Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2016 – 06:17 PM EDT

PDB ID	:	5D4T
Title	:	SeMet-labelled HcgC from Methanocaldococcus jannaschii in space group P212121
Authors	:	Fujishiro, T.; Ermler, U.; Shima, S.
Deposited on	:	2015-08-09
Resolution	:	2.90 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 ⓘ symbol.

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

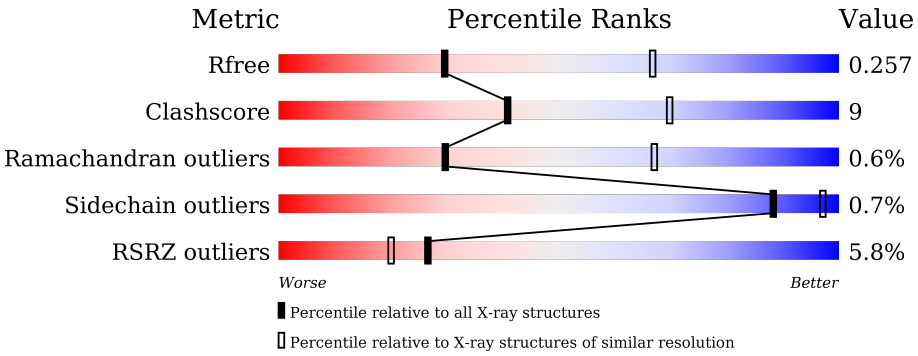
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	268	9% 69% 19% • • 9%
1	B	268	2% 75% 16% • 8%
1	C	268	7% 72% 18% 9%
1	D	268	2% 74% 17% 9%
1	E	268	10% 68% 20% • • 9%
1	F	268	4% 73% 16% • 9%

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Mol	Chain	Length	Quality of chain
1	G	268	6% 78% 12% • 9%
1	H	268	3% 74% 16% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15781 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 Uncharacterized protein MJ0489.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	Se	0	0	0
			1961	1274	309	375	3			
1	B	246	Total	C	N	O	Se	0	0	0
			1983	1285	314	381	3			
1	C	243	Total	C	N	O	Se	0	0	0
			1961	1274	309	375	3			
1	D	244	Total	C	N	O	Se	0	0	0
			1967	1277	310	377	3			
1	E	243	Total	C	N	O	Se	0	1	0
			1967	1278	309	377	3			
1	F	244	Total	C	N	O	Se	0	0	0
			1967	1277	310	377	3			
1	G	244	Total	C	N	O	Se	0	1	0
			1973	1281	310	379	3			
1	H	247	Total	C	N	O	Se	0	0	0
			1991	1289	316	383	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q57913
B	1	MSE	-	initiating methionine	UNP Q57913
C	1	MSE	-	initiating methionine	UNP Q57913
D	1	MSE	-	initiating methionine	UNP Q57913
E	1	MSE	-	initiating methionine	UNP Q57913
F	1	MSE	-	initiating methionine	UNP Q57913
G	1	MSE	-	initiating methionine	UNP Q57913
H	1	MSE	-	initiating methionine	UNP Q57913

- Molecule 2 is water.

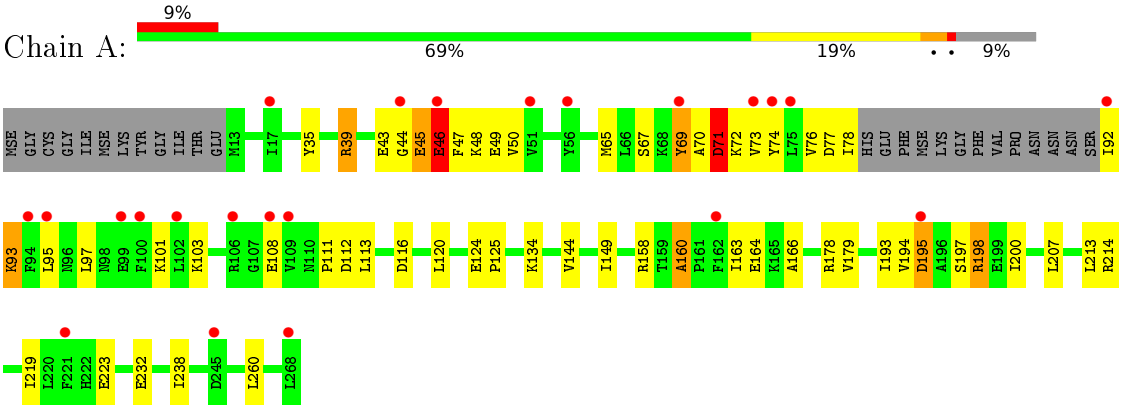
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	B	3	Total O 3 3	0	0
2	C	1	Total O 1 1	0	0
2	D	2	Total O 2 2	0	0
2	F	1	Total O 1 1	0	0
2	G	1	Total O 1 1	0	0
2	H	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

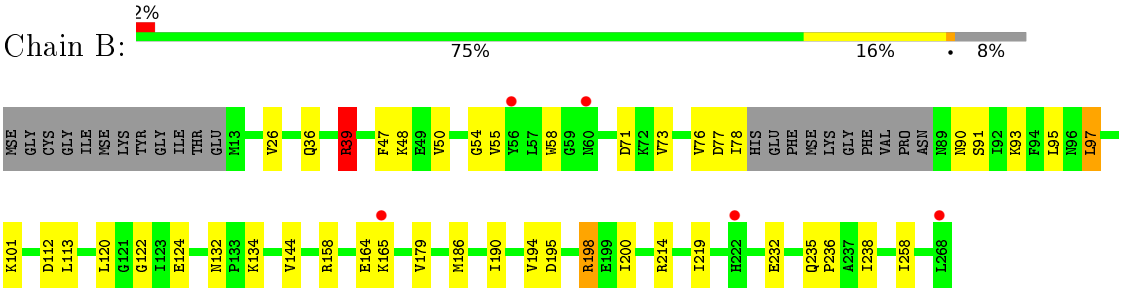
- Molecule 1: Uncharacterized protein MJ0489

Chain A:



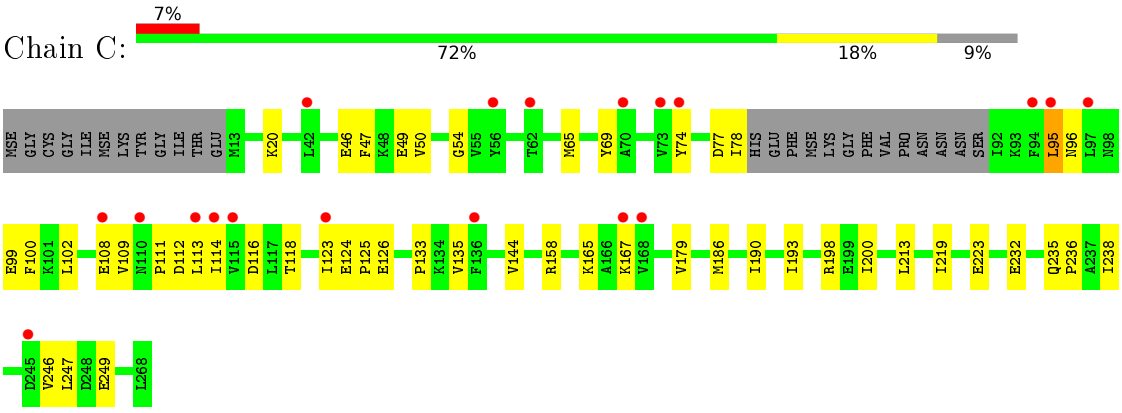
- Molecule 1: Uncharacterized protein MJ0489

Chain B:



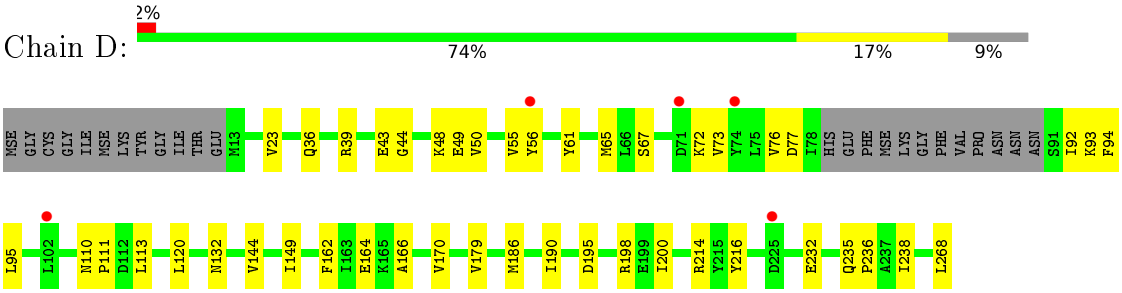
- Molecule 1: Uncharacterized protein MJ0489

Chain C:



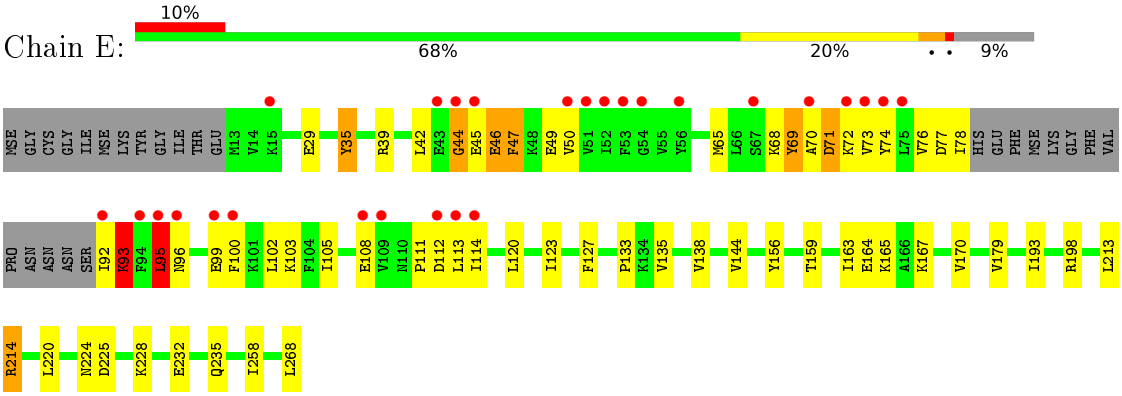
- Molecule 1: Uncharacterized protein MJ0489

Chain D:



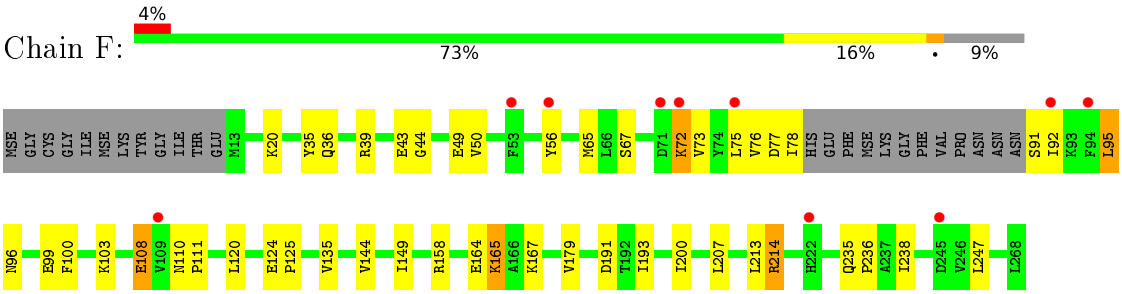
• Molecule 1: Uncharacterized protein MJ0489

Chain E:



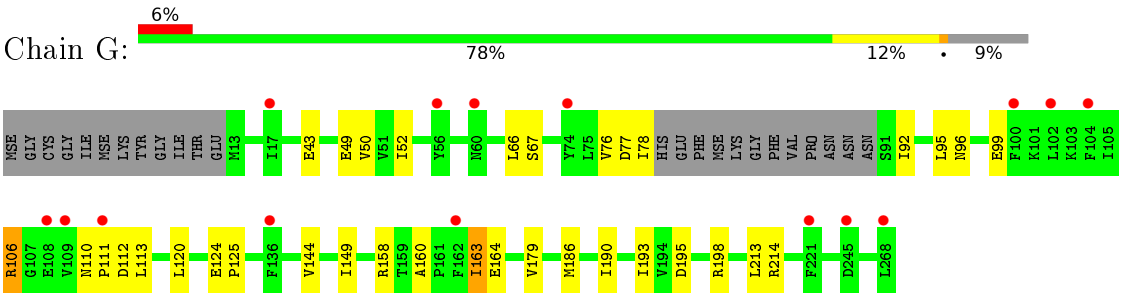
• Molecule 1: Uncharacterized protein MJ0489

