



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:48 PM UTC

PDB ID : 4LUY / pdb_00004luy
Title : Crystal structure of CdALR mutant K 271 T
Authors : Asojo, O.A.
Deposited on : 2013-07-25
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

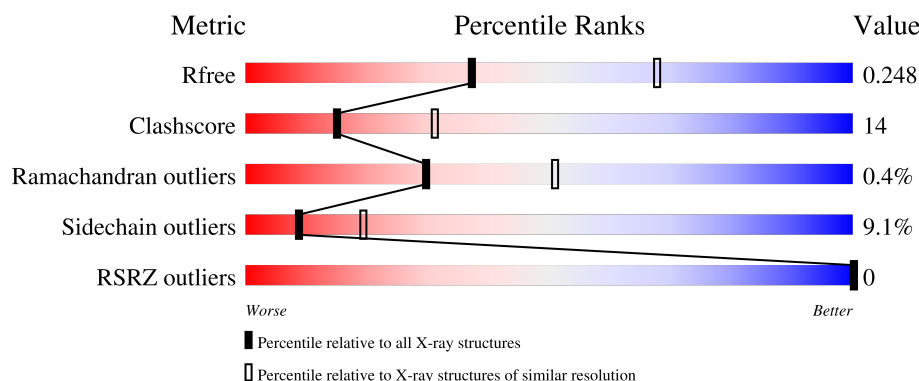
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

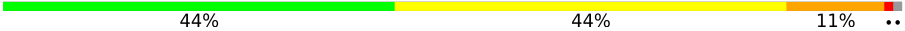
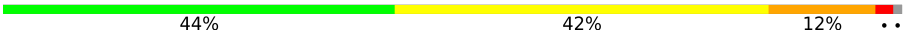
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	385	 44% 44% 11% ..
1	B	385	 44% 42% 12% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	LLP	B	39	-	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6158 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 Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	P	S	0	0	0
			3036	1927	505	587	1	16			
1	B	383	Total	C	N	O	P	S	0	0	0
			3036	1927	505	587	1	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	THR	LYS	engineered mutation	UNP Q180W0
B	271	THR	LYS	engineered mutation	UNP Q180W0

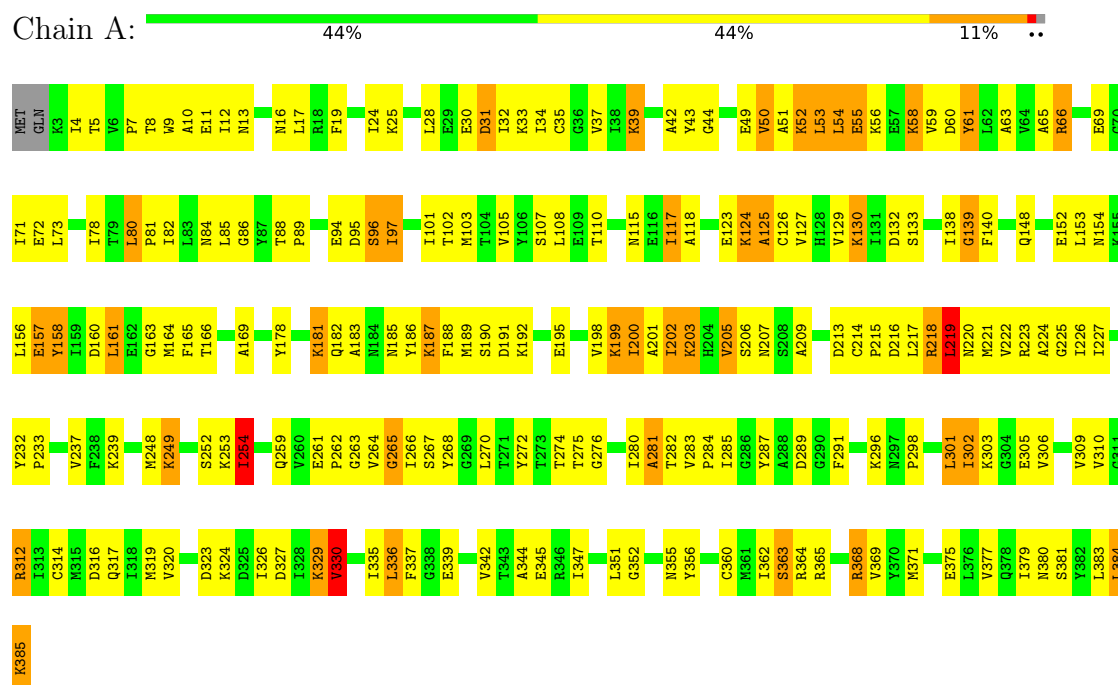
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	42	Total	O	0	0
			42	42		

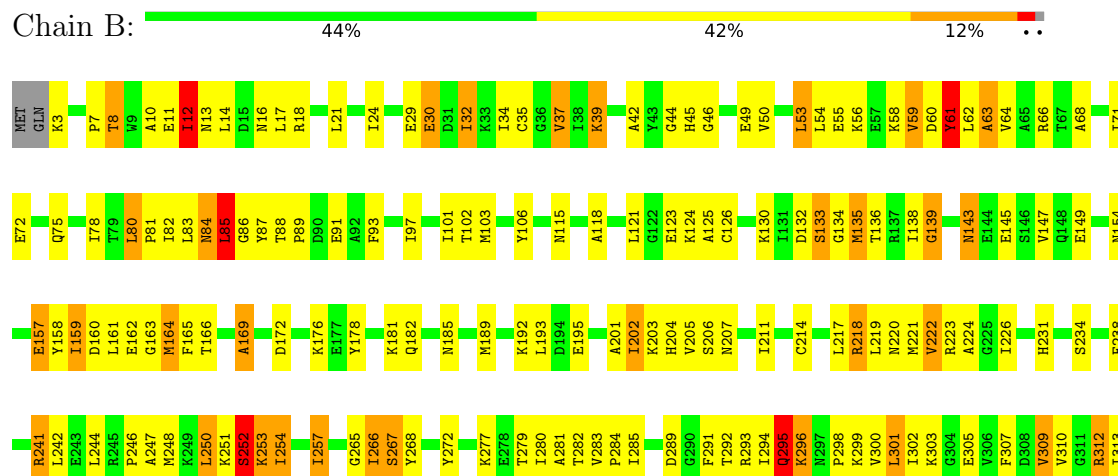
3 Residue-property plots

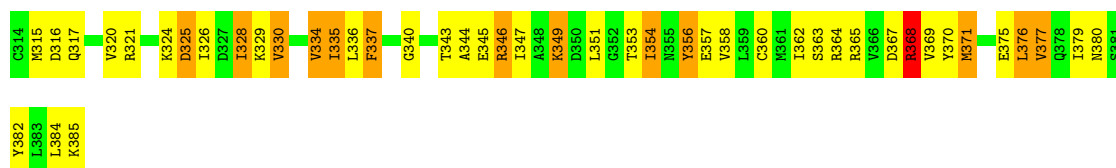
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alanine racemase



