



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2026 – 03:16 PM JST

PDB ID : 25MN / pdb_000025mn
Title : Lysine racemase TM1597
Authors : Nitta, S.; Miyamoto, T.; Fushinobu, S.
Deposited on : 2026-04-09
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.2
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.2
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

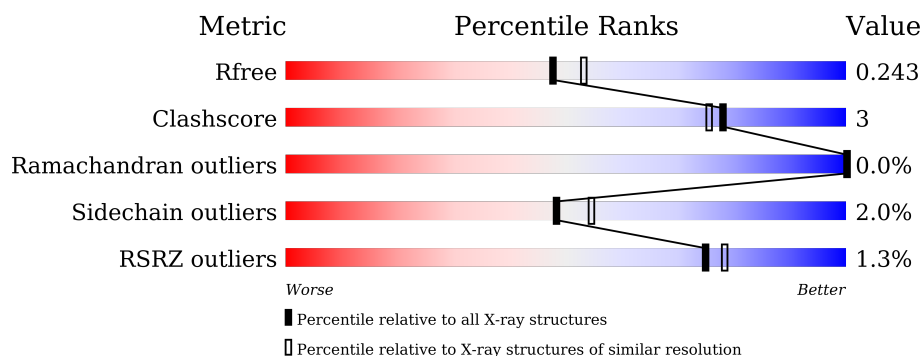
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	364	% 84% 11% ..
1	B	364	% 84% 12% ..
1	C	364	83% 12% ..
1	D	364	2% 85% 11% ..
1	E	364	2% 82% 12% • 5%
1	F	364	% 81% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17190 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 Lysine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	P	S	0	0	0
			2794	1776	485	518	1	14			
1	C	351	Total	C	N	O	P	S	0	0	0
			2780	1767	483	515	1	14			
1	F	349	Total	C	N	O	P	S	0	0	0
			2770	1762	481	513	1	13			
1	D	353	Total	C	N	O	P	S	0	0	0
			2794	1776	485	518	1	14			
1	E	344	Total	C	N	O	P	S	0	0	0
			2723	1730	472	506	1	14			
1	B	353	Total	C	N	O	P	S	0	0	0
			2794	1776	485	518	1	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	LEU	-	expression tag	UNP Q9X1T3
A	356	GLU	-	expression tag	UNP Q9X1T3
A	357	HIS	-	expression tag	UNP Q9X1T3
A	358	HIS	-	expression tag	UNP Q9X1T3
A	359	HIS	-	expression tag	UNP Q9X1T3
A	360	HIS	-	expression tag	UNP Q9X1T3
A	361	HIS	-	expression tag	UNP Q9X1T3
A	362	HIS	-	expression tag	UNP Q9X1T3
A	363	HIS	-	expression tag	UNP Q9X1T3
A	364	HIS	-	expression tag	UNP Q9X1T3
C	355	LEU	-	expression tag	UNP Q9X1T3
C	356	GLU	-	expression tag	UNP Q9X1T3
C	357	HIS	-	expression tag	UNP Q9X1T3
C	358	HIS	-	expression tag	UNP Q9X1T3
C	359	HIS	-	expression tag	UNP Q9X1T3
C	360	HIS	-	expression tag	UNP Q9X1T3
C	361	HIS	-	expression tag	UNP Q9X1T3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	362	HIS	-	expression tag	UNP Q9X1T3
C	363	HIS	-	expression tag	UNP Q9X1T3
C	364	HIS	-	expression tag	UNP Q9X1T3
F	355	LEU	-	expression tag	UNP Q9X1T3
F	356	GLU	-	expression tag	UNP Q9X1T3
F	357	HIS	-	expression tag	UNP Q9X1T3
F	358	HIS	-	expression tag	UNP Q9X1T3
F	359	HIS	-	expression tag	UNP Q9X1T3
F	360	HIS	-	expression tag	UNP Q9X1T3
F	361	HIS	-	expression tag	UNP Q9X1T3
F	362	HIS	-	expression tag	UNP Q9X1T3
F	363	HIS	-	expression tag	UNP Q9X1T3
F	364	HIS	-	expression tag	UNP Q9X1T3
D	355	LEU	-	expression tag	UNP Q9X1T3
D	356	GLU	-	expression tag	UNP Q9X1T3
D	357	HIS	-	expression tag	UNP Q9X1T3
D	358	HIS	-	expression tag	UNP Q9X1T3
D	359	HIS	-	expression tag	UNP Q9X1T3
D	360	HIS	-	expression tag	UNP Q9X1T3
D	361	HIS	-	expression tag	UNP Q9X1T3
D	362	HIS	-	expression tag	UNP Q9X1T3
D	363	HIS	-	expression tag	UNP Q9X1T3
D	364	HIS	-	expression tag	UNP Q9X1T3
E	355	LEU	-	expression tag	UNP Q9X1T3
E	356	GLU	-	expression tag	UNP Q9X1T3
E	357	HIS	-	expression tag	UNP Q9X1T3
E	358	HIS	-	expression tag	UNP Q9X1T3
E	359	HIS	-	expression tag	UNP Q9X1T3
E	360	HIS	-	expression tag	UNP Q9X1T3
E	361	HIS	-	expression tag	UNP Q9X1T3
E	362	HIS	-	expression tag	UNP Q9X1T3
E	363	HIS	-	expression tag	UNP Q9X1T3
E	364	HIS	-	expression tag	UNP Q9X1T3
B	355	LEU	-	expression tag	UNP Q9X1T3
B	356	GLU	-	expression tag	UNP Q9X1T3
B	357	HIS	-	expression tag	UNP Q9X1T3
B	358	HIS	-	expression tag	UNP Q9X1T3
B	359	HIS	-	expression tag	UNP Q9X1T3
B	360	HIS	-	expression tag	UNP Q9X1T3
B	361	HIS	-	expression tag	UNP Q9X1T3
B	362	HIS	-	expression tag	UNP Q9X1T3
B	363	HIS	-	expression tag	UNP Q9X1T3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	364	HIS	-	expression tag	UNP Q9X1T3

