Mn 1	0	0
2	R	1	Total 1	Mn 1	0	0
2	L	1	Total 1	Mn 1	0	0
2	S	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0
2	M	1	Total 1	Mn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total 84	O 84	0	0
3	B	104	Total 104	O 104	0	0
3	C	93	Total 93	O 93	0	0
3	D	112	Total 112	O 112	0	0

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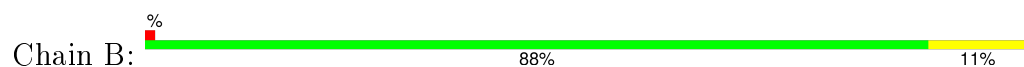| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	85	Total 85	O 85	0	0
3	F	96	Total 96	O 96	0	0
3	G	87	Total 87	O 87	0	0
3	H	77	Total 77	O 77	0	0
3	I	82	Total 82	O 82	0	0
3	J	70	Total 70	O 70	0	0
3	K	94	Total 94	O 94	0	0
3	L	86	Total 86	O 86	0	0
3	M	76	Total 76	O 76	0	0
3	N	90	Total 90	O 90	0	0
3	O	78	Total 78	O 78	0	0
3	P	89	Total 89	O 89	0	0
3	Q	71	Total 71	O 71	0	0
3	R	76	Total 76	O 76	0	0
3	S	54	Total 54	O 54	0	0
3	T	62	Total 62	O 62	0	0

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 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.
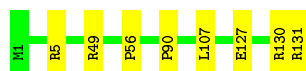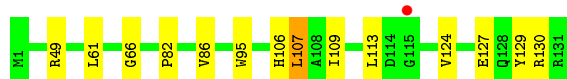
- Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

- Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

- Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN
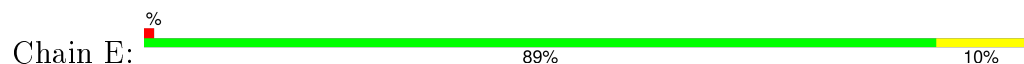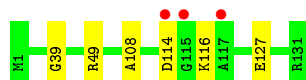

- Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

- Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

- Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain G:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain H:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain I:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain J:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain K:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain L:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain M:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain N:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain O:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain P:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN
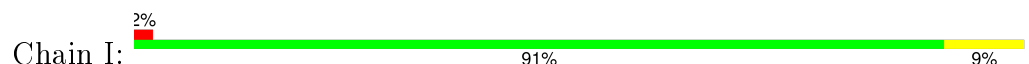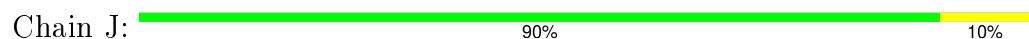
Chain Q:

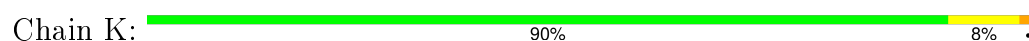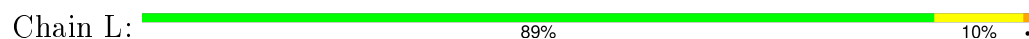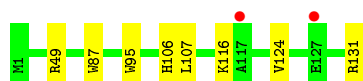• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain R:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain S:

