Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:16 am BST

PDB ID	:	5EXV
Title	:	Crystal structure of heme binding protein HutX from Vibrio cholerae
Authors	:	Sekine, Y.; Tanaka, Y.; Uchida, T.
Deposited on	:	2015-11-24
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 following versions of software and data (see references ①) were used in the production of this report:

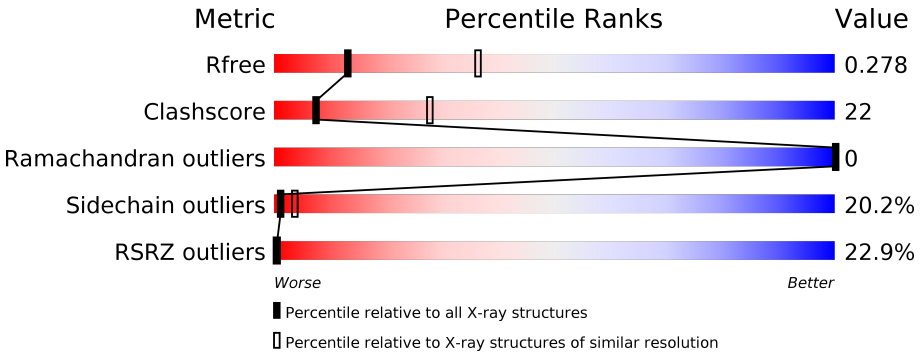
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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	189	15% 38% 36% 13% 14%
1	B	189	57% 26% 5% 12%
1	C	189	8% 50% 27% 10% • 13%
1	D	189	% 55% 26% 6% • 13%
1	E	189	52% 41% 38% 9% 12%
1	F	189	46% 39% 40% 10% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7856 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 Hemin-degrading HemS.ChuX domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1286	823	221	236	6			
1	B	167	Total	C	N	O	S	0	0	0
			1321	844	227	243	7			
1	C	165	Total	C	N	O	S	0	0	0
			1303	833	223	240	7			
1	D	165	Total	C	N	O	S	0	0	0
			1304	834	224	240	6			
1	E	167	Total	C	N	O	S	0	0	0
			1321	844	227	243	7			
1	F	167	Total	C	N	O	S	0	0	0
			1321	844	227	243	7			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A0A085SE34
A	-20	GLY	-	expression tag	UNP A0A085SE34
A	-19	SER	-	expression tag	UNP A0A085SE34
A	-18	SER	-	expression tag	UNP A0A085SE34
A	-17	HIS	-	expression tag	UNP A0A085SE34
A	-16	HIS	-	expression tag	UNP A0A085SE34
A	-15	HIS	-	expression tag	UNP A0A085SE34
A	-14	HIS	-	expression tag	UNP A0A085SE34
A	-13	HIS	-	expression tag	UNP A0A085SE34
A	-12	HIS	-	expression tag	UNP A0A085SE34
A	-11	SER	-	expression tag	UNP A0A085SE34
A	-10	SER	-	expression tag	UNP A0A085SE34
A	-9	GLY	-	expression tag	UNP A0A085SE34
A	-8	LEU	-	expression tag	UNP A0A085SE34
A	-7	GLU	-	expression tag	UNP A0A085SE34
A	-6	VAL	-	expression tag	UNP A0A085SE34
A	-5	LEU	-	expression tag	UNP A0A085SE34

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PHE	-	expression tag	UNP A0A085SE34
A	-3	GLN	-	expression tag	UNP A0A085SE34
A	-2	GLY	-	expression tag	UNP A0A085SE34
A	-1	PRO	-	expression tag	UNP A0A085SE34
A	0	HIS	-	expression tag	UNP A0A085SE34
B	-21	MET	-	expression tag	UNP A0A085SE34
B	-20	GLY	-	expression tag	UNP A0A085SE34
B	-19	SER	-	expression tag	UNP A0A085SE34
B	-18	SER	-	expression tag	UNP A0A085SE34
B	-17	HIS	-	expression tag	UNP A0A085SE34
B	-16	HIS	-	expression tag	UNP A0A085SE34
B	-15	HIS	-	expression tag	UNP A0A085SE34
B	-14	HIS	-	expression tag	UNP A0A085SE34
B	-13	HIS	-	expression tag	UNP A0A085SE34
B	-12	HIS	-	expression tag	UNP A0A085SE34
B	-11	SER	-	expression tag	UNP A0A085SE34
B	-10	SER	-	expression tag	UNP A0A085SE34
B	-9	GLY	-	expression tag	UNP A0A085SE34
B	-8	LEU	-	expression tag	UNP A0A085SE34
B	-7	GLU	-	expression tag	UNP A0A085SE34
B	-6	VAL	-	expression tag	UNP A0A085SE34
B	-5	LEU	-	expression tag	UNP A0A085SE34
B	-4	PHE	-	expression tag	UNP A0A085SE34
B	-3	GLN	-	expression tag	UNP A0A085SE34
B	-2	GLY	-	expression tag	UNP A0A085SE34
B	-1	PRO	-	expression tag	UNP A0A085SE34
B	0	HIS	-	expression tag	UNP A0A085SE34
C	-21	MET	-	expression tag	UNP A0A085SE34
C	-20	GLY	-	expression tag	UNP A0A085SE34
C	-19	SER	-	expression tag	UNP A0A085SE34
C	-18	SER	-	expression tag	UNP A0A085SE34
C	-17	HIS	-	expression tag	UNP A0A085SE34
C	-16	HIS	-	expression tag	UNP A0A085SE34
C	-15	HIS	-	expression tag	UNP A0A085SE34
C	-14	HIS	-	expression tag	UNP A0A085SE34
C	-13	HIS	-	expression tag	UNP A0A085SE34
C	-12	HIS	-	expression tag	UNP A0A085SE34
C	-11	SER	-	expression tag	UNP A0A085SE34
C	-10	SER	-	expression tag	UNP A0A085SE34
C	-9	GLY	-	expression tag	UNP A0A085SE34
C	-8	LEU	-	expression tag	UNP A0A085SE34
C	-7	GLU	-	expression tag	UNP A0A085SE34

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	VAL	-	expression tag	UNP A0A085SE34
C	-5	LEU	-	expression tag	UNP A0A085SE34
C	-4	PHE	-	expression tag	UNP A0A085SE34
C	-3	GLN	-	expression tag	UNP A0A085SE34
C	-2	GLY	-	expression tag	UNP A0A085SE34
C	-1	PRO	-	expression tag	UNP A0A085SE34
C	0	HIS	-	expression tag	UNP A0A085SE34
D	-21	MET	-	expression tag	UNP A0A085SE34
D	-20	GLY	-	expression tag	UNP A0A085SE34
D	-19	SER	-	expression tag	UNP A0A085SE34
D	-18	SER	-	expression tag	UNP A0A085SE34
D	-17	HIS	-	expression tag	UNP A0A085SE34
D	-16	HIS	-	expression tag	UNP A0A085SE34
D	-15	HIS	-	expression tag	UNP A0A085SE34
D	-14	HIS	-	expression tag	UNP A0A085SE34
D	-13	HIS	-	expression tag	UNP A0A085SE34
D	-12	HIS	-	expression tag	UNP A0A085SE34
D	-11	SER	-	expression tag	UNP A0A085SE34
D	-10	SER	-	expression tag	UNP A0A085SE34
D	-9	GLY	-	expression tag	UNP A0A085SE34
D	-8	LEU	-	expression tag	UNP A0A085SE34
D	-7	GLU	-	expression tag	UNP A0A085SE34
D	-6	VAL	-	expression tag	UNP A0A085SE34
D	-5	LEU	-	expression tag	UNP A0A085SE34
D	-4	PHE	-	expression tag	UNP A0A085SE34
D	-3	GLN	-	expression tag	UNP A0A085SE34
D	-2	GLY	-	expression tag	UNP A0A085SE34
D	-1	PRO	-	expression tag	UNP A0A085SE34
D	0	HIS	-	expression tag	UNP A0A085SE34
E	-21	MET	-	expression tag	UNP A0A085SE34
E	-20	GLY	-	expression tag	UNP A0A085SE34
E	-19	SER	-	expression tag	UNP A0A085SE34
E	-18	SER	-	expression tag	UNP A0A085SE34
E	-17	HIS	-	expression tag	UNP A0A085SE34
E	-16	HIS	-	expression tag	UNP A0A085SE34
E	-15	HIS	-	expression tag	UNP A0A085SE34
E	-14	HIS	-	expression tag	UNP A0A085SE34
E	-13	HIS	-	expression tag	UNP A0A085SE34
E	-12	HIS	-	expression tag	UNP A0A085SE34
E	-11	SER	-	expression tag	UNP A0A085SE34
E	-10	SER	-	expression tag	UNP A0A085SE34
E	-9	GLY	-	expression tag	UNP A0A085SE34