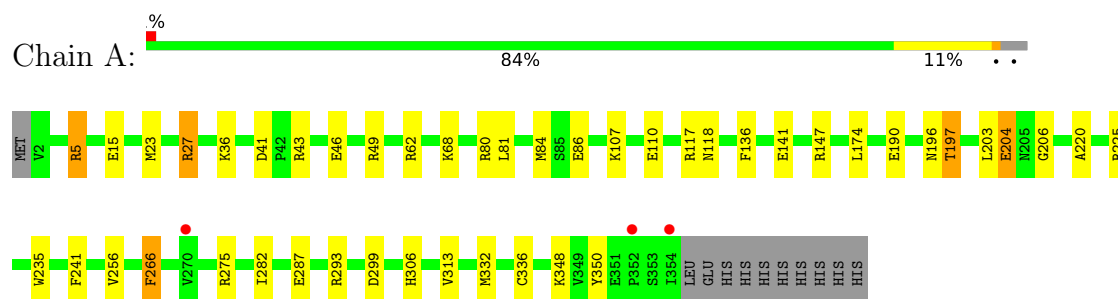
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total 106	O 106	0	0
2	C	93	Total 93	O 93	0	0
2	F	51	Total 51	O 51	0	0
2	D	105	Total 105	O 105	0	0
2	E	68	Total 68	O 68	0	0
2	B	112	Total 112	O 112	0	0

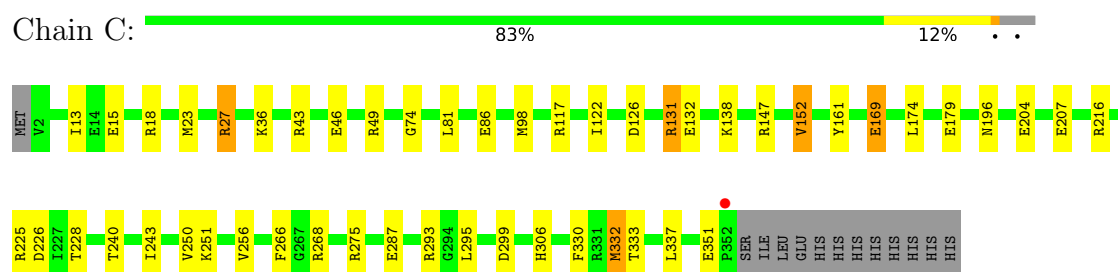
3 Residue-property plots [i](#)