• Molecule 1: CUPIN 2 CONSERVED BARREL DOMAIN PROTEIN

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.81Å　　93.17Å　　146.67Å 90.00°　　111.93°　　90.00°	Depositor
Resolution (Å)	58.28　　–　　2.10 58.28　　–　　2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (58.28-2.10) 99.6 (58.28-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.181　　,　　0.234 0.186　　,　　0.234	Depositor DCC
R_{free} test set	8937 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.9	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	2 of 178787 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21980	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.57	0/1047	0.73	0/1428
1	B	0.66	0/1071	0.75	0/1460
1	C	0.65	0/1047	0.76	0/1428
1	D	0.68	0/1047	0.76	0/1428
1	E	0.63	0/1047	0.73	0/1428
1	F	0.65	0/1047	0.77	0/1428
1	G	0.63	0/1047	0.73	0/1428
1	H	0.65	0/1047	0.74	0/1428
1	I	0.59	0/1047	0.72	0/1428
1	J	0.66	0/1047	0.73	0/1428
1	K	0.63	0/1047	0.76	0/1428
1	L	0.66	0/1058	0.78	0/1442
1	M	0.56	0/1047	0.72	0/1428
1	N	0.60	0/1047	0.76	2/1428 (0.1%)
1	O	0.65	0/1047	0.75	0/1428
1	P	0.68	0/1047	0.75	0/1428
1	Q	0.60	0/1047	0.74	0/1428
1	R	0.60	0/1047	0.73	0/1428
1	S	0.60	0/1047	0.77	2/1428 (0.1%)
1	T	0.59	0/1047	0.73	0/1428
All	All	0.63	0/20975	0.74	4/28606 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	24	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	S	24	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	N	130	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	N	17	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1013	0	956	2	0
1	B	1036	0	977	8	0
1	C	1013	0	956	2	0
1	D	1013	0	956	5	0
1	E	1013	0	956	7	0
1	F	1013	0	956	6	0
1	G	1013	0	956	2	0
1	H	1013	0	956	2	0
1	I	1013	0	956	6	0
1	J	1013	0	956	8	0
1	K	1013	0	956	5	0
1	L	1024	0	968	4	1
1	M	1013	0	956	2	0
1	N	1013	0	956	9	0
1	O	1013	0	956	0	0
1	P	1013	0	956	2	0
1	Q	1013	0	956	4	0
1	R	1013	0	956	5	0
1	S	1013	0	956	2	0
1	T	1013	0	956	4	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	A	84	0	0	0	0
3	B	104	0	0	2	0
3	C	93	0	0	0	0
3	D	112	0	0	2	0
3	E	85	0	0	1	0
3	F	96	0	0	2	0
3	G	87	0	0	1	0
3	H	77	0	0	0	0
3	I	82	0	0	2	0
3	J	70	0	0	2	0
3	K	94	0	0	1	0
3	L	86	0	0	1	0
3	M	76	0	0	0	0
3	N	90	0	0	2	0
3	O	78	0	0	0	0
3	P	89	0	0	2	0
3	Q	71	0	0	1	0
3	R	76	0	0	3	0
3	S	54	0	0	1	0
3	T	62	0	0	1	0
All	All	21980	0	19153	79	1

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.

