



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 10:10 AM JST

PDB ID : 7CQJ
Title : Peroxiredoxin from *Aeropyrum pernix* K1 (ApPrx) C50S/K84A/C207S/C213
S mutant (ApPrx*K84A)
Authors : Himiyama, T.; Nakamura, T.
Deposited on : 2020-08-11
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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

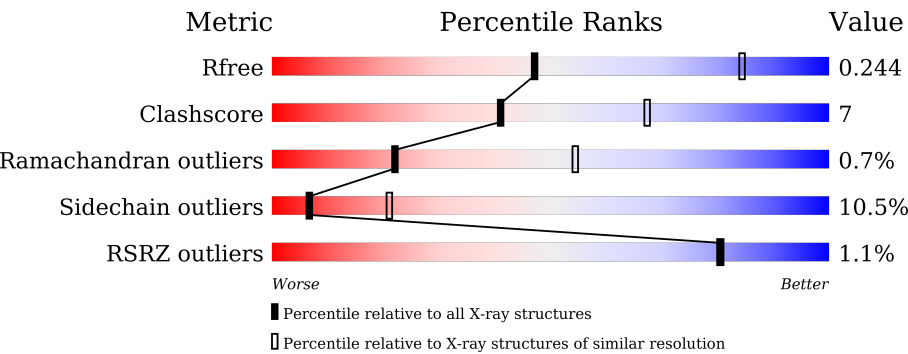
1 Overall quality at a glance i

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 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	250	<div><div>2%</div><div><div></div><div>72%</div><div>24%</div><div>..</div></div></div>
1	B	250	<div><div>%</div><div><div></div><div>75%</div><div>21%</div><div>..</div></div></div>
1	C	250	<div><div></div><div><div></div><div>75%</div><div>20%</div><div>..</div></div></div>
1	D	250	<div><div>2%</div><div><div></div><div>75%</div><div>22%</div><div>..</div></div></div>
1	E	250	<div><div></div><div><div></div><div>76%</div><div>18%</div><div>..</div></div></div>
1	F	250	<div><div>%</div><div><div></div><div>69%</div><div>25%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	250	<div><div></div><div>70%25%<div><div></div><div></div></div></div></div>
1	H	250	<div>%<div><div></div><div>75%20%<div><div></div><div></div></div></div></div></div>
1	I	250	<div><div></div><div>71%24%<div><div></div><div></div></div></div></div>
1	J	250	<div>%<div><div></div><div>73%22%<div><div></div><div></div></div></div></div></div>
1	K	250	<div>3%<div><div></div><div>70%24%<div><div></div><div></div></div></div></div></div>
1	L	250	<div><div></div><div>78%17%<div><div></div><div></div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23675 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	B	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	C	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	D	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	E	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	F	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	G	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	H	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	I	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	J	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	K	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0
1	L	244	Total 1969	C 1265	N 346	O 354	S 4	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	SER	CYS	engineered mutation	UNP Q9Y9L0
A	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
A	207	SER	CYS	engineered mutation	UNP Q9Y9L0
A	213	SER	CYS	engineered mutation	UNP Q9Y9L0
B	50	SER	CYS	engineered mutation	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
B	207	SER	CYS	engineered mutation	UNP Q9Y9L0
B	213	SER	CYS	engineered mutation	UNP Q9Y9L0
C	50	SER	CYS	engineered mutation	UNP Q9Y9L0
C	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
C	207	SER	CYS	engineered mutation	UNP Q9Y9L0
C	213	SER	CYS	engineered mutation	UNP Q9Y9L0
D	50	SER	CYS	engineered mutation	UNP Q9Y9L0
D	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
D	207	SER	CYS	engineered mutation	UNP Q9Y9L0
D	213	SER	CYS	engineered mutation	UNP Q9Y9L0
E	50	SER	CYS	engineered mutation	UNP Q9Y9L0
E	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
E	207	SER	CYS	engineered mutation	UNP Q9Y9L0
E	213	SER	CYS	engineered mutation	UNP Q9Y9L0
F	50	SER	CYS	engineered mutation	UNP Q9Y9L0
F	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
F	207	SER	CYS	engineered mutation	UNP Q9Y9L0
F	213	SER	CYS	engineered mutation	UNP Q9Y9L0
G	50	SER	CYS	engineered mutation	UNP Q9Y9L0
G	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
G	207	SER	CYS	engineered mutation	UNP Q9Y9L0
G	213	SER	CYS	engineered mutation	UNP Q9Y9L0
H	50	SER	CYS	engineered mutation	UNP Q9Y9L0
H	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
H	207	SER	CYS	engineered mutation	UNP Q9Y9L0
H	213	SER	CYS	engineered mutation	UNP Q9Y9L0
I	50	SER	CYS	engineered mutation	UNP Q9Y9L0
I	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
I	207	SER	CYS	engineered mutation	UNP Q9Y9L0
I	213	SER	CYS	engineered mutation	UNP Q9Y9L0
J	50	SER	CYS	engineered mutation	UNP Q9Y9L0
J	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
J	207	SER	CYS	engineered mutation	UNP Q9Y9L0
J	213	SER	CYS	engineered mutation	UNP Q9Y9L0
K	50	SER	CYS	engineered mutation	UNP Q9Y9L0
K	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
K	207	SER	CYS	engineered mutation	UNP Q9Y9L0
K	213	SER	CYS	engineered mutation	UNP Q9Y9L0
L	50	SER	CYS	engineered mutation	UNP Q9Y9L0
L	84	ALA	LYS	engineered mutation	UNP Q9Y9L0
L	207	SER	CYS	engineered mutation	UNP Q9Y9L0

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Chain	Residue	Modelled	Actual	Comment	Reference
L	213	SER	CYS	engineered mutation	UNP Q9Y9L0

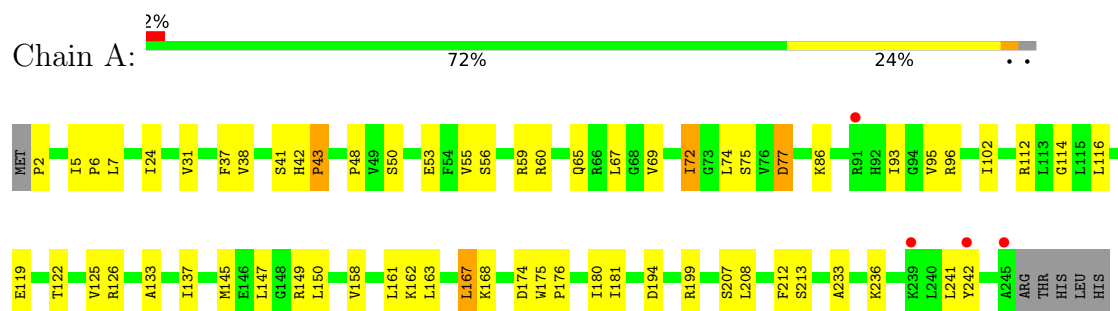
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	8	Total O 8 8	0	0
2	C	3	Total O 3 3	0	0
2	D	5	Total O 5 5	0	0
2	E	4	Total O 4 4	0	0
2	F	2	Total O 2 2	0	0
2	G	2	Total O 2 2	0	0
2	H	7	Total O 7 7	0	0
2	I	3	Total O 3 3	0	0
2	J	4	Total O 4 4	0	0
2	L	3	Total O 3 3	0	0

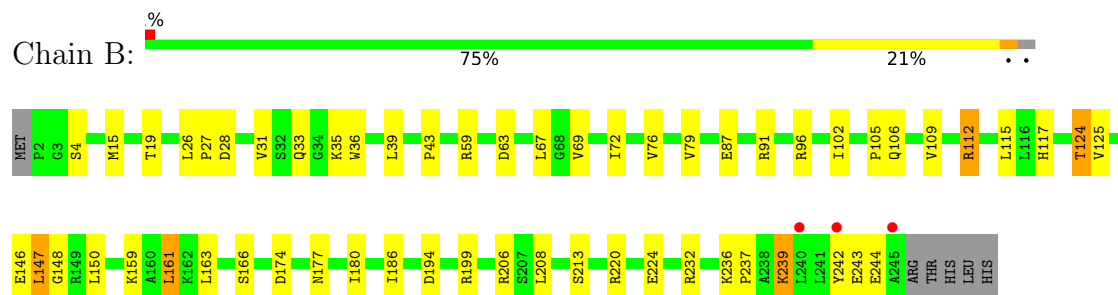
3 Residue-property plots

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.

