Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:38 PM GMT

PDB ID	:	4FO8
Title	:	Pseudomonas aeruginosa MetAP with Met, in Mn form
Authors	:	Ye, Q.Z.; Lu, J.P.
Deposited on	:	2012-06-20
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

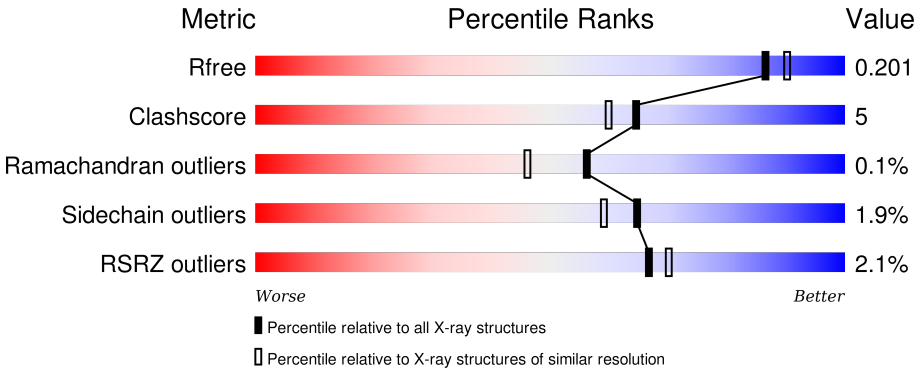
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	280	2% 81% 10% • 8%
1	B	280	% 83% 10% 7%
1	C	280	3% 85% 9% • 5%
1	D	280	2% 82% 10% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9002 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 Methionine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	3	0
			2059	1301	357	389	12			
1	B	261	Total	C	N	O	S	0	2	0
			2059	1299	358	390	12			
1	C	266	Total	C	N	O	S	0	1	0
			2093	1322	361	398	12			
1	D	259	Total	C	N	O	S	0	3	0
			2053	1294	359	387	13			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	GLU	-	EXPRESSION TAG	UNP Q9HXY1
A	263	PHE	-	EXPRESSION TAG	UNP Q9HXY1
A	264	GLU	-	EXPRESSION TAG	UNP Q9HXY1
A	265	LEU	-	EXPRESSION TAG	UNP Q9HXY1
A	266	VAL	-	EXPRESSION TAG	UNP Q9HXY1
A	267	ASP	-	EXPRESSION TAG	UNP Q9HXY1
A	268	LYS	-	EXPRESSION TAG	UNP Q9HXY1
A	269	LEU	-	EXPRESSION TAG	UNP Q9HXY1
A	270	ALA	-	EXPRESSION TAG	UNP Q9HXY1
A	271	ALA	-	EXPRESSION TAG	UNP Q9HXY1
A	272	ALA	-	EXPRESSION TAG	UNP Q9HXY1
A	273	LEU	-	EXPRESSION TAG	UNP Q9HXY1
A	274	GLU	-	EXPRESSION TAG	UNP Q9HXY1
A	275	HIS	-	EXPRESSION TAG	UNP Q9HXY1
A	276	HIS	-	EXPRESSION TAG	UNP Q9HXY1
A	277	HIS	-	EXPRESSION TAG	UNP Q9HXY1
A	278	HIS	-	EXPRESSION TAG	UNP Q9HXY1
A	279	HIS	-	EXPRESSION TAG	UNP Q9HXY1
A	280	HIS	-	EXPRESSION TAG	UNP Q9HXY1
B	262	GLU	-	EXPRESSION TAG	UNP Q9HXY1
B	263	PHE	-	EXPRESSION TAG	UNP Q9HXY1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	GLU	-	EXPRESSION TAG	UNP Q9HXY1
B	265	LEU	-	EXPRESSION TAG	UNP Q9HXY1
B	266	VAL	-	EXPRESSION TAG	UNP Q9HXY1
B	267	ASP	-	EXPRESSION TAG	UNP Q9HXY1
B	268	LYS	-	EXPRESSION TAG	UNP Q9HXY1
B	269	LEU	-	EXPRESSION TAG	UNP Q9HXY1
B	270	ALA	-	EXPRESSION TAG	UNP Q9HXY1
B	271	ALA	-	EXPRESSION TAG	UNP Q9HXY1
B	272	ALA	-	EXPRESSION TAG	UNP Q9HXY1
B	273	LEU	-	EXPRESSION TAG	UNP Q9HXY1
B	274	GLU	-	EXPRESSION TAG	UNP Q9HXY1
B	275	HIS	-	EXPRESSION TAG	UNP Q9HXY1
B	276	HIS	-	EXPRESSION TAG	UNP Q9HXY1
B	277	HIS	-	EXPRESSION TAG	UNP Q9HXY1
B	278	HIS	-	EXPRESSION TAG	UNP Q9HXY1
B	279	HIS	-	EXPRESSION TAG	UNP Q9HXY1
B	280	HIS	-	EXPRESSION TAG	UNP Q9HXY1
C	262	GLU	-	EXPRESSION TAG	UNP Q9HXY1
C	263	PHE	-	EXPRESSION TAG	UNP Q9HXY1
C	264	GLU	-	EXPRESSION TAG	UNP Q9HXY1
C	265	LEU	-	EXPRESSION TAG	UNP Q9HXY1
C	266	VAL	-	EXPRESSION TAG	UNP Q9HXY1
C	267	ASP	-	EXPRESSION TAG	UNP Q9HXY1
C	268	LYS	-	EXPRESSION TAG	UNP Q9HXY1
C	269	LEU	-	EXPRESSION TAG	UNP Q9HXY1
C	270	ALA	-	EXPRESSION TAG	UNP Q9HXY1
C	271	ALA	-	EXPRESSION TAG	UNP Q9HXY1
C	272	ALA	-	EXPRESSION TAG	UNP Q9HXY1
C	273	LEU	-	EXPRESSION TAG	UNP Q9HXY1
C	274	GLU	-	EXPRESSION TAG	UNP Q9HXY1
C	275	HIS	-	EXPRESSION TAG	UNP Q9HXY1
C	276	HIS	-	EXPRESSION TAG	UNP Q9HXY1
C	277	HIS	-	EXPRESSION TAG	UNP Q9HXY1
C	278	HIS	-	EXPRESSION TAG	UNP Q9HXY1
C	279	HIS	-	EXPRESSION TAG	UNP Q9HXY1
C	280	HIS	-	EXPRESSION TAG	UNP Q9HXY1
D	262	GLU	-	EXPRESSION TAG	UNP Q9HXY1
D	263	PHE	-	EXPRESSION TAG	UNP Q9HXY1
D	264	GLU	-	EXPRESSION TAG	UNP Q9HXY1
D	265	LEU	-	EXPRESSION TAG	UNP Q9HXY1
D	266	VAL	-	EXPRESSION TAG	UNP Q9HXY1
D	267	ASP	-	EXPRESSION TAG	UNP Q9HXY1

