



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 05:44 PM EDT

PDB ID : 1SFT  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

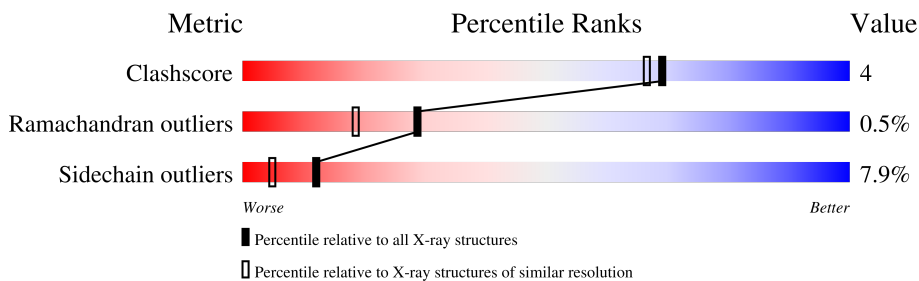
# 1 Overall quality at a glance

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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  $\geq 3$ , 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	

## 2 Entry composition [i](#)

There are 4 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.

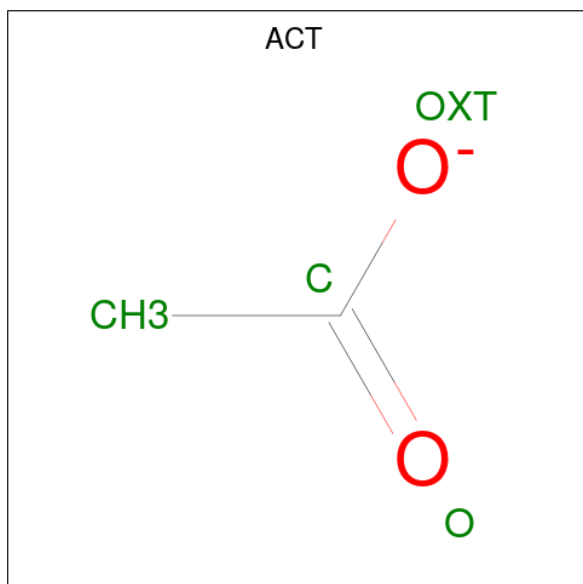
- Molecule 1 is a protein called ALANINE RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	Total 3030	C 1940	N 538	O 539	S 13	0	0	0
1	B	380	Total 3021	C 1935	N 536	O 537	S 13	0	0	0

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 (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



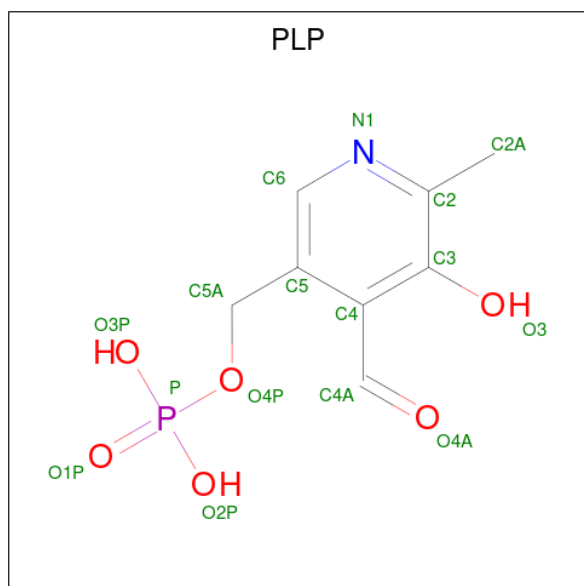
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0
3	B	1	15	8	1	5	1	0	0

- Molecule 4 is water.