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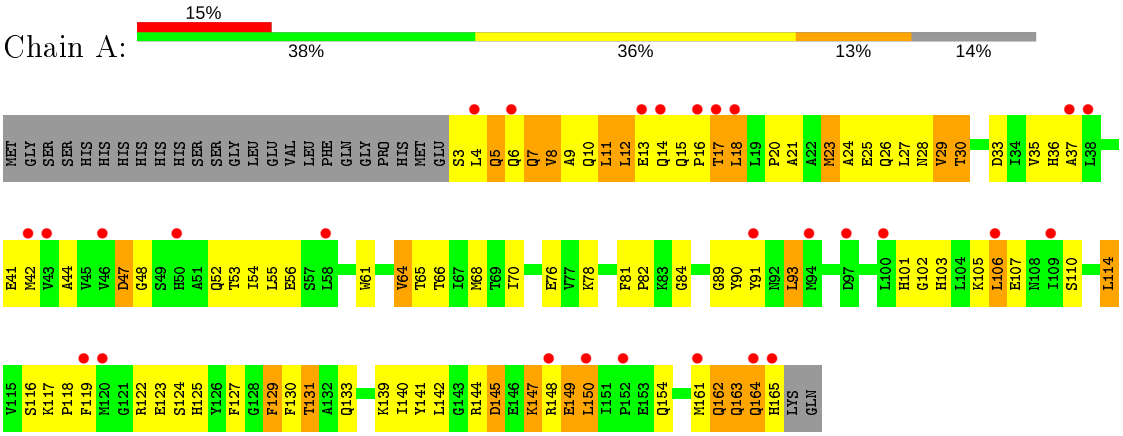
Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	LEU	-	expression tag	UNP A0A085SE34
E	-7	GLU	-	expression tag	UNP A0A085SE34
E	-6	VAL	-	expression tag	UNP A0A085SE34
E	-5	LEU	-	expression tag	UNP A0A085SE34
E	-4	PHE	-	expression tag	UNP A0A085SE34
E	-3	GLN	-	expression tag	UNP A0A085SE34
E	-2	GLY	-	expression tag	UNP A0A085SE34
E	-1	PRO	-	expression tag	UNP A0A085SE34
E	0	HIS	-	expression tag	UNP A0A085SE34
F	-21	MET	-	expression tag	UNP A0A085SE34
F	-20	GLY	-	expression tag	UNP A0A085SE34
F	-19	SER	-	expression tag	UNP A0A085SE34
F	-18	SER	-	expression tag	UNP A0A085SE34
F	-17	HIS	-	expression tag	UNP A0A085SE34
F	-16	HIS	-	expression tag	UNP A0A085SE34
F	-15	HIS	-	expression tag	UNP A0A085SE34
F	-14	HIS	-	expression tag	UNP A0A085SE34
F	-13	HIS	-	expression tag	UNP A0A085SE34
F	-12	HIS	-	expression tag	UNP A0A085SE34
F	-11	SER	-	expression tag	UNP A0A085SE34
F	-10	SER	-	expression tag	UNP A0A085SE34
F	-9	GLY	-	expression tag	UNP A0A085SE34
F	-8	LEU	-	expression tag	UNP A0A085SE34
F	-7	GLU	-	expression tag	UNP A0A085SE34
F	-6	VAL	-	expression tag	UNP A0A085SE34
F	-5	LEU	-	expression tag	UNP A0A085SE34
F	-4	PHE	-	expression tag	UNP A0A085SE34
F	-3	GLN	-	expression tag	UNP A0A085SE34
F	-2	GLY	-	expression tag	UNP A0A085SE34
F	-1	PRO	-	expression tag	UNP A0A085SE34
F	0	HIS	-	expression tag	UNP A0A085SE34

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 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.

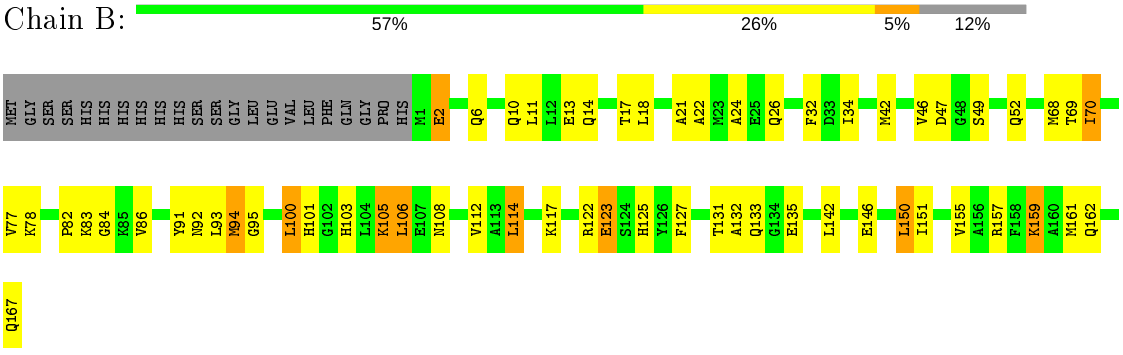
- Molecule 1: Hemin-degrading HemS.ChuX domain protein

Chain A:



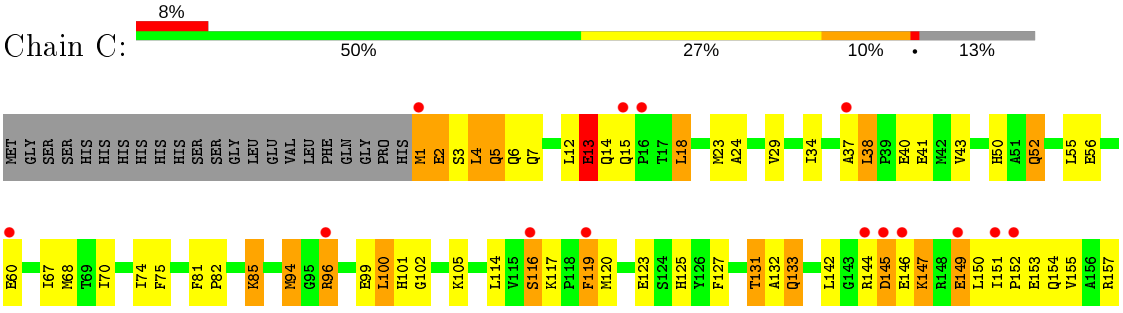
- Molecule 1: Hemin-degrading HemS.ChuX domain protein

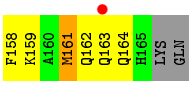
Chain B:



- Molecule 1: Hemin-degrading HemS.ChuX domain protein

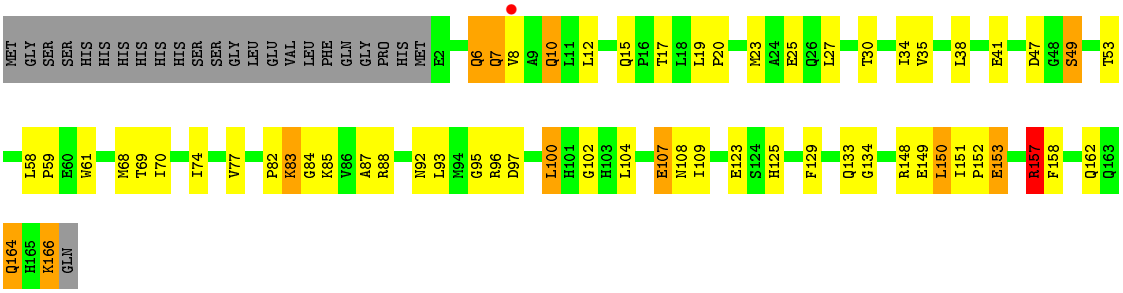
Chain C:





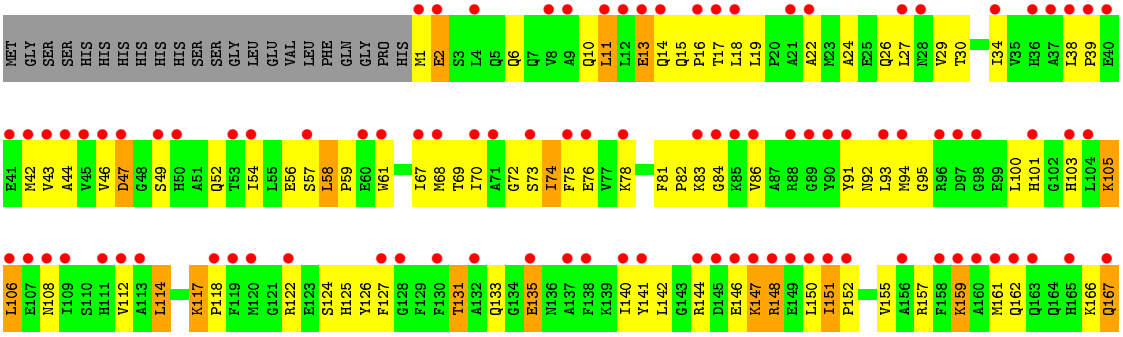
• Molecule 1: Hemin-degrading HemS.ChuX domain protein

Chain D:



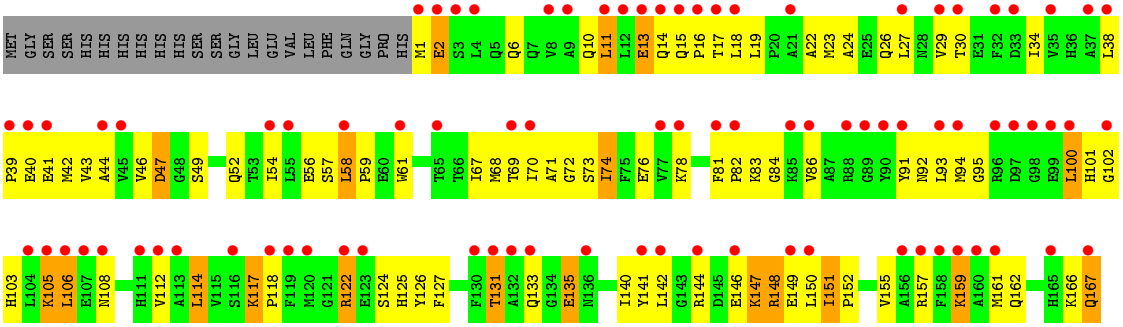
• Molecule 1: Hemin-degrading HemS.ChuX domain protein

Chain E:



• Molecule 1: Hemin-degrading HemS.ChuX domain protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.20Å 80.88Å 111.09Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	48.66 – 2.90 48.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.66-2.90) 98.3 (48.66-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.246 , 0.278 0.249 , 0.278	Depositor DCC
R_{free} test set	1186 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 80.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7856	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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

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	0.39	0/1316	0.65	0/1780
1	B	0.30	0/1351	0.52	0/1825
1	C	0.39	1/1333 (0.1%)	0.59	0/1802
1	D	0.41	0/1334	0.63	1/1803 (0.1%)
1	E	0.66	4/1351 (0.3%)	0.67	6/1825 (0.3%)
1	F	0.66	4/1351 (0.3%)	0.68	6/1825 (0.3%)
All	All	0.49	9/8036 (0.1%)	0.63	13/10860 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	39	PRO	N-CD	5.34	1.55	1.47
1	F	39	PRO	N-CD	5.28	1.55	1.47
1	E	16	PRO	N-CD	5.23	1.55	1.47
1	C	13	GLU	CB-CG	-5.18	1.42	1.52
1	E	152	PRO	N-CD	5.17	1.55	1.47
1	F	152	PRO	N-CD	5.16	1.55	1.47
1	F	16	PRO	N-CD	5.13	1.55	1.47
1	F	118	PRO	N-CD	5.09	1.54	1.47
1	E	118	PRO	N-CD	5.05	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	ARG	NE-CZ-NH1	-11.27	114.66	120.30
1	F	19	LEU	C-N-CD	5.87	140.73	128.40
1	E	58	LEU	C-N-CD	5.86	140.70	128.40
1	E	19	LEU	C-N-CD	5.83	140.64	128.40
1	F	58	LEU	C-N-CD	5.82	140.62	128.40
1	F	15	GLN	C-N-CD	5.68	140.33	128.40
1	E	151	ILE	C-N-CD	5.67	140.30	128.40
1	E	15	GLN	C-N-CD	5.66	140.28	128.40
1	F	151	ILE	C-N-CD	5.66	140.28	128.40
1	F	117	LYS	C-N-CD	5.61	140.19	128.40
1	E	117	LYS	C-N-CD	5.61	140.18	128.40
1	E	38	LEU	C-N-CD	5.46	139.86	128.40
1	F	38	LEU	C-N-CD	5.45	139.85	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	GLU	Peptide
1	C	4	LEU	Peptide
1	D	8	VAL	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	1286	0	1275	80	0
1	B	1321	0	1314	31	1
1	C	1303	0	1293	51	1
1	D	1304	0	1294	37	0
1	E	1321	0	1313	90	0
1	F	1321	0	1313	102	0
All	All	7856	0	7802	347	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 22.