• Molecule 1: Alanine racemase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.97 Å 154.33 Å 55.77 Å 90.00° 113.63° 90.00°	Depositor
Resolution (Å)	28.83 – 2.60 28.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.83-2.60) 97.1 (28.83-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.181 , 0.252 0.182 , 0.248	Depositor DCC
R_{free} test set	1182 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6158	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: KCX, 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	2.32	124/3041 (4.1%)	1.25	24/4102 (0.6%)
1	B	2.33	121/3041 (4.0%)	1.20	20/4102 (0.5%)
All	All	2.33	245/6082 (4.0%)	1.23	44/8204 (0.5%)

All (245) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	ILE	C-O	-8.56	1.15	1.24
1	A	362	ILE	C-O	-8.42	1.15	1.24
1	B	317	GLN	C-O	-8.35	1.13	1.23
1	B	316	ASP	C-O	-7.64	1.14	1.24
1	B	35	CYS	C-O	-7.63	1.14	1.24
1	A	66	ARG	C-O	-7.43	1.14	1.23
1	B	313	ILE	C-O	-7.41	1.16	1.24
1	B	82	ILE	C-O	-7.38	1.16	1.24
1	A	356	TYR	C-O	-7.37	1.15	1.24
1	B	334	VAL	C-O	-7.35	1.16	1.24
1	A	102	THR	C-O	-7.25	1.15	1.23
1	A	54	LEU	C-O	-7.24	1.15	1.24
1	B	362	ILE	C-O	-7.23	1.17	1.24
1	B	382	TYR	C-O	-7.18	1.14	1.24
1	B	380	ASN	C-O	-7.10	1.15	1.24
1	A	37	VAL	C-O	-7.00	1.16	1.24
1	B	8	THR	C-O	-6.97	1.16	1.24
1	A	103	MET	C-O	-6.96	1.15	1.23
1	A	189	MET	C-O	-6.88	1.16	1.24
1	A	164	MET	C-O	-6.87	1.15	1.23
1	B	356	TYR	C-O	-6.84	1.16	1.24
1	A	344	ALA	C-O	-6.77	1.16	1.24
1	B	344	ALA	C-O	-6.71	1.15	1.24
1	A	84	ASN	C-O	-6.70	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	ILE	C-O	-6.68	1.16	1.24
1	B	246	PRO	C-O	-6.66	1.16	1.23
1	A	12	ILE	C-O	-6.62	1.17	1.24
1	A	345	GLU	C-O	-6.56	1.16	1.24
1	A	82	ILE	C-O	-6.55	1.17	1.24
1	A	34	ILE	C-O	-6.45	1.17	1.24
1	B	312	ARG	C-O	-6.44	1.16	1.24
1	B	335	ILE	C-O	-6.43	1.17	1.24
1	B	17	LEU	C-O	-6.41	1.16	1.24
1	B	283	VAL	C-O	-6.41	1.18	1.23
1	A	35	CYS	C-O	-6.36	1.16	1.24
1	A	335	ILE	C-O	-6.33	1.17	1.24
1	B	37	VAL	C-O	-6.32	1.16	1.23
1	A	49	GLU	C-O	-6.31	1.16	1.24
1	B	159	ILE	C-O	-6.31	1.17	1.24
1	A	380	ASN	C-O	-6.30	1.16	1.24
1	A	8	THR	C-O	-6.29	1.16	1.24
1	A	94	GLU	C-O	-6.28	1.16	1.24
1	B	291	PHE	C-O	-6.24	1.15	1.23
1	B	360	CYS	C-O	-6.23	1.16	1.24
1	B	353	THR	C-O	-6.21	1.16	1.24
1	B	42	ALA	C-O	-6.17	1.15	1.23
1	A	342	VAL	C-O	-6.15	1.17	1.24
1	B	369	VAL	C-O	-6.13	1.17	1.24
1	A	86	GLY	C-O	-6.13	1.17	1.23
1	A	302	ILE	C-O	-6.10	1.17	1.24
1	A	226	ILE	C-O	-6.10	1.17	1.24
1	A	224	ALA	C-O	-6.04	1.16	1.24
1	A	202	ILE	C-O	-6.04	1.17	1.24
1	A	227	ILE	C-O	-6.04	1.16	1.24
1	A	285	ILE	C-O	-6.04	1.17	1.23
1	A	225	GLY	C-O	-6.03	1.15	1.23
1	B	254	ILE	C-O	-6.03	1.17	1.24
1	A	187	LYS	C-O	-6.00	1.17	1.24
1	B	13	ASN	C-O	-6.00	1.16	1.24
1	A	160	ASP	C-O	-5.98	1.17	1.24
1	A	248	MET	C-O	-5.98	1.16	1.24
1	A	371	MET	C-O	-5.98	1.16	1.24
1	B	102	THR	C-O	-5.98	1.16	1.23
1	A	81	PRO	C-O	-5.97	1.17	1.23
1	B	330	VAL	C-O	-5.96	1.17	1.24
1	B	309	VAL	C-O	-5.95	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	SER	C-O	-5.94	1.15	1.23
1	B	72	GLU	C-O	-5.91	1.17	1.24
1	A	88	THR	C-O	-5.91	1.17	1.24
1	B	59	VAL	C-O	-5.90	1.16	1.24
1	A	59	VAL	C-O	-5.89	1.16	1.24
1	A	364	ARG	C-O	-5.89	1.17	1.24
1	A	16	ASN	C-O	-5.89	1.17	1.24
1	B	101	ILE	C-O	-5.88	1.17	1.24
1	A	203	LYS	C-O	-5.87	1.17	1.24
1	A	347	ILE	C-O	-5.86	1.17	1.24
1	A	43	TYR	C-O	-5.85	1.16	1.23
1	A	117	ILE	C-O	-5.84	1.17	1.24
1	B	34	ILE	C-O	-5.84	1.17	1.24
1	B	75	GLN	C-O	-5.83	1.16	1.24
1	B	328	ILE	C-O	-5.83	1.18	1.24
1	B	81	PRO	C-O	-5.83	1.17	1.23
1	A	126	CYS	C-O	-5.81	1.17	1.24
1	A	17	LEU	C-O	-5.79	1.17	1.24
1	B	12	ILE	C-O	-5.79	1.17	1.24
1	A	89	PRO	C-O	-5.76	1.17	1.23
1	A	138	ILE	C-O	-5.76	1.17	1.23