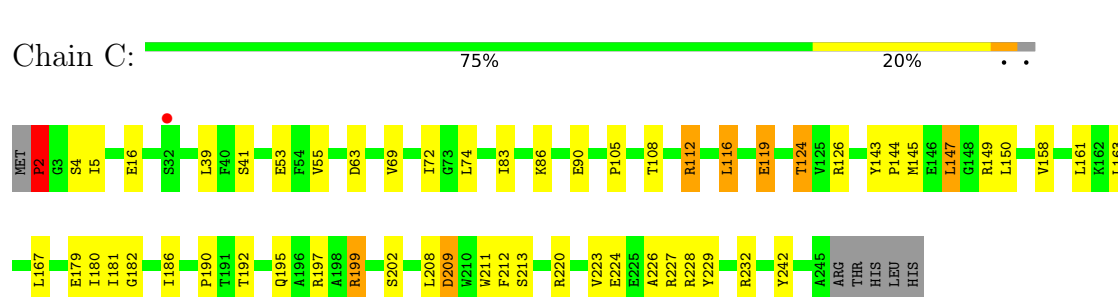
• Molecule 1: Peroxiredoxin



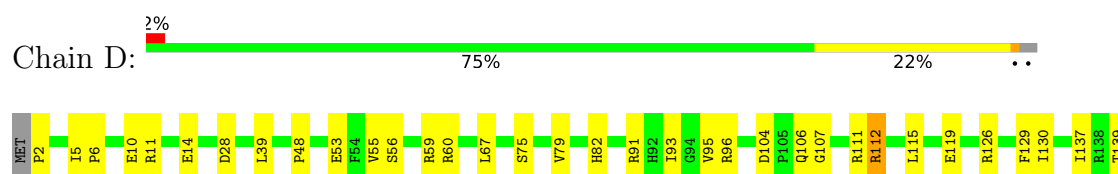
• Molecule 1: Peroxiredoxin



• Molecule 1: Peroxiredoxin



• Molecule 1: Peroxiredoxin

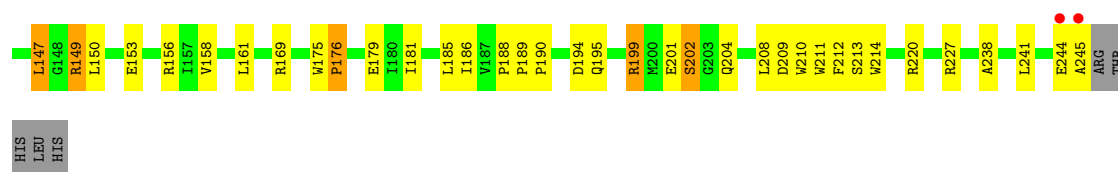
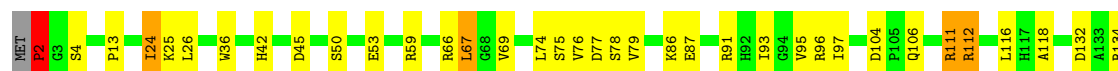




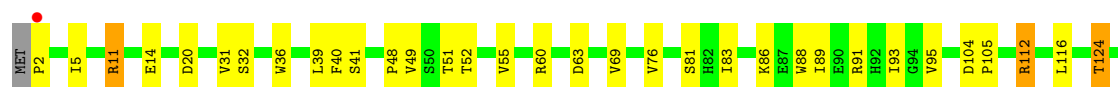
• Molecule 1: Peroxiredoxin



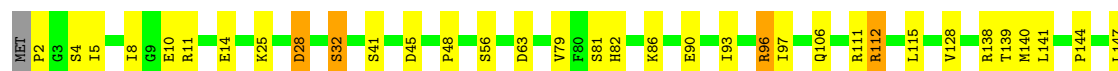
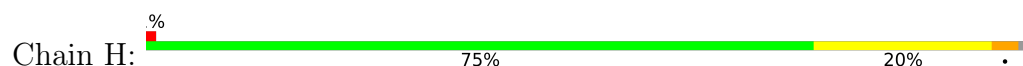
• Molecule 1: Peroxiredoxin