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

### 3 Residue-property plots

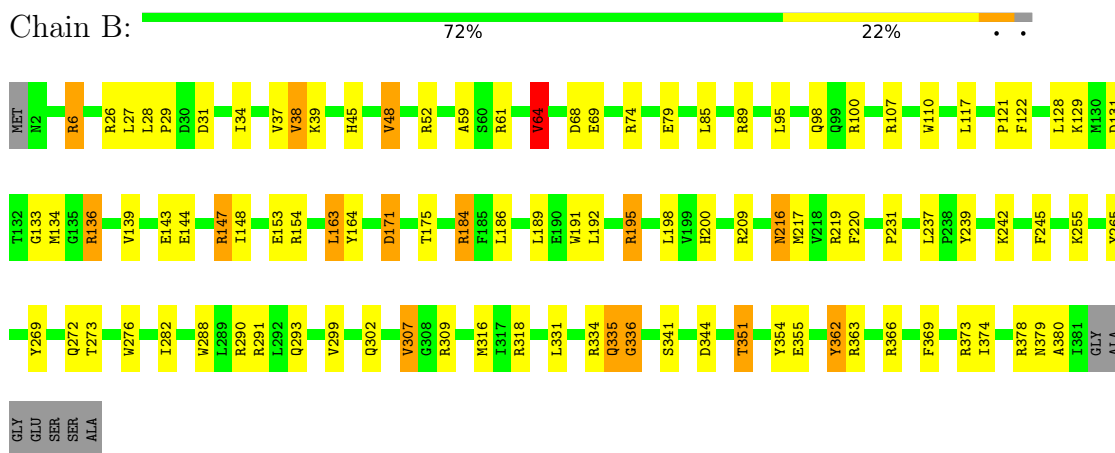
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: ALANINE RACEMASE



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	6295	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.98	1/3108 (0.0%)	1.79	86/4225 (2.0%)
1	B	0.99	0/3099	1.82	83/4213 (2.0%)
All	All	0.99	1/6207 (0.0%)	1.81	169/8438 (2.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	LYS	CE-NZ	-5.72	1.34	1.49