1	A	249	LYS	C-O	-5.75	1.17	1.24
1	B	71	ILE	C-O	-5.75	1.17	1.24
1	B	295	GLN	N-CA	-5.74	1.39	1.46
1	B	301	LEU	C-O	-5.74	1.17	1.24
1	B	337	PHE	C-O	-5.74	1.17	1.23
1	A	13	ASN	C-O	-5.73	1.17	1.24
1	B	46	GLY	C-O	-5.73	1.16	1.23
1	A	291	PHE	C-O	-5.72	1.16	1.23
1	B	50	VAL	C-O	-5.72	1.17	1.24
1	B	293	ARG	C-O	-5.71	1.16	1.24
1	B	53	LEU	C-O	-5.70	1.17	1.24
1	B	223	ARG	C-O	-5.66	1.17	1.24
1	A	223	ARG	C-O	-5.65	1.17	1.24
1	B	226	ILE	C-O	-5.65	1.17	1.24
1	A	207	ASN	C-O	-5.65	1.16	1.24
1	A	51	ALA	C-O	-5.65	1.17	1.24
1	B	93	PHE	C-O	-5.64	1.17	1.24
1	B	61	TYR	C-O	-5.64	1.17	1.23
1	A	259	GLN	CA-C	-5.63	1.46	1.52
1	A	305	GLU	C-O	-5.63	1.17	1.24
1	A	368	ARG	C-O	-5.63	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	VAL	C-O	-5.63	1.17	1.23
1	B	125	ALA	C-O	-5.63	1.17	1.24
1	B	207	ASN	C-O	-5.59	1.17	1.23
1	A	220	ASN	C-O	-5.59	1.17	1.24
1	A	97	ILE	C-O	-5.59	1.17	1.24
1	A	139	GLY	C-O	-5.59	1.16	1.23
1	B	367	ASP	C-O	-5.59	1.17	1.23
1	A	9	TRP	C-O	-5.58	1.17	1.23
1	A	24	ILE	C-O	-5.58	1.17	1.24
1	B	252	SER	C-O	-5.58	1.17	1.23
1	B	78	ILE	C-O	-5.57	1.17	1.24
1	B	44	GLY	C-O	-5.57	1.16	1.24
1	B	300	VAL	C-O	-5.56	1.17	1.23
1	B	358	VAL	C-O	-5.56	1.17	1.24
1	B	66	ARG	C-O	-5.56	1.17	1.23
1	B	370	TYR	C-O	-5.56	1.17	1.24
1	A	365	ARG	C-O	-5.55	1.16	1.24
1	B	202	ILE	C-O	-5.55	1.18	1.24
1	B	126	CYS	C-O	-5.54	1.17	1.24
1	B	347	ILE	C-O	-5.53	1.17	1.24
1	A	10	ALA	C-O	-5.53	1.17	1.24
1	A	125	ALA	C-O	-5.53	1.17	1.24
1	A	282	THR	C-O	-5.51	1.17	1.24
1	A	11	GLU	C-O	-5.51	1.17	1.24
1	B	103	MET	C-O	-5.51	1.17	1.23
1	A	384	LEU	C-O	-5.50	1.16	1.23
1	B	16	ASN	C-O	-5.50	1.17	1.24
1	B	343	THR	C-O	-5.50	1.16	1.23
1	A	63	ALA	C-O	-5.50	1.17	1.24
1	B	64	VAL	C-O	-5.50	1.17	1.23
1	B	163	GLY	C-O	-5.50	1.17	1.24
1	B	222	VAL	C-O	-5.50	1.17	1.23
1	B	88	THR	C-O	-5.49	1.20	1.25
1	A	53	LEU	C-O	-5.48	1.17	1.24
1	B	267	SER	C-O	-5.48	1.17	1.24
1	B	315	MET	C-O	-5.47	1.17	1.24
1	B	320	VAL	C-O	-5.47	1.18	1.24
1	A	233	PRO	C-O	-5.46	1.17	1.24
1	B	247	ALA	C-O	-5.46	1.16	1.24
1	B	162	GLU	C-O	-5.46	1.17	1.24
1	B	49	GLU	C-O	-5.45	1.17	1.24
1	B	376	LEU	C-O	-5.45	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	GLU	C-O	-5.45	1.17	1.24
1	A	50	VAL	C-O	-5.44	1.17	1.24
1	A	281	ALA	C-O	-5.43	1.17	1.23
1	B	253	LYS	C-O	-5.43	1.17	1.23
1	B	205	VAL	C-O	-5.43	1.17	1.24
1	A	381	SER	C-O	-5.42	1.17	1.24
1	B	124	LYS	C-O	-5.42	1.17	1.24
1	A	95	ASP	C-O	-5.42	1.17	1.24
1	B	224	ALA	C-O	-5.42	1.17	1.24
1	B	349	LYS	C-O	-5.42	1.17	1.24
1	A	105	VAL	C-O	-5.41	1.18	1.24
1	A	71	ILE	C-O	-5.40	1.17	1.24
1	A	72	GLU	C-O	-5.40	1.17	1.24
1	A	73	LEU	C-O	-5.40	1.17	1.24
1	A	78	ILE	C-O	-5.38	1.18	1.24
1	B	321	ARG	C-O	-5.38	1.17	1.24
1	A	364	ARG	CZ-NH2	-5.36	1.26	1.33
1	A	5	THR	C-O	-5.35	1.17	1.24
1	B	63	ALA	C-O	-5.34	1.17	1.24
1	A	209	ALA	C-O	-5.34	1.17	1.24
1	A	183	ALA	C-O	-5.34	1.17	1.24
1	A	383	LEU	C-O	-5.34	1.17	1.24
1	B	368	ARG	C-O	-5.32	1.17	1.24
1	A	310	VAL	C-O	-5.32	1.18	1.24
1	A	52	LYS	N-CA	-5.31	1.40	1.46
1	A	280	ILE	C-O	-5.30	1.18	1.24
1	B	164	MET	C-O	-5.30	1.17	1.23
1	B	91	GLU	C-O	-5.30	1.17	1.24
1	B	282	THR	C-O	-5.30	1.17	1.24
1	B	354	ILE	C-O	-5.29	1.17	1.23
1	B	364	ARG	CZ-NH2	-5.29	1.26	1.33
1	B	251	LYS	C-O	-5.28	1.17	1.23
1	A	52	LYS	CA-C	-5.28	1.46	1.52
1	A	355	ASN	C-O	-5.27	1.17	1.24
1	B	203	LYS	C-O	-5.27	1.17	1.24
1	B	11	GLU	C-O	-5.26	1.17	1.24
1	B	346	ARG	C-O	-5.26	1.18	1.24
1	B	364	ARG	C-O	-5.26	1.17	1.24
1	B	66	ARG	CZ-NH2	-5.26	1.26	1.33
1	A	55	GLU	C-O	-5.25	1.18	1.24
1	A	7	PRO	C-O	-5.24	1.18	1.24
1	A	283	VAL	C-O	-5.24	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	LEU	C-O	-5.23	1.17	1.24
1	A	198	VAL	C-O	-5.23	1.18	1.24
1	B	62	LEU	C-O	-5.22	1.17	1.24
1	A	88	THR	CA-C	-5.21	1.47	1.52