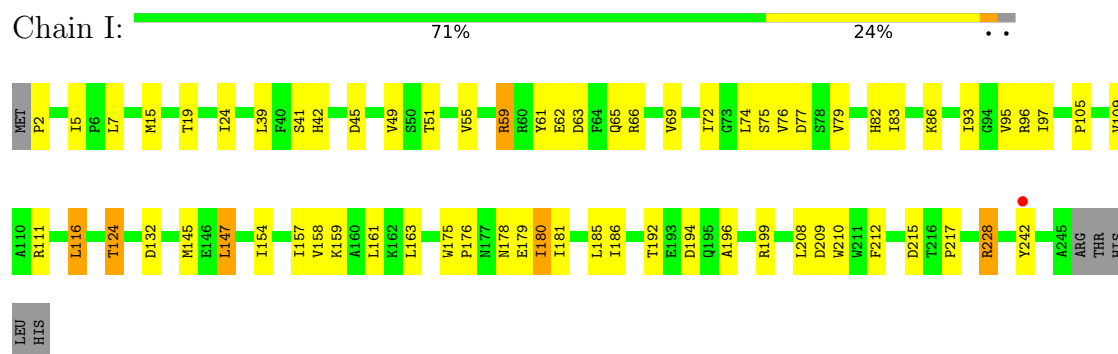
• Molecule 1: Peroxiredoxin



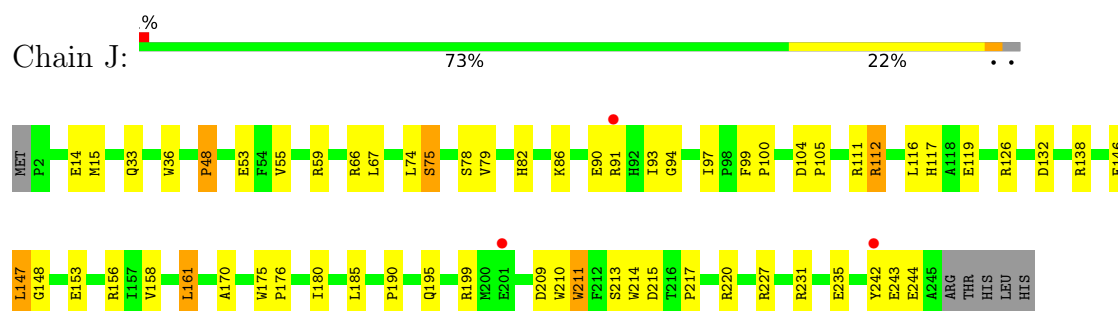
• Molecule 1: Peroxiredoxin



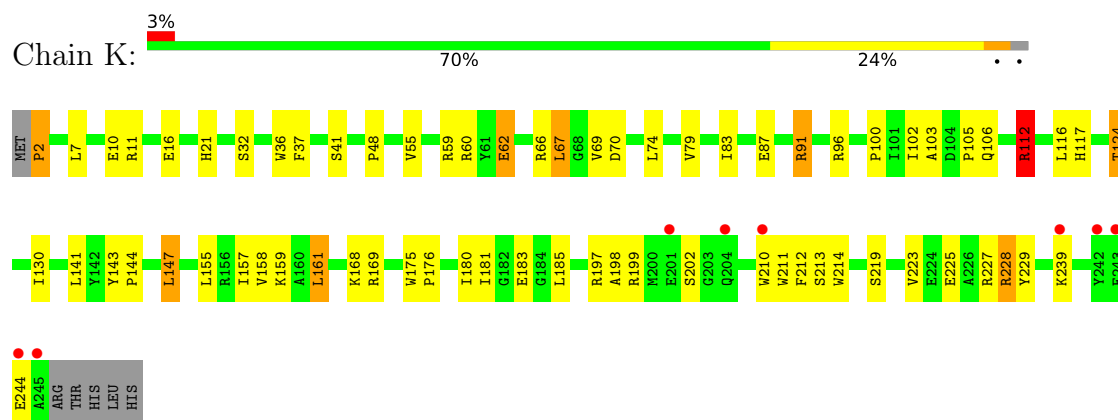
● Molecule 1: Peroxiredoxin



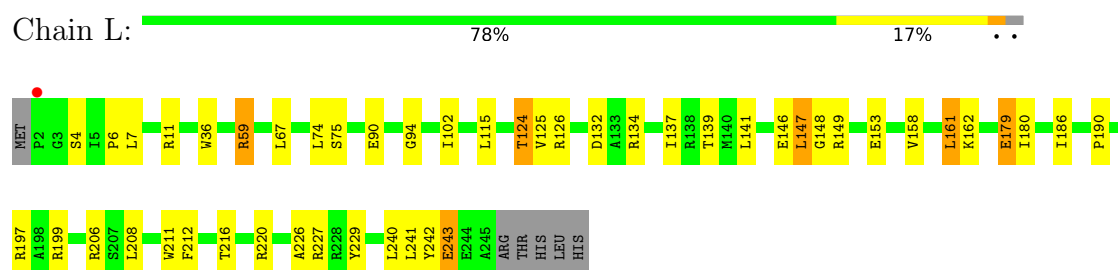
● Molecule 1: Peroxiredoxin



● Molecule 1: Peroxiredoxin



● Molecule 1: Peroxiredoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.01Å 210.57Å 308.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 2.90 49.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.48-2.90) 99.8 (49.48-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.179 , 0.256 0.171 , 0.244	Depositor DCC
R_{free} test set	4355 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23675	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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 20.61 % 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 8.3704e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.68	0/2024	0.92	1/2753 (0.0%)
1	B	0.69	0/2024	0.94	0/2753
1	C	0.71	1/2024 (0.0%)	0.92	1/2753 (0.0%)
1	D	0.70	0/2024	0.92	0/2753
1	E	0.71	0/2024	0.94	0/2753
1	F	0.70	0/2024	0.94	2/2753 (0.1%)
1	G	0.70	0/2024	0.92	0/2753
1	H	0.72	0/2024	0.95	1/2753 (0.0%)
1	I	0.69	0/2024	0.89	2/2753 (0.1%)
1	J	0.69	0/2024	0.87	0/2753
1	K	0.71	0/2024	0.92	2/2753 (0.1%)
1	L	0.71	0/2024	0.92	0/2753
All	All	0.70	1/24288 (0.0%)	0.92	9/33036 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	GLU	CD-OE1	5.20	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2	PRO	CA-N-CD	-5.91	103.23	111.50
1	A	2	PRO	CA-N-CD	-5.79	103.39	111.50
1	K	2	PRO	CA-N-CD	-5.59	103.68	111.50
1	F	2	PRO	CA-N-CD	-5.52	103.78	111.50
1	F	149	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	H	156	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	I	228	ARG	CB-CA-C	5.18	120.77	110.40
1	C	2	PRO	CA-N-CD	-5.17	104.25	111.50
1	K	112	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1969	0	1951	31	0
1	B	1969	0	1951	26	0
1	C	1969	0	1951	29	0
1	D	1969	0	1951	30	0
1	E	1969	0	1951	30	0
1	F	1969	0	1951	35	0
1	G	1969	0	1951	40	0
1	H	1969	0	1951	29	0
1	I	1969	0	1951	36	0
1	J	1969	0	1951	31	0
1	K	1969	0	1951	41	0
1	L	1969	0	1951	30	0
2	A	6	0	0	0	0
2	B	8	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
2	E	4	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	7	0	0	0	0
2	I	3	0	0	0	0
2	J	4	0	0	0	0
2	L	3	0	0	0	0
All	All	23675	0	23412	334	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (334) 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:C:2:PRO:HB2	1:D:10:GLU:OE2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:OG	1:A:77:ASP:OD1	1.98	0.80
1:A:69:VAL:HG21	1:A:158:VAL:HG11	1.67	0.76
1:I:69:VAL:HG21	1:I:158:VAL:HG11	1.67	0.75
1:G:69:VAL:HG21	1:G:158:VAL:HG11	1.67	0.75
1:F:24:ILE:HD11	1:F:26:LEU:HD21	1.70	0.74
1:A:37:PHE:HD2	1:A:72:ILE:HD11	1.52	0.73
1:K:67:LEU:HD21	1:K:159:LYS:HD2	1.71	0.73
1:C:69:VAL:HG21	1:C:158:VAL:HG11	1.70	0.72
1:F:69:VAL:HG21	1:F:158:VAL:HG21	1.73	0.71
1:K:69:VAL:HG21	1:K:158:VAL:HG11	1.72	0.71
1:J:74:LEU:HD13	1:J:75:SER:N	2.07	0.69
1:A:31:VAL:HG13	1:A:133:ALA:O	1.91	0.69
1:I:215:ASP:OD1	1:I:217:PRO:HD3	1.93	0.69
1:C:199:ARG:HH11	1:C:199:ARG:HG3	1.57	0.68
1:L:216:THR:OG1	1:L:216:THR:O	2.11	0.68
1:K:2:PRO:O	1:L:7:LEU:HG	1.94	0.68
1:A:74:LEU:HD23	1:A:102:ILE:HB	1.75	0.67
1:G:144:PRO:HG3	1:H:138:ARG:O	1.95	0.66
1:D:158:VAL:O	1:D:162:LYS:HG3	1.97	0.65
1:D:106:GLN:O	1:D:111:ARG:NH2	2.29	0.64
1:F:156:ARG:HD2	1:F:175:TRP:O	1.97	0.63
1:D:188:PRO:O	1:D:199:ARG:NH2	2.31	0.63
1:J:147:LEU:HD22	1:J:148:GLY:O	1.98	0.63
1:G:2:PRO:HB2	1:H:10:GLU:OE2	2.00	0.62
1:L:67:LEU:HD13	1:L:158:VAL:HG23	1.80	0.62
1:C:55:VAL:HG21	1:D:180:ILE:HD11	1.83	0.61
1:G:49:VAL:O	1:G:52:THR:OG1	2.19	0.60
1:K:69:VAL:CG2	1:K:158:VAL:HG11	2.31	0.60
1:C:199:ARG:HH11	1:C:199:ARG:CG	2.15	0.60
1:D:67:LEU:HD13	1:D:158:VAL:HG23	1.84	0.60
1:F:93:ILE:HG22	1:F:95:VAL:HG23	1.84	0.59
1:I:93:ILE:CG2	1:I:95:VAL:HG23	2.33	0.59
1:J:55:VAL:O	1:J:59:ARG:HG3	2.03	0.59
1:K:112:ARG:HH11	1:K:112:ARG:HG3	1.66	0.59
1:A:150:LEU:HD12	1:B:174:ASP:HA	1.84	0.59
1:K:112:ARG:CG	1:K:112:ARG:HH11	2.16	0.58
1:G:41:SER:HB2	1:G:124:THR:CG2	2.34	0.58
1:G:93:ILE:HG22	1:G:95:VAL:HG23	1.85	0.58
1:L:146:GLU:OE2	1:L:146:GLU:N	2.36	0.58
1:E:11:ARG:HG2	1:E:11:ARG:NH1	2.18	0.58
1:A:175:TRP:CG	1:A:176:PRO:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:VAL:HG21	1:J:170:ALA:HB1	1.86	0.58
