



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:17 AM UTC

PDB ID : 1OS2 / pdb_00001os2
Title : Ternary enzyme-product-inhibitor complexes of human MMP12
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Mangani, S.; Terni, B.
Deposited on : 2003-03-18
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

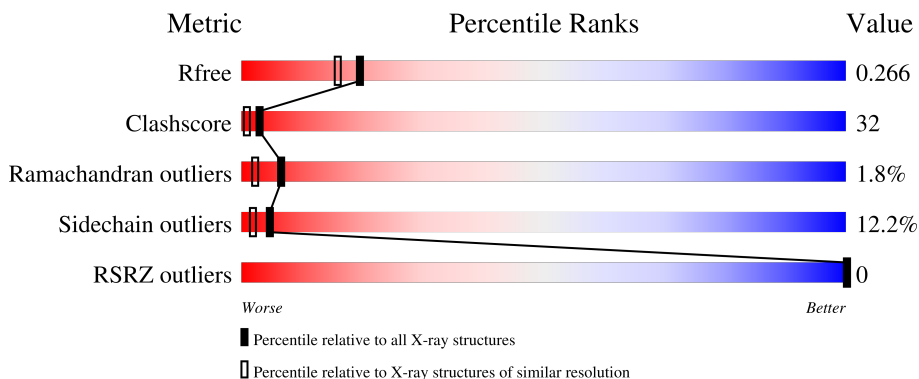
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	 49% 42% 7% .
1	B	165	 44% 39% 15% .
1	C	165	 48% 33% 15% .
1	D	165	 53% 37% 7% .
1	E	165	 45% 38% 15% .

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Mol	Chain	Length	Quality of chain
1	F	165	

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
5	ACT	B	374	-	X	-	-
6	AZI	C	474	-	X	-	-
6	AZI	F	774	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8132 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 Macrophage metalloelastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1295	823	225	242	5	0	7	0
1	B	165	1295	823	225	242	5	0	7	0
1	C	165	1295	823	225	242	5	0	6	0
1	D	165	1295	823	225	242	5	0	7	0
1	E	165	1295	823	225	242	5	0	7	0
1	F	165	1295	823	225	242	5	0	7	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	MET	-	cloning artifact	UNP P39900
A	105	MET	-	cloning artifact	UNP P39900
A	171	ASP	PHE	engineered mutation	UNP P39900
B	104	MET	-	cloning artifact	UNP P39900
B	105	MET	-	cloning artifact	UNP P39900
B	171	ASP	PHE	engineered mutation	UNP P39900
C	104	MET	-	cloning artifact	UNP P39900
C	105	MET	-	cloning artifact	UNP P39900
C	171	ASP	PHE	engineered mutation	UNP P39900
D	104	MET	-	cloning artifact	UNP P39900
D	105	MET	-	cloning artifact	UNP P39900
D	171	ASP	PHE	engineered mutation	UNP P39900
E	104	MET	-	cloning artifact	UNP P39900
E	105	MET	-	cloning artifact	UNP P39900
E	171	ASP	PHE	engineered mutation	UNP P39900
F	104	MET	-	cloning artifact	UNP P39900
F	105	MET	-	cloning artifact	UNP P39900

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Chain	Residue	Modelled	Actual	Comment	Reference
F	171	ASP	PHE	engineered mutation	UNP P39900

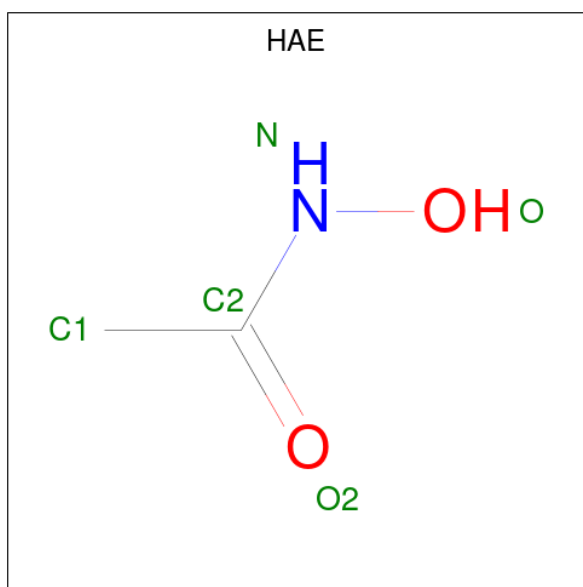
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