1	B	7	PRO	C-O	-5.21	1.18	1.24
1	B	14	LEU	C-O	-5.21	1.18	1.24
1	A	96	SER	C-O	-5.20	1.18	1.24
1	A	330	VAL	C-O	-5.20	1.18	1.24
1	A	181	LYS	C-O	-5.19	1.18	1.24
1	A	205	VAL	C-O	-5.18	1.18	1.24
1	B	292	THR	C-O	-5.18	1.17	1.23
1	B	307	PHE	C-O	-5.18	1.17	1.23
1	B	85	LEU	C-O	-5.18	1.17	1.24
1	B	97	ILE	C-O	-5.17	1.18	1.24
1	A	320	VAL	C-O	-5.15	1.18	1.24
1	A	108	LEU	C-O	-5.15	1.18	1.24
1	B	248	MET	C-O	-5.14	1.17	1.24
1	A	52	LYS	C-O	-5.14	1.18	1.24
1	A	285	ILE	N-CA	-5.14	1.40	1.46
1	B	160	ASP	C-O	-5.13	1.18	1.24
1	A	329	LYS	C-O	-5.12	1.17	1.23
1	A	42	ALA	C-O	-5.11	1.17	1.23
1	B	310	VAL	C-O	-5.11	1.18	1.24
1	B	377	VAL	C-O	-5.10	1.19	1.24
1	A	69	GLU	C-O	-5.10	1.18	1.24
1	A	19	PHE	N-CA	-5.09	1.40	1.46
1	B	10	ALA	C-O	-5.09	1.18	1.24
1	A	133	SER	C-O	-5.09	1.17	1.24
1	B	68	ALA	C-O	-5.09	1.18	1.24
1	B	45	HIS	C-O	-5.08	1.17	1.24
1	B	53	LEU	N-CA	-5.08	1.40	1.46
1	A	314	CYS	C-O	-5.08	1.17	1.23
1	A	379	ILE	C-O	-5.07	1.18	1.24
1	B	305	GLU	C-O	-5.07	1.17	1.24
1	A	252	SER	C-O	-5.07	1.17	1.24
1	A	363	SER	CA-C	-5.07	1.46	1.53
1	B	250	LEU	C-O	-5.07	1.17	1.24
1	B	340	GLY	C-O	-5.07	1.17	1.24
1	B	80	LEU	C-O	-5.07	1.17	1.23
1	A	165	PHE	C-O	-5.06	1.17	1.23
1	B	281	ALA	C-O	-5.06	1.17	1.24
1	B	154	ASN	C-O	-5.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ILE	C-O	-5.06	1.18	1.24
1	A	44	GLY	C-O	-5.05	1.17	1.24
1	A	306	VAL	C-O	-5.05	1.17	1.24
1	B	18	ARG	C-O	-5.05	1.18	1.24
1	A	163	GLY	C-O	-5.05	1.17	1.24
1	A	190	SER	C-O	-5.04	1.18	1.24
1	A	148	GLN	CA-C	-5.03	1.46	1.52
1	A	352	GLY	C-O	-5.03	1.17	1.24
1	A	218	ARG	CA-C	-5.02	1.46	1.52
1	A	132	ASP	C-O	-5.02	1.17	1.24
1	A	32	ILE	C-O	-5.01	1.19	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	N-CA-CB	-12.37	93.12	111.43
1	A	158	TYR	N-CA-C	-10.28	96.60	111.30
1	A	199	LYS	N-CA-C	9.52	121.74	111.36
1	A	169	ALA	N-CA-C	9.11	121.29	111.36
1	A	60	ASP	N-CA-C	9.09	121.27	111.36
1	B	60	ASP	N-CA-C	8.18	120.28	111.36
1	A	201	ALA	N-CA-C	7.68	119.65	111.28
1	A	157	GLU	N-CA-C	7.51	120.54	111.82
1	B	139	GLY	N-CA-C	7.24	119.40	112.08
1	A	218	ARG	N-CA-C	-7.17	100.39	110.50
1	A	336	LEU	N-CA-C	6.90	118.59	111.14
1	B	295	GLN	N-CA-C	6.72	118.30	110.97
1	A	380	ASN	N-CA-C	6.46	118.93	108.41
1	A	58	LYS	N-CA-C	6.05	119.73	111.39
1	B	202	ILE	N-CA-C	5.97	116.47	107.75
1	A	330	VAL	N-CA-C	-5.92	101.11	109.63
1	B	384	LEU	N-CA-C	5.84	118.92	109.40
1	A	86	GLY	N-CA-C	5.80	122.76	112.55
1	B	169	ALA	N-CA-C	5.78	117.66	111.36
1	A	324	LYS	N-CA-C	-5.73	102.97	110.53
1	B	324	LYS	N-CA-C	-5.71	103.16	110.53
1	B	58	LYS	N-CA-C	5.70	119.43	111.74
1	A	219	LEU	N-CA-C	-5.67	98.72	110.80
1	A	200	ILE	N-CA-C	5.67	121.13	109.34
1	B	192	LYS	N-CA-C	5.65	117.25	111.14
1	B	244	LEU	N-CA-C	5.52	118.46	109.24
1	B	134	GLY	N-CA-C	5.46	122.65	114.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	N-CA-C	5.45	117.30	111.36
1	B	201	ALA	N-CA-C	5.40	117.17	111.28
1	B	220	ASN	N-CA-C	5.38	117.14	111.28
1	A	287	TYR	N-CA-C	5.31	117.98	111.82
1	A	360	CYS	N-CA-C	5.27	117.93	111.82
1	B	162	GLU	N-CA-C	5.26	117.09	111.36
1	B	376	LEU	N-CA-C	-5.25	101.22	109.25
1	B	218	ARG	N-CA-C	5.25	116.85	111.03
1	B	266	ILE	N-CA-C	5.21	115.41	108.11
1	B	292	THR	N-CA-C	5.21	117.78	110.23
1	B	280	ILE	N-CA-C	5.21	115.35	107.75
1	A	44	GLY	N-CA-C	5.17	121.93	115.21
1	A	206	SER	N-CA-C	5.14	118.32	110.20
1	A	265	GLY	N-CA-C	5.13	118.52	111.54
1	A	317	GLN	N-CA-C	5.08	117.10	109.23
1	B	49	GLU	N-CA-C	5.08	116.89	111.36
1	A	356	TYR	CA-CB-CG	5.05	122.98	113.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3036	0	3083	84	0
1	B	3036	0	3083	86	0
2	A	44	0	0	2	0
2	B	42	0	0	2	0
All	All	6158	0	6166	168	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 14.

