



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 06:48 AM UTC

PDB ID : 5D4T / pdb_00005d4t
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

<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

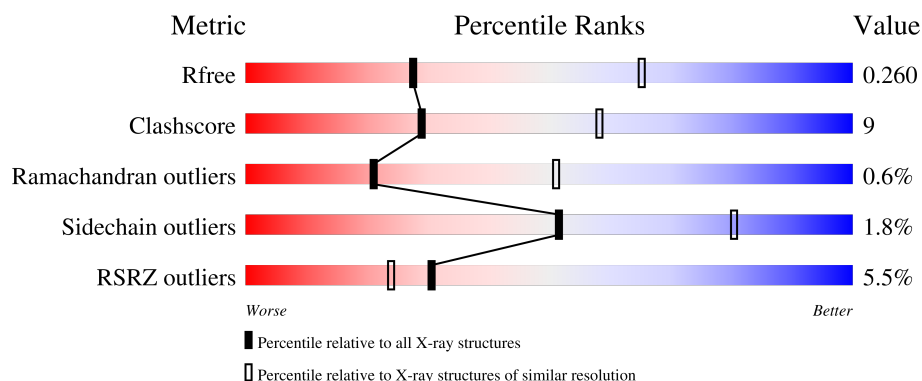
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	268	5% 67% 19% • • 9%
1	B	268	3% 72% 18% • 8%
1	C	268	6% 69% 21% 9%
1	D	268	4% 72% 18% • 9%
1	E	268	9% 65% 22% • 9%

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Mol	Chain	Length	Quality of chain
1	F	268	 3% 69% 20% • 9%
1	G	268	 3% 77% 13% • 9%
1	H	268	 6% 72% 17% • 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

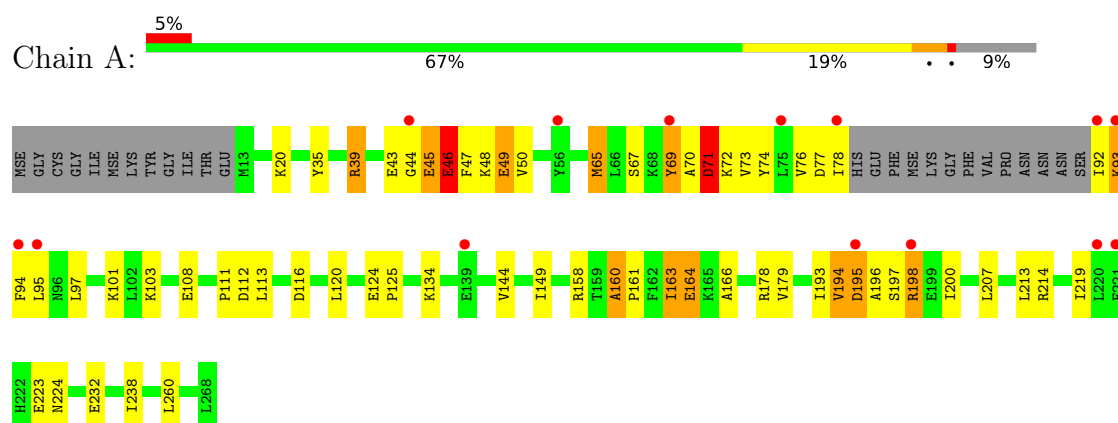
- Molecule 2 is water.

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

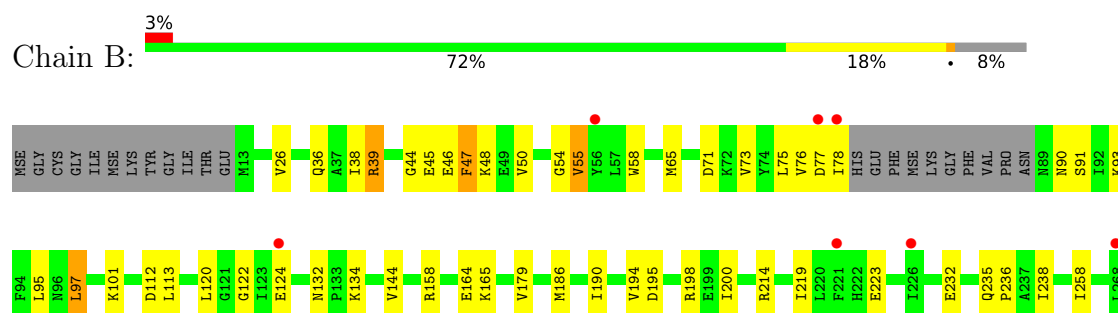
3 Residue-property plots [i](#)

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.

