



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 10:30 PM EST

PDB ID : 4I5F
Title : Crystal structure of Ralstonia sp. alcohol dehydrogenase mutant N15G, G37D, R38V, R39S
Authors : Jarasch, A.; Lerchner, A.; Meining, W.; Schiefner, A.; Skerra, A.
Deposited on : unknown
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

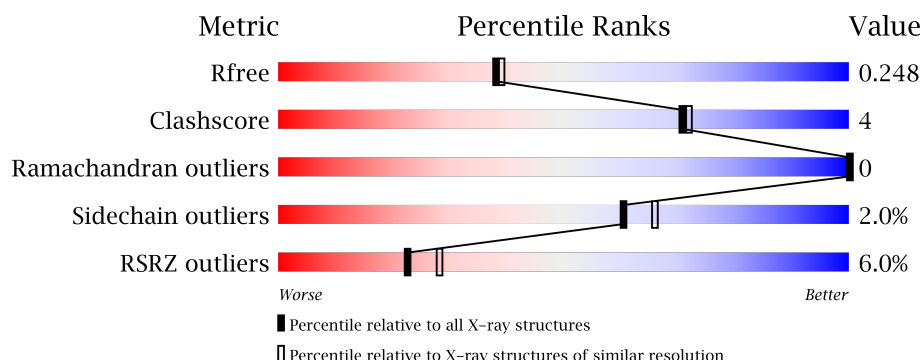
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	262	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div> </div>
1	B	262	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>11%</div> </div> </div>
1	C	262	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>7%</div> <div>11%</div> </div> </div>
1	D	262	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>11%</div> </div> </div>
1	E	262	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	262	<div><div></div><div>5%</div><div>77%</div><div>11%</div><div>•</div><div>11%</div></div>
1	G	262	<div><div></div><div>8%</div><div>81%</div><div>7%</div><div></div><div>11%</div></div>
1	H	262	<div><div></div><div>6%</div><div>80%</div><div>8%</div><div>•</div><div>11%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14580 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 Alcohol dehydrogenase/short-chain dehydrogenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	B	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	C	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	D	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	E	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	F	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	G	233	Total	C	N	O	0	0	0
			1743	1100	307	336			
1	H	233	Total	C	N	O	0	0	0
			1743	1100	307	336			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP C0IR58
A	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
A	-10	SER	-	EXPRESSION TAG	UNP C0IR58
A	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
A	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
A	-7	SER	-	EXPRESSION TAG	UNP C0IR58
A	-6	HIS	-	EXPRESSION TAG	UNP C0IR58
A	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
A	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
A	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
A	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
A	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
A	0	GLY	-	EXPRESSION TAG	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP C0IR58
A	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
A	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
A	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
A	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58
B	-12	MET	-	EXPRESSION TAG	UNP C0IR58
B	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
B	-10	SER	-	EXPRESSION TAG	UNP C0IR58
B	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
B	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
B	-7	SER	-	EXPRESSION TAG	UNP C0IR58
B	-6	HIS	-	EXPRESSION TAG	UNP C0IR58
B	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
B	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
B	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
B	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
B	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
B	0	GLY	-	EXPRESSION TAG	UNP C0IR58
B	1	ALA	-	EXPRESSION TAG	UNP C0IR58
B	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
B	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
B	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
B	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58
C	-12	MET	-	EXPRESSION TAG	UNP C0IR58
C	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
C	-10	SER	-	EXPRESSION TAG	UNP C0IR58
C	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
C	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
C	-7	SER	-	EXPRESSION TAG	UNP C0IR58
C	-6	HIS	-	EXPRESSION TAG	UNP C0IR58
C	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
C	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
C	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
C	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
C	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
C	0	GLY	-	EXPRESSION TAG	UNP C0IR58
C	1	ALA	-	EXPRESSION TAG	UNP C0IR58
C	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
C	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
C	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
C	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58