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

• Molecule 1: Lysine racemase



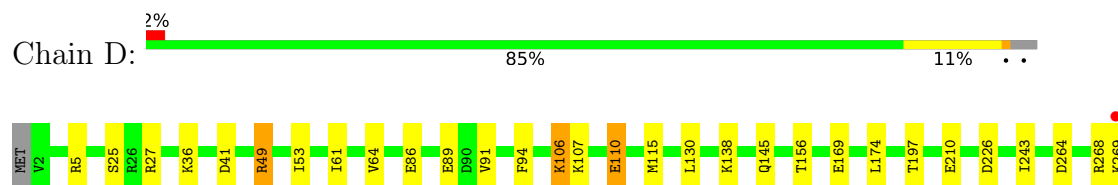
• Molecule 1: Lysine racemase



• Molecule 1: Lysine racemase

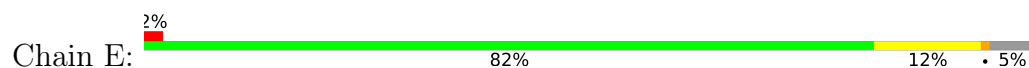


• Molecule 1: Lysine racemase

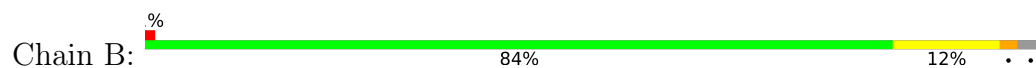




- Molecule 1: Lysine racemase



- Molecule 1: Lysine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.91Å 138.47Å 174.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.15 48.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.92-2.15) 100.0 (48.92-2.15)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.177 , 0.240 0.186 , 0.243	Depositor DCC
R_{free} test set	5917 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.0	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	0.96	EDS
Total number of atoms	17190	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 4.20% 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

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	1.01	1/2810 (0.0%)	1.48	23/3782 (0.6%)
1	B	1.08	2/2810 (0.1%)	1.47	15/3782 (0.4%)
1	C	1.01	1/2796 (0.0%)	1.47	23/3763 (0.6%)
1	D	0.97	1/2810 (0.0%)	1.43	19/3782 (0.5%)
1	E	0.98	2/2737 (0.1%)	1.45	17/3683 (0.5%)
1	F	0.90	1/2785 (0.0%)	1.51	25/3747 (0.7%)
All	All	0.99	8/16748 (0.0%)	1.47	122/22539 (0.5%)

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	6
1	B	0	6
1	C	0	8
1	D	0	2
1	E	0	6
1	F	0	4
All	All	0	32

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	329	ARG	NE-CZ	6.64	1.40	1.33
1	C	27	ARG	NE-CZ	5.85	1.39	1.33
1	A	197	THR	C-O	-5.68	1.19	1.24
1	B	293	ARG	NE-CZ	5.53	1.39	1.33
1	F	329	ARG	NE-CZ	5.44	1.39	1.33
1	E	85	SER	C-O	-5.17	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	320	GLY	C-O	-5.15	1.21	1.24
1	D	347	GLU	CD-OE1	5.03	1.34	1.25

