



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:38 AM UTC

PDB ID : 1PRE / pdb_00001pre
Title : PROAEROLYSIN
Authors : Parker, M.W.; Buckley, J.T.; Postma, J.P.M.; Tucker, A.D.; Tsernoglou, D.
Deposited on : 1995-09-15
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
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

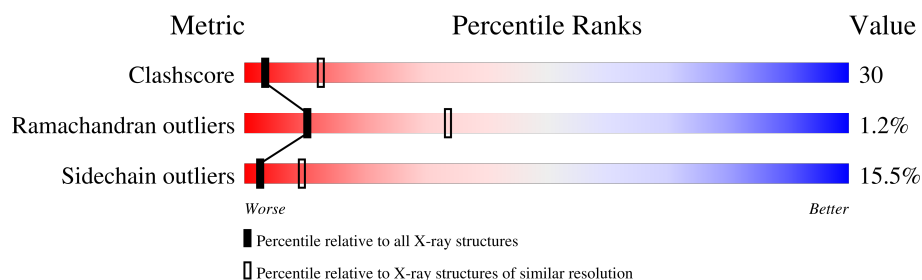
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

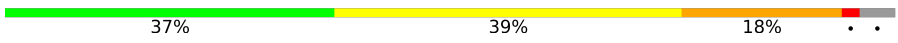
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	470	
1	B	470	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7089 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 PROAEROLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3523	2228	607	679	9			
1	B	451	Total	C	N	O	S	0	0	0
			3533	2234	607	683	9			

- Molecule 2 is water.

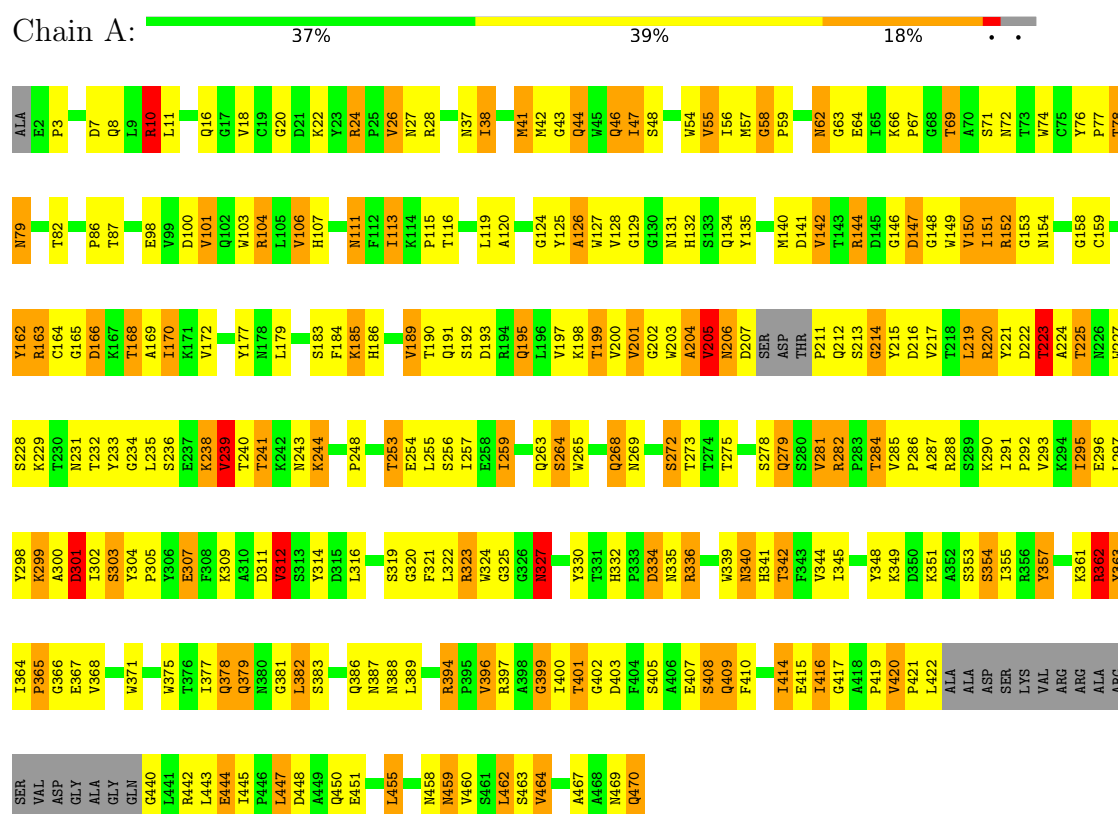
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	15	Total	O	0	0
			15	15		

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: PROAEROLYSIN



• Molecule 1: PROAEROLYSIN



GLY	ALA	K367	Y368	K294	T218
	GLY	K369	L295	L219	
GLN	GLY	W370	E296	R220	
	GLY	W371	L297	Y221	
L441	R442	I372	Y298	D222	
	L443	W373	K299	T223	
E444	L445	K374	A300	A224	
		W375	D301	T225	
D448	A449	T376	I302	N226	
	Q450	I377	S303		
E451	L452	Q378	Y304	T230	
		Q379	E307		
L455	G456	N380	F308	Y233	
	F457	S383	K309	G234	
V460	S461	T384	A310	L235	
		M385	D311	S236	
V464		N388	V312	E237	
		L389	S313	K238	
L468	ASN	R390	G326	V239	
	GLN	A391	R327	T240	
		K392	Y330	T241	
		V396	T331	K242	
		A398	H332	N243	
		G399	Y332	K244	
		I400	R336	F245	
		T401	P337	K246	
		G402	N338	W247	
		Q409	W339	P248	
		G412	N340	E252	
		N413	H341	T253	
		I416	T342	E254	
		G417		E258	
		A418		Q263	
		P419		A266	
		W420		T273	
		P421		T274	
		L422		T275	
		A423		S276	
		A424		L277	
		ASP		S278	
		SER		Q279	
		LYS		S280	
		VAL		V281	
		ARG		R282	
		ARG		P283	
		ARG		T284	
		ALA		V285	
		ALA		P286	
		R362		A287	
		Y363		R288	
		I364		S289	
		SER		K290	
		VAL		I291	
		VAL		P292	
		ASP		V293	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.00Å 104.00Å 222.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.0 (6.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7089	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.88	2/3620 (0.1%)	2.27	179/4938 (3.6%)
1	B	0.85	0/3631	2.24	188/4957 (3.8%)
All	All	0.87	2/7251 (0.0%)	2.26	367/9895 (3.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	HIS	C-O	-6.09	1.20	1.23
1	A	397	ARG	NE-CZ	5.16	1.38	1.33