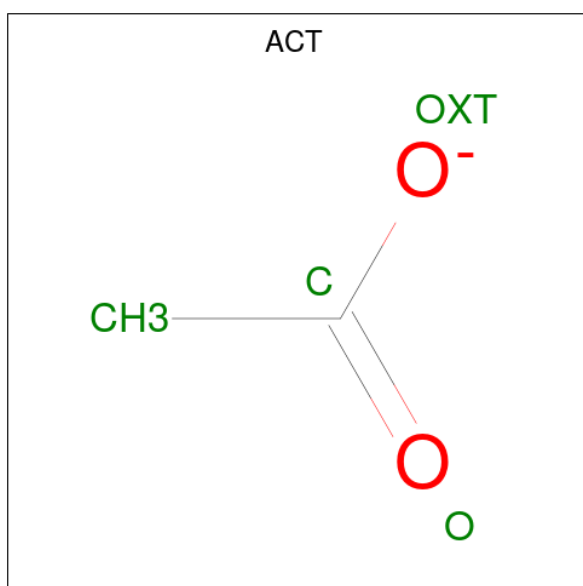
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	B	3	Total Ca 3 3	0	0
3	C	3	Total Ca 3 3	0	0
3	D	3	Total Ca 3 3	0	0
3	E	3	Total Ca 3 3	0	0
3	F	3	Total Ca 3 3	0	0

- Molecule 4 is ACETOHYDROXAMIC ACID (CCD ID: HAE) (formula: C₂H₅NO₂).



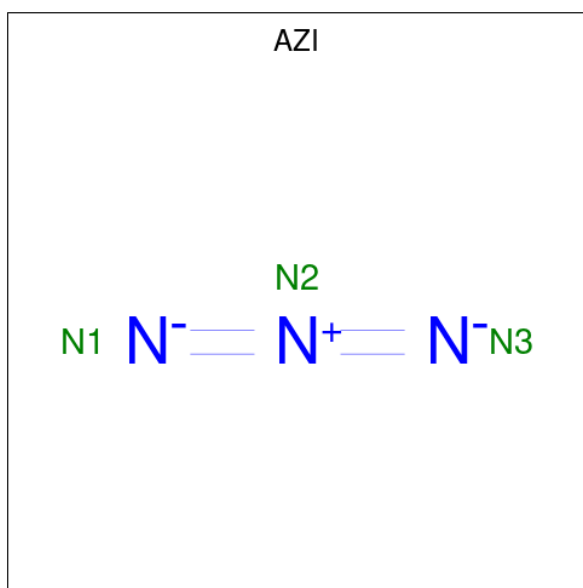
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	5	2	1	2	0	0
4	D	1	5	2	1	2	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
5	B	1	4	2 2	0	0
5	E	1	4	2 2	0	0

- Molecule 6 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total N 3 3	0	0
6	F	1	Total N 3 3	0	0

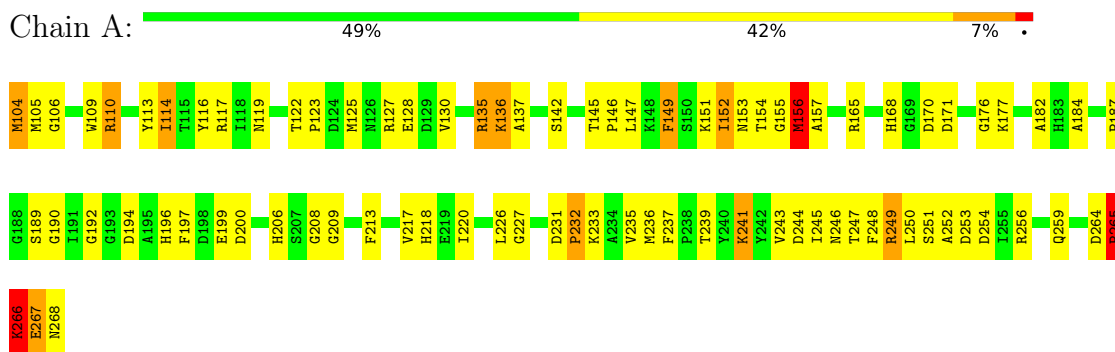
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	46	Total O 46 46	0	0
7	B	67	Total O 67 67	0	0
7	C	51	Total O 51 51	0	0
7	D	44	Total O 44 44	0	0
7	E	59	Total O 59 59	0	0
7	F	41	Total O 41 41	0	0