Chain F:



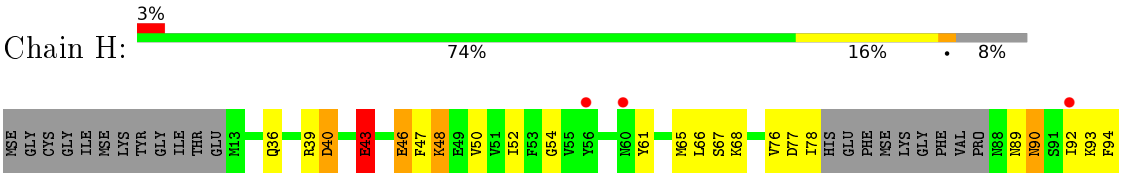
• Molecule 1: Uncharacterized protein MJ0489

Chain G:



• Molecule 1: Uncharacterized protein MJ0489

Chain H:




L95
N96
L97
N98
E99
L102
K103
R106
G107
E108
L113
E124
P125
E126
V144
I163
E164
K165
V179
M186
I190
I193
R198
E199
I200
L213
R214
L220
F221
H222
E223
N224
D225
I226
I238
E267
L268

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.43Å 145.00Å 150.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.90 48.56 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.56-2.90) 100.0 (48.56-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.259 0.229 , 0.257	Depositor DCC
R_{free} test set	3494 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	81.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15781	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.55 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.4662e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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	0.74	9/1994 (0.5%)	1.17	28/2694 (1.0%)
1	B	0.36	0/2016	0.73	4/2724 (0.1%)
1	C	0.38	0/1994	0.78	4/2694 (0.1%)
1	D	0.35	0/2000	0.68	0/2702
1	E	0.47	1/2003 (0.0%)	0.94	13/2706 (0.5%)
1	F	0.42	0/2000	0.86	5/2702 (0.2%)
1	G	0.34	0/2009	0.67	2/2714 (0.1%)
1	H	0.52	1/2024 (0.0%)	0.96	12/2735 (0.4%)
All	All	0.46	11/16040 (0.1%)	0.86	68/21671 (0.3%)

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	2
1	E	0	1
1	F	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ARG	CZ-NH2	-14.91	1.13	1.33
1	A	198	ARG	CG-CD	-10.39	1.25	1.51
1	H	43	GLU	CD-OE2	-9.48	1.15	1.25
1	A	39	ARG	CG-CD	-6.81	1.34	1.51
1	A	69	TYR	C-O	6.38	1.35	1.23
1	A	46	GLU	CD-OE1	-5.64	1.19	1.25
1	E	46	GLU	CG-CD	-5.58	1.43	1.51
1	A	71	ASP	CB-CG	-5.53	1.40	1.51
1	A	198	ARG	CA-CB	-5.35	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ARG	CD-NE	5.09	1.55	1.46
1	A	46	GLU	CB-CG	5.05	1.61	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	40	ASP	CB-CG-OD1	-16.38	103.56	118.30
1	A	198	ARG	CG-CD-NE	-16.28	77.61	111.80
1	E	214	ARG	NE-CZ-NH2	-14.80	112.90	120.30
1	A	71	ASP	CB-CG-OD2	-13.92	105.77	118.30
1	A	39	ARG	NE-CZ-NH2	12.89	126.75	120.30
1	A	195	ASP	CB-CG-OD1	12.34	129.41	118.30
1	F	214	ARG	NE-CZ-NH2	-11.79	114.40	120.30
1	H	40	ASP	CB-CG-OD2	11.16	128.34	118.30
1	A	198	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	A	198	ARG	N-CA-CB	-10.70	91.33	110.60
1	A	195	ASP	OD1-CG-OD2	-9.78	104.71	123.30
1	A	198	ARG	NH1-CZ-NH2	-9.43	109.03	119.40
1	H	48	LYS	CB-CA-C	8.90	128.20	110.40
1	E	47	PHE	N-CA-C	-8.84	87.12	111.00
1	A	69	TYR	O-C-N	8.75	136.70	122.70
1	A	71	ASP	CB-CG-OD1	8.37	125.83	118.30
1	E	69	TYR	CB-CG-CD2	8.31	125.98	121.00
1	F	214	ARG	CG-CD-NE	-8.23	94.52	111.80
1	H	48	LYS	CA-CB-CG	-8.09	95.60	113.40
1	A	195	ASP	CB-CA-C	7.87	126.13	110.40
1	A	71	ASP	CB-CA-C	-7.71	94.97	110.40
1	A	69	TYR	C-N-CA	7.69	140.93	121.70
1	A	198	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	F	95	LEU	CB-CG-CD2	-7.55	98.16	111.00
1	E	69	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	H	46	GLU	OE1-CD-OE2	7.37	132.15	123.30
1	A	39	ARG	NE-CZ-NH1	-7.25	116.68	120.30
1	A	69	TYR	CB-CG-CD1	-7.24	116.66	121.00
1	E	47	PHE	CB-CG-CD1	-7.09	115.84	120.80
1	H	224	ASN	N-CA-C	7.07	130.10	111.00
1	B	198	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	A	69	TYR	CB-CG-CD2	6.72	125.03	121.00
1	C	165	LYS	N-CA-C	-6.72	92.87	111.00
1	H	163	ILE	N-CA-C	-6.62	93.14	111.00
1	H	48	LYS	CB-CG-CD	6.59	128.75	111.60
1	A	46	GLU	CG-CD-OE1	-6.56	105.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	163	ILE	N-CA-C	-6.43	93.64	111.00
1	E	47	PHE	CB-CG-CD2	6.41	125.29	120.80
1	E	214	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	46	GLU	CA-CB-CG	6.19	127.02	113.40
1	A	198	ARG	CD-NE-CZ	6.18	132.25	123.60
1	E	165	LYS	N-CA-C	-6.13	94.44	111.00
1	A	71	ASP	N-CA-CB	-6.07	99.68	110.60
1	C	95	LEU	CB-CG-CD2	-6.01	100.79	111.00
1	E	35	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	B	93	LYS	CB-CG-CD	5.85	126.81	111.60
1	F	95	LEU	CA-CB-CG	5.80	128.65	115.30
1	H	46	GLU	CA-CB-CG	5.77	126.10	113.40
1	A	71	ASP	N-CA-C	5.73	126.48	111.00
1	A	198	ARG	CA-CB-CG	-5.65	100.98	113.40
1	E	35	TYR	CB-CG-CD2	5.49	124.29	121.00
1	A	69	TYR	CA-CB-CG	5.46	123.78	113.40
1	B	39	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	97	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	108	GLU	CA-CB-CG	5.34	125.15	113.40
1	A	39	ARG	CA-CB-CG	-5.28	101.79	113.40
1	H	40	ASP	CB-CA-C	5.26	120.93	110.40
1	E	95	LEU	CA-CB-CG	5.25	127.36	115.30
1	F	72	LYS	CB-CA-C	-5.20	99.99	110.40
1	G	43	GLU	CA-CB-CG	5.19	124.82	113.40
1	A	160	ALA	C-N-CD	5.15	139.21	128.40
1	E	214	ARG	CG-CD-NE	-5.15	100.99	111.80
1	E	71	ASP	N-CA-C	-5.14	97.11	111.00
1	H	220	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	70	ALA	N-CA-C	5.10	124.78	111.00
1	C	47	PHE	N-CA-C	-5.06	97.34	111.00
1	A	45	GLU	C-N-CA	5.03	134.27	121.70
1	H	224	ASN	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	GLU	Sidechain
1	A	71	ASP	Sidechain
1	E	93	LYS	Peptide
1	F	108	GLU	Sidechain