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ARG	NE-CZ-NH1	-14.33	107.17	121.50
1	A	5	ARG	NE-CZ-NH2	12.51	130.46	119.20
1	C	169	GLU	CB-CG-CD	10.34	130.18	112.60
1	F	152	VAL	N-CA-CB	-9.84	99.56	112.26
1	B	207	GLU	CB-CA-C	9.61	126.41	110.17
1	C	152	VAL	N-CA-CB	-9.54	101.72	112.21
1	A	15	GLU	CB-CA-C	8.76	125.34	110.79
1	B	141	GLU	CB-CG-CD	8.62	127.26	112.60
1	D	145	GLN	CB-CA-C	8.29	125.13	110.37
1	F	240	THR	OG1-CB-CG2	-8.05	93.20	109.30
1	B	107	LYS	CB-CA-C	8.02	123.47	110.88
1	A	107	LYS	CB-CA-C	7.94	123.97	110.79
1	A	117	ARG	CA-C-N	-7.74	112.42	122.79
1	A	117	ARG	C-N-CA	-7.74	112.42	122.79
1	F	107	LYS	CB-CA-C	7.71	123.96	110.85
1	F	141	GLU	CB-CG-CD	7.71	125.70	112.60
1	B	207	GLU	N-CA-CB	-7.65	99.05	110.61
1	E	300	LYS	CB-CA-C	7.65	123.61	109.54
1	E	264	ASP	CA-CB-CG	7.62	120.22	112.60
1	F	205	ASN	CB-CA-C	7.44	121.48	111.14
1	E	226	ASP	CA-CB-CG	7.39	119.99	112.60
1	F	3	TYR	O-C-N	-7.28	115.54	121.80
1	B	115	MET	CG-SD-CE	-7.08	85.33	100.90
1	D	86	GLU	N-CA-CB	-7.04	99.36	110.98
1	B	86	GLU	N-CA-CB	-7.00	99.88	110.73
1	F	172	GLU	CB-CG-CD	6.88	124.30	112.60
1	A	141	GLU	CB-CG-CD	6.88	124.29	112.60
1	F	207	GLU	CA-C-N	-6.85	117.94	122.60
1	F	207	GLU	C-N-CA	-6.85	117.94	122.60
1	A	204	GLU	CB-CA-C	-6.82	99.09	110.68
1	D	347	GLU	CG-CD-OE2	-6.80	102.75	118.40
1	C	306	HIS	CA-CB-CG	6.77	120.57	113.80
1	E	146	CYS	CB-CA-C	6.76	122.73	111.23
1	D	347	GLU	CG-CD-OE1	6.71	133.83	118.40
1	D	210	GLU	CB-CA-C	6.61	120.70	109.72
1	A	84	MET	CG-SD-CE	6.60	115.42	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	117	ARG	NE-CZ-NH2	6.54	125.09	119.20
1	E	329	ARG	CD-NE-CZ	6.42	133.38	124.40
1	A	299	ASP	CA-CB-CG	6.41	119.01	112.60
1	E	30	GLU	CG-CD-OE2	-6.38	103.73	118.40
1	C	13	ILE	N-CA-C	-6.33	104.58	110.53
1	D	110	GLU	CB-CA-C	6.33	120.81	110.88
1	C	86	GLU	N-CA-CB	-6.32	100.56	110.98
1	F	351	GLU	CB-CA-C	6.19	122.36	110.17
1	F	117	ARG	CA-C-N	-6.18	114.51	122.79
1	F	117	ARG	C-N-CA	-6.18	114.51	122.79
1	A	46	GLU	N-CA-CB	6.16	119.71	110.22
1	C	226	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	266	PHE	CA-CB-CG	-6.15	107.65	113.80
1	C	275	ARG	CG-CD-NE	-6.13	98.52	112.00
1	F	84	MET	CG-SD-CE	6.12	114.36	100.90
1	C	240	THR	CA-CB-OG1	-6.08	100.48	109.60
1	D	306	HIS	CA-CB-CG	6.06	119.86	113.80
1	E	2	VAL	N-CA-CB	6.02	121.73	111.50
1	A	141	GLU	N-CA-CB	6.01	119.60	110.28
1	C	126	ASP	CA-CB-CG	5.96	118.56	112.60
1	E	172	GLU	CB-CG-CD	5.95	122.72	112.60
1	C	117	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	D	41	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	138	LYS	CB-CA-C	-5.83	100.32	110.17
1	E	188	ASN	CB-CA-C	5.82	120.62	111.77
1	C	333	THR	CA-CB-OG1	-5.80	100.91	109.60
1	D	300	LYS	CB-CG-CD	5.77	124.57	111.30
1	A	86	GLU	N-CA-CB	-5.69	101.59	110.98
1	E	228	THR	CA-CB-OG1	-5.69	101.07	109.60
1	C	332	MET	CG-SD-CE	-5.66	88.44	100.90
1	F	310	ASP	CA-CB-CG	5.66	118.25	112.60
1	F	161	TYR	CB-CA-C	5.63	120.80	110.10
1	B	107	LYS	N-CA-CB	-5.63	101.85	110.01
1	A	174	LEU	N-CA-CB	5.61	118.14	110.01
1	D	5	ARG	CG-CD-NE	-5.61	99.67	112.00
1	B	141	GLU	CG-CD-OE1	5.61	131.29	118.40
1	E	69	LYS	CB-CA-C	-5.60	101.85	110.81
1	B	18	ARG	CD-NE-CZ	5.60	132.24	124.40
1	C	131	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	C	15	GLU	CB-CG-CD	5.57	122.06	112.60
1	D	321	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	228	THR	CA-CB-OG1	-5.55	101.28	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	138	LYS	CB-CA-C	5.55	119.31	109.65
1	E	141	GLU	CB-CG-CD	5.54	122.01	112.60
1	C	27	ARG	CD-NE-CZ	5.49	132.09	124.40
1	F	98	MET	CG-SD-CE	-5.48	88.84	100.90
1	F	117	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	B	126	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	207	GLU	N-CA-CB	-5.43	102.59	110.47
1	A	62	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	107	LYS	N-CA-CB	-5.41	102.17	110.12
1	B	291	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	299	ASP	CA-CB-CG	5.40	118.00	112.60
1	D	145	GLN	N-CA-CB	-5.38	102.67	110.47
1	D	89	GLU	CB-CG-CD	5.35	121.70	112.60
1	C	74	GLY	O-C-N	-5.34	117.61	122.42
1	C	275	ARG	CB-CA-C	5.33	119.73	110.94
1	A	136	PHE	CA-CB-CG	5.32	119.12	113.80
1	F	131	ARG	CB-CG-CD	5.29	123.48	111.30
1	D	295	LEU	N-CA-CB	-5.29	101.79	110.42
1	B	5	ARG	CG-CD-NE	-5.28	100.38	112.00
1	C	256	VAL	N-CA-CB	5.26	118.58	111.21
1	D	226	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	348	LYS	CB-CG-CD	5.25	123.38	111.30
1	B	62	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	A	147	ARG	CB-CA-C	5.24	118.07	109.90
1	E	204	GLU	N-CA-CB	5.23	118.39	110.28
1	A	68	LYS	CB-CG-CD	5.23	123.32	111.30
1	A	118	ASN	CB-CA-C	5.23	119.72	111.72
1	D	299	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	174	LEU	N-CA-CB	5.20	117.61	110.07
1	F	270	VAL	N-CA-CB	5.20	116.70	110.31
1	E	351	GLU	CB-CA-C	5.19	120.39	110.17
1	D	272	PHE	CA-CB-CG	-5.17	108.63	113.80
1	F	333	THR	CA-CB-OG1	-5.17	101.85	109.60
1	C	295	LEU	N-CA-CB	-5.16	102.02	110.42
1	D	107	LYS	CB-CA-C	5.15	119.34	110.79
1	E	22	GLU	N-CA-CB	5.14	117.53	110.07
1	F	329	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	F	41	ASP	CA-CB-CG	5.11	117.70	112.60
1	A	190	GLU	CG-CD-OE1	-5.10	106.67	118.40
1	B	46	GLU	CB-CG-CD	-5.07	103.98	112.60
1	C	351	GLU	CB-CG-CD	5.06	121.21	112.60
1	E	179	GLU	N-CA-C	-5.04	105.67	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	150	ASN	CB-CA-C	5.04	118.64	111.74
1	F	92	LYS	CB-CA-C	5.01	118.82	110.81

