



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:22 PM UTC

PDB ID : 1AT1 / pdb_00001at1
Title : CRYSTAL STRUCTURES OF PHOSPHONOACETAMIDE LIGATED T AND PHOSPHONOACETAMIDE AND MALONATE LIGATED R STATES OF ASPARTATE CARBAMOYLTRANSFERASE AT 2.8-ANGSTROMS RESOLUTION AND NEUTRAL P*H
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Deposited on : 1989-09-22
Resolution : 2.80 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

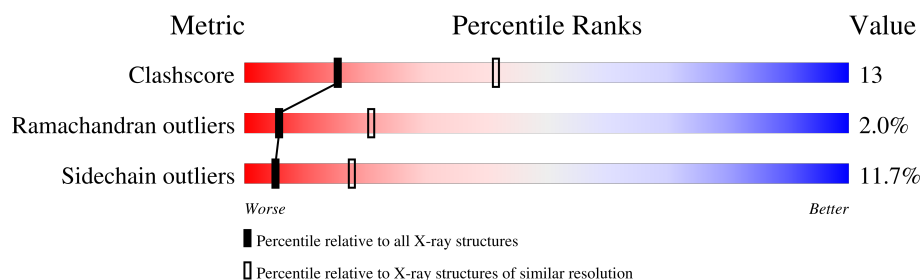
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	310	
1	C	310	
2	B	153	
2	D	153	

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
3	MLI	A	312	-	X	-	-
4	PCT	A	311	-	X	-	-
4	PCT	C	311	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7138 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 ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
C	60	GLN	GLU	conflict	UNP P0A786
C	147	GLN	GLU	conflict	UNP P0A786
C	149	GLU	GLN	conflict	UNP P0A786
C	196	GLU	GLN	conflict	UNP P0A786

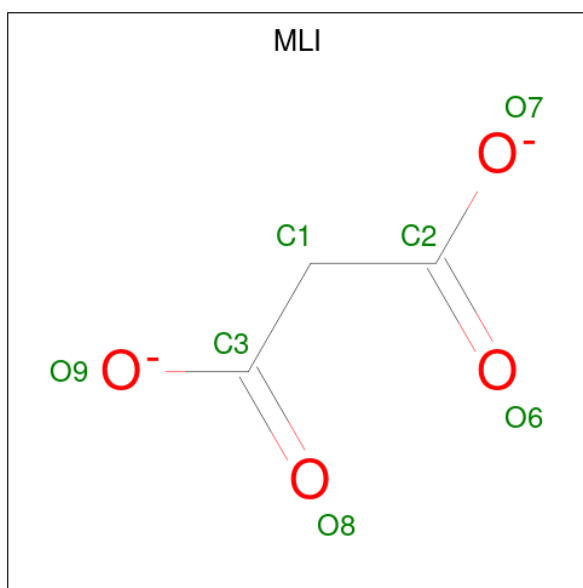
- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

There are 2 discrepancies between the modelled and reference sequences:

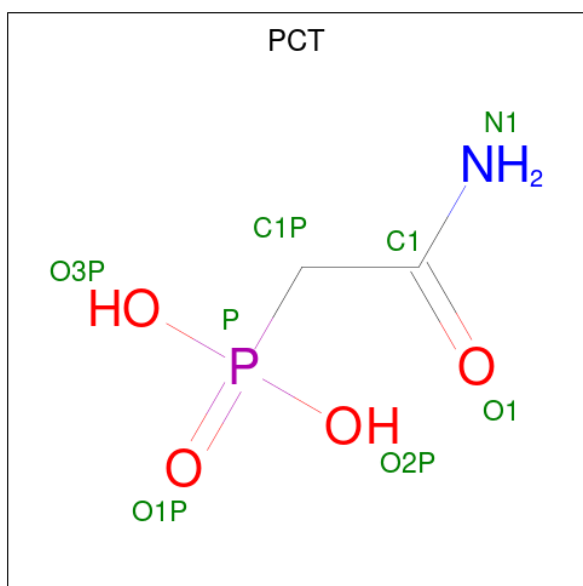
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3
D	8	GLY	GLN	conflict	UNP P0A7F3

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is PHOSPHONOACETAMIDE (CCD ID: PCT) (formula: $\text{C}_2\text{H}_6\text{NO}_4\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			8	2	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			8	2	1	4	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

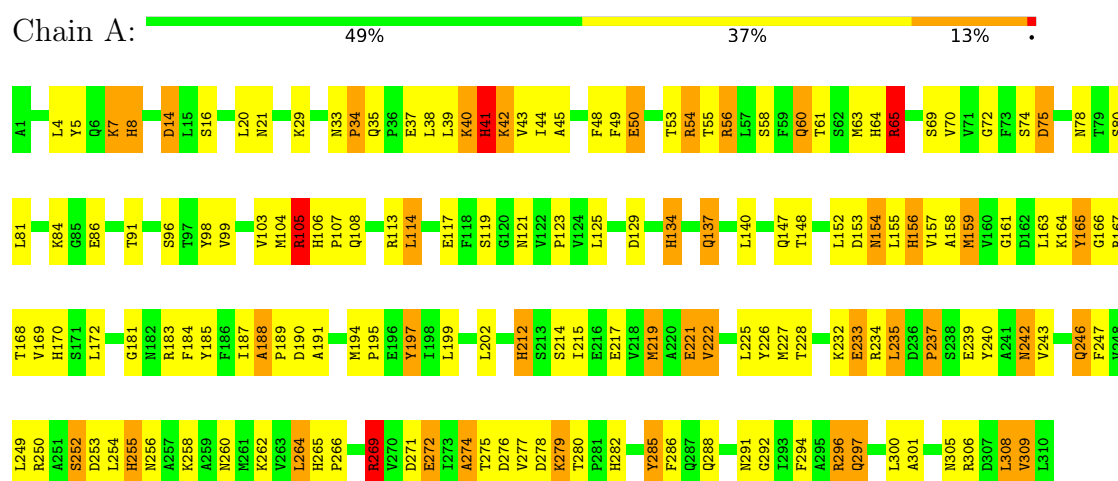
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