D	-12	MET	-	EXPRESSION TAG	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
D	-10	SER	-	EXPRESSION TAG	UNP C0IR58
D	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
D	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
D	-7	SER	-	EXPRESSION TAG	UNP C0IR58
D	-6	HIS	-	EXPRESSION TAG	UNP C0IR58
D	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
D	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
D	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
D	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
D	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
D	0	GLY	-	EXPRESSION TAG	UNP C0IR58
D	1	ALA	-	EXPRESSION TAG	UNP C0IR58
D	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
D	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
D	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
D	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58
E	-12	MET	-	EXPRESSION TAG	UNP C0IR58
E	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
E	-10	SER	-	EXPRESSION TAG	UNP C0IR58
E	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
E	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
E	-7	SER	-	EXPRESSION TAG	UNP C0IR58
E	-6	HIS	-	EXPRESSION TAG	UNP C0IR58
E	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
E	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
E	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
E	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
E	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
E	0	GLY	-	EXPRESSION TAG	UNP C0IR58
E	1	ALA	-	EXPRESSION TAG	UNP C0IR58
E	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
E	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
E	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
E	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58
F	-12	MET	-	EXPRESSION TAG	UNP C0IR58
F	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
F	-10	SER	-	EXPRESSION TAG	UNP C0IR58
F	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
F	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
F	-7	SER	-	EXPRESSION TAG	UNP C0IR58
F	-6	HIS	-	EXPRESSION TAG	UNP C0IR58

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
F	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
F	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
F	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
F	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
F	0	GLY	-	EXPRESSION TAG	UNP C0IR58
F	1	ALA	-	EXPRESSION TAG	UNP C0IR58
F	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
F	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
F	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
F	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58
G	-12	MET	-	EXPRESSION TAG	UNP C0IR58
G	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
G	-10	SER	-	EXPRESSION TAG	UNP C0IR58
G	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
G	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
G	-7	SER	-	EXPRESSION TAG	UNP C0IR58
G	-6	HIS	-	EXPRESSION TAG	UNP C0IR58
G	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
G	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
G	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
G	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
G	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
G	0	GLY	-	EXPRESSION TAG	UNP C0IR58
G	1	ALA	-	EXPRESSION TAG	UNP C0IR58
G	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
G	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
G	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
G	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58
H	-12	MET	-	EXPRESSION TAG	UNP C0IR58
H	-11	ALA	-	EXPRESSION TAG	UNP C0IR58
H	-10	SER	-	EXPRESSION TAG	UNP C0IR58
H	-9	ARG	-	EXPRESSION TAG	UNP C0IR58
H	-8	GLY	-	EXPRESSION TAG	UNP C0IR58
H	-7	SER	-	EXPRESSION TAG	UNP C0IR58
H	-6	HIS	-	EXPRESSION TAG	UNP C0IR58
H	-5	HIS	-	EXPRESSION TAG	UNP C0IR58
H	-4	HIS	-	EXPRESSION TAG	UNP C0IR58
H	-3	HIS	-	EXPRESSION TAG	UNP C0IR58
H	-2	HIS	-	EXPRESSION TAG	UNP C0IR58
H	-1	HIS	-	EXPRESSION TAG	UNP C0IR58
H	0	GLY	-	EXPRESSION TAG	UNP C0IR58

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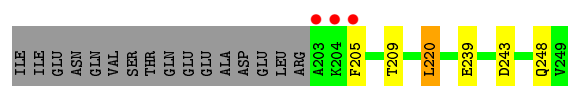
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	ALA	-	EXPRESSION TAG	UNP C0IR58
H	15	GLY	ASN	ENGINEERED MUTATION	UNP C0IR58
H	37	ASP	GLY	ENGINEERED MUTATION	UNP C0IR58
H	38	VAL	ARG	ENGINEERED MUTATION	UNP C0IR58
H	39	SER	ARG	ENGINEERED MUTATION	UNP C0IR58

- Molecule 2 is water.