All (367) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	15.43	146.01	124.40
1	A	382	LEU	CA-C-O	-12.40	107.80	120.82
1	A	323	ARG	CD-NE-CZ	12.05	141.27	124.40
1	B	55	VAL	CA-C-O	-11.53	110.22	121.63
1	B	24	ARG	NE-CZ-NH2	11.34	129.41	119.20
1	B	62	ASN	CA-CB-CG	-11.31	101.29	112.60
1	B	417	GLY	CA-C-O	10.90	133.09	121.53
1	B	252	GLU	N-CA-C	-10.82	100.21	113.41
1	B	301	ASP	CA-CB-CG	-10.58	102.02	112.60
1	A	379	GLN	OE1-CD-NE2	10.45	133.05	122.60
1	A	24	ARG	CD-NE-CZ	9.78	138.09	124.40
1	A	340	ASN	OD1-CG-ND2	-9.76	112.84	122.60
1	A	345	ILE	N-CA-CB	-9.74	102.61	112.06
1	B	160	ASP	CA-CB-CG	-9.50	103.10	112.60
1	A	87	THR	CA-C-O	-9.47	108.32	120.25
1	A	147	ASP	N-CA-CB	9.40	121.17	110.35
1	B	4	VAL	N-CA-CB	9.12	122.75	110.26
1	B	300	ALA	CA-C-O	-8.97	111.64	121.33
1	B	78	THR	CA-C-N	8.84	132.79	122.89
1	B	78	THR	C-N-CA	8.84	132.79	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	PRO	CA-C-O	-8.74	111.02	121.95
1	B	336	ARG	CB-CA-C	-8.73	103.41	111.00
1	B	311	ASP	CA-C-O	-8.68	112.10	121.56
1	A	201	VAL	CA-C-O	-8.58	111.63	121.75
1	A	243	ASN	OD1-CG-ND2	8.56	131.16	122.60
1	A	394	ARG	NE-CZ-NH2	8.39	126.75	119.20
1	A	104	ARG	CA-C-O	-8.39	110.62	120.10
1	B	347	PRO	CA-C-O	-8.38	111.83	121.56
1	A	166	ASP	CA-CB-CG	-8.37	104.23	112.60
1	A	256	SER	CA-C-O	8.33	129.38	120.63
1	A	420	VAL	N-CA-CB	8.32	117.57	111.83
1	A	464	VAL	CA-C-O	8.23	128.58	120.27
1	B	413	ASN	OD1-CG-ND2	8.23	130.83	122.60
1	B	72	ASN	CA-C-O	-8.22	111.88	121.16
1	B	82	THR	N-CA-C	8.17	122.55	110.46
1	A	79	ASN	N-CA-CB	-8.15	96.33	111.24
1	B	307	GLU	CA-C-O	-8.12	108.89	120.51
1	A	348	TYR	CA-C-O	-8.11	111.67	120.92
1	A	163	ARG	CD-NE-CZ	8.08	135.71	124.40
1	A	132	HIS	CA-CB-CG	-8.07	105.73	113.80
1	A	206	ASN	CA-CB-CG	8.04	120.64	112.60
1	A	410	PHE	CA-CB-CG	7.98	121.78	113.80
1	A	362	ARG	CD-NE-CZ	-7.97	113.24	124.40
1	B	141	ASP	CA-CB-CG	7.94	120.54	112.60
1	A	332	HIS	N-CA-CB	-7.93	102.86	111.66
1	A	151	ILE	O-C-N	-7.83	114.33	123.03
1	B	84	GLU	CA-C-O	-7.80	112.60	121.81
1	B	142	VAL	N-CA-CB	7.80	121.50	111.67
1	B	302	ILE	CB-CA-C	-7.80	96.75	110.71
1	A	16	GLN	N-CA-C	7.78	120.73	108.67
1	A	78	THR	N-CA-C	-7.74	103.29	112.89
1	B	308	PHE	CA-CB-CG	7.74	121.54	113.80
1	B	79	ASN	N-CA-CB	-7.73	98.62	110.75
1	A	320	GLY	CA-C-O	-7.72	113.84	121.48
1	A	42	MET	N-CA-C	7.68	122.16	109.95
1	A	154	ASN	OD1-CG-ND2	7.67	130.26	122.60
1	A	152	ARG	CB-CA-C	7.65	123.64	109.86
1	B	354	SER	CA-C-O	-7.62	112.01	120.70
1	A	419	PRO	CA-C-O	-7.60	112.19	121.31
1	A	170	ILE	CA-C-O	-7.53	112.00	120.74
1	A	303	SER	CA-CB-OG	-7.53	96.04	111.10
1	B	49	GLY	N-CA-C	7.42	123.28	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	268	GLN	OE1-CD-NE2	-7.37	115.23	122.60
1	A	448	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	219	LEU	CA-C-O	-7.35	112.60	120.46
1	B	384	THR	O-C-N	7.34	130.56	122.11
1	B	187	GLY	CA-C-O	-7.34	114.54	122.76
1	B	23	TYR	CA-C-O	-7.30	112.56	121.11
1	B	27	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	256	SER	CA-C-N	7.24	132.62	123.14
1	A	256	SER	C-N-CA	7.24	132.62	123.14
1	B	92	ASP	CA-C-N	7.23	129.69	123.04
1	B	92	ASP	C-N-CA	7.23	129.69	123.04
1	A	101	VAL	N-CA-CB	7.21	121.39	110.58
1	B	82	THR	CA-C-O	-7.16	112.79	121.89
1	B	140	MET	CA-C-O	-7.16	112.86	120.80
1	A	357	TYR	N-CA-C	-7.13	103.20	110.97
1	A	69	THR	CA-CB-OG1	-7.12	98.92	109.60
1	A	297	LEU	CA-C-O	-7.11	112.63	120.38
1	A	312	VAL	N-CA-CB	7.11	118.47	110.72
1	A	244	LYS	CA-C-O	-7.09	112.96	121.05
1	B	98	GLU	CA-C-O	-7.09	113.03	120.55
1	B	321	PHE	CA-CB-CG	7.09	120.89	113.80
1	B	398	ALA	CA-C-O	-7.07	113.21	120.71
1	B	397	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	A	379	GLN	CB-CA-C	-7.01	99.87	110.88
1	B	365	PRO	N-CD-CG	-7.01	92.69	103.20
1	B	358	GLN	CA-C-O	-6.99	112.20	120.10
1	B	212	GLN	CA-C-O	6.99	129.06	121.16
1	B	384	THR	CA-C-O	-6.99	113.09	120.92
1	B	321	PHE	CA-C-O	-6.98	113.48	121.72
1	B	298	TYR	N-CA-C	6.91	120.78	109.85
1	A	148	GLY	CA-C-O	-6.91	114.36	121.61
1	A	134	GLN	CA-C-O	-6.88	111.47	119.59
1	B	364	ILE	CA-C-N	6.88	128.43	119.84
1	B	364	ILE	C-N-CA	6.88	128.43	119.84
1	B	208	SER	N-CA-C	6.87	120.62	110.46
1	A	335	ASN	OD1-CG-ND2	6.87	129.47	122.60
1	B	195	GLN	CB-CG-CD	6.84	124.22	112.60
1	A	362	ARG	NE-CZ-NH2	6.83	125.35	119.20
1	B	394	ARG	NH1-CZ-NH2	6.82	128.17	119.30
1	A	152	ARG	NE-CZ-NH2	-6.82	113.06	119.20
1	B	308	PHE	CA-C-O	-6.80	113.65	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	ASN	CA-CB-CG	-6.80	105.80	112.60
1	A	8	GLN	OE1-CD-NE2	6.80	129.40	122.60
1	B	211	PRO	CA-C-O	-6.77	113.71	121.56
1	A	464	VAL	N-CA-CB	6.74	120.99	111.82
1	A	335	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	115	PRO	CA-C-N	6.69	129.55	120.38
1	A	115	PRO	C-N-CA	6.69	129.55	120.38
1	B	464	VAL	N-CA-CB	6.66	121.25	111.52
1	B	320	GLY	CA-C-O	-6.65	114.96	121.75
1	A	332	HIS	CA-C-O	-6.63	114.96	120.26
1	B	114	LYS	CA-C-N	6.63	126.41	119.05
1	B	114	LYS	C-N-CA	6.63	126.41	119.05
1	B	293	VAL	N-CA-CB	6.61	121.17	111.52
1	B	28	ARG	CB-CA-C	-6.60	100.51	110.88
1	A	147	ASP	N-CA-C	-6.58	102.36	110.65
1	B	385	MET	CA-C-O	-6.58	113.45	120.42
1	B	413	ASN	O-C-N	6.56	130.72	122.65
1	A	111	ASN	CA-CB-CG	-6.56	106.04	112.60
1	A	79	ASN	O-C-N	-6.56	115.45	121.42
1	A	361	LYS	CA-C-N	6.55	130.27	120.31
1	A	361	LYS	C-N-CA	6.55	130.27	120.31
1	A	150	VAL	CA-CB-CG1	6.52	121.49	110.40
1	B	464	VAL	CA-C-O	-6.51	113.45	120.36
1	B	351	LYS	N-CA-C	6.50	119.18	111.71
1	A	367	GLU	N-CA-C	6.49	120.46	112.54
1	A	241	THR	CA-C-O	-6.48	113.21	120.66
1	A	189	VAL	N-CA-CB	6.45	117.97	110.82
1	B	236	SER	CB-CA-C	-6.44	97.61	110.42
1	B	391	ARG	CD-NE-CZ	6.41	133.37	124.40
1	B	82	THR	N-CA-CB	-6.40	100.53	110.46
1	B	394	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	A	309	LYS	CA-C-O	-6.37	113.33	120.66
1	B	28	ARG	N-CA-CB	6.36	119.23	110.01
1	A	330	TYR	CA-C-O	-6.33	113.11	120.20
1	B	355	ILE	CA-C-O	6.31	127.52	120.95
1	B	383	SER	CA-CB-OG	-6.30	98.51	111.10
1	A	165	GLY	N-CA-C	-6.29	104.67	115.61
1	A	311	ASP	CA-C-N	-6.25	114.30	122.37
1	A	311	ASP	C-N-CA	-6.25	114.30	122.37
1	A	106	VAL	O-C-N	-6.25	114.76	122.57
1	B	105	LEU	CA-C-O	6.24	127.32	120.90
1	B	56	ILE	O-C-N	-6.23	116.43	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	CYS	N-CA-C	6.23	117.64	108.86
1	A	168	THR	CA-C-O	-6.22	113.96	121.05
1	A	223	THR	CA-C-O	-6.22	114.86	121.88
1	B	464	VAL	N-CA-C	-6.21	99.17	108.12
1	A	44	GLN	N-CA-C	6.21	118.56	111.11
1	A	355	ILE	CA-C-N	6.21	128.60	120.28
1	A	355	ILE	C-N-CA	6.21	128.60	120.28
1	B	388	ASN	OD1-CG-ND2	6.19	128.79	122.60
1	B	350	ASP	CA-C-O	-6.17	114.84	121.38
1	A	177	TYR	CA-C-O	-6.17	113.67	120.33
1	A	379	GLN	CA-C-O	-6.17	114.34	120.82
1	A	79	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	126	ALA	N-CA-C	6.16	120.11	110.32
1	B	184	PHE	N-CA-C	6.13	118.88	110.24
1	A	265	TRP	N-CA-C	-6.12	104.60	111.28
1	B	193	ASP	CA-CB-CG	-6.12	106.48	112.60
1	A	259	ILE	CA-C-O	6.11	127.95	120.74
1	B	152	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	A	299	LYS	CA-C-O	6.11	127.79	120.28
1	A	279	GLN	CA-C-O	-6.11	114.24	120.71
1	A	379	GLN	CB-CG-CD	-6.09	102.25	112.60
1	B	370	TRP	CA-C-O	-6.09	111.81	120.51
1	A	264	SER	CA-CB-OG	-6.08	98.94	111.10
1	A	238	LYS	CA-C-O	-6.07	112.55	119.41
1	B	155	ASN	OD1-CG-ND2	6.07	128.67	122.60
1	B	358	GLN	OE1-CD-NE2	6.06	128.66	122.60
1	A	298	TYR	N-CA-C	6.05	117.77	109.18
1	B	377	ILE	CA-C-O	-6.04	114.77	121.17
1	A	327	ASN	CA-C-O	-6.04	114.56	121.68
1	B	154	ASN	OD1-CG-ND2	6.04	128.64	122.60
1	A	158	GLY	CA-C-O	-6.03	114.43	121.61
1	B	79	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	A	104	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	A	387	ASN	O-C-N	-6.00	114.29	122.33
1	B	205	VAL	N-CA-C	5.99	117.99	108.89
1	B	51	ALA	CA-C-N	5.98	131.94	122.61
1	B	51	ALA	C-N-CA	5.98	131.94	122.61
1	A	295	ILE	CA-C-O	-5.98	114.33	120.25
1	A	402	GLY	CA-C-O	-5.97	115.57	121.48