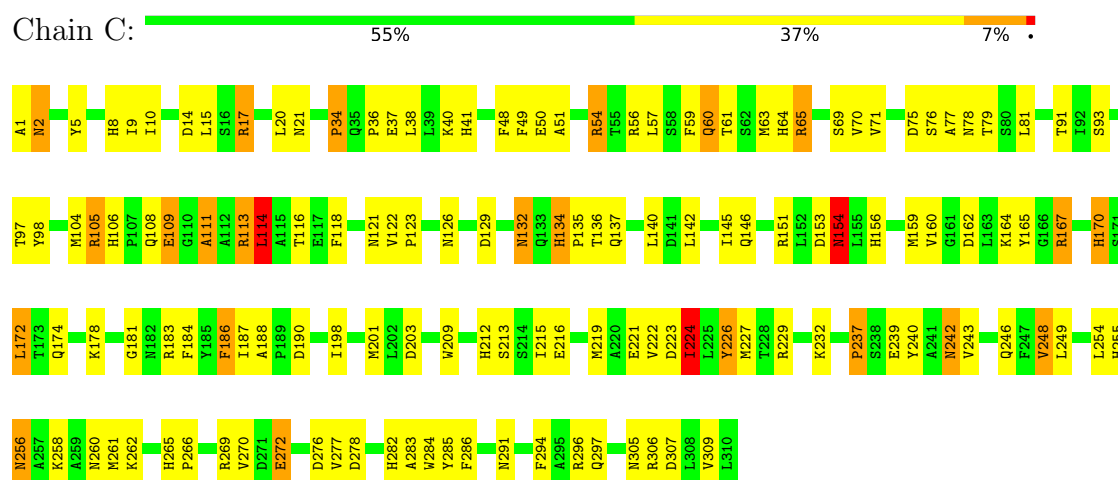
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

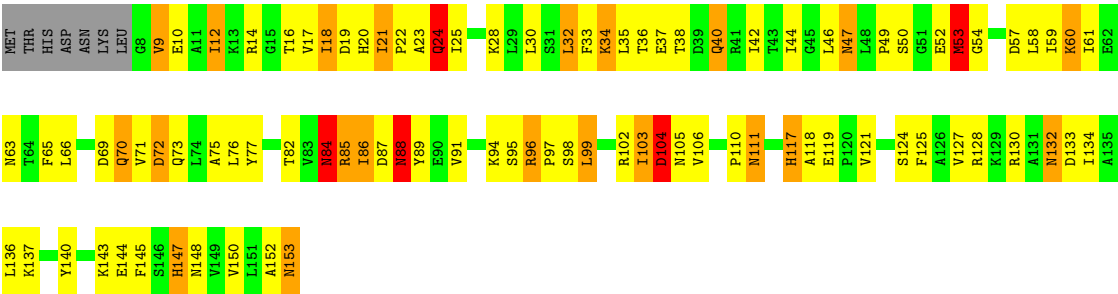


• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN

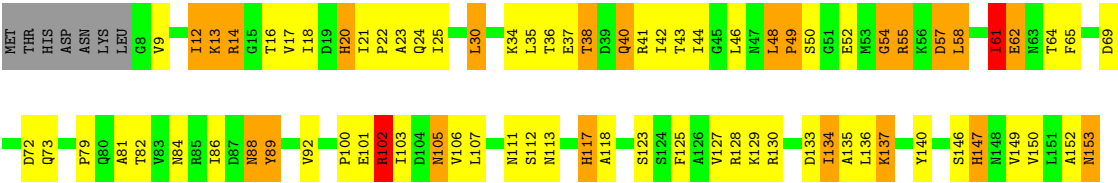


• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.30Å 122.30Å 156.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7138	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: MLI, PCT, ZN

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	1.22	17/2461 (0.7%)	2.10	95/3339 (2.8%)
1	C	1.26	19/2461 (0.8%)	2.08	86/3339 (2.6%)
2	B	1.08	5/1155 (0.4%)	2.01	36/1561 (2.3%)
2	D	1.05	5/1155 (0.4%)	1.97	25/1561 (1.6%)
All	All	1.19	46/7232 (0.6%)	2.06	242/9800 (2.5%)

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	3
1	C	0	6
2	B	0	2
2	D	0	2
All	All	0	13

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	106	VAL	CA-CB	9.11	1.66	1.54
1	A	265	HIS	CD2-NE2	-7.92	1.29	1.37
1	C	64	HIS	CD2-NE2	-7.84	1.29	1.37
1	C	156	HIS	CD2-NE2	-7.64	1.29	1.37
1	C	265	HIS	CD2-NE2	-7.54	1.29	1.37
2	B	12	ILE	CA-CB	7.52	1.64	1.54
1	C	134	HIS	CD2-NE2	-7.43	1.29	1.37
1	A	64	HIS	CD2-NE2	-7.33	1.29	1.37
1	C	106	HIS	CD2-NE2	-7.25	1.29	1.37
1	C	170	HIS	CD2-NE2	-7.22	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	134	HIS	CD2-NE2	-6.69	1.30	1.37
1	C	212	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	156	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	170	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	106	HIS	CG-ND1	-6.13	1.31	1.38
1	A	282	HIS	CD2-NE2	-6.12	1.31	1.37
1	C	224	ILE	CA-CB	6.11	1.62	1.54
2	B	20	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	134	HIS	CG-ND1	-6.07	1.31	1.38
1	A	44	ILE	CA-CB	6.06	1.61	1.54
2	D	117	HIS	CD2-NE2	-6.02	1.31	1.37
2	B	147	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	34	PRO	CA-CB	-5.97	1.45	1.53
2	D	147	HIS	CD2-NE2	-5.95	1.31	1.37
1	C	8	HIS	CD2-NE2	-5.92	1.31	1.37
2	D	117	HIS	CG-ND1	-5.91	1.31	1.38
1	C	41	HIS	CD2-NE2	-5.86	1.31	1.37
1	C	91	THR	CA-CB	5.81	1.62	1.53
1	A	255	HIS	CD2-NE2	-5.76	1.31	1.37
1	C	255	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	8	HIS	CD2-NE2	-5.57	1.31	1.37
1	C	167	ARG	CA-CB	5.41	1.62	1.53
2	B	117	HIS	CD2-NE2	-5.38	1.31	1.37
1	C	156	HIS	CG-ND1	-5.36	1.32	1.38
1	A	212	HIS	CG-ND1	-5.35	1.32	1.38
2	D	12	ILE	CA-CB	5.21	1.60	1.55
1	C	265	HIS	CG-ND1	-5.12	1.32	1.38
1	A	64	HIS	CG-ND1	-5.12	1.32	1.38
1	C	34	PRO	CA-CB	-5.09	1.48	1.54
1	C	212	HIS	CG-ND1	-5.05	1.32	1.38
1	C	41	HIS	CA-CB	5.05	1.60	1.54
2	D	20	HIS	CD2-NE2	-5.04	1.32	1.37
1	A	148	THR	CA-CB	5.03	1.60	1.53