5.2 Too-close contacts

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	1961	0	1990	54	1
1	B	1983	0	2007	35	0
1	C	1961	0	1990	31	0
1	D	1967	0	1995	26	1
1	E	1967	0	1996	52	1
1	F	1967	0	1995	49	0
1	G	1973	0	2001	22	0
1	H	1991	0	2013	32	1
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	1	0
All	All	15781	0	15987	273	2

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 9.

All (273) 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:39:ARG:NE	1:A:69:TYR:OH	1.77	1.17
1:A:46:GLU:OE1	1:A:46:GLU:N	1.91	1.02
1:A:198:ARG:HH21	1:B:198:ARG:NH1	1.59	0.97
1:G:67:SER:HB3	1:G:92:ILE:HD11	1.51	0.92
1:A:214:ARG:NH2	1:B:232:GLU:OE1	2.03	0.92
1:G:195:ASP:OD1	1:G:198:ARG:NH2	2.04	0.90
1:F:95:LEU:HD21	1:F:100:PHE:HB2	1.55	0.89
1:A:198:ARG:NH2	1:B:198:ARG:NH1	2.22	0.87
1:A:39:ARG:HE	1:A:69:TYR:HH	1.21	0.85
1:D:67:SER:HB3	1:D:92:ILE:HD11	1.60	0.82
1:G:213:LEU:O	1:G:214:ARG:NH1	2.13	0.81
1:F:67:SER:HB3	1:F:92:ILE:HD11	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:OE1	1:A:46:GLU:CA	2.31	0.77
1:F:95:LEU:HG	1:F:99:GLU:HB2	1.67	0.76
1:E:95:LEU:HD21	1:E:100:PHE:HB2	1.67	0.76
1:G:163:ILE:O	1:G:164:GLU:HB2	1.86	0.75
1:H:164:GLU:OE2	1:H:165:LYS:NZ	2.18	0.74
1:H:36:GLN:HG2	1:H:39:ARG:NH2	2.02	0.74
1:D:195:ASP:OD1	1:D:198:ARG:NH2	2.22	0.73
1:F:103:LYS:HG3	1:F:108:GLU:OE1	1.89	0.72
1:A:198:ARG:NH2	1:B:198:ARG:CZ	2.52	0.72
1:C:198:ARG:HG3	1:D:198:ARG:NH1	2.04	0.72
1:C:20:LYS:HE3	1:C:247:LEU:HD21	1.71	0.71
1:E:76:VAL:HG22	1:E:95:LEU:HD22	1.73	0.70
1:A:49:GLU:HB3	1:A:111:PRO:HA	1.73	0.70
1:A:77:ASP:OD1	1:A:78:ILE:N	2.23	0.69
1:F:49:GLU:HA	1:F:72:LYS:HB3	1.74	0.69
1:G:50:VAL:HG22	1:G:113:LEU:HB3	1.75	0.69
1:F:96:ASN:OD1	1:F:99:GLU:HG3	1.91	0.69
1:B:165:LYS:HG3	1:B:165:LYS:O	1.91	0.69
1:C:144:VAL:HG11	1:C:179:VAL:HG13	1.75	0.68
1:A:194:VAL:O	1:A:198:ARG:HG2	1.93	0.68
1:F:43:GLU:CD	1:F:44:GLY:H	1.97	0.68
1:E:214:ARG:NH2	1:F:214:ARG:NE	2.43	0.67
1:E:68:LYS:HE3	1:E:69:TYR:CE2	2.30	0.67
1:B:77:ASP:OD1	1:B:78:ILE:N	2.28	0.66
1:C:118:THR:HG21	1:C:123:ILE:HG12	1.75	0.66
1:A:35:TYR:HH	1:A:69:TYR:HE2	1.43	0.66
1:B:144:VAL:HG11	1:B:179:VAL:HG13	1.78	0.66
1:H:213:LEU:O	1:H:214:ARG:NH1	2.28	0.66
1:C:124:GLU:HG3	1:C:126:GLU:OE1	1.95	0.66
1:G:49:GLU:OE2	1:G:110:ASN:N	2.26	0.65
1:F:77:ASP:OD1	1:F:78:ILE:N	2.29	0.65
1:H:144:VAL:HG11	1:H:179:VAL:HG13	1.78	0.65
1:B:186:MSE:HE3	1:B:190:ILE:HD11	1.79	0.65
1:G:198:ARG:NH1	1:H:198:ARG:HG3	2.11	0.65
1:A:197:SER:OG	1:A:198:ARG:HG2	1.97	0.64
1:D:144:VAL:HG11	1:D:179:VAL:HG13	1.79	0.64
1:A:195:ASP:HA	1:A:198:ARG:HB2	1.79	0.63
1:A:35:TYR:OH	1:A:69:TYR:HE2	1.80	0.63
1:B:90:ASN:ND2	1:B:91:SER:H	1.97	0.63
1:E:213:LEU:O	1:E:214:ARG:NH1	2.32	0.62
1:H:47:PHE:C	1:H:48:LYS:HG3	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:NH2	1:B:198:ARG:HH12	1.96	0.62
1:D:56:TYR:CE1	1:D:94:PHE:HB3	2.34	0.62
1:F:144:VAL:HG11	1:F:179:VAL:HG13	1.82	0.62
1:A:48:LYS:HA	1:A:71:ASP:OD2	2.00	0.61
1:E:214:ARG:HH21	1:F:214:ARG:NH2	1.98	0.61
1:G:144:VAL:HG11	1:G:179:VAL:HG13	1.82	0.61
1:B:132:ASN:HD21	1:B:165:LYS:HE2	1.65	0.60
