



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:33 AM UTC

PDB ID : 1SFT / pdb_00001sft
Title : ALANINE RACEMASE
Authors : Shaw, J.P.; Petsko, G.A.; Ringe, D.
Deposited on : 1996-09-20
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

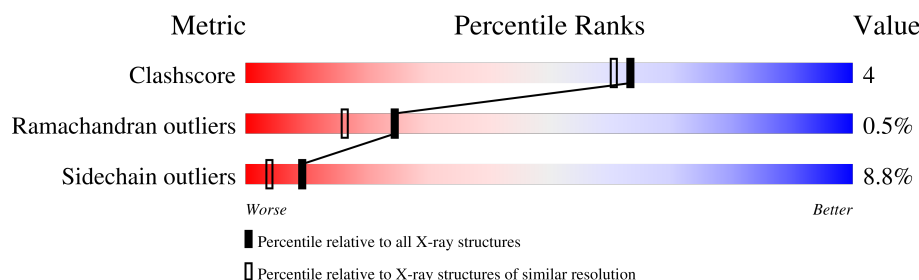
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	
1	B	388	

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
2	ACT	B	400	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6295 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.

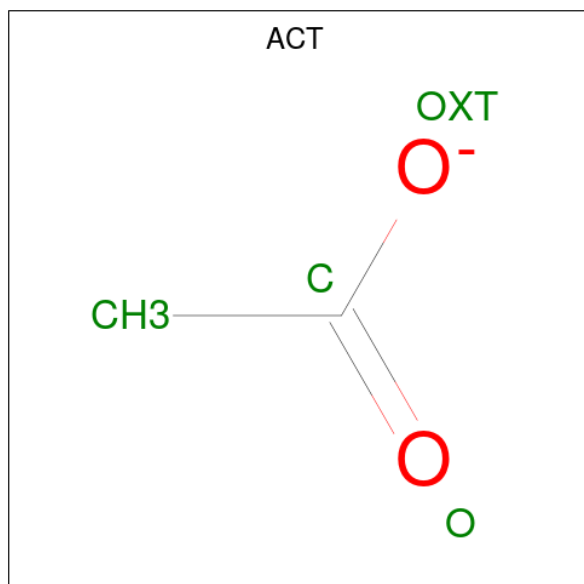
- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	P	S	0	0	0
			3045	1948	539	544	1	13			
1	B	380	Total	C	N	O	P	S	0	0	0
			3036	1943	537	542	1	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	ALA	ARG	conflict	UNP P10724
B	383	ALA	ARG	conflict	UNP P10724

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	91	Total	O	0	0
			91	91		

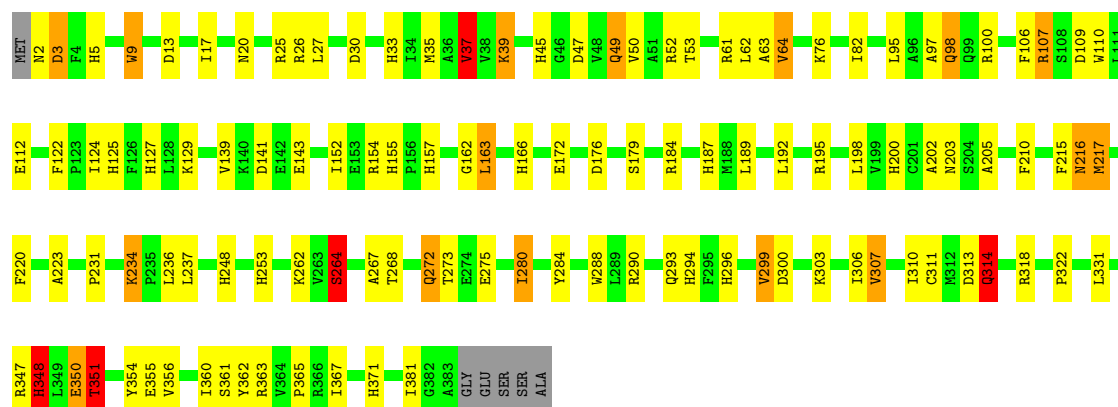
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