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	VAL	N-CA-C	12.83	124.71	110.21
1	C	14	ASP	CA-CB-CG	9.89	122.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2	ASN	CA-CB-CG	9.54	122.14	112.60
2	B	133	ASP	CA-CB-CG	9.22	121.82	112.60
1	C	75	ASP	CA-CB-CG	9.09	121.69	112.60
1	A	81	LEU	N-CA-C	-9.05	101.49	111.36
1	A	272	GLU	N-CA-C	8.96	123.21	111.75
1	C	190	ASP	CA-CB-CG	8.91	121.51	112.60
1	A	246	GLN	N-CA-C	-8.82	101.24	111.03
2	D	153	ASN	OD1-CG-ND2	-8.75	113.85	122.60
1	A	91	THR	CA-CB-OG1	-8.74	96.50	109.60
1	C	65	ARG	NE-CZ-NH2	8.73	127.06	119.20
2	B	84	ASN	CA-CB-CG	-8.68	103.92	112.60
1	A	309	VAL	O-C-N	8.60	133.32	122.57
2	B	21	ILE	N-CA-C	-8.57	101.26	108.63
1	C	60	GLN	CA-CB-CG	-8.38	97.33	114.10
1	C	243	VAL	N-CA-C	8.33	118.42	110.42
2	B	152	ALA	N-CA-C	8.22	128.31	110.80
1	A	271	ASP	CA-CB-CG	8.21	120.81	112.60
1	C	167	ARG	CB-CG-CD	8.16	130.06	111.30
1	C	291	ASN	CB-CG-ND2	8.07	128.51	116.40
1	C	51	ALA	N-CA-C	8.00	121.52	110.24
1	A	56	ARG	NE-CZ-NH1	-7.77	113.73	121.50
2	B	10	GLU	N-CA-C	7.71	120.78	109.07
1	C	305	ASN	CA-CB-CG	-7.68	104.92	112.60
1	C	122	VAL	CA-C-N	7.67	127.43	119.76
1	C	122	VAL	C-N-CA	7.67	127.43	119.76
1	C	291	ASN	OD1-CG-ND2	-7.66	114.94	122.60
2	B	130	ARG	NE-CZ-NH2	7.63	126.07	119.20
1	A	276	ASP	CA-CB-CG	7.63	120.23	112.60
1	A	242	ASN	CA-CB-CG	7.58	120.18	112.60
1	C	129	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	58	SER	CA-C-O	-7.50	112.95	120.82
2	B	47	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	A	242	ASN	CB-CG-ND2	7.45	127.58	116.40
1	C	109	GLU	CA-C-O	7.45	129.38	120.81
2	B	104	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	49	PHE	N-CA-C	-7.42	104.12	113.02
1	C	269	ARG	CA-CB-CG	7.40	128.91	114.10
2	D	105	ASN	N-CA-C	7.30	126.34	110.80
2	D	127	VAL	N-CA-C	7.28	116.79	106.53
1	A	33	ASN	CA-C-N	7.25	128.90	119.84
1	A	33	ASN	C-N-CA	7.25	128.90	119.84
1	C	278	ASP	CA-CB-CG	7.24	119.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	A	33	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	C	48	PHE	CA-C-O	7.22	128.18	120.46
1	C	54	ARG	NE-CZ-NH2	7.21	125.69	119.20
1	C	297	GLN	OE1-CD-NE2	-7.17	115.43	122.60
2	D	102	ARG	NE-CZ-NH2	7.12	125.61	119.20
2	D	14	ARG	NE-CZ-NH2	7.08	125.57	119.20
1	A	105	ARG	CA-CB-CG	-7.07	99.95	114.10
2	B	153	ASN	CA-CB-CG	7.07	119.67	112.60
2	B	119	GLU	N-CA-C	7.03	119.53	110.39
1	C	56	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	C	126	ASN	N-CA-C	7.00	119.52	108.67
1	A	75	ASP	CA-CB-CG	6.99	119.59	112.60
1	C	105	ARG	NE-CZ-NH2	6.93	125.43	119.20
1	A	106	HIS	CA-C-N	6.91	126.54	119.56
1	A	106	HIS	C-N-CA	6.91	126.54	119.56
2	D	61	ILE	CA-CB-CG2	-6.82	98.91	110.50
1	A	21	ASN	CA-CB-CG	-6.81	105.79	112.60
1	A	54	ARG	N-CA-C	6.80	119.32	111.02
1	A	91	THR	CA-CB-CG2	6.73	121.94	110.50
1	A	137	GLN	N-CA-C	-6.72	103.88	111.14
1	A	121	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	C	54	ARG	CA-C-O	-6.67	113.73	121.07
1	C	269	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	A	288	GLN	OE1-CD-NE2	-6.62	115.98	122.60
2	B	105	ASN	OD1-CG-ND2	-6.61	115.99	122.60
2	D	84	ASN	N-CA-C	6.58	119.53	108.02
1	A	242	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	A	14	ASP	O-C-N	-6.52	113.98	122.39
1	A	256	ASN	CA-CB-CG	6.47	119.07	112.60
2	B	53	MET	N-CA-C	-6.45	99.79	110.17
2	B	37	GLU	CA-CB-CG	-6.42	101.25	114.10
1	C	172	LEU	CA-C-O	-6.40	113.63	120.42
1	A	234	ARG	NE-CZ-NH2	6.39	124.96	119.20
1	A	72	GLY	N-CA-C	6.39	119.20	110.58
1	A	153	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	157	VAL	N-CA-C	6.37	116.80	107.37
1	C	276	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	215	ILE	N-CA-C	-6.37	104.29	110.72
1	A	235	LEU	N-CA-C	6.36	119.47	110.50
2	D	153	ASN	CB-CG-ND2	6.35	125.93	116.40
2	D	134	ILE	N-CA-CB	-6.28	104.07	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	VAL	O-C-N	6.27	129.50	122.98
1	C	123	PRO	N-CA-CB	6.27	109.17	103.34
1	C	17	ARG	NE-CZ-NH2	6.23	124.81	119.20
2	B	111	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	C	111	ALA	CA-C-N	6.19	129.40	120.79
1	C	111	ALA	C-N-CA	6.19	129.40	120.79
1	A	60	GLN	O-C-N	-6.19	114.66	122.27
1	A	234	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	A	104	MET	N-CA-CB	-6.16	100.14	110.80
1	C	154	ASN	CB-CG-ND2	6.16	125.64	116.40
1	A	157	VAL	N-CA-CB	-6.15	103.92	111.67
1	C	54	ARG	N-CA-C	6.15	118.52	111.02
1	A	42	LYS	O-C-N	-6.14	116.03	123.16
2	B	148	ASN	OD1-CG-ND2	-6.11	116.49	122.60
2	B	60	LYS	N-CA-C	-6.11	98.44	108.76
1	A	14	ASP	CA-CB-CG	6.09	118.69	112.60
2	D	152	ALA	CA-C-O	6.08	128.01	121.02
2	B	21	ILE	N-CA-CB	6.06	116.71	110.23
1	C	98	TYR	N-CA-C	6.06	121.18	113.55
1	A	60	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	C	203	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	54	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	C	77	ALA	CA-C-O	6.03	126.94	120.55
2	B	47	ASN	CB-CG-ND2	6.02	125.43	116.40
2	D	57	ASP	CA-CB-CG	6.00	118.61	112.60
1	A	297	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	C	132	ASN	CA-CB-CG	5.97	118.57	112.60
1	C	104	MET	N-CA-C	5.97	119.21	109.06
1	A	98	TYR	CA-CB-CG	5.96	124.63	113.90
1	A	191	ALA	O-C-N	5.96	129.19	122.22
1	A	265	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	A	147	GLN	OE1-CD-NE2	-5.91	116.69	122.60
2	B	33	PHE	N-CA-C	-5.87	99.16	108.73
2	B	99	LEU	N-CA-C	-5.87	102.38	109.83
1	A	86	GLU	CA-CB-CG	5.84	125.78	114.10
1	C	186	PHE	CA-CB-CG	-5.84	107.96	113.80