1:E:214:ARG:HH21	1:F:214:ARG:CZ	2.14	0.60
1:C:219:ILE:HA	1:C:223:GLU:HG2	1.82	0.60
1:C:74:TYR:HE2	1:C:109:VAL:HG11	1.66	0.60
1:F:95:LEU:CD2	1:F:100:PHE:HB2	2.28	0.60
1:H:124:GLU:HG3	1:H:126:GLU:OE1	2.02	0.60
1:E:42:LEU:O	1:E:44:GLY:N	2.30	0.60
1:E:29:GLU:HG2	1:E:258:ILE:HG21	1.83	0.60
1:D:50:VAL:HG22	1:D:113:LEU:HB3	1.83	0.59
1:F:49:GLU:OE2	1:F:110:ASN:N	2.28	0.59
1:B:36:GLN:OE1	1:B:39:ARG:NH2	2.35	0.59
1:H:163:ILE:O	1:H:164:GLU:HB3	2.01	0.59
1:F:235:GLN:HG3	1:F:236:PRO:HD2	1.84	0.59
1:E:77:ASP:OD1	1:E:78:ILE:N	2.32	0.59
1:C:95:LEU:HD22	1:C:100:PHE:HB2	1.84	0.59
1:H:186:MSE:HE3	1:H:190:ILE:HD11	1.84	0.59
1:A:195:ASP:O	1:A:198:ARG:HB2	2.02	0.59
1:A:144:VAL:HG11	1:A:179:VAL:HG13	1.84	0.58
1:C:95:LEU:HD21	1:C:100:PHE:N	2.18	0.58
1:A:232:GLU:OE1	1:B:214:ARG:NH2	2.36	0.58
1:G:77:ASP:OD1	1:G:78:ILE:N	2.35	0.58
1:H:93:LYS:HE3	1:H:95:LEU:HD21	1.84	0.58
1:A:160:ALA:O	1:A:163:ILE:HG22	2.04	0.58
1:E:193:ILE:HD12	1:E:213:LEU:HD21	1.85	0.58
1:E:214:ARG:NH2	1:F:214:ARG:NH2	2.52	0.58
1:E:214:ARG:NH2	1:F:214:ARG:HE	2.01	0.57
1:E:95:LEU:HG	1:E:99:GLU:HB2	1.87	0.57
1:E:123:ILE:HD11	1:E:127:PHE:CD2	2.39	0.57
1:E:144:VAL:HG11	1:E:179:VAL:HG13	1.86	0.57
1:G:49:GLU:HG2	1:G:111:PRO:HA	1.87	0.57
1:C:74:TYR:HE2	1:C:109:VAL:CG1	2.18	0.57
1:F:56:TYR:HD1	1:F:75:LEU:HD22	1.70	0.57
1:H:102:LEU:HD11	1:H:106:ARG:HH12	1.69	0.56
1:E:39:ARG:NH2	1:E:69:TYR:HE2	2.03	0.56
1:H:67:SER:HB3	1:H:92:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:HA	1:A:69:TYR:O	2.05	0.56
1:H:103:LYS:HG2	1:H:108:GLU:HB2	1.88	0.56
1:F:49:GLU:HB2	1:F:72:LYS:HD2	1.88	0.56
1:H:164:GLU:OE1	1:H:165:LYS:HG2	2.06	0.56
1:E:39:ARG:HH21	1:E:69:TYR:HE2	1.55	0.55
1:G:76:VAL:HA	1:G:95:LEU:O	2.07	0.55
1:A:35:TYR:CE2	1:A:65:MSE:HG2	2.42	0.55
1:H:96:ASN:OD1	1:H:99:GLU:HG3	2.07	0.55
1:G:120:LEU:HD11	1:G:149:ILE:HG23	1.88	0.55
1:C:50:VAL:HG22	1:C:113:LEU:HB3	1.88	0.54
1:C:135:VAL:HG22	1:C:167:LYS:HB3	1.88	0.54
1:D:186:MSE:HE3	1:D:190:ILE:HD11	1.89	0.54
1:H:225:ASP:HB3	2:H:302:HOH:O	2.07	0.54
1:B:48:LYS:HG2	1:B:71:ASP:OD2	2.08	0.54
1:A:219:ILE:HA	1:A:223:GLU:HG2	1.88	0.54
1:H:36:GLN:HG2	1:H:39:ARG:HH22	1.72	0.54
1:D:49:GLU:CG	1:D:111:PRO:HA	2.38	0.53
1:D:170:VAL:HG23	1:D:268:LEU:HD11	1.90	0.53
1:E:123:ILE:HD11	1:E:127:PHE:HD2	1.73	0.53
1:F:120:LEU:HD11	1:F:149:ILE:HG23	1.91	0.53
1:H:93:LYS:HG3	1:H:94:PHE:N	2.23	0.53
1:D:72:LYS:HZ1	1:D:93:LYS:HG3	1.72	0.53
1:F:56:TYR:CD1	1:F:75:LEU:HD22	2.43	0.53
1:D:162:PHE:HB3	1:D:166:ALA:HB3	1.91	0.53
1:E:214:ARG:NH2	1:F:214:ARG:HG3	2.24	0.53
1:C:95:LEU:HD21	1:C:100:PHE:H	1.74	0.53
1:C:95:LEU:HD23	1:C:96:ASN:O	2.09	0.53
1:G:186:MSE:HE3	1:G:190:ILE:HD11	1.89	0.53
1:E:214:ARG:NH2	1:F:214:ARG:HH21	2.07	0.52
1:G:96:ASN:OD1	1:G:99:GLU:HG3	2.10	0.52
1:F:35:TYR:CZ	1:F:65:MSE:HB3	2.45	0.52
1:B:124:GLU:N	1:B:124:GLU:OE1	2.43	0.52
1:E:72:LYS:HE3	1:E:74:TYR:CZ	2.44	0.52
1:C:46:GLU:OE1	1:C:69:TYR:HA	2.09	0.52
1:D:120:LEU:HD11	1:D:149:ILE:HG23	1.90	0.52
1:C:49:GLU:HG3	1:C:111:PRO:HA	1.92	0.51
1:F:36:GLN:HG2	1:F:39:ARG:NH2	2.24	0.51