1:D:39:LEU:HD23	1:D:39:LEU:C	2.25	0.57
1:B:147:LEU:HD22	1:B:148:GLY:O	2.02	0.57
1:H:86:LYS:HD3	1:H:97:ILE:HB	1.87	0.57
1:I:93:ILE:HG22	1:I:95:VAL:HG23	1.87	0.57
1:I:55:VAL:HG21	1:J:180:ILE:HD11	1.87	0.57
1:B:87:GLU:OE2	1:C:209:ASP:OD1	2.22	0.56
1:F:36:TRP:HB2	1:F:69:VAL:HG22	1.88	0.56
1:F:45:ASP:N	1:F:77:ASP:OD2	2.21	0.56
1:J:243:GLU:HB2	1:J:244:GLU:OE1	2.05	0.56
1:G:14:GLU:O	1:G:112:ARG:NH2	2.38	0.56
1:I:45:ASP:OD2	1:I:82:HIS:ND1	2.33	0.56
1:F:132:ASP:OD2	1:F:134:ARG:NH1	2.39	0.56
1:C:53:GLU:OE2	1:C:149:ARG:NE	2.34	0.55
1:I:41:SER:HB2	1:I:124:THR:HG21	1.89	0.55
1:D:175:TRP:CG	1:D:176:PRO:HA	2.41	0.55
1:A:72:ILE:H	1:A:72:ILE:HD12	1.72	0.55
1:I:157:ILE:O	1:I:161:LEU:HB2	2.06	0.54
1:K:36:TRP:HH2	1:K:161:LEU:HB3	1.71	0.54
1:A:233:ALA:O	1:B:177:ASN:ND2	2.35	0.54
1:D:180:ILE:HG22	1:D:181:ILE:HG23	1.88	0.54
1:F:244:GLU:O	1:F:245:ALA:C	2.46	0.54
1:E:20:ASP:OD2	1:E:86:LYS:NZ	2.26	0.54
1:A:72:ILE:N	1:A:72:ILE:HD12	2.23	0.54
1:C:112:ARG:HG3	1:C:112:ARG:HH11	1.72	0.54
1:G:132:ASP:OD2	1:G:134:ARG:NH1	2.41	0.54
1:D:153:GLU:OE1	1:D:153:GLU:HA	2.08	0.53
1:K:143:TYR:OH	1:L:153:GLU:OE2	2.23	0.53
1:B:15:MET:SD	1:B:109:VAL:HG13	2.47	0.53
1:C:179:GLU:OE2	1:D:59:ARG:HD3	2.08	0.53
1:F:202:SER:OG	1:F:204:GLN:NE2	2.42	0.53
1:A:41:SER:HB3	1:A:74:LEU:HD12	1.89	0.53
1:A:93:ILE:HG22	1:A:95:VAL:HG23	1.89	0.53
1:D:55:VAL:O	1:D:59:ARG:HG3	2.08	0.53
1:F:36:TRP:CD2	1:F:132:ASP:HA	2.44	0.53
1:I:69:VAL:CG2	1:I:158:VAL:HG11	2.37	0.53
1:B:27:PRO:O	1:B:31:VAL:HG23	2.08	0.53
1:G:20:ASP:OD2	1:G:86:LYS:HE3	2.09	0.53
1:D:93:ILE:HG22	1:D:95:VAL:HG23	1.90	0.53
1:K:21:HIS:ND1	1:K:100:PRO:HB3	2.23	0.53
1:H:56:SER:HB3	1:H:151:VAL:HG21	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:SER:HB2	1:C:124:THR:HG21	1.89	0.52
1:I:42:HIS:CE1	1:I:75:SER:HB2	2.44	0.52
1:E:147:LEU:HD22	1:E:148:GLY:O	2.09	0.52
1:L:36:TRP:CD2	1:L:132:ASP:HA	2.45	0.52
1:H:90:GLU:OE2	1:H:96:ARG:NH2	2.43	0.52
1:B:39:LEU:HA	1:B:72:ILE:O	2.10	0.52
1:C:150:LEU:HD12	1:D:174:ASP:HA	1.91	0.52
1:E:161:LEU:HD13	1:F:147:LEU:HG	1.91	0.52
1:I:180:ILE:HD12	1:J:93:ILE:HD13	1.92	0.52
1:I:178:ASN:HB3	1:I:181:ILE:O	2.10	0.52
1:C:143:TYR:HD2	1:C:147:LEU:HD13	1.76	0.51
1:G:175:TRP:CG	1:G:176:PRO:HA	2.46	0.51
1:L:59:ARG:HH12	1:L:241:LEU:HD11	1.74	0.51
1:E:14:GLU:HA	1:E:26:LEU:O	2.11	0.51
1:C:83:ILE:HB	1:H:210:TRP:CZ2	2.45	0.51
1:L:190:PRO:HD2	1:L:211:TRP:HA	1.91	0.51
1:D:210:TRP:CE2	1:G:83:ILE:HG22	2.46	0.51
1:D:56:SER:OG	1:D:60:ARG:NH1	2.45	0.50
1:L:90:GLU:O	1:L:94:GLY:HA2	2.11	0.50
1:J:74:LEU:HD13	1:J:74:LEU:C	2.30	0.50
1:K:183:GLU:HG3	1:K:183:GLU:O	2.12	0.50
1:E:41:SER:HB2	1:E:124:THR:HG21	1.93	0.50
1:G:11:ARG:HH11	1:G:11:ARG:HG2	1.77	0.50
1:H:156:ARG:HD2	1:H:175:TRP:O	2.11	0.50
1:K:7:LEU:O	1:K:10:GLU:HB2	2.12	0.49
1:D:112:ARG:HH11	1:D:112:ARG:CG	2.25	0.49
1:J:99:PHE:HB2	1:J:100:PRO:HD2	1.93	0.49
1:D:53:GLU:OE1	1:D:126:ARG:NH2	2.45	0.49
1:G:39:LEU:HD23	1:G:39:LEU:C	2.32	0.49
1:J:175:TRP:CG	1:J:176:PRO:HA	2.48	0.49
1:L:6:PRO:HB2	1:L:137:ILE:HD13	1.94	0.49
1:B:239:LYS:NZ	1:B:243:GLU:HB2	2.28	0.49
1:I:154:ILE:O	1:I:158:VAL:HG23	2.12	0.49
1:J:153:GLU:OE1	1:J:153:GLU:HA	2.13	0.49
1:J:67:LEU:HD13	1:J:158:VAL:HG23	1.94	0.49
1:C:223:VAL:HG12	1:C:227:ARG:HH12	1.77	0.49
1:C:69:VAL:CG2	1:C:158:VAL:HG11	2.41	0.49
1:F:175:TRP:CG	1:F:176:PRO:HA	2.47	0.49
1:G:5:ILE:HD13	1:H:5:ILE:HD13	1.95	0.49
1:L:74:LEU:HD23	1:L:102:ILE:HB	1.95	0.48
1:L:243:GLU:OE2	1:L:243:GLU:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:SER:HB2	1:G:124:THR:HG21	1.95	0.48
1:I:196:ALA:HB1	1:I:210:TRP:HB3	1.96	0.48
1:L:147:LEU:HD22	1:L:148:GLY:O	2.13	0.48
1:C:180:ILE:HG22	1:C:181:ILE:HG23	1.95	0.48
1:F:188:PRO:O	1:F:199:ARG:NH2	2.42	0.48
1:I:7:LEU:HD13	1:J:117:HIS:HA	1.95	0.48
1:J:86:LYS:HE3	1:J:97:ILE:HB	1.95	0.48
1:K:74:LEU:HD23	1:K:102:ILE:HB	1.95	0.48
1:K:62:GLU:HA	1:K:62:GLU:OE2	2.12	0.48
1:E:11:ARG:HG2	1:E:11:ARG:HH11	1.79	0.48
1:J:185:LEU:O	1:J:214:TRP:HB2	2.14	0.48
1:K:175:TRP:CG	1:K:176:PRO:HA	2.49	0.48
1:F:153:GLU:OE1	1:F:153:GLU:HA	2.14	0.48
1:G:142:TYR:O	1:H:8:ILE:HD11	2.14	0.48
1:G:196:ALA:HB1	1:G:210:TRP:HB3	1.95	0.48
1:H:45:ASP:OD2	1:H:82:HIS:ND1	2.40	0.48
1:F:111:ARG:HG3	1:F:116:LEU:HD12	1.95	0.48
1:H:199:ARG:HD2	1:H:205:TYR:CD2	2.49	0.48
1:G:141:LEU:HD22	1:H:141:LEU:HD22	1.95	0.47
1:E:180:ILE:HA	1:F:241:LEU:HB2	1.96	0.47
1:F:13:PRO:HB3	1:F:112:ARG:NH2	2.29	0.47