All (347) 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:E:159:LYS:NZ	1:E:162:GLN:OE1	1.88	1.05
1:F:159:LYS:NZ	1:F:162:GLN:OE1	1.87	1.05
1:E:131:THR:HG21	1:E:135:GLU:HG2	1.44	1.00
1:F:131:THR:HG21	1:F:135:GLU:HG2	1.44	0.99
1:F:105:LYS:CD	1:F:108:ASN:HB3	1.94	0.98
1:E:105:LYS:CD	1:E:108:ASN:HB3	1.93	0.98
1:F:105:LYS:HD2	1:F:108:ASN:HB3	1.47	0.97
1:C:13:GLU:CD	1:F:122:ARG:HH21	1.69	0.95
1:E:105:LYS:HD2	1:E:108:ASN:HB3	1.47	0.94
1:E:76:GLU:N	1:F:101:HIS:O	2.00	0.94
1:E:72:GLY:C	1:F:105:LYS:HG2	1.88	0.93
1:E:74:ILE:HG23	1:F:103:HIS:H	1.32	0.90
1:F:18:LEU:O	1:F:117:LYS:NZ	2.08	0.87
1:E:18:LEU:O	1:E:117:LYS:NZ	2.08	0.86
1:E:74:ILE:CG2	1:F:103:HIS:HB2	2.06	0.86
1:E:105:LYS:HE3	1:F:71:ALA:O	1.76	0.84
1:E:67:ILE:HD12	1:E:141:TYR:CD2	2.15	0.82
1:F:67:ILE:HD12	1:F:141:TYR:CD2	2.15	0.81
1:E:131:THR:CG2	1:E:135:GLU:HG2	2.13	0.79
1:E:74:ILE:HG22	1:F:103:HIS:O	1.83	0.78
1:B:18:LEU:O	1:B:117:LYS:NZ	2.17	0.78
1:F:131:THR:CG2	1:F:135:GLU:HG2	2.13	0.78
1:D:30:THR:HB	1:D:134:GLY:HA3	1.66	0.77
1:F:124:SER:C	1:F:125:HIS:HD1	1.88	0.76
1:E:105:LYS:HG2	1:F:72:GLY:O	1.86	0.76
1:E:124:SER:C	1:E:125:HIS:HD1	1.88	0.76
1:C:123:GLU:HB3	1:C:125:HIS:HE1	1.50	0.76
1:E:124:SER:O	1:E:125:HIS:ND1	2.16	0.76
1:E:105:LYS:HG2	1:F:72:GLY:C	2.07	0.76
1:E:74:ILE:HG23	1:F:103:HIS:N	2.01	0.75
1:A:11:LEU:O	1:A:15:GLN:N	2.20	0.74
1:E:10:GLN:O	1:E:14:GLN:HG3	1.88	0.74
1:E:72:GLY:CA	1:F:105:LYS:HG2	2.18	0.74
1:E:72:GLY:C	1:F:105:LYS:CG	2.56	0.74
1:C:125:HIS:HB2	1:C:142:LEU:HD22	1.70	0.73
1:F:10:GLN:O	1:F:14:GLN:HG3	1.88	0.73
1:E:105:LYS:CE	1:F:71:ALA:O	2.36	0.73
1:A:144:ARG:HD2	1:A:148:ARG:O	1.87	0.73
1:B:159:LYS:NZ	1:B:162:GLN:OE1	2.21	0.73
1:F:124:SER:O	1:F:125:HIS:ND1	2.16	0.73
1:E:108:ASN:ND2	1:F:71:ALA:O	2.21	0.72
1:C:123:GLU:HB3	1:C:125:HIS:CE1	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:HG3	1:A:8:VAL:HG22	1.72	0.71
1:A:6:GLN:NE2	1:F:1:MET:O	2.24	0.71
1:E:105:LYS:HD3	1:E:108:ASN:HB3	1.72	0.71
1:E:92:ASN:OD1	1:E:103:HIS:ND1	2.24	0.71
1:E:72:GLY:O	1:F:105:LYS:HG2	1.89	0.71
1:F:105:LYS:HD3	1:F:108:ASN:HB3	1.72	0.70
1:E:73:SER:OG	1:F:105:LYS:NZ	2.25	0.70
1:F:92:ASN:OD1	1:F:103:HIS:ND1	2.24	0.70
1:A:61:TRP:CD1	1:A:154:GLN:HG2	2.26	0.69
1:E:146:GLU:CD	1:E:146:GLU:H	1.95	0.69
1:C:13:GLU:OE2	1:F:122:ARG:NH2	2.26	0.69
1:F:146:GLU:H	1:F:146:GLU:CD	1.95	0.69
1:B:105:LYS:HD2	1:B:108:ASN:HB3	1.74	0.68
1:F:52:GLN:HB2	1:F:106:LEU:HD23	1.75	0.68
1:E:52:GLN:HB2	1:E:106:LEU:HD23	1.76	0.68
1:A:61:TRP:HD1	1:A:154:GLN:HG2	1.57	0.68
1:E:72:GLY:HA3	1:F:105:LYS:HG2	1.75	0.68
1:F:105:LYS:O	1:F:105:LYS:HD2	1.94	0.68
1:A:125:HIS:HB2	1:A:142:LEU:HD22	1.76	0.67
1:E:105:LYS:HG3	1:F:73:SER:OG	1.93	0.67
1:F:114:LEU:N	1:F:114:LEU:HD23	2.09	0.67
1:F:1:MET:HG3	1:F:1:MET:O	1.95	0.67
1:E:105:LYS:O	1:E:105:LYS:HD2	1.94	0.67
1:E:114:LEU:HD23	1:E:114:LEU:N	2.09	0.66
1:F:24:ALA:HA	1:F:34:ILE:HD11	1.78	0.66
1:C:151:ILE:HB	1:F:41:GLU:HB2	1.77	0.66
1:A:93:LEU:HB3	1:A:102:GLY:HA2	1.78	0.66
1:E:1:MET:O	1:E:1:MET:HG3	1.95	0.66
1:D:133:GLN:N	1:D:133:GLN:OE1	2.30	0.65
1:A:107:GLU:N	1:A:107:GLU:OE1	2.29	0.65
1:C:116:SER:OG	1:C:162:GLN:OE1	2.15	0.65
1:A:118:PRO:HA	1:A:123:GLU:HA	1.78	0.65
1:E:24:ALA:HA	1:E:34:ILE:HD11	1.78	0.65
1:C:52:GLN:NE2	1:C:56:GLU:OE2	2.30	0.64
1:F:124:SER:C	1:F:125:HIS:ND1	2.51	0.64
1:E:67:ILE:HD12	1:E:141:TYR:HD2	1.63	0.64
1:E:151:ILE:O	1:E:155:VAL:HG23	1.98	0.63
1:A:123:GLU:OE1	1:A:123:GLU:N	2.28	0.63
1:D:7:GLN:HG2	1:D:27:LEU:HD22	1.80	0.63
1:F:151:ILE:O	1:F:155:VAL:HG23	1.98	0.62
1:E:124:SER:C	1:E:125:HIS:ND1	2.51	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ILE:HD12	1:F:141:TYR:HD2	1.63	0.62
1:F:125:HIS:HB2	1:F:142:LEU:HD13	1.81	0.62
1:E:125:HIS:HB2	1:E:142:LEU:HD13	1.81	0.61
1:F:162:GLN:O	1:F:166:LYS:HG3	2.01	0.61
1:E:162:GLN:O	1:E:166:LYS:HG3	2.00	0.61
1:E:166:LYS:C	1:E:167:GLN:HG3	2.20	0.61
1:D:82:PRO:HB3	1:D:95:GLY:HA2	1.83	0.60
1:F:166:LYS:C	1:F:167:GLN:HG3	2.20	0.60
1:D:6:GLN:O	1:D:10:GLN:HB2	2.01	0.60
1:D:151:ILE:HG22	1:D:153:GLU:HG2	1.84	0.60
1:C:151:ILE:HB	1:F:41:GLU:CB	2.31	0.59
1:F:54:ILE:O	1:F:57:SER:OG	2.20	0.59
1:B:24:ALA:HA	1:B:34:ILE:HD11	1.83	0.59
1:C:145:ASP:N	1:C:146:GLU:HA	2.17	0.59
1:A:66:THR:HG23	1:A:140:ILE:HD13	1.85	0.59
1:A:47:ASP:N	1:A:47:ASP:OD1	2.36	0.59
1:F:67:ILE:CD1	1:F:141:TYR:CD2	2.86	0.59
1:C:153:GLU:HG3	1:C:154:GLN:HG2	1.85	0.59
1:B:92:ASN:OD1	1:B:103:HIS:ND1	2.32	0.59
1:E:54:ILE:O	1:E:57:SER:OG	2.20	0.58
1:C:40:GLU:HB2	1:F:149:GLU:OE2	2.03	0.58
1:A:145:ASP:HB3	1:A:147:LYS:HG3	1.85	0.58
1:A:93:LEU:N	1:A:102:GLY:O	2.37	0.58
1:A:20:PRO:HA	1:A:23:MET:HG3	1.86	0.58
1:D:157:ARG:HG2	1:D:157:ARG:HH21	1.69	0.58
1:C:119:PHE:CZ	1:C:120:MET:HG2	2.39	0.58
1:A:3:SER:O	1:A:7:GLN:HB3	2.04	0.58
1:E:105:LYS:HD3	1:F:71:ALA:O	2.04	0.58
1:A:89:GLY:O	1:A:105:LYS:NZ	2.36	0.58
1:F:83:LYS:HB2	1:F:94:MET:HE2	1.86	0.58
1:E:67:ILE:CD1	1:E:141:TYR:CD2	2.86	0.58
1:A:11:LEU:HD13	1:A:11:LEU:H	1.68	0.57