1:C:124:GLU:OE2	1:C:125:PRO:HD2	2.11	0.51
1:E:198:ARG:NH1	1:F:191:ASP:OD1	2.38	0.51
1:F:73:VAL:HB	1:F:92:ILE:HD12	1.91	0.51
1:A:47:PHE:CE2	1:A:113:LEU:HD22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:VAL:HG22	1:B:113:LEU:HB3	1.93	0.51
1:A:103:LYS:HG2	1:A:108:GLU:OE1	2.11	0.51
1:E:47:PHE:HB3	1:E:112:ASP:HB2	1.92	0.50
1:E:95:LEU:CD2	1:E:100:PHE:HB2	2.38	0.50
1:G:49:GLU:CG	1:G:111:PRO:HA	2.41	0.50
1:E:72:LYS:HE3	1:E:74:TYR:CE2	2.46	0.50
1:A:198:ARG:HD3	1:B:194:VAL:HG11	1.94	0.50
1:H:78:ILE:HG22	1:H:97:LEU:HB2	1.93	0.50
1:A:76:VAL:HA	1:A:95:LEU:O	2.11	0.49
1:F:20:LYS:HE2	1:F:247:LEU:HD21	1.94	0.49
1:A:134:LYS:O	1:A:166:ALA:HB1	2.13	0.49
1:F:91:SER:OG	1:F:92:ILE:N	2.45	0.49
1:H:52:ILE:HD11	1:H:66:LEU:HD12	1.95	0.48
1:B:200:ILE:HD12	1:B:238:ILE:HD13	1.95	0.48
1:E:102:LEU:O	1:E:105:ILE:HG13	2.13	0.48
1:F:95:LEU:HD21	1:F:100:PHE:CB	2.33	0.48
1:A:214:ARG:HH22	1:B:232:GLU:CD	2.16	0.48
1:A:198:ARG:HH21	1:B:198:ARG:CZ	2.17	0.48
1:A:198:ARG:CZ	1:A:198:ARG:HB3	2.42	0.48
1:E:214:ARG:NH2	1:F:214:ARG:CZ	2.77	0.48
1:C:186:MSE:HE3	1:C:190:ILE:HD11	1.95	0.48
1:C:74:TYR:CE2	1:C:109:VAL:HG11	2.47	0.48
1:E:214:ARG:HH22	1:F:214:ARG:HG3	1.78	0.48
1:A:193:ILE:HD12	1:A:213:LEU:HD21	1.96	0.47
1:C:54:GLY:O	1:C:77:ASP:HA	2.13	0.47
1:E:214:ARG:HH21	1:F:214:ARG:NE	2.12	0.47
1:D:49:GLU:HG3	1:D:111:PRO:HA	1.96	0.47
1:D:49:GLU:OE2	1:D:110:ASN:N	2.33	0.47
1:G:160:ALA:O	1:G:163:ILE:HG22	2.13	0.47
1:A:163:ILE:O	1:A:164:GLU:HB3	2.14	0.47
1:A:200:ILE:HD12	1:A:238:ILE:HD13	1.95	0.47
1:G:193:ILE:HD12	1:G:213:LEU:HD21	1.96	0.47
1:D:36:GLN:HG2	1:D:39:ARG:NH2	2.29	0.47
1:G:52:ILE:HD11	1:G:66:LEU:HD12	1.95	0.47
1:B:235:GLN:HG3	1:B:236:PRO:HD2	1.97	0.47
1:H:106:ARG:HG3	1:H:106:ARG:HH11	1.80	0.47
1:A:178:ARG:HG3	1:A:260:LEU:HD13	1.97	0.47
1:D:55:VAL:HA	1:D:77:ASP:OD2	2.14	0.47
1:H:54:GLY:O	1:H:77:ASP:HA	2.15	0.47
1:A:47:PHE:CD2	1:A:113:LEU:HD22	2.50	0.46
1:B:195:ASP:OD1	1:B:198:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:C	1:A:93:LYS:HD3	2.36	0.46
1:D:73:VAL:HB	1:D:92:ILE:HD12	1.98	0.46
1:C:193:ILE:HD12	1:C:213:LEU:HD21	1.97	0.46
1:F:76:VAL:HA	1:F:95:LEU:O	2.16	0.46
1:E:96:ASN:OD1	1:E:99:GLU:HG2	2.15	0.46
1:F:193:ILE:HD12	1:F:213:LEU:HD21	1.99	0.45
1:D:200:ILE:HD12	1:D:238:ILE:HD13	1.99	0.45
1:B:54:GLY:O	1:B:77:ASP:HA	2.16	0.45
1:C:77:ASP:OD1	1:C:78:ILE:N	2.50	0.45
1:D:214:ARG:HG3	1:D:232:GLU:OE1	2.17	0.45
1:E:49:GLU:HG3	1:E:111:PRO:HA	1.98	0.45
1:A:195:ASP:OD1	1:A:198:ARG:CB	2.65	0.45
1:E:45:GLU:HG3	1:E:46:GLU:N	2.32	0.45
1:A:50:VAL:HG22	1:A:113:LEU:HB3	1.99	0.45
1:C:116:ASP:OD2	1:C:158:ARG:NH1	2.40	0.45
1:F:43:GLU:CD	1:F:44:GLY:N	2.69	0.45
1:H:76:VAL:HA	1:H:95:LEU:O	2.17	0.45
1:E:50:VAL:HG22	1:E:113:LEU:HB3	1.98	0.45
1:B:50:VAL:HB	1:B:73:VAL:HG22	1.98	0.45
1:D:214:ARG:NH1	1:D:232:GLU:OE1	2.50	0.44
1:E:220:LEU:O	1:E:224:ASN:HA	2.16	0.44
1:E:135:VAL:HG22	1:E:167:LYS:HB3	1.99	0.44
1:E:232:GLU:OE2	1:F:214:ARG:NH2	2.50	0.44
1:H:200:ILE:HD12	1:H:238:ILE:HD13	1.99	0.44
1:C:232:GLU:OE1	1:D:214:ARG:NH2	2.50	0.44
1:E:103:LYS:HG3	1:E:108:GLU:OE1	2.17	0.44
