



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:50 AM UTC

PDB ID : 1QU4 / pdb_00001qu4
Title : CRYSTAL STRUCTURE OF TRYPANOSOMA BRUCEI ORNITHINE DE-CARBOXYLASE
Authors : Grishin, N.V.; Osterman, A.L.; Brooks, H.B.; Phillips, M.A.; Goldsmith, E.J.
Deposited on : 1999-07-06
Resolution : 2.90 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

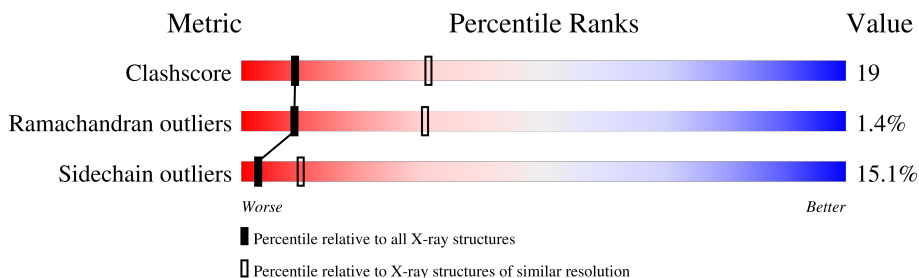
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	425	 43% 28% 10% • 16%
1	B	425	 41% 28% 13% • 16%
1	C	425	 45% 28% 9% • 16%
1	D	425	 43% 29% 10% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11176 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 ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2779	1786	460	518	15			
1	B	356	Total	C	N	O	S	0	0	0
			2779	1786	460	518	15			
1	C	356	Total	C	N	O	S	0	0	0
			2779	1786	460	518	15			
1	D	356	Total	C	N	O	S	0	0	0
			2779	1786	460	518	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	LYS	engineered mutation	UNP P07805
A	2	ALA	SER	engineered mutation	UNP P07805
B	1	GLY	LYS	engineered mutation	UNP P07805
B	2	ALA	SER	engineered mutation	UNP P07805
C	1	GLY	LYS	engineered mutation	UNP P07805
C	2	ALA	SER	engineered mutation	UNP P07805
D	1	GLY	LYS	engineered mutation	UNP P07805
D	2	ALA	SER	engineered mutation	UNP P07805

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



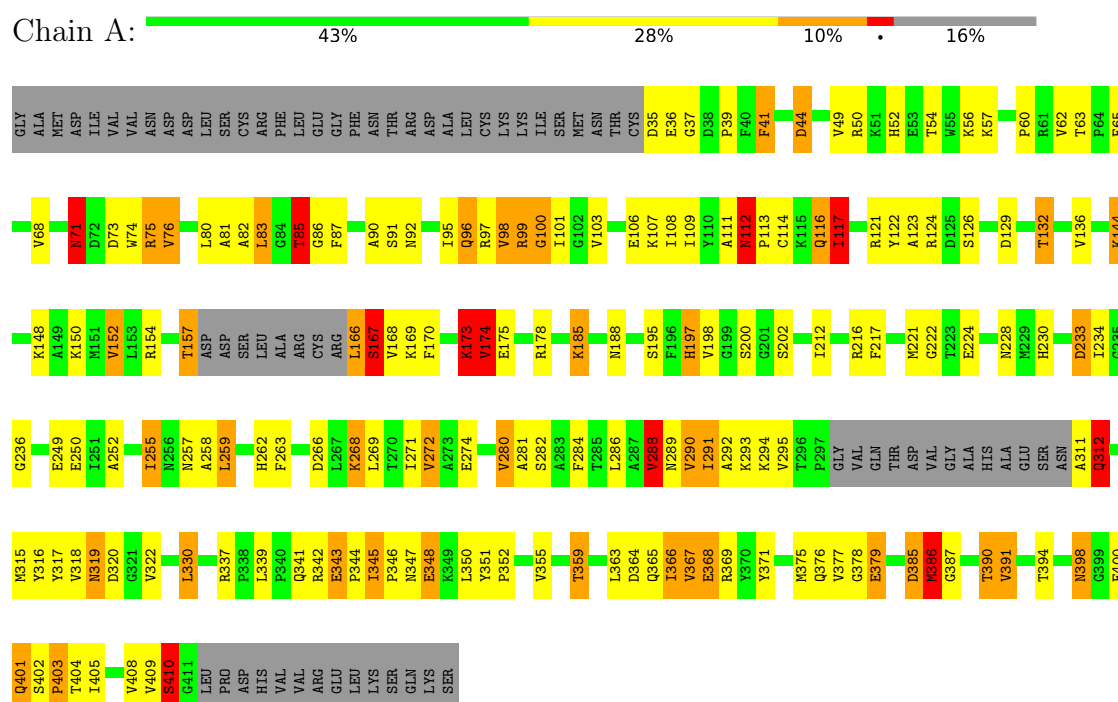
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

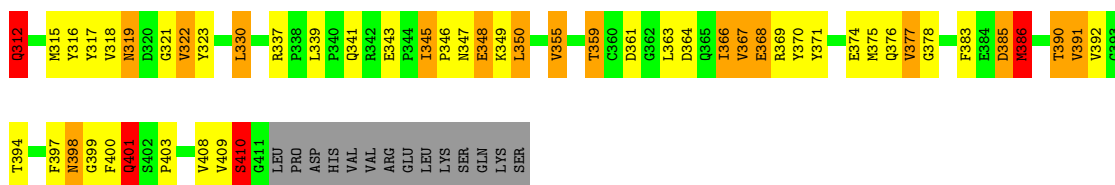
3 Residue-property plots

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.

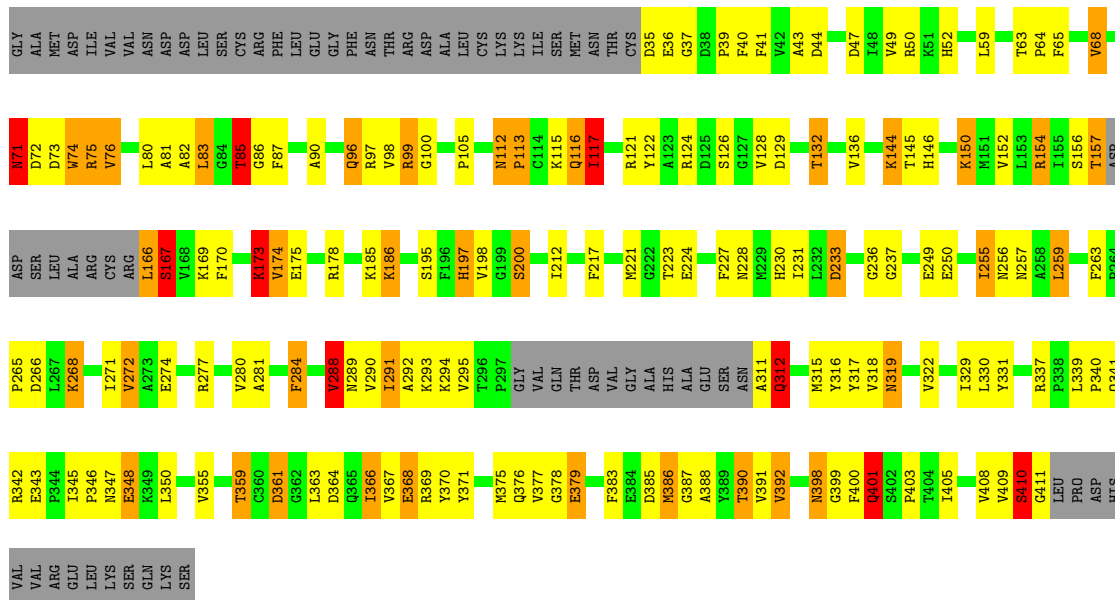
Note EDS was not executed.

• Molecule 1: ORNITHINE DECARBOXYLASE

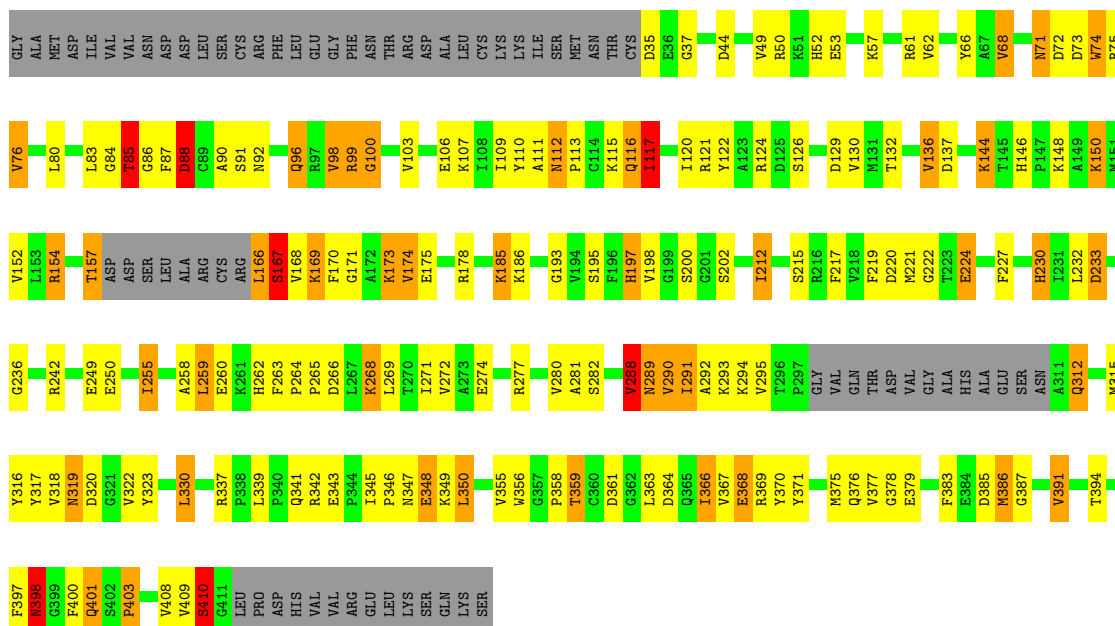




- Molecule 1: ORNITHINE DECARBOXYLASE



- Molecule 1: ORNITHINE DECARBOXYLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.80Å 151.70Å 85.35Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.245 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11176	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: 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	0.83	0/2848	2.00	88/3867 (2.3%)
1	B	0.84	0/2848	2.01	90/3867 (2.3%)
1	C	0.85	0/2848	1.97	80/3867 (2.1%)
1	D	0.86	0/2848	1.97	74/3867 (1.9%)
All	All	0.84	0/11392	1.99	332/15468 (2.1%)