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	ARG	Sidechain
1	A	27	ARG	Sidechain
1	A	275	ARG	Sidechain
1	A	43	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	5	ARG	Sidechain
1	B	147	ARG	Sidechain
1	B	225	ARG	Sidechain
1	B	275	ARG	Sidechain
1	B	43	ARG	Sidechain
1	B	49	ARG	Sidechain
1	B	5	ARG	Sidechain
1	C	131	ARG	Sidechain
1	C	147	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	225	ARG	Sidechain
1	C	268	ARG	Sidechain
1	C	27	ARG	Sidechain
1	C	43	ARG	Sidechain
1	C	49	ARG	Sidechain
1	D	27	ARG	Sidechain
1	D	49	ARG	Sidechain
1	E	147	ARG	Sidechain
1	E	225	ARG	Sidechain
1	E	27	ARG	Sidechain
1	E	329	ARG	Sidechain
1	E	331	ARG	Sidechain
1	E	49	ARG	Sidechain
1	F	117	ARG	Sidechain
1	F	268	ARG	Sidechain
1	F	331	ARG	Sidechain
1	F	5	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2794	0	2874	19	0
1	B	2794	0	2874	22	0
1	C	2780	0	2858	16	0
1	D	2794	0	2873	13	0
1	E	2723	0	2796	14	0
1	F	2770	0	2849	20	0
2	A	106	0	0	1	0
2	B	112	0	0	0	0
2	C	93	0	0	0	0
2	D	105	0	0	0	0
2	E	68	0	0	1	0
2	F	51	0	0	0	0
All	All	17190	0	17124	96	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 3.