1	A	269	ARG	CB-CG-CD	-5.83	97.89	111.30
1	C	255	HIS	N-CA-C	5.81	119.19	111.75
2	B	85	ARG	N-CA-C	-5.80	99.82	109.46
1	C	54	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	C	97	THR	N-CA-C	-5.78	106.00	113.16
2	D	147	HIS	CA-CB-CG	5.75	119.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	88	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	65	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	A	255	HIS	CA-CB-CG	5.75	119.55	113.80
1	A	264	LEU	O-C-N	-5.74	115.93	123.16
1	A	33	ASN	CB-CG-ND2	5.74	125.01	116.40
1	A	106	HIS	O-C-N	5.74	125.87	121.85
1	A	55	THR	CA-CB-OG1	-5.73	101.00	109.60
2	B	47	ASN	CA-CB-CG	5.73	118.33	112.60
1	C	256	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	C	65	ARG	CB-CG-CD	5.71	124.43	111.30
1	C	151	ARG	NE-CZ-NH2	5.71	124.33	119.20
1	C	111	ALA	CA-C-O	5.70	126.47	120.42
1	A	232	LYS	N-CA-CB	-5.70	100.49	109.78
1	A	219	MET	N-CA-C	5.69	120.75	111.37
1	C	126	ASN	CA-CB-CG	5.68	118.28	112.60
1	A	134	HIS	CA-CB-CG	5.67	119.47	113.80
1	C	126	ASN	CA-C-O	5.64	126.97	120.60
1	A	86	GLU	N-CA-C	5.62	118.14	110.55
1	A	286	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	129	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	78	ASN	N-CA-CB	-5.61	101.69	110.44
1	A	243	VAL	CA-C-O	5.60	123.83	118.90
1	A	221	GLU	CA-C-O	-5.60	114.94	120.82
2	D	9	VAL	CA-C-N	5.60	132.23	121.54
2	D	9	VAL	C-N-CA	5.60	132.23	121.54
1	C	224	ILE	CA-CB-CG2	5.58	119.99	110.50
1	C	269	ARG	CG-CD-NE	-5.58	99.73	112.00
2	B	34	LYS	N-CA-C	5.57	122.66	110.80
1	C	98	TYR	CB-CA-C	-5.56	100.73	109.34
1	C	113	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	C	162	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	132	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	A	165	TYR	CA-C-O	5.52	125.81	119.35
1	A	260	ASN	OD1-CG-ND2	-5.51	117.08	122.60
2	B	96	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	C	209	TRP	CB-CG-CD1	-5.51	118.63	126.90
1	A	53	THR	N-CA-C	-5.51	103.13	111.34
2	D	118	ALA	N-CA-C	5.50	118.04	111.71
2	B	52	GLU	N-CA-C	-5.49	104.99	110.97
2	D	24	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	C	282	HIS	N-CA-C	-5.47	107.26	114.04
2	D	153	ASN	CA-CB-CG	5.47	118.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	LEU	N-CA-C	-5.46	105.22	111.07
1	C	21	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	C	246	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	C	113	ARG	NE-CZ-NH1	-5.44	116.06	121.50
2	B	118	ALA	N-CA-C	5.43	117.20	111.28
1	C	248	VAL	O-C-N	-5.39	117.80	123.03
1	A	239	GLU	CA-CB-CG	-5.39	103.32	114.10
1	C	188	ALA	O-C-N	-5.37	117.36	121.55
2	D	61	ILE	CA-CB-CG1	5.37	119.52	110.40
2	B	18	ILE	N-CA-C	-5.36	99.37	107.73
1	C	242	ASN	CB-CG-ND2	5.35	124.42	116.40
2	B	9	VAL	CA-C-O	-5.34	114.10	120.78
1	A	105	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	A	191	ALA	N-CA-C	5.33	117.84	111.71
1	C	284	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	A	258	LYS	CB-CG-CD	-5.32	99.07	111.30
1	C	209	TRP	CE2-CD2-CG	-5.31	100.83	107.20
2	B	153	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	269	ARG	N-CA-C	-5.28	100.57	109.07
2	B	140	TYR	O-C-N	-5.27	115.58	122.59
2	B	70	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	165	TYR	N-CA-CB	-5.26	102.70	110.49
1	A	37	GLU	N-CA-C	-5.26	106.09	112.88
1	A	84	LYS	CG-CD-CE	5.26	123.39	111.30
2	D	12	ILE	CB-CA-C	-5.25	104.50	111.80
2	D	37	GLU	N-CA-C	-5.25	99.20	108.23
1	A	58	SER	N-CA-C	-5.25	105.45	111.07
1	C	269	ARG	CB-CG-CD	5.25	123.36	111.30
1	A	121	ASN	CB-CG-ND2	5.24	124.25	116.40
1	A	274	ALA	CA-C-O	-5.23	116.00	121.55
2	D	88	ASN	CA-CB-CG	-5.23	107.37	112.60
1	C	294	PHE	CA-CB-CG	-5.22	108.58	113.80
1	C	269	ARG	N-CA-C	-5.22	101.37	109.72
1	C	121	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	C	57	LEU	CA-C-O	-5.21	115.03	120.55
1	A	56	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	159	MET	CA-C-O	5.21	125.87	120.40
2	B	40	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	265	HIS	CA-CB-CG	5.20	119.00	113.80
1	C	61	THR	N-CA-C	-5.19	105.53	111.14
1	A	105	ARG	O-C-N	-5.18	117.17	123.29
1	C	126	ASN	OD1-CG-ND2	-5.18	117.42	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	CA-CB-CG	-5.18	103.74	114.10
1	A	291	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	C	153	ASP	N-CA-C	-5.17	101.69	109.85
1	C	114	LEU	CA-CB-CG	5.17	134.38	116.30
2	D	105	ASN	O-C-N	-5.16	115.73	122.59
1	A	7	LYS	CG-CD-CE	5.16	123.16	111.30
1	C	216	GLU	N-CA-C	-5.14	106.27	112.54
2	D	9	VAL	O-C-N	5.14	128.99	122.57
2	B	148	ASN	N-CA-C	-5.13	105.60	111.14
1	C	272	GLU	CA-CB-CG	5.13	124.35	114.10
1	C	260	ASN	CB-CG-ND2	5.12	124.08	116.40
1	C	309	VAL	N-CA-C	-5.12	98.64	107.24
1	A	167	ARG	N-CA-C	-5.12	105.70	111.28
1	A	167	ARG	CB-CG-CD	5.11	123.05	111.30
1	A	190	ASP	CA-CB-CG	5.10	117.70	112.60
2	D	102	ARG	N-CA-CB	-5.10	102.24	110.81
1	A	154	ASN	OD1-CG-ND2	-5.09	117.50	122.60
1	C	2	ASN	CA-C-O	-5.09	114.28	120.54
2	D	37	GLU	CA-CB-CG	-5.09	103.92	114.10
1	A	153	ASP	N-CA-C	-5.09	101.58	109.72
1	A	103	VAL	O-C-N	-5.08	117.39	123.03
2	B	60	LYS	O-C-N	5.07	129.24	123.31
1	C	229	ARG	O-C-N	-5.06	117.30	123.16
1	A	256	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	C	224	ILE	CA-CB-CG1	-5.04	101.84	110.40
1	A	309	VAL	CA-C-N	5.02	130.73	121.70
1	A	309	VAL	C-N-CA	5.02	130.73	121.70
1	C	8	HIS	O-C-N	-5.02	117.50	123.22
1	C	93	SER	CB-CA-C	-5.02	102.94	110.92
2	B	49	PRO	CB-CA-C	5.00	117.01	111.56