All (168) 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:115:ASN:ND2	1:B:157:GLU:O	1.83	1.10
1:A:264:VAL:H	1:A:274:THR:HG22	1.18	1.08
1:B:295:GLN:O	1:B:296:LYS:HB2	1.49	1.06
1:A:52:LYS:O	1:A:56:LYS:HD2	1.65	0.96
1:A:261:GLU:O	1:A:274:THR:HG21	1.65	0.95
1:A:52:LYS:O	1:A:56:LYS:CD	2.19	0.89
1:B:149:GLU:OE1	2:B:422:HOH:O	1.88	0.88
1:A:214:CYS:HB3	1:A:217:LEU:HD12	1.56	0.86
1:B:133:SER:HG	1:B:166:THR:HG1	1.22	0.80
1:A:214:CYS:HB3	1:A:217:LEU:CD1	2.12	0.78
1:B:118:ALA:HB1	1:B:123:GLU:O	1.84	0.77
1:A:195:GLU:OE2	2:A:529:HOH:O	2.04	0.75
1:A:202:ILE:HG21	1:A:221:MET:HE3	1.68	0.75
1:A:53:LEU:C	1:A:53:LEU:HD23	2.14	0.72
1:B:214:CYS:HB3	1:B:217:LEU:HD12	1.70	0.72
1:A:298:PRO:HB2	1:A:309:VAL:HB	1.71	0.72
1:A:55:GLU:HG2	1:A:80:LEU:HD22	1.72	0.72
1:A:214:CYS:CB	1:A:217:LEU:HD12	2.20	0.72
1:B:135:MET:O	1:B:136:THR:OG1	2.08	0.71
1:A:262:PRO:HA	1:A:274:THR:HG23	1.71	0.70
1:A:266:ILE:HD12	1:A:272:TYR:CD2	2.27	0.69
1:A:107:SER:OG	1:A:110:THR:HG23	1.91	0.69
1:B:211:ILE:HD11	1:B:222:VAL:HB	1.75	0.68
1:B:84:ASN:C	1:B:84:ASN:HD22	2.00	0.67
1:A:52:LYS:O	1:A:56:LYS:HD3	1.95	0.66
1:A:312:ARG:HH11	1:A:312:ARG:HG2	1.59	0.66
1:A:266:ILE:HD12	1:A:272:TYR:HD2	1.60	0.66
1:B:61:TYR:HB2	1:B:221:MET:CE	2.26	0.66
1:A:213:ASP:C	1:A:215:PRO:HD3	2.21	0.65
1:A:261:GLU:O	1:A:274:THR:CG2	2.43	0.65
1:A:53:LEU:HD23	1:A:53:LEU:O	1.97	0.65
1:B:143:ASN:OD1	1:B:145:GLU:N	2.28	0.64
1:A:264:VAL:N	1:A:274:THR:HG22	2.03	0.64
1:B:61:TYR:HB2	1:B:221:MET:HE1	1.79	0.64
1:B:61:TYR:HD2	1:B:221:MET:HE1	1.64	0.63
1:B:84:ASN:ND2	1:B:86:GLY:H	1.96	0.63
1:B:84:ASN:HD22	1:B:85:LEU:N	1.98	0.62
1:A:263:GLY:N	1:A:274:THR:O	2.26	0.62
1:A:267:SER:OG	1:A:268:TYR:N	2.29	0.62
1:B:161:LEU:O	1:B:161:LEU:HG	1.98	0.62
1:A:336:LEU:H	1:A:336:LEU:HD22	1.65	0.62
1:B:157:GLU:O	1:B:158:TYR:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD22	1:A:336:LEU:N	2.15	0.61
1:B:325:ASP:OD1	1:B:325:ASP:N	2.31	0.61
1:B:214:CYS:CB	1:B:217:LEU:HD12	2.30	0.61
1:A:267:SER:HA	1:B:135:MET:HE2	1.84	0.59
1:B:106:TYR:HB3	1:B:139:GLY:HA2	1.84	0.59
1:B:84:ASN:C	1:B:84:ASN:ND2	2.59	0.58
1:A:312:ARG:HH11	1:A:312:ARG:CG	2.17	0.58
1:A:375:GLU:O	1:A:377:VAL:HG13	2.04	0.58
1:B:61:TYR:CD2	1:B:221:MET:HE1	2.39	0.57
1:B:55:GLU:HG2	1:B:80:LEU:HG	1.86	0.57
1:B:181:LYS:O	1:B:185:ASN:ND2	2.37	0.57
1:B:325:ASP:C	1:B:326:ILE:HG23	2.29	0.57
1:B:178:TYR:O	1:B:182:GLN:HG3	2.05	0.56
1:A:213:ASP:O	1:A:215:PRO:HD3	2.05	0.56
1:B:30:GLU:H	1:B:30:GLU:CD	2.12	0.56
1:B:371:MET:HA	1:B:375:GLU:O	2.06	0.56
1:B:135:MET:C	1:B:136:THR:OG1	2.47	0.55
1:A:50:VAL:O	1:A:54:LEU:HG	2.07	0.55
1:B:295:GLN:O	1:B:296:LYS:CB	2.36	0.55
1:B:63:ALA:HB1	1:B:85:LEU:HD22	1.89	0.54
1:B:87:TYR:CE2	1:B:89:PRO:HD3	2.43	0.54
1:B:298:PRO:HG2	1:B:309:VAL:HB	1.90	0.54
1:B:337:PHE:CD1	1:B:337:PHE:C	2.85	0.54
1:A:185:ASN:O	1:A:188:PHE:HB3	2.08	0.54
1:B:115:ASN:ND2	1:B:158:TYR:HB2	2.22	0.53
1:A:249:LYS:NZ	1:A:339:GLU:OE2	2.42	0.53
1:B:165:PHE:HB3	1:B:204:HIS:CE1	2.44	0.52
1:B:32:ILE:CD1	1:B:32:ILE:N	2.73	0.52
1:B:268:TYR:O	1:B:312:ARG:HD2	2.10	0.52
1:A:203:LYS:HB3	1:A:219:LEU:HD23	1.90	0.52
1:B:250:LEU:HG	1:B:336:LEU:HD23	1.91	0.52
1:A:384:LEU:O	1:A:385:LYS:HB2	2.09	0.52
1:A:30:GLU:HA	1:A:30:GLU:OE1	2.09	0.51
1:B:164:MET:HE1	1:B:193:LEU:CD1	2.41	0.51
1:A:65:ALA:C	1:A:66:ARG:HG2	2.36	0.51
1:A:154:ASN:HB2	1:A:161:LEU:HD12	1.92	0.50
1:B:157:GLU:O	1:B:158:TYR:CB	2.57	0.50
1:A:61:TYR:CD2	1:A:221:MET:HE1	2.47	0.50
1:B:115:ASN:HD22	1:B:159:ILE:HG12	1.76	0.50
1:B:267:SER:OG	1:B:268:TYR:N	2.42	0.50
1:A:337:PHE:CD1	1:A:337:PHE:C	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:HD11	1:B:279:THR:CG2	2.42	0.50
1:A:263:GLY:N	1:A:274:THR:CG2	2.74	0.50
1:A:268:TYR:CD1	1:B:135:MET:HE1	2.47	0.49
1:B:185:ASN:HD22	1:B:185:ASN:H	1.59	0.49