All (96) 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:23:MET:HE1	1:C:204:GLU:HB3	1.64	0.79
1:B:88:VAL:HG13	1:B:115:MET:HE1	1.71	0.72
1:C:23:MET:HE1	1:C:204:GLU:CB	2.31	0.60
1:D:156:THR:HG22	1:D:174:LEU:HD11	1.85	0.59
1:A:23:MET:HE2	1:A:203:LEU:HG	1.84	0.59
1:F:27:ARG:NH2	1:F:208:ILE:O	2.35	0.59
1:B:159:GLY:HA2	1:B:163:GLY:HA2	1.83	0.59
1:B:184:ASN:HD22	1:B:184:ASN:N	2.01	0.58
1:F:332:MET:HG2	1:F:336:CYS:SG	2.43	0.58
1:C:293:ARG:HH11	1:D:268:ARG:HH21	1.51	0.58
1:B:350:TYR:O	1:B:352:PRO:HD3	2.05	0.56
1:F:341:MET:HA	1:F:348:LYS:HE3	1.87	0.56
1:A:27:ARG:HD2	1:A:203:LEU:HD11	1.89	0.55
1:D:106:LYS:HE3	1:D:110:GLU:OE2	2.07	0.55
1:A:23:MET:CE	1:A:204:GLU:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ARG:CG	1:B:27:ARG:HH11	2.22	0.53
1:C:23:MET:HE1	1:C:204:GLU:CA	2.39	0.53
1:A:197:THR:HG23	1:A:220:ALA:HB2	1.91	0.52
1:E:225:ARG:NH2	2:E:403:HOH:O	2.42	0.51
1:B:114:GLU:OE1	1:B:114:GLU:C	2.53	0.51
1:C:266:PHE:CZ	1:C:287:GLU:HG3	2.46	0.51
1:A:204:GLU:CD	1:A:235:TRP:HE1	2.19	0.51
1:B:178:LYS:HG3	1:B:189:ILE:HB	1.93	0.50
1:B:49:ARG:HD3	1:B:53:ILE:O	2.12	0.50
1:C:23:MET:CE	1:C:204:GLU:HA	2.42	0.50
1:B:332:MET:HE1	1:B:337:LEU:HD13	1.94	0.50
1:A:293:ARG:HD2	2:A:401:HOH:O	2.13	0.49
1:E:6:LEU:CD1	1:E:332:MET:HE1	2.43	0.49
1:D:332:MET:HB2	1:D:336:CYS:HB3	1.95	0.49
1:A:27:ARG:HD2	1:A:203:LEU:CD1	2.44	0.48
1:F:244:GLU:OE2	1:F:329:ARG:NE	2.46	0.48
1:F:279:LYS:HD2	1:F:316:VAL:HG23	1.96	0.48
1:E:196:ASN:HA	1:E:216:ARG:O	2.14	0.48
1:F:144:ALA:HB1	1:F:185:HIS:ND1	2.29	0.48
1:C:332:MET:HE3	1:C:332:MET:HB2	1.43	0.48
1:F:107:LYS:HD2	1:F:107:LYS:HA	1.68	0.48
1:B:196:ASN:HA	1:B:216:ARG:O	2.14	0.47
1:A:80:ARG:O	1:A:81:LEU:C	2.58	0.47
1:A:110:GLU:OE2	1:C:299:ASP:HA	2.15	0.47
1:C:332:MET:HE1	1:C:337:LEU:HD13	1.96	0.46
1:A:23:MET:HE1	1:A:204:GLU:N	2.31	0.46
1:E:243:ILE:HB	1:E:332:MET:HE1	1.98	0.46
1:F:49:ARG:HD3	1:F:53:ILE:O	2.16	0.46
1:D:106:LYS:CE	1:D:110:GLU:OE2	2.64	0.45
1:D:341:MET:HA	1:D:348:LYS:HE3	1.98	0.45
1:A:266:PHE:CZ	1:A:287:GLU:HG3	2.51	0.45
1:B:14:GLU:HB2	1:B:47:THR:HG23	1.97	0.45
1:F:161:TYR:CD2	1:E:306:HIS:HB3	2.51	0.45
1:A:196:ASN:OD1	1:A:196:ASN:N	2.50	0.45
1:A:23:MET:HE1	1:A:204:GLU:CA	2.47	0.45
1:C:161:TYR:HA	1:D:306:HIS:CE1	2.51	0.45
1:F:86:GLU:OE2	1:F:90:ASP:OD1	2.34	0.45
1:D:290:ILE:HD12	1:D:290:ILE:C	2.42	0.45
1:F:80:ARG:O	1:F:81:LEU:C	2.60	0.44
1:F:233:ILE:HG21	1:F:236:LEU:HD12	1.99	0.44
1:E:49:ARG:HD3	1:E:53:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HG12	1:A:313:VAL:HG22	1.99	0.43
1:C:23:MET:HE1	1:C:204:GLU:HA	2.00	0.43
1:F:183:LYS:C	1:F:184:ASN:OD1	2.61	0.43
1:B:9:ASN:C	1:B:9:ASN:HD22	2.25	0.43
1:B:332:MET:HE3	1:B:332:MET:HB2	1.79	0.43
1:A:332:MET:HG2	1:A:336:CYS:SG	2.58	0.43
1:A:41:ASP:OD2	1:A:350:TYR:OH	2.24	0.43
1:B:27:ARG:CG	1:B:27:ARG:NH1	2.80	0.42
1:B:164:ILE:HD13	1:B:164:ILE:HA	1.86	0.42
1:F:14:GLU:OE1	1:F:50:LYS:HD2	2.20	0.42
1:E:144:ALA:O	1:E:147:ARG:HD3	2.20	0.42
1:B:39:LEU:HD12	1:B:39:LEU:N	2.34	0.42
1:E:6:LEU:HD11	1:E:241:PHE:HB3	2.00	0.42
1:B:266:PHE:CZ	1:B:287:GLU:HG3	2.54	0.42
1:D:354:ILE:HD12	1:D:354:ILE:HA	1.94	0.42
1:F:229:ASN:O	1:F:230:ASN:C	2.63	0.42
1:C:250:VAL:O	1:C:251:LYS:HG3	2.19	0.41
1:D:243:ILE:HG22	1:D:330:PHE:HB2	2.02	0.41
1:C:196:ASN:HA	1:C:216:ARG:O	2.20	0.41
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.86	0.41
1:A:241:PHE:HB3	1:A:332:MET:HE1	2.01	0.41
1:E:197:THR:HG23	1:E:220:ALA:HB2	2.02	0.41
1:F:184:ASN:OD1	1:F:184:ASN:N	2.53	0.41
1:E:80:ARG:O	1:E:81:LEU:C	2.63	0.41
1:E:107:LYS:HE3	1:E:107:LYS:HB2	1.90	0.41
1:F:80:ARG:HD3	1:E:310:ASP:HB3	2.02	0.41
1:F:239:ASN:O	1:F:239:ASN:ND2	2.49	0.41
1:D:264:ASP:OD1	1:D:264:ASP:C	2.64	0.41
1:A:80:ARG:CZ	1:B:284:ALA:HB1	2.51	0.41
1:E:350:TYR:O	1:E:352:PRO:HD3	2.21	0.41
1:C:81:LEU:HD11	1:C:132:GLU:HB2	2.02	0.40
1:D:64:VAL:HG21	1:D:94:PHE:CE1	2.56	0.40
1:D:49:ARG:HD3	1:D:53:ILE:O	2.21	0.40
1:C:98:MET:HA	1:C:122:ILE:O	2.22	0.40
1:C:243:ILE:HG22	1:C:330:PHE:HB2	2.04	0.40
1:F:167:THR:O	1:F:168:ARG:C	2.65	0.40
1:B:27:ARG:HH11	1:B:27:ARG:HG2	1.86	0.40
1:B:243:ILE:HG22	1:B:330:PHE:HB2	2.03	0.40
1:A:306:HIS:HB3	1:B:161:TYR:CE2	2.57	0.40
1:F:306:HIS:HB3	1:E:161:TYR:CE2	2.57	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	350/364 (96%)	333 (95%)	16 (5%)	1 (0%)	36	34
1	B	350/364 (96%)	336 (96%)	14 (4%)	0	100	100
1	C	348/364 (96%)	339 (97%)	9 (3%)	0	100	100
1	D	350/364 (96%)	338 (97%)	12 (3%)	0	100	100
1	E	339/364 (93%)	323 (95%)	16 (5%)	0	100	100
1	F	344/364 (94%)	328 (95%)	16 (5%)	0	100	100
All	All	2081/2184 (95%)	1997 (96%)	83 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	GLY