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ALA	Peptide
1	A	197	TYR	Sidechain
1	A	285	TYR	Sidechain
2	B	77	TYR	Sidechain
2	B	89	TYR	Sidechain
1	C	118	PHE	Sidechain
1	C	226	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	240	TYR	Sidechain
1	C	285	TYR	Sidechain
1	C	286	PHE	Sidechain
1	C	5	TYR	Sidechain
2	D	140	TYR	Sidechain
2	D	89	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	2415	0	2422	62	0
1	C	2415	0	2422	44	0
2	B	1138	0	1154	50	0
2	D	1138	0	1154	45	0
3	A	7	0	2	0	0
3	C	7	0	2	0	0
4	A	8	0	4	1	0
4	C	8	0	4	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
All	All	7138	0	7164	193	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 13.

All (193) 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:254:LEU:HD22	1:C:261:MET:HE1	1.51	0.91
2:B:14:ARG:HG3	2:B:87:ASP:HA	1.53	0.91
2:D:146:SER:HB3	2:D:149:VAL:HG23	1.55	0.88
2:B:22:PRO:HB2	2:B:25:ILE:HD12	1.63	0.81
2:D:102:ARG:HH21	2:D:102:ARG:HB3	1.45	0.81
1:C:145:ILE:HG12	1:C:224:ILE:HD13	1.61	0.80
1:A:292:GLY:O	1:A:296:ARG:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:PRO:HA	2:D:55:ARG:HA	1.67	0.75
1:C:154:ASN:HA	1:C:181:GLY:O	1.89	0.72
2:D:13:LYS:HG3	2:D:88:ASN:HA	1.73	0.71
2:D:130:ARG:HD2	2:D:135:ALA:HB2	1.74	0.69
2:B:84:ASN:HD21	2:B:91:VAL:HG13	1.59	0.67
2:D:106:VAL:HG23	2:D:107:LEU:HD12	1.76	0.66
1:A:43:VAL:HG22	1:A:69:SER:HB2	1.78	0.66
1:A:154:ASN:HA	1:A:181:GLY:O	1.96	0.66
1:C:10:ILE:HD11	1:C:116:THR:HG21	1.79	0.65
2:B:30:LEU:HD11	2:B:59:ILE:HG21	1.77	0.65
2:B:42:ILE:HB	2:D:46:LEU:HB2	1.79	0.65
1:A:159:MET:HE2	1:A:169:VAL:HG12	1.78	0.65
1:A:4:LEU:HD23	1:A:7:LYS:HD3	1.78	0.64
1:C:54:ARG:HE	4:C:311:PCT:H1P2	1.61	0.64
2:B:66:LEU:HD12	2:B:71:VAL:HG22	1.81	0.63
2:B:16:THR:OG1	2:B:65:PHE:HA	1.98	0.63
2:B:75:ALA:HB2	2:B:97:PRO:HB2	1.79	0.63
2:B:53:MET:SD	2:B:54:GLY:N	2.72	0.63
2:B:30:LEU:HD12	2:B:35:LEU:HD13	1.79	0.62
2:D:72:ASP:HB3	2:D:100:PRO:HG3	1.80	0.62
2:B:134:ILE:O	2:B:147:HIS:HB3	1.99	0.61
1:C:248:VAL:HG22	1:C:272:GLU:HA	1.82	0.61
1:C:9:ILE:HD12	1:C:15:LEU:HD11	1.84	0.60
1:C:76:SER:HA	1:C:79:THR:HG23	1.83	0.60
2:D:111:ASN:O	2:D:117:HIS:HE1	1.84	0.60
2:B:44:ILE:HB	2:D:44:ILE:HD13	1.83	0.60
1:A:63:MET:SD	1:A:70:VAL:HG22	2.43	0.59
1:A:254:LEU:HD12	1:A:280:THR:HG21	1.84	0.59
1:A:219:MET:HE1	1:A:225:LEU:HD22	1.84	0.58
1:C:137:GLN:O	1:C:140:LEU:HG	2.03	0.58
2:B:46:LEU:HB2	2:D:42:ILE:HB	1.85	0.58
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.85	0.57
2:D:38:THR:HG23	2:D:40:GLN:H	1.71	0.56
1:A:114:LEU:HD22	2:B:121:VAL:HG11	1.88	0.56
2:B:44:ILE:HG23	2:B:59:ILE:HG13	1.85	0.56
2:B:104:ASP:HA	2:B:124:SER:HA	1.87	0.55
1:A:35:GLN:HB3	1:A:38:LEU:HD13	1.88	0.55
1:C:50:GLU:HB3	1:C:105:ARG:HG2	1.88	0.55
1:A:235:LEU:HB2	1:A:240:TYR:HE2	1.72	0.55
2:D:14:ARG:HG3	2:D:65:PHE:CE1	2.41	0.55
1:C:50:GLU:HB3	1:C:105:ARG:CG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASN:HD22	1:C:181:GLY:HA3	1.73	0.54
1:C:63:MET:SD	1:C:70:VAL:HG22	2.48	0.53
1:C:160:VAL:HB	1:C:227:MET:SD	2.49	0.53
1:A:4:LEU:HA	1:A:7:LYS:HD2	1.90	0.52
1:C:254:LEU:CD2	1:C:261:MET:HE1	2.34	0.52
1:A:185:TYR:HD2	1:A:212:HIS:NE2	2.07	0.52
2:B:136:LEU:HD12	2:B:150:VAL:HG21	1.92	0.52
1:C:49:PHE:HD2	1:C:76:SER:HB3	1.75	0.52
2:D:125:PHE:HA	2:D:137:LYS:O	2.10	0.52
2:D:107:LEU:HD23	2:D:150:VAL:HG11	1.92	0.52
2:B:103:ILE:HD11	2:B:127:VAL:HG22	1.92	0.51
2:D:14:ARG:HA	2:D:86:ILE:O	2.10	0.51
2:D:14:ARG:HG3	2:D:65:PHE:HE1	1.75	0.51
2:B:50:SER:HB3	2:B:53:MET:O	2.10	0.51
1:A:185:TYR:HB3	1:A:212:HIS:CD2	2.46	0.51
2:B:72:ASP:HA	2:B:97:PRO:HB3	1.92	0.51
1:C:1:ALA:HA	1:C:306:ARG:HG2	1.91	0.51
2:B:23:ALA:HA	2:B:57:ASP:CG	2.35	0.50
1:C:134:HIS:HB2	1:C:167:ARG:HD3	1.92	0.50
2:B:38:THR:HG21	2:B:42:ILE:HD11	1.92	0.50
1:A:301:ALA:O	1:A:305:ASN:HB2	2.12	0.50
1:A:56:ARG:HE	1:A:60:GLN:NE2	2.08	0.50
2:B:23:ALA:O	2:B:24:GLN:HB2	2.11	0.50
1:A:214:SER:HB3	1:A:217:GLU:HG3	1.93	0.49
2:B:91:VAL:HG11	2:B:94:LYS:NZ	2.27	0.49
1:A:161:GLY:HA3	1:A:228:THR:OG1	2.12	0.49
2:D:12:ILE:HG23	2:D:41:ARG:NH1	2.28	0.49
2:D:102:ARG:HA	2:D:125:PHE:O	2.12	0.49
2:B:18:ILE:HD12	2:B:18:ILE:N	2.27	0.49
1:A:159:MET:HE3	1:A:172:LEU:HD23	1.93	0.49
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.94	0.49
1:C:219:MET:HE1	1:C:249:LEU:HD11	1.94	0.49
2:B:21:ILE:HD13	2:B:58:LEU:HA	1.93	0.49
1:C:159:MET:HE3	1:C:172:LEU:HD23	1.95	0.49
1:A:189:PRO:HD3	1:A:247:PHE:HE1	1.78	0.49
1:A:137:GLN:O	1:A:140:LEU:HG	2.13	0.49
1:C:249:LEU:HD21	1:C:254:LEU:HD21	1.94	0.49
2:D:16:THR:OG1	2:D:65:PHE:HA	2.13	0.49
1:A:278:ASP:HB2	1:A:279:LYS:NZ	2.27	0.48
1:C:136:THR:HB	1:C:296:ARG:NH2	2.28	0.48
1:C:239:GLU:O	1:C:242:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:HIS:O	1:C:174:GLN:HG3	2.12	0.48
2:D:12:ILE:HD11	2:D:17:VAL:HG23	1.95	0.48
1:A:183:ARG:NH2	1:A:184:PHE:O	2.46	0.48
2:B:40:GLN:NE2	2:B:63:ASN:HB2	2.28	0.48
2:D:13:LYS:CG	2:D:88:ASN:HA	2.42	0.48