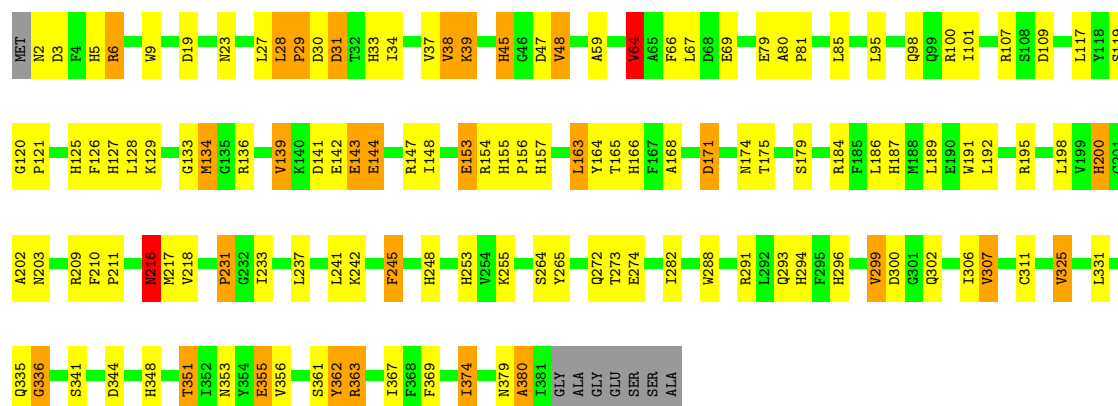
• Molecule 1: Alanine racemase

Chain A: 



• Molecule 1: Alanine racemase

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.59Å 90.13Å 85.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	83.0 (10.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.193 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6295	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	1.28	23/3098 (0.7%)	1.95	98/4211 (2.3%)
1	B	1.28	18/3089 (0.6%)	1.98	107/4199 (2.5%)
All	All	1.28	41/6187 (0.7%)	1.97	205/8410 (2.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	HIS	CD2-NE2	-7.09	1.30	1.37
1	B	294	HIS	CD2-NE2	-7.08	1.30	1.37
1	B	125	HIS	CD2-NE2	-6.92	1.30	1.37
1	B	157	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	33	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	33	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	200	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	248	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	45	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	200	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	348	HIS	CD2-NE2	-6.13	1.31	1.37
1	B	127	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	166	HIS	CD2-NE2	-6.11	1.31	1.37
1	B	155	HIS	CD2-NE2	-6.07	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	253	HIS	CD2-NE2	-6.01	1.31	1.37
1	B	5	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	371	HIS	CG-ND1	-5.96	1.31	1.38
1	A	125	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	45	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	166	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	5	HIS	CD2-NE2	-5.90	1.31	1.37
1	B	253	HIS	CD2-NE2	-5.89	1.31	1.37
1	B	296	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	296	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	187	HIS	CD2-NE2	-5.60	1.31	1.37
1	B	187	HIS	CD2-NE2	-5.56	1.31	1.37
1	A	296	HIS	CG-ND1	-5.53	1.32	1.38
1	B	81	PRO	CA-CB	-5.52	1.46	1.53
1	A	253	HIS	CG-ND1	-5.51	1.32	1.38
1	B	200	HIS	CG-ND1	-5.49	1.32	1.38
1	A	310	ILE	CA-CB	5.47	1.61	1.54
1	A	157	HIS	CD2-NE2	-5.37	1.31	1.37
1	B	9	TRP	NE1-CE2	-5.30	1.31	1.37
1	B	155	HIS	CG-ND1	-5.29	1.32	1.38
1	A	166	HIS	CG-ND1	-5.28	1.32	1.38
1	A	348	HIS	CG-ND1	-5.19	1.32	1.38
1	A	152	ILE	CA-CB	5.18	1.61	1.54
1	A	143	GLU	CA-CB	5.17	1.61	1.53
1	B	348	HIS	CD2-NE2	-5.17	1.32	1.37
1	A	163	LEU	CB-CG	-5.03	1.43	1.53

