wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 07:49 PM EDT

PDB ID	:	2AF7
Title	:	Crystal structure of the gamma-carboxymuconolactone decarboxylase from Methanobacterium thermoautotrophicum. Northeast Structural Genomics Consortium target TT747.
Authors	:	Vorobiev, S.M.; Kuzin, A.; Skarina, T.; Savchenko, A.; Semesi, A.; Arrowsmith, C.; Edwards, A.; Montelione, G.T.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2005-07-25
Resolution	:	2.81 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 (i) 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 (i)) were used in the production of this report:

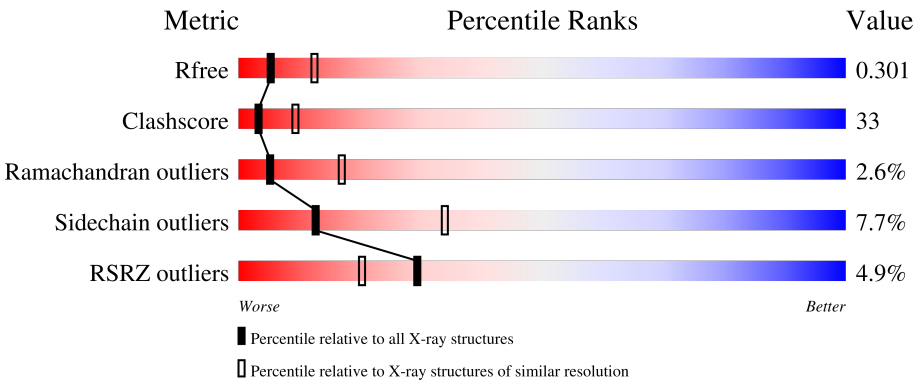
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 2.81 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	125	2%, 54%, 35%, 5%, • 5%
1	B	125	3%, 51%, 41%, • 6%
1	C	125	3%, 48%, 41%, • • 6%
1	D	125	6%, 46%, 42%, 9%, • •

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Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
1	E	125	5% 50% 39% 7% •
1	F	125	6% 48% 44% • •
1	G	125	9% 43% 44% 7% 6%
1	H	125	2% 53% 39% • 5%
1	I	125	5% 47% 43% 6% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8293 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 gamma-carboxymuconolactone decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	119	909	576	162	165	1	5	0	0	0
1	B	118	900	571	158	166	1	4	0	0	0
1	C	118	910	576	161	168	1	4	0	0	0
1	D	122	935	590	166	173	1	5	0	0	0
1	E	120	908	575	160	167	1	5	0	0	0
1	F	120	888	566	153	164	1	4	0	0	0
1	G	118	914	578	161	170	1	4	0	0	0
1	H	119	922	582	163	172	1	4	0	0	0
1	I	120	913	578	161	169	1	4	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
A	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
A	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
A	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
A	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
B	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
B	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
B	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
B	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
B	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
C	1	MSE	MET	MODIFIED RESIDUE	UNP O26336

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
C	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
C	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
C	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
D	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
D	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
D	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
D	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
D	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
E	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
E	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
E	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
E	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
E	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
F	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
F	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
F	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
F	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
F	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
G	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
G	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
G	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
G	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
G	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
H	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
H	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
H	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
H	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
H	97	MSE	MET	MODIFIED RESIDUE	UNP O26336
I	1	MSE	MET	MODIFIED RESIDUE	UNP O26336
I	8	MSE	MET	MODIFIED RESIDUE	UNP O26336
I	14	MSE	MET	MODIFIED RESIDUE	UNP O26336
I	94	MSE	MET	MODIFIED RESIDUE	UNP O26336
I	97	MSE	MET	MODIFIED RESIDUE	UNP O26336

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	8	Total O 8 8	0	0

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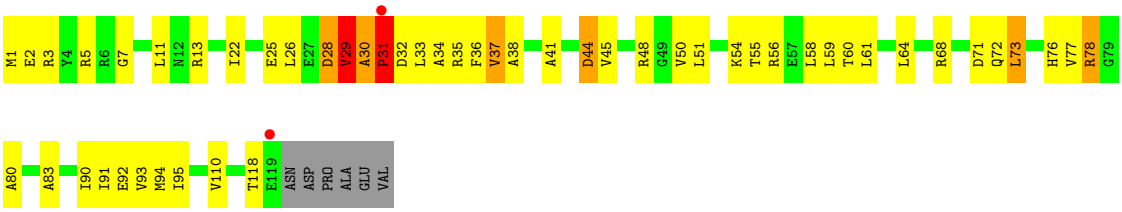
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	C	12	12	12	0	0
			Total	O		
2	D	11	11	11	0	0
			Total	O		
2	E	5	5	5	0	0
			Total	O		
2	F	9	9	9	0	0
			Total	O		
2	G	10	10	10	0	0
			Total	O		
2	H	13	13	13	0	0
			Total	O		
2	I	13	13	13	0	0

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.