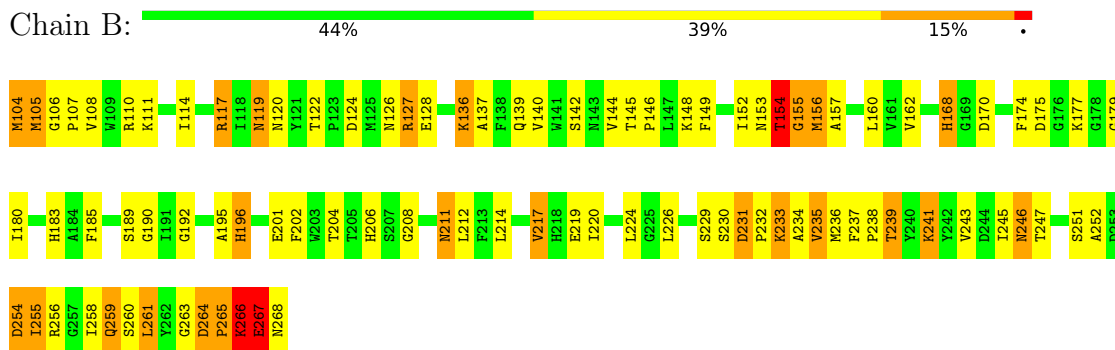
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

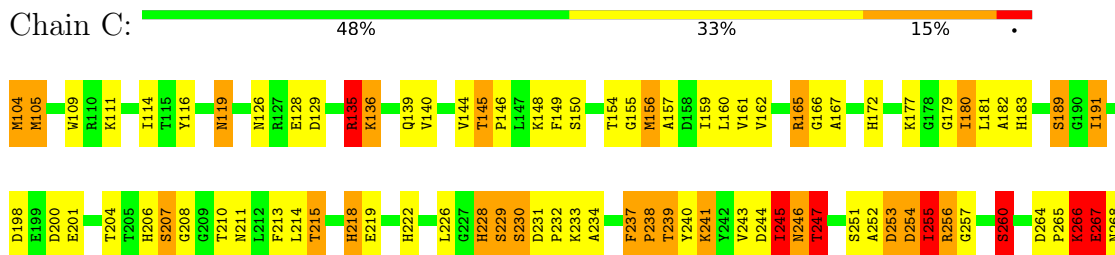
- Molecule 1: Macrophage metalloelastase



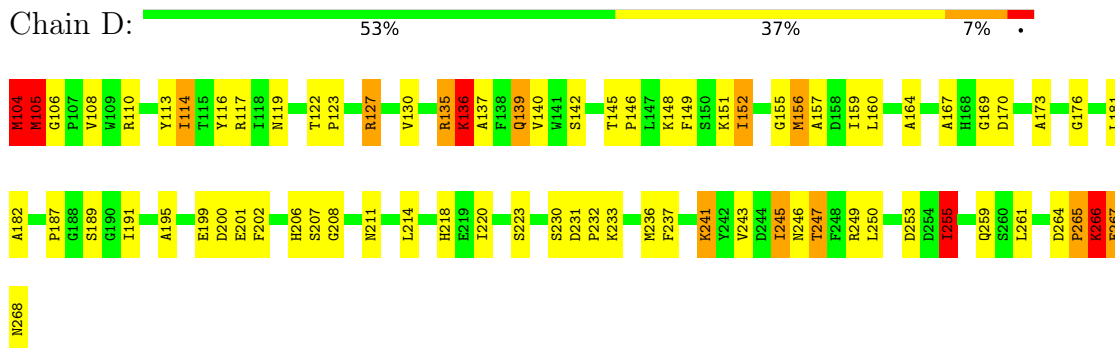
- Molecule 1: Macrophage metalloelastase