1:A:45:GLU:HG2	1:A:47:PHE:CZ	2.51	0.44
1:A:125:PRO:HG3	1:A:158:ARG:HG2	1.99	0.44
1:F:50:VAL:HB	1:F:73:VAL:HG22	1.99	0.44
1:H:193:ILE:HD12	1:H:213:LEU:HD21	2.00	0.44
1:A:116:ASP:OD2	1:A:158:ARG:NH1	2.41	0.44
1:A:97:LEU:HG	1:A:101:LYS:HE3	2.00	0.44
1:B:47:PHE:CE2	1:B:113:LEU:HD22	2.53	0.44
1:B:55:VAL:HG21	1:B:58:TRP:CD1	2.53	0.44
1:F:164:GLU:O	1:F:165:LYS:HB2	2.17	0.44
1:H:163:ILE:O	1:H:164:GLU:CB	2.66	0.44
1:E:35:TYR:OH	1:E:39:ARG:NE	2.51	0.43
1:F:49:GLU:HG2	1:F:111:PRO:HA	2.01	0.43
1:A:207:LEU:HD21	1:B:120:LEU:HD12	2.00	0.43
1:E:70:ALA:HB3	1:E:73:VAL:HG23	1.98	0.43
1:F:200:ILE:HD12	1:F:238:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:PRO:HG3	1:G:158:ARG:HG2	2.01	0.43
1:B:76:VAL:HA	1:B:95:LEU:O	2.19	0.43
1:C:246:VAL:HA	1:C:249:GLU:OE1	2.18	0.43
1:E:163:ILE:O	1:E:164:GLU:HB2	2.18	0.43
1:B:214:ARG:HG2	1:B:219:ILE:HD11	2.00	0.43
1:C:102:LEU:HD23	1:C:102:LEU:HA	1.90	0.43
1:A:124:GLU:HA	1:A:125:PRO:HD3	1.86	0.43
1:E:170:VAL:HG23	1:E:268:LEU:HD11	2.00	0.42
1:E:95:LEU:HD23	1:E:95:LEU:C	2.39	0.42
1:A:194:VAL:O	1:A:198:ARG:CG	2.63	0.42
1:H:65:MSE:O	1:H:68:LYS:HE2	2.18	0.42
1:A:72:LYS:NZ	1:A:74:TYR:OH	2.46	0.42
1:E:92:ILE:O	1:E:93:LYS:HD2	2.19	0.42
1:F:135:VAL:HG22	1:F:167:LYS:HB3	2.01	0.42
1:A:45:GLU:O	1:A:46:GLU:O	2.36	0.42
1:F:124:GLU:HA	1:F:125:PRO:HD3	1.87	0.42
1:H:61:TYR:CE1	1:H:65:MSE:HE3	2.54	0.42
1:H:89:ASN:O	1:H:90:ASN:HB2	2.20	0.42
1:E:96:ASN:OD1	1:E:96:ASN:N	2.51	0.42
1:F:125:PRO:HG3	1:F:158:ARG:HG2	2.01	0.42
1:B:122:GLY:H	1:B:158:ARG:HH22	1.68	0.42
1:B:90:ASN:HD22	1:B:91:SER:H	1.66	0.42
1:C:235:GLN:HG3	1:C:236:PRO:HD2	2.01	0.42
1:C:124:GLU:CD	1:C:125:PRO:HD2	2.41	0.42
1:C:200:ILE:HD12	1:C:238:ILE:HD13	2.02	0.42
1:E:138:VAL:HG11	1:E:159:THR:CG2	2.50	0.42
1:H:50:VAL:HG22	1:H:113:LEU:HB3	2.02	0.42
1:D:23:VAL:HG11	1:D:216:TYR:OH	2.20	0.41
1:G:106:ARG:HG3	1:G:106:ARG:O	2.20	0.41
1:A:198:ARG:NH2	1:B:198:ARG:NH2	2.67	0.41
1:H:43:GLU:OE2	1:H:43:GLU:HA	2.20	0.41
1:D:61:TYR:CE1	1:D:65:MSE:HE3	2.55	0.41
1:F:49:GLU:CG	1:F:111:PRO:HA	2.50	0.41
1:G:124:GLU:CD	1:G:124:GLU:H	2.24	0.41
1:B:26:VAL:HG22	1:B:258:ILE:HD11	2.01	0.41
1:E:114:ILE:HD12	1:E:133:PRO:HG3	2.03	0.41
1:E:235:GLN:HE22	1:F:214:ARG:CZ	2.34	0.41
1:E:156:TYR:HA	1:E:159:THR:OG1	2.21	0.41
1:B:112:ASP:HB3	1:B:134:LYS:HE2	2.03	0.41
1:C:114:ILE:HD12	1:C:133:PRO:HG3	2.02	0.41
1:A:49:GLU:N	1:A:112:ASP:OD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:CE1	1:A:65:MSE:HB3	2.55	0.41
1:F:76:VAL:HG22	1:F:95:LEU:HD22	2.02	0.41
1:G:106:ARG:HD2	1:G:106:ARG:HH11	1.76	0.41
1:A:67:SER:HA	1:A:73:VAL:HG21	2.01	0.41
1:C:96:ASN:OD1	1:C:99:GLU:HG3	2.20	0.41
1:E:225:ASP:OD2	1:E:228:LYS:HB2	2.21	0.41
1:F:43:GLU:CG	1:F:44:GLY:H	2.33	0.41
1:B:97:LEU:O	1:B:101:LYS:HG3	2.21	0.41
1:H:46:GLU:OE2	1:H:48:LYS:NZ	2.51	0.41
1:D:76:VAL:HA	1:D:95:LEU:O	2.21	0.40
1:D:49:GLU:HG2	1:D:111:PRO:HA	2.02	0.40
1:E:120:LEU:HD12	1:F:207:LEU:HD21	2.04	0.40
1:A:120:LEU:HD11	1:A:149:ILE:HG23	2.03	0.40
1:D:235:GLN:HG3	1:D:236:PRO:HD2	2.03	0.40
1:E:42:LEU:HA	1:E:42:LEU:HD23	1.86	0.40