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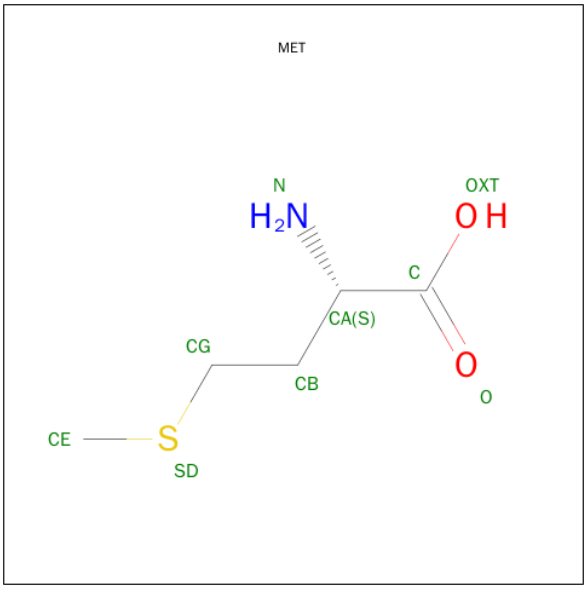
Chain	Residue	Modelled	Actual	Comment	Reference
D	268	LYS	-	EXPRESSION TAG	UNP Q9HXY1
D	269	LEU	-	EXPRESSION TAG	UNP Q9HXY1
D	270	ALA	-	EXPRESSION TAG	UNP Q9HXY1
D	271	ALA	-	EXPRESSION TAG	UNP Q9HXY1
D	272	ALA	-	EXPRESSION TAG	UNP Q9HXY1
D	273	LEU	-	EXPRESSION TAG	UNP Q9HXY1
D	274	GLU	-	EXPRESSION TAG	UNP Q9HXY1
D	275	HIS	-	EXPRESSION TAG	UNP Q9HXY1
D	276	HIS	-	EXPRESSION TAG	UNP Q9HXY1
D	277	HIS	-	EXPRESSION TAG	UNP Q9HXY1
D	278	HIS	-	EXPRESSION TAG	UNP Q9HXY1
D	279	HIS	-	EXPRESSION TAG	UNP Q9HXY1
D	280	HIS	-	EXPRESSION TAG	UNP Q9HXY1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mn 3 3	0	0
2	A	4	Total Mn 4 4	0	0
2	D	3	Total Mn 3 3	0	0
2	C	3	Total Mn 3 3	0	0