1:D:157:ARG:H	1:D:157:ARG:HD3	1.69	0.57
1:A:119:PHE:N	1:A:122:ARG:O	2.34	0.57
1:A:17:THR:HG1	1:A:119:PHE:HE1	1.52	0.57
1:E:83:LYS:HB2	1:E:94:MET:HE2	1.87	0.57
1:F:29:VAL:HG23	1:F:34:ILE:HD11	1.87	0.57
1:A:116:SER:HB2	1:A:125:HIS:ND1	2.20	0.57
1:D:30:THR:CB	1:D:134:GLY:HA3	2.34	0.57
1:E:29:VAL:HG23	1:E:34:ILE:HD11	1.87	0.57
1:C:41:GLU:N	1:F:149:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ILE:HG22	1:F:103:HIS:HB2	1.85	0.56
1:F:144:ARG:HG2	1:F:144:ARG:HH11	1.71	0.56
1:A:93:LEU:HD23	1:A:101:HIS:HB3	1.88	0.56
1:F:131:THR:HG22	1:F:135:GLU:O	2.06	0.56
1:F:146:GLU:N	1:F:146:GLU:OE1	2.37	0.56
1:B:84:GLY:HA3	1:B:91:TYR:CZ	2.41	0.56
1:C:149:GLU:HG2	1:F:40:GLU:HB3	1.88	0.56
1:A:25:GLU:HB3	1:D:85:LYS:HB3	1.89	0.55
1:B:146:GLU:CD	1:B:146:GLU:H	2.10	0.55
1:A:105:LYS:HD2	1:A:107:GLU:HB2	1.87	0.55
1:B:105:LYS:CD	1:B:108:ASN:HB3	2.36	0.55
1:E:144:ARG:HH11	1:E:144:ARG:HG2	1.71	0.55
1:C:3:SER:OG	1:C:5:GLN:O	2.11	0.55
1:C:2:GLU:HB3	1:C:6:GLN:OE1	2.07	0.55
1:E:131:THR:HG22	1:E:135:GLU:O	2.06	0.55
1:D:34:ILE:HG13	1:D:35:VAL:N	2.21	0.54
1:F:95:GLY:HA3	1:F:101:HIS:CD2	2.42	0.54
1:D:157:ARG:HG2	1:D:157:ARG:NH2	2.21	0.54
1:D:157:ARG:N	1:D:157:ARG:HD3	2.22	0.54
1:E:95:GLY:HA3	1:E:101:HIS:CD2	2.42	0.54
1:D:87:ALA:O	1:D:92:ASN:ND2	2.37	0.54
1:C:154:GLN:HB3	1:C:157:ARG:HG3	1.88	0.54
1:F:131:THR:CG2	1:F:135:GLU:CG	2.86	0.54
1:B:123:GLU:HG2	1:B:150:LEU:HD23	1.89	0.54
1:E:131:THR:CG2	1:E:135:GLU:CG	2.85	0.54
1:E:146:GLU:N	1:E:146:GLU:OE1	2.38	0.53
1:D:157:ARG:CG	1:D:157:ARG:HH21	2.21	0.53
1:A:4:LEU:HD11	1:A:29:VAL:HG21	1.90	0.53
1:D:123:GLU:OE1	1:D:150:LEU:HD23	2.08	0.53
1:F:67:ILE:HG21	1:F:74:ILE:HD11	1.91	0.53
1:A:14:GLN:O	1:A:16:PRO:HD3	2.09	0.53
1:D:58:LEU:O	1:D:61:TRP:HB2	2.08	0.53
1:A:44:ALA:HB3	1:A:114:LEU:HB2	1.91	0.52
1:A:30:THR:N	1:A:33:ASP:OD2	2.40	0.52
1:E:74:ILE:CG2	1:F:103:HIS:CB	2.83	0.52
1:A:84:GLY:HA3	1:A:91:TYR:CE2	2.45	0.52
1:D:23:MET:HB2	1:D:34:ILE:HD13	1.91	0.52
1:E:147:LYS:O	1:E:148:ARG:HB2	2.09	0.52
1:E:67:ILE:HG21	1:E:74:ILE:HD11	1.91	0.52
1:E:74:ILE:O	1:F:102:GLY:HA3	2.09	0.52
1:E:72:GLY:O	1:F:105:LYS:CG	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LYS:O	1:F:148:ARG:HB2	2.09	0.52
1:E:105:LYS:CD	1:F:71:ALA:O	2.58	0.52
1:C:13:GLU:CD	1:F:122:ARG:NH2	2.51	0.51
1:C:15:GLN:HE22	1:C:18:LEU:HD22	1.74	0.51
1:D:107:GLU:N	1:D:107:GLU:OE1	2.41	0.51
1:C:1:MET:HE3	1:C:1:MET:O	2.10	0.51
1:C:2:GLU:OE2	1:C:2:GLU:N	2.43	0.51
1:A:66:THR:O	1:A:76:GLU:HA	2.10	0.51
1:E:74:ILE:CG2	1:F:103:HIS:O	2.58	0.51
1:C:102:GLY:HA3	1:D:74:ILE:O	2.11	0.51
1:B:125:HIS:HB2	1:B:142:LEU:HD13	1.92	0.51
1:C:1:MET:N	1:C:2:GLU:OE2	2.38	0.51
1:C:74:ILE:O	1:D:102:GLY:HA3	2.11	0.51
1:B:77:VAL:HG11	1:B:100:LEU:HB2	1.93	0.50
1:C:14:GLN:O	1:C:15:GLN:HG3	2.12	0.50
1:F:131:THR:HG23	1:F:135:GLU:H	1.77	0.50
1:A:8:VAL:HG11	1:A:27:LEU:HD21	1.93	0.50
1:A:117:LYS:O	1:A:124:SER:OG	2.21	0.50
1:E:30:THR:O	1:E:34:ILE:HD12	2.12	0.50
1:E:131:THR:HG23	1:E:135:GLU:H	1.77	0.49
1:A:64:VAL:HG12	1:A:141:TYR:O	2.12	0.49
1:F:30:THR:O	1:F:34:ILE:HD12	2.12	0.49
1:A:55:LEU:HD21	1:A:129:PHE:CE2	2.46	0.49
1:E:56:GLU:O	1:E:59:PRO:HD2	2.12	0.49
1:E:22:ALA:O	1:E:26:GLN:HG2	2.13	0.49
1:F:56:GLU:O	1:F:59:PRO:HD2	2.12	0.49
1:C:38:LEU:HD21	1:C:43:VAL:CG2	2.42	0.49
1:C:145:ASP:OD1	1:C:145:ASP:N	2.44	0.49
1:E:46:VAL:HG13	1:E:112:VAL:HB	1.95	0.49
1:F:13:GLU:HG3	1:F:14:GLN:HG2	1.94	0.49
1:A:24:ALA:O	1:A:28:ASN:N	2.46	0.49
1:A:84:GLY:HA3	1:A:91:TYR:HE2	1.78	0.48
1:A:5:GLN:HB3	1:A:37:ALA:O	2.13	0.48
1:C:150:LEU:O	1:C:152:PRO:HD3	2.13	0.48
1:A:114:LEU:HD22	1:A:127:PHE:CD1	2.49	0.48
1:A:70:ILE:HB	1:B:70:ILE:CD1	2.44	0.48
1:E:13:GLU:HG3	1:E:14:GLN:HG2	1.94	0.48
1:F:22:ALA:O	1:F:26:GLN:HG2	2.13	0.48
1:A:133:GLN:OE1	1:A:133:GLN:N	2.25	0.48
1:A:53:THR:HA	1:A:56:GLU:OE2	2.14	0.48
1:F:46:VAL:HG13	1:F:112:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:CD	1:A:163:GLN:HA	2.33	0.48
1:A:48:GLY:HA3	1:A:110:SER:O	2.14	0.48
1:A:55:LEU:HD21	1:A:129:PHE:CZ	2.49	0.48
1:C:5:GLN:HB3	1:C:37:ALA:O	2.13	0.48
1:D:162:GLN:O	1:D:166:LYS:HB2	2.14	0.48
1:A:105:LYS:HD3	1:A:105:LYS:HA	1.64	0.47
1:B:10:GLN:O	1:B:14:GLN:HG3	2.14	0.47
1:C:125:HIS:HB3	1:C:158:PHE:CE2	2.50	0.47
1:A:29:VAL:HB	1:A:33:ASP:CB	2.44	0.47
1:A:150:LEU:H	1:A:150:LEU:HD22	1.78	0.47
1:A:127:PHE:HB3	1:A:129:PHE:HE1	1.80	0.47
1:A:12:LEU:HA	1:A:13:GLU:HA	1.41	0.47
1:C:144:ARG:HA	1:C:145:ASP:HA	1.71	0.47
1:A:18:LEU:O	1:A:117:LYS:NZ	2.31	0.47
1:A:29:VAL:HB	1:A:33:ASP:HB2	1.96	0.47
1:D:153:GLU:CD	1:D:153:GLU:H	2.17	0.47
1:B:2:GLU:H	1:B:2:GLU:HG2	1.65	0.46
1:F:127:PHE:HB2	1:F:140:ILE:HB	1.97	0.46
1:A:91:TYR:CD1	1:A:106:LEU:HD11	2.49	0.46
1:B:105:LYS:O	1:B:105:LYS:HD2	2.15	0.46
1:B:46:VAL:HG13	1:B:112:VAL:HB	1.98	0.46
1:B:83:LYS:HB2	1:B:94:MET:HE2	1.97	0.46
1:D:109:ILE:HD12	1:D:129:PHE:HB3	1.97	0.46
1:D:19:LEU:O	1:D:23:MET:HG3	2.15	0.46
1:A:129:PHE:N	1:A:129:PHE:HD1	2.13	0.46
1:B:32:PHE:CD2	1:D:164:GLN:HG2	2.49	0.46