2:B:18:ILE:HD12	2:B:18:ILE:H	1.78	0.48
2:D:22:PRO:O	2:D:25:ILE:HB	2.13	0.47
2:D:134:ILE:HB	2:D:147:HIS:HB3	1.96	0.47
2:D:130:ARG:CD	2:D:135:ALA:HB2	2.44	0.47
1:C:10:ILE:HD11	1:C:116:THR:CG2	2.45	0.47
2:B:14:ARG:HA	2:B:86:ILE:HG22	1.95	0.47
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.15	0.47
1:C:60:GLN:HG2	1:C:70:VAL:HG21	1.96	0.47
1:A:134:HIS:CD2	1:A:137:GLN:HB2	2.50	0.46
1:C:10:ILE:O	1:C:135:PRO:HG3	2.16	0.46
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.96	0.46
1:A:39:LEU:O	1:A:42:LYS:HB2	2.16	0.46
1:A:194:MET:SD	1:A:195:PRO:HD2	2.55	0.46
1:A:233:GLU:H	1:A:233:GLU:CD	2.23	0.46
1:A:254:LEU:HD11	1:A:277:VAL:HG13	1.97	0.46
1:A:158:ALA:HB2	1:A:222:VAL:HG11	1.98	0.46
1:A:275:THR:O	1:A:279:LYS:NZ	2.46	0.46
1:C:20:LEU:HD11	1:C:178:LYS:HD2	1.97	0.46
1:A:38:LEU:HD11	1:A:309:VAL:HG21	1.98	0.46
2:B:70:GLN:HA	2:B:73:GLN:OE1	2.16	0.46
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.97	0.46
1:C:164:LYS:HD3	1:C:165:TYR:CE2	2.51	0.46
2:D:61:ILE:CG2	2:D:64:THR:HB	2.46	0.46
1:A:250:ARG:HG2	1:A:274:ALA:CB	2.45	0.46
2:B:136:LEU:HD12	2:B:150:VAL:HG11	1.98	0.46
1:A:294:PHE:HA	1:A:297:GLN:HG2	1.97	0.45
1:A:61:THR:O	1:A:65:ARG:HG3	2.16	0.45
2:B:69:ASP:O	2:B:73:GLN:HG3	2.17	0.45
2:B:110:PRO:HG2	2:B:145:PHE:CG	2.51	0.45
1:A:269:ARG:NH1	1:A:278:ASP:OD2	2.49	0.45
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.16	0.45
2:D:23:ALA:HB3	2:D:55:ARG:NH2	2.31	0.45
1:A:156:HIS:HA	1:A:183:ARG:HB3	1.99	0.45
1:A:199:LEU:O	1:A:202:LEU:HB2	2.17	0.45
2:B:36:THR:HG23	2:D:46:LEU:HD13	1.97	0.45
2:D:100:PRO:HG2	2:D:103:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASN:ND2	2:B:91:VAL:HG13	2.29	0.45
2:B:102:ARG:HA	2:B:125:PHE:O	2.17	0.45
1:C:183:ARG:NH2	1:C:184:PHE:O	2.50	0.45
1:C:223:ASP:O	1:C:261:MET:HA	2.16	0.45
1:A:164:LYS:HD3	1:A:165:TYR:CE2	2.51	0.45
2:B:16:THR:HG21	2:B:66:LEU:HG	1.99	0.45
1:C:49:PHE:CD2	1:C:76:SER:HB3	2.52	0.44
1:A:5:TYR:CZ	1:A:306:ARG:HG2	2.52	0.44
2:D:30:LEU:HD13	2:D:35:LEU:HB2	1.99	0.44
2:D:49:PRO:HA	2:D:54:GLY:O	2.17	0.44
1:A:96:SER:OG	1:A:119:SER:HA	2.17	0.44
2:B:17:VAL:HG13	2:B:60:LYS:HG2	2.00	0.44
2:B:99:LEU:HA	2:B:99:LEU:HD23	1.84	0.44
2:B:137:LYS:HG3	2:B:144:GLU:HG2	1.99	0.44
2:B:84:ASN:ND2	2:B:91:VAL:HG22	2.33	0.43
2:D:48:LEU:O	2:D:55:ARG:HA	2.19	0.43
1:A:40:LYS:O	1:A:41:HIS:HB2	2.18	0.43
2:D:12:ILE:HG22	2:D:62:GLU:HG3	1.99	0.43
1:A:4:LEU:HD23	1:A:7:LYS:CD	2.46	0.43
1:A:16:SER:O	1:A:20:LEU:HG	2.19	0.43
2:B:66:LEU:HB2	2:B:71:VAL:HG23	2.00	0.43
1:C:108:GLN:HA	2:D:113:ASN:ND2	2.32	0.43
2:D:38:THR:HG21	2:D:42:ILE:HD11	2.00	0.43
2:D:69:ASP:O	2:D:73:GLN:HG3	2.19	0.43
2:D:20:HIS:HB2	2:D:81:ALA:HA	2.01	0.43
1:A:48:PHE:CD2	1:A:105:ARG:HB2	2.54	0.43
1:C:34:PRO:O	1:C:36:PRO:HD3	2.19	0.43
2:D:13:LYS:HB2	2:D:89:TYR:OH	2.19	0.42
1:A:227:MET:HE1	1:A:249:LEU:HB2	2.00	0.42
1:A:262:LYS:HA	1:A:262:LYS:HD3	1.90	0.42
2:D:129:LYS:HD2	2:D:129:LYS:N	2.35	0.42
1:C:277:VAL:O	1:C:283:ALA:HB2	2.19	0.42
1:A:8:HIS:ND1	1:A:123:PRO:HA	2.35	0.42
1:C:186:PHE:C	1:C:187:ILE:HD12	2.45	0.42
1:A:152:LEU:HA	1:A:155:LEU:HD11	2.01	0.42
1:C:227:MET:HE2	1:C:249:LEU:HB2	2.02	0.42
2:D:18:ILE:O	2:D:58:LEU:HD12	2.20	0.42
2:B:127:VAL:HA	2:B:136:LEU:HD23	2.00	0.41
1:A:29:LYS:HZ1	1:A:308:LEU:HD21	1.85	0.41
1:A:252:SER:O	1:A:255:HIS:HB3	2.21	0.41
1:A:226:TYR:CZ	1:A:266:PRO:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:PRO:HG2	2:B:145:PHE:CD2	2.54	0.41
2:B:136:LEU:O	2:B:144:GLU:HA	2.19	0.41
2:D:61:ILE:HG22	2:D:64:THR:HB	2.02	0.41
1:A:50:GLU:HG3	1:A:107:PRO:HD3	2.02	0.41
2:B:28:LYS:O	2:B:32:LEU:HB2	2.20	0.41
1:C:201:MET:SD	1:C:201:MET:C	3.03	0.41
2:D:125:PHE:HB3	2:D:136:LEU:HD22	2.02	0.41
1:A:45:ALA:HB2	1:A:99:VAL:HG21	2.02	0.41
1:A:197:TYR:HE2	2:B:143:LYS:HD3	1.85	0.41
2:B:111:ASN:O	2:B:117:HIS:CE1	2.74	0.41
1:C:109:GLU:OE2	2:D:113:ASN:HB3	2.20	0.41
1:A:54:ARG:HE	4:A:311:PCT:H1P2	1.86	0.41
1:C:160:VAL:HG11	1:C:215:ILE:HD11	2.02	0.41
2:D:21:ILE:HB	2:D:57:ASP:O	2.20	0.41
1:A:296:ARG:O	1:A:300:LEU:HG	2.21	0.41
2:B:30:LEU:HA	2:B:35:LEU:HD12	2.02	0.41
2:B:96:ARG:HA	2:B:97:PRO:HD3	1.89	0.41
1:A:237:PRO:HA	1:A:240:TYR:CD1	2.57	0.40
1:C:256:ASN:OD1	1:C:256:ASN:N	2.54	0.40
1:C:111:ALA:O	1:C:114:LEU:HB3	2.21	0.40
1:A:189:PRO:HD3	1:A:247:PHE:CE1	2.56	0.40
2:D:50:SER:N	2:D:54:GLY:O	2.54	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	308/310 (99%)	283 (92%)	23 (8%)	2 (1%)	21	51
1	C	308/310 (99%)	285 (92%)	19 (6%)	4 (1%)	9	31
2	B	144/153 (94%)	120 (83%)	18 (12%)	6 (4%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	144/153 (94%)	113 (78%)	25 (17%)	6 (4%)	2	7
All	All	904/926 (98%)	801 (89%)	85 (9%)	18 (2%)	6	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	34	LYS
2	D	105	ASN
2	B	24	GLN
2	B	132	ASN
2	D	54	GLY
2	B	9	VAL
2	B	88	ASN
2	B	47	ASN
1	C	154	ASN
2	D	48	LEU
2	D	133	ASP
1	A	41	HIS
2	D	13	LYS
1	C	132	ASN
2	D	49	PRO
1	C	237	PRO
1	A	166	GLY
1	C	270	VAL