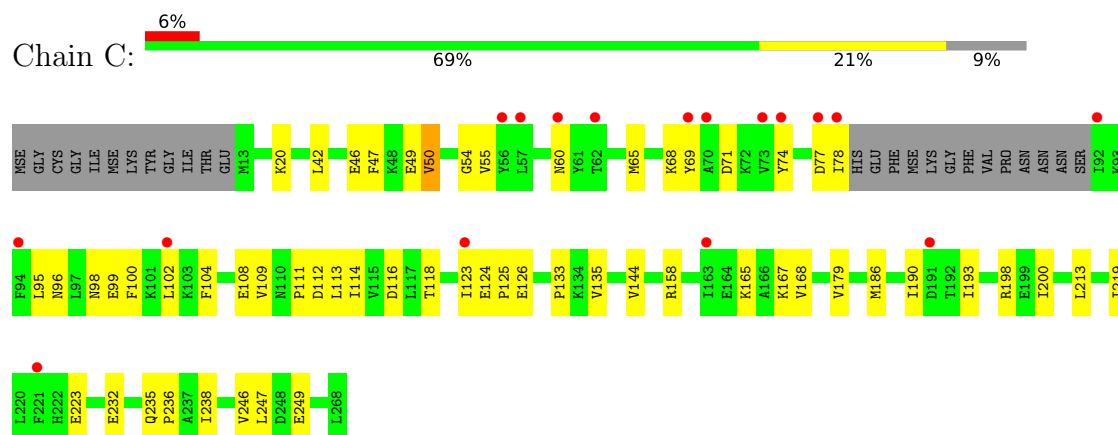
• Molecule 1: Uncharacterized protein MJ0489



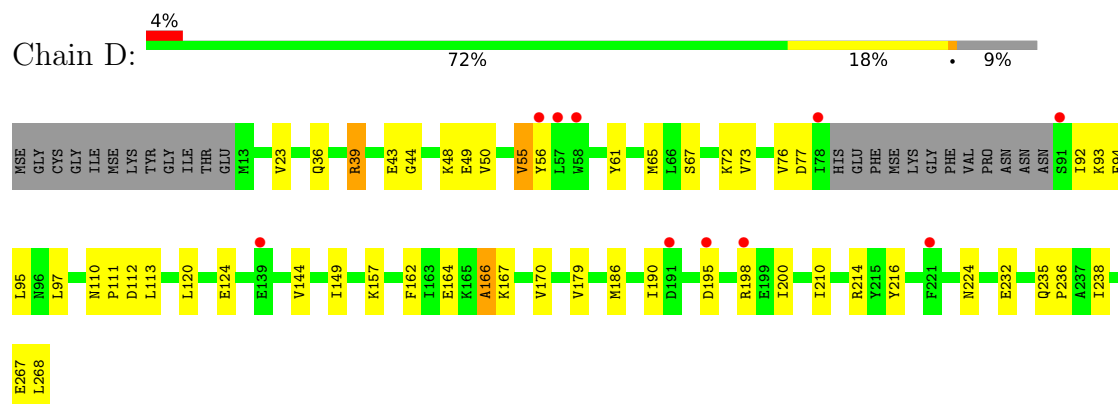
• Molecule 1: Uncharacterized protein MJ0489