1:K:74:LEU:HD23	1:K:102:ILE:CG2	2.45	0.47
1:D:14:GLU:O	1:D:112:ARG:NH2	2.48	0.47
1:A:180:ILE:HG22	1:A:181:ILE:HG23	1.97	0.47
1:C:190:PRO:HD2	1:C:211:TRP:HA	1.96	0.47
1:K:175:TRP:CE2	1:K:176:PRO:HB3	2.50	0.47
1:K:60:ARG:HG2	1:K:155:LEU:HD11	1.97	0.47
1:K:144:PRO:HD3	1:L:139:THR:OG1	2.14	0.47
1:L:226:ALA:HA	1:L:229:TYR:CD2	2.50	0.47
1:E:36:TRP:CD2	1:E:132:ASP:HA	2.50	0.47
1:I:175:TRP:CG	1:I:176:PRO:HA	2.50	0.47
1:K:112:ARG:CG	1:K:112:ARG:NH1	2.78	0.47
1:B:236:LYS:HG3	1:B:237:PRO:CD	2.45	0.47
1:D:14:GLU:OE1	1:D:28:ASP:OD1	2.32	0.47
1:E:215:ASP:OD1	1:E:217:PRO:HD3	2.15	0.47
1:I:79:VAL:O	1:I:82:HIS:HB2	2.15	0.47
1:A:59:ARG:HH22	1:A:241:LEU:HD21	1.80	0.47
1:K:37:PHE:HA	1:K:70:ASP:O	2.14	0.47
1:E:9:GLY:HA3	1:F:118:ALA:HB3	1.97	0.46
1:G:156:ARG:HD2	1:G:175:TRP:O	2.15	0.46
1:G:139:THR:OG1	1:H:144:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:MET:HB3	1:J:112:ARG:NH2	2.30	0.46
1:A:37:PHE:CD2	1:A:72:ILE:HD11	2.42	0.46
1:A:174:ASP:HA	1:B:150:LEU:HD12	1.96	0.46
1:H:112:ARG:HG3	1:H:112:ARG:HH11	1.80	0.46
1:A:53:GLU:OE1	1:A:126:ARG:NH2	2.49	0.46
1:G:31:VAL:HG13	1:G:133:ALA:O	2.15	0.46
1:K:180:ILE:HG22	1:K:181:ILE:HG23	1.97	0.46
1:A:6:PRO:HB2	1:A:137:ILE:CD1	2.46	0.46
1:F:150:LEU:HD23	1:F:153:GLU:HB2	1.97	0.46
1:H:175:TRP:CG	1:H:176:PRO:HA	2.51	0.46
1:H:228:ARG:HA	1:H:231:ARG:HG3	1.97	0.46
1:I:61:TYR:CE1	1:I:65:GLN:NE2	2.84	0.46
1:C:86:LYS:HD3	1:H:193:GLU:OE1	2.16	0.45
1:E:172:PRO:HG3	1:E:181:ILE:HD11	1.98	0.45
1:L:115:LEU:O	1:L:124:THR:HA	2.15	0.45
1:D:130:ILE:HD13	1:D:139:THR:HB	1.98	0.45
1:E:175:TRP:CG	1:E:176:PRO:HA	2.52	0.45
1:E:185:LEU:O	1:E:214:TRP:HB2	2.16	0.45
1:E:42:HIS:CE1	1:E:75:SER:HB2	2.51	0.45
1:H:41:SER:HB3	1:H:115:LEU:HD13	1.98	0.45
1:L:153:GLU:OE1	1:L:153:GLU:HA	2.17	0.45
1:A:7:LEU:HD13	1:B:117:HIS:HA	1.98	0.45
1:J:90:GLU:O	1:J:94:GLY:HA2	2.16	0.45
1:K:180:ILE:HG22	1:K:181:ILE:CG2	2.46	0.45
1:D:115:LEU:HD21	1:D:129:PHE:HE1	1.81	0.45
1:G:104:ASP:N	1:G:105:PRO:HD3	2.32	0.45
1:H:11:ARG:NH1	1:H:14:GLU:OE2	2.49	0.45
1:I:39:LEU:HA	1:I:72:ILE:O	2.17	0.45
1:L:126:ARG:HB3	1:L:149:ARG:CZ	2.47	0.45
1:A:55:VAL:HG21	1:B:180:ILE:HD11	1.98	0.45
1:K:67:LEU:HD11	1:K:229:TYR:OH	2.17	0.45
1:D:175:TRP:CD1	1:D:176:PRO:HA	2.52	0.45
1:I:74:LEU:HD13	1:I:74:LEU:C	2.37	0.45
1:J:104:ASP:N	1:J:105:PRO:HD3	2.32	0.45
1:F:76:VAL:HA	1:F:104:ASP:O	2.17	0.45
1:E:48:PRO:HG2	1:F:186:ILE:HG21	1.98	0.44
1:B:63:ASP:OD2	1:B:232:ARG:NH1	2.46	0.44
1:C:63:ASP:OD2	1:C:232:ARG:NH2	2.39	0.44
1:G:41:SER:HB2	1:G:124:THR:HG23	1.99	0.44
1:J:119:GLU:OE1	1:J:146:GLU:OE2	2.35	0.44
1:F:53:GLU:CD	1:F:149:ARG:HH21	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:LEU:HG	1:L:161:LEU:HD13	1.98	0.44
1:E:188:PRO:HA	1:E:189:PRO:HD2	1.87	0.44
1:A:56:SER:OG	1:A:60:ARG:NH1	2.51	0.44
1:K:198:ALA:O	1:K:202:SER:HB3	2.18	0.44
1:E:59:ARG:NH1	1:F:179:GLU:OE1	2.50	0.44
1:G:147:LEU:HD22	1:G:148:GLY:O	2.17	0.44
1:I:42:HIS:O	1:I:124:THR:HG22	2.18	0.44
1:K:141:LEU:HD22	1:L:141:LEU:HD22	2.00	0.44
1:E:226:ALA:HA	1:E:229:TYR:CD2	2.52	0.44
1:F:190:PRO:HB3	1:F:195:GLN:HB3	2.00	0.44
1:D:112:ARG:CG	1:D:112:ARG:NH1	2.80	0.43
1:G:40:PHE:HA	1:G:127:GLY:O	2.17	0.43
1:I:15:MET:SD	1:I:109:VAL:HG13	2.58	0.43
1:J:111:ARG:HG3	1:J:116:LEU:HD12	1.98	0.43
1:K:225:GLU:O	1:K:228:ARG:HG2	2.18	0.43
1:F:87:GLU:OE2	1:G:209:ASP:OD1	2.36	0.43
1:G:163:LEU:HA	1:G:163:LEU:HD12	1.80	0.43
1:K:48:PRO:CG	1:L:186:ILE:HG21	2.48	0.43
1:C:143:TYR:CD2	1:C:147:LEU:HD13	2.54	0.43
1:F:42:HIS:HB2	1:F:50:SER:OG	2.19	0.43
1:H:112:ARG:CG	1:H:112:ARG:HH11	2.31	0.43
1:B:112:ARG:O	1:B:112:ARG:HG3	2.18	0.43
1:F:86:LYS:HG2	1:F:97:ILE:HB	2.00	0.43
1:L:158:VAL:O	1:L:162:LYS:HG3	2.19	0.43
1:A:175:TRP:CD1	1:A:176:PRO:HA	2.54	0.43
1:C:105:PRO:O	1:G:105:PRO:O	2.37	0.43
1:A:67:LEU:O	1:A:162:LYS:NZ	2.31	0.43
1:E:190:PRO:HB3	1:E:195:GLN:HB3	1.99	0.43
1:G:51:THR:O	1:G:55:VAL:HG23	2.18	0.43
1:I:76:VAL:O	1:I:105:PRO:HA	2.19	0.43
1:J:190:PRO:HA	1:J:195:GLN:NE2	2.34	0.43
1:J:36:TRP:CD2	1:J:132:ASP:HA	2.54	0.43
1:B:67:LEU:HD21	1:B:159:LYS:HD2	2.01	0.42
1:E:228:ARG:CG	1:E:228:ARG:HH11	2.32	0.42
1:I:63:ASP:OD1	1:I:66:ARG:NH1	2.52	0.42
1:K:103:ALA:C	1:K:105:PRO:HD3	2.39	0.42
1:L:11:ARG:HG2	1:L:11:ARG:HH11	1.83	0.42
1:A:163:LEU:HG	1:A:167:LEU:CD2	2.48	0.42
1:E:242:TYR:CD1	1:F:214:TRP:HH2	2.37	0.42
1:E:26:LEU:HA	1:E:27:PRO:HA	1.84	0.42
1:I:93:ILE:CG2	1:I:95:VAL:CG2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:THR:OG1	1:J:211:TRP:HZ3	2.02	0.42