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
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	SER	CA-C-O	10.80	132.51	120.31
1	A	288	VAL	N-CA-CB	-10.49	96.20	111.52
1	B	167	SER	CA-C-O	10.15	131.78	120.31
1	A	167	SER	CA-C-O	9.59	131.75	120.43
1	C	319	ASN	CA-CB-CG	9.52	122.12	112.60
1	C	284	PHE	CA-C-O	-9.46	110.68	120.71
1	D	255	ILE	CA-C-O	-9.33	111.28	121.17
1	B	319	ASN	CA-CB-CG	9.27	121.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	ASN	CA-CB-CG	9.24	121.84	112.60
1	B	52	HIS	CA-CB-CG	-9.21	104.59	113.80
1	D	288	VAL	N-CA-CB	-9.21	98.07	111.52
1	C	288	VAL	N-CA-CB	-9.05	96.59	111.44
1	A	82	ALA	CA-C-O	-9.00	111.01	120.55
1	C	167	SER	CA-C-O	8.93	130.96	120.43
1	D	87	PHE	CA-CB-CG	-8.86	104.94	113.80
1	B	154	ARG	NE-CZ-NH1	-8.74	112.76	121.50
1	D	154	ARG	NE-CZ-NH1	-8.71	112.79	121.50
1	D	233	ASP	CA-CB-CG	8.52	121.12	112.60
1	A	319	ASN	CA-CB-CG	8.36	120.96	112.60
1	A	173	LYS	CA-C-O	-8.34	112.71	121.55
1	B	288	VAL	N-CA-CB	-8.23	99.50	111.52
1	B	87	PHE	CA-CB-CG	-8.15	105.65	113.80
1	C	266	ASP	O-C-N	-8.03	114.01	123.41
1	C	295	VAL	CA-C-O	-7.98	112.09	120.39
1	A	167	SER	N-CA-C	7.97	121.46	108.55
1	A	56	LYS	CA-C-O	-7.97	112.00	120.92
1	D	193	GLY	O-C-N	-7.94	116.29	123.92
1	D	386	MET	CA-C-N	7.86	128.70	119.98
1	D	386	MET	C-N-CA	7.86	128.70	119.98
1	C	154	ARG	NE-CZ-NH1	-7.73	113.77	121.50
1	B	386	MET	CA-C-N	7.71	128.48	120.00
1	B	386	MET	C-N-CA	7.71	128.48	120.00
1	D	52	HIS	CA-CB-CG	-7.56	106.24	113.80
1	C	257	ASN	OD1-CG-ND2	-7.55	115.05	122.60
1	B	65	PHE	CA-C-O	-7.52	112.42	120.46
1	D	167	SER	N-CA-C	7.51	119.81	108.46
1	B	368	GLU	CB-CG-CD	7.50	125.36	112.60
1	A	266	ASP	O-C-N	-7.50	114.64	123.41
1	B	167	SER	N-CA-C	7.47	119.75	108.46
1	B	233	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	368	GLU	CB-CG-CD	7.36	125.11	112.60
1	D	368	GLU	CB-CG-CD	7.36	125.10	112.60
1	B	154	ARG	CD-NE-CZ	-7.33	114.14	124.40
1	C	52	HIS	CA-CB-CG	-7.31	106.49	113.80
1	D	96	GLN	CA-CB-CG	7.30	128.70	114.10
1	A	272	VAL	N-CA-CB	-7.25	98.95	112.36
1	A	132	THR	CA-CB-OG1	-7.24	98.73	109.60
1	A	216	ARG	NE-CZ-NH1	7.22	128.72	121.50
1	C	82	ALA	CA-C-O	-7.21	112.91	120.55
1	D	154	ARG	NE-CZ-NH2	7.20	125.68	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ASP	CA-C-O	-7.17	113.27	121.65
1	A	85	THR	N-CA-CB	-7.16	100.12	110.36
1	A	188	ASN	OD1-CG-ND2	7.12	129.72	122.60
1	D	400	PHE	CA-CB-CG	-7.03	106.77	113.80
1	C	112	ASN	CA-CB-CG	7.03	119.63	112.60
1	C	167	SER	N-CA-C	7.02	119.92	108.55
1	C	173	LYS	CA-C-O	-6.97	114.16	121.55
1	B	112	ASN	CA-CB-CG	6.96	119.56	112.60
1	B	152	VAL	CA-C-O	-6.95	113.13	120.57
1	A	96	GLN	CA-CB-CG	6.94	127.98	114.10
1	D	107	LYS	CB-CG-CD	6.92	127.23	111.30
1	A	52	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	116	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	B	256	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	D	99	ARG	CD-NE-CZ	-6.75	114.94	124.40
1	A	255	ILE	CA-C-O	-6.70	114.30	121.27
1	B	82	ALA	CA-C-O	-6.68	113.47	120.55
1	A	174	VAL	CA-C-N	6.68	130.13	120.38
1	A	174	VAL	C-N-CA	6.68	130.13	120.38
1	B	368	GLU	N-CA-CB	6.67	120.20	110.26
1	C	368	GLU	CB-CG-CD	6.66	123.93	112.60
1	B	117	ILE	N-CA-CB	6.64	120.55	110.58
1	C	116	GLN	CA-C-O	-6.64	113.89	121.19
1	A	152	VAL	O-C-N	-6.61	115.69	123.03
1	A	320	ASP	CA-C-O	-6.59	114.21	121.33
1	A	39	PRO	CA-C-O	-6.54	114.02	122.12
1	A	272	VAL	CB-CA-C	6.53	121.34	110.30
1	A	44	ASP	CA-C-O	6.52	127.88	120.84
1	D	277	ARG	CD-NE-CZ	6.48	133.48	124.40
1	B	211	ALA	O-C-N	6.46	128.96	122.12
1	A	390	THR	CA-C-O	-6.45	111.29	120.51
1	B	230	HIS	CA-CB-CG	-6.44	107.36	113.80
1	A	96	GLN	N-CA-CB	6.43	119.33	110.01
1	B	366	ILE	N-CA-C	-6.42	106.29	111.81
1	A	295	VAL	CA-C-O	-6.42	113.68	120.48
1	A	263	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	295	VAL	CA-C-O	-6.40	113.70	120.48
1	C	289	ASN	CA-CB-CG	-6.38	106.22	112.60
1	B	367	VAL	CA-C-O	-6.38	114.07	120.90
1	A	112	ASN	CA-CB-CG	6.37	118.97	112.60
1	B	400	PHE	CA-CB-CG	-6.36	107.44	113.80
1	B	40	PHE	O-C-N	6.36	130.60	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	GLU	CA-C-O	-6.35	113.81	120.55
1	B	101	ILE	CA-C-O	6.33	126.47	120.14
1	C	117	ILE	CB-CG1-CD1	-6.31	100.54	113.80
1	A	330	LEU	CA-C-O	-6.31	114.20	120.70
1	B	193	GLY	O-C-N	-6.30	117.87	123.92
1	D	391	VAL	O-C-N	-6.30	115.71	121.89
1	B	96	GLN	CA-CB-CG	6.29	126.68	114.10
1	B	321	GLY	CA-C-O	-6.28	114.49	121.21
1	D	230	HIS	CA-CB-CG	-6.27	107.53	113.80
1	B	197	HIS	CA-CB-CG	-6.27	107.53	113.80
1	C	379	GLU	O-C-N	-6.25	113.92	122.23
1	D	255	ILE	O-C-N	6.24	128.02	121.91
1	C	59	LEU	CA-C-O	6.19	127.61	121.29
1	B	228	ASN	CA-CB-CG	6.19	118.79	112.60
1	B	99	ARG	CD-NE-CZ	-6.18	115.74	124.40
1	A	371	TYR	CA-CB-CG	-6.17	102.80	113.90
1	B	371	TYR	CA-CB-CG	-6.15	102.83	113.90
1	C	228	ASN	CA-CB-CG	6.13	118.73	112.60
1	D	197	HIS	CA-CB-CG	-6.12	107.68	113.80
1	B	99	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	D	85	THR	N-CA-CB	-6.10	101.38	110.17
1	A	95	ILE	CA-C-O	-6.07	114.73	121.05
1	C	40	PHE	CA-C-O	-6.07	114.77	121.33
1	C	366	ILE	N-CA-C	-6.07	106.59	111.81
1	A	60	PRO	CB-CA-C	6.05	120.51	111.68
1	A	99	ARG	O-C-N	-6.05	115.84	122.07
1	B	132	THR	CA-CB-OG1	-6.05	100.53	109.60
1	C	124	ARG	CD-NE-CZ	6.05	132.87	124.40
1	D	74	TRP	CA-C-O	-6.02	114.12	120.63
1	C	113	PRO	CA-C-O	-6.00	110.49	119.86
1	D	72	ASP	CA-CB-CG	-6.00	106.59	112.60
1	C	197	HIS	CA-CB-CG	-5.99	107.81	113.80
1	D	323	TYR	N-CA-C	-5.97	105.76	113.16
1	B	385	ASP	CA-C-O	-5.96	114.67	121.65
1	C	43	ALA	CA-C-O	-5.96	113.98	120.36
1	A	106	GLU	CA-C-O	-5.96	112.28	119.49
1	C	366	ILE	CA-C-O	-5.94	113.79	120.32
1	B	49	VAL	O-C-N	-5.92	115.84	121.94
1	A	57	LYS	CA-C-O	-5.91	114.16	120.42
1	B	62	VAL	N-CA-C	5.90	116.36	107.80
1	D	117	ILE	N-CA-CB	5.89	118.56	110.54
1	D	319	ASN	CA-CB-CG	5.89	118.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	ASP	CA-C-O	-5.88	114.42	120.54
1	A	378	GLY	N-CA-C	-5.88	107.28	114.92
1	C	75	ARG	CA-C-N	-5.87	112.08	120.42
1	C	75	ARG	C-N-CA	-5.87	112.08	120.42
1	C	265	PRO	O-C-N	5.87	130.57	122.64
1	A	252	ALA	N-CA-CB	5.86	118.73	110.12
1	C	284	PHE	O-C-N	5.86	130.65	123.21
1	A	233	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	397	PHE	CA-CB-CG	5.86	119.66	113.80
1	D	249	GLU	CA-C-O	-5.86	114.34	120.55
1	D	100	GLY	CA-C-O	-5.84	110.40	120.57
1	B	289	ASN	CA-C-N	-5.83	113.73	122.01
1	B	289	ASN	C-N-CA	-5.83	113.73	122.01
1	D	262	HIS	CA-C-O	5.83	125.20	118.97
1	A	345	ILE	CB-CA-C	5.81	116.69	110.53
1	C	186	LYS	N-CA-CB	5.81	118.67	110.12
1	A	258	ALA	CA-C-O	5.80	126.91	120.82
1	A	75	ARG	CA-C-N	-5.79	112.19	120.42
1	A	75	ARG	C-N-CA	-5.79	112.19	120.42
1	D	92	ASN	CA-CB-CG	5.78	118.38	112.60
1	D	366	ILE	CA-C-O	-5.78	113.96	120.32
1	B	277	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	A	117	ILE	N-CA-CB	5.77	118.39	110.54
1	A	386	MET	CA-C-O	5.77	127.75	120.65
1	C	361	ASP	O-C-N	-5.77	116.75	123.27
1	D	368	GLU	N-CA-CB	5.76	118.85	110.26
1	C	96	GLN	N-CA-CB	5.76	118.36	110.01
1	A	280	VAL	N-CA-C	5.76	119.18	113.71
1	D	387	GLY	CA-C-O	-5.74	114.83	120.75
1	C	59	LEU	O-C-N	-5.74	116.38	121.20
1	A	289	ASN	CA-CB-CG	-5.74	106.86	112.60
1	C	85	THR	N-CA-CB	-5.74	102.15	110.36