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	D	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 4 is water.

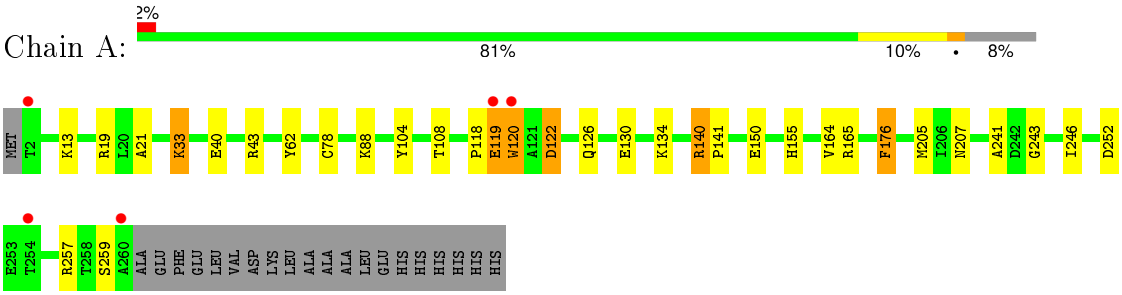
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total	O	0	0
			170	170		
4	B	188	Total	O	0	0
			188	188		
4	C	174	Total	O	0	0
			174	174		
4	D	157	Total	O	0	0
			157	157		

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.

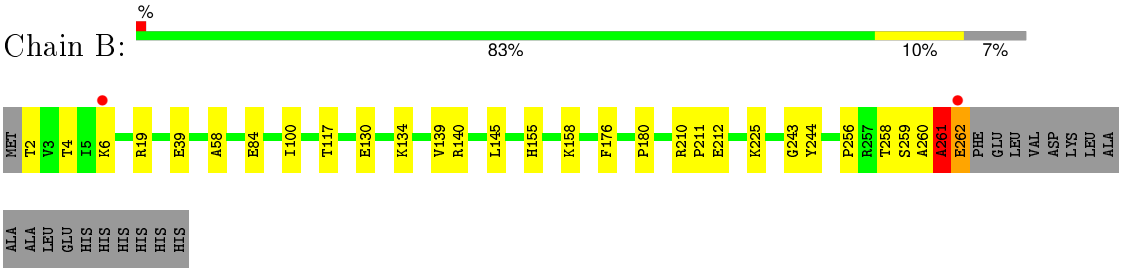
- Molecule 1: Methionine aminopeptidase

Chain A:



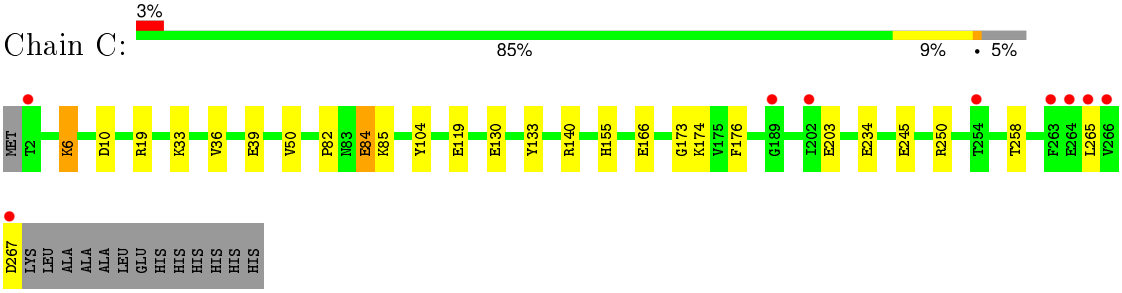
- Molecule 1: Methionine aminopeptidase

Chain B:



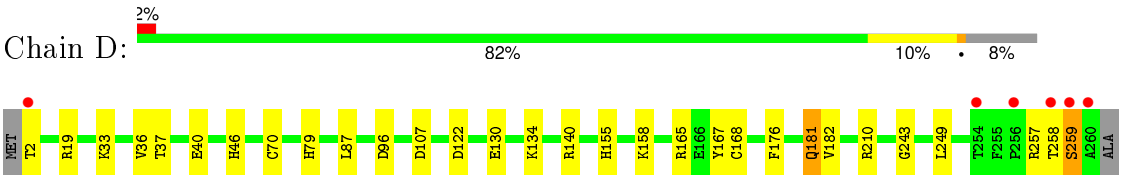
- Molecule 1: Methionine aminopeptidase

Chain C:



- Molecule 1: Methionine aminopeptidase

Chain D:




GLU
PHE
GLU
LEU
VAL
ASP
LYS
LEU
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.65Å 105.66Å 133.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.77 – 1.90 30.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.3 (30.77-1.90) 88.3 (30.77-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.47 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.157 , 0.200 0.158 , 0.201	Depositor DCC
R_{free} test set	4516 reflections (5.96%)	DCC
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 79778 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9002	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: 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	1.20	6/2103 (0.3%)	0.98	8/2847 (0.3%)
1	B	1.18	4/2101 (0.2%)	0.98	2/2842 (0.1%)
1	C	1.14	6/2136 (0.3%)	0.96	5/2891 (0.2%)
1	D	1.10	0/2095	0.92	4/2834 (0.1%)
All	All	1.16	16/8435 (0.2%)	0.96	19/11414 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	ALA	CA-CB	-6.38	1.39	1.52
1	A	88	LYS	CE-NZ	6.05	1.64	1.49
1	A	119	GLU	CB-CG	5.93	1.63	1.52
1	C	250	ARG	CZ-NH1	5.85	1.40	1.33
1	A	78	CYS	CB-SG	5.68	1.92	1.82
1	C	39	GLU	CG-CD	5.66	1.60	1.51
1	C	166	GLU	CB-CG	5.51	1.62	1.52
1	B	244	TYR	CG-CD2	5.50	1.46	1.39
1	A	119	GLU	CG-CD	5.40	1.60	1.51
1	A	150	GLU	CB-CG	5.28	1.62	1.52
1	B	139	VAL	CB-CG2	5.23	1.63	1.52
1	C	50	VAL	CB-CG1	5.21	1.63	1.52
1	A	62	TYR	CD2-CE2	5.09	1.47	1.39
1	C	133	TYR	CD1-CE1	5.09	1.47	1.39
1	B	84	GLU	CG-CD	5.04	1.59	1.51
1	C	104	TYR	CD2-CE2	5.00	1.46	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	250	ARG	NE-CZ-NH2	-10.20	115.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	165	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	B	140	ARG	CG-CD-NE	-8.16	94.66	111.80
1	B	19	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	A	19	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	120[A]	TRP	CB-CA-C	6.29	122.97	110.40
1	A	120[B]	TRP	CB-CA-C	6.29	122.97	110.40
1	A	122	ASP	CB-CA-C	-6.04	98.32	110.40
1	C	140	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	140	ARG	CG-CD-NE	-5.72	99.80	111.80
1	A	19	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	252	ASP	CB-CG-OD2	5.47	123.23	118.30
1	D	107	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	165	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	10	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	D	122	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	181	GLN	CB-CA-C	-5.25	99.89	110.40
1	C	6	LYS	CD-CE-NZ	5.09	123.40	111.70
1	C	19	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2059	0	2046	24	0
1	B	2059	0	2055	36	0
1	C	2093	0	2082	8	1
1	D	2053	0	2048	26	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	9	0	8	1	0
3	B	9	0	8	0	0
3	C	9	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	9	0	8	0	0
4	A	170	0	0	13	0
4	B	188	0	0	1	0
4	C	174	0	0	0	0
4	D	157	0	0	2	1
All	All	9002	0	8263	85	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 5.