1:B:106:GLN:OE1	1:B:106:GLN:HA	2.19	0.42
1:E:21:HIS:HE1	1:E:98:PRO:O	2.02	0.42
1:I:147:LEU:HG	1:J:161:LEU:HD13	2.01	0.42
1:J:210:TRP:CE2	1:J:211:TRP:HD1	2.38	0.42
1:B:115:LEU:HB3	1:B:124:THR:HG22	2.01	0.42
1:G:76:VAL:O	1:G:105:PRO:HA	2.20	0.42
1:I:111:ARG:HG3	1:I:116:LEU:HD23	2.00	0.42
1:A:5:ILE:HG22	1:A:114:GLY:HA3	2.00	0.42
1:F:210:TRP:CZ3	1:F:211:TRP:HB3	2.54	0.42
1:D:156:ARG:HD2	1:D:175:TRP:O	2.19	0.42
1:E:210:TRP:CE2	1:E:211:TRP:HD1	2.38	0.42
1:J:53:GLU:OE1	1:J:126:ARG:NH2	2.53	0.42
1:L:240:LEU:N	1:L:240:LEU:HD23	2.34	0.42
1:B:19:THR:HG22	1:B:102:ILE:HG12	2.02	0.42
1:C:226:ALA:HA	1:C:229:TYR:CD2	2.55	0.42
1:F:169:ARG:HB3	1:F:185:LEU:HB3	2.01	0.42
1:G:36:TRP:CD2	1:G:132:ASP:HA	2.54	0.42
1:H:138:ARG:O	1:H:139:THR:OG1	2.35	0.42
1:H:28:ASP:O	1:H:32:SER:OG	2.35	0.42
1:C:53:GLU:OE1	1:C:126:ARG:NH2	2.54	0.41
1:J:156:ARG:HD2	1:J:175:TRP:O	2.20	0.41
1:B:76:VAL:O	1:B:105:PRO:HA	2.20	0.41
1:C:5:ILE:HD11	1:D:5:ILE:HG21	2.02	0.41
1:D:104:ASP:OD2	1:D:107:GLY:HA2	2.19	0.41
1:K:41:SER:HB2	1:K:124:THR:HG21	2.01	0.41
1:A:42:HIS:CD2	1:A:50:SER:HB3	2.56	0.41
1:D:119:GLU:OE2	1:D:145:MET:HG2	2.20	0.41
1:G:161:LEU:HA	1:G:161:LEU:HD12	1.90	0.41
1:G:171:VAL:HG22	1:G:185:LEU:HD22	2.01	0.41
1:I:132:ASP:OD1	1:I:132:ASP:C	2.59	0.41
1:K:117:HIS:HA	1:L:7:LEU:HD13	2.02	0.41
1:A:48:PRO:HG2	1:B:186:ILE:HG21	2.02	0.41
1:A:65:GLN:NE2	1:A:65:GLN:HA	2.34	0.41
1:B:72:ILE:HD11	1:B:102:ILE:CG1	2.51	0.41
1:H:106:GLN:O	1:H:111:ARG:NH2	2.53	0.41
1:L:132:ASP:OD2	1:L:134:ARG:NH1	2.54	0.41
1:F:67:LEU:HD13	1:F:158:VAL:CG2	2.51	0.41
1:I:41:SER:HB2	1:I:124:THR:CG2	2.49	0.41
1:J:215:ASP:C	1:J:217:PRO:HD3	2.41	0.41
1:K:87:GLU:O	1:K:91:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:HE3	1:B:163:LEU:HD21	2.03	0.41
1:E:5:ILE:O	1:F:2:PRO:HB3	2.21	0.41
1:F:189:PRO:HA	1:F:190:PRO:HD3	1.94	0.41
1:K:55:VAL:HG11	1:L:180:ILE:HD11	2.02	0.41
1:G:88:TRP:HE3	1:G:89:ILE:N	2.17	0.41
1:I:83:ILE:HG22	1:K:210:TRP:CE2	2.56	0.41
1:F:210:TRP:CZ2	1:K:83:ILE:CG2	3.04	0.41
1:A:38:VAL:O	1:A:72:ILE:HD12	2.21	0.41
1:B:26:LEU:HA	1:B:27:PRO:HA	1.85	0.41
1:D:6:PRO:HB2	1:D:137:ILE:CD1	2.51	0.41
1:J:138:ARG:HA	1:J:138:ARG:HD2	1.88	0.41
1:A:43:PRO:HD2	1:A:126:ARG:NH2	2.36	0.41
1:I:186:ILE:HG21	1:J:48:PRO:HG2	2.03	0.41
1:K:48:PRO:HG2	1:L:186:ILE:HG21	2.03	0.41
1:L:161:LEU:HD12	1:L:161:LEU:HA	1.78	0.41
1:L:179:GLU:H	1:L:179:GLU:CD	2.24	0.41
1:C:39:LEU:HA	1:C:72:ILE:HG23	2.01	0.41
1:G:157:ILE:O	1:G:161:LEU:HB2	2.21	0.41
1:G:63:ASP:OD2	1:G:232:ARG:NH1	2.51	0.41
1:G:186:ILE:HG21	1:H:48:PRO:HG2	2.03	0.41
1:H:112:ARG:CG	1:H:112:ARG:NH1	2.83	0.40
1:H:128:VAL:O	1:H:140:MET:HA	2.21	0.40
1:I:49:VAL:CG2	1:J:170:ALA:HB1	2.49	0.40
1:C:116:LEU:HA	1:C:116:LEU:HD12	1.92	0.40
1:E:163:LEU:HD12	1:E:163:LEU:HA	1.82	0.40
1:E:190:PRO:HB3	1:E:195:GLN:CB	2.51	0.40
1:I:180:ILE:HD11	1:I:212:PHE:CZ	2.57	0.40
1:B:36:TRP:HB2	1:B:69:VAL:HG22	2.02	0.40
1:C:186:ILE:HG21	1:D:48:PRO:HG2	2.04	0.40
1:E:242:TYR:CD1	1:F:214:TRP:CH2	3.09	0.40
1:G:60:ARG:HD3	1:G:151:VAL:HG12	2.03	0.40
1:K:130:ILE:HD13	1:K:157:ILE:HG21	2.03	0.40
1:K:169:ARG:CB	1:K:185:LEU:HB3	2.51	0.40
1:K:223:VAL:HG12	1:K:227:ARG:NH1	2.36	0.40
1:C:41:SER:HB2	1:C:124:THR:CG2	2.51	0.40
1:C:53:GLU:CD	1:C:149:ARG:HH21	2.25	0.40
1:G:208:LEU:O	1:G:209:ASP:HB2	2.21	0.40
1:G:241:LEU:HB2	1:H:180:ILE:HA	2.02	0.40
1:H:190:PRO:HG2	1:H:210:TRP:HE3	1.86	0.40
1:H:63:ASP:OD2	1:H:232:ARG:NH2	2.50	0.40
1:A:53:GLU:OE2	1:A:149:ARG:NE	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HA	1:B:161:LEU:HD12	1.96	0.40
1:B:33:GLN:HB3	1:B:35:LYS:HG3	2.04	0.40
1:I:86:LYS:HG2	1:I:97:ILE:HB	2.04	0.40
1:E:122:THR:HG22	1:K:106:GLN:HG3	2.04	0.40
1:K:41:SER:HB2	1:K:124:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	A	242/250 (97%)	224 (93%)	16 (7%)	2 (1%)	19	51	
1	B	242/250 (97%)	227 (94%)	13 (5%)	2 (1%)	19	51	
1	C	242/250 (97%)	225 (93%)	15 (6%)	2 (1%)	19	51	
1	D	242/250 (97%)	224 (93%)	17 (7%)	1 (0%)	34	66	
1	E	242/250 (97%)	227 (94%)	14 (6%)	1 (0%)	34	66	
1	F	242/250 (97%)	227 (94%)	11 (4%)	4 (2%)	9	31	
1	G	242/250 (97%)	227 (94%)	14 (6%)	1 (0%)	34	66	
1	H	242/250 (97%)	221 (91%)	19 (8%)	2 (1%)	19	51	
1	I	242/250 (97%)	224 (93%)	16 (7%)	2 (1%)	19	51	
1	J	242/250 (97%)	221 (91%)	20 (8%)	1 (0%)	34	66	
1	K	242/250 (97%)	225 (93%)	17 (7%)	0	100	100	
1	L	242/250 (97%)	221 (91%)	20 (8%)	1 (0%)	34	66	
All	All	2904/3000 (97%)	2693 (93%)	192 (7%)	19 (1%)	22	54	