1	D	116	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	B	322	VAL	CA-C-O	-5.73	112.31	119.70
1	A	391	VAL	N-CA-C	5.73	116.37	110.36
1	A	148	LYS	CA-CB-CG	5.72	125.54	114.10
1	C	63	THR	CA-C-O	-5.72	115.06	119.46
1	D	62	VAL	N-CA-C	5.71	115.83	107.37
1	A	319	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	C	96	GLN	CA-CB-CG	5.70	125.51	114.10
1	D	220	ASP	CA-C-O	-5.70	114.51	120.55
1	A	252	ALA	CA-C-O	-5.70	114.51	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	GLN	N-CA-CB	5.70	118.33	110.07
1	D	289	ASN	CA-C-N	-5.69	113.93	122.01
1	D	289	ASN	C-N-CA	-5.69	113.93	122.01
1	C	249	GLU	CA-C-O	-5.69	114.52	120.55
1	C	231	ILE	CB-CA-C	-5.68	102.22	110.63
1	B	385	ASP	CA-CB-CG	-5.68	106.92	112.60
1	C	272	VAL	N-CA-CB	-5.68	101.85	112.36
1	A	124	ARG	CD-NE-CZ	5.68	132.35	124.40
1	A	63	THR	CA-C-O	-5.66	115.14	119.32
1	A	234	ILE	O-C-N	-5.66	115.50	122.57
1	B	272	VAL	CB-CA-C	5.65	119.84	110.30
1	B	88	ASP	CA-C-O	-5.64	114.67	120.54
1	D	366	ILE	N-CA-C	-5.63	106.97	111.81
1	D	148	LYS	O-C-N	-5.63	115.34	122.26
1	C	400	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	403	PRO	N-CA-CB	-5.61	98.18	103.17
1	A	400	PHE	CA-CB-CG	-5.61	108.19	113.80
1	D	398	ASN	CA-C-N	-5.61	116.77	123.44
1	D	398	ASN	C-N-CA	-5.61	116.77	123.44
1	D	193	GLY	CA-C-O	5.60	127.23	121.35
1	C	383	PHE	CA-CB-CG	-5.60	108.20	113.80
1	C	271	ILE	O-C-N	-5.60	116.99	122.93
1	D	167	SER	O-C-N	-5.60	117.36	123.52
1	C	340	PRO	CA-C-O	-5.59	114.60	121.31
1	C	41	PHE	CA-C-N	-5.59	115.75	122.90
1	C	41	PHE	C-N-CA	-5.59	115.75	122.90
1	C	233	ASP	CA-CB-CG	5.59	118.19	112.60
1	D	99	ARG	CA-CB-CG	-5.57	102.97	114.10
1	B	262	HIS	CA-C-O	5.55	124.91	118.97
1	C	99	ARG	O-C-N	-5.54	116.11	122.09
1	C	255	ILE	CA-C-O	-5.52	115.32	121.17
1	C	390	THR	CA-C-O	-5.52	112.62	120.51
1	B	64	PRO	CA-C-N	-5.50	115.30	123.11
1	B	64	PRO	C-N-CA	-5.50	115.30	123.11
1	A	123	ALA	CA-C-O	-5.50	114.72	120.55
1	D	295	VAL	CA-C-O	-5.50	114.65	120.48
1	D	289	ASN	CA-CB-CG	-5.50	107.10	112.60
1	D	371	TYR	CA-CB-CG	-5.50	104.01	113.90
1	A	117	ILE	CA-C-O	-5.49	115.24	120.95
1	D	154	ARG	CD-NE-CZ	-5.49	116.72	124.40
1	C	81	ALA	CA-C-N	5.49	127.64	120.28
1	C	81	ALA	C-N-CA	5.49	127.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	ASP	N-CA-CB	-5.48	101.20	111.13
1	A	97	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	B	289	ASN	CA-CB-CG	-5.47	107.13	112.60
1	C	227	PHE	CA-C-O	-5.47	114.81	121.05
1	C	47	ASP	CA-CB-CG	-5.45	107.15	112.60
1	B	391	VAL	N-CA-C	5.45	116.83	110.62
1	A	107	LYS	CB-CG-CD	5.43	123.79	111.30
1	A	92	ASN	CA-CB-CG	5.42	118.03	112.60
1	C	72	ASP	CA-CB-CG	-5.42	107.18	112.60
1	D	403	PRO	CA-C-O	-5.42	115.58	121.27
1	C	371	TYR	CA-CB-CG	-5.42	104.15	113.90
1	C	361	ASP	CA-C-N	5.42	126.91	120.14
1	C	361	ASP	C-N-CA	5.42	126.91	120.14
1	B	266	ASP	O-C-N	-5.42	117.07	123.41
1	C	99	ARG	CB-CA-C	5.41	119.44	110.90
1	A	124	ARG	O-C-N	-5.41	116.50	122.07
1	B	330	LEU	N-CA-C	5.39	117.02	111.03
1	C	392	VAL	O-C-N	-5.39	115.91	122.06
1	A	87	PHE	CA-CB-CG	-5.39	108.41	113.80
1	B	290	VAL	N-CA-CB	5.39	117.64	111.39
1	C	68	VAL	O-C-N	-5.39	116.43	121.87
1	D	266	ASP	N-CA-CB	-5.38	101.47	110.99
1	A	262	HIS	CA-C-O	5.38	124.73	118.97
1	C	331	TYR	CA-CB-CG	5.37	123.57	113.90
1	D	171	GLY	O-C-N	-5.36	115.73	122.70
1	B	181	LEU	CA-C-O	-5.36	113.81	119.97
1	A	365	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	B	92	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	D	146	HIS	CA-C-O	5.34	127.47	120.16
1	C	378	GLY	CA-C-O	-5.33	113.56	119.27
1	A	402	SER	CB-CA-C	5.32	117.94	109.96
1	B	96	GLN	N-CA-CB	5.32	117.72	110.01
1	B	53	GLU	CB-CA-C	5.32	119.32	110.81
1	B	155	ILE	CA-C-O	-5.31	114.66	121.40
1	C	132	THR	CA-CB-OG1	-5.31	101.64	109.60
1	D	130	VAL	CA-C-O	-5.30	114.59	120.74
1	B	151	MET	CA-C-O	-5.29	114.67	120.43
1	D	227	PHE	CA-C-O	-5.29	115.02	121.36
1	C	105	PRO	O-C-N	-5.28	115.89	122.23
1	A	36	GLU	CB-CG-CD	5.28	121.58	112.60
1	B	401	GLN	CA-C-N	-5.28	113.92	122.48
1	B	401	GLN	C-N-CA	-5.28	113.92	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	PHE	CA-C-O	-5.27	115.41	121.47
1	A	379	GLU	CB-CG-CD	5.26	121.55	112.60
1	B	147	PRO	CA-C-O	-5.26	111.61	118.86
1	A	62	VAL	N-CA-C	5.25	115.41	107.75
1	A	255	ILE	O-C-N	5.25	127.19	121.94
1	A	41	PHE	CA-C-N	-5.24	115.82	122.37
1	A	41	PHE	C-N-CA	-5.24	115.82	122.37
1	A	255	ILE	N-CA-CB	5.23	116.32	110.51
1	C	256	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	D	258	ALA	CA-C-O	5.23	126.31	120.82
1	C	378	GLY	N-CA-C	-5.22	108.47	114.69
1	B	272	VAL	N-CA-CB	-5.22	102.70	112.36
1	B	345	ILE	CA-C-O	5.22	122.58	119.19
1	B	390	THR	CA-C-O	-5.22	113.04	120.51
1	B	273	ALA	N-CA-CB	5.22	119.92	111.21
1	B	169	LYS	CA-C-O	-5.21	115.33	120.70
1	C	36	GLU	CB-CG-CD	5.21	121.45	112.60
1	C	97	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	B	323	TYR	N-CA-CB	5.20	118.40	110.44
1	B	288	VAL	O-C-N	-5.20	117.59	123.20
1	D	320	ASP	CA-C-O	-5.20	115.72	121.33
1	D	397	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	64	PRO	CB-CA-C	-5.19	105.03	111.11
1	D	124	ARG	O-C-N	-5.19	116.72	122.07
1	A	228	ASN	CA-CB-CG	5.18	117.78	112.60
1	D	53	GLU	O-C-N	-5.17	116.71	122.09
1	D	84	GLY	CA-C-N	5.17	129.06	120.94
1	D	84	GLY	C-N-CA	5.17	129.06	120.94
1	D	330	LEU	N-CA-C	5.17	116.72	111.14
1	B	101	ILE	O-C-N	-5.17	116.78	122.05
1	B	154	ARG	CA-C-O	-5.16	114.81	120.43
1	D	263	PHE	CA-CB-CG	5.16	118.96	113.80
1	D	57	LYS	CA-C-O	-5.16	114.52	120.24
1	C	401	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	B	41	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	345	ILE	CB-CA-C	5.11	115.95	110.53
1	B	107	LYS	CB-CG-CD	5.11	123.05	111.30
1	B	81	ALA	CA-C-N	5.10	127.12	120.28
1	B	81	ALA	C-N-CA	5.10	127.12	120.28
1	C	385	ASP	CA-C-O	-5.10	115.68	121.65
1	A	197	HIS	CA-CB-CG	-5.09	108.71	113.80
1	B	85	THR	N-CA-CB	-5.09	102.56	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ALA	CA-C-N	5.08	127.09	120.28
1	A	81	ALA	C-N-CA	5.08	127.09	120.28
1	C	47	ASP	O-C-N	5.07	127.50	122.12
1	A	404	THR	CA-C-O	-5.07	115.97	121.44
1	B	200	SER	CA-C-O	-5.07	113.36	119.59
1	A	54	THR	O-C-N	5.06	127.49	122.12
1	B	97	ARG	CA-C-O	-5.06	115.50	121.07
1	B	36	GLU	CB-CG-CD	5.06	121.21	112.60
1	B	125	ASP	CA-C-O	-5.06	112.47	119.05
1	B	263	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	366	ILE	CA-C-O	-5.06	114.76	120.32
1	D	224	GLU	CA-C-O	-5.06	115.49	120.90
1	C	74	TRP	O-C-N	-5.05	116.77	122.12
1	D	169	LYS	CA-C-O	-5.05	115.50	120.70
1	B	366	ILE	CA-C-O	-5.05	114.77	120.32
1	D	212	ILE	O-C-N	5.05	127.03	121.83
1	A	257	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	C	87	PHE	CA-CB-CG	-5.04	108.76	113.80
1	C	383	PHE	CA-C-N	-5.04	112.50	122.02
1	C	383	PHE	C-N-CA	-5.04	112.50	122.02
1	D	383	PHE	CA-CB-CG	-5.04	108.76	113.80
1	B	383	PHE	CA-CB-CG	-5.03	108.77	113.80
1	C	263	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	249	GLU	CA-C-O	-5.03	115.22	120.55
1	A	99	ARG	CB-CA-C	5.02	118.77	110.88
1	A	367	VAL	CA-C-O	-5.02	115.27	120.64
1	B	99	ARG	CA-CB-CG	-5.02	104.06	114.10
1	A	289	ASN	CA-C-N	-5.01	114.89	122.01
1	A	289	ASN	C-N-CA	-5.01	114.89	122.01
1	C	329	ILE	CA-C-O	-5.00	115.87	121.17