All (2) 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:D:48:LYS:NZ	1:E:71:ASP:OD1[4_465]	2.00	0.20
1:A:46:GLU:OE2	1:H:39:ARG:NH2[3_655]	2.03	0.17

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	239/268 (89%)	233 (98%)	3 (1%)	3 (1%)	15 46
1	B	242/268 (90%)	240 (99%)	1 (0%)	1 (0%)	39 74
1	C	239/268 (89%)	233 (98%)	6 (2%)	0	100 100
1	D	240/268 (90%)	233 (97%)	4 (2%)	3 (1%)	15 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	240/268 (90%)	232 (97%)	7 (3%)	1 (0%)	39 74
1	F	240/268 (90%)	231 (96%)	8 (3%)	1 (0%)	39 74
1	G	241/268 (90%)	238 (99%)	3 (1%)	0	100 100
1	H	243/268 (91%)	237 (98%)	4 (2%)	2 (1%)	24 60
All	All	1924/2144 (90%)	1877 (98%)	36 (2%)	11 (1%)	30 67

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	46	GLU
1	D	164	GLU
1	H	90	ASN
1	B	164	GLU
1	D	44	GLY
1	F	165	LYS
1	H	164	GLU
1	D	43	GLU
1	E	44	GLY
1	A	44	GLY

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	218/233 (94%)	216 (99%)	2 (1%)	84 96
1	B	221/233 (95%)	220 (100%)	1 (0%)	92 98
1	C	218/233 (94%)	216 (99%)	2 (1%)	84 96
1	D	219/233 (94%)	218 (100%)	1 (0%)	92 98
1	E	219/233 (94%)	216 (99%)	3 (1%)	74 93
1	F	219/233 (94%)	219 (100%)	0	100 100
1	G	220/233 (94%)	218 (99%)	2 (1%)	84 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	222/233 (95%)	220 (99%)	2 (1%)	84 96
All	All	1756/1864 (94%)	1743 (99%)	13 (1%)	88 97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	93	LYS
1	B	39	ARG
1	C	65	MSE
1	C	112	ASP
1	D	132	ASN
1	E	65	MSE
1	E	93	LYS
1	E	95	LEU
1	G	106	ARG
1	G	112	ASP
1	H	40	ASP
1	H	43	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	132	ASN
1	E	36	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	240/268 (89%)	0.53	23 (9%) 10 6	54, 82, 112, 134	0
1	B	243/268 (90%)	0.12	5 (2%) 67 62	55, 72, 98, 117	0
1	C	240/268 (89%)	0.47	19 (7%) 15 10	61, 92, 141, 166	0
1	D	241/268 (89%)	0.13	5 (2%) 67 62	57, 78, 108, 133	0
1	E	240/268 (89%)	0.68	27 (11%) 7 4	62, 97, 161, 180	0
1	F	241/268 (89%)	0.25	10 (4%) 41 34	60, 82, 108, 133	0
1	G	241/268 (89%)	0.41	15 (6%) 24 17	49, 78, 112, 129	0
1	H	244/268 (91%)	0.27	7 (2%) 55 49	53, 76, 107, 135	0
All	All	1930/2144 (90%)	0.36	111 (5%) 26 20	49, 81, 128, 180	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	56	TYR	9.2
1	E	74	TYR	6.4
1	E	100	PHE	5.5
1	H	268	LEU	5.3
1	E	92	ILE	5.2
1	C	74	TYR	5.1
1	A	92	ILE	5.1
1	E	94	PHE	5.0
1	G	56	TYR	4.9
1	A	56	TYR	4.8
1	A	69	TYR	4.8
1	G	162	PHE	4.5
1	C	70	ALA	4.5
1	E	75	LEU	4.4
1	B	268	LEU	4.3
1	E	114	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	73	VAL	4.1
1	E	53	PHE	4.0
1	B	56	TYR	3.9
1	A	99	GLU	3.9
1	E	70	ALA	3.8
1	E	95	LEU	3.8
1	C	56	TYR	3.8
1	E	108	GLU	3.8
1	A	109	VAL	3.7
1	E	99	GLU	3.6
1	C	114	ILE	3.5
1	F	56	TYR	3.5
1	H	222	HIS	3.5
1	F	71	ASP	3.4
1	G	245	ASP	3.4
1	G	111	PRO	3.3
1	C	136	PHE	3.2
1	F	92	ILE	3.2
1	G	109	VAL	3.2
1	F	72	LYS	3.1
1	C	115	VAL	3.1
1	C	108	GLU	3.1
1	H	56	TYR	3.0
1	D	74	TYR	3.0
1	A	106	ARG	3.0
1	H	92	ILE	3.0
1	C	97	LEU	2.9
1	H	226	ILE	2.9
1	H	267	GLU	2.8
1	G	108	GLU	2.8
1	D	225	ASP	2.8
1	A	94	PHE	2.7
1	G	221	PHE	2.7
1	C	113	LEU	2.7
1	D	56	TYR	2.7
1	E	54	GLY	2.7
1	E	113	LEU	2.7
1	B	222	HIS	2.6
1	G	74	TYR	2.6
1	E	52	ILE	2.6
1	D	71	ASP	2.6
1	E	67	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	109	VAL	2.6
1	A	75	LEU	2.5
1	C	110	ASN	2.5
1	G	17	ILE	2.5
1	G	102	LEU	2.5
1	A	245	ASP	2.5
1	A	44	GLY	2.5
1	A	195	ASP	2.4
1	A	73	VAL	2.4
1	C	168	VAL	2.4
1	E	96	ASN	2.4
1	E	44	GLY	2.4
1	E	51	VAL	2.4
1	C	123	ILE	2.4
1	C	42	LEU	2.3
1	E	50	VAL	2.3
1	C	95	LEU	2.3
1	G	268	LEU	2.3
1	A	221	PHE	2.3
1	E	43	GLU	2.3
1	C	62	THR	2.2
1	F	109	VAL	2.2
1	F	245	ASP	2.2
1	G	104	PHE	2.2
1	C	245	ASP	2.2
1	A	108	GLU	2.2
1	E	15	LYS	2.2
1	A	268	LEU	2.2
1	E	45	GLU	2.2
1	A	74	TYR	2.2
1	A	46	GLU	2.2
1	C	167	LYS	2.2
1	B	60	ASN	2.2
1	E	112	ASP	2.2
1	F	53	PHE	2.2
1	A	95	LEU	2.2
1	G	100	PHE	2.2
1	F	94	PHE	2.1
1	A	100	PHE	2.1
1	H	60	ASN	2.1
1	F	222	HIS	2.1
1	C	94	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	2.1
1	C	73	VAL	2.1
1	G	60	ASN	2.1
1	A	51	VAL	2.1
1	F	75	LEU	2.1
1	A	102	LEU	2.1
1	A	17	ILE	2.1
1	B	165	LYS	2.1
1	G	136	PHE	2.1
1	E	72	LYS	2.0
1	A	162	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.