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	GLN
1	I	59	ARG
1	I	194	ASP
1	D	209	ASP
1	E	107	GLY
1	F	201	GLU
1	F	202	SER
1	F	209	ASP
1	F	238	ALA
1	H	209	ASP
1	H	182	GLY
1	L	125	VAL
1	A	43	PRO
1	A	125	VAL
1	G	48	PRO
1	C	182	GLY
1	B	43	PRO
1	B	125	VAL
1	J	48	PRO

5.3.2 Protein sidechains ⓘ

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	209/215 (97%)	187 (90%)	22 (10%)	7	21
1	B	209/215 (97%)	187 (90%)	22 (10%)	7	21
1	C	209/215 (97%)	181 (87%)	28 (13%)	4	11
1	D	209/215 (97%)	190 (91%)	19 (9%)	9	28
1	E	209/215 (97%)	188 (90%)	21 (10%)	7	23
1	F	209/215 (97%)	182 (87%)	27 (13%)	4	13
1	G	209/215 (97%)	188 (90%)	21 (10%)	7	23
1	H	209/215 (97%)	189 (90%)	20 (10%)	8	25
1	I	209/215 (97%)	187 (90%)	22 (10%)	7	21
1	J	209/215 (97%)	189 (90%)	20 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	209/215 (97%)	183 (88%)	26 (12%)	4	14
1	L	209/215 (97%)	193 (92%)	16 (8%)	13	35
All	All	2508/2580 (97%)	2244 (90%)	264 (10%)	7	21

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	72	ILE
1	A	77	ASP
1	A	86	LYS
1	A	96	ARG
1	A	112	ARG
1	A	116	LEU
1	A	119	GLU
1	A	122	THR
1	A	145	MET
1	A	147	LEU
1	A	161	LEU
1	A	167	LEU
1	A	168	LYS
1	A	194	ASP
1	A	199	ARG
1	A	207	SER
1	A	208	LEU
1	A	212	PHE
1	A	213	SER
1	A	236	LYS
1	A	242	TYR
1	B	4	SER
1	B	28	ASP
1	B	59	ARG
1	B	79	VAL
1	B	91	ARG
1	B	96	ARG
1	B	112	ARG
1	B	124	THR
1	B	146	GLU
1	B	147	LEU
1	B	161	LEU
1	B	166	SER

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Mol	Chain	Res	Type
1	B	194	ASP
1	B	199	ARG
1	B	206	ARG
1	B	208	LEU
1	B	213	SER
1	B	220	ARG
1	B	224	GLU
1	B	239	LYS
1	B	242	TYR
1	B	244	GLU
1	C	2	PRO
1	C	4	SER
1	C	16	GLU
1	C	74	LEU
1	C	90	GLU
1	C	108	THR
1	C	112	ARG
1	C	116	LEU
1	C	119	GLU
1	C	124	THR
1	C	144	PRO
1	C	145	MET
1	C	147	LEU
1	C	161	LEU
1	C	163	LEU
1	C	167	LEU
1	C	192	THR
1	C	197	ARG
1	C	199	ARG
1	C	202	SER
1	C	208	LEU
1	C	209	ASP
1	C	212	PHE
1	C	213	SER
1	C	220	ARG
1	C	224	GLU
1	C	228	ARG
1	C	242	TYR
1	D	2	PRO
1	D	11	ARG
1	D	75	SER
1	D	79	VAL