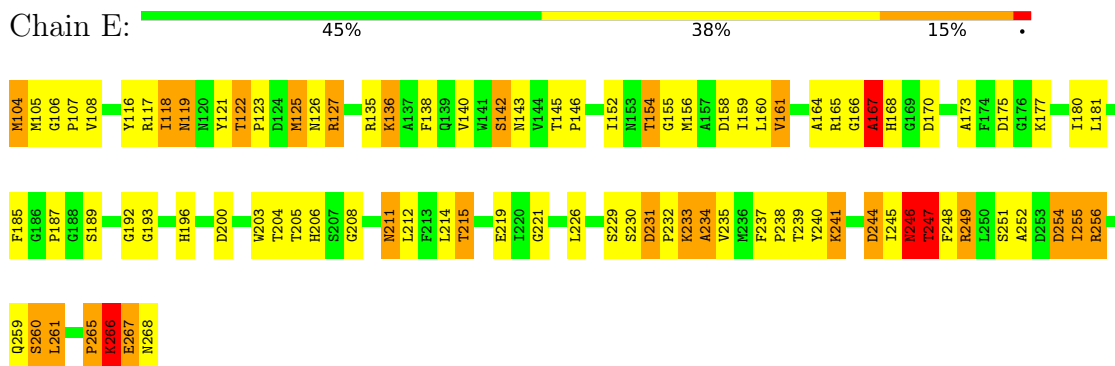
- Molecule 1: Macrophage metalloelastase



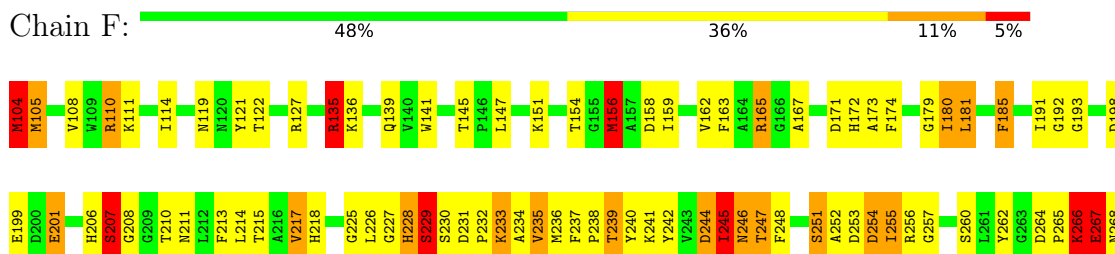
- Molecule 1: Macrophage metalloelastase



- Molecule 1: Macrophage metalloelastase



- Molecule 1: Macrophage metalloelastase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.84Å 123.84Å 69.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.01 – 2.15 69.01 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (69.01-2.15) 100.0 (69.01-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.1.80	Depositor
R, R_{free}	0.212 , 0.271 0.216 , 0.266	Depositor DCC
R_{free} test set	3296 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.007	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for -h,-k,l 0.488 for h,-h-k,-l 0.029 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8132	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, AZI, HAE, CA, ZN

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	1.90	26/1333 (2.0%)	1.74	25/1805 (1.4%)
1	B	2.01	28/1333 (2.1%)	1.81	31/1805 (1.7%)
1	C	1.91	25/1333 (1.9%)	1.83	33/1805 (1.8%)
1	D	1.85	31/1333 (2.3%)	1.70	22/1805 (1.2%)
1	E	2.05	36/1333 (2.7%)	1.97	40/1805 (2.2%)
1	F	1.84	21/1333 (1.6%)	1.77	25/1805 (1.4%)
All	All	1.93	167/7998 (2.1%)	1.81	176/10830 (1.6%)

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	A	1	2
1	B	0	2
1	C	0	2
1	E	0	4
1	F	1	2
All	All	2	12

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	MET	C-O	12.73	1.39	1.23
1	E	167	ALA	C-O	-9.28	1.11	1.23
1	F	252	ALA	CA-CB	9.24	1.67	1.53
1	A	137	ALA	CA-CB	9.11	1.67	1.53
1	E	166	GLY	C-N	8.96	1.45	1.33