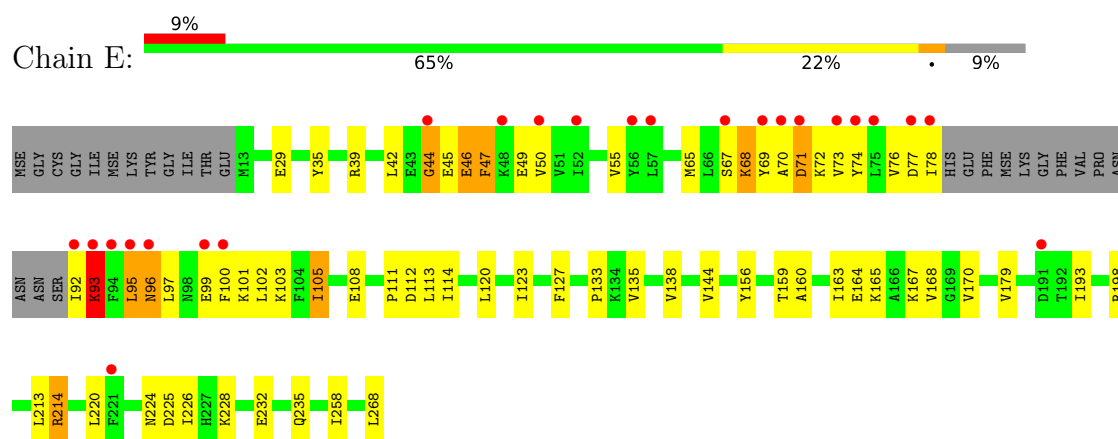
• Molecule 1: Uncharacterized protein MJ0489



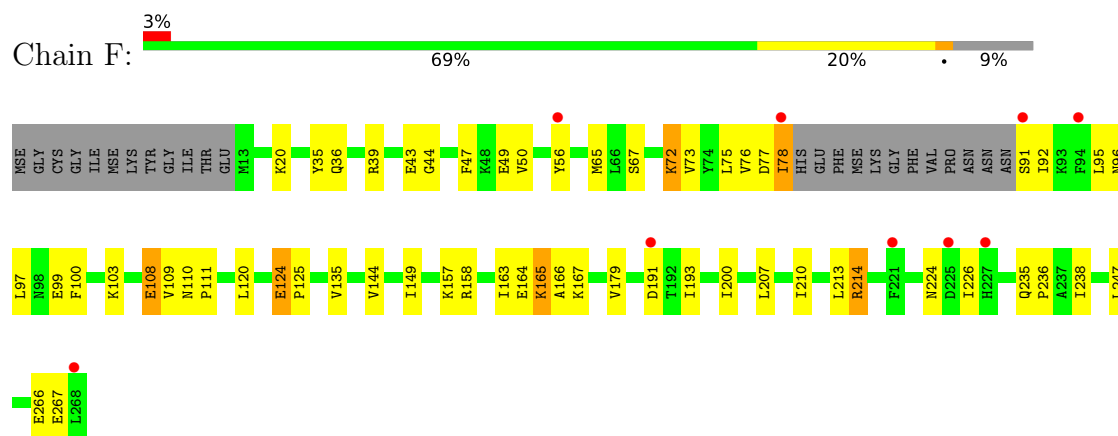
• Molecule 1: Uncharacterized protein MJ0489



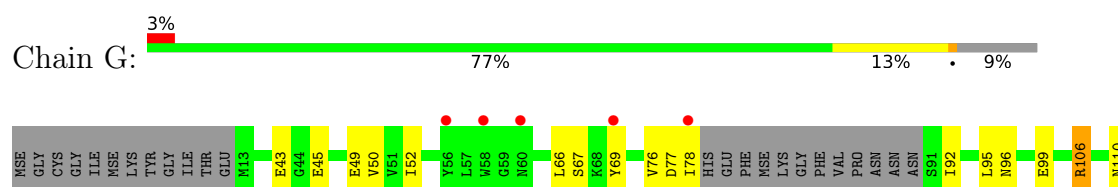
• Molecule 1: Uncharacterized protein MJ0489