1	B	163	ARG	NE-CZ-NH2	-5.95	113.84	119.20
1	B	391	ARG	NE-CZ-NH1	5.95	127.45	121.50
1	A	222	ASP	CB-CA-C	-5.94	101.18	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	GLU	CA-C-O	-5.92	113.80	120.43
1	A	11	LEU	CA-C-N	-5.92	112.46	123.05
1	A	11	LEU	C-N-CA	-5.92	112.46	123.05
1	A	220	ARG	CA-C-O	-5.91	113.94	120.38
1	B	356	ARG	CD-NE-CZ	-5.91	116.12	124.40
1	B	455	LEU	N-CA-C	-5.91	105.83	113.16
1	B	399	GLY	CA-C-N	5.91	130.96	123.10
1	B	399	GLY	C-N-CA	5.91	130.96	123.10
1	B	26	VAL	CA-C-O	-5.90	114.12	120.85
1	B	348	TYR	CA-CB-CG	5.90	124.52	113.90
1	A	345	ILE	CB-CG1-CD1	5.89	126.17	113.80
1	B	16	GLN	N-CA-C	5.89	118.73	109.96
1	B	77	PRO	CA-C-O	-5.88	114.84	121.43
1	B	87	THR	N-CA-CB	5.88	120.46	110.87
1	B	442	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	A	254	GLU	CA-C-N	5.88	132.68	122.81
1	A	254	GLU	C-N-CA	5.88	132.68	122.81
1	B	172	VAL	N-CA-CB	-5.87	104.34	111.21
1	B	43	GLY	N-CA-C	-5.86	104.17	112.37
1	A	142	VAL	CA-C-O	-5.85	114.28	120.48
1	A	134	GLN	N-CA-CB	5.84	119.79	110.73
1	B	276	SER	CA-C-O	5.84	126.70	120.46
1	B	18	VAL	CA-C-O	-5.81	114.25	120.59
1	B	210	THR	N-CA-CB	5.80	119.80	109.94
1	B	368	VAL	CA-C-N	5.78	131.28	122.37
1	B	368	VAL	C-N-CA	5.78	131.28	122.37
1	B	374	ASN	CA-CB-CG	5.78	118.38	112.60
1	B	248	PRO	N-CA-C	5.77	120.27	111.15
1	A	56	ILE	CB-CA-C	5.77	119.17	110.63
1	B	418	ALA	O-C-N	5.76	126.21	121.31
1	A	204	ALA	N-CA-C	-5.76	100.44	109.25
1	A	301	ASP	CA-CB-CG	-5.75	106.85	112.60
1	A	388	ASN	CA-C-O	-5.75	114.78	120.70
1	A	401	THR	CB-CA-C	-5.75	100.13	110.36
1	B	55	VAL	N-CA-CB	-5.75	101.73	112.36
1	B	191	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	B	341	HIS	N-CA-C	5.75	118.58	109.50
1	B	219	LEU	CA-C-O	-5.75	114.50	120.70
1	B	216	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	327	ASN	CB-CG-ND2	5.72	124.99	116.40
1	B	104	ARG	CD-NE-CZ	-5.72	116.39	124.40
1	B	114	LYS	CB-CA-C	5.71	122.35	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ASN	CA-C-O	-5.71	114.25	120.36
1	B	263	GLN	CB-CA-C	5.69	119.25	110.14
1	A	354	SER	O-C-N	-5.69	115.87	122.87
1	A	241	THR	N-CA-CB	5.68	121.29	111.00
1	A	353	SER	CA-C-O	-5.68	112.92	119.56
1	A	150	VAL	N-CA-CB	5.67	120.77	111.58
1	A	386	GLN	CA-C-O	-5.67	113.44	119.97
1	A	82	THR	N-CA-CB	-5.67	101.38	110.51
1	A	214	GLY	CA-C-O	5.65	126.87	119.69
1	A	263	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	B	184	PHE	O-C-N	-5.65	116.07	122.97
1	A	131	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	416	ILE	CB-CA-C	-5.65	103.11	111.19
1	B	3	PRO	CA-C-O	-5.64	114.97	121.86
1	A	41	MET	CA-C-O	-5.64	112.45	119.28
1	B	97	ASP	CA-C-O	-5.62	115.58	121.99
1	B	148	GLY	CA-C-N	5.61	131.82	122.73
1	B	148	GLY	C-N-CA	5.61	131.82	122.73
1	B	110	ALA	N-CA-C	5.61	117.39	111.28
1	B	171	LYS	CA-C-O	5.61	126.65	120.71
1	A	462	LEU	CA-C-O	-5.59	114.67	120.70
1	A	336	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	B	400	ILE	N-CA-CB	5.57	118.88	111.64
1	B	362	ARG	CD-NE-CZ	-5.57	116.61	124.40
1	B	388	ASN	CA-C-O	-5.55	114.98	120.70
1	B	391	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	B	338	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	222	ASP	CA-C-O	-5.54	114.59	120.40
1	A	309	LYS	O-C-N	5.53	130.01	123.27
1	B	21	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	302	ILE	N-CA-CB	5.51	122.23	111.92
1	B	331	THR	N-CA-CB	5.51	119.38	110.40
1	A	205	VAL	N-CA-C	5.50	115.87	108.17
1	A	387	ASN	CA-C-N	5.50	127.92	120.44
1	A	387	ASN	C-N-CA	5.50	127.92	120.44
1	A	268	GLN	CG-CD-NE2	5.49	124.64	116.40
1	B	409	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	A	259	ILE	O-C-N	-5.49	116.69	122.83
1	A	459	ASN	N-CA-CB	-5.47	103.98	112.30
1	A	56	ILE	N-CA-CB	5.47	118.96	111.41
1	B	380	ASN	N-CA-C	5.46	120.07	113.41
1	B	93	ILE	CB-CA-C	-5.44	104.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	CA-C-O	5.44	126.39	120.57
1	A	243	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	334	ASP	CA-C-N	-5.43	113.81	122.66
1	A	334	ASP	C-N-CA	-5.43	113.81	122.66
1	A	146	GLY	CA-C-O	-5.43	113.86	122.28
1	B	340	ASN	N-CA-CB	-5.43	102.41	110.71
1	B	56	ILE	N-CA-C	-5.42	100.38	108.46
1	A	296	GLU	CB-CG-CD	-5.42	103.38	112.60
1	A	87	THR	O-C-N	5.42	130.19	123.14
1	A	382	LEU	CB-CA-C	-5.41	102.39	110.88
1	A	345	ILE	O-C-N	-5.40	116.37	122.36
1	A	403	ASP	CA-CB-CG	-5.40	107.20	112.60
1	B	417	GLY	O-C-N	-5.39	115.52	122.80
1	A	18	VAL	CB-CA-C	-5.38	103.78	111.31
1	B	330	TYR	CB-CA-C	5.38	119.99	110.85
1	A	185	LYS	CA-C-O	-5.37	114.98	120.89
1	A	46	GLN	OE1-CD-NE2	5.37	127.97	122.60
1	B	131	ASN	N-CA-CB	5.36	118.34	110.57
1	B	282	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	A	166	ASP	CA-C-O	-5.36	113.79	122.20
1	B	199	THR	CA-C-N	5.35	129.29	121.80
1	B	199	THR	C-N-CA	5.35	129.29	121.80
1	B	443	LEU	CA-C-O	5.35	126.26	120.43
1	B	47	ILE	CA-C-O	-5.34	115.07	120.31
1	B	388	ASN	N-CA-CB	5.34	117.81	110.07
1	A	141	ASP	CA-C-O	-5.33	114.57	120.38
1	B	24	ARG	CB-CG-CD	5.32	123.54	111.30
1	A	383	SER	CA-CB-OG	-5.32	100.47	111.10
1	B	413	ASN	CA-C-O	-5.29	115.85	121.94
1	B	291	ILE	N-CA-CB	5.29	118.62	111.21
1	A	20	GLY	N-CA-C	-5.29	104.10	112.66
1	B	384	THR	N-CA-CB	5.28	118.39	109.78
1	B	243	ASN	OD1-CG-ND2	5.28	127.88	122.60
1	B	119	LEU	N-CA-C	-5.27	105.44	111.14
1	B	366	GLY	N-CA-C	-5.27	108.42	115.32
1	B	299	LYS	N-CA-C	-5.26	100.82	109.40
1	A	10	ARG	CG-CD-NE	5.26	123.57	112.00
1	B	309	LYS	CA-C-O	-5.25	115.03	120.70
1	A	394	ARG	NH1-CZ-NH2	-5.25	112.48	119.30
1	B	254	GLU	CA-C-O	-5.25	115.44	121.47
1	B	292	PRO	CA-C-O	-5.24	115.19	121.48
1	A	394	ARG	CG-CD-NE	5.24	123.53	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	VAL	N-CA-CB	-5.24	104.86	111.41
1	A	420	VAL	CB-CA-C	-5.24	103.46	111.89
1	B	50	LEU	CA-C-O	-5.24	115.50	121.68
1	B	100	ASP	N-CA-C	-5.24	105.25	111.69
1	A	166	ASP	OD1-CG-OD2	5.23	135.46	122.90
1	B	57	MET	N-CA-CB	-5.23	102.48	110.85
1	A	410	PHE	CA-C-O	-5.23	115.51	121.68
1	B	15	GLY	CA-C-O	-5.23	116.51	122.78
1	A	221	TYR	CA-C-O	-5.22	115.76	121.14
1	A	301	ASP	OD1-CG-OD2	5.22	135.43	122.90
1	A	399	GLY	CA-C-O	5.21	126.43	121.64
1	B	145	ASP	CA-CB-CG	-5.21	107.39	112.60
1	B	417	GLY	CA-C-N	5.21	128.49	121.20
1	B	417	GLY	C-N-CA	5.21	128.49	121.20
1	B	24	ARG	CA-CB-CG	5.21	124.51	114.10
1	A	241	THR	CB-CA-C	-5.19	99.07	109.35
1	A	323	ARG	N-CA-CB	-5.19	102.41	110.29
1	A	71	SER	N-CA-CB	-5.17	103.42	110.56
1	B	241	THR	CA-C-O	-5.17	115.06	120.80
1	B	73	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	239	VAL	N-CA-CB	5.15	118.16	110.13
1	A	293	VAL	CB-CA-C	-5.15	102.95	110.62
1	B	210	THR	N-CA-C	-5.15	101.61	109.64
1	A	409	GLN	CB-CG-CD	-5.14	103.86	112.60
1	A	382	LEU	N-CA-C	5.14	116.57	111.07
1	A	38	ILE	N-CA-C	-5.14	105.32	110.30
1	A	104	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	B	27	ASN	CA-C-O	-5.13	115.61	121.82
1	B	412	GLY	O-C-N	5.13	127.22	122.81
1	A	37	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	B	152	ARG	CA-C-O	-5.11	114.47	120.60
1	B	67	PRO	O-C-N	-5.10	116.63	122.85
1	B	298	TYR	CA-C-O	5.08	127.41	121.46
1	B	442	ARG	CA-CB-CG	5.08	124.26	114.10
1	B	107	HIS	N-CA-C	-5.05	106.80	113.17
1	B	280	SER	N-CA-C	5.05	116.75	108.76
1	A	363	TYR	CA-C-N	5.05	131.48	122.13
1	A	363	TYR	C-N-CA	5.05	131.48	122.13
1	A	152	ARG	CD-NE-CZ	5.05	131.47	124.40
1	B	16	GLN	CA-C-O	5.04	126.50	120.70
1	B	172	VAL	CB-CA-C	5.04	117.89	110.98
1	A	199	THR	CA-C-N	-5.04	114.13	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	THR	C-N-CA	-5.04	114.13	120.98
1	B	313	SER	CA-CB-OG	-5.03	101.04	111.10
1	B	64	GLU	O-C-N	-5.03	117.08	123.01
1	B	74	TRP	CA-C-O	-5.02	114.99	120.36
1	A	27	ASN	CA-C-N	5.02	127.25	120.38
1	A	27	ASN	C-N-CA	5.02	127.25	120.38
1	B	217	VAL	N-CA-CB	5.01	117.98	111.67
1	B	299	LYS	CA-C-O	-5.01	115.29	120.70
1	A	399	GLY	O-C-N	-5.00	117.86	122.96
1	B	394	ARG	CD-NE-CZ	-5.00	117.40	124.40
1	B	409	GLN	CG-CD-NE2	-5.00	108.90	116.40