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	SER	Peptide
1	B	167	SER	Peptide
1	C	167	SER	Peptide
1	D	167	SER	Peptide

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	2779	0	2729	108	0
1	B	2779	0	2729	123	0
1	C	2779	0	2729	105	0
1	D	2779	0	2729	109	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
All	All	11176	0	10944	412	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 19.

All (412) 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:A:166:LEU:HD13	1:A:167:SER:H	1.22	1.04
1:C:166:LEU:HD13	1:C:167:SER:H	1.20	1.03
1:A:366:ILE:HG22	1:A:367:VAL:HG23	1.42	1.01
1:D:166:LEU:HD13	1:D:167:SER:H	1.24	0.98
1:D:366:ILE:HG22	1:D:367:VAL:HG23	1.42	0.98
1:A:173:LYS:HZ1	1:A:174:VAL:H	1.11	0.97
1:B:166:LEU:HD13	1:B:167:SER:H	1.25	0.96
1:B:366:ILE:HG22	1:B:367:VAL:HG23	1.47	0.95
1:A:319:ASN:HD22	1:B:116:GLN:NE2	1.64	0.94
1:C:366:ILE:HG22	1:C:367:VAL:HG23	1.49	0.94
1:C:173:LYS:HZ2	1:C:174:VAL:H	1.06	0.94
1:A:319:ASN:HD22	1:B:116:GLN:HE22	1.14	0.93
1:B:173:LYS:HZ1	1:B:174:VAL:H	1.12	0.92
1:C:319:ASN:HD22	1:D:116:GLN:NE2	1.66	0.92
1:C:319:ASN:HD22	1:D:116:GLN:HE22	1.14	0.91
1:A:116:GLN:NE2	1:B:319:ASN:HD22	1.67	0.91
1:D:173:LYS:HZ1	1:D:174:VAL:H	1.18	0.89
1:C:116:GLN:NE2	1:D:319:ASN:HD22	1.70	0.88
1:A:116:GLN:HE22	1:B:319:ASN:HD22	1.21	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLN:HE22	1:D:319:ASN:HD22	1.19	0.87
1:B:288:VAL:HG13	1:B:318:VAL:HB	1.57	0.85
1:D:117:ILE:HD11	1:D:121:ARG:NH2	1.92	0.85
1:D:73:ASP:HB3	1:D:76:VAL:HG13	1.60	0.83
1:A:73:ASP:HB3	1:A:76:VAL:HG13	1.61	0.82
1:A:359:THR:HB	1:A:364:ASP:OD2	1.79	0.82
1:D:288:VAL:HG13	1:D:318:VAL:HB	1.62	0.81
1:B:292:ALA:HB3	1:B:317:TYR:HB2	1.60	0.81
1:C:359:THR:HB	1:C:364:ASP:OD2	1.80	0.81
1:A:117:ILE:HD11	1:A:121:ARG:NH2	1.94	0.81
1:A:217:PHE:CE2	1:A:221:MET:HE2	2.15	0.81
1:A:288:VAL:HG13	1:A:318:VAL:HB	1.61	0.81
1:A:173:LYS:HE3	1:A:175:GLU:OE2	1.83	0.79
1:B:359:THR:HB	1:B:364:ASP:OD2	1.83	0.78
1:A:292:ALA:HB3	1:A:317:TYR:HB2	1.64	0.78
1:B:117:ILE:HD11	1:B:121:ARG:NH2	1.99	0.78
1:C:288:VAL:HG13	1:C:318:VAL:HB	1.66	0.78
1:B:73:ASP:HB3	1:B:76:VAL:HG13	1.66	0.77
1:D:359:THR:HB	1:D:364:ASP:OD2	1.85	0.77
1:C:73:ASP:HB3	1:C:76:VAL:HG13	1.66	0.77
1:B:113:PRO:HG2	1:B:170:PHE:CD2	2.21	0.76
1:A:217:PHE:HE2	1:A:221:MET:HE2	1.51	0.74
1:C:157:THR:H	1:C:166:LEU:HD11	1.53	0.73
1:D:173:LYS:HE3	1:D:175:GLU:OE2	1.88	0.73
1:A:113:PRO:HG2	1:A:170:PHE:CD2	2.23	0.72
1:A:294:LYS:HB2	1:A:315:MET:HB2	1.73	0.70
1:C:292:ALA:HB3	1:C:317:TYR:HB2	1.72	0.70
1:A:166:LEU:CD1	1:A:167:SER:H	2.03	0.70
1:B:173:LYS:HE3	1:B:175:GLU:OE2	1.92	0.69
1:B:293:LYS:HE2	1:B:375:MET:O	1.92	0.69
1:C:166:LEU:HD13	1:C:167:SER:N	2.02	0.69
1:A:71:ASN:C	1:A:71:ASN:HD22	2.00	0.69
1:B:217:PHE:CE2	1:B:221:MET:HE2	2.28	0.69
1:B:217:PHE:HE2	1:B:221:MET:HE2	1.58	0.69
1:C:175:GLU:CD	1:C:175:GLU:H	2.01	0.69
1:D:113:PRO:HG2	1:D:170:PHE:CD2	2.28	0.69
1:D:217:PHE:CE2	1:D:221:MET:HE2	2.28	0.69
1:A:166:LEU:HD13	1:A:167:SER:N	2.04	0.68
1:D:157:THR:H	1:D:166:LEU:HD11	1.57	0.68
1:C:117:ILE:HD11	1:C:121:ARG:NH2	2.08	0.68
1:D:293:LYS:HE2	1:D:375:MET:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:H	1:A:166:LEU:HD11	1.59	0.67
1:C:173:LYS:HZ2	1:C:174:VAL:N	1.86	0.67
1:A:293:LYS:HE2	1:A:375:MET:O	1.95	0.67
1:C:217:PHE:CE2	1:C:221:MET:HE2	2.30	0.67
1:D:157:THR:HG21	1:D:198:VAL:HA	1.77	0.67
1:B:157:THR:H	1:B:166:LEU:HD11	1.58	0.67
1:B:71:ASN:C	1:B:71:ASN:HD22	2.03	0.66
1:B:132:THR:HG22	1:B:152:VAL:HB	1.78	0.66
1:B:167:SER:HB2	1:B:169:LYS:H	1.60	0.66
1:C:346:PRO:O	1:C:347:ASN:HB2	1.95	0.66
1:D:132:THR:HG22	1:D:152:VAL:HB	1.77	0.66
1:D:255:ILE:HG22	1:D:259:LEU:HD22	1.78	0.66
1:C:294:LYS:HB2	1:C:315:MET:HB2	1.79	0.65
1:D:217:PHE:HE2	1:D:221:MET:HE2	1.62	0.65
1:A:346:PRO:O	1:A:347:ASN:HB2	1.96	0.65
1:D:175:GLU:CD	1:D:175:GLU:H	2.05	0.65
1:D:292:ALA:HB3	1:D:317:TYR:HB2	1.78	0.64
1:A:132:THR:HG22	1:A:152:VAL:HB	1.80	0.64
1:C:293:LYS:HE2	1:C:375:MET:O	1.98	0.63
1:A:175:GLU:CD	1:A:175:GLU:H	2.07	0.63
1:D:85:THR:HG23	1:D:86:GLY:O	1.98	0.63
1:B:157:THR:HG21	1:B:198:VAL:HA	1.81	0.63
1:A:117:ILE:HD12	1:A:117:ILE:O	1.98	0.63
1:D:348:GLU:HG2	1:D:350:LEU:HD13	1.80	0.63
1:C:113:PRO:HG2	1:C:170:PHE:CD2	2.34	0.63
1:C:85:THR:HG23	1:C:86:GLY:O	1.99	0.63
1:C:255:ILE:HG22	1:C:259:LEU:HD22	1.78	0.62
1:A:348:GLU:HG2	1:A:350:LEU:HD13	1.81	0.62
1:D:197:HIS:CD2	1:D:236:GLY:H	2.17	0.62
1:A:157:THR:HG21	1:A:198:VAL:HA	1.81	0.62
1:D:212:ILE:HD13	1:D:259:LEU:HD13	1.81	0.62
1:B:230:HIS:HB2	1:B:268:LYS:O	1.99	0.62
1:D:80:LEU:HB3	1:D:85:THR:HG21	1.81	0.62
1:A:316:TYR:CE2	1:A:375:MET:HB2	2.35	0.61
1:B:294:LYS:HB2	1:B:315:MET:HB2	1.82	0.61
1:D:166:LEU:HD13	1:D:167:SER:N	2.07	0.61
1:D:346:PRO:O	1:D:347:ASN:HB2	2.00	0.61
1:A:80:LEU:HB3	1:A:85:THR:HG21	1.81	0.61
1:C:167:SER:HB2	1:C:169:LYS:H	1.65	0.61
1:C:212:ILE:HD13	1:C:259:LEU:HD13	1.82	0.61
1:B:269:LEU:HD21	1:B:271:ILE:HD11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:VAL:CG1	1:B:318:VAL:HB	2.29	0.60
1:C:132:THR:HG22	1:C:152:VAL:HB	1.83	0.60
1:C:167:SER:HB2	1:C:169:LYS:N	2.16	0.60
1:B:175:GLU:CD	1:B:175:GLU:H	2.09	0.60
1:A:212:ILE:HD13	1:A:259:LEU:HD13	1.84	0.60
1:C:197:HIS:CD2	1:C:236:GLY:H	2.20	0.60
1:B:167:SER:HB2	1:B:169:LYS:N	2.17	0.60
1:C:157:THR:HG21	1:C:198:VAL:HA	1.83	0.60
1:C:173:LYS:HE3	1:C:175:GLU:OE2	2.02	0.60
1:D:166:LEU:HD22	1:D:167:SER:OG	2.02	0.59
1:A:166:LEU:HD22	1:A:167:SER:OG	2.01	0.59
1:C:316:TYR:CE2	1:C:375:MET:HB2	2.37	0.59
1:D:316:TYR:CE2	1:D:375:MET:HB2	2.37	0.59
1:A:85:THR:HG23	1:A:86:GLY:O	2.02	0.59
1:C:166:LEU:CD1	1:C:167:SER:H	2.04	0.59
1:B:346:PRO:O	1:B:347:ASN:HB2	2.01	0.59
1:A:230:HIS:HB2	1:A:268:LYS:O	2.02	0.59
1:C:288:VAL:CG1	1:C:318:VAL:HB	2.33	0.59
1:D:230:HIS:HB2	1:D:268:LYS:O	2.03	0.59
1:A:90:ALA:HB3	1:B:398:ASN:ND2	2.17	0.59
1:D:50:ARG:HH12	1:D:410:SER:HB3	1.67	0.59
1:D:71:ASN:HD22	1:D:71:ASN:C	2.09	0.59
1:D:269:LEU:HD21	1:D:271:ILE:HD11	1.85	0.59
1:A:197:HIS:CD2	1:A:236:GLY:H	2.22	0.58
1:C:166:LEU:HD22	1:C:167:SER:OG	2.03	0.58
1:C:230:HIS:HB2	1:C:268:LYS:O	2.03	0.58
1:B:197:HIS:CD2	1:B:236:GLY:H	2.20	0.58
1:B:85:THR:HG23	1:B:86:GLY:O	2.03	0.58
1:C:99:ARG:HH11	1:C:126:SER:HB3	1.68	0.58
1:A:167:SER:HB2	1:A:169:LYS:N	2.19	0.58