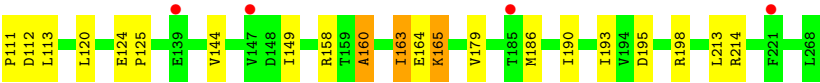


• Molecule 1: Uncharacterized protein MJ0489

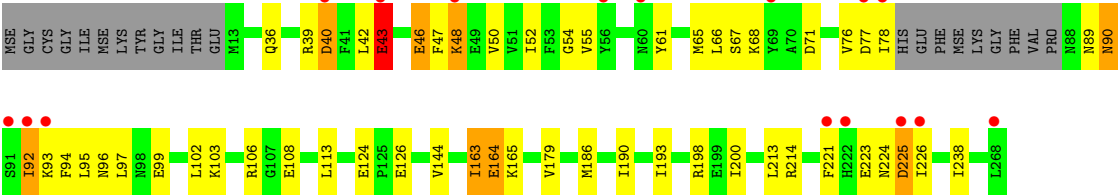


• Molecule 1: Uncharacterized protein MJ0489





● Molecule 1: Uncharacterized protein MJ0489



4 Data and refinement statistics

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) 99.9 (48.56-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.259 0.231 , 0.260	Depositor DCC
R_{free} test set	3501 reflections (5.06%)	wwPDB-VP
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 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.86	11/1994 (0.6%)	1.41	36/2694 (1.3%)
1	B	0.46	0/2016	1.05	9/2724 (0.3%)
1	C	0.47	0/1994	1.15	11/2694 (0.4%)
1	D	0.42	0/2000	0.99	8/2702 (0.3%)
1	E	0.55	0/2003	1.26	15/2706 (0.6%)
1	F	0.53	0/2000	1.16	17/2702 (0.6%)
1	G	0.42	0/2009	0.99	7/2714 (0.3%)
1	H	0.60	2/2024 (0.1%)	1.23	22/2735 (0.8%)
All	All	0.56	13/16040 (0.1%)	1.16	125/21671 (0.6%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ARG	CZ-NH2	-15.22	1.13	1.33
1	A	198	ARG	CG-CD	-8.83	1.25	1.52
1	A	69	TYR	C-O	8.31	1.35	1.24
1	A	198	ARG	CA-CB	-6.98	1.42	1.53
1	A	70	ALA	CA-C	6.71	1.61	1.52
1	A	198	ARG	N-CA	-6.66	1.38	1.46
1	A	198	ARG	CD-NE	6.33	1.55	1.46
1	A	70	ALA	N-CA	5.91	1.53	1.45
1	A	39	ARG	CG-CD	-5.84	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	46	GLU	CA-C	-5.78	1.45	1.52
1	A	46	GLU	CA-C	-5.59	1.45	1.52
1	H	43	GLU	CD-OE2	-5.33	1.15	1.25
1	A	46	GLU	N-CA	5.18	1.52	1.46