1:B:253:LYS:O	1:B:284:PRO:HD2	2.12	0.49
1:B:214:CYS:HB3	1:B:217:LEU:CD1	2.42	0.49
1:A:124:LYS:HE3	1:A:157:GLU:O	2.13	0.48
1:B:325:ASP:C	1:B:326:ILE:CG2	2.85	0.48
1:A:385:LYS:HA	1:A:385:LYS:HD2	1.66	0.48
1:A:124:LYS:CE	1:A:157:GLU:O	2.61	0.48
1:A:253:LYS:O	1:A:284:PRO:HD2	2.14	0.48
1:A:53:LEU:C	1:A:53:LEU:CD2	2.85	0.48
1:A:4:ILE:HD11	1:A:369:VAL:HG11	1.96	0.47
1:B:294:ILE:HG22	1:B:294:ILE:O	2.14	0.47
1:B:143:ASN:O	1:B:147:VAL:HG23	2.15	0.47
1:B:302:ILE:HG12	1:B:334:VAL:HG22	1.96	0.47
1:A:97:ILE:HG12	1:A:125:ALA:HB2	1.97	0.47
1:A:130:KCX:HE2	1:A:166:THR:HA	1.97	0.46
1:B:132:ASP:OD2	1:B:136:THR:HA	2.15	0.46
1:A:301:LEU:C	1:A:302:ILE:HG13	2.40	0.46
1:A:39:LLP:C2	1:A:85:LEU:HD13	2.45	0.46
1:A:254:ILE:HD13	1:A:281:ALA:HB1	1.97	0.46
1:B:238:PHE:HB3	1:B:241:ARG:HG3	1.98	0.46
1:B:135:MET:HE3	1:B:169:ALA:HA	1.98	0.46
1:A:33:LYS:CB	1:A:221:MET:HG3	2.46	0.45
1:B:8:THR:HG1	1:B:252:SER:HG	1.64	0.45
1:B:32:ILE:N	1:B:32:ILE:HD12	2.31	0.45
1:A:96:SER:HB3	1:A:101:ILE:HB	1.96	0.45
1:A:263:GLY:N	1:A:274:THR:HG23	2.30	0.45
1:B:39:LLP:C2'	1:B:85:LEU:HG	2.46	0.45
1:B:266:ILE:O	1:B:267:SER:HB3	2.17	0.45
1:A:166:THR:HG22	1:A:205:VAL:HG12	1.98	0.45
1:A:192:LYS:HD3	1:A:192:LYS:HA	1.74	0.45
1:B:53:LEU:C	1:B:53:LEU:HD23	2.41	0.45
1:B:301:LEU:HB3	1:B:335:ILE:HB	1.98	0.45
1:A:214:CYS:N	1:A:215:PRO:HD3	2.28	0.45
1:A:115:ASN:OD1	1:A:158:TYR:HB2	2.16	0.45
1:A:268:TYR:O	1:A:312:ARG:HD2	2.16	0.45
1:B:303:LYS:HB2	1:B:326:ILE:HD12	2.00	0.44
1:B:37:VAL:HG11	1:B:39:LLP:HE3	2.00	0.44
1:B:21:LEU:O	1:B:24:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ARG:CG	1:A:312:ARG:NH1	2.79	0.44
1:B:135:MET:CE	1:B:169:ALA:HA	2.48	0.44
1:B:354:ILE:HD12	1:B:356:TYR:CD1	2.53	0.44
1:A:262:PRO:HG3	1:A:276:GLY:C	2.43	0.43
1:A:266:ILE:O	1:A:267:SER:HB3	2.18	0.43
1:B:164:MET:HE1	1:B:193:LEU:HD11	2.00	0.43
1:A:153:LEU:O	1:A:156:LEU:HD12	2.18	0.43
1:B:54:LEU:HD22	1:B:59:VAL:HG11	2.00	0.43
1:A:129:VAL:HG13	1:A:140:PHE:CE2	2.54	0.43
1:B:371:MET:HE2	1:B:376:LEU:HA	1.99	0.43
1:B:206:SER:HB2	1:B:222:VAL:HG12	2.00	0.42
1:A:39:LLP:C2'	1:A:85:LEU:HD13	2.49	0.42
1:B:231:HIS:HD2	1:B:345:GLU:OE2	2.01	0.42
1:A:130:KCX:HB2	1:A:139:GLY:HA2	2.01	0.42
1:B:3:LYS:HD2	1:B:3:LYS:HA	1.62	0.42
1:B:218:ARG:NH1	2:B:411:HOH:O	2.52	0.42
1:A:329:LYS:O	1:A:330:VAL:C	2.62	0.42
1:A:178:TYR:O	1:A:182:GLN:HG3	2.19	0.42
1:B:218:ARG:O	1:B:219:LEU:HB2	2.18	0.42
1:A:289:ASP:HA	1:A:363:SER:HB2	2.01	0.42
1:A:263:GLY:N	1:A:274:THR:HG22	2.34	0.42
1:A:263:GLY:H	1:A:274:THR:HG23	1.85	0.42
1:B:189:MET:HE3	1:B:189:MET:HB3	1.83	0.42
1:B:257:ILE:HD11	1:B:279:THR:HG22	2.02	0.42
1:A:187:LYS:NZ	1:A:191:ASP:OD2	2.46	0.41
1:A:186:TYR:CD1	1:A:186:TYR:C	2.97	0.41
1:A:232:TYR:CD2	1:A:239:LYS:HE2	2.55	0.41
1:A:265:GLY:HA3	1:A:270:LEU:HD22	2.02	0.41
1:B:326:ILE:HG13	1:B:328:ILE:HG23	2.01	0.41
1:A:118:ALA:HB1	1:A:123:GLU:O	2.20	0.41
1:B:12:ILE:CD1	1:B:368:ARG:HG2	2.51	0.41
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.84	0.41
1:B:265:GLY:HA2	1:B:272:TYR:O	2.21	0.41
1:B:172:ASP:HB2	1:B:234:SER:HB3	2.02	0.41
1:A:302:ILE:O	1:A:303:LYS:C	2.62	0.41
1:B:29:GLU:HB2	1:B:32:ILE:HD13	2.02	0.41
1:A:218:ARG:H	1:A:218:ARG:HG2	1.74	0.40
1:B:289:ASP:HA	1:B:363:SER:OG	2.21	0.40
1:A:262:PRO:CA	1:A:274:THR:HG23	2.47	0.40
1:B:138:ILE:HD13	1:B:138:ILE:HG21	1.85	0.40
1:A:216:ASP:OD1	1:A:216:ASP:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD12	2:A:525:HOH:O	2.21	0.40
1:B:169:ALA:H	1:B:182:GLN:HE22	1.68	0.40
1:B:254:ILE:HG22	1:B:330:VAL:HA	2.04	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	379/385 (98%)	365 (96%)	12 (3%)	2 (0%)	24	46
1	B	379/385 (98%)	369 (97%)	9 (2%)	1 (0%)	36	58
All	All	758/770 (98%)	734 (97%)	21 (3%)	3 (0%)	30	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	LYS
1	A	200	ILE
1	A	31	ASP