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	VAL	N-CA-CB	-11.13	96.05	111.41
1	A	64	VAL	N-CA-CB	-10.41	97.94	112.52
1	B	307	VAL	N-CA-CB	-9.99	92.73	111.21
1	B	30	ASP	CA-CB-CG	9.69	122.29	112.60
1	B	64	VAL	N-CA-CB	-9.66	99.00	112.52
1	B	203	ASN	CA-CB-CG	9.48	122.08	112.60
1	B	171	ASP	CA-CB-CG	9.29	121.89	112.60
1	B	48	VAL	CB-CA-C	-8.97	99.84	112.22
1	B	38	VAL	N-CA-CB	-8.89	96.39	111.50
1	B	216	ASN	CA-CB-CG	8.82	121.42	112.60
1	B	307	VAL	CB-CA-C	8.81	124.21	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLU	CA-CB-CG	8.79	131.67	114.10
1	B	31	ASP	CA-CB-CG	8.67	121.27	112.60
1	B	98	GLN	CA-CB-CG	8.53	131.16	114.10
1	B	200	HIS	CA-CB-CG	8.30	122.10	113.80
1	A	203	ASN	CA-CB-CG	8.22	120.82	112.60
1	A	176	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	347	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	A	361	SER	N-CA-C	8.02	121.42	110.35
1	B	109	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	3	ASP	N-CA-C	7.82	121.05	109.24
1	A	110	TRP	CG-CD2-CE3	7.61	141.51	133.90
1	A	33	HIS	CB-CG-CD2	-7.58	121.35	131.20
1	A	9	TRP	CG-CD2-CE3	7.57	141.47	133.90
1	B	47	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	37	VAL	CA-C-O	7.46	128.52	120.53
1	B	294	HIS	CA-CB-CG	-7.36	106.44	113.80
1	B	195	ARG	CA-C-N	7.35	127.95	120.38
1	B	195	ARG	C-N-CA	7.35	127.95	120.38
1	A	307	VAL	CB-CA-C	7.34	121.49	110.63
1	B	294	HIS	CB-CG-CD2	-7.33	121.67	131.20
1	B	6	ARG	CB-CG-CD	-7.25	94.61	111.30
1	A	20	ASN	OD1-CG-ND2	-7.17	115.44	122.60
1	A	210	PHE	CA-C-N	7.03	127.02	119.28
1	A	210	PHE	C-N-CA	7.03	127.02	119.28
1	B	129	LYS	CA-CB-CG	6.98	128.06	114.10
1	B	29	PRO	N-CA-C	6.92	122.08	111.15
1	A	216	ASN	CA-CB-CG	6.90	119.50	112.60
1	B	27	LEU	N-CA-CB	-6.90	98.94	110.39
1	A	268	THR	N-CA-CB	-6.88	100.03	110.01
1	B	45	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	B	242	LYS	CA-CB-CG	6.83	127.76	114.10
1	B	174	ASN	CA-CB-CG	6.79	119.39	112.60
1	B	6	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	B	380	ALA	N-CA-C	6.78	119.51	111.71
1	B	66	PHE	CA-CB-CG	6.75	120.55	113.80
1	A	49	GLN	OE1-CD-NE2	-6.75	115.85	122.60
1	B	379	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	B	154	ARG	CA-CB-CG	6.72	127.54	114.10
1	B	47	ASP	N-CA-C	6.71	118.25	111.07
1	B	191	TRP	CA-C-O	6.71	127.17	119.18
1	A	30	ASP	CA-CB-CG	6.70	119.30	112.60
1	B	153	GLU	CB-CG-CD	6.69	123.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	VAL	CB-CA-C	-6.62	101.12	110.12
1	B	288	TRP	CG-CD2-CE3	6.59	140.49	133.90
1	A	195	ARG	CA-CB-CG	6.59	127.27	114.10
1	A	202	ALA	N-CA-C	6.53	119.95	110.28
1	A	217	MET	CG-SD-CE	-6.51	86.58	100.90
1	A	125	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	B	216	ASN	N-CA-C	6.45	120.79	112.41
1	A	112	GLU	CA-CB-CG	6.44	126.97	114.10
1	B	379	ASN	CB-CG-ND2	6.43	126.05	116.40
1	A	284	TYR	N-CA-C	6.42	120.21	112.38
1	B	23	ASN	CB-CG-ND2	6.39	125.99	116.40
1	B	2	ASN	CA-CB-CG	6.36	118.96	112.60
1	A	25	ARG	CA-CB-CG	6.35	126.80	114.10
1	A	299	VAL	CB-CA-C	-6.33	101.52	110.12
1	A	112	GLU	N-CA-C	-6.32	104.31	111.14