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	166	GLY	CA-C-N	-19.57	89.94	122.82
1	E	166	GLY	C-N-CA	-19.57	89.94	122.82
1	C	155	GLY	CA-C-N	-11.12	107.32	122.99
1	C	155	GLY	C-N-CA	-11.12	107.32	122.99
1	F	246	ASN	N-CA-C	10.84	127.82	113.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	266	LYS	CA
1	F	246	ASN	CA

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	MET	Mainchain
1	A	265	PRO	Peptide
1	B	265	PRO	Peptide
1	B	266	LYS	Peptide
1	C	245	ILE	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	1295	0	1210	59	0
1	B	1295	0	1210	122	1
1	C	1295	0	1212	108	0
1	D	1295	0	1210	48	0
1	E	1295	0	1210	78	1
1	F	1295	0	1210	113	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	5	0	4	0	0
4	D	5	0	4	0	0
5	B	4	0	3	1	0
5	E	4	0	3	1	0
6	C	3	0	0	1	0
6	F	3	0	0	1	0
7	A	46	0	0	11	0
7	B	67	0	0	10	0
7	C	51	0	0	2	0
7	D	44	0	0	4	0
7	E	59	0	0	9	0
7	F	41	0	0	5	0
All	All	8132	0	7276	483	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 32.

The worst 5 of 483 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:F:136:LYS:CE	1:F:245:ILE:HD11	1.33	1.58
1:C:136:LYS:CE	1:C:245:ILE:HD11	1.32	1.55
1:F:136:LYS:HE2	1:F:245:ILE:CD1	1.42	1.49
1:C:136:LYS:HE2	1:C:245:ILE:CD1	1.58	1.32
1:C:136:LYS:CE	1:C:245:ILE:CD1	2.08	1.31

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:B:233:LYS:NZ	1:E:249:ARG:NH1[1_554]	2.07	0.13

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	163/165 (99%)	155 (95%)	6 (4%)	2 (1%)	10	5
1	B	163/165 (99%)	153 (94%)	7 (4%)	3 (2%)	6	2
1	C	163/165 (99%)	152 (93%)	7 (4%)	4 (2%)	4	1
1	D	163/165 (99%)	158 (97%)	3 (2%)	2 (1%)	10	5
1	E	163/165 (99%)	153 (94%)	7 (4%)	3 (2%)	6	2
1	F	163/165 (99%)	151 (93%)	8 (5%)	4 (2%)	4	1
All	All	978/990 (99%)	922 (94%)	38 (4%)	18 (2%)	6	2

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	LYS
1	B	266	LYS
1	C	245	ILE
1	C	266	LYS
1	C	267	GLU

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	134/134 (100%)	122 (91%)	12 (9%)	9	5
1	B	134/134 (100%)	117 (87%)	17 (13%)	4	1
1	C	134/134 (100%)	116 (87%)	18 (13%)	4	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	134/134 (100%)	119 (89%)	15 (11%)	6	2
1	E	134/134 (100%)	115 (86%)	19 (14%)	3	1
1	F	134/134 (100%)	117 (87%)	17 (13%)	4	1
All	All	804/804 (100%)	706 (88%)	98 (12%)	5	2

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	191	ILE
1	E	239	THR
1	D	247	THR
1	E	142[A]	SER
1	E	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	211[A]	ASN
1	F	211[A]	ASN
1	D	206	HIS
1	F	119	ASN
1	D	143	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 30 are monoatomic - leaving 6 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
5	ACT	E	674	2	3,3,3	2.14	1 (33%)	3,3,3	0.89	0
6	AZI	C	474	2	2,2,2	2.38	2 (100%)	0,1,1	-	-
4	HAE	A	874	2	4,4,4	1.20	0	2,4,4	4.42	2 (100%)
6	AZI	F	774	2	2,2,2	2.34	2 (100%)	0,1,1	-	-
4	HAE	D	574	2	4,4,4	1.35	1 (25%)	2,4,4	5.88	2 (100%)
5	ACT	B	374	2	3,3,3	1.84	1 (33%)	3,3,3	5.32	3 (100%)