5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/332 (99%)	302 (92%)	28 (8%)	10	22
1	B	330/332 (99%)	298 (90%)	32 (10%)	8	17
All	All	660/664 (99%)	600 (91%)	60 (9%)	9	19

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	28	LEU
1	A	31	ASP
1	A	58	LYS
1	A	61	TYR
1	A	80	LEU
1	A	117	ILE
1	A	124	LYS
1	A	127	VAL
1	A	152	GLU
1	A	161	LEU
1	A	181	LYS
1	A	199	LYS
1	A	219	LEU
1	A	237	VAL
1	A	254	ILE
1	A	275	THR
1	A	301	LEU
1	A	312	ARG
1	A	316	ASP
1	A	319	MET
1	A	323	ASP
1	A	326	ILE
1	A	327	ASP
1	A	330	VAL
1	A	351	LEU
1	A	368	ARG
1	A	385	LYS
1	B	12	ILE
1	B	30	GLU
1	B	32	ILE
1	B	56	LYS

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Mol	Chain	Res	Type
1	B	61	TYR
1	B	84	ASN
1	B	85	LEU
1	B	121	LEU
1	B	133	SER
1	B	135	MET
1	B	143	ASN
1	B	157	GLU
1	B	176	LYS
1	B	195	GLU
1	B	202	ILE
1	B	241	ARG
1	B	242	LEU
1	B	252	SER
1	B	257	ILE
1	B	277	LYS
1	B	295	GLN
1	B	299	LYS
1	B	325	ASP
1	B	329	LYS
1	B	346	ARG
1	B	349	LYS
1	B	351	LEU
1	B	365	ARG
1	B	368	ARG
1	B	371	MET
1	B	377	VAL
1	B	385	LYS