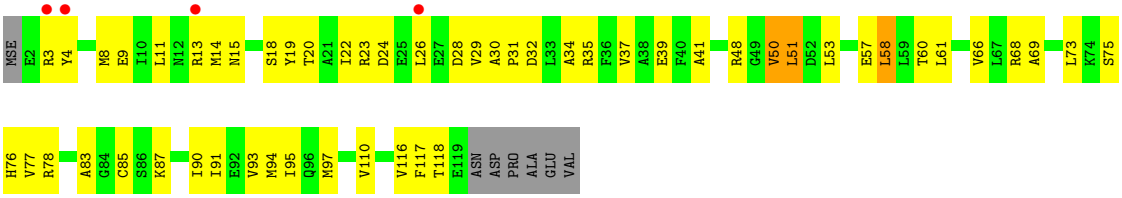
• Molecule 1: gamma-carboxymuconolactone decarboxylase

Chain A:



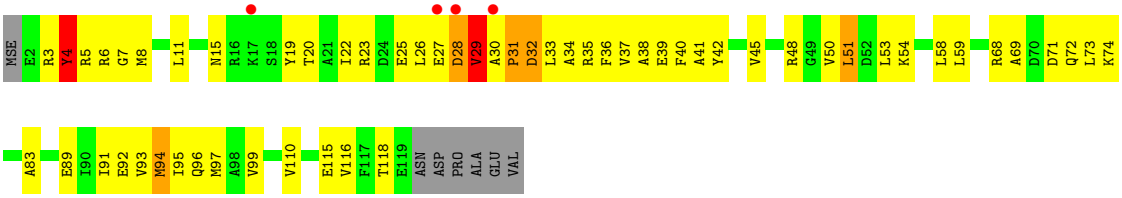
• Molecule 1: gamma-carboxymuconolactone decarboxylase

Chain B:



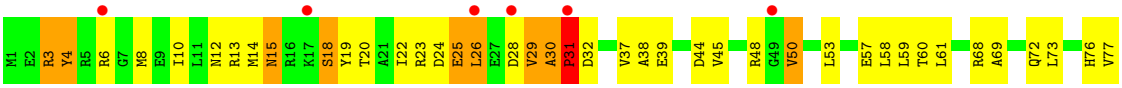
• Molecule 1: gamma-carboxymuconolactone decarboxylase

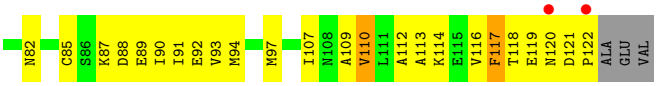
Chain C:



• Molecule 1: gamma-carboxymuconolactone decarboxylase

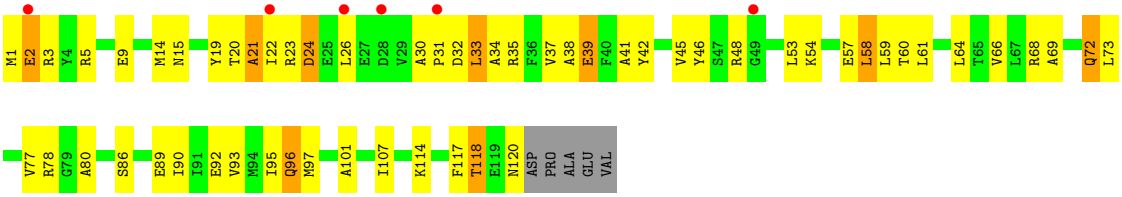
Chain D:





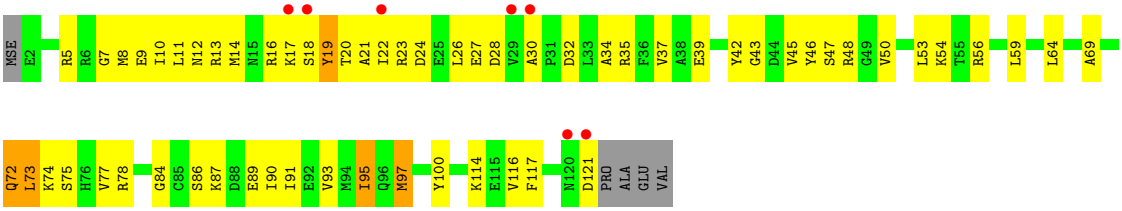
• Molecule 1: gamma-carboxymuconolactone decarboxylase

Chain E:



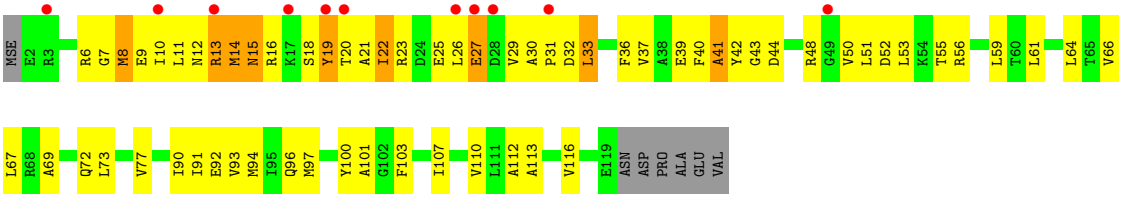
• Molecule 1: gamma-carboxymuconolactone decarboxylase

Chain F:



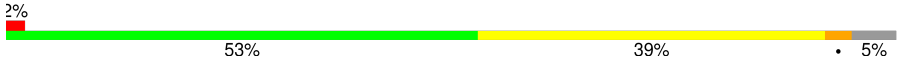
• Molecule 1: gamma-carboxymuconolactone decarboxylase

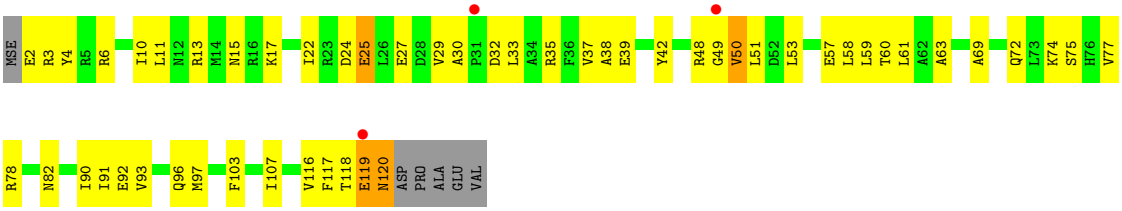
Chain G:



• Molecule 1: gamma-carboxymuconolactone decarboxylase

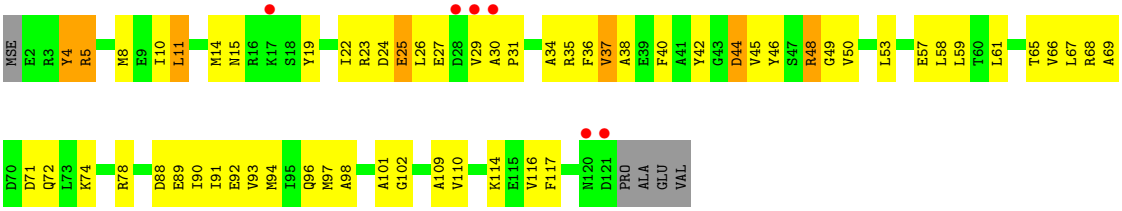
Chain H:





• Molecule 1: gamma-carboxymuconolactone decarboxylase

Chain I:


MSE
E2
R3
Y4
R5
M8
E9
I10
L11
M14
N15
R16
K17
S18
Y19
I22
R23
D24
E25
L26
E27
D28
V29
A30
P31
A34
R35
F36
V37
A38
E39
F40
A41
Y42
G43
D44
V45
Y46
S47
R48
G49
V50
L53
E57
L58
L59
T60
L61
T65
V66
L67
R68
A69
D70
D71
Q72
L73
K74
R78
D88
E89
I90
I91
E92
V93
M94
I95
Q96
M97
A98
A101
G102
A109
V110
K114
E115
V116
F117
N120
D121
PRO
ALA
GLU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	183.31Å 119.11Å 73.62Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	29.97 – 2.81 29.97 – 2.81	Depositor EDS
% Data completeness (in resolution range)	80.3 (29.97-2.81) 96.4 (29.97-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.292 0.254 , 0.301	Depositor DCC
R_{free} test set	2928 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8293	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.64	2/916 (0.2%)	0.90	5/1229 (0.4%)
1	B	0.38	0/907	0.69	0/1219
1	C	0.42	0/917	0.80	1/1231 (0.1%)
1	D	0.51	0/943	0.85	5/1267 (0.4%)
1	E	0.45	0/915	0.77	2/1231 (0.2%)
1	F	0.45	0/895	0.75	1/1207 (0.1%)
1	G	0.40	0/921	0.68	0/1236
1	H	0.47	0/929	0.75	2/1247 (0.2%)
1	I	0.44	0/920	0.73	1/1237 (0.1%)
All	All	0.47	2/8263 (0.0%)	0.77	17/11104 (0.2%)