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	CG-CD-NE	-15.63	77.61	112.00
1	E	165	LYS	N-CA-C	-15.40	94.44	114.31
1	C	165	LYS	N-CA-C	-15.29	92.87	114.12
1	E	47	PHE	N-CA-C	-14.45	87.12	109.52
1	H	224	ASN	N-CA-C	13.82	130.10	111.30
1	E	71	ASP	N-CA-C	-13.36	97.11	113.41
1	H	163	ILE	N-CA-C	-12.75	93.14	109.58
1	A	198	ARG	N-CA-CB	-12.72	91.33	110.16
1	A	69	TYR	O-C-N	12.15	136.70	122.25
1	A	160	ALA	CA-C-N	-11.83	107.32	120.45
1	A	160	ALA	C-N-CA	-11.83	107.32	120.45
1	A	69	TYR	CA-C-N	11.61	140.93	122.36
1	A	69	TYR	C-N-CA	11.61	140.93	122.36
1	G	163	ILE	N-CA-C	-11.53	93.64	109.55
1	A	70	ALA	N-CA-C	10.50	124.78	109.14
1	H	48	LYS	CB-CA-C	10.39	128.20	109.29
1	E	160	ALA	CA-C-N	-10.25	109.07	120.45
1	E	160	ALA	C-N-CA	-10.25	109.07	120.45
1	A	71	ASP	N-CA-C	10.09	126.48	112.45
1	H	48	LYS	CA-CB-CG	-9.25	95.60	114.10
1	E	68	LYS	N-CA-C	-8.89	101.86	112.89
1	C	98	ASN	N-CA-C	8.44	122.07	111.69
1	A	39	ARG	NE-CZ-NH2	8.38	126.75	119.20
1	A	195	ASP	CB-CA-C	8.38	126.13	110.63
1	F	224	ASN	CA-C-N	-8.18	111.60	123.05
1	F	224	ASN	C-N-CA	-8.18	111.60	123.05
1	A	71	ASP	CB-CA-C	-8.01	94.97	110.11
1	F	214	ARG	CG-CD-NE	-7.95	94.52	112.00
1	C	47	PHE	N-CA-C	-7.94	97.34	109.41
1	A	198	ARG	NH1-CZ-NH2	-7.90	109.03	119.30
1	C	68	LYS	N-CA-C	-7.89	103.10	112.89
1	H	226	ILE	N-CA-C	7.82	118.59	110.62
1	E	101	LYS	N-CA-C	7.63	119.60	111.28
1	H	221	PHE	N-CA-C	7.62	123.73	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLU	N-CA-C	7.59	120.68	110.35
1	H	48	LYS	CB-CG-CD	7.58	128.75	111.30
1	A	195	ASP	OD1-CG-OD2	-7.58	104.71	122.90
1	A	196	ALA	N-CA-C	-7.17	103.46	111.28
1	A	163	ILE	N-CA-C	-7.12	100.33	109.80
1	A	71	ASP	N-CA-CB	-7.10	99.68	110.26
1	H	223	GLU	CA-C-N	7.03	132.38	122.46
1	H	223	GLU	C-N-CA	7.03	132.38	122.46
1	H	224	ASN	N-CA-CB	-7.01	101.59	111.62
1	E	214	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	D	224	ASN	N-CA-C	6.94	120.97	111.54
1	A	94	PHE	N-CA-C	6.92	120.20	109.07
1	D	166	ALA	N-CA-C	6.83	119.45	109.07
1	F	226	ILE	N-CA-C	6.81	117.57	110.62
1	A	224	ASN	N-CA-C	6.77	120.75	111.54
1	B	93	LYS	CB-CG-CD	6.74	126.81	111.30
1	A	45	GLU	CA-C-N	6.67	134.27	121.54
1	A	45	GLU	C-N-CA	6.67	134.27	121.54
1	B	47	PHE	N-CA-C	-6.58	99.33	109.52
1	A	198	ARG	CA-CB-CG	-6.56	100.98	114.10
1	A	46	GLU	CA-CB-CG	6.46	127.02	114.10
1	H	40	ASP	CB-CG-OD1	-6.45	103.56	118.40
1	C	60	ASN	N-CA-C	6.40	119.07	111.33
1	F	97	LEU	N-CA-C	6.32	119.84	111.75
1	E	67	SER	N-CA-C	6.25	120.17	112.54
1	H	223	GLU	N-CA-C	-6.25	105.59	113.72
1	F	267	GLU	N-CA-C	6.22	119.65	109.76
1	F	224	ASN	N-CA-C	6.21	124.03	110.80
1	H	225	ASP	CA-C-N	6.18	128.92	120.46
1	H	225	ASP	C-N-CA	6.18	128.92	120.46
1	A	39	ARG	CA-CB-CG	-6.15	101.79	114.10
1	C	71	ASP	N-CA-C	-6.12	105.64	113.23
1	D	97	LEU	N-CA-C	6.05	119.49	111.75
1	E	46	GLU	N-CA-C	6.03	119.87	110.17
1	H	46	GLU	CA-CB-CG	6.00	126.10	114.10
1	C	50	VAL	N-CA-C	5.98	116.48	108.11
1	D	167	LYS	N-CA-C	-5.95	100.14	109.25
1	H	71	ASP	N-CA-C	-5.91	105.90	113.23
1	F	109	VAL	N-CA-C	5.86	117.13	108.45
1	G	160	ALA	CA-C-N	-5.80	114.02	120.45
1	G	160	ALA	C-N-CA	-5.80	114.02	120.45
1	B	223	GLU	N-CA-C	-5.79	106.19	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	47	PHE	N-CA-C	-5.79	100.61	109.41
1	F	72	LYS	CB-CA-C	-5.77	99.99	109.80
1	A	46	GLU	CG-CD-OE1	-5.75	105.18	118.40
1	D	210	ILE	N-CA-C	5.75	113.57	107.76
1	B	44	GLY	CA-C-N	-5.73	114.34	122.94
1	B	44	GLY	C-N-CA	-5.73	114.34	122.94
1	E	97	LEU	N-CA-C	5.72	119.07	111.75
1	F	210	ILE	N-CA-C	5.64	113.45	107.76
1	F	124	GLU	CA-C-N	5.62	125.46	119.28
1	F	124	GLU	C-N-CA	5.62	125.46	119.28
1	A	198	ARG	CD-NE-CZ	5.61	132.25	124.40
1	A	69	TYR	CB-CA-C	-5.56	101.33	110.72
1	G	165	LYS	CA-CB-CG	-5.54	103.02	114.10
1	C	108	GLU	CA-CB-CG	5.52	125.15	114.10
1	C	104	PHE	N-CA-C	-5.51	105.35	111.36
1	E	96	ASN	N-CA-CB	-5.50	101.94	110.29
1	E	71	ASP	N-CA-CB	5.49	118.49	110.47
1	A	71	ASP	CB-CG-OD2	-5.49	105.77	118.40
1	A	69	TYR	CA-CB-CG	5.49	123.78	113.90
1	A	198	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	F	72	LYS	N-CA-C	5.47	118.33	108.48
1	A	164	GLU	N-CA-CB	-5.47	103.94	112.41
1	D	267	GLU	N-CA-C	5.46	118.44	109.76
1	D	124	GLU	CA-C-N	5.41	125.23	119.28
1	D	124	GLU	C-N-CA	5.41	125.23	119.28
1	G	43	GLU	CA-CB-CG	5.36	124.82	114.10
1	A	194	VAL	CB-CA-C	-5.35	105.13	111.97
1	H	40	ASP	CB-CA-C	5.34	120.93	110.67
1	F	214	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	G	45	GLU	N-CA-C	-5.29	101.08	109.96
1	H	92	ILE	CA-C-N	-5.26	114.40	122.87
1	H	92	ILE	C-N-CA	-5.26	114.40	122.87
1	A	39	ARG	CB-CG-CD	5.25	123.36	111.30
1	A	161	PRO	CA-C-N	-5.22	114.39	122.49
1	A	161	PRO	C-N-CA	-5.22	114.39	122.49
1	H	223	GLU	CB-CA-C	5.21	118.31	109.55
1	E	168	VAL	N-CA-C	5.21	115.46	108.17
1	B	38	ILE	N-CA-C	5.20	115.92	110.62
1	B	45	GLU	CA-C-N	5.18	128.57	120.75
1	B	45	GLU	C-N-CA	5.18	128.57	120.75
1	C	42	LEU	N-CA-C	-5.17	106.92	113.18
1	H	48	LYS	N-CA-CB	-5.17	102.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	42	LEU	N-CA-C	-5.13	106.97	113.18
1	C	168	VAL	N-CA-C	5.09	115.30	108.17
1	G	69	TYR	CB-CA-C	-5.07	102.85	111.02
1	A	71	ASP	CA-C-O	5.05	126.16	120.00
1	F	166	ALA	N-CA-C	5.05	116.74	109.07
1	F	266	GLU	CB-CA-C	5.04	118.07	109.80
1	E	214	ARG	CG-CD-NE	-5.00	100.99	112.00