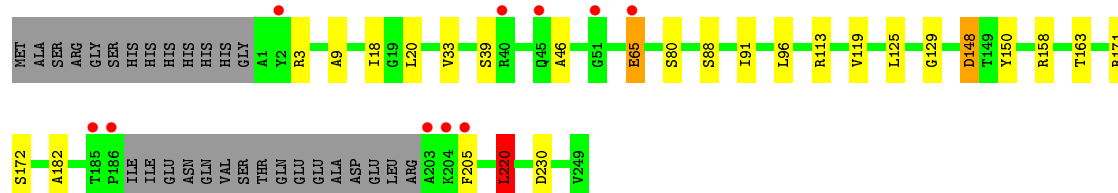
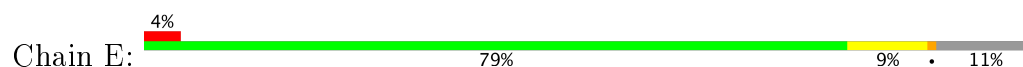
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	89	Total O 89 89	0	0
2	B	84	Total O 84 84	0	0
2	C	80	Total O 80 80	0	0
2	D	85	Total O 85 85	0	0
2	E	87	Total O 87 87	0	0
2	F	74	Total O 74 74	0	0
2	G	65	Total O 65 65	0	0
2	H	72	Total O 72 72	0	0

- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase

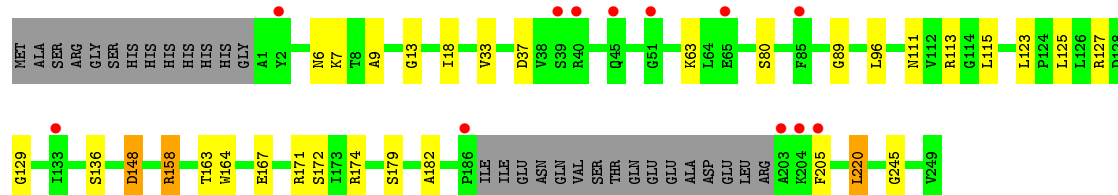




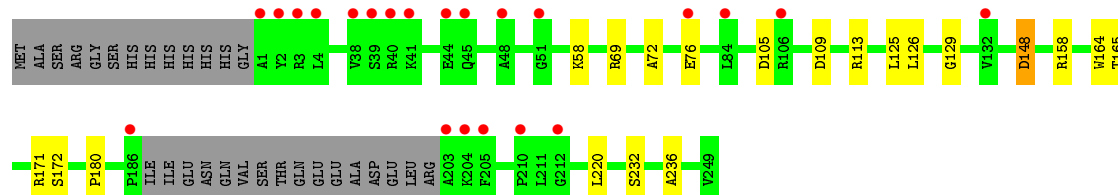
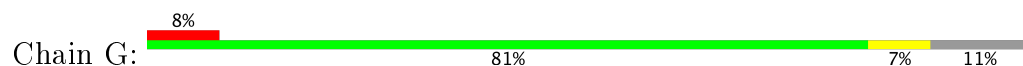
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



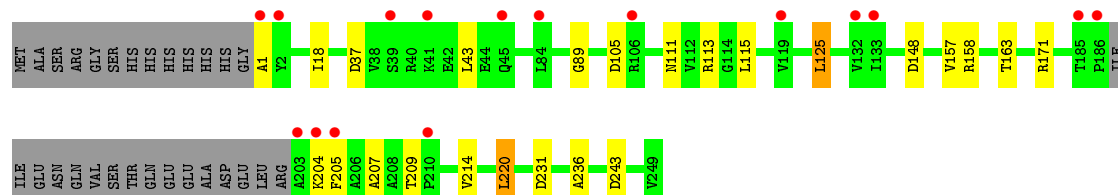
- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



- Molecule 1: Alcohol dehydrogenase/short-chain dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.80 Å 72.97 Å 132.89 Å 80.74° 86.53° 64.18°	Depositor
Resolution (Å)	29.58 – 2.10 29.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.58-2.10) 91.7 (29.58-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.244 0.208 , 0.248	Depositor DCC
R_{free} test set	6862 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14580	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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	1.03	1/1765 (0.1%)	1.06	5/2392 (0.2%)
1	B	0.95	3/1765 (0.2%)	0.96	2/2392 (0.1%)
1	C	1.01	3/1765 (0.2%)	1.00	2/2392 (0.1%)
1	D	0.98	2/1765 (0.1%)	1.02	6/2392 (0.3%)
1	E	1.04	1/1765 (0.1%)	1.09	4/2392 (0.2%)
1	F	0.96	1/1765 (0.1%)	1.00	7/2392 (0.3%)
1	G	0.94	2/1765 (0.1%)	0.91	0/2392
1	H	0.92	0/1765	0.96	6/2392 (0.3%)
All	All	0.98	13/14120 (0.1%)	1.00	32/19136 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	TRP	CD2-CE2	7.30	1.50	1.41
1	C	239	GLU	CD-OE1	7.22	1.33	1.25
1	B	232	SER	CB-OG	5.93	1.50	1.42
1	D	164	TRP	CD2-CE2	5.83	1.48	1.41
1	B	164	TRP	CD2-CE2	5.73	1.48	1.41
1	B	218	GLU	CD-OE2	5.55	1.31	1.25
1	G	232	SER	CB-OG	5.53	1.49	1.42
1	G	164	TRP	CD2-CE2	5.51	1.48	1.41
1	F	164	TRP	CD2-CE2	5.29	1.47	1.41
1	A	164	TRP	CD2-CE2	5.28	1.47	1.41
1	C	158	ARG	CZ-NH1	5.11	1.39	1.33
1	D	239	GLU	CD-OE1	5.05	1.31	1.25