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ARG	NE-CZ-NH2	-16.79	111.91	120.30
1	B	6	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	A	347	ARG	NE-CZ-NH1	13.85	127.22	120.30
1	B	107	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	B	6	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	B	100	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	B	363	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	A	100	ARG	NE-CZ-NH2	-11.05	114.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	B	334	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	B	209	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	B	366	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	B	363	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	B	100	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	B	209	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	B	318	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	B	52	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	B	61	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	9	TRP	CE2-CD2-CG	-9.58	99.64	107.30
1	B	288	TRP	CD1-CG-CD2	9.55	113.94	106.30
1	B	61	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	A	250	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	B	290	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	288	TRP	CD1-CG-CD2	9.20	113.66	106.30
1	A	288	TRP	CE2-CD2-CG	-9.09	100.03	107.30
1	A	373	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	288	TRP	CE2-CD2-CG	-8.81	100.25	107.30
1	A	110	TRP	CE2-CD2-CG	-8.79	100.27	107.30
1	A	9	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	A	318	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	A	107	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	307	VAL	N-CA-CB	-8.53	92.73	111.50
1	A	217	MET	CG-SD-CE	-8.51	86.58	100.20
1	A	110	TRP	CG-CD2-CE3	8.45	141.51	133.90
1	A	110	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	A	61	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	9	TRP	CG-CD2-CE3	8.41	141.47	133.90
1	B	378	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	B	184	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	143	GLU	CA-CB-CG	8.31	131.67	113.40
1	B	378	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	98	GLN	CA-CB-CG	8.07	131.16	113.40
1	A	100	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	B	74	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	136	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	B	219	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	276	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	B	195	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	184	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	26	ARG	NE-CZ-NH1	7.54	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	351	THR	CA-CB-CG2	-7.48	101.93	112.40
1	B	136	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	334	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	192	LEU	CA-CB-CG	7.38	132.27	115.30
1	B	110	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	B	288	TRP	CG-CD2-CE3	7.32	140.49	133.90
1	A	110	TRP	CB-CG-CD1	-7.28	117.53	127.00
1	A	147	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	378	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	276	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	A	26	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	213	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	B	366	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	61	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	B	309	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	184	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	369	PHE	CB-CG-CD2	-7.06	115.86	120.80
1	A	354	TYR	CB-CG-CD2	-7.05	116.77	121.00
1	A	307	VAL	N-CA-CB	-7.02	96.05	111.50
1	A	276	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	A	316	MET	CG-SD-CE	6.95	111.31	100.20
1	B	191	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	A	6	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	288	TRP	CG-CD2-CE3	6.87	140.08	133.90
1	B	38	VAL	N-CA-CB	-6.87	96.39	111.50
1	A	209	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	373	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	316	MET	CG-SD-CE	6.75	111.00	100.20
1	B	307	VAL	CB-CA-C	6.74	124.21	111.40
1	A	366	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	110	TRP	CD1-CG-CD2	6.67	111.63	106.30
1	A	378	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	129	LYS	CA-CB-CG	6.66	128.06	113.40
1	B	136	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	219	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	191	TRP	CD1-CG-CD2	6.57	111.55	106.30
1	B	89	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	107	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	27	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	25	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	6	ARG	CB-CG-CD	-6.53	94.61	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	LYS	CA-CB-CG	6.53	127.76	113.40
1	A	290	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	154	ARG	CA-CB-CG	6.43	127.54	113.40
1	A	39	LYS	CA-CB-CG	6.41	127.49	113.40
1	A	25	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	195	ARG	CA-CB-CG	6.31	127.27	113.40
1	B	52	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	370	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	276	TRP	CD1-CG-CD2	6.21	111.27	106.30
1	B	307	VAL	CG1-CB-CG2	6.20	120.82	110.90
1	A	154	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	112	GLU	CA-CB-CG	6.17	126.97	113.40
1	A	64	VAL	N-CA-CB	-6.16	97.94	111.50
1	A	25	ARG	CA-CB-CG	6.09	126.80	113.40
1	B	318	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	48	VAL	CB-CA-C	-6.08	99.84	111.40
1	B	373	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	164	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	A	343	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	141	ASP	CB-CA-C	-5.99	98.42	110.40
1	A	64	VAL	CG1-CB-CG2	5.97	120.46	110.90
1	A	39	LYS	CG-CD-CE	5.96	129.77	111.90
1	B	239	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	B	265	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	A	195	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	293	GLN	CA-C-N	5.79	129.93	117.20
1	A	366	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	191	TRP	CE2-CD2-CG	-5.76	102.69	107.30
1	B	27	LEU	N-CA-CB	-5.73	98.94	110.40
1	B	89	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	309	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	64	VAL	N-CA-CB	-5.68	99.00	111.50
1	A	191	TRP	CE2-CD2-CG	-5.66	102.77	107.30
1	A	158	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	B	288	TRP	CB-CG-CD1	-5.62	119.70	127.00
1	B	131	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	147	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	9	TRP	CB-CG-CD1	-5.59	119.73	127.00
1	A	182	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	A	293	GLN	CA-CB-CG	5.54	125.59	113.40
1	B	64	VAL	CA-CB-CG2	-5.54	102.59	110.90
1	B	316	MET	CA-CB-CG	5.51	122.66	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	CYS	CA-CB-SG	5.46	123.84	114.00
1	B	171	ASP	CB-CG-OD1	5.45	123.21	118.30
1	B	38	VAL	CB-CA-C	5.43	121.72	111.40
1	A	382	GLY	CA-C-N	-5.43	105.25	117.20
1	A	284	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	299	VAL	CB-CA-C	-5.41	101.12	111.40
1	A	268	THR	N-CA-CB	-5.41	100.03	110.30
1	B	335	GLN	CA-C-N	-5.40	105.41	116.20
1	A	47	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	307	VAL	CB-CA-C	5.31	121.49	111.40
1	A	314	GLN	CA-CB-CG	5.31	125.08	113.40
1	B	154	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	171	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	334	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	288	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	A	280	ILE	CA-CB-CG2	-5.26	100.38	110.90
1	B	26	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	269	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	288	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	B	336	GLY	CA-C-N	-5.22	105.72	117.20
1	A	107	ARG	CA-CB-CG	5.22	124.88	113.40
1	B	122	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	A	299	VAL	CB-CA-C	-5.20	101.52	111.40
1	B	220	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	A	76	LYS	CB-CG-CD	-5.12	98.30	111.60
1	A	288	TRP	CB-CG-CD1	-5.10	120.37	127.00
1	A	318	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	164	TYR	CA-CB-CG	5.10	123.09	113.40
1	B	191	TRP	CG-CD2-CE3	5.07	138.46	133.90
1	B	354	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	316	MET	CA-CB-CG	5.06	121.90	113.30
1	B	79	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	269	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	A	331	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	381	ILE	CA-CB-CG2	-5.00	100.89	110.90