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
4	HAE	A	874	2	-	0/1/2/2	-
4	HAE	D	574	2	-	0/1/2/2	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	674	ACT	O-C	3.03	1.35	1.22
6	F	774	AZI	N1-N2	-2.59	1.17	1.23
5	B	374	ACT	OXT-C	-2.56	1.19	1.30
6	C	474	AZI	N1-N2	-2.49	1.18	1.23
6	C	474	AZI	N3-N2	-2.26	1.18	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	374	ACT	OXT-C-O	-7.67	93.56	122.03
4	D	574	HAE	C1-C2-N	5.93	125.96	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	574	HAE	O2-C2-C1	-5.84	111.66	122.05
4	A	874	HAE	C1-C2-N	4.99	124.39	116.10
5	B	374	ACT	OXT-C-CH3	4.46	133.73	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	674	ACT	1	0
6	C	474	AZI	1	0
6	F	774	AZI	1	0
5	B	374	ACT	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 [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	165/165 (100%)	-1.19	0 100 100	18, 36, 52, 62	9 (5%)
1	B	165/165 (100%)	-1.19	0 100 100	11, 30, 51, 82	9 (5%)
1	C	165/165 (100%)	-1.15	0 100 100	13, 34, 56, 86	8 (4%)
1	D	165/165 (100%)	-1.19	0 100 100	17, 36, 52, 66	9 (5%)
1	E	165/165 (100%)	-1.22	0 100 100	11, 30, 52, 89	9 (5%)
1	F	165/165 (100%)	-1.13	0 100 100	14, 34, 56, 82	9 (5%)
All	All	990/990 (100%)	-1.18	0 100 100	11, 34, 54, 89	53 (5%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	AZI	C	474	3/3	0.98	0.05	29,29,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	873	1/1	0.99	0.03	47,47,47,47	0
3	CA	B	372	1/1	0.99	0.03	35,35,35,35	0
3	CA	D	572	1/1	0.99	0.02	40,40,40,40	0
3	CA	D	573	1/1	0.99	0.03	51,51,51,51	0
3	CA	E	672	1/1	0.99	0.03	32,32,32,32	0
3	CA	A	872	1/1	0.99	0.02	39,39,39,39	0
6	AZI	F	774	3/3	0.99	0.03	29,29,44,48	0
2	ZN	E	669	1/1	1.00	0.01	33,33,33,33	0
2	ZN	E	670	1/1	1.00	0.01	30,30,30,30	0
2	ZN	F	769	1/1	1.00	0.02	33,33,33,33	0
2	ZN	F	770	1/1	1.00	0.01	33,33,33,33	0
3	CA	A	871	1/1	1.00	0.01	44,44,44,44	0
2	ZN	A	869	1/1	1.00	0.01	29,29,29,29	0
2	ZN	A	870	1/1	1.00	0.01	43,43,43,43	0
3	CA	B	371	1/1	1.00	0.01	26,26,26,26	0
2	ZN	B	369	1/1	1.00	0.01	34,34,34,34	0
3	CA	B	373	1/1	1.00	0.01	28,28,28,28	0
3	CA	C	471	1/1	1.00	0.02	28,28,28,28	0
3	CA	C	472	1/1	1.00	0.01	31,31,31,31	0
3	CA	C	473	1/1	1.00	0.01	38,38,38,38	0
3	CA	D	571	1/1	1.00	0.01	43,43,43,43	0
2	ZN	B	370	1/1	1.00	0.01	29,29,29,29	0
2	ZN	C	469	1/1	1.00	0.02	32,32,32,32	0
3	CA	E	671	1/1	1.00	0.01	27,27,27,27	0
2	ZN	C	470	1/1	1.00	0.01	33,33,33,33	0
3	CA	E	673	1/1	1.00	0.01	30,30,30,30	0
3	CA	F	771	1/1	1.00	0.02	29,29,29,29	0
3	CA	F	772	1/1	1.00	0.02	30,30,30,30	0
3	CA	F	773	1/1	1.00	0.01	37,37,37,37	0
4	HAE	A	874	5/5	1.00	0.06	27,34,38,43	0
4	HAE	D	574	5/5	1.00	0.04	28,34,42,43	0
5	ACT	B	374	4/4	1.00	0.04	33,35,37,40	0
5	ACT	E	674	4/4	1.00	0.04	28,33,36,36	0
2	ZN	D	569	1/1	1.00	0.01	28,28,28,28	0
2	ZN	D	570	1/1	1.00	0.01	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.