There are no chirality outliers.

There are no planarity outliers.

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	3523	0	3357	198	0
1	B	3533	0	3366	227	0
2	A	18	0	0	5	0
2	B	15	0	0	2	0
All	All	7089	0	6723	415	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 30.

All (415) 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:LYS:HD3	1:B:357:TYR:CE2	1.88	1.09
1:B:362:ARG:HG3	1:B:374:ASN:ND2	1.69	1.06
1:B:100:ASP:O	1:B:104:ARG:HG3	1.59	1.03
1:B:292:PRO:HG2	1:B:417:GLY:HA3	1.45	0.97
1:A:47:ILE:HD13	1:A:57:MET:HE3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ILE:HD13	1:A:382:LEU:HD13	1.47	0.95
1:B:14:LEU:HB2	1:B:18:VAL:CG1	1.97	0.95
1:B:14:LEU:HB2	1:B:18:VAL:HG11	1.46	0.93
1:A:116:THR:HG21	1:A:170:ILE:HG21	1.52	0.90
1:B:362:ARG:HG3	1:B:374:ASN:HD21	1.31	0.90
1:A:26:VAL:HG23	1:A:74:TRP:O	1.73	0.87
1:A:100:ASP:O	1:A:104:ARG:HG3	1.75	0.86
1:A:225:THR:HG23	1:A:408:SER:HB3	1.58	0.85
1:B:302:ILE:N	1:B:302:ILE:HD13	1.90	0.85
1:B:351:LYS:HD3	1:B:357:TYR:CZ	2.13	0.82
1:A:43:GLY:HA3	1:B:10:ARG:HH21	1.41	0.82
1:A:57:MET:HG3	1:A:64:GLU:O	1.80	0.81
1:A:219:LEU:HB3	1:A:279:GLN:HB2	1.63	0.80
1:B:91:LEU:HD23	1:B:396:VAL:HG22	1.64	0.79
1:A:377:ILE:HD13	1:A:382:LEU:CD1	2.13	0.79
1:A:47:ILE:HD13	1:A:57:MET:CE	2.14	0.78
1:A:197:VAL:CG1	1:A:455:LEU:HD23	2.13	0.78
1:A:301:ASP:HB3	1:A:407:GLU:HB2	1.65	0.78
1:A:3:PRO:HD2	2:A:476:HOH:O	1.82	0.78
1:A:206:ASN:ND2	1:A:286:PRO:O	2.19	0.77
1:B:191:GLN:H	1:B:303:SER:HB2	1.48	0.76
1:A:128:VAL:O	1:A:128:VAL:HG12	1.85	0.76
1:A:290:LYS:HG3	1:A:420:VAL:HG23	1.65	0.76
1:A:120:ALA:O	1:A:125:TYR:HB2	1.85	0.75
1:B:285:VAL:CG1	1:B:441:LEU:HD11	2.17	0.75
1:A:213:SER:O	1:A:215:TYR:HD1	1.69	0.75
1:B:193:ASP:CG	1:B:195:GLN:HE22	1.94	0.75
1:A:351:LYS:HD3	1:A:357:TYR:CE2	2.23	0.73
1:B:420:VAL:HG13	1:B:421:PRO:HD2	1.71	0.73
1:B:422:LEU:HD12	1:B:423:ALA:H	1.54	0.73
1:B:292:PRO:CG	1:B:417:GLY:HA3	2.17	0.73
1:A:162:TYR:CE1	1:A:163:ARG:HG3	2.24	0.73
1:A:197:VAL:HG12	1:A:455:LEU:HD23	1.71	0.73
1:A:43:GLY:HA3	1:B:10:ARG:NH2	2.04	0.72
1:B:178:ASN:ND2	1:B:242:LYS:HD3	2.04	0.72
1:B:292:PRO:HG2	1:B:417:GLY:CA	2.19	0.72
1:B:171:LYS:NZ	1:B:173:SER:HB3	2.04	0.72
1:A:444:GLU:O	1:A:444:GLU:HG3	1.89	0.71
1:A:111:ASN:HD21	1:B:252:GLU:HG2	1.53	0.71
1:A:290:LYS:HG3	1:A:420:VAL:CG2	2.19	0.71
1:A:312:VAL:HG13	1:A:396:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HD2	1:A:186:HIS:H	1.55	0.71
1:A:22:LYS:HB3	1:A:79:ASN:HD21	1.55	0.71
1:B:220:ARG:O	1:B:460:VAL:HA	1.89	0.71
1:B:222:ASP:HA	1:B:275:THR:O	1.91	0.71
1:A:363:TYR:O	1:A:365:PRO:HD3	1.91	0.70
1:A:323:ARG:HA	1:A:323:ARG:NE	2.06	0.70
1:B:442:ARG:NH2	1:B:444:GLU:OE2	2.24	0.69
1:A:204:ALA:HB3	1:A:291:ILE:HG22	1.74	0.69
1:A:281:VAL:HG21	1:A:414:ILE:HG12	1.76	0.68
1:B:322:LEU:HB3	1:B:327:ASN:HD22	1.58	0.68
1:A:205:VAL:HG11	1:A:442:ARG:NH2	2.09	0.68
1:B:171:LYS:HZ2	1:B:173:SER:HB3	1.56	0.68
1:B:162:TYR:CE1	1:B:163:ARG:HB2	2.30	0.67
1:B:285:VAL:HG11	1:B:441:LEU:HD11	1.74	0.67
1:B:162:TYR:CD1	1:B:163:ARG:HB2	2.29	0.67
1:A:291:ILE:HD11	1:A:417:GLY:O	1.94	0.67
1:B:351:LYS:NZ	1:B:357:TYR:OH	2.17	0.67
1:A:116:THR:CG2	1:A:170:ILE:HG21	2.22	0.67
1:B:48:SER:CB	1:B:72:ASN:HD21	2.08	0.67
1:A:204:ALA:HB3	1:A:291:ILE:CG2	2.25	0.66
1:B:230:THR:O	1:B:402:GLY:HA3	1.95	0.66
1:B:47:ILE:HG12	1:B:57:MET:HG2	1.75	0.66
1:B:221:TYR:HD2	1:B:223:THR:HG23	1.60	0.66
1:B:354:SER:HB3	1:B:357:TYR:HB3	1.78	0.66
1:B:352:ALA:O	1:B:358:GLN:NE2	2.29	0.66
1:B:364:ILE:HG22	1:B:367:GLU:HG2	1.76	0.66
1:A:444:GLU:O	1:A:444:GLU:CG	2.42	0.66
1:A:447:LEU:HD21	1:A:460:VAL:HG12	1.77	0.65
1:A:291:ILE:HG13	1:A:292:PRO:HD2	1.78	0.65
1:B:284:THR:HG22	1:B:284:THR:O	1.96	0.65
1:A:107:HIS:HB2	2:A:477:HOH:O	1.96	0.65
1:A:290:LYS:CG	1:A:420:VAL:HG23	2.26	0.65
1:A:54:TRP:CZ3	1:A:67:PRO:HD3	2.32	0.64
1:B:127:TRP:CE2	1:B:164:CYS:HA	2.31	0.64
1:A:152:ARG:HD2	1:A:169:ALA:HB2	1.78	0.64
1:A:212:GLN:OE1	1:A:215:TYR:CZ	2.51	0.64
1:A:322:LEU:HG	1:A:339:TRP:HB2	1.80	0.64
1:B:6:PRO:HG3	1:B:34:VAL:CG1	2.27	0.64
1:B:222:ASP:OD1	1:B:276:SER:OG	2.14	0.64
1:B:4:VAL:CG2	1:B:34:VAL:HG21	2.28	0.64
1:B:191:GLN:HB2	1:B:303:SER:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:O	1:B:278:SER:HA	1.98	0.64
1:A:163:ARG:HB3	1:A:166:ASP:OD2	1.98	0.64
1:B:47:ILE:HG23	1:B:55:VAL:HG13	1.78	0.64
1:A:354:SER:HB3	1:A:357:TYR:HB3	1.80	0.63
1:B:103:TRP:CD1	1:B:103:TRP:C	2.76	0.63
1:A:202:GLY:HA3	1:A:445:ILE:HG12	1.80	0.63
1:B:27:ASN:OD1	1:B:30:GLU:HG3	1.99	0.63
1:B:216:ASP:OD1	1:B:282:ARG:HD3	1.99	0.63
1:B:331:THR:O	1:B:332:HIS:HB2	1.98	0.63
1:A:377:ILE:O	1:A:381:GLY:N	2.29	0.62
1:B:14:LEU:HB2	1:B:18:VAL:HG12	1.78	0.62
1:B:275:THR:HG22	1:B:276:SER:N	2.15	0.62