1	B	361	SER	N-CA-C	6.32	119.07	110.35
1	B	293	GLN	O-C-N	-6.31	115.43	122.12
1	A	9	TRP	CE2-CD2-CG	-6.30	99.64	107.20
1	B	335	GLN	O-C-N	6.29	131.61	123.06
1	A	110	TRP	CB-CG-CD1	-6.25	117.53	126.90
1	A	356	VAL	CA-C-O	-6.24	111.59	119.95
1	B	101	ILE	N-CA-CB	-6.20	103.96	111.21
1	B	245	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	288	TRP	CG-CD2-CE3	6.18	140.08	133.90
1	A	141	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	64	VAL	CB-CA-C	6.15	119.93	110.82
1	A	350	GLU	CB-CG-CD	6.14	123.03	112.60
1	B	98	GLN	CB-CG-CD	-6.12	102.20	112.60
1	A	33	HIS	CB-CG-ND1	6.10	131.84	122.70
1	B	307	VAL	O-C-N	-6.07	116.95	123.14
1	B	48	VAL	N-CA-CB	6.06	119.67	110.58
1	A	268	THR	CA-CB-OG1	-6.06	100.52	109.60
1	A	290	ARG	N-CA-C	6.01	119.45	111.75
1	B	300	ASP	CA-CB-CG	5.99	118.58	112.60
1	A	288	TRP	CE2-CD2-CG	-5.98	100.03	107.20
1	A	280	ILE	CA-CB-CG2	-5.95	100.38	110.50
1	A	154	ARG	N-CA-C	5.95	117.84	111.36
1	B	6	ARG	NE-CZ-NH2	-5.93	113.86	119.20
1	A	95	LEU	N-CA-CB	-5.92	101.40	110.16
1	B	33	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	B	325	VAL	N-CA-CB	-5.88	102.25	110.13
1	A	45	HIS	CB-CG-CD2	-5.87	123.57	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	144	GLU	N-CA-C	-5.86	104.48	111.69
1	B	157	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	B	141	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	79	GLU	CB-CG-CD	5.85	122.54	112.60
1	B	19	ASP	N-CA-C	5.83	117.64	111.28
1	B	288	TRP	CE2-CD2-CG	-5.79	100.25	107.20
1	B	3	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	110	TRP	CE2-CD2-CG	-5.78	100.27	107.20
1	A	155	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	B	210	PHE	CA-C-N	5.75	125.43	119.56
1	B	210	PHE	C-N-CA	5.75	125.43	119.56
1	A	293	GLN	CA-CB-CG	5.75	125.59	114.10
1	B	294	HIS	N-CA-C	5.73	119.26	112.72
1	A	360	ILE	N-CA-C	-5.73	101.27	108.84
1	B	218	VAL	N-CA-CB	-5.73	104.12	110.99
1	A	47	ASP	N-CA-C	5.72	117.20	111.07
1	A	347	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	A	106	PHE	CA-CB-CG	5.69	119.49	113.80
1	A	314	GLN	N-CA-C	5.68	117.91	108.99
1	B	143	GLU	CB-CG-CD	5.67	122.24	112.60
1	A	76	LYS	CB-CG-CD	-5.65	98.30	111.30
1	A	354	TYR	CB-CA-C	-5.65	101.07	110.68
1	A	381	ILE	CA-CB-CG2	-5.65	100.89	110.50
1	A	27	LEU	N-CA-C	5.65	117.11	111.07
1	A	216	ASN	N-CA-C	5.63	120.88	112.94
1	B	67	LEU	N-CA-C	5.62	118.17	111.71
1	A	162	GLY	O-C-N	5.62	129.24	123.29
1	B	241	LEU	O-C-N	-5.61	116.83	123.22
1	B	306	ILE	N-CA-C	-5.61	100.24	108.54
1	B	293	GLN	CA-C-O	-5.60	114.58	120.63
1	B	195	ARG	CA-C-O	-5.59	113.95	119.49
1	A	248	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	B	100	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	A	294	HIS	CA-CB-CG	5.56	119.36	113.80
1	A	237	LEU	N-CA-C	5.55	116.65	109.65
1	B	28	LEU	CA-C-N	5.54	125.55	119.90
1	B	28	LEU	C-N-CA	5.54	125.55	119.90
1	B	174	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	45	HIS	CB-CG-ND1	5.52	130.98	122.70
1	B	165	THR	CA-CB-OG1	-5.51	101.33	109.60