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	303/314 (96%)	302 (100%)	1 (0%)	86	91
1	B	303/314 (96%)	299 (99%)	4 (1%)	61	68
1	C	301/314 (96%)	296 (98%)	5 (2%)	53	60
1	D	303/314 (96%)	293 (97%)	10 (3%)	33	34
1	E	295/314 (94%)	288 (98%)	7 (2%)	43	47
1	F	300/314 (96%)	290 (97%)	10 (3%)	33	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1805/1884 (96%)	1768 (98%)	37 (2%)	48 54

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	VAL
1	C	46	GLU
1	C	138	LYS
1	C	152	VAL
1	C	169	GLU
1	C	179	GLU
1	F	2	VAL
1	F	53	ILE
1	F	81	LEU
1	F	107	LYS
1	F	141	GLU
1	F	152	VAL
1	F	239	ASN
1	F	240	THR
1	F	279	LYS
1	F	351	GLU
1	D	25	SER
1	D	61	ILE
1	D	91	VAL
1	D	106	LYS
1	D	115	MET
1	D	130	LEU
1	D	169	GLU
1	D	197	THR
1	D	269	LYS
1	D	271	ASP
1	E	2	VAL
1	E	50	LYS
1	E	120	LYS
1	E	138	LYS
1	E	147	ARG
1	E	273	VAL
1	E	277	ILE
1	B	27	ARG
1	B	107	LYS
1	B	184	ASN
1	B	308	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	311	HIS
1	C	214	GLN
1	C	229	ASN
1	C	311	HIS
1	F	214	GLN
1	F	311	HIS
1	D	145	GLN
1	D	214	GLN
1	E	214	GLN
1	E	239	ASN
1	B	184	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	B	36	1	23,24,25	0.92	2 (8%)	25,32,34	0.94	0
1	LLP	C	36	1	23,24,25	1.04	1 (4%)	25,32,34	0.97	1 (4%)
1	LLP	F	36	1	23,24,25	1.33	2 (8%)	25,32,34	1.49	3 (12%)
1	LLP	D	36	1	23,24,25	0.74	0	25,32,34	1.07	2 (8%)
1	LLP	A	36	1	23,24,25	0.96	2 (8%)	25,32,34	1.02	0
1	LLP	E	36	1	23,24,25	1.18	1 (4%)	25,32,34	1.08	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	36	1	-	4/16/17/19	0/1/1/1
1	LLP	C	36	1	-	3/16/17/19	0/1/1/1
1	LLP	F	36	1	-	7/16/17/19	0/1/1/1
1	LLP	D	36	1	-	4/16/17/19	0/1/1/1
1	LLP	A	36	1	-	5/16/17/19	0/1/1/1
1	LLP	E	36	1	-	2/16/17/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	36	LLP	C3-C2	4.28	1.45	1.40
1	A	36	LLP	CD-CE	-2.79	1.41	1.51
1	E	36	LLP	P-OP1	2.50	1.58	1.50
1	C	36	LLP	C3-C2	2.38	1.43	1.40
1	F	36	LLP	C4-C4'	2.29	1.51	1.46
1	A	36	LLP	P-OP4	2.19	1.67	1.60
1	B	36	LLP	P-OP3	-2.11	1.46	1.54
1	B	36	LLP	C3-C2	-2.00	1.38	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	36	LLP	C3-C4-C4'	3.33	126.62	120.41
1	F	36	LLP	C5-C4-C4'	-3.15	116.37	121.56
1	F	36	LLP	OP3-P-OP4	-2.68	99.61	106.73
1	C	36	LLP	O3-C3-C2	2.55	123.05	117.49
1	D	36	LLP	CD-CG-CB	2.53	122.58	113.62
1	E	36	LLP	OP3-P-OP2	2.48	117.12	107.64
1	D	36	LLP	OP3-P-OP2	2.29	116.41	107.64
1	E	36	LLP	CD-CE-NZ	2.17	116.24	110.93