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	261/261 (100%)	234 (90%)	27 (10%)	7	23
1	C	261/261 (100%)	238 (91%)	23 (9%)	9	29
2	B	129/136 (95%)	109 (84%)	20 (16%)	2	9
2	D	129/136 (95%)	108 (84%)	21 (16%)	2	8
All	All	780/794 (98%)	689 (88%)	91 (12%)	5	18

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	34	PRO
1	A	40	LYS
1	A	50	GLU
1	A	65	ARG
1	A	74	SER
1	A	75	ASP
1	A	80	SER
1	A	105	ARG
1	A	108	GLN
1	A	113	ARG
1	A	114	LEU
1	A	117	GLU
1	A	125	LEU
1	A	221	GLU
1	A	233	GLU
1	A	237	PRO
1	A	242	ASN
1	A	246	GLN
1	A	252	SER
1	A	253	ASP
1	A	264	LEU
1	A	269	ARG
1	A	279	LYS
1	A	285	TYR
1	A	296	ARG
1	A	308	LEU
2	B	12	ILE
2	B	19	ASP
2	B	24	GLN
2	B	32	LEU
2	B	53	MET
2	B	61	ILE
2	B	72	ASP
2	B	76	LEU
2	B	82	THR
2	B	84	ASN
2	B	85	ARG
2	B	86	ILE
2	B	88	ASN
2	B	95	SER
2	B	98	SER