All (79) 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:B:130[A]:ARG:NH2	3:B:2103:HOH:O	1.92	0.88
1:R:119:ASP:HB3	3:R:2068:HOH:O	1.79	0.81
1:J:4:LYS:HE2	3:J:2002:HOH:O	1.87	0.74
1:I:4:LYS:HD2	3:I:2010:HOH:O	1.89	0.72
1:I:115:GLY:HA3	3:I:2080:HOH:O	1.92	0.70
1:R:4:LYS:HE3	3:R:2030:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:ASP:HB3	3:L:2077:HOH:O	1.94	0.67
1:K:116:LYS:NZ	1:K:119:ASP:OD1	2.28	0.63
1:J:4:LYS:CE	3:J:2002:HOH:O	2.45	0.62
1:P:4:LYS:HE2	3:P:2006:HOH:O	2.02	0.60
1:F:131:ARG:OXT	1:F:131:ARG:HG2	2.03	0.58
1:R:130:ARG:HB2	1:R:131:ARG:HG3	1.85	0.57
1:A:127:GLU:O	1:A:130:ARG:NE	2.39	0.56
1:B:55:HIS:CD2	1:B:59:GLN:HB2	2.41	0.56
1:R:130:ARG:NH1	3:R:2075:HOH:O	2.39	0.55
1:S:72:ARG:HD3	3:S:2045:HOH:O	2.07	0.54
1:F:131:ARG:OXT	1:F:131:ARG:CG	2.56	0.53
1:E:129:TYR:O	1:E:130:ARG:HG3	2.08	0.53
1:D:98:ALA:HB1	1:D:102:THR:O	2.09	0.53
1:F:66:GLY:O	1:F:82:PRO:HD3	2.09	0.52
1:F:131:ARG:NH2	3:F:2067:HOH:O	2.42	0.52
1:M:95:TRP:CG	1:M:124:VAL:HG21	2.46	0.50
1:B:6:VAL:O	1:J:130:ARG:NH2	2.44	0.50
1:T:95:TRP:CG	1:T:124:VAL:HG21	2.47	0.50
1:M:87:TRP:O	1:N:1:MET:HA	2.11	0.50
1:A:5:ARG:NH2	1:N:131:ARG:HG3	2.26	0.49
1:Q:13:LYS:NZ	3:Q:2016:HOH:O	2.45	0.49
1:C:127:GLU:O	1:C:130:ARG:HG3	2.13	0.49
1:J:98:ALA:HB1	1:J:102:THR:O	2.13	0.48
1:E:107:LEU:HD13	1:E:109:ILE:HD11	1.95	0.48
1:J:95:TRP:CG	1:J:124:VAL:HG21	2.49	0.47
1:N:15:PRO:HG2	1:N:18:TRP:CE3	2.49	0.47
1:G:114:ASP:HB2	3:G:2076:HOH:O	2.14	0.47
1:I:77:VAL:HG21	1:I:130:ARG:O	2.15	0.47
1:T:4:LYS:HE3	3:T:2023:HOH:O	2.14	0.46
1:G:39:GLY:HA2	1:G:108:ALA:O	2.15	0.46
1:L:98:ALA:HB1	1:L:102:THR:O	2.16	0.45
1:B:4:LYS:HE3	3:B:2039:HOH:O	2.16	0.45
1:D:4:LYS:HE3	3:D:2044:HOH:O	2.16	0.45
1:S:95:TRP:CG	1:S:124:VAL:HG21	2.50	0.45
1:B:98:ALA:HB1	1:B:102:THR:O	2.16	0.45
1:K:66:GLY:O	1:K:82:PRO:HD3	2.17	0.45
1:H:56:PRO:O	1:H:90:PRO:HB3	2.17	0.45
1:E:113:LEU:HA	3:E:2073:HOH:O	2.17	0.45
1:N:55:HIS:CD2	1:N:59:GLN:HB2	2.51	0.44
1:P:131:ARG:O	3:P:2089:HOH:O	2.21	0.44
1:B:61:LEU:HB2	1:B:86:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:61:LEU:HB2	1:N:86:VAL:HB	2.00	0.44
3:K:2078:HOH:O	1:L:4:LYS:HE2	2.17	0.44
1:H:95:TRP:CG	1:H:124:VAL:HG21	2.53	0.44
1:C:56:PRO:O	1:C:90:PRO:HB3	2.18	0.44
1:L:66:GLY:O	1:L:82:PRO:HD3	2.18	0.44
1:Q:13:LYS:HA	1:Q:13:LYS:HE3	2.00	0.43
1:E:66:GLY:O	1:E:82:PRO:HD3	2.19	0.43
1:E:61:LEU:HB2	1:E:86:VAL:HB	2.01	0.43
1:D:18:TRP:HE3	3:D:2022:HOH:O	2.01	0.43
1:E:95:TRP:CG	1:E:124:VAL:HG21	2.53	0.43
1:F:130:ARG:HG2	3:F:2095:HOH:O	2.18	0.43
1:K:38:ALA:HB2	1:K:112:ARG:HH11	1.84	0.42
1:T:98:ALA:HB1	1:T:102:THR:O	2.20	0.42
1:I:66:GLY:O	1:I:82:PRO:HD3	2.20	0.42
1:D:66:GLY:O	1:D:82:PRO:HD3	2.20	0.42
1:B:66:GLY:O	1:B:82:PRO:HD3	2.20	0.42
1:I:87:TRP:O	1:J:1:MET:HA	2.20	0.41
1:K:127:GLU:HA	1:K:130:ARG:HH21	1.84	0.41
1:K:112:ARG:HG2	1:K:117:ALA:HB2	2.02	0.41
1:N:95:TRP:CG	1:N:124:VAL:HG21	2.55	0.41
1:D:30:GLN:HE21	1:D:112:ARG:NE	2.18	0.41
1:E:127:GLU:O	1:E:130:ARG:NH2	2.54	0.41
1:B:130[B]:ARG:HD2	1:N:79:GLU:OE2	2.20	0.41
1:R:95:TRP:CG	1:R:124:VAL:HG21	2.55	0.41
1:I:72:ARG:HG2	1:J:1:MET:HB3	2.03	0.41
1:Q:72:ARG:HD3	1:Q:92:GLU:OE2	2.21	0.41
1:J:66:GLY:O	1:J:82:PRO:HD3	2.20	0.41
1:N:116:LYS:NZ	3:N:2083:HOH:O	2.54	0.40
1:Q:36:LEU:O	1:Q:112:ARG:HG2	2.22	0.40
1:T:66:GLY:O	1:T:82:PRO:HD3	2.20	0.40
1:F:106:HIS:C	1:F:106:HIS:HD1	2.24	0.40
1:N:72:ARG:HD3	3:N:2073:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:ARG:NH2	1:T:130:ARG:O[1_565]	2.09	0.11

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	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
1	B	131/131 (100%)	128 (98%)	2 (2%)	1 (1%)	24	17
1	C	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	D	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	E	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	F	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	G	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	H	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
1	I	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	J	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	K	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	L	130/131 (99%)	127 (98%)	3 (2%)	0	100	100
1	M	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	N	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	O	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
1	P	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	Q	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
1	R	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
1	S	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
1	T	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
All	All	2583/2620 (99%)	2520 (98%)	62 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	ASP