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	45	HIS
1	A	148	GLN
1	A	154	ASN
1	A	378	GLN
1	B	84	ASN
1	B	141	GLN
1	B	182	GLN
1	B	185	ASN
1	B	231	HIS
1	B	256	HIS

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Mol	Chain	Res	Type
1	B	259	GLN
1	B	317	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	KCX	B	130	1	10,11,12	1.30	2 (20%)	6,12,14	1.66	1 (16%)
1	KCX	A	130	1	10,11,12	1.73	3 (30%)	6,12,14	1.09	1 (16%)
1	LLP	A	39	1	23,24,25	2.61	8 (34%)	25,32,34	1.63	7 (28%)
1	LLP	B	39	1	23,24,25	2.75	12 (52%)	25,32,34	2.30	8 (32%)

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	KCX	B	130	1	-	3/9/10/12	-
1	KCX	A	130	1	-	5/9/10/12	-
1	LLP	A	39	1	-	6/16/17/19	0/1/1/1
1	LLP	B	39	1	-	11/16/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	LLP	C4'-NZ	5.80	1.46	1.27
1	B	39	LLP	C4'-NZ	5.52	1.45	1.27
1	B	39	LLP	C3-C2	5.43	1.46	1.41
1	B	39	LLP	C4-C5	4.84	1.48	1.42
1	A	39	LLP	P-OP2	-4.56	1.37	1.54
1	A	39	LLP	P-OP3	-4.54	1.37	1.54
1	B	39	LLP	P-OP1	-4.17	1.37	1.50
1	A	39	LLP	P-OP1	-4.11	1.37	1.50
1	A	39	LLP	C4-C5	4.05	1.47	1.42
1	B	39	LLP	C4-C3	3.76	1.47	1.41
1	B	39	LLP	P-OP3	-3.63	1.41	1.54
1	B	39	LLP	P-OP2	-3.52	1.41	1.54
1	A	130	KCX	CX-NZ	-3.33	1.29	1.35
1	A	39	LLP	C4-C3	3.18	1.46	1.41
1	A	39	LLP	P-OP4	-3.03	1.50	1.60
1	B	130	KCX	OQ1-CX	-2.73	1.16	1.21
1	A	130	KCX	OQ1-CX	-2.55	1.17	1.21
1	B	39	LLP	C2'-C2	-2.49	1.46	1.50
1	A	39	LLP	O3-C3	-2.44	1.31	1.36
1	B	130	KCX	CX-NZ	-2.44	1.30	1.35
1	B	39	LLP	P-OP4	-2.23	1.53	1.60
1	A	130	KCX	CB-CA	-2.16	1.50	1.53
1	B	39	LLP	CA-N	-2.16	1.42	1.48
1	B	39	LLP	C6-N1	-2.12	1.30	1.34
1	B	39	LLP	C4-C4'	2.07	1.51	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	LLP	C4-C3-C2	-8.03	115.62	120.14
1	B	130	KCX	CE-NZ-CX	3.72	128.29	121.98
1	B	39	LLP	OP4-P-OP1	-3.65	96.58	106.44
1	A	39	LLP	C4-C4'-NZ	-3.30	108.81	124.04
1	A	39	LLP	C6-N1-C2	3.05	124.74	119.20
1	B	39	LLP	C4-C4'-NZ	-3.04	110.03	124.04
1	B	39	LLP	CD-CE-NZ	2.86	118.40	110.83
1	A	39	LLP	OP3-P-OP2	2.78	118.23	107.80
1	B	39	LLP	C6-N1-C2	2.64	123.98	119.20
1	B	39	LLP	OP3-P-OP2	2.63	117.66	107.80
1	B	39	LLP	OP4-C5'-C5	2.63	114.28	109.36
1	A	39	LLP	OP4-P-OP1	2.41	112.96	106.44
1	A	39	LLP	C4-C3-C2	-2.35	118.82	120.14
1	A	39	LLP	C2'-C2-N1	2.13	121.66	117.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	LLP	O3-C3-C2	2.10	121.93	117.58
1	A	39	LLP	OP2-P-OP4	-2.02	101.39	106.67
1	A	130	KCX	CD-CE-NZ	-2.02	106.52	112.20

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	39	LLP	C4-C4'-NZ-CE
1	A	130	KCX	N-CA-CB-CG
1	A	130	KCX	C-CA-CB-CG
1	B	39	LLP	C4-C4'-NZ-CE
1	B	39	LLP	C5'-OP4-P-OP2
1	B	39	LLP	C5'-OP4-P-OP3
1	B	130	KCX	N-CA-CB-CG
1	B	130	KCX	C-CA-CB-CG
1	A	39	LLP	CG-CD-CE-NZ
1	B	39	LLP	CG-CD-CE-NZ
1	A	39	LLP	C5-C4-C4'-NZ
1	A	130	KCX	CA-CB-CG-CD
1	A	39	LLP	C3-C4-C4'-NZ
1	B	39	LLP	C3-C4-C4'-NZ
1	B	39	LLP	C5'-OP4-P-OP1
1	B	39	LLP	C5-C4-C4'-NZ
1	A	130	KCX	CG-CD-CE-NZ
1	B	39	LLP	C4-C5-C5'-OP4
1	A	39	LLP	CE-CD-CG-CB
1	B	39	LLP	C-CA-CB-CG
1	A	130	KCX	CE-CD-CG-CB
1	B	130	KCX	CA-CB-CG-CD
1	A	39	LLP	CD-CE-NZ-C4'
1	B	39	LLP	C6-C5-C5'-OP4
1	B	39	LLP	CD-CE-NZ-C4'

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	130	KCX	2	0
1	A	39	LLP	2	0
1	B	39	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	381/385 (98%)	-0.47	0 100 100	26, 39, 58, 79	0
1	B	381/385 (98%)	-0.54	0 100 100	23, 39, 59, 67	0
All	All	762/770 (98%)	-0.50	0 100 100	23, 39, 59, 79	0

There are no RSRZ outliers to report.

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	KCX	B	130	12/13	0.93	0.10	42,47,57,61	0
1	KCX	A	130	12/13	0.95	0.07	29,31,42,42	0
1	LLP	B	39	24/25	0.96	0.07	30,35,38,38	0
1	LLP	A	39	24/25	0.97	0.06	29,33,37,42	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.