All (85) 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:6:LYS:H	1:D:181:GLN:NE2	1.51	1.08
1:B:258:THR:OG1	1:B:261:ALA:HB1	1.56	1.06
1:B:260:ALA:CA	1:B:261:ALA:HB2	1.91	1.00
1:B:260:ALA:N	1:B:261:ALA:HB2	1.78	0.98
1:B:6:LYS:H	1:D:181:GLN:HE22	0.96	0.95
1:B:260:ALA:N	1:B:261:ALA:CB	2.30	0.95
1:B:260:ALA:CB	1:B:261:ALA:HB2	2.00	0.90
4:A:567:HOH:O	1:D:158:LYS:HD2	1.71	0.89
1:B:260:ALA:HB3	1:B:261:ALA:HB2	1.52	0.88
1:A:118:PRO:O	4:A:562:HOH:O	1.92	0.88
1:A:246:ILE:O	1:A:257:ARG:NH1	2.08	0.87
1:B:6:LYS:N	1:D:181:GLN:HE22	1.74	0.86
1:A:120[B]:TRP:HB2	4:A:539:HOH:O	1.77	0.84
1:D:158:LYS:HE2	4:D:492:HOH:O	1.77	0.84
1:B:258:THR:OG1	1:B:261:ALA:CB	2.26	0.83
1:A:126:GLN:HG2	4:A:492:HOH:O	1.77	0.82
1:B:260:ALA:CA	1:B:261:ALA:CB	2.57	0.81
1:D:37:THR:OG1	1:D:40[B]:GLU:HG3	1.86	0.75
1:B:2:THR:N	1:D:79:HIS:HE2	1.84	0.75
1:B:260:ALA:N	1:B:261:ALA:HB3	2.04	0.71
1:B:258:THR:HG1	1:B:261:ALA:HB1	1.57	0.69
1:B:256:PRO:HB3	1:B:262:GLU:HA	1.74	0.68
1:A:122:ASP:CB	4:A:532:HOH:O	2.41	0.68
4:B:453:HOH:O	1:C:85:LYS:HE3	1.94	0.67
1:A:120[A]:TRP:O	4:A:539:HOH:O	2.14	0.66
1:D:46:HIS:HE1	4:D:488:HOH:O	1.77	0.66
1:B:260:ALA:H	1:B:261:ALA:HB2	1.57	0.65
1:D:243:GLY:HA3	1:D:259:SER:OG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:HB2	4:A:532:HOH:O	1.97	0.64
1:B:6:LYS:N	1:D:181:GLN:NE2	2.36	0.61
1:C:203:GLU:HB3	1:C:234:GLU:HG3	1.84	0.59
1:A:140:ARG:NH1	4:A:564:HOH:O	2.14	0.58
1:A:122:ASP:CG	4:A:532:HOH:O	2.44	0.56
1:B:155:HIS:HD2	1:B:158:LYS:NZ	2.04	0.55
1:A:140:ARG:HB3	1:A:243:GLY:HA2	1.89	0.55
1:B:134:LYS:HE3	1:B:155:HIS:CD2	2.42	0.54
1:A:13:LYS:HD3	1:A:104:TYR:CE2	2.42	0.54
1:C:245:GLU:HG3	1:C:258:THR:HG22	1.89	0.54
1:C:6:LYS:HE3	1:C:173:GLY:HA3	1.89	0.53
1:B:2:THR:HG22	1:D:79:HIS:NE2	2.25	0.52
1:D:37:THR:HG1	1:D:40[B]:GLU:HG3	1.74	0.52
1:B:2:THR:HG22	1:D:79:HIS:CE1	2.44	0.52
1:D:130:GLU:OE1	1:D:155:HIS:HE1	1.92	0.51