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	101/101 (100%)	96 (95%)	5 (5%)	30	27
1	B	103/101 (102%)	97 (94%)	6 (6%)	25	21
1	C	101/101 (100%)	97 (96%)	4 (4%)	38	38
1	D	101/101 (100%)	96 (95%)	5 (5%)	30	27
1	E	101/101 (100%)	98 (97%)	3 (3%)	48	51
1	F	101/101 (100%)	97 (96%)	4 (4%)	38	38
1	G	101/101 (100%)	98 (97%)	3 (3%)	48	51
1	H	101/101 (100%)	95 (94%)	6 (6%)	24	20
1	I	101/101 (100%)	97 (96%)	4 (4%)	38	38
1	J	101/101 (100%)	97 (96%)	4 (4%)	38	38
1	K	101/101 (100%)	94 (93%)	7 (7%)	19	15
1	L	102/101 (101%)	94 (92%)	8 (8%)	16	11
1	M	101/101 (100%)	96 (95%)	5 (5%)	30	27
1	N	101/101 (100%)	97 (96%)	4 (4%)	38	38
1	O	101/101 (100%)	96 (95%)	5 (5%)	30	27
1	P	101/101 (100%)	96 (95%)	5 (5%)	30	27
1	Q	101/101 (100%)	94 (93%)	7 (7%)	19	15
1	R	101/101 (100%)	98 (97%)	3 (3%)	48	51
1	S	101/101 (100%)	94 (93%)	7 (7%)	19	15
1	T	101/101 (100%)	98 (97%)	3 (3%)	48	51
All	All	2023/2020 (100%)	1925 (95%)	98 (5%)	31	29

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	49	ARG
1	A	106	HIS

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Mol	Chain	Res	Type
1	A	114	ASP
1	A	119	ASP
1	B	49	ARG
1	B	106	HIS
1	B	107	LEU
1	B	127	GLU
1	B	130[A]	ARG
1	B	130[B]	ARG
1	C	5	ARG
1	C	49	ARG
1	C	107	LEU
1	C	131	ARG
1	D	2	GLU
1	D	49	ARG
1	D	96	HIS
1	D	107	LEU
1	D	127	GLU
1	E	49	ARG
1	E	106	HIS
1	E	107	LEU
1	F	49	ARG
1	F	78	GLU
1	F	106	HIS
1	F	107	LEU
1	G	49	ARG
1	G	116	LYS
1	G	127	GLU
1	H	33	ASP
1	H	49	ARG
1	H	106	HIS
1	H	107	LEU
1	H	116	LYS
1	H	130	ARG
1	I	49	ARG
1	I	107	LEU
1	I	112	ARG
1	I	116	LYS
1	J	2	GLU
1	J	30	GLN
1	J	49	ARG
1	J	107	LEU
1	K	2	GLU

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Mol	Chain	Res	Type
1	K	49	ARG
1	K	107	LEU
1	K	119	ASP
1	K	127	GLU
1	K	130	ARG
1	K	131	ARG
1	L	49	ARG
1	L	100	PRO
1	L	106	HIS
1	L	107	LEU
1	L	110	HIS
1	L	114	ASP
1	L	127	GLU
1	L	131	ARG
1	M	49	ARG
1	M	106	HIS
1	M	107	LEU
1	M	116	LYS
1	M	131	ARG
1	N	49	ARG
1	N	106	HIS
1	N	107	LEU
1	N	110	HIS
1	O	49	ARG
1	O	106	HIS
1	O	107	LEU
1	O	130	ARG
1	O	131	ARG
1	P	49	ARG
1	P	106	HIS
1	P	107	LEU
1	P	127	GLU
1	P	131	ARG
1	Q	13	LYS
1	Q	33	ASP
1	Q	49	ARG
1	Q	96	HIS
1	Q	100	PRO
1	Q	107	LEU
1	Q	110	HIS
1	R	49	ARG
1	R	107	LEU