1	B	179	SER	CA-CB-OG	5.50	122.11	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	GLN	CA-CB-CG	5.49	125.08	114.10
1	B	64	VAL	CB-CA-C	5.49	118.94	110.82
1	A	351	THR	CB-CA-C	-5.47	99.62	111.11
1	B	353	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	5	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	B	187	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	33	HIS	N-CA-C	5.44	117.89	110.55
1	B	38	VAL	CB-CA-C	5.43	121.72	111.40
1	B	216	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	107	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	B	336	GLY	O-C-N	5.41	129.73	122.70
1	A	187	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	B	120	GLY	O-C-N	-5.41	116.36	121.77
1	A	107	ARG	CA-CB-CG	5.39	124.88	114.10
1	A	215	PHE	CA-C-N	-5.37	114.10	122.37
1	A	215	PHE	C-N-CA	-5.37	114.10	122.37
1	A	264	SER	N-CA-C	5.36	122.22	110.80
1	B	356	VAL	CA-C-O	-5.36	112.77	119.95
1	A	272	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	B	30	ASP	CA-C-N	5.33	128.41	120.31
1	B	30	ASP	C-N-CA	5.33	128.41	120.31
1	A	53	THR	CA-C-O	5.33	126.19	120.55
1	A	33	HIS	CA-CB-CG	5.32	119.12	113.80
1	B	126	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	211	PRO	N-CA-C	5.29	120.72	113.84
1	A	237	LEU	CA-C-N	5.28	124.61	118.85
1	A	237	LEU	C-N-CA	5.28	124.61	118.85
1	B	367	ILE	N-CA-C	-5.28	100.78	108.17
1	B	98	GLN	CG-CD-NE2	5.27	124.30	116.40
1	B	218	VAL	O-C-N	-5.25	117.20	123.03
1	A	141	ASP	CB-CA-C	-5.24	98.42	109.38
1	A	195	ARG	CA-C-O	-5.23	114.39	119.51
1	B	355	GLU	CA-CB-CG	-5.22	103.66	114.10
1	B	296	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	13	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	274	GLU	CA-CB-CG	-5.20	103.70	114.10
1	B	363	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	166	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	A	35	MET	O-C-N	-5.18	116.71	122.93
1	A	365	PRO	CA-C-O	-5.17	115.57	121.56
1	B	248	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	306	ILE	N-CA-C	-5.17	102.07	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	202	ALA	N-CA-C	5.16	118.03	109.46
1	A	125	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	200	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	80	ALA	CA-C-O	-5.12	115.15	120.88
1	A	234	LYS	CA-C-N	5.12	124.73	119.56
1	A	234	LYS	C-N-CA	5.12	124.73	119.56
1	B	164	TYR	CA-CB-CG	5.11	123.09	113.90
1	B	144	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	179	SER	N-CA-C	5.09	116.91	111.36
1	B	139	VAL	CB-CA-C	5.07	119.23	111.68
1	A	294	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	142	GLU	N-CA-C	5.07	116.49	111.07
1	B	231	PRO	CA-C-N	5.05	125.55	120.00
1	B	231	PRO	C-N-CA	5.05	125.55	120.00
1	A	351	THR	CA-CB-CG2	-5.04	101.93	110.50
1	B	139	VAL	N-CA-CB	-5.04	101.58	110.95
1	A	100	ARG	N-CA-C	5.04	118.54	111.74
1	A	275	GLU	N-CA-C	5.04	117.45	109.50
1	B	264	SER	N-CA-C	5.03	121.51	110.80
1	B	129	LYS	CB-CG-CD	5.02	122.85	111.30
1	B	156	PRO	N-CA-C	5.02	120.43	113.65
1	A	157	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	A	205	ALA	N-CA-C	5.01	116.43	111.07