1:D:140:ARG:HB3	1:D:243:GLY:HA2	1.93	0.51
1:A:130:GLU:OE1	1:A:155:HIS:HE1	1.93	0.51
1:B:212:GLU:CB	1:B:225:LYS:HD2	2.41	0.51
1:B:4:THR:HG22	1:D:167:TYR:CE1	2.46	0.50
1:B:130:GLU:OE1	1:B:155:HIS:HE1	1.94	0.50
1:A:155:HIS:HD2	4:A:533:HOH:O	1.94	0.50
1:C:84:GLU:CD	1:C:84:GLU:H	2.15	0.50
1:B:261:ALA:H	1:D:210:ARG:HH22	1.58	0.49
1:C:130:GLU:OE1	1:C:155:HIS:HE1	1.97	0.48
1:B:212:GLU:HB3	1:B:225:LYS:HD2	1.96	0.48
1:C:33:LYS:O	1:C:36:VAL:HG12	2.13	0.47
1:A:207:ASN:HB3	4:A:442:HOH:O	2.15	0.47
1:A:43:ARG:HD2	4:A:510:HOH:O	2.14	0.47
1:B:260:ALA:HB3	1:B:261:ALA:CB	2.34	0.47
1:A:120[B]:TRP:N	1:A:120[B]:TRP:CE3	2.77	0.47
1:A:119:GLU:OE2	1:A:119:GLU:O	2.32	0.46
1:D:134:LYS:HE3	1:D:155:HIS:CD2	2.52	0.45
1:B:243:GLY:HA3	1:B:259:SER:OG	2.17	0.45
1:D:158:LYS:HE3	1:D:158:LYS:HB3	1.67	0.44
1:B:58:ALA:HB2	1:B:100:ILE:CG1	2.47	0.44
1:B:258:THR:O	1:B:261:ALA:HB3	2.18	0.44
1:D:257:ARG:HG2	1:D:258:THR:HG23	2.00	0.44
1:B:145:LEU:HD11	1:B:180:PRO:HB2	1.99	0.44
1:D:19:ARG:HD2	1:D:19:ARG:HA	1.83	0.44
1:B:260:ALA:H	1:B:261:ALA:CB	2.18	0.44
1:A:126:GLN:CG	4:A:492:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:HB	1:A:205:MET:HB2	2.00	0.44
1:D:168[A]:CYS:HB2	1:D:182:VAL:O	2.18	0.43
1:D:33:LYS:O	1:D:36:VAL:HG12	2.17	0.43
1:C:203:GLU:HB3	1:C:234:GLU:CG	2.48	0.43
1:A:33:LYS:HB3	1:A:33:LYS:HE3	1.61	0.43
1:D:36:VAL:CG1	1:D:87:LEU:HD12	2.49	0.43
1:A:141:PRO:HG2	1:A:241:ALA:O	2.19	0.43
1:A:176:PHE:CZ	3:A:305:MET:HB2	2.54	0.42
1:B:155:HIS:HD2	1:B:158:LYS:HZ1	1.67	0.42
1:A:21:ALA:HB1	1:A:108:THR:HG22	2.01	0.42
1:D:70:CYS:HB2	1:D:96:ASP:HB3	2.01	0.41
1:B:210:ARG:HB3	1:B:211:PRO:HD2	2.02	0.41
1:B:262:GLU:CD	1:B:262:GLU:H	2.24	0.41
1:B:158:LYS:HE3	1:B:158:LYS:HB2	1.93	0.41
1:A:134:LYS:HE3	1:A:155:HIS:CD2	2.55	0.41
1:D:249:LEU:HD22	1:D:257:ARG:HB2	2.02	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:C:174:LYS:NZ	4:D:524:HOH:O[3_654]	2.13	0.07