1	E	65	GLU	CD-OE2	5.03	1.31	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	113	ARG	NE-CZ-NH2	-9.61	115.49	120.30
1	E	220	LEU	CA-CB-CG	-8.96	94.69	115.30
1	F	171	ARG	NE-CZ-NH2	-8.42	116.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	220	LEU	CA-CB-CG	-6.80	99.67	115.30
1	E	171	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	F	113	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	H	171	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	243	ASP	CB-CG-OD1	6.23	123.90	118.30
1	F	7	LYS	CD-CE-NZ	-6.09	97.70	111.70
1	D	171	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	H	231	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	H	243	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	128	ASP	CB-CG-OD1	5.84	123.56	118.30
1	F	174	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	H	231	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	128	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	F	171	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	88	SER	N-CA-C	-5.60	95.88	111.00
1	A	227	LEU	CB-CG-CD1	-5.59	101.49	111.00
1	B	246	LEU	CB-CG-CD1	5.56	120.46	111.00
1	H	125	LEU	CB-CG-CD1	-5.50	101.66	111.00
1	A	69	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	C	171	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	220	LEU	CA-CB-CG	-5.25	103.22	115.30
1	D	171	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	1	ALA	N-CA-C	-5.23	96.89	111.00
1	B	88	SER	N-CA-C	-5.20	96.97	111.00
1	A	60	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	E	230	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	37	ASP	CB-CG-OD2	5.06	122.86	118.30
1	H	220	LEU	CA-CB-CG	-5.03	103.72	115.30
1	F	113	ARG	NE-CZ-NH1	5.03	122.81	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	1743	0	1785	14	0
1	B	1743	0	1785	21	0
1	C	1743	0	1785	17	0
1	D	1743	0	1785	15	0
1	E	1743	0	1785	14	0
1	F	1743	0	1785	23	0
1	G	1743	0	1785	12	0
1	H	1743	0	1785	14	0
2	A	89	0	0	1	0
2	B	84	0	0	1	0
2	C	80	0	0	0	0
2	D	85	0	0	1	0
2	E	87	0	0	2	0
2	F	74	0	0	4	0
2	G	65	0	0	2	0
2	H	72	0	0	2	0
All	All	14580	0	14280	115	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 4.