1	A	109	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	268	THR	CA-CB-CG2	5.00	119.01	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	TYR	Sidechain
1	B	362	TYR	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	3045	0	3026	29	0
1	B	3036	0	3019	23	0
2	A	4	0	3	0	0
2	B	4	0	3	2	0
3	A	115	0	0	3	0
3	B	91	0	0	1	0
All	All	6295	0	6051	49	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 (49) 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:351:THR:HG21	1:B:355:GLU:OE1	1.69	0.92
1:A:163:LEU:HD21	1:A:189:LEU:HD22	1.68	0.73
1:A:163:LEU:HD21	1:A:189:LEU:CD2	2.19	0.73
1:A:350:GLU:HB2	1:B:291:ARG:HH22	1.53	0.73
1:A:351:THR:HG21	1:A:355:GLU:OE1	1.95	0.65
1:B:198:LEU:HA	1:B:216:ASN:HD21	1.61	0.65
1:A:198:LEU:HA	1:A:216:ASN:HD21	1.61	0.64
1:A:129:LYS:NZ	3:A:474:HOH:O	2.36	0.59
1:B:37:VAL:HG12	1:B:39:LLP:HG3	1.87	0.57
1:B:163:LEU:HD13	1:B:192:LEU:HD11	1.87	0.55
1:A:61:ARG:HD2	1:A:217:MET:HE1	1.90	0.53
1:A:220:PHE:CE1	1:A:223:ALA:HB3	2.44	0.52
1:A:97:ALA:HB2	1:A:124:ILE:HG12	1.92	0.51
1:B:200:HIS:HB3	1:B:217:MET:HB3	1.94	0.50
1:A:129:LYS:O	1:A:139:VAL:HG22	2.12	0.49
1:A:98:GLN:HG2	1:A:122:PHE:CE2	2.48	0.49
1:A:163:LEU:CD2	1:A:189:LEU:HD22	2.40	0.48
1:A:37:VAL:HB	1:A:63:ALA:HB3	1.95	0.48
1:A:314:GLN:HG3	1:B:136:ARG:HD2	1.96	0.48
1:A:350:GLU:HB2	1:B:291:ARG:NH2	2.25	0.48
1:B:175:THR:HA	3:B:481:HOH:O	2.15	0.46
1:B:128:LEU:HD13	1:B:148:ILE:HG21	1.97	0.46
1:B:134:MET:HE2	1:B:168:ALA:HA	1.98	0.46
1:A:39:LLP:H4'1	2:B:400:ACT:H1	1.98	0.45
1:A:348:HIS:CE1	3:A:412:HOH:O	2.70	0.45
1:A:163:LEU:HD22	1:A:192:LEU:HD11	1.99	0.45
1:B:64:VAL:HG13	1:B:69:GLU:HB2	1.99	0.45
1:B:34:ILE:HB	1:B:59:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:HB3	1:A:267:ALA:HB1	2.00	0.44
1:B:39:LLP:C3	1:B:85:LEU:HD13	2.47	0.43
1:B:362:TYR:O	1:B:380:ALA:HB3	2.17	0.43
1:A:220:PHE:CZ	1:A:223:ALA:HB3	2.54	0.42
1:B:45:HIS:NE2	1:B:245:PHE:HB2	2.34	0.42
1:A:311:CYS:HB2	1:A:314:GLN:O	2.18	0.42
1:B:198:LEU:HA	1:B:216:ASN:ND2	2.32	0.42
1:B:186:LEU:HA	1:B:189:LEU:HD12	2.01	0.42
1:A:49:GLN:HG3	1:A:52:ARG:HH21	1.84	0.42
1:A:348:HIS:CE1	3:A:478:HOH:O	2.71	0.42
1:A:9:TRP:CD1	1:A:367:ILE:HD12	2.54	0.42
1:B:369:PHE:CE2	1:B:374:ILE:HG12	2.55	0.42
1:B:265:TYR:CE2	1:B:311:CYS:SG	3.13	0.42
1:B:282:ILE:HG21	1:B:331:LEU:HD21	2.02	0.42
1:A:39:LLP:C4'	2:B:400:ACT:H1	2.50	0.41
1:A:61:ARG:CD	1:A:217:MET:HE1	2.50	0.41
1:A:17:ILE:HD13	1:A:50:VAL:HG22	2.03	0.41
1:A:231:PRO:HA	1:A:234:LYS:HG3	2.03	0.40
1:B:28:LEU:HA	1:B:29:PRO:HD2	1.87	0.40
1:B:341:SER:O	1:B:344:ASP:HB2	2.20	0.40
1:A:62:LEU:O	1:A:82:ILE:HA	2.22	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	379/388 (98%)	364 (96%)	13 (3%)	2 (0%)	24	16
1	B	377/388 (97%)	365 (97%)	10 (3%)	2 (0%)	24	16
All	All	756/776 (97%)	729 (96%)	23 (3%)	4 (0%)	24	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	SER
1	B	133	GLY
1	B	336	GLY
1	A	322	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/321 (99%)	294 (93%)	23 (7%)	13	6
1	B	317/321 (99%)	284 (90%)	33 (10%)	7	2
All	All	634/642 (99%)	578 (91%)	56 (9%)	9	4