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Mol	Chain	Res	Type
1	D	82	HIS
1	D	91	ARG
1	D	96	ARG
1	D	112	ARG
1	D	147	LEU
1	D	161	LEU
1	D	191	THR
1	D	194	ASP
1	D	199	ARG
1	D	202	SER
1	D	208	LEU
1	D	209	ASP
1	D	212	PHE
1	D	242	TYR
1	D	244	GLU
1	E	11	ARG
1	E	59	ARG
1	E	62	GLU
1	E	78	SER
1	E	108	THR
1	E	116	LEU
1	E	124	THR
1	E	147	LEU
1	E	161	LEU
1	E	163	LEU
1	E	167	LEU
1	E	174	ASP
1	E	179	GLU
1	E	188	PRO
1	E	194	ASP
1	E	199	ARG
1	E	208	LEU
1	E	213	SER
1	E	228	ARG
1	E	235	GLU
1	E	242	TYR
1	F	2	PRO
1	F	4	SER
1	F	24	ILE
1	F	25	LYS
1	F	59	ARG
1	F	66	ARG

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Mol	Chain	Res	Type
1	F	67	LEU
1	F	74	LEU
1	F	75	SER
1	F	78	SER
1	F	79	VAL
1	F	91	ARG
1	F	96	ARG
1	F	106	GLN
1	F	111	ARG
1	F	112	ARG
1	F	147	LEU
1	F	161	LEU
1	F	176	PRO
1	F	181	ILE
1	F	194	ASP
1	F	199	ARG
1	F	208	LEU
1	F	212	PHE
1	F	213	SER
1	F	220	ARG
1	F	227	ARG
1	G	11	ARG
1	G	32	SER
1	G	81	SER
1	G	91	ARG
1	G	112	ARG
1	G	116	LEU
1	G	124	THR
1	G	147	LEU
1	G	161	LEU
1	G	163	LEU
1	G	167	LEU
1	G	199	ARG
1	G	206	ARG
1	G	208	LEU
1	G	212	PHE
1	G	220	ARG
1	G	221	ASP
1	G	227	ARG
1	G	228	ARG
1	G	239	LYS
1	G	242	TYR

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Mol	Chain	Res	Type
1	H	2	PRO
1	H	4	SER
1	H	25	LYS
1	H	28	ASP
1	H	32	SER
1	H	79	VAL
1	H	81	SER
1	H	93	ILE
1	H	96	ARG
1	H	112	ARG
1	H	147	LEU
1	H	161	LEU
1	H	176	PRO
1	H	199	ARG
1	H	202	SER
1	H	208	LEU
1	H	212	PHE
1	H	213	SER
1	H	220	ARG
1	H	242	TYR
1	I	5	ILE
1	I	19	THR
1	I	24	ILE
1	I	59	ARG
1	I	62	GLU
1	I	77	ASP
1	I	96	ARG
1	I	116	LEU
1	I	124	THR
1	I	145	MET
1	I	147	LEU
1	I	159	LYS
1	I	163	LEU
1	I	179	GLU
1	I	180	ILE
1	I	185	LEU
1	I	192	THR
1	I	199	ARG
1	I	208	LEU
1	I	209	ASP
1	I	228	ARG
1	I	242	TYR

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Mol	Chain	Res	Type
1	J	14	GLU
1	J	33	GLN
1	J	66	ARG
1	J	75	SER
1	J	78	SER
1	J	79	VAL
1	J	82	HIS
1	J	91	ARG
1	J	112	ARG
1	J	147	LEU
1	J	161	LEU
1	J	199	ARG
1	J	209	ASP
1	J	211	TRP
1	J	213	SER
1	J	220	ARG
1	J	227	ARG
1	J	231	ARG
1	J	235	GLU
1	J	242	TYR
1	K	11	ARG
1	K	16	GLU
1	K	32	SER
1	K	59	ARG
1	K	62	GLU
1	K	66	ARG
1	K	67	LEU
1	K	79	VAL
1	K	91	ARG
1	K	96	ARG
1	K	112	ARG
1	K	116	LEU
1	K	124	THR
1	K	147	LEU
1	K	161	LEU
1	K	168	LYS
1	K	197	ARG
1	K	199	ARG
1	K	211	TRP
1	K	212	PHE
1	K	213	SER
1	K	214	TRP

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Mol	Chain	Res	Type
1	K	219	SER
1	K	228	ARG
1	K	239	LYS
1	K	244	GLU
1	L	4	SER
1	L	59	ARG
1	L	75	SER
1	L	124	THR
1	L	147	LEU
1	L	161	LEU
1	L	179	GLU
1	L	197	ARG
1	L	199	ARG
1	L	206	ARG
1	L	208	LEU
1	L	212	PHE
1	L	220	ARG
1	L	227	ARG
1	L	242	TYR
1	L	243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	65	GLN
1	A	92	HIS
1	A	204	GLN
1	B	65	GLN
1	C	29	HIS
1	C	33	GLN
1	C	195	GLN
1	D	106	GLN
1	D	204	GLN
1	E	21	HIS
1	E	33	GLN
1	E	42	HIS
1	E	195	GLN
1	E	204	GLN
1	F	65	GLN
1	F	204	GLN
1	G	195	GLN

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Mol	Chain	Res	Type
1	H	42	HIS
1	H	106	GLN
1	H	195	GLN
1	I	65	GLN
1	I	204	GLN
1	J	195	GLN
1	K	42	HIS
1	K	204	GLN
1	L	21	HIS
1	L	65	GLN
1	L	204	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	244/250 (97%)	-0.29	4 (1%) 72 71	41, 59, 88, 111	0
1	B	244/250 (97%)	-0.35	3 (1%) 79 79	39, 56, 82, 119	0
1	C	244/250 (97%)	-0.39	1 (0%) 92 93	35, 50, 75, 108	0
1	D	244/250 (97%)	-0.41	5 (2%) 65 63	33, 48, 76, 120	0
1	E	244/250 (97%)	-0.47	1 (0%) 92 93	33, 47, 76, 105	0
1	F	244/250 (97%)	-0.45	2 (0%) 86 86	30, 46, 81, 109	0
1	G	244/250 (97%)	-0.46	1 (0%) 92 93	32, 46, 71, 96	0
1	H	244/250 (97%)	-0.44	2 (0%) 86 86	30, 49, 77, 108	0
1	I	244/250 (97%)	-0.34	1 (0%) 92 93	40, 56, 81, 107	0
1	J	244/250 (97%)	-0.31	3 (1%) 79 79	39, 57, 87, 112	0
1	K	244/250 (97%)	-0.20	8 (3%) 46 41	36, 58, 88, 116	0
1	L	244/250 (97%)	-0.37	1 (0%) 92 93	41, 57, 82, 119	0
All	All	2928/3000 (97%)	-0.37	32 (1%) 80 80	30, 53, 82, 120	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	ALA	3.7
1	A	245	ALA	3.6
1	D	245	ALA	3.5
1	K	244	GLU	3.2
1	B	242	TYR	3.2
1	K	245	ALA	3.1
1	K	204	GLN	2.8
1	J	242	TYR	2.7
1	L	2	PRO	2.6
1	J	91	ARG	2.6
1	K	210	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	201	GLU	2.5
1	A	239	LYS	2.5
1	H	245	ALA	2.5
1	D	239	LYS	2.4
1	K	242	TYR	2.4
1	F	245	ALA	2.4
1	B	240	LEU	2.3
1	I	242	TYR	2.3
1	C	32	SER	2.3
1	A	242	TYR	2.3
1	D	242	TYR	2.3
1	J	201	GLU	2.2
1	G	2	PRO	2.2
1	D	244	GLU	2.2
1	K	243	GLU	2.2
1	A	91	ARG	2.2
1	K	239	LYS	2.1
1	E	245	ALA	2.1
1	F	244	GLU	2.1
1	H	242	TYR	2.1
1	D	201	GLU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.