All (115) 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:B:40:ARG:HH11	1:B:40:ARG:HG2	1.46	0.80
1:B:18:ILE:HG21	1:B:220:LEU:HD23	1.63	0.80
1:D:18:ILE:HD12	1:D:220:LEU:HD22	1.64	0.80
1:D:18:ILE:HD12	1:D:220:LEU:CD2	2.14	0.78
1:B:72:ALA:O	1:B:76:GLU:HG3	1.86	0.75
1:H:214:VAL:HG22	2:H:345:HOH:O	1.88	0.72
1:A:18:ILE:HD12	1:A:220:LEU:CD2	2.20	0.71
1:C:18:ILE:HB	1:C:220:LEU:HD23	1.74	0.70
1:C:18:ILE:HD12	1:C:220:LEU:CD2	2.23	0.68
1:C:18:ILE:HG21	1:C:220:LEU:HD22	1.74	0.68
1:C:18:ILE:CD1	1:C:220:LEU:CD2	2.74	0.66
1:B:180:PRO:HG3	1:B:220:LEU:HD21	1.78	0.64
1:G:236:ALA:HB1	2:G:321:HOH:O	1.99	0.62
1:F:18:ILE:HD12	1:F:220:LEU:CD2	2.31	0.61
1:F:18:ILE:HD12	1:F:220:LEU:HD22	1.82	0.61
1:H:18:ILE:HD12	1:H:220:LEU:HD22	1.81	0.60
1:A:64:LEU:HD22	1:A:121:LYS:HE3	1.82	0.60
1:H:1:ALA:N	2:H:372:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:LEU:HD12	1:H:125:LEU:N	2.18	0.58
1:B:40:ARG:HG2	1:B:40:ARG:NH1	2.17	0.58
1:H:115:LEU:HD22	1:H:157:VAL:HG22	1.85	0.58
1:E:91:ILE:HB	1:E:150:TYR:CD1	2.38	0.58
1:E:129:GLY:HA2	1:E:172:SER:O	2.05	0.57
1:E:18:ILE:HD12	1:E:220:LEU:HD22	1.86	0.57
1:D:61:VAL:HG12	1:D:67:LEU:HD21	1.87	0.57
1:B:119:VAL:HG21	1:B:164:TRP:CZ3	2.40	0.56
1:H:18:ILE:HD12	1:H:220:LEU:CD2	2.36	0.56
1:F:89:GLY:HA2	1:F:111:ASN:OD1	2.06	0.56
1:G:72:ALA:O	1:G:76:GLU:HG3	2.06	0.55
1:B:18:ILE:HG21	1:B:220:LEU:CD2	2.35	0.55
1:D:18:ILE:CD1	1:D:220:LEU:HD22	2.34	0.55
1:E:20:LEU:HD13	1:E:46:ALA:HB1	1.86	0.55
1:D:182:ALA:HB2	1:D:205:PHE:HD2	1.72	0.55
1:E:148:ASP:OD1	1:F:167:GLU:OE2	2.25	0.55
1:B:180:PRO:CG	1:B:220:LEU:HD21	2.37	0.54
1:A:115:LEU:HD22	1:A:157:VAL:HG22	1.90	0.54
1:A:76:GLU:HG3	2:A:313:HOH:O	2.06	0.54
1:G:125:LEU:HD12	1:G:125:LEU:N	2.23	0.54
1:F:80:SER:HB2	1:F:125:LEU:O	2.08	0.53
1:G:58:LYS:O	1:G:69:ARG:NH2	2.40	0.53
1:D:126:LEU:O	1:D:171:ARG:NH2	2.42	0.52
1:A:104:TYR:CE2	1:C:113:ARG:HB2	2.44	0.52
1:G:109:ASP:HA	1:G:113:ARG:HB3	1.91	0.51
1:G:105:ASP:OD1	1:H:113:ARG:NH2	2.44	0.51
1:F:18:ILE:CD1	1:F:220:LEU:HD22	2.39	0.51
1:F:63:LYS:HA	2:F:358:HOH:O	2.11	0.50
1:B:88:SER:HA	2:B:352:HOH:O	2.11	0.49
1:F:13:GLY:N	2:F:347:HOH:O	2.44	0.49
1:B:167:GLU:OE2	1:D:148:ASP:OD1	2.30	0.49
1:F:136:SER:HB3	1:F:179:SER:OG	2.12	0.49
1:C:79:GLY:O	1:F:6:ASN:HB3	2.12	0.49