1:C:99:ARG:NH1	1:C:126:SER:HB3	2.19	0.58
1:B:348:GLU:HG2	1:B:350:LEU:HD13	1.85	0.57
1:C:348:GLU:HG2	1:C:350:LEU:HD13	1.86	0.57
1:B:255:ILE:HG22	1:B:259:LEU:HD22	1.87	0.57
1:C:117:ILE:HD12	1:C:117:ILE:O	2.04	0.57
1:C:157:THR:H	1:C:166:LEU:CD1	2.17	0.57
1:D:154:ARG:HA	1:D:195:SER:O	2.04	0.57
1:D:167:SER:HB2	1:D:169:LYS:H	1.69	0.57
1:A:173:LYS:HZ1	1:A:174:VAL:N	1.93	0.57
1:A:398:ASN:ND2	1:B:90:ALA:HB3	2.20	0.57
1:B:80:LEU:HB3	1:B:85:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:MET:HE3	1:B:390:THR:HG21	1.87	0.56
1:C:319:ASN:ND2	1:D:116:GLN:NE2	2.48	0.56
1:B:212:ILE:HD13	1:B:259:LEU:HD13	1.88	0.56
1:B:316:TYR:CE2	1:B:375:MET:HB2	2.40	0.56
1:D:99:ARG:HH11	1:D:126:SER:HB3	1.71	0.56
1:C:178:ARG:HH22	1:C:224:GLU:CD	2.13	0.56
1:B:166:LEU:HD22	1:B:167:SER:OG	2.06	0.56
1:C:121:ARG:HH12	1:D:35:ASP:CG	2.14	0.56
1:A:99:ARG:HH11	1:A:126:SER:HB3	1.71	0.55
1:D:294:LYS:HB2	1:D:315:MET:HB2	1.89	0.55
1:D:96:GLN:HG2	1:D:122:TYR:OH	2.06	0.55
1:A:99:ARG:NH1	1:A:126:SER:HB3	2.22	0.55
1:A:255:ILE:HG22	1:A:259:LEU:HD22	1.89	0.55
1:C:280:VAL:O	1:C:281:ALA:C	2.49	0.55
1:D:167:SER:HB2	1:D:169:LYS:N	2.22	0.55
1:C:49:VAL:HG22	1:C:83:LEU:HD21	1.88	0.55
1:D:157:THR:H	1:D:166:LEU:CD1	2.19	0.55
1:B:96:GLN:HG2	1:B:122:TYR:OH	2.07	0.55
1:C:99:ARG:O	1:C:100:GLY:C	2.49	0.55
1:D:288:VAL:CG1	1:D:318:VAL:HB	2.36	0.55
1:A:157:THR:H	1:A:166:LEU:CD1	2.20	0.54
1:C:398:ASN:ND2	1:D:90:ALA:HB3	2.22	0.54
1:B:65:PHE:O	1:B:274:GLU:HA	2.08	0.54
1:A:288:VAL:CG1	1:A:318:VAL:HB	2.34	0.54
1:B:157:THR:H	1:B:166:LEU:CD1	2.20	0.54
1:A:121:ARG:HH12	1:B:35:ASP:CG	2.16	0.54
1:C:71:ASN:C	1:C:71:ASN:HD22	2.16	0.54
1:C:157:THR:HB	1:C:166:LEU:HG	1.90	0.54
1:D:280:VAL:O	1:D:281:ALA:C	2.51	0.53
1:B:50:ARG:HH12	1:B:410:SER:HB3	1.73	0.53
1:B:99:ARG:HH11	1:B:126:SER:HB3	1.73	0.53
1:C:90:ALA:HB3	1:D:398:ASN:ND2	2.23	0.53
1:A:167:SER:HB2	1:A:169:LYS:H	1.73	0.53
1:A:178:ARG:HH22	1:A:224:GLU:CD	2.17	0.53
1:B:178:ARG:HH22	1:B:224:GLU:CD	2.17	0.53
1:A:90:ALA:CB	1:B:398:ASN:HD21	2.22	0.53
1:B:280:VAL:O	1:B:281:ALA:C	2.52	0.53
1:D:166:LEU:CD1	1:D:167:SER:H	2.11	0.52
1:B:99:ARG:NH1	1:B:126:SER:HB3	2.25	0.52
1:B:173:LYS:HZ1	1:B:174:VAL:N	1.95	0.52
1:A:99:ARG:O	1:A:100:GLY:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:ILE:CG2	1:D:259:LEU:HD22	2.39	0.52
1:A:291:ILE:HD13	1:A:319:ASN:HB3	1.91	0.51
1:B:349:LYS:HD3	1:B:350:LEU:H	1.75	0.51
1:A:50:ARG:HH12	1:A:410:SER:HB3	1.75	0.51
1:C:217:PHE:HE2	1:C:221:MET:HE2	1.73	0.51
1:B:359:THR:HG22	1:B:361:ASP:H	1.75	0.51
1:A:280:VAL:O	1:A:281:ALA:C	2.53	0.51
1:A:359:THR:O	1:B:169:LYS:NZ	2.38	0.51
1:B:157:THR:HB	1:B:166:LEU:HG	1.92	0.51
1:B:166:LEU:CD1	1:B:167:SER:H	2.11	0.51
1:C:169:LYS:HB2	1:D:356:TRP:CZ3	2.46	0.51
1:A:348:GLU:HG2	1:A:350:LEU:CD1	2.41	0.50
1:B:401:GLN:HA	1:B:401:GLN:HE21	1.77	0.50
1:D:409:VAL:O	1:D:409:VAL:HG22	2.11	0.50
1:C:274:GLU:O	2:C:600:PLP:H6	2.11	0.50
1:C:50:ARG:HH12	1:C:410:SER:HB3	1.76	0.50
1:D:178:ARG:HH22	1:D:224:GLU:CD	2.20	0.50
1:C:280:VAL:O	1:C:387:GLY:HA3	2.11	0.50
1:D:359:THR:HG22	1:D:361:ASP:H	1.75	0.50
1:D:348:GLU:HG2	1:D:350:LEU:CD1	2.42	0.50
1:D:157:THR:HB	1:D:166:LEU:HG	1.94	0.49
1:C:173:LYS:NZ	1:C:174:VAL:H	1.93	0.49
1:D:391:VAL:O	1:D:394:THR:HG23	2.12	0.49
1:C:71:ASN:HD22	1:C:73:ASP:H	1.58	0.49
1:A:274:GLU:O	2:A:600:PLP:H6	2.13	0.49
1:C:96:GLN:HG2	1:C:122:TYR:OH	2.13	0.49
1:C:348:GLU:HG2	1:C:350:LEU:CD1	2.41	0.49
1:A:157:THR:HB	1:A:166:LEU:HG	1.95	0.49
1:B:129:ASP:O	1:B:150:LYS:N	2.41	0.49
1:A:269:LEU:HD21	1:A:271:ILE:HD11	1.94	0.49
1:B:376:GLN:O	1:B:377:VAL:C	2.56	0.49
1:A:41:PHE:CZ	1:A:286:LEU:HD13	2.48	0.48
1:B:154:ARG:HA	1:B:195:SER:O	2.13	0.48
1:B:44:ASP:HA	1:B:408:VAL:HG13	1.95	0.48
1:A:195:SER:HB3	1:A:233:ASP:HB3	1.96	0.48
1:B:322:VAL:HB	1:B:330:LEU:CD2	2.44	0.48
1:B:166:LEU:HD13	1:B:167:SER:N	2.09	0.48
1:B:289:ASN:HD21	1:B:378:GLY:HA2	1.77	0.48
1:C:80:LEU:HB3	1:C:85:THR:HG21	1.95	0.48
1:D:195:SER:HA	1:D:233:ASP:O	2.13	0.48
1:D:274:GLU:O	2:D:600:PLP:H6	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:VAL:O	1:D:358:PRO:HD3	2.13	0.48
1:A:71:ASN:HD22	1:A:73:ASP:H	1.62	0.47
1:D:44:ASP:HA	1:D:408:VAL:HG13	1.95	0.47
1:A:90:ALA:HB3	1:B:398:ASN:HD21	1.78	0.47
1:A:98:VAL:HG23	1:A:103:VAL:HB	1.96	0.47
1:B:144:LYS:HD3	1:B:144:LYS:N	2.30	0.47
1:C:117:ILE:HD13	1:C:145:THR:OG1	2.15	0.47
1:A:319:ASN:ND2	1:B:116:GLN:NE2	2.47	0.47
1:B:195:SER:HA	1:B:233:ASP:O	2.13	0.47
1:C:322:VAL:HB	1:C:330:LEU:CD2	2.45	0.47
1:D:99:ARG:NH1	1:D:126:SER:HB3	2.30	0.47
1:A:255:ILE:CG2	1:A:259:LEU:HD22	2.44	0.47
1:A:376:GLN:O	1:A:379:GLU:HG3	2.15	0.47
1:B:156:SER:OG	1:B:173:LYS:HD2	2.14	0.47
1:D:376:GLN:O	1:D:379:GLU:HG3	2.15	0.47
1:B:185:LYS:HD2	1:B:185:LYS:HA	1.73	0.47
1:B:391:VAL:O	1:B:394:THR:HG23	2.15	0.47
1:A:154:ARG:HA	1:A:195:SER:O	2.15	0.47
1:A:391:VAL:O	1:A:394:THR:HG23	2.15	0.47
1:B:157:THR:N	1:B:166:LEU:HD11	2.29	0.47
1:C:116:GLN:HA	1:D:291:ILE:HB	1.96	0.47
1:D:136:VAL:O	1:D:137:ASP:C	2.58	0.47
1:B:274:GLU:O	2:B:600:PLP:H6	2.16	0.46
1:C:154:ARG:HA	1:C:195:SER:O	2.15	0.46
1:D:185:LYS:HA	1:D:185:LYS:HD2	1.74	0.46
1:A:109:ILE:HG22	1:A:111:ALA:HB2	1.97	0.46
1:A:116:GLN:HA	1:B:291:ILE:HB	1.96	0.46
1:C:376:GLN:O	1:C:377:VAL:C	2.58	0.46
1:A:337:ARG:HH21	1:A:337:ARG:HG3	1.81	0.46
1:D:88:ASP:OD1	1:D:88:ASP:C	2.58	0.46
1:A:96:GLN:HG2	1:A:122:TYR:OH	2.16	0.46
1:A:322:VAL:HB	1:A:330:LEU:CD2	2.46	0.46
1:C:195:SER:CB	1:C:233:ASP:HB3	2.45	0.46
1:B:367:VAL:HG11	1:B:370:TYR:HB2	1.98	0.46
1:A:386:MET:HE3	1:A:390:THR:HG21	1.98	0.46
1:B:349:LYS:HD3	1:B:350:LEU:N	2.29	0.46
1:B:41:PHE:CZ	1:B:286:LEU:HD13	2.51	0.46
1:B:66:TYR:CE2	1:B:68:VAL:HA	2.50	0.46
1:B:255:ILE:CG2	1:B:259:LEU:HD22	2.45	0.46
1:B:316:TYR:O	1:B:355:VAL:HA	2.16	0.46
1:C:311:ALA:O	1:C:312:GLN:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLN:O	1:C:379:GLU:HG3	2.15	0.46
1:D:290:VAL:HG22	1:D:377:VAL:HA	1.98	0.46
1:C:391:VAL:HG23	1:C:392:VAL:N	2.30	0.45
1:A:173:LYS:NZ	1:A:174:VAL:H	1.97	0.45
1:A:398:ASN:HD21	1:B:90:ALA:HB3	1.81	0.45
1:C:35:ASP:CG	1:D:121:ARG:HH12	2.25	0.45
1:A:195:SER:CB	1:A:233:ASP:HB3	2.46	0.45
1:A:311:ALA:O	1:A:312:GLN:C	2.60	0.45
1:C:44:ASP:HA	1:C:408:VAL:HG13	1.98	0.45
1:B:71:ASN:HD22	1:B:73:ASP:H	1.63	0.45