1:B:163:ARG:O	1:B:166:ASP:HB2	1.99	0.61
1:A:28:ARG:HD3	1:A:54:TRP:CE2	2.36	0.61
1:B:47:ILE:HG23	1:B:55:VAL:CG1	2.30	0.61
1:B:28:ARG:HD2	1:B:54:TRP:CE2	2.36	0.61
1:B:34:VAL:HG12	1:B:37:ASN:HB2	1.81	0.61
1:B:4:VAL:HG22	1:B:34:VAL:HG21	1.83	0.61
1:B:364:ILE:O	1:B:367:GLU:HB2	2.01	0.60
1:A:214:GLY:O	1:A:467:ALA:N	2.34	0.60
1:B:11:LEU:HD12	1:B:73:THR:O	2.00	0.60
1:B:162:TYR:HE1	1:B:163:ARG:HE	1.50	0.60
1:A:215:TYR:HH	1:A:440:GLY:N	1.99	0.59
1:A:205:VAL:HG11	1:A:442:ARG:CZ	2.33	0.59
1:A:399:GLY:O	1:A:400:ILE:HD13	2.02	0.59
1:A:206:ASN:HB3	1:A:285:VAL:CG1	2.33	0.59
1:B:91:LEU:HB2	1:B:394:ARG:HE	1.67	0.59
1:B:162:TYR:CD1	1:B:162:TYR:C	2.81	0.58
1:A:144:ARG:NH2	1:A:147:ASP:OD1	2.36	0.58
1:A:216:ASP:HA	1:A:281:VAL:O	2.03	0.58
1:B:18:VAL:HG12	1:B:18:VAL:O	2.04	0.58
1:B:364:ILE:CG2	1:B:367:GLU:HG2	2.32	0.58
1:A:288:ARG:O	1:A:288:ARG:HG2	2.02	0.58
1:B:422:LEU:HD12	1:B:423:ALA:N	2.18	0.58
1:B:191:GLN:HB2	1:B:303:SER:CB	2.32	0.58
1:A:168:THR:HG23	1:A:319:SER:O	2.04	0.58
1:A:189:VAL:HA	1:A:304:TYR:HB3	1.84	0.58
1:B:57:MET:HE2	1:B:61:TYR:CG	2.38	0.58
1:B:178:ASN:HD21	1:B:242:LYS:HD3	1.67	0.58
1:B:375:TRP:O	1:B:379:GLN:HG2	2.04	0.57
1:B:130:GLY:HA3	1:B:139:ASP:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ILE:HD13	1:B:302:ILE:H	1.70	0.57
1:A:124:GLY:HA3	1:A:327:ASN:HA	1.87	0.57
1:B:336:ARG:HG3	1:B:336:ARG:HH11	1.70	0.57
1:B:189:VAL:HG12	1:B:189:VAL:O	2.04	0.56
1:A:135:TYR:CE2	1:B:294:LYS:HD3	2.40	0.56
1:A:185:LYS:HD2	1:A:186:HIS:N	2.21	0.56
1:B:368:VAL:HG22	1:B:368:VAL:O	2.04	0.56
1:B:354:SER:O	1:B:358:GLN:HG3	2.06	0.55
1:B:94:PRO:O	1:B:104:ARG:NH1	2.37	0.55
1:A:57:MET:O	1:A:63:GLY:HA2	2.06	0.55
1:B:302:ILE:N	1:B:302:ILE:CD1	2.67	0.55
1:A:48:SER:HA	1:A:72:ASN:OD1	2.07	0.55
1:B:99:VAL:O	1:B:103:TRP:HB2	2.06	0.55
1:A:375:TRP:CZ2	1:A:379:GLN:HG3	2.42	0.55
1:A:304:TYR:HB2	1:A:305:PRO:HD2	1.88	0.55
1:B:223:THR:HG21	1:B:409:GLN:O	2.06	0.55
1:A:43:GLY:O	1:A:59:PRO:HD2	2.06	0.55
1:A:126:ALA:HB2	1:A:323:ARG:CD	2.36	0.54
1:A:206:ASN:HB3	1:A:285:VAL:HG11	1.87	0.54
1:A:231:ASN:O	1:A:232:THR:C	2.48	0.54
1:B:193:ASP:CB	1:B:195:GLN:HE22	2.19	0.54
1:A:291:ILE:HG12	1:A:416:ILE:HG22	1.89	0.54
1:B:246:LYS:HD3	1:B:258:GLU:HB3	1.89	0.54
1:A:223:THR:HG22	1:A:224:ALA:H	1.72	0.54
1:A:253:THR:HB	1:A:300:ALA:CB	2.36	0.54
1:B:221:TYR:CD2	1:B:223:THR:HG23	2.42	0.54
1:B:275:THR:CG2	1:B:276:SER:N	2.71	0.54
1:A:162:TYR:CD1	1:A:163:ARG:HG3	2.43	0.54
1:A:57:MET:SD	1:A:66:LYS:HE3	2.48	0.54
1:A:229:LYS:NZ	1:A:268:GLN:O	2.41	0.54
1:A:307:GLU:HB2	1:A:401:THR:HG22	1.90	0.54
1:A:416:ILE:HG22	1:A:417:GLY:N	2.23	0.54
1:A:22:LYS:HB3	1:A:79:ASN:ND2	2.22	0.53
1:A:201:VAL:HG12	1:A:202:GLY:N	2.22	0.53
1:A:291:ILE:HG12	1:A:416:ILE:CG2	2.38	0.53
1:B:202:GLY:HA3	1:B:445:ILE:HB	1.90	0.53
1:B:224:ALA:HA	1:B:274:THR:HA	1.91	0.53
1:B:383:SER:O	1:B:384:THR:C	2.51	0.53
1:B:389:LEU:HA	1:B:392:VAL:HG13	1.90	0.53
1:B:194:ARG:O	1:B:194:ARG:HG3	2.09	0.53
1:A:204:ALA:N	1:A:291:ILE:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HB	1:A:300:ALA:HB3	1.90	0.52
1:B:66:LYS:HB2	1:B:67:PRO:HD2	1.91	0.52
1:A:217:VAL:CG2	1:A:414:ILE:HD11	2.39	0.52
1:A:219:LEU:HD22	1:A:295:ILE:HD13	1.90	0.52
1:B:220:ARG:HA	1:B:277:LEU:O	2.09	0.52
1:B:336:ARG:HG3	1:B:336:ARG:NH1	2.24	0.52
1:B:200:VAL:HG12	1:B:445:ILE:CD1	2.40	0.52
1:A:321:PHE:HE1	1:A:323:ARG:NH1	2.06	0.52
1:A:451:GLU:HG2	1:A:455:LEU:HD13	1.91	0.52
1:B:72:ASN:C	1:B:72:ASN:ND2	2.66	0.52
1:B:287:ALA:O	1:B:288:ARG:C	2.49	0.52
1:B:6:PRO:HG3	1:B:34:VAL:HG11	1.90	0.52
1:A:195:GLN:NE2	1:A:299:LYS:O	2.35	0.52
1:A:206:ASN:CB	1:A:285:VAL:HG11	2.39	0.52
1:B:200:VAL:CG1	1:B:445:ILE:HD11	2.39	0.52
1:A:98:GLU:OE1	1:A:238:LYS:NZ	2.42	0.52
1:A:234:GLY:O	1:A:235:LEU:C	2.52	0.52
1:B:351:LYS:CD	1:B:357:TYR:CE2	2.80	0.52
1:A:206:ASN:O	1:A:422:LEU:HD22	2.10	0.51
1:B:35:LYS:HZ2	1:B:65:ILE:HD12	1.74	0.51
1:B:206:ASN:ND2	1:B:287:ALA:HA	2.25	0.51
1:B:285:VAL:HG12	1:B:441:LEU:HD11	1.92	0.51
1:A:365:PRO:O	1:A:368:VAL:HG22	2.11	0.51
1:B:357:TYR:CE1	1:B:361:LYS:NZ	2.79	0.51
1:A:217:VAL:HG23	1:A:414:ILE:HD11	1.93	0.51
1:A:126:ALA:HB2	1:A:323:ARG:HD3	1.93	0.51
1:A:239:VAL:HG23	1:A:240:THR:N	2.25	0.50
1:A:284:THR:O	1:A:286:PRO:HD3	2.11	0.50
1:A:399:GLY:C	1:A:400:ILE:HD13	2.36	0.50
1:B:220:ARG:HG2	1:B:461:SER:OG	2.11	0.50
1:B:301:ASP:OD1	1:B:301:ASP:C	2.52	0.50
1:A:140:MET:HE3	1:A:151:ILE:HG22	1.93	0.50
1:A:203:TRP:HB2	1:A:444:GLU:HG3	1.93	0.50
1:B:236:SER:HB2	1:B:266:ALA:HB2	1.93	0.50
1:B:114:LYS:NZ	1:B:138:GLU:OE2	2.44	0.50
1:B:200:VAL:HG11	1:B:445:ILE:HD11	1.94	0.50
1:A:101:VAL:HG21	1:A:235:LEU:CD2	2.41	0.50
1:A:54:TRP:CZ3	1:A:67:PRO:CD	2.95	0.50