1:B:129:GLY:HA2	1:B:172:SER:O	2.13	0.49
1:E:163:THR:HG21	1:F:148:ASP:HA	1.95	0.48
1:D:125:LEU:HD12	1:D:125:LEU:N	2.29	0.48
1:A:82:ASP:OD1	1:A:127:ARG:NE	2.22	0.48
1:F:13:GLY:HA2	2:F:347:HOH:O	2.13	0.48
1:B:40:ARG:HH11	1:B:40:ARG:CG	2.19	0.48
1:A:18:ILE:CD1	1:A:220:LEU:HD22	2.44	0.47
1:C:18:ILE:HD12	1:C:220:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:LEU:O	1:G:171:ARG:NH2	2.48	0.47
1:G:180:PRO:HG3	1:G:220:LEU:HD21	1.96	0.47
1:E:148:ASP:HA	1:F:163:THR:HG21	1.96	0.47
1:B:18:ILE:CG2	1:B:220:LEU:HD23	2.39	0.47
1:D:182:ALA:HB2	1:D:205:PHE:CD2	2.50	0.47
1:G:148:ASP:HA	1:H:163:THR:HG21	1.96	0.47
1:A:18:ILE:HD12	1:A:220:LEU:HD22	1.96	0.46
1:H:204:LYS:O	1:H:207:ALA:HB3	2.15	0.46
1:D:89:GLY:HA3	2:D:373:HOH:O	2.15	0.46
1:H:205:PHE:O	1:H:209:THR:OG1	2.25	0.46
1:E:3:ARG:HD3	2:E:326:HOH:O	2.16	0.46
1:E:119:VAL:HG12	1:F:96:LEU:HD21	1.96	0.46
1:C:139:ALA:HB1	1:C:151:SER:OG	2.16	0.45
1:C:182:ALA:HB2	1:C:205:PHE:HD2	1.81	0.45
1:D:205:PHE:O	1:D:209:THR:OG1	2.25	0.45
1:F:129:GLY:HA2	1:F:172:SER:O	2.16	0.45
1:B:18:ILE:CD1	1:B:220:LEU:HD23	2.46	0.45
1:E:9:ALA:HB3	1:E:33:VAL:HG22	1.99	0.45
1:C:18:ILE:HD12	1:C:220:LEU:HD21	1.97	0.45
1:G:113:ARG:NH2	1:H:105:ASP:OD1	2.50	0.45
1:E:182:ALA:HB2	1:E:205:PHE:HD2	1.81	0.45
1:A:115:LEU:HD11	1:A:134:LEU:HD22	2.00	0.44
1:C:127:ARG:CZ	1:F:127:ARG:NH1	2.80	0.44
1:A:182:ALA:O	1:A:183:ILE:HD13	2.17	0.44
1:B:12:THR:O	1:B:87:ASN:HB3	2.17	0.44
1:E:96:LEU:HD23	1:F:123:LEU:HD11	2.00	0.44
1:F:158:ARG:C	1:F:158:ARG:HD3	2.38	0.44
1:F:182:ALA:HB2	1:F:205:PHE:HB3	1.99	0.44
1:C:180:PRO:HB3	1:C:220:LEU:HD13	1.99	0.44
1:D:139:ALA:O	1:D:151:SER:HB3	2.17	0.44
1:F:9:ALA:HB3	1:F:33:VAL:HG22	2.00	0.44
1:B:125:LEU:N	1:B:125:LEU:HD12	2.33	0.43
1:E:80:SER:HB2	1:E:125:LEU:O	2.17	0.43
1:B:20:LEU:HD13	1:B:46:ALA:HB1	2.00	0.43
1:G:129:GLY:HA2	1:G:172:SER:O	2.18	0.43
1:A:64:LEU:HD21	1:A:117:PHE:CG	2.54	0.43
1:C:11:ILE:HD12	1:C:23:ALA:HB2	2.01	0.43
1:B:109:ASP:HA	1:B:113:ARG:HB3	1.99	0.43
1:C:162:ARG:HD3	1:D:248:GLN:O	2.18	0.43
1:H:37:ASP:O	1:H:43:LEU:HD11	2.18	0.43
1:A:18:ILE:CD1	1:A:220:LEU:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:THR:O	1:A:87:ASN:HB3	2.19	0.42
1:B:9:ALA:HA	1:B:83:VAL:O	2.19	0.42
1:A:158:ARG:HD3	1:A:158:ARG:C	2.39	0.42