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	53	1
1	B	1983	0	2007	36	0
1	C	1961	0	1990	32	0
1	D	1967	0	1995	26	1
1	E	1967	0	1996	53	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	275	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 (275) 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:N	1:A:46:GLU:OE1	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
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:43:GLU:CD	1:F:44:GLY:H	1.97	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:O	1:B:165:LYS:HG3	1.91	0.69
1:H:47:PHE:C	1:H:48:LYS:HG3	2.18	0.68
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:HG21	1:C:123:ILE:HG12	1.75	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:H:102:LEU:HD11	1:H:106:ARG:HH12	1.69	0.56
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:D:72:LYS:HZ2	1:D:93:LYS:HG3	1.71	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:F:56:TYR:CD1	1:F:75:LEU:HD22	2.43	0.53
1:A:214:ARG:HH22	1:B:232:GLU:CD	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:B:124:GLU:N	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
1:B:50:VAL:HG22	1:B:113:LEU:HB3	1.93	0.51
1:A:92:ILE:C	1:A:93:LYS:HD3	2.36	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:43:GLU:CD	1:F:44:GLY:N	2.69	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:198:ARG:HH21	1:B:198:ARG:CZ	2.17	0.48
1:A:198:ARG:HB3	1:A:198:ARG:CZ	2.42	0.48
1:E:214:ARG:NH2	1:F:214:ARG:CZ	2.77	0.48
1:C:74:TYR:CE2	1:C:109:VAL:HG11	2.47	0.48
1:C:186:MSE:HE3	1:C:190:ILE:HD11	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:95:LEU:HD23	1:E:95:LEU:C	2.39	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: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:G:193:ILE:HD12	1:G:213:LEU:HD21	1.96	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:C:124:GLU:CD	1:C:125:PRO:HD2	2.41	0.46
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
1:G:124:GLU:CD	1:G:124:GLU:H	2.24	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: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:124:GLU:CD	1:B:124:GLU:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:LEU:HG	1:A:101:LYS:HE3	2.00	0.44
1:A:116:ASP:OD2	1:A:158:ARG:NH1	2.41	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
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: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:90:ASN:HD22	1:B:91:SER:H	1.66	0.42
1:B:122:GLY:H	1:B:158:ARG:HH22	1.68	0.42
1:C:235:GLN:HG3	1:C:236:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:G:106:ARG:HG3	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: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:46:GLU:CD	1:E:69:TYR:HA	2.45	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:95:LEU:HD23	1:C:95:LEU:C	2.46	0.41
1:C:114:ILE:HD12	1:C:133:PRO:HG3	2.02	0.41
1:A:35:TYR:CE1	1:A:65:MSE:HB3	2.55	0.41
1:A:49:GLU:N	1:A:112:ASP:OD1	2.50	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:76:VAL:HG22	1:F:95:LEU:HD22	2.02	0.41
1:G:106:ARG:HH11	1:G:106:ARG:HD2	1.76	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:HD23	1:E:42:LEU:HA	1.86	0.40
1:F:43:GLU:CG	1:F:44:GLY:H	2.33	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%)	9	32
1	B	242/268 (90%)	240 (99%)	1 (0%)	1 (0%)	30	59
1	C	239/268 (89%)	233 (98%)	6 (2%)	0	100	100
1	D	240/268 (90%)	233 (97%)	4 (2%)	3 (1%)	9	32
1	E	240/268 (90%)	232 (97%)	7 (3%)	1 (0%)	30	59
1	F	240/268 (90%)	231 (96%)	8 (3%)	1 (0%)	30	59
1	G	241/268 (90%)	238 (99%)	3 (1%)	0	100	100
1	H	243/268 (91%)	237 (98%)	4 (2%)	2 (1%)	16	44
All	All	1924/2144 (90%)	1877 (98%)	36 (2%)	11 (1%)	21	51