1:E:84:GLY:HA3	1:E:91:TYR:CZ	2.51	0.46
1:A:81:PHE:CG	1:A:82:PRO:HD2	2.50	0.46
1:B:108:ASN:OD1	1:D:53:THR:HG21	2.15	0.46
1:E:27:LEU:N	1:E:27:LEU:HD23	2.31	0.46
1:A:131:THR:HB	1:A:133:GLN:OE1	2.16	0.46
1:E:43:VAL:HG22	1:E:44:ALA:N	2.31	0.46
1:B:22:ALA:O	1:B:26:GLN:HG2	2.16	0.46
1:E:127:PHE:HB2	1:E:140:ILE:HB	1.97	0.46
1:E:29:VAL:HG23	1:E:34:ILE:CD1	2.46	0.46
1:A:61:TRP:C	1:A:154:GLN:HE21	2.20	0.46
1:A:30:THR:HG1	1:A:33:ASP:CG	2.18	0.45
1:D:157:ARG:N	1:D:157:ARG:CD	2.79	0.45
1:D:59:PRO:HG2	1:D:83:LYS:HG2	1.98	0.45
1:A:65:THR:HG23	1:A:78:LYS:HG3	1.99	0.45
1:E:131:THR:CG2	1:E:135:GLU:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:CD1	1:A:129:PHE:N	2.84	0.45
1:F:84:GLY:HA3	1:F:91:TYR:CZ	2.51	0.45
1:A:116:SER:HB2	1:A:125:HIS:CE1	2.51	0.45
1:B:34:ILE:H	1:B:34:ILE:HD12	1.81	0.45
1:F:27:LEU:HD23	1:F:27:LEU:N	2.31	0.45
1:A:164:GLN:OE1	1:A:164:GLN:HA	2.16	0.45
1:C:114:LEU:CD2	1:C:161:MET:HB3	2.47	0.45
1:F:81:PHE:CG	1:F:82:PRO:HD2	2.52	0.45
1:E:2:GLU:HB2	1:E:6:GLN:HB2	1.99	0.45
1:E:58:LEU:O	1:E:61:TRP:HB2	2.17	0.45
1:E:81:PHE:CG	1:E:82:PRO:HD2	2.52	0.45
1:F:131:THR:CG2	1:F:135:GLU:H	2.30	0.45
1:A:17:THR:OG1	1:A:119:PHE:HE1	1.98	0.45
1:A:3:SER:O	1:A:6:GLN:HG2	2.17	0.45
1:F:29:VAL:HG23	1:F:34:ILE:CD1	2.46	0.45
1:C:96:ARG:HG2	1:C:96:ARG:H	1.43	0.45
1:E:75:PHE:HB3	1:F:100:LEU:HD11	1.98	0.45
1:F:13:GLU:HG3	1:F:14:GLN:N	2.32	0.45
1:A:24:ALA:HB1	1:A:29:VAL:O	2.16	0.44
1:A:5:GLN:HA	1:A:37:ALA:HB1	1.98	0.44
1:A:9:ALA:HA	1:A:12:LEU:HD23	1.99	0.44
1:B:151:ILE:O	1:B:155:VAL:HG23	2.17	0.44
1:B:21:ALA:O	1:B:24:ALA:HB3	2.17	0.44
1:F:114:LEU:N	1:F:114:LEU:CD2	2.78	0.44
1:F:2:GLU:HB2	1:F:6:GLN:HB2	1.99	0.44
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.77	0.44
1:C:4:LEU:HB3	1:C:37:ALA:HB1	1.99	0.44
1:F:157:ARG:HA	1:F:157:ARG:HD2	1.76	0.44
1:C:38:LEU:HD21	1:C:43:VAL:HG23	1.97	0.44
1:E:74:ILE:HG21	1:F:103:HIS:HB2	1.91	0.44
1:F:58:LEU:O	1:F:61:TRP:HB2	2.17	0.44
1:C:85:LYS:HB2	1:C:94:MET:CE	2.47	0.44
1:E:142:LEU:N	1:E:142:LEU:HD12	2.33	0.44
1:F:43:VAL:HG22	1:F:44:ALA:N	2.31	0.44
1:C:67:ILE:HA	1:C:75:PHE:O	2.18	0.43
1:D:125:HIS:HB3	1:D:158:PHE:CE2	2.52	0.43
1:F:142:LEU:HD12	1:F:142:LEU:N	2.32	0.43
1:D:96:ARG:HD3	1:D:96:ARG:HA	1.56	0.43
1:E:2:GLU:HB3	1:E:6:GLN:OE1	2.18	0.43
1:C:100:LEU:H	1:C:100:LEU:HD23	1.83	0.43
1:E:101:HIS:O	1:F:76:GLU:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:LEU:HA	1:E:11:LEU:HD23	1.80	0.43
1:E:13:GLU:HG3	1:E:14:GLN:N	2.32	0.43
1:E:114:LEU:N	1:E:114:LEU:CD2	2.78	0.43
1:E:74:ILE:O	1:F:103:HIS:N	2.50	0.43
1:F:2:GLU:HB3	1:F:6:GLN:OE1	2.18	0.43
1:B:114:LEU:HD22	1:B:127:PHE:CD1	2.54	0.43
1:A:41:GLU:HG3	1:A:42:MET:N	2.34	0.43
1:C:131:THR:HG23	1:C:133:GLN:OE1	2.19	0.43
1:C:18:LEU:HA	1:C:18:LEU:HD12	1.84	0.43
1:F:147:LYS:HA	1:F:147:LYS:HD2	1.85	0.43
1:A:10:GLN:HG3	1:F:14:GLN:HE22	1.83	0.43
1:A:21:ALA:O	1:A:24:ALA:HB3	2.19	0.42
1:B:157:ARG:HA	1:B:157:ARG:HD2	1.82	0.42
1:F:82:PRO:HG2	1:F:93:LEU:HD22	2.01	0.42
1:A:161:MET:HA	1:A:165:HIS:CE1	2.53	0.42
1:D:47:ASP:OD2	1:D:49:SER:OG	2.30	0.42
1:E:166:LYS:C	1:E:167:GLN:CG	2.86	0.42
1:F:67:ILE:CG2	1:F:74:ILE:HD11	2.49	0.42
1:C:24:ALA:HB1	1:C:29:VAL:O	2.20	0.42
1:B:52:GLN:HB2	1:B:106:LEU:HD23	2.00	0.42
1:C:131:THR:OG1	1:C:132:ALA:N	2.53	0.42
1:B:131:THR:OG1	1:B:132:ALA:N	2.53	0.42
1:E:157:ARG:HD2	1:E:157:ARG:HA	1.76	0.42
1:C:142:LEU:HD23	1:C:155:VAL:HG22	2.00	0.42
1:E:67:ILE:CG2	1:E:74:ILE:HD11	2.49	0.42
1:E:82:PRO:HG2	1:E:93:LEU:HD22	2.01	0.42
1:A:161:MET:O	1:A:164:GLN:HA	2.20	0.41
1:B:82:PRO:HG2	1:B:93:LEU:HD22	2.03	0.41
1:C:23:MET:HE3	1:C:34:ILE:HG21	2.03	0.41
1:F:105:LYS:HD3	1:F:108:ASN:HD22	1.86	0.41
1:A:90:TYR:CD1	1:A:90:TYR:N	2.89	0.41
1:C:120:MET:O	1:C:120:MET:HG3	2.19	0.41
1:A:122:ARG:HD2	1:A:149:GLU:OE1	2.21	0.41
1:A:35:VAL:HG21	1:A:130:PHE:CZ	2.55	0.41
1:A:35:VAL:HG21	1:A:130:PHE:HZ	1.86	0.41
1:A:8:VAL:HG21	1:A:27:LEU:HD13	2.02	0.41
1:D:95:GLY:HA3	1:D:100:LEU:O	2.20	0.41
1:A:133:GLN:CD	1:A:133:GLN:H	2.16	0.41
1:B:95:GLY:HA3	1:B:101:HIS:CD2	2.56	0.41
1:F:166:LYS:C	1:F:167:GLN:CG	2.86	0.41
1:C:147:LYS:HD3	1:C:149:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:SER:O	1:C:7:GLN:HB2	2.21	0.41
1:B:2:GLU:HB2	1:B:6:GLN:HB2	2.03	0.41
1:C:60:GLU:HG2	1:C:157:ARG:HH12	1.85	0.41
1:D:20:PRO:HA	1:D:34:ILE:HD11	2.01	0.41
1:F:46:VAL:HG22	1:F:47:ASP:N	2.36	0.40
1:E:105:LYS:HD3	1:E:108:ASN:HD22	1.86	0.40
1:E:46:VAL:HG22	1:E:47:ASP:N	2.36	0.40
1:A:11:LEU:O	1:A:14:GLN:N	2.54	0.40
1:D:58:LEU:HA	1:D:61:TRP:CD1	2.57	0.40
1:D:84:GLY:O	1:D:85:LYS:HD2	2.21	0.40
1:F:105:LYS:HZ2	1:F:105:LYS:HG3	1.73	0.40
1:E:126:TYR:CD1	1:E:126:TYR:C	2.94	0.40
1:F:11:LEU:HD13	1:F:23:MET:HG2	2.03	0.40
1:A:101:HIS:HA	1:A:102:GLY:HA2	1.94	0.40
1:C:159:LYS:NZ	1:C:162:GLN:HE22	2.19	0.40
1:C:81:PHE:HA	1:C:82:PRO:HD3	1.87	0.40
1:D:151:ILE:HA	1:D:152:PRO:HD3	1.92	0.40
1:F:126:TYR:C	1:F:126:TYR:CD1	2.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:NH2	1:C:133:GLN:O[2_557]	2.12	0.08