1:D:180:PRO:HB3	1:D:220:LEU:HD13	2.01	0.42
1:F:245:GLY:HA2	1:H:236:ALA:O	2.20	0.42
1:C:123:LEU:HB2	1:C:124:PRO:HD3	2.01	0.41
1:C:18:ILE:HD13	1:C:220:LEU:CD2	2.47	0.41
1:H:89:GLY:HA2	1:H:111:ASN:OD1	2.20	0.41
1:D:136:SER:OG	1:D:154:LYS:O	2.36	0.41
1:G:165:THR:HG23	2:G:321:HOH:O	2.19	0.41
1:E:88:SER:HA	2:E:379:HOH:O	2.21	0.40
1:C:127:ARG:NH2	1:F:127:ARG:NH1	2.69	0.40
1:F:13:GLY:CA	2:F:347:HOH:O	2.67	0.40
1:B:40:ARG:CG	1:B:40:ARG:NH1	2.77	0.40
1:B:20:LEU:HG	1:B:24:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	229/262 (87%)	218 (95%)	11 (5%)	0	100	100
1	B	229/262 (87%)	219 (96%)	10 (4%)	0	100	100
1	C	229/262 (87%)	217 (95%)	12 (5%)	0	100	100
1	D	229/262 (87%)	222 (97%)	7 (3%)	0	100	100
1	E	229/262 (87%)	217 (95%)	12 (5%)	0	100	100
1	F	229/262 (87%)	219 (96%)	10 (4%)	0	100	100
1	G	229/262 (87%)	218 (95%)	11 (5%)	0	100	100
1	H	229/262 (87%)	221 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1832/2096 (87%)	1751 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	179/204 (88%)	175 (98%)	4 (2%)	57	62
1	B	179/204 (88%)	176 (98%)	3 (2%)	66	72
1	C	179/204 (88%)	174 (97%)	5 (3%)	49	52
1	D	179/204 (88%)	175 (98%)	4 (2%)	57	62
1	E	179/204 (88%)	174 (97%)	5 (3%)	49	52
1	F	179/204 (88%)	175 (98%)	4 (2%)	57	62
1	G	179/204 (88%)	177 (99%)	2 (1%)	78	83
1	H	179/204 (88%)	177 (99%)	2 (1%)	78	83
All	All	1432/1632 (88%)	1403 (98%)	29 (2%)	60	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	148	ASP
1	A	158	ARG
1	A	205	PHE
1	B	37	ASP
1	B	148	ASP
1	B	158	ARG
1	C	37	ASP
1	C	88	SER
1	C	148	ASP
1	C	158	ARG
1	C	180	PRO

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Mol	Chain	Res	Type
1	D	40	ARG
1	D	115	LEU
1	D	148	ASP
1	D	158	ARG
1	E	39	SER
1	E	65	GLU
1	E	148	ASP
1	E	158	ARG
1	E	220	LEU
1	F	37	ASP
1	F	115	LEU
1	F	148	ASP
1	F	158	ARG
1	G	148	ASP
1	G	158	ARG
1	H	148	ASP
1	H	158	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 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	233/262 (88%)	0.04	13 (5%)	25	31	16, 26, 52, 175	0
1	B	233/262 (88%)	0.19	19 (8%)	12	16	18, 34, 57, 126	0
1	C	233/262 (88%)	0.03	10 (4%)	36	43	17, 29, 50, 129	0
1	D	233/262 (88%)	0.03	10 (4%)	36	43	17, 30, 50, 117	0
1	E	233/262 (88%)	0.04	10 (4%)	36	43	18, 27, 51, 109	0