1:C:359:THR:O	1:D:169:LYS:NZ	2.37	0.45
1:D:215:SER:O	1:D:219:PHE:HB2	2.17	0.45
1:A:343:GLU:HA	1:A:344:PRO:HD3	1.89	0.45
1:D:322:VAL:HB	1:D:330:LEU:CD2	2.47	0.45
1:A:351:TYR:HB3	1:A:352:PRO:HD2	1.99	0.45
1:B:348:GLU:HG2	1:B:350:LEU:CD1	2.47	0.45
1:A:116:GLN:NE2	1:B:319:ASN:ND2	2.51	0.45
1:B:117:ILE:HD12	1:B:145:THR:HG21	1.99	0.45
1:C:359:THR:HG22	1:C:361:ASP:H	1.81	0.45
1:B:282:SER:HA	1:B:385:ASP:HA	1.99	0.45
1:C:401:GLN:HA	1:C:401:GLN:HE21	1.82	0.45
1:D:106:GLU:CD	1:D:106:GLU:H	2.26	0.44
1:A:409:VAL:HG22	1:A:409:VAL:O	2.16	0.44
1:B:71:ASN:C	1:B:71:ASN:ND2	2.73	0.44
1:B:386:MET:HE3	1:B:386:MET:HB3	1.76	0.44
1:C:195:SER:HA	1:C:233:ASP:O	2.18	0.44
1:C:359:THR:CG2	1:C:361:ASP:H	2.31	0.44
1:D:120:ILE:O	1:D:121:ARG:C	2.60	0.44
1:D:129:ASP:O	1:D:150:LYS:N	2.45	0.44
1:D:337:ARG:HH21	1:D:337:ARG:HG3	1.82	0.44
1:A:376:GLN:O	1:A:377:VAL:C	2.61	0.44
1:C:386:MET:HE3	1:C:386:MET:HB3	1.76	0.44
1:A:280:VAL:O	1:A:387:GLY:HA3	2.17	0.44
1:C:200:SER:HB3	1:C:277:ARG:HE	1.83	0.44
1:A:44:ASP:HA	1:A:408:VAL:HG13	1.99	0.44
1:C:128:VAL:O	1:C:146:HIS:HE1	2.01	0.44
1:D:61:ARG:NH2	1:D:260:GLU:OE1	2.44	0.44
1:B:88:ASP:OD1	1:B:88:ASP:C	2.61	0.43
1:B:173:LYS:NZ	1:B:174:VAL:H	1.99	0.43
1:D:98:VAL:HG23	1:D:103:VAL:HB	2.00	0.43
1:B:52:HIS:O	1:B:53:GLU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LEU:HD22	1:C:330:LEU:H	1.84	0.43
1:B:113:PRO:HG2	1:B:170:PHE:CE2	2.54	0.43
1:D:173:LYS:NZ	1:D:174:VAL:H	2.02	0.43
1:D:221:MET:O	1:D:222:GLY:C	2.58	0.43
1:A:35:ASP:CG	1:B:121:ARG:HH12	2.27	0.43
1:A:71:ASN:ND2	1:A:73:ASP:H	2.15	0.43
1:B:157:THR:HG22	1:B:166:LEU:HD12	1.99	0.43
1:C:223:THR:O	1:C:224:GLU:C	2.62	0.43
1:D:71:ASN:HD22	1:D:73:ASP:H	1.64	0.43
1:D:144:LYS:HD3	1:D:144:LYS:N	2.33	0.43
1:D:330:LEU:H	1:D:330:LEU:HD22	1.82	0.43
1:C:398:ASN:HD21	1:D:90:ALA:HB3	1.82	0.43
1:D:376:GLN:O	1:D:377:VAL:C	2.61	0.43
1:B:50:ARG:HH12	1:B:410:SER:CB	2.32	0.43
1:B:367:VAL:CG1	1:B:370:TYR:HB2	2.47	0.43
1:D:117:ILE:HD12	1:D:117:ILE:O	2.19	0.43
1:D:282:SER:HA	1:D:385:ASP:HA	2.01	0.43
1:A:386:MET:HE3	1:A:386:MET:HB3	1.83	0.43
1:B:99:ARG:O	1:B:100:GLY:C	2.60	0.43
1:D:99:ARG:HH11	1:D:99:ARG:HD3	1.72	0.43
1:B:99:ARG:HH11	1:B:99:ARG:HD3	1.58	0.43
1:C:284:PHE:HE2	1:C:405:ILE:HD13	1.84	0.43
1:D:50:ARG:HH12	1:D:410:SER:CB	2.32	0.43
1:D:359:THR:CG2	1:D:361:ASP:H	2.31	0.43
1:C:399:GLY:HA3	1:D:91:SER:OG	2.19	0.43
1:A:49:VAL:HG22	1:A:83:LEU:HD21	2.01	0.42
1:A:99:ARG:O	1:A:101:ILE:N	2.52	0.42
1:C:255:ILE:CG2	1:C:259:LEU:HD22	2.45	0.42
1:D:386:MET:HE3	1:D:386:MET:HB3	1.76	0.42
1:A:195:SER:HA	1:A:233:ASP:O	2.18	0.42
1:A:401:GLN:HE21	1:A:401:GLN:HA	1.84	0.42
1:B:71:ASN:ND2	1:B:73:ASP:H	2.17	0.42
1:B:98:VAL:HG23	1:B:103:VAL:HB	2.01	0.42
1:B:195:SER:CB	1:B:233:ASP:HB3	2.49	0.42
1:A:99:ARG:HH11	1:A:99:ARG:HD3	1.67	0.42
1:C:169:LYS:HE3	1:D:356:TRP:HB3	2.02	0.42
1:C:185:LYS:HA	1:C:185:LYS:HD2	1.85	0.42
1:B:337:ARG:HH21	1:B:337:ARG:HG3	1.84	0.42
1:B:409:VAL:O	1:B:409:VAL:HG22	2.19	0.42
1:C:388:ALA:O	1:C:390:THR:HG23	2.19	0.42
1:C:200:SER:HA	1:C:237:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:GLN:HE21	1:D:401:GLN:HA	1.85	0.42
1:B:189:ILE:HD13	1:B:189:ILE:HA	1.92	0.42
1:B:264:PRO:O	1:B:265:PRO:C	2.62	0.42
1:C:144:LYS:HD3	1:C:144:LYS:N	2.34	0.42
1:D:157:THR:HG22	1:D:166:LEU:HD12	2.00	0.42
1:A:98:VAL:HG22	1:A:108:ILE:HD11	2.02	0.42
1:C:65:PHE:O	1:C:274:GLU:HA	2.18	0.42
1:C:178:ARG:NH2	1:C:224:GLU:OE1	2.51	0.42
1:D:49:VAL:HG22	1:D:83:LEU:HD21	2.02	0.42
1:D:289:ASN:HD21	1:D:378:GLY:HA2	1.84	0.42
1:A:290:VAL:HG22	1:A:377:VAL:HA	2.02	0.42
1:C:157:THR:N	1:C:166:LEU:HD11	2.28	0.42
1:B:92:ASN:H	1:B:119:HIS:CD2	2.38	0.42
1:B:200:SER:HB3	1:B:277:ARG:HH21	1.85	0.42
1:D:367:VAL:HG11	1:D:370:TYR:HB2	2.02	0.42
1:D:66:TYR:CG	1:D:80:LEU:HD13	2.54	0.42
1:D:264:PRO:O	1:D:265:PRO:C	2.62	0.42
1:A:217:PHE:CD2	1:A:221:MET:HE2	2.55	0.41
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.86	0.41
1:A:284:PHE:HE2	1:A:405:ILE:HD13	1.85	0.41
1:D:195:SER:HB3	1:D:233:ASP:HB3	2.02	0.41
1:A:73:ASP:CB	1:A:76:VAL:HG13	2.43	0.41
1:B:391:VAL:HG23	1:B:392:VAL:N	2.36	0.41
1:C:115:LYS:HE2	1:C:115:LYS:HB2	1.88	0.41
1:C:116:GLN:NE2	1:D:319:ASN:ND2	2.53	0.41
1:A:112:ASN:ND2	1:A:114:CYS:H	2.17	0.41
1:B:293:LYS:NZ	1:B:374:GLU:OE1	2.53	0.41
1:B:311:ALA:O	1:B:312:GLN:C	2.64	0.41
1:C:90:ALA:CB	1:D:398:ASN:HD21	2.34	0.41
1:D:109:ILE:HG22	1:D:111:ALA:HB2	2.02	0.41
1:B:106:GLU:CD	1:B:106:GLU:H	2.27	0.41
1:B:136:VAL:O	1:B:140:GLU:HG3	2.21	0.41
1:D:232:LEU:HD23	1:D:271:ILE:HD12	2.02	0.41
1:A:112:ASN:C	1:A:112:ASN:HD22	2.29	0.41
1:A:282:SER:HA	1:A:385:ASP:HA	2.01	0.41
1:C:157:THR:HG22	1:C:166:LEU:HD12	2.02	0.41
1:A:221:MET:O	1:A:222:GLY:C	2.60	0.41
1:D:195:SER:CB	1:D:233:ASP:HB3	2.50	0.41
1:B:41:PHE:CE2	1:B:286:LEU:HD13	2.55	0.41
1:C:367:VAL:CG1	1:C:370:TYR:HB2	2.50	0.41
1:A:65:PHE:O	1:A:274:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:VAL:O	1:B:50:ARG:C	2.64	0.41
1:B:196:PHE:CD1	1:B:196:PHE:C	2.99	0.41
1:C:409:VAL:O	1:C:411:GLY:N	2.54	0.41
1:D:367:VAL:CG1	1:D:370:TYR:HB2	2.50	0.41
1:A:117:ILE:HD12	1:A:117:ILE:C	2.45	0.41
1:A:129:ASP:O	1:A:150:LYS:N	2.51	0.40
1:B:128:VAL:O	1:B:146:HIS:HE1	2.04	0.40
1:C:39:PRO:HD3	1:C:319:ASN:ND2	2.36	0.40
1:C:291:ILE:HD13	1:C:319:ASN:HB3	2.02	0.40
1:D:110:TYR:CZ	1:D:115:LYS:HG2	2.57	0.40
1:A:71:ASN:C	1:A:71:ASN:ND2	2.70	0.40
1:A:91:SER:OG	1:B:399:GLY:HA3	2.21	0.40
1:B:112:ASN:C	1:B:112:ASN:HD22	2.29	0.40
1:B:195:SER:HB3	1:B:233:ASP:HB3	2.03	0.40
1:C:73:ASP:CB	1:C:76:VAL:HG13	2.45	0.40
1:C:156:SER:OG	1:C:173:LYS:HD2	2.21	0.40
1:C:337:ARG:HH21	1:C:337:ARG:HG3	1.87	0.40
1:A:144:LYS:N	1:A:144:LYS:HD3	2.36	0.40
1:B:78:GLY:O	1:B:79:THR:C	2.63	0.40
1:B:243:ASP:OD1	1:B:243:ASP:N	2.53	0.40
1:B:263:PHE:N	1:B:264:PRO:CD	2.84	0.40
1:D:66:TYR:CE2	1:D:68:VAL:HA	2.56	0.40
1:C:129:ASP:O	1:C:150:LYS:N	2.52	0.40
1:B:66:TYR:CG	1:B:80:LEU:HD13	2.56	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	350/425 (82%)	324 (93%)	21 (6%)	5 (1%)	9 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	350/425 (82%)	319 (91%)	26 (7%)	5 (1%)	9	30
1	C	350/425 (82%)	325 (93%)	21 (6%)	4 (1%)	11	36
1	D	350/425 (82%)	324 (93%)	21 (6%)	5 (1%)	9	30
All	All	1400/1700 (82%)	1292 (92%)	89 (6%)	19 (1%)	9	30