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%)	213 (98%)	5 (2%)	44	76
1	B	221/233 (95%)	216 (98%)	5 (2%)	44	76
1	C	218/233 (94%)	215 (99%)	3 (1%)	59	85
1	D	219/233 (94%)	215 (98%)	4 (2%)	51	80
1	E	219/233 (94%)	213 (97%)	6 (3%)	39	73
1	F	219/233 (94%)	216 (99%)	3 (1%)	59	85
1	G	220/233 (94%)	217 (99%)	3 (1%)	59	85
1	H	222/233 (95%)	219 (99%)	3 (1%)	59	85
All	All	1756/1864 (94%)	1724 (98%)	32 (2%)	51	80

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	46	GLU
1	A	49	GLU
1	A	65	MSE
1	A	93	LYS
1	B	39	ARG
1	B	55	VAL
1	B	65	MSE
1	B	75	LEU
1	B	97	LEU
1	C	55	VAL
1	C	65	MSE
1	C	112	ASP
1	D	39	ARG
1	D	55	VAL
1	D	112	ASP
1	D	157	LYS
1	E	55	VAL
1	E	65	MSE
1	E	93	LYS
1	E	95	LEU
1	E	105	ILE
1	E	226	ILE
1	F	78	ILE

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Mol	Chain	Res	Type
1	F	157	LYS
1	F	163	ILE
1	G	106	ARG
1	G	112	ASP
1	G	165	LYS
1	H	40	ASP
1	H	43	GLU
1	H	55	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	B	90	ASN
1	B	132	ASN
1	C	222	HIS
1	E	36	GLN
1	G	212	ASN
1	H	60	ASN
1	H	212	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](#)