1	F	233/262 (88%)	0.18	12 (5%)	28	34	19, 32, 58, 127	0
1	G	233/262 (88%)	0.38	22 (9%)	9	12	18, 36, 95, 119	0
1	H	233/262 (88%)	0.13	16 (6%)	18	22	20, 33, 60, 159	0
All	All	1864/2096 (88%)	0.13	112 (6%)	23	28	16, 31, 60, 175	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	186	PRO	10.0
1	H	186	PRO	7.8
1	F	186	PRO	7.8
1	B	186	PRO	7.6
1	F	205	PHE	7.1
1	A	186	PRO	6.3
1	G	203	ALA	6.3
1	C	186	PRO	5.9
1	E	204	LYS	5.8
1	D	186	PRO	5.4
1	G	186	PRO	5.0
1	G	40	ARG	4.9
1	C	203	ALA	4.9
1	G	41	LYS	4.8
1	B	203	ALA	4.8
1	G	205	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	203	ALA	4.5
1	E	203	ALA	4.4
1	C	205	PHE	4.4
1	B	2	TYR	4.3
1	C	204	LYS	4.3
1	A	203	ALA	4.3
1	G	84	LEU	4.1
1	G	2	TYR	4.0
1	B	1	ALA	4.0
1	B	205	PHE	3.9
1	E	40	ARG	3.8
1	G	1	ALA	3.8
1	G	204	LYS	3.7
1	H	41	LYS	3.6
1	H	2	TYR	3.5
1	A	204	LYS	3.5
1	H	84	LEU	3.4
1	F	40	ARG	3.4
1	H	205	PHE	3.4
1	E	205	PHE	3.4
1	D	84	LEU	3.4
1	D	205	PHE	3.3
1	E	2	TYR	3.3
1	D	41	LYS	3.2
1	A	40	ARG	3.2
1	G	39	SER	3.2
1	H	210	PRO	3.2
1	D	203	ALA	3.1
1	G	44	GLU	3.1
1	B	207	ALA	3.0
1	H	204	LYS	3.0
1	G	38	VAL	3.0
1	H	45	GLN	3.0
1	D	185	THR	2.9
1	H	185	THR	2.9
1	B	204	LYS	2.9
1	B	45	GLN	2.8
1	D	2	TYR	2.8
1	H	203	ALA	2.8
1	A	2	TYR	2.8
1	B	212	GLY	2.8
1	G	48	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	204	LYS	2.8
1	F	204	LYS	2.7
1	D	1	ALA	2.7
1	F	39	SER	2.7
1	A	45	GLN	2.7
1	A	212	GLY	2.7
1	E	185	THR	2.7
1	D	132	VAL	2.7
1	G	132	VAL	2.7
1	B	206	ALA	2.7
1	G	51	GLY	2.6
1	A	41	LYS	2.6
1	H	1	ALA	2.6
1	A	133	ILE	2.5
1	B	40	ARG	2.5
1	B	132	VAL	2.5
1	B	84	LEU	2.5
1	A	205	PHE	2.5
1	A	84	LEU	2.5
1	F	45	GLN	2.4
1	G	3	ARG	2.3
1	G	210	PRO	2.3
1	G	212	GLY	2.3
1	C	45	GLN	2.3
1	G	106	ARG	2.3
1	G	45	GLN	2.3
1	H	132	VAL	2.2
1	C	48	ALA	2.2
1	C	88	SER	2.2
1	A	208	ALA	2.2
1	H	39	SER	2.2
1	H	119	VAL	2.2
1	B	76	GLU	2.2
1	E	51	GLY	2.2
1	F	51	GLY	2.2
1	B	133	ILE	2.1
1	H	106	ARG	2.1
1	E	65	GLU	2.1
1	A	185	THR	2.1
1	C	206	ALA	2.1
1	F	2	TYR	2.1
1	B	41	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	89	GLY	2.1
1	B	106	ARG	2.1
1	E	45	GLN	2.1
1	G	4	LEU	2.0
1	H	133	ILE	2.0
1	C	41	LYS	2.0
1	B	184	ASP	2.0
1	F	65	GLU	2.0
1	F	85	PHE	2.0
1	B	88	SER	2.0
1	G	76	GLU	2.0
1	F	133	ILE	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.