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	260/280 (93%)	253 (97%)	7 (3%)	0	100 100
1	B	261/280 (93%)	252 (97%)	8 (3%)	1 (0%)	39 27
1	C	265/280 (95%)	258 (97%)	7 (3%)	0	100 100
1	D	260/280 (93%)	255 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1046/1120 (93%)	1018 (97%)	27 (3%)	1 (0%)	56 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	ALA

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	224/238 (94%)	219 (98%)	5 (2%)	60 53
1	B	224/238 (94%)	220 (98%)	4 (2%)	66 61
1	C	228/238 (96%)	222 (97%)	6 (3%)	54 45
1	D	224/238 (94%)	221 (99%)	3 (1%)	76 73
All	All	900/952 (94%)	882 (98%)	18 (2%)	65 57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	40[A]	GLU
1	A	40[B]	GLU
1	A	176	PHE
1	A	259	SER
1	B	39	GLU
1	B	117	THR
1	B	176	PHE
1	B	262	GLU
1	C	82	PRO
1	C	84	GLU
1	C	119	GLU
1	C	176	PHE
1	C	265	LEU

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Mol	Chain	Res	Type
1	C	267	ASP
1	D	2	THR
1	D	176	PHE
1	D	259	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	155	HIS
1	B	46	HIS
1	B	155	HIS
1	B	232	GLN
1	C	46	HIS
1	C	51	ASN
1	C	155	HIS
1	D	46	HIS
1	D	155	HIS
1	D	181	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

Of 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MET	A	305	2	5,8,8	0.56	0	3,9,9	0.61	0
3	MET	B	304	2	5,8,8	0.54	0	3,9,9	1.08	0
3	MET	C	304	2	5,8,8	0.24	0	3,9,9	0.52	0
3	MET	D	304	2	5,8,8	0.64	0	3,9,9	1.24	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MET	A	305	2	-	0/4/8/8	0/0/0/0
3	MET	B	304	2	-	0/4/8/8	0/0/0/0
3	MET	C	304	2	-	0/4/8/8	0/0/0/0
3	MET	D	304	2	-	0/4/8/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	304	MET	CB-CG-SD	-2.06	104.48	113.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	MET	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	259/280 (92%)	-0.31	5 (1%)	70 73	7, 15, 29, 47	0
1	B	261/280 (93%)	-0.39	2 (0%)	87 88	8, 15, 30, 49	0
1	C	266/280 (95%)	-0.08	9 (3%)	49 52	10, 17, 33, 66	0
1	D	259/280 (92%)	-0.22	6 (2%)	64 67	9, 16, 33, 54	0
All	All	1045/1120 (93%)	-0.25	22 (2%)	67 70	7, 16, 32, 66	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	265	LEU	7.5
1	C	263	PHE	6.6
1	D	2	THR	6.5
1	D	260	ALA	6.4
1	C	266	VAL	6.2
1	A	2	THR	4.8
1	D	259	SER	4.0
1	A	254	THR	4.0
1	D	254	THR	4.0
1	D	258	THR	3.2
1	C	254	THR	3.1
1	C	267	ASP	3.0
1	C	2	THR	3.0
1	A	260	ALA	2.9
1	B	262	GLU	2.8
1	A	120[A]	TRP	2.8
1	B	6	LYS	2.3
1	C	202	ILE	2.3
1	D	256	PRO	2.3
1	C	189	GLY	2.2
1	C	264	GLU	2.1
1	A	119	GLU	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, 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	MET	D	304	9/9	0.97	0.14	1.34	16,19,25,29	0
3	MET	C	304	9/9	0.99	0.11	0.50	14,17,21,23	0
2	MN	B	303	1/1	0.98	0.08	0.03	20,20,20,20	1
3	MET	A	305	9/9	0.98	0.10	-0.00	8,13,19,22	0
3	MET	B	304	9/9	0.99	0.09	-0.03	10,13,17,20	0
2	MN	C	303	1/1	1.00	0.06	-1.16	16,16,16,16	1
2	MN	A	301	1/1	1.00	0.08	-1.19	10,10,10,10	0
2	MN	D	303	1/1	0.99	0.05	-1.53	20,20,20,20	1
2	MN	C	301	1/1	1.00	0.06	-1.93	14,14,14,14	0
2	MN	D	301	1/1	1.00	0.07	-2.05	13,13,13,13	0
2	MN	C	302	1/1	1.00	0.08	-2.09	13,13,13,13	0
2	MN	A	303	1/1	1.00	0.03	-2.10	19,19,19,19	0
2	MN	A	304	1/1	0.99	0.05	-2.15	17,17,17,17	1
2	MN	B	302	1/1	1.00	0.07	-2.17	10,10,10,10	0
2	MN	B	301	1/1	1.00	0.06	-2.19	10,10,10,10	0
2	MN	A	302	1/1	1.00	0.07	-3.48	10,10,10,10	0
2	MN	D	302	1/1	1.00	0.08	-4.92	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.