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	B	312	GLN
1	C	312	GLN
1	D	312	GLN
1	A	37	GLY
1	A	410	SER
1	B	37	GLY
1	B	410	SER
1	C	37	GLY
1	C	410	SER
1	D	100	GLY
1	D	410	SER
1	A	71	ASN
1	A	100	GLY
1	D	37	GLY
1	C	71	ASN
1	D	242	ARG
1	B	377	VAL
1	B	100	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/362 (83%)	258 (85%)	44 (15%)	3	10
1	B	302/362 (83%)	253 (84%)	49 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	302/362 (83%)	259 (86%)	43 (14%)	3	11
1	D	302/362 (83%)	255 (84%)	47 (16%)	2	9
All	All	1208/1448 (83%)	1025 (85%)	183 (15%)	3	10

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	71	ASN
1	A	74	TRP
1	A	75	ARG
1	A	76	VAL
1	A	83	LEU
1	A	85	THR
1	A	98	VAL
1	A	112	ASN
1	A	117	ILE
1	A	136	VAL
1	A	144	LYS
1	A	157	THR
1	A	166	LEU
1	A	168	VAL
1	A	173	LYS
1	A	174	VAL
1	A	185	LYS
1	A	200	SER
1	A	202	SER
1	A	250	GLU
1	A	259	LEU
1	A	268	LYS
1	A	272	VAL
1	A	288	VAL
1	A	290	VAL
1	A	291	ILE
1	A	312	GLN
1	A	339	LEU
1	A	341	GLN
1	A	342	ARG
1	A	343	GLU
1	A	345	ILE
1	A	348	GLU