1:B:66:LYS:HB2	1:B:67:PRO:CD	2.41	0.50
1:B:98:GLU:CD	1:B:238:LYS:HD3	2.37	0.50
1:A:324:TRP:O	1:A:325:GLY:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLN:HG2	1:A:379:GLN:N	2.27	0.49
1:B:6:PRO:HG3	1:B:34:VAL:HG13	1.94	0.49
1:B:321:PHE:CE1	1:B:336:ARG:HD3	2.47	0.49
1:A:206:ASN:HD21	1:A:287:ALA:HA	1.76	0.49
1:A:323:ARG:NE	1:A:323:ARG:CA	2.73	0.49
1:A:127:TRP:CE2	1:A:164:CYS:HA	2.47	0.49
1:A:321:PHE:CE1	1:A:323:ARG:NH1	2.80	0.49
1:B:4:VAL:HG11	1:B:30:GLU:HB3	1.92	0.49
1:B:350:ASP:C	1:B:350:ASP:OD1	2.55	0.49
1:B:136:VAL:HG23	1:B:137:GLY:N	2.26	0.49
1:A:193:ASP:O	1:A:300:ALA:HA	2.13	0.49
1:A:303:SER:HB2	1:A:405:SER:CB	2.43	0.49
1:A:227:TRP:CE2	1:A:257:ILE:HG23	2.48	0.49
1:A:239:VAL:HG11	1:A:400:ILE:HG13	1.94	0.49
1:A:225:THR:HG23	1:A:408:SER:CB	2.38	0.48
1:A:54:TRP:HZ3	1:A:67:PRO:HD3	1.76	0.48
1:B:191:GLN:N	1:B:303:SER:HB2	2.24	0.48
1:A:203:TRP:CE3	1:A:290:LYS:HD3	2.49	0.48
1:A:211:PRO:HB3	1:A:286:PRO:HA	1.96	0.48
1:A:215:TYR:O	1:A:282:ARG:HA	2.13	0.48
1:B:127:TRP:NE1	1:B:164:CYS:HA	2.29	0.48
1:A:378:GLN:CG	1:A:379:GLN:N	2.77	0.47
1:B:128:VAL:HG23	2:B:479:HOH:O	2.13	0.47
1:A:304:TYR:HB2	1:A:305:PRO:CD	2.44	0.47
1:B:91:LEU:HD23	1:B:396:VAL:CG2	2.41	0.47
1:B:193:ASP:C	1:B:193:ASP:OD1	2.57	0.47
1:B:388:ASN:O	1:B:392:VAL:HG12	2.14	0.47
1:A:106:VAL:HG13	1:A:151:ILE:HD11	1.96	0.47
1:B:142:VAL:O	1:B:142:VAL:HG22	2.14	0.47
1:A:44:GLN:CB	1:B:7:ASP:HB2	2.45	0.47
1:A:287:ALA:O	1:A:288:ARG:C	2.57	0.47
1:A:323:ARG:NH2	1:A:336:ARG:HH11	2.12	0.47
1:B:205:VAL:HG22	1:B:290:LYS:HB3	1.97	0.47
1:A:111:ASN:HD21	1:B:252:GLU:CG	2.25	0.47
1:B:200:VAL:HG12	1:B:445:ILE:HD12	1.97	0.47
1:A:162:TYR:CE1	1:A:163:ARG:CG	2.95	0.47
1:B:44:GLN:HA	1:B:59:PRO:HD2	1.97	0.47
1:B:273:THR:O	1:B:273:THR:OG1	2.26	0.47
1:B:322:LEU:CB	1:B:327:ASN:HD22	2.25	0.47
1:A:217:VAL:HG22	1:A:281:VAL:HB	1.96	0.47
1:B:193:ASP:OD1	1:B:195:GLN:NE2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:VAL:O	1:B:368:VAL:CG2	2.63	0.47
1:B:420:VAL:CG1	1:B:421:PRO:HD2	2.43	0.47
1:A:316:LEU:O	1:A:342:THR:HA	2.15	0.47
1:A:415:GLU:OE1	1:B:114:LYS:CE	2.63	0.47
1:B:9:LEU:CD1	1:B:38:ILE:HG12	2.45	0.47
1:B:209:ASP:OD1	1:B:209:ASP:N	2.47	0.47
1:B:451:GLU:O	1:B:455:LEU:HD13	2.15	0.47
1:B:193:ASP:HB2	1:B:195:GLN:HE22	1.80	0.46
1:A:107:HIS:CD2	2:A:477:HOH:O	2.68	0.46
1:B:57:MET:HE2	1:B:61:TYR:HB3	1.96	0.46
1:B:178:ASN:ND2	1:B:242:LYS:HG2	2.30	0.46
1:B:191:GLN:HB2	1:B:303:SER:OG	2.15	0.46
1:B:163:ARG:O	1:B:166:ASP:N	2.46	0.46
1:A:44:GLN:HB3	1:B:7:ASP:HB2	1.97	0.46
1:A:140:MET:HA	1:A:153:GLY:HA2	1.96	0.46
1:A:295:ILE:HG12	1:A:414:ILE:HB	1.96	0.46
1:B:37:ASN:O	1:B:41:MET:HG3	2.16	0.46
1:B:297:LEU:HD22	1:B:457:PHE:CE2	2.50	0.46
1:B:341:HIS:CD2	1:B:371:TRP:HE1	2.34	0.46
1:A:229:LYS:HE3	1:A:268:GLN:O	2.15	0.45
1:A:292:PRO:HG2	1:A:417:GLY:HA3	1.98	0.45
1:B:448:ASP:OD1	1:B:448:ASP:C	2.59	0.45
1:B:299:LYS:HG3	1:B:409:GLN:HG3	1.98	0.45
1:A:469:ASN:ND2	1:A:470:GLN:HE22	2.15	0.45
1:A:183:SER:O	1:A:184:PHE:C	2.60	0.45
1:B:122:TYR:HE2	2:B:475:HOH:O	1.99	0.45
1:A:28:ARG:HD3	1:A:54:TRP:CZ2	2.50	0.45
1:A:314:TYR:CD1	1:A:314:TYR:N	2.85	0.45
1:A:414:ILE:HG21	1:A:414:ILE:HD13	1.57	0.45
1:B:48:SER:CA	1:B:72:ASN:HD21	2.30	0.45
1:B:178:ASN:CG	1:B:242:LYS:HG2	2.41	0.45
1:B:192:SER:O	1:B:193:ASP:HB3	2.17	0.45
1:B:281:VAL:HG13	1:B:283:PRO:HD3	1.99	0.45
1:B:349:LYS:HE2	1:B:349:LYS:HB2	1.70	0.45
1:B:448:ASP:O	1:B:449:ALA:C	2.58	0.45
1:A:57:MET:HG3	1:A:64:GLU:HG3	1.97	0.45
1:B:99:VAL:O	1:B:103:TRP:CB	2.64	0.45
1:A:225:THR:O	1:A:272:SER:HA	2.16	0.45
1:B:409:GLN:HE21	1:B:409:GLN:HB2	1.29	0.45
1:A:24:ARG:O	1:A:24:ARG:HG3	2.15	0.45
1:A:362:ARG:HH11	1:A:362:ARG:HD2	1.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:O	1:B:120:ALA:C	2.60	0.45
1:A:47:ILE:HG22	1:A:55:VAL:HG13	1.99	0.44
1:B:281:VAL:HG22	1:B:282:ARG:N	2.31	0.44
1:B:373:TRP:O	1:B:377:ILE:HG13	2.17	0.44
1:B:246:LYS:CE	1:B:258:GLU:HB3	2.47	0.44
1:B:291:ILE:HG21	1:B:291:ILE:HD13	1.71	0.44
1:B:298:TYR:O	1:B:409:GLN:HA	2.18	0.44
1:B:322:LEU:HD22	1:B:339:TRP:HB2	1.98	0.44
1:A:192:SER:O	1:A:193:ASP:HB3	2.17	0.44
1:A:220:ARG:HG3	1:A:278:SER:OG	2.18	0.44
1:B:416:ILE:H	1:B:416:ILE:HG12	1.46	0.44
1:B:421:PRO:O	1:B:422:LEU:C	2.60	0.44
1:A:458:ASN:O	1:A:459:ASN:HB2	2.18	0.44
1:A:126:ALA:HB2	1:A:323:ARG:HD2	2.00	0.44
1:B:104:ARG:HH11	1:B:104:ARG:HD2	1.55	0.44
1:B:178:ASN:ND2	1:B:242:LYS:CD	2.76	0.44
1:B:242:LYS:HD2	1:B:242:LYS:HA	1.58	0.44
1:B:72:ASN:C	1:B:72:ASN:HD22	2.26	0.44
1:B:131:ASN:HD22	1:B:159:CYS:HB3	1.83	0.43
1:A:191:GLN:O	1:A:302:ILE:HA	2.18	0.43
1:B:394:ARG:HH11	1:B:394:ARG:HD2	1.44	0.43
1:A:228:SER:HA	1:A:269:ASN:O	2.18	0.43
1:A:415:GLU:OE1	1:B:114:LYS:NZ	2.50	0.43