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	26	ARG
1	A	37	VAL
1	A	64	VAL
1	A	98	GLN
1	A	107	ARG
1	A	172	GLU
1	A	184	ARG
1	A	236	LEU
1	A	264	SER
1	A	272	GLN
1	A	273	THR
1	A	280	ILE
1	A	299	VAL
1	A	303	LYS
1	A	307	VAL
1	A	313	ASP
1	A	314	GLN
1	A	318	ARG

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Mol	Chain	Res	Type
1	A	331	LEU
1	A	348	HIS
1	A	351	THR
1	A	363	ARG
1	B	6	ARG
1	B	31	ASP
1	B	38	VAL
1	B	48	VAL
1	B	64	VAL
1	B	95	LEU
1	B	117	LEU
1	B	119	SER
1	B	121	PRO
1	B	134	MET
1	B	139	VAL
1	B	143	GLU
1	B	144	GLU
1	B	147	ARG
1	B	153	GLU
1	B	163	LEU
1	B	171	ASP
1	B	184	ARG
1	B	209	ARG
1	B	216	ASN
1	B	231	PRO
1	B	233	ILE
1	B	237	LEU
1	B	255	LYS
1	B	272	GLN
1	B	273	THR
1	B	299	VAL
1	B	302	GLN
1	B	307	VAL
1	B	325	VAL
1	B	351	THR
1	B	363	ARG
1	B	374	ILE