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Mol	Chain	Res	Type
1	R	127	GLU
1	S	36	LEU
1	S	49	ARG
1	S	107	LEU
1	S	110	HIS
1	S	116	LYS
1	S	127	GLU
1	S	130	ARG
1	T	49	ARG
1	T	107	LEU
1	T	131	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	30	GLN
1	G	123	HIS
1	H	30	GLN
1	J	30	GLN
1	J	123	HIS
1	K	40	HIS
1	M	123	HIS
1	N	123	HIS
1	T	30	GLN
1	T	123	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	131/131 (100%)	-0.31	3 (2%)	64	70	28, 40, 60, 73	0
1	B	131/131 (100%)	-0.28	1 (0%)	87	90	24, 32, 52, 77	0
1	C	131/131 (100%)	-0.40	0	100	100	27, 35, 54, 68	0
1	D	131/131 (100%)	-0.18	0	100	100	22, 30, 48, 58	0
1	E	131/131 (100%)	-0.29	1 (0%)	87	90	27, 38, 53, 70	0
1	F	131/131 (100%)	-0.27	0	100	100	26, 34, 55, 72	0
1	G	131/131 (100%)	-0.30	3 (2%)	64	70	26, 33, 56, 80	0
1	H	131/131 (100%)	-0.18	0	100	100	27, 35, 53, 66	0
1	I	131/131 (100%)	-0.17	3 (2%)	64	70	29, 41, 62, 77	0
1	J	131/131 (100%)	-0.28	0	100	100	26, 36, 55, 69	0
1	K	131/131 (100%)	-0.42	0	100	100	26, 35, 54, 66	0
1	L	131/131 (100%)	-0.24	0	100	100	26, 33, 52, 64	0
1	M	131/131 (100%)	-0.17	2 (1%)	76	81	29, 43, 65, 78	0
1	N	131/131 (100%)	-0.31	1 (0%)	87	90	24, 33, 53, 70	0
1	O	131/131 (100%)	-0.44	0	100	100	26, 35, 53, 65	0
1	P	131/131 (100%)	-0.20	0	100	100	24, 30, 47, 61	0
1	Q	131/131 (100%)	0.03	4 (3%)	52	61	32, 44, 67, 74	0
1	R	131/131 (100%)	-0.13	1 (0%)	87	90	29, 39, 62, 74	0
1	S	131/131 (100%)	0.03	3 (2%)	64	70	31, 43, 63, 81	0
1	T	131/131 (100%)	-0.06	0	100	100	27, 39, 62, 78	0
All	All	2620/2620 (100%)	-0.23	22 (0%)	87	90	22, 37, 58, 81	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	115	GLY	4.6
1	G	117	ALA	3.6
1	Q	117	ALA	3.4
1	E	115	GLY	3.4
1	I	115	GLY	3.1
1	R	115	GLY	2.8
1	I	114	ASP	2.7
1	A	114	ASP	2.5
1	N	115	GLY	2.5
1	G	114	ASP	2.4
1	B	115	GLY	2.4
1	A	115	GLY	2.3
1	A	117	ALA	2.3
1	M	117	ALA	2.3
1	S	117	ALA	2.1
1	Q	34	PRO	2.1
1	Q	127	GLU	2.1
1	S	127	GLU	2.1
1	I	113	LEU	2.1
1	M	127	GLU	2.1
1	Q	120	TRP	2.0
1	S	114	ASP	2.0

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 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, 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	LLDF	B-factors(Å²)	Q<0.9
2	MN	F	200	1/1	0.99	0.09	1.27	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	MN	D	200	1/1	0.99	0.10	0.96	30,30,30,30	0
2	MN	L	200	1/1	1.00	0.09	0.42	40,40,40,40	0
2	MN	K	200	1/1	0.99	0.08	-0.23	35,35,35,35	0
2	MN	J	200	1/1	0.99	0.08	-0.52	39,39,39,39	0
2	MN	R	200	1/1	0.99	0.09	-0.85	45,45,45,45	0
2	MN	T	200	1/1	0.99	0.08	-1.08	43,43,43,43	0
2	MN	P	200	1/1	0.99	0.08	-1.16	34,34,34,34	0
2	MN	B	200	1/1	0.99	0.07	-1.58	39,39,39,39	0
2	MN	H	200	1/1	1.00	0.07	-1.63	38,38,38,38	0
2	MN	N	200	1/1	0.99	0.07	-1.66	40,40,40,40	0
2	MN	E	200	1/1	0.99	0.06	-2.36	40,40,40,40	0
2	MN	I	200	1/1	0.99	0.05	-3.52	48,48,48,48	0
2	MN	O	200	1/1	0.99	0.06	-3.61	40,40,40,40	0
2	MN	G	200	1/1	0.99	0.06	-3.97	44,44,44,44	0
2	MN	M	200	1/1	0.99	0.04	-4.06	50,50,50,50	0
2	MN	Q	200	1/1	0.99	0.05	-4.91	47,47,47,47	0
2	MN	A	200	1/1	0.99	0.06	-4.98	44,44,44,44	0
2	MN	S	200	1/1	1.00	0.05	-6.42	47,47,47,47	0
2	MN	C	200	1/1	0.99	0.03	-6.78	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.