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	0	1
1	D	0	1
1	G	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	VAL	CA-C	-8.35	1.31	1.52
1	A	30	ALA	CA-CB	-8.31	1.34	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	VAL	N-CA-C	9.74	137.30	111.00
1	A	28	ASP	N-CA-C	-7.94	89.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	32	ASP	N-CA-C	-7.02	92.05	111.00
1	A	29	VAL	CB-CA-C	-6.87	98.35	111.40
1	A	30	ALA	C-N-CA	-6.51	94.65	122.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	VAL	Mainchain
1	D	28	ASP	Peptide
1	G	100	TYR	Sidechain

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	909	0	919	84	0
1	B	900	0	905	58	0
1	C	910	0	920	72	0
1	D	935	0	938	71	0
1	E	908	0	908	71	0
1	F	888	0	872	67	0
1	G	914	0	924	82	0
1	H	922	0	930	62	0
1	I	913	0	913	66	0
2	A	13	0	0	1	0
2	B	8	0	0	0	0
2	C	12	0	0	1	0
2	D	11	0	0	0	0
2	E	5	0	0	1	0
2	F	9	0	0	1	0
2	G	10	0	0	2	0
2	H	13	0	0	0	0
2	I	13	0	0	2	0
All	All	8293	0	8229	540	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 33.

The worst 5 of 540 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ALA:HB1	1:A:33:LEU:H	1.01	1.10
1:B:29:VAL:HG22	1:B:30:ALA:H	1.16	1.05
1:F:91:ILE:HD11	1:F:117:PHE:HE2	1.22	1.03
1:A:30:ALA:HB1	1:A:33:LEU:N	1.76	1.01
1:A:56:ARG:NH2	1:C:96:GLN:HB2	1.73	1.00

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	117/125 (94%)	108 (92%)	7 (6%)	2 (2%)	9 27
1	B	116/125 (93%)	99 (85%)	15 (13%)	2 (2%)	9 27
1	C	116/125 (93%)	95 (82%)	18 (16%)	3 (3%)	5 17
1	D	120/125 (96%)	96 (80%)	20 (17%)	4 (3%)	4 12
1	E	118/125 (94%)	96 (81%)	20 (17%)	2 (2%)	9 27
1	F	118/125 (94%)	92 (78%)	23 (20%)	3 (2%)	5 18
1	G	116/125 (93%)	95 (82%)	14 (12%)	7 (6%)	1 4
1	H	117/125 (94%)	105 (90%)	11 (9%)	1 (1%)	17 44
1	I	118/125 (94%)	101 (86%)	14 (12%)	3 (2%)	5 18
All	All	1056/1125 (94%)	887 (84%)	142 (13%)	27 (3%)	5 17

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	28	ASP
1	B	50	VAL
1	D	29	VAL
1	F	27	GLU
1	G	41	ALA

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	89/96 (93%)	83 (93%)	6 (7%)	16	41
1	B	89/96 (93%)	84 (94%)	5 (6%)	21	49
1	C	91/96 (95%)	81 (89%)	10 (11%)	6	18
1	D	93/96 (97%)	87 (94%)	6 (6%)	17	43
1	E	89/96 (93%)	82 (92%)	7 (8%)	12	33
1	F	84/96 (88%)	77 (92%)	7 (8%)	11	31
1	G	92/96 (96%)	86 (94%)	6 (6%)	17	43
1	H	93/96 (97%)	86 (92%)	7 (8%)	13	35
1	I	90/96 (94%)	82 (91%)	8 (9%)	9	27
All	All	810/864 (94%)	748 (92%)	62 (8%)	13	34

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	15	ASN
1	I	5	ARG
1	F	35	ARG
1	I	4	TYR
1	I	25	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	72	GLN
1	G	15	ASN
1	H	120	ASN
1	F	76	HIS
1	G	72	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	114/125 (91%)	-0.22	2 (1%)	68	61	11, 39, 75, 102	0
1	B	114/125 (91%)	0.03	4 (3%)	44	34	20, 55, 95, 102	0
1	C	114/125 (91%)	-0.15	4 (3%)	44	34	11, 42, 91, 101	0
1	D	117/125 (93%)	0.16	8 (6%)	17	10	17, 48, 102, 102	0
1	E	115/125 (92%)	0.10	6 (5%)	27	18	13, 52, 102, 102	0
1	F	116/125 (92%)	-0.06	7 (6%)	21	14	18, 48, 95, 102	0
1	G	114/125 (91%)	0.22	11 (9%)	8	4	15, 49, 102, 102	0
1	H	115/125 (92%)	-0.14	3 (2%)	56	46	14, 39, 81, 102	0
1	I	116/125 (92%)	0.11	6 (5%)	27	18	21, 50, 96, 102	0
All	All	1035/1125 (92%)	0.01	51 (4%)	29	20	11, 46, 97, 102	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	28	ASP	5.1
1	G	49	GLY	4.0
1	G	19	TYR	4.0
1	G	20	THR	3.9
1	H	31	PRO	3.8

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.