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	216	ASN

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Mol	Chain	Res	Type
1	A	253	HIS
1	A	272	GLN
1	A	293	GLN
1	B	5	HIS
1	B	23	ASN
1	B	203	ASN
1	B	216	ASN
1	B	258	GLN
1	B	296	HIS
1	B	371	HIS
1	B	379	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	39	1	23,24,25	1.45	3 (13%)	25,32,34	2.51	8 (32%)
1	LLP	A	39	1	23,24,25	2.44	8 (34%)	25,32,34	2.03	10 (40%)

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	39	1	-	2/16/17/19	0/1/1/1
1	LLP	A	39	1	-	3/16/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	LLP	C4-C4'	5.86	1.59	1.46
1	A	39	LLP	CE-NZ	-5.38	1.34	1.46
1	A	39	LLP	C3-C2	-5.19	1.35	1.41
1	B	39	LLP	C4-C4'	3.45	1.54	1.46
1	A	39	LLP	CD-CE	3.13	1.62	1.51
1	A	39	LLP	C6-C5	-3.03	1.31	1.37
1	A	39	LLP	C2-N1	2.90	1.39	1.33
1	A	39	LLP	P-OP3	-2.32	1.46	1.54
1	B	39	LLP	C2-N1	2.27	1.37	1.33
1	A	39	LLP	P-OP2	-2.16	1.46	1.54
1	B	39	LLP	CB-CA	-2.15	1.50	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	LLP	CE-NZ-C4'	-8.41	91.80	118.72
1	B	39	LLP	C4-C4'-NZ	4.93	146.81	124.04
1	A	39	LLP	CG-CD-CE	4.71	129.77	113.38
1	A	39	LLP	C4-C4'-NZ	4.19	143.38	124.04
1	B	39	LLP	CG-CD-CE	3.52	125.62	113.38
1	B	39	LLP	CD-CG-CB	-3.25	101.35	113.62
1	A	39	LLP	OP2-P-OP4	-2.73	99.56	106.67
1	A	39	LLP	CD-CE-NZ	2.68	117.93	110.83
1	A	39	LLP	C5-C6-N1	-2.48	119.80	123.83
1	A	39	LLP	C3-C2-N1	-2.41	117.91	120.96
1	B	39	LLP	OP2-P-OP4	-2.37	100.50	106.67
1	A	39	LLP	C6-N1-C2	2.32	123.40	119.20
1	B	39	LLP	OP3-P-OP2	2.31	116.48	107.80
1	B	39	LLP	C5-C6-N1	-2.30	120.09	123.83
1	A	39	LLP	C2'-C2-N1	2.27	121.92	117.64
1	A	39	LLP	CE-NZ-C4'	2.25	125.93	118.72
1	B	39	LLP	C5-C4-C4'	-2.24	118.01	121.47
1	A	39	LLP	OP3-P-OP2	2.23	116.15	107.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	39	LLP	C4-C4'-NZ-CE
1	B	39	LLP	C4-C4'-NZ-CE
1	A	39	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
1	B	39	LLP	C4-C5-C5'-OP4
1	A	39	LLP	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
2	ACT	B	400	-	3,3,3	1.04	0	3,3,3	1.17	0
2	ACT	A	401	-	3,3,3	1.06	0	3,3,3	1.73	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	401	ACT	OXT-C-CH3	2.35	124.92	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.