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Mol	Chain	Res	Type
1	A	355	VAL
1	A	359	THR
1	A	363	LEU
1	A	368	GLU
1	A	369	ARG
1	A	386	MET
1	A	398	ASN
1	A	401	GLN
1	A	403	PRO
1	A	410	SER
1	B	68	VAL
1	B	71	ASN
1	B	74	TRP
1	B	75	ARG
1	B	76	VAL
1	B	83	LEU
1	B	85	THR
1	B	98	VAL
1	B	112	ASN
1	B	117	ILE
1	B	136	VAL
1	B	144	LYS
1	B	150	LYS
1	B	157	THR
1	B	166	LEU
1	B	168	VAL
1	B	173	LYS
1	B	174	VAL
1	B	185	LYS
1	B	186	LYS
1	B	200	SER
1	B	202	SER
1	B	250	GLU
1	B	259	LEU
1	B	268	LYS
1	B	272	VAL
1	B	288	VAL
1	B	290	VAL
1	B	291	ILE
1	B	293	LYS
1	B	296	THR
1	B	297	PRO

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Mol	Chain	Res	Type
1	B	312	GLN
1	B	339	LEU
1	B	341	GLN
1	B	343	GLU
1	B	345	ILE
1	B	348	GLU
1	B	350	LEU
1	B	355	VAL
1	B	359	THR
1	B	363	LEU
1	B	368	GLU
1	B	369	ARG
1	B	386	MET
1	B	398	ASN
1	B	401	GLN
1	B	403	PRO
1	B	410	SER
1	C	68	VAL
1	C	71	ASN
1	C	74	TRP
1	C	75	ARG
1	C	76	VAL
1	C	83	LEU
1	C	85	THR
1	C	98	VAL
1	C	112	ASN
1	C	117	ILE
1	C	136	VAL
1	C	144	LYS
1	C	150	LYS
1	C	157	THR
1	C	166	LEU
1	C	173	LYS
1	C	174	VAL
1	C	186	LYS
1	C	200	SER
1	C	250	GLU
1	C	259	LEU
1	C	268	LYS
1	C	272	VAL
1	C	288	VAL
1	C	290	VAL

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Mol	Chain	Res	Type
1	C	291	ILE
1	C	312	GLN
1	C	339	LEU
1	C	341	GLN
1	C	342	ARG
1	C	343	GLU
1	C	345	ILE
1	C	348	GLU
1	C	355	VAL
1	C	359	THR
1	C	363	LEU
1	C	368	GLU
1	C	369	ARG
1	C	386	MET
1	C	398	ASN
1	C	401	GLN
1	C	403	PRO
1	C	410	SER
1	D	68	VAL
1	D	71	ASN
1	D	74	TRP
1	D	75	ARG
1	D	76	VAL
1	D	85	THR
1	D	88	ASP
1	D	98	VAL
1	D	112	ASN
1	D	117	ILE
1	D	136	VAL
1	D	144	LYS
1	D	150	LYS
1	D	157	THR
1	D	166	LEU
1	D	168	VAL
1	D	173	LYS
1	D	174	VAL
1	D	185	LYS
1	D	186	LYS
1	D	200	SER
1	D	202	SER
1	D	250	GLU
1	D	259	LEU

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Mol	Chain	Res	Type
1	D	268	LYS
1	D	272	VAL
1	D	288	VAL
1	D	290	VAL
1	D	291	ILE
1	D	312	GLN
1	D	339	LEU
1	D	341	GLN
1	D	342	ARG
1	D	343	GLU
1	D	345	ILE
1	D	348	GLU
1	D	349	LYS
1	D	350	LEU
1	D	355	VAL
1	D	359	THR
1	D	363	LEU
1	D	368	GLU
1	D	369	ARG
1	D	398	ASN
1	D	401	GLN
1	D	403	PRO
1	D	410	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	112	ASN
1	A	116	GLN
1	A	197	HIS
1	A	210	GLN
1	A	228	ASN
1	A	256	ASN
1	A	262	HIS
1	A	289	ASN
1	A	312	GLN
1	A	341	GLN
1	A	398	ASN
1	B	71	ASN
1	B	112	ASN
1	B	116	GLN

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Mol	Chain	Res	Type
1	B	197	HIS
1	B	262	HIS
1	B	289	ASN
1	B	341	GLN
1	B	398	ASN
1	B	401	GLN
1	C	71	ASN
1	C	112	ASN
1	C	116	GLN
1	C	197	HIS
1	C	210	GLN
1	C	228	ASN
1	C	256	ASN
1	C	262	HIS
1	C	341	GLN
1	C	398	ASN
1	C	401	GLN
1	D	71	ASN
1	D	112	ASN
1	D	116	GLN
1	D	197	HIS
1	D	256	ASN
1	D	262	HIS
1	D	289	ASN
1	D	312	GLN
1	D	341	GLN
1	D	398	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	PLP	A	600	1	15,15,16	2.81	4 (26%)	21,22,23	2.61	8 (38%)
2	PLP	D	600	1	15,15,16	2.77	4 (26%)	21,22,23	3.36	6 (28%)
2	PLP	B	600	1	15,15,16	2.50	5 (33%)	21,22,23	3.24	5 (23%)
2	PLP	C	600	1	15,15,16	2.75	6 (40%)	21,22,23	2.34	5 (23%)

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
2	PLP	A	600	1	-	0/6/6/8	0/1/1/1
2	PLP	D	600	1	-	0/6/6/8	0/1/1/1
2	PLP	B	600	1	-	0/6/6/8	0/1/1/1
2	PLP	C	600	1	-	0/6/6/8	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	PLP	C4A-C4	7.04	1.65	1.51
2	D	600	PLP	C5-C4	7.01	1.48	1.40
2	C	600	PLP	C5-C4	6.77	1.48	1.40
2	D	600	PLP	C4A-C4	6.36	1.64	1.51
2	C	600	PLP	C4A-C4	6.15	1.63	1.51
2	B	600	PLP	C4A-C4	6.10	1.63	1.51
2	A	600	PLP	C5-C4	5.89	1.47	1.40
2	B	600	PLP	C5-C4	5.36	1.46	1.40
2	A	600	PLP	O3-C3	3.32	1.44	1.36
2	B	600	PLP	P-O4P	3.25	1.70	1.60
2	D	600	PLP	P-O4P	3.07	1.70	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	PLP	O3-C3	2.51	1.42	1.36
2	A	600	PLP	C2-N1	2.46	1.38	1.33
2	C	600	PLP	P-O4P	2.40	1.67	1.60
2	B	600	PLP	C2-N1	2.27	1.37	1.33
2	C	600	PLP	C2-N1	2.26	1.37	1.33
2	D	600	PLP	C2-N1	2.20	1.37	1.33
2	B	600	PLP	O3-C3	2.07	1.41	1.36
2	C	600	PLP	C3-C4	2.05	1.44	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	PLP	C4A-C4-C5	11.83	133.13	120.94
2	B	600	PLP	C4A-C4-C5	11.48	132.77	120.94
2	A	600	PLP	C4A-C4-C5	7.58	128.75	120.94
2	C	600	PLP	C4A-C4-C5	6.74	127.89	120.94
2	B	600	PLP	O3-C3-C2	5.53	129.04	117.58
2	D	600	PLP	C4A-C4-C3	-5.13	111.97	120.52
2	B	600	PLP	C4A-C4-C3	-5.13	111.98	120.52
2	D	600	PLP	O3-C3-C2	4.96	127.87	117.58
2	C	600	PLP	O3-C3-C2	4.86	127.65	117.58
2	A	600	PLP	O3-C3-C2	4.45	126.81	117.58
2	A	600	PLP	C4A-C4-C3	-3.64	114.45	120.52
2	B	600	PLP	O3-C3-C4	-3.44	109.14	118.10
2	C	600	PLP	C4A-C4-C3	-3.27	115.07	120.52
2	D	600	PLP	C3-C4-C5	-3.09	114.88	118.59
2	D	600	PLP	O3-C3-C4	-3.03	110.19	118.10
2	C	600	PLP	C2A-C2-C3	3.03	124.35	120.80
2	A	600	PLP	O2P-P-O4P	-3.03	98.78	106.67
2	D	600	PLP	O2P-P-O4P	-2.90	99.10	106.67
2	A	600	PLP	C6-C5-C4	2.84	120.42	118.10
2	B	600	PLP	C3-C4-C5	-2.79	115.24	118.59
2	A	600	PLP	C2A-C2-C3	2.78	124.05	120.80
2	A	600	PLP	O3P-P-O4P	2.59	113.43	106.67
2	C	600	PLP	O4P-P-O1P	2.37	112.86	106.44
2	A	600	PLP	O4P-P-O1P	2.01	111.88	106.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	PLP	1	0
2	D	600	PLP	1	0
2	B	600	PLP	1	0
2	C	600	PLP	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.