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	36	LLP	C4-C4'-NZ-CE
1	A	36	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	C	36	LLP	C4-C4'-NZ-CE
1	F	36	LLP	C4-C4'-NZ-CE
1	F	36	LLP	O-C-CA-CB
1	D	36	LLP	C4-C4'-NZ-CE
1	D	36	LLP	O-C-CA-CB
1	E	36	LLP	C4-C4'-NZ-CE
1	E	36	LLP	CG-CD-CE-NZ
1	B	36	LLP	C4-C4'-NZ-CE
1	A	36	LLP	CG-CD-CE-NZ
1	C	36	LLP	CG-CD-CE-NZ
1	F	36	LLP	CG-CD-CE-NZ
1	D	36	LLP	CG-CD-CE-NZ
1	B	36	LLP	CG-CD-CE-NZ
1	F	36	LLP	CE-CD-CG-CB
1	C	36	LLP	CE-CD-CG-CB
1	D	36	LLP	CE-CD-CG-CB
1	B	36	LLP	CE-CD-CG-CB
1	A	36	LLP	C5'-OP4-P-OP1
1	F	36	LLP	C3-C4-C4'-NZ
1	F	36	LLP	C5'-OP4-P-OP1
1	F	36	LLP	CD-CE-NZ-C4'
1	A	36	LLP	CE-CD-CG-CB
1	B	36	LLP	C4-C5-C5'-OP4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	352/364 (96%)	-0.41	3 (0%) 81 83	17, 28, 50, 89	0
1	B	352/364 (96%)	-0.41	3 (0%) 81 83	18, 28, 48, 89	0
1	C	350/364 (96%)	-0.38	1 (0%) 90 91	20, 30, 50, 93	0
1	D	352/364 (96%)	-0.32	6 (1%) 69 73	18, 30, 55, 101	0
1	E	343/364 (94%)	-0.22	9 (2%) 57 61	19, 32, 56, 118	0
1	F	348/364 (95%)	0.16	5 (1%) 73 77	23, 40, 64, 94	0
All	All	2097/2184 (96%)	-0.26	27 (1%) 75 78	17, 31, 57, 118	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	263	LEU	6.0
1	A	354	ILE	5.2
1	D	354	ILE	5.2
1	F	352	PRO	4.7
1	D	352	PRO	4.5
1	F	161	TYR	4.4
1	B	354	ILE	4.4
1	B	352	PRO	4.3
1	C	352	PRO	4.3
1	E	273	VAL	4.0
1	E	352	PRO	3.9
1	E	272	PHE	3.7
1	B	353	SER	3.7
1	F	2	VAL	3.5
1	E	2	VAL	3.4
1	D	270	VAL	3.3
1	A	352	PRO	3.2
1	D	353	SER	3.1
1	D	269	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	262	GLY	2.9
1	A	270	VAL	2.4
1	E	147	ARG	2.3
1	F	162	GLY	2.2
1	E	300	LYS	2.2
1	D	272	PHE	2.1
1	F	201	TYR	2.0
1	E	148	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	F	36	24/25	0.96	0.09	26,38,46,49	0
1	LLP	C	36	24/25	0.97	0.07	18,25,35,40	0
1	LLP	A	36	24/25	0.97	0.06	18,26,31,40	0
1	LLP	D	36	24/25	0.97	0.06	19,24,31,36	0
1	LLP	E	36	24/25	0.97	0.07	19,27,34,36	0
1	LLP	B	36	24/25	0.98	0.05	14,21,27,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.