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

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, 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	240/268 (89%)	0.51	14 (5%) 29 22	54, 82, 112, 134	0
1	B	243/268 (90%)	0.13	7 (2%) 53 45	55, 72, 98, 117	0
1	C	240/268 (89%)	0.49	17 (7%) 22 17	61, 92, 141, 166	0
1	D	241/268 (89%)	0.31	10 (4%) 41 33	57, 78, 108, 133	0
1	E	240/268 (89%)	0.76	24 (10%) 12 10	59, 97, 161, 180	1 (0%)
1	F	241/268 (89%)	0.37	9 (3%) 45 37	60, 82, 108, 133	0
1	G	241/268 (89%)	0.29	9 (3%) 45 37	45, 78, 112, 129	1 (0%)
1	H	244/268 (91%)	0.34	16 (6%) 24 19	53, 76, 107, 135	0
All	All	1930/2144 (90%)	0.40	106 (5%) 30 24	45, 81, 128, 180	2 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	56	TYR	8.5
1	E	94	PHE	7.5
1	E	75	LEU	5.8
1	C	56	TYR	5.8
1	A	56	TYR	5.5
1	F	78	ILE	5.3
1	E	92	ILE	5.3
1	E	191	ASP	5.2
1	F	56	TYR	5.2
1	B	56	TYR	5.2
1	A	92	ILE	5.1
1	E	73	VAL	4.8
1	E	74	TYR	4.5
1	E	95	LEU	4.4
1	E	67	SER	4.4
1	A	195	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	91	SER	4.4
1	H	56	TYR	4.3
1	H	226	ILE	4.3
1	C	94	PHE	4.0
1	G	56	TYR	3.9
1	B	221	PHE	3.8
1	G	139	GLU	3.8
1	G	78	ILE	3.8
1	D	91	SER	3.8
1	D	198	ARG	3.7
1	H	221	PHE	3.7
1	D	56	TYR	3.6
1	A	78	ILE	3.6
1	C	60	ASN	3.5
1	B	78	ILE	3.5
1	A	94	PHE	3.4
1	E	70	ALA	3.3
1	D	57	LEU	3.3
1	A	69	TYR	3.2
1	A	221	PHE	3.1
1	E	44	GLY	3.1
1	C	78	ILE	3.1
1	C	74	TYR	3.1
1	H	40	ASP	3.1
1	F	94	PHE	3.0
1	H	92	ILE	3.0
1	C	57	LEU	3.0
1	E	100	PHE	3.0
1	C	69	TYR	2.9
1	F	191	ASP	2.9
1	E	99	GLU	2.8
1	H	48	LYS	2.8
1	E	69	TYR	2.8
1	H	60	ASN	2.8
1	H	77	ASP	2.8
1	A	198	ARG	2.8
1	G	221	PHE	2.7
1	E	78	ILE	2.7
1	E	57	LEU	2.7
1	C	191	ASP	2.7
1	C	123	ILE	2.7
1	H	91	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	78	ILE	2.6
1	D	221	PHE	2.6
1	A	220	LEU	2.5
1	D	195	ASP	2.5
1	H	43	GLU	2.5
1	C	70	ALA	2.5
1	F	268	LEU	2.4
1	C	92	ILE	2.4
1	C	62	THR	2.4
1	G	60	ASN	2.3
1	H	268	LEU	2.3
1	C	102	LEU	2.3
1	H	222	HIS	2.3
1	F	221	PHE	2.3
1	A	93	LYS	2.3
1	E	48	LYS	2.3
1	G	58	TRP	2.3
1	G	185	THR	2.3
1	A	75	LEU	2.2
1	D	191	ASP	2.2
1	E	77	ASP	2.2
1	B	226	ILE	2.2
1	H	78	ILE	2.2
1	B	77	ASP	2.2
1	D	58	TRP	2.2
1	A	139	GLU	2.2
1	B	124	GLU	2.2
1	E	96	ASN	2.2
1	C	73	VAL	2.2
1	G	69	TYR	2.2
1	G	147	VAL	2.1
1	E	71	ASP	2.1
1	E	93	LYS	2.1
1	H	69	TYR	2.1
1	F	227	HIS	2.1
1	H	93	LYS	2.1
1	E	221	PHE	2.1
1	E	50	VAL	2.1
1	B	268	LEU	2.1
1	E	52	ILE	2.1
1	C	221	PHE	2.1
1	C	163	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	139	GLU	2.1
1	A	95	LEU	2.0
1	C	77	ASP	2.0
1	F	225	ASP	2.0
1	A	44	GLY	2.0
1	H	225	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.