1:B:193:ASP:HB2	1:B:195:GLN:NE2	2.33	0.43
1:A:101:VAL:HG21	1:A:235:LEU:HD21	1.99	0.43
1:A:216:ASP:OD1	1:A:282:ARG:HB2	2.18	0.43
1:B:321:PHE:HA	1:B:338:ASN:HA	2.00	0.43
1:B:220:ARG:CG	1:B:461:SER:OG	2.66	0.43
1:A:129:GLY:O	1:A:153:GLY:HA3	2.18	0.43
1:B:35:LYS:HZ2	1:B:35:LYS:HG3	1.71	0.43
1:B:72:ASN:ND2	1:B:72:ASN:O	2.52	0.43
1:B:189:VAL:HA	1:B:304:TYR:HB3	2.01	0.43
1:A:323:ARG:HH22	1:A:336:ARG:HH11	1.66	0.43
1:B:96:GLY:HA2	1:B:233:TYR:CG	2.54	0.43
1:B:330:TYR:O	1:B:332:HIS:HD2	2.02	0.43
1:A:303:SER:HB2	1:A:405:SER:HB3	2.00	0.43
1:A:341:HIS:CD2	1:A:371:TRP:HE1	2.37	0.43
1:A:206:ASN:ND2	1:A:287:ALA:HA	2.33	0.42
1:A:324:TRP:HD1	1:A:334:ASP:HB2	1.84	0.42
1:B:346:GLY:HA3	1:B:347:PRO:HD2	1.84	0.42
1:B:389:LEU:O	1:B:393:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:VAL:HG13	2:A:484:HOH:O	2.19	0.42
1:B:34:VAL:HG12	1:B:34:VAL:O	2.20	0.42
1:B:442:ARG:CZ	1:B:444:GLU:OE2	2.68	0.42
1:B:452:LEU:HD13	1:B:460:VAL:HG11	2.02	0.42
1:A:103:TRP:HE3	1:A:149:TRP:CH2	2.37	0.42
1:A:416:ILE:HG22	1:A:417:GLY:H	1.82	0.42
1:B:57:MET:HE2	1:B:61:TYR:CB	2.49	0.42
1:A:7:ASP:O	1:A:10:ARG:NH2	2.52	0.42
1:A:206:ASN:CB	1:A:285:VAL:CG1	2.97	0.42
1:B:208:SER:OG	1:B:210:THR:O	2.37	0.42
1:A:62:ASN:HD22	1:A:62:ASN:HA	1.67	0.42
1:A:113:ILE:HG23	1:A:151:ILE:HG21	2.02	0.42
1:A:364:ILE:O	1:A:365:PRO:C	2.62	0.42
1:B:194:ARG:HA	1:B:299:LYS:O	2.20	0.42
1:B:352:ALA:HB2	1:B:370:TRP:NE1	2.35	0.42
1:A:163:ARG:NE	1:A:166:ASP:OD2	2.48	0.42
1:A:184:PHE:CG	1:A:248:PRO:HG3	2.54	0.42
1:B:12:PHE:CE1	1:B:20:GLY:HA3	2.54	0.42
1:B:47:ILE:CG2	1:B:55:VAL:HG13	2.48	0.42
1:B:164:CYS:C	1:B:166:ASP:H	2.27	0.42
1:A:232:THR:CG2	1:A:233:TYR:CE2	3.03	0.42
1:B:163:ARG:HG2	1:B:166:ASP:HB2	2.00	0.42
1:B:352:ALA:C	1:B:358:GLN:NE2	2.78	0.42
1:A:119:LEU:HD13	1:A:389:LEU:CD2	2.50	0.41
1:A:162:TYR:CE1	1:A:163:ARG:HD3	2.55	0.41
1:A:223:THR:HG22	1:A:224:ALA:N	2.35	0.41
1:A:323:ARG:CZ	1:A:336:ARG:HD3	2.50	0.41
1:A:375:TRP:CE2	1:A:379:GLN:HG3	2.54	0.41
1:A:444:GLU:O	1:A:444:GLU:CD	2.63	0.41
1:B:253:THR:H	1:B:253:THR:HG22	1.48	0.41
1:B:354:SER:CB	1:B:357:TYR:HB3	2.48	0.41
1:A:162:TYR:CE1	1:A:163:ARG:CD	3.03	0.41
1:A:420:VAL:HB	1:A:421:PRO:HD2	2.01	0.41
1:B:234:GLY:O	1:B:235:LEU:C	2.62	0.41
1:B:364:ILE:CG2	1:B:367:GLU:CG	2.97	0.41
1:A:284:THR:O	1:A:284:THR:HG22	2.19	0.41
1:B:103:TRP:CD1	1:B:103:TRP:O	2.74	0.41
1:B:216:ASP:OD1	1:B:282:ARG:NH1	2.52	0.41
1:B:330:TYR:O	1:B:332:HIS:CD2	2.74	0.41
1:A:38:ILE:HG23	1:A:74:TRP:CE2	2.56	0.41
1:A:162:TYR:CD1	1:A:162:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:N	1:A:442:ARG:O	2.46	0.41
1:A:46:GLN:O	1:A:58:GLY:N	2.48	0.41
1:B:322:LEU:CG	1:B:327:ASN:HD22	2.33	0.41
1:A:244:LYS:HB2	1:A:259:ILE:O	2.20	0.41
1:A:407:GLU:HG2	1:A:408:SER:N	2.36	0.41
1:A:206:ASN:HB3	1:A:285:VAL:HG12	2.01	0.41
1:B:57:MET:O	1:B:63:GLY:HA2	2.19	0.41
1:B:162:TYR:CD1	1:B:163:ARG:CB	3.02	0.41
1:B:178:ASN:OD1	1:B:242:LYS:HG2	2.20	0.41
1:A:232:THR:HG21	1:A:233:TYR:CE2	2.56	0.41
1:B:144:ARG:HG3	1:B:145:ASP:H	1.85	0.41
1:A:111:ASN:ND2	1:B:252:GLU:OE2	2.54	0.41
1:A:364:ILE:O	1:A:364:ILE:HG22	2.21	0.41
1:A:365:PRO:O	1:A:366:GLY:C	2.64	0.41
1:B:171:LYS:HZ1	1:B:173:SER:HB3	1.82	0.41
1:B:178:ASN:HD21	1:B:242:LYS:N	2.19	0.41
1:B:208:SER:O	1:B:288:ARG:HG2	2.21	0.41
1:B:246:LYS:CD	1:B:258:GLU:HB3	2.49	0.41
1:B:286:PRO:O	1:B:289:SER:HB2	2.21	0.41
1:B:362:ARG:HH11	1:B:362:ARG:HD2	1.54	0.41
1:B:47:ILE:CG2	1:B:55:VAL:CG1	2.98	0.41
1:B:319:SER:HB3	1:B:340:ASN:OD1	2.21	0.41
1:A:368:VAL:HG22	1:A:368:VAL:H	1.55	0.40
1:B:237:GLU:HG2	1:B:266:ALA:CB	2.51	0.40
1:B:364:ILE:HA	1:B:365:PRO:HD2	1.73	0.40
1:B:400:ILE:C	1:B:401:THR:HG23	2.47	0.40
1:A:107:HIS:HD2	2:A:477:HOH:O	2.02	0.40
1:A:229:LYS:CE	1:A:268:GLN:O	2.69	0.40
1:B:24:ARG:HH22	1:B:30:GLU:CD	2.28	0.40
1:B:194:ARG:O	1:B:194:ARG:CG	2.69	0.40
1:B:246:LYS:HD3	1:B:246:LYS:HA	1.87	0.40
1:B:307:GLU:HG2	1:B:307:GLU:O	2.21	0.40
1:B:22:LYS:HD3	1:B:22:LYS:HA	1.24	0.40
1:B:279:GLN:HE21	1:B:279:GLN:HB2	1.57	0.40
1:B:301:ASP:OD1	1:B:301:ASP:O	2.40	0.40
1:A:76:TYR:CG	1:A:77:PRO:HD2	2.55	0.40
1:A:198:LYS:CG	1:A:199:THR:N	2.84	0.40
1:A:54:TRP:CE3	1:A:66:LYS:C	3.00	0.40
1:B:114:LYS:N	1:B:115:PRO:HD2	2.36	0.40
1:B:200:VAL:CG1	1:B:445:ILE:CD1	2.98	0.40
1:B:361:LYS:HA	1:B:361:LYS:HD3	1.80	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	443/470 (94%)	401 (90%)	39 (9%)	3 (1%)	18	47
1	B	447/470 (95%)	404 (90%)	35 (8%)	8 (2%)	6	23
All	All	890/940 (95%)	805 (90%)	74 (8%)	11 (1%)	10	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	B	190	THR
1	B	362	ARG
1	A	236	SER
1	B	58	GLY
1	B	193	ASP
1	A	58	GLY
1	B	236	SER
1	B	244	LYS
1	B	189	VAL
1	B	326	GLY