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 [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	3030	0	3020	25	0
1	B	3021	0	3012	22	0
2	A	4	0	3	0	0
2	B	4	0	3	1	0
3	A	15	0	6	1	0
3	B	15	0	7	2	0
4	A	115	0	0	3	0
4	B	91	0	0	1	0
All	All	6295	0	6051	45	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 (45) 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	4:A:474:HOH:O	2.36	0.59
1:B:37:VAL:HG12	1:B:39:LYS:HG2	1.87	0.57
1:B:163:LEU:HD13	1:B:192:LEU:HD11	1.87	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:THR:HA	4:B:481:HOH:O	2.15	0.46
1:B:85:LEU:HD22	3:B:401:PLP:H2A3	1.96	0.46
1:B:128:LEU:HD13	1:B:148:ILE:HG21	1.97	0.46
1:A:348:HIS:CE1	4: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
1:A:262:LYS:HB3	1:A:267:ALA:HB1	2.00	0.44
1:B:85:LEU:HD13	3:B:401:PLP:C3	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	4: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:282:ILE:HG21	1:B:331:LEU:HD21	2.02	0.42
3:A:402:PLP:C4A	2:B:400:ACT:H1	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 [\(i\)](#)

### 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	380/388 (98%)	365 (96%)	13 (3%)	2 (0%)	29	18
1	B	378/388 (97%)	366 (97%)	10 (3%)	2 (0%)	29	18
All	All	758/776 (98%)	731 (96%)	23 (3%)	4 (0%)	29	18

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 [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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/322 (99%)	298 (94%)	20 (6%)	18	8
1	B	318/322 (99%)	288 (91%)	30 (9%)	8	3
All	All	636/644 (99%)	586 (92%)	50 (8%)	12	5

All (50) 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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	291	ARG
1	A	299	VAL
1	A	307	VAL
1	A	313	ASP
1	A	314	GLN
1	A	318	ARG
1	A	331	LEU
1	A	351	THR
1	B	6	ARG
1	B	31	ASP
1	B	38	VAL
1	B	48	VAL
1	B	64	VAL
1	B	68	ASP
1	B	95	LEU
1	B	117	LEU
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	195	ARG
1	B	216	ASN
1	B	231	PRO
1	B	237	LEU
1	B	255	LYS
1	B	272	GLN
1	B	273	THR
1	B	302	GLN
1	B	307	VAL
1	B	335	GLN
1	B	351	THR
1	B	379	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	253	HIS
1	A	272	GLN
1	A	293	GLN
1	A	314	GLN
1	B	216	ASN
1	B	258	GLN
1	B	294	HIS
1	B	296	HIS
1	B	379	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	0.99	0	3,3,3	1.17	0
3	PLP	A	402	1	15,15,16	2.16	6 (40%)	20,22,23	1.57	7 (35%)
3	PLP	B	401	1	15,15,16	1.25	1 (6%)	20,22,23	1.46	5 (25%)
2	ACT	A	401	-	3,3,3	1.00	0	3,3,3	1.74	1 (33%)



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
3	PLP	B	401	1	-	1/6/6/8	0/1/1/1
3	PLP	A	402	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	PLP	C3-C2	-5.32	1.35	1.40
3	A	402	PLP	C4A-C4	3.59	1.59	1.51
3	A	402	PLP	C6-C5	-2.84	1.31	1.37
3	A	402	PLP	C2-N1	2.74	1.39	1.33
3	A	402	PLP	P-O3P	-2.25	1.46	1.54
3	B	401	PLP	C2-N1	2.15	1.37	1.33
3	A	402	PLP	P-O2P	-2.09	1.46	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	PLP	C4A-C4-C5	-2.84	118.01	120.94
3	A	402	PLP	C6-C5-C4	2.74	120.32	118.16
3	A	402	PLP	O2P-P-O4P	-2.70	99.56	106.73
3	B	401	PLP	C6-C5-C4	2.66	120.25	118.16
3	A	402	PLP	C5-C6-N1	-2.41	119.80	123.82
2	A	401	ACT	OXT-C-CH3	2.36	124.92	115.18
3	B	401	PLP	O2P-P-O4P	-2.34	100.50	106.73
3	B	401	PLP	O3P-P-O2P	2.31	116.48	107.64
3	A	402	PLP	C6-N1-C2	2.28	123.40	119.17
3	B	401	PLP	C5-C6-N1	-2.24	120.09	123.82
3	A	402	PLP	O3P-P-O2P	2.23	116.15	107.64
3	A	402	PLP	C3-C2-N1	-2.21	117.91	120.77
3	A	402	PLP	C2A-C2-N1	2.17	121.92	117.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	PLP	C4-C5-C5A-O4P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	ACT	1	0
3	A	402	PLP	1	0
3	B	401	PLP	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.