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	161/189 (85%)	147 (91%)	14 (9%)	0	100	100
1	B	165/189 (87%)	159 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	163/189 (86%)	153 (94%)	10 (6%)	0	100	100
1	D	163/189 (86%)	157 (96%)	6 (4%)	0	100	100
1	E	165/189 (87%)	159 (96%)	6 (4%)	0	100	100
1	F	165/189 (87%)	159 (96%)	6 (4%)	0	100	100
All	All	982/1134 (87%)	934 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	136/159 (86%)	106 (78%)	30 (22%)	1	3
1	B	140/159 (88%)	116 (83%)	24 (17%)	2	6
1	C	138/159 (87%)	107 (78%)	31 (22%)	1	2
1	D	138/159 (87%)	109 (79%)	29 (21%)	1	3
1	E	140/159 (88%)	113 (81%)	27 (19%)	1	4
1	F	140/159 (88%)	113 (81%)	27 (19%)	1	4
All	All	832/954 (87%)	664 (80%)	168 (20%)	1	4

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	GLN
1	A	8	VAL
1	A	11	LEU
1	A	12	LEU
1	A	17	THR
1	A	18	LEU
1	A	23	MET
1	A	26	GLN

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Mol	Chain	Res	Type
1	A	29	VAL
1	A	30	THR
1	A	36	HIS
1	A	47	ASP
1	A	52	GLN
1	A	54	ILE
1	A	64	VAL
1	A	68	MET
1	A	93	LEU
1	A	103	HIS
1	A	106	LEU
1	A	114	LEU
1	A	129	PHE
1	A	131	THR
1	A	139	LYS
1	A	145	ASP
1	A	147	LYS
1	A	150	LEU
1	A	162	GLN
1	A	163	GLN
1	A	164	GLN
1	B	2	GLU
1	B	13	GLU
1	B	17	THR
1	B	42	MET
1	B	47	ASP
1	B	49	SER
1	B	68	MET
1	B	69	THR
1	B	70	ILE
1	B	78	LYS
1	B	86	VAL
1	B	94	MET
1	B	100	LEU
1	B	105	LYS
1	B	106	LEU
1	B	114	LEU
1	B	122	ARG
1	B	123	GLU
1	B	133	GLN
1	B	135	GLU
1	B	150	LEU

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Mol	Chain	Res	Type
1	B	159	LYS
1	B	161	MET
1	B	167	GLN
1	C	1	MET
1	C	2	GLU
1	C	5	GLN
1	C	12	LEU
1	C	13	GLU
1	C	18	LEU
1	C	38	LEU
1	C	50	HIS
1	C	52	GLN
1	C	55	LEU
1	C	68	MET
1	C	70	ILE
1	C	85	LYS
1	C	94	MET
1	C	96	ARG
1	C	99	GLU
1	C	100	LEU
1	C	101	HIS
1	C	105	LYS
1	C	116	SER
1	C	117	LYS
1	C	119	PHE
1	C	127	PHE
1	C	131	THR
1	C	133	GLN
1	C	145	ASP
1	C	147	LYS
1	C	149	GLU
1	C	161	MET
1	C	163	GLN
1	C	164	GLN
1	D	6	GLN
1	D	7	GLN
1	D	10	GLN
1	D	12	LEU
1	D	15	GLN
1	D	17	THR
1	D	25	GLU
1	D	38	LEU

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Mol	Chain	Res	Type
1	D	41	GLU
1	D	49	SER
1	D	68	MET
1	D	69	THR
1	D	70	ILE
1	D	77	VAL
1	D	83	LYS
1	D	88	ARG
1	D	93	LEU
1	D	97	ASP
1	D	100	LEU
1	D	104	LEU
1	D	107	GLU
1	D	108	ASN
1	D	148	ARG
1	D	149	GLU
1	D	150	LEU
1	D	153	GLU
1	D	157	ARG
1	D	164	GLN
1	D	166	LYS
1	E	2	GLU
1	E	11	LEU
1	E	13	GLU
1	E	17	THR
1	E	42	MET
1	E	47	ASP
1	E	49	SER
1	E	68	MET
1	E	69	THR
1	E	70	ILE
1	E	74	ILE
1	E	78	LYS
1	E	86	VAL
1	E	100	LEU
1	E	105	LYS
1	E	106	LEU
1	E	114	LEU
1	E	122	ARG
1	E	131	THR
1	E	133	GLN
1	E	135	GLU

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Mol	Chain	Res	Type
1	E	147	LYS
1	E	148	ARG
1	E	150	LEU
1	E	159	LYS
1	E	161	MET
1	E	167	GLN
1	F	2	GLU
1	F	11	LEU
1	F	13	GLU
1	F	17	THR
1	F	42	MET
1	F	47	ASP
1	F	49	SER
1	F	68	MET
1	F	69	THR
1	F	70	ILE
1	F	74	ILE
1	F	78	LYS
1	F	86	VAL
1	F	100	LEU
1	F	105	LYS
1	F	106	LEU
1	F	114	LEU
1	F	122	ARG
1	F	131	THR
1	F	133	GLN
1	F	135	GLU
1	F	147	LYS
1	F	148	ARG
1	F	150	LEU
1	F	159	LYS
1	F	161	MET
1	F	167	GLN