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Mol	Chain	Res	Type
2	B	103	ILE
2	B	104	ASP
2	B	128	ARG
2	B	132	ASN
2	B	153	ASN
1	C	2	ASN
1	C	17	ARG
1	C	37	GLU
1	C	38	LEU
1	C	40	LYS
1	C	59	PHE
1	C	65	ARG
1	C	69	SER
1	C	71	VAL
1	C	81	LEU
1	C	113	ARG
1	C	114	LEU
1	C	146	GLN
1	C	154	ASN
1	C	198	ILE
1	C	213	SER
1	C	221	GLU
1	C	224	ILE
1	C	232	LYS
1	C	237	PRO
1	C	258	LYS
1	C	262	LYS
1	C	307	ASP
2	D	30	LEU
2	D	34	LYS
2	D	36	THR
2	D	38	THR
2	D	40	GLN
2	D	43	THR
2	D	52	GLU
2	D	55	ARG
2	D	58	LEU
2	D	61	ILE
2	D	62	GLU
2	D	79	PRO
2	D	82	THR
2	D	92	VAL

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Mol	Chain	Res	Type
2	D	101	GLU
2	D	102	ARG
2	D	112	SER
2	D	123	SER
2	D	128	ARG
2	D	137	LYS
2	D	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	21	ASN
1	A	60	GLN
1	A	108	GLN
1	A	134	HIS
1	A	231	GLN
1	A	242	ASN
2	B	40	GLN
2	B	63	ASN
2	B	113	ASN
2	B	117	HIS
2	B	153	ASN
1	C	13	ASN
1	C	60	GLN
1	C	64	HIS
1	C	154	ASN
2	D	80	GLN
2	D	111	ASN
2	D	117	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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
3	MLI	A	312	-	6,6,6	3.91	3 (50%)	7,7,7	3.97	3 (42%)
4	PCT	C	311	-	7,7,7	3.27	5 (71%)	9,10,10	1.95	2 (22%)
3	MLI	C	312	-	6,6,6	2.22	2 (33%)	7,7,7	4.91	4 (57%)
4	PCT	A	311	-	7,7,7	3.09	3 (42%)	9,10,10	2.14	5 (55%)

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	MLI	A	312	-	-	1/4/4/4	-
4	PCT	C	311	-	-	4/4/5/5	-
3	MLI	C	312	-	-	0/4/4/4	-
4	PCT	A	311	-	-	4/4/5/5	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	312	MLI	C1-C3	7.85	1.63	1.51
4	C	311	PCT	P-O1P	5.61	1.61	1.50
4	A	311	PCT	P-C1P	5.21	1.87	1.79
4	A	311	PCT	P-O1P	5.06	1.60	1.50
4	C	311	PCT	P-C1P	4.76	1.87	1.79
3	A	312	MLI	O9-C3	-4.26	1.16	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	312	MLI	O9-C3	-3.89	1.18	1.30
4	C	311	PCT	P-O3P	3.19	1.62	1.55
3	C	312	MLI	O7-C2	-2.94	1.21	1.30
4	A	311	PCT	C1P-C1	2.78	1.54	1.51
3	A	312	MLI	O7-C2	-2.53	1.22	1.30
4	C	311	PCT	P-O2P	2.32	1.60	1.55
4	C	311	PCT	C1P-C1	2.13	1.54	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	312	MLI	O9-C3-O8	-8.79	100.74	123.33
3	C	312	MLI	O6-C2-C1	-7.69	100.21	122.11
3	C	312	MLI	O7-C2-O6	6.99	141.32	123.33
3	C	312	MLI	O9-C3-O8	-6.37	106.95	123.33
3	A	312	MLI	O9-C3-C1	4.85	129.53	114.51
4	C	311	PCT	O1-C1-C1P	4.03	124.11	119.86
3	C	312	MLI	O8-C3-C1	3.88	133.17	122.11
4	A	311	PCT	O1P-P-C1P	-3.27	103.54	111.10
4	A	311	PCT	O3P-P-O2P	2.95	116.37	107.96
4	C	311	PCT	O1P-P-C1P	-2.80	104.62	111.10
3	A	312	MLI	O8-C3-C1	2.66	129.69	122.11
4	A	311	PCT	O1-C1-C1P	2.44	122.43	119.86
4	A	311	PCT	C1P-C1-N1	2.36	118.23	115.41
4	A	311	PCT	O3P-P-C1P	2.29	111.66	106.84

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	311	PCT	C1-C1P-P-O1P
4	A	311	PCT	C1-C1P-P-O3P
4	C	311	PCT	C1-C1P-P-O1P
4	A	311	PCT	C1-C1P-P-O2P
4	C	311	PCT	C1-C1P-P-O2P
4	A	311	PCT	O1-C1-C1P-P
4	C	311	PCT	O1-C1-C1P-P
4	C	311	PCT	C1-C1P-P-O3P
3	A	312	MLI	C3-C1-C2-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	311	PCT	1	0
4	A	311	PCT	1	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.