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	378/392 (96%)	322 (85%)	56 (15%)	3	10
1	B	379/392 (97%)	318 (84%)	61 (16%)	2	8
All	All	757/784 (97%)	640 (84%)	117 (16%)	2	9

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	26	VAL
1	A	41	MET
1	A	47	ILE
1	A	55	VAL
1	A	62	ASN
1	A	69	THR
1	A	78	THR
1	A	113	ILE
1	A	142	VAL
1	A	144	ARG
1	A	150	VAL
1	A	162	TYR
1	A	172	VAL
1	A	179	LEU
1	A	190	THR
1	A	195	GLN
1	A	200	VAL
1	A	205	VAL
1	A	223	THR
1	A	225	THR
1	A	239	VAL
1	A	241	THR
1	A	253	THR
1	A	255	LEU
1	A	264	SER
1	A	272	SER
1	A	273	THR
1	A	275	THR
1	A	281	VAL
1	A	282	ARG
1	A	284	THR
1	A	301	ASP
1	A	307	GLU
1	A	312	VAL

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Mol	Chain	Res	Type
1	A	327	ASN
1	A	340	ASN
1	A	342	THR
1	A	349	LYS
1	A	362	ARG
1	A	365	PRO
1	A	378	GLN
1	A	394	ARG
1	A	396	VAL
1	A	408	SER
1	A	409	GLN
1	A	414	ILE
1	A	443	LEU
1	A	444	GLU
1	A	447	LEU
1	A	450	GLN
1	A	455	LEU
1	A	462	LEU
1	A	463	SER
1	A	464	VAL
1	A	470	GLN
1	B	2	GLU
1	B	10	ARG
1	B	14	LEU
1	B	16	GLN
1	B	18	VAL
1	B	21	ASP
1	B	22	LYS
1	B	24	ARG
1	B	28	ARG
1	B	35	LYS
1	B	36	SER
1	B	42	MET
1	B	55	VAL
1	B	62	ASN
1	B	66	LYS
1	B	71	SER
1	B	72	ASN
1	B	78	THR
1	B	87	THR
1	B	89	SER
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	128	VAL
1	B	136	VAL
1	B	140	MET
1	B	142	VAL
1	B	143	THR
1	B	150	VAL
1	B	172	VAL
1	B	182	ASP
1	B	195	GLN
1	B	199	THR
1	B	209	ASP
1	B	212	GLN
1	B	220	ARG
1	B	225	THR
1	B	236	SER
1	B	239	VAL
1	B	241	THR
1	B	243	ASN
1	B	253	THR
1	B	273	THR
1	B	282	ARG
1	B	284	THR
1	B	288	ARG
1	B	293	VAL
1	B	302	ILE
1	B	307	GLU
1	B	322	LEU
1	B	327	ASN
1	B	342	THR
1	B	353	SER
1	B	362	ARG
1	B	368	VAL
1	B	383	SER
1	B	392	VAL
1	B	409	GLN
1	B	413	ASN
1	B	416	ILE
1	B	441	LEU
1	B	445	ILE
1	B	460	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	32	GLN
1	A	44	GLN
1	A	62	ASN
1	A	79	ASN
1	A	111	ASN
1	A	132	HIS
1	A	206	ASN
1	A	341	HIS
1	A	378	GLN
1	A	386	GLN
1	A	413	ASN
1	A	450	GLN
1	A	470	GLN
1	B	62	ASN
1	B	72	ASN
1	B	131	ASN
1	B	178	ASN
1	B	195	GLN
1	B	206	ASN
1	B	212	GLN
1	B	226	ASN
1	B	279	GLN
1	B	327	ASN
1	B	332	HIS
1	B	341	HIS
1	B	374	ASN
1	B	379	GLN
1	B	387	ASN
1	B	409	GLN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.