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

Mol	Chain	Res	Type
1	A	92	ASN
1	A	165	HIS
1	B	111	HIS
1	C	15	GLN
1	C	154	GLN

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Mol	Chain	Res	Type
1	C	162	GLN
1	D	10	GLN
1	D	164	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	163/189 (86%)	1.09	28 (17%) 1 1	42, 98, 138, 155	0
1	B	167/189 (88%)	0.10	0 100 100	23, 41, 66, 90	0
1	C	165/189 (87%)	0.62	15 (9%) 9 6	27, 62, 116, 148	0
1	D	165/189 (87%)	0.17	1 (0%) 89 89	28, 47, 87, 127	0
1	E	167/189 (88%)	2.88	98 (58%) 0 0	122, 152, 168, 184	0
1	F	167/189 (88%)	2.29	86 (51%) 0 0	117, 157, 172, 185	0
All	All	994/1134 (87%)	1.20	228 (22%) 0 0	23, 89, 167, 185	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	119	PHE	14.2
1	E	112	VAL	12.8
1	E	84	GLY	11.3
1	E	1	MET	10.6
1	E	120	MET	10.4
1	E	147	LYS	8.6
1	F	104	LEU	8.5
1	F	15	GLN	8.3
1	E	44	ALA	8.3
1	E	21	ALA	7.5
1	E	161	MET	7.5
1	F	85	LYS	7.5
1	F	120	MET	7.1
1	E	113	ALA	7.1
1	E	45	VAL	6.9
1	F	16	PRO	6.9
1	C	145	ASP	6.7
1	F	38	LEU	6.7
1	E	89	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	F	1	MET	6.4
1	E	46	VAL	6.4
1	F	156	ALA	6.1
1	F	150	LEU	6.0
1	E	94	MET	5.8
1	E	165	HIS	5.7
1	E	22	ALA	5.7
1	F	133	GLN	5.6
1	E	146	GLU	5.6
1	E	86	VAL	5.5
1	E	109	ILE	5.4
1	E	148	ARG	5.4
1	F	119	PHE	5.4
1	A	37	ALA	5.4
1	E	71	ALA	5.3
1	A	38	LEU	5.2
1	E	11	LEU	5.2
1	F	61	TRP	5.1
1	E	8	VAL	5.1
1	C	151	ILE	5.1
1	F	58	LEU	5.0
1	A	17	THR	5.0
1	A	120	MET	4.9
1	E	70	ILE	4.9
1	E	16	PRO	4.9
1	E	61	TRP	4.9
1	E	54	ILE	4.8
1	F	89	GLY	4.8
1	E	163	GLN	4.8
1	A	13	GLU	4.7
1	F	37	ALA	4.7
1	F	8	VAL	4.6
1	E	38	LEU	4.6
1	E	90	TYR	4.5
1	E	96	ARG	4.5
1	F	167	GLN	4.5
1	F	35	VAL	4.5
1	F	112	VAL	4.3
1	A	165	HIS	4.3
1	E	98	GLY	4.3
1	F	17	THR	4.3
1	E	93	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	94	MET	4.2
1	E	162	GLN	4.2
1	F	40	GLU	4.2
1	E	130	PHE	4.1
1	F	132	ALA	4.1
1	F	14	GLN	4.0
1	E	12	LEU	4.0
1	F	96	ARG	4.0
1	A	50	HIS	4.0
1	E	135	GLU	4.0
1	F	27	LEU	4.0
1	F	158	PHE	4.0
1	F	77	VAL	3.9
1	F	149	GLU	3.9
1	F	78	LYS	3.9
1	E	128	GLY	3.8
1	E	156	ALA	3.8
1	E	27	LEU	3.8
1	F	70	ILE	3.8
1	A	150	LEU	3.8
1	F	116	SER	3.7
1	E	150	LEU	3.6
1	A	91	TYR	3.6
1	F	142	LEU	3.6
1	E	73	SER	3.6
1	E	138	PHE	3.6
1	F	144	ARG	3.6
1	E	67	ILE	3.6
1	F	165	HIS	3.5
1	F	86	VAL	3.5
1	C	96	ARG	3.5
1	E	151	ILE	3.5
1	E	13	GLU	3.5
1	E	42	MET	3.4
1	C	37	ALA	3.4
1	E	101	HIS	3.4
1	F	107	GLU	3.4
1	E	91	TYR	3.4
1	F	94	MET	3.3
1	E	97	ASP	3.3
1	F	157	ARG	3.3
1	F	3	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	2	GLU	3.3
1	E	107	GLU	3.3
1	F	93	LEU	3.3
1	E	111	HIS	3.2
1	E	85	LYS	3.2
1	E	68	MET	3.2
1	A	148	ARG	3.1
1	F	122	ARG	3.1
1	F	12	LEU	3.1
1	E	17	THR	3.1
1	E	152	PRO	3.1
1	E	14	GLN	3.1
1	F	55	LEU	3.1
1	F	44	ALA	3.0
1	F	131	THR	3.0
1	A	152	PRO	3.0
1	F	105	LYS	3.0
1	C	16	PRO	3.0
1	E	53	THR	3.0
1	A	6	GLN	3.0
1	E	145	ASP	3.0
1	C	144	ARG	3.0
1	E	122	ARG	2.9
1	F	106	LEU	2.9
1	E	132	ALA	2.9
1	C	116	SER	2.9
1	A	58	LEU	2.9
1	F	160	ALA	2.9
1	F	81	PHE	2.9
1	F	69	THR	2.9
1	F	91	TYR	2.9
1	F	32	PHE	2.8
1	E	76	GLU	2.8
1	F	161	MET	2.8
1	E	141	TYR	2.8
1	F	100	LEU	2.8
1	C	163	GLN	2.8
1	E	43	VAL	2.8
1	A	119	PHE	2.7
1	E	118	PRO	2.7
1	F	146	GLU	2.7
1	F	4	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	119	PHE	2.7
1	F	111	HIS	2.7
1	E	158	PHE	2.7
1	A	100	LEU	2.7
1	C	149	GLU	2.7
1	E	60	GLU	2.7
1	E	167	GLN	2.6
1	F	113	ALA	2.6
1	F	33	ASP	2.6
1	E	18	LEU	2.6
1	E	106	LEU	2.6
1	E	83	LYS	2.6
1	E	144	ARG	2.6
1	A	164	GLN	2.6
1	F	65	THR	2.6
1	E	160	ALA	2.6
1	F	136	ASN	2.6
1	A	161	MET	2.5
1	C	146	GLU	2.5
1	C	15	GLN	2.5
1	E	104	LEU	2.5
1	F	29	VAL	2.5
1	E	47	ASP	2.5
1	A	4	LEU	2.5
1	E	36	HIS	2.5
1	E	41	GLU	2.5
1	F	90	TYR	2.5
1	F	30	THR	2.5
1	F	41	GLU	2.5
1	E	149	GLU	2.4
1	A	14	GLN	2.4
1	F	9	ALA	2.4
1	E	28	ASN	2.4
1	F	21	ALA	2.4
1	A	43	VAL	2.4
1	F	45	VAL	2.4
1	E	4	LEU	2.4
1	F	97	ASP	2.4
1	E	88	ARG	2.4
1	A	18	LEU	2.4
1	F	141	TYR	2.4
1	E	49	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	159	LYS	2.4
1	C	60	GLU	2.4
1	E	40	GLU	2.4
1	C	1	MET	2.4
1	F	159	LYS	2.4
1	F	130	PHE	2.3
1	D	8	VAL	2.3
1	A	106	LEU	2.3
1	E	75	PHE	2.3
1	F	2	GLU	2.3
1	F	13	GLU	2.3
1	F	102	GLY	2.3
1	F	39	PRO	2.3
1	F	88	ARG	2.3
1	E	140	ILE	2.3
1	E	37	ALA	2.3
1	F	54	ILE	2.3
1	E	137	ALA	2.2
1	E	34	ILE	2.2
1	E	39	PRO	2.2
1	E	78	LYS	2.2
1	E	9	ALA	2.2
1	A	16	PRO	2.2
1	A	46	VAL	2.2
1	E	57	SER	2.2
1	F	98	GLY	2.2
1	F	18	LEU	2.2
1	E	108	ASN	2.2
1	F	108	ASN	2.1
1	F	123	GLU	2.1
1	E	103	HIS	2.1
1	A	97	ASP	2.1
1	F	118	PRO	2.1
1	F	82	PRO	2.1
1	E	50	HIS	2.1
1	F	11	LEU	2.0
1	A	42	MET	2.0
1	C	152	PRO	2.0
1	A	109	ILE	2.0
1	F	99	GLU	2.0
1	E	127	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.