



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:31 AM UTC

PDB ID : 5RUB / pdb_00005rub
Title : CRYSTALLOGRAPHIC REFINEMENT AND STRUCTURE OF RIBULO
SE-1,5-BISPHOSPHATE CARBOXYLASE FROM RHODOSPIRILLUM
RUBRUM AT 1.7 ANGSTROMS RESOLUTION
Authors : Schneider, G.; Lindqvist, Y.; Lundqvist, T.
Deposited on : 1990-05-29
Resolution : 1.70 Å(reported)

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

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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

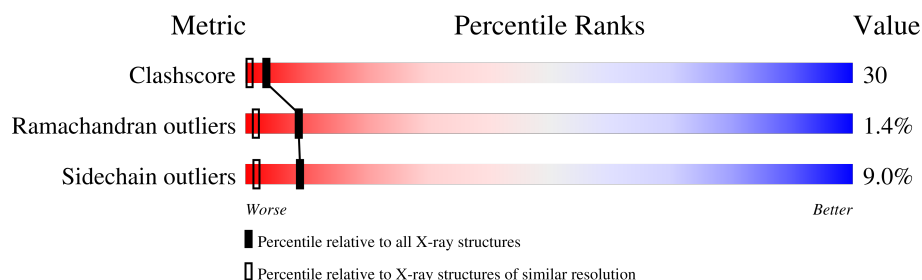
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

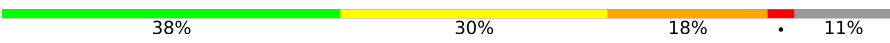
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	490	 38% 30% 18% • 11%
1	B	490	 40% 33% 12% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7377 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 RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	18	0	0
			3330	2110	588	617	15			
1	B	433	Total	C	N	O	S	9	0	0
			3311	2100	585	611	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	conflict	UNP P04718
B	91	ASP	HIS	conflict	UNP P04718

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	342	Total	O	0	0
			342	342		
2	B	394	Total	O	0	0
			394	394		

L424	D425	Y426	A427	R428	E429	H430	K431	A434	R435	A436	F437	G442	D443	A444	D445	Q446	I447	Y448	P449	G450	W451	R452	K453	A454	L455	G456	V457	GLU	ASP	THR	ARG	SER	ALA	LEU	PRO	ALA																
T344	E347	F352	Y353	R354	Q355	S356	K361	A362	C363	T364	S368	N371	N372	A373	L374	R375	M376	P377	G378	F379	F380	N382	N385	A386	N387	T391	A392	G393	G394	G395	A396	F397	G398	H399	I400	D401	G402	P403	V404	A405	K411	Q412	Q415	D419	G420	V421	P422	V423				
R277	R278	F279	N282	F283	L284	H285	Y286	H287	R288	A289	G290	H291	G292	A293	V294	T295	Q298	S299	K300	R301	G302	Y303	T304	V307	H308	C309	K310	M311	Q315	G316	A317	S318	G319	I320	H321	T322	G323	THR	MET	GLY	PHE	GLY	GLY	LYS	MET	GLU	GLY	SER	D336	R337	A338	Y341
G197	N198	Q199	A202	P203	L204	R205	A209	L210	V211	A212	D213	A214	M215	R216	R217	A218	Q219	Y222	G223	E224	A225	K226	S229	A230	N231	L232	T233	A234	D235	D236	V247	T250	N254	H257	V258	A259	L260	L261	V262	D263	G264	Y265	G268	A269	A270	A271	T274	A275	R276			
F126	E130	R133	F136	D137	G138	P139	S140	V141	M142	I143	S144	A145	L146	W147	K148	V149	L150	G151	R152	P153	E154	G157	G158	L159	V160	W161	G162	T163	I164	I165	K166	P167	K168	L169	R172	P173	K174	P175	F176	A177	E178	A179	C180	H181	D188	F189	I190	D193	E194	P195	Q196	

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	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	5.50 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (5.50-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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	1.38	12/3410 (0.4%)	2.59	291/4620 (6.3%)
1	B	1.38	8/3391 (0.2%)	2.48	232/4594 (5.1%)
All	All	1.38	20/6801 (0.3%)	2.54	523/9214 (5.7%)

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	B	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	LYS	N-CA	7.66	1.52	1.46
1	A	317	ALA	CA-C	6.63	1.61	1.52
1	A	279	PHE	N-CA	6.62	1.54	1.46
1	B	259	ALA	CA-C	6.40	1.60	1.52
1	B	102	ALA	N-CA	6.21	1.53	1.46
1	A	106	THR	N-CA	5.89	1.53	1.46
1	B	222	THR	CA-CB	5.67	1.62	1.53
1	A	142	ASN	CA-C	5.41	1.58	1.53
1	A	273	THR	CA-CB	5.37	1.62	1.53
1	A	275	ALA	N-CA	5.32	1.52	1.46
1	A	315	GLN	C-N	5.29	1.40	1.32
1	A	91	ASP	C-O	5.27	1.30	1.23
1	A	222	THR	CA-CB	5.20	1.61	1.53
1	B	279	PHE	N-CA	5.19	1.52	1.46
1	B	193	ASP	CA-C	5.16	1.59	1.52
1	A	211	VAL	C-N	-5.15	1.27	1.33
1	B	163	THR	CA-CB	5.13	1.61	1.53
1	A	83	ILE	CA-CB	5.09	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	ALA	N-CA	5.08	1.52	1.46
1	B	412	GLN	N-CA	5.04	1.52	1.46

All (523) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	CD-NE-CZ	16.85	147.99	124.40
1	A	2	ASP	CA-CB-CG	14.30	126.90	112.60
1	B	316	GLY	CA-C-O	-13.23	106.33	118.77
1	B	172	ARG	CD-NE-CZ	12.66	142.13	124.40
1	A	425	ASP	CA-CB-CG	-11.59	101.01	112.60
1	A	288	ARG	NE-CZ-NH2	11.40	129.46	119.20
1	B	126	PHE	CA-CB-CG	11.26	125.06	113.80
1	A	431	LYS	CA-CB-CG	10.97	136.05	114.10
1	B	111	ASN	OD1-CG-ND2	10.86	133.46	122.60
1	A	67	VAL	CB-CA-C	10.69	122.16	110.62
1	A	126	PHE	CA-CB-CG	10.51	124.31	113.80
1	B	301	ARG	NE-CZ-NH2	10.40	128.56	119.20
1	A	243	ARG	CA-C-N	10.13	131.44	119.99
1	A	243	ARG	C-N-CA	10.13	131.44	119.99
1	A	152	ARG	NH1-CZ-NH2	10.09	132.42	119.30
1	A	194	GLU	CB-CG-CD	10.00	129.60	112.60
1	B	287	HIS	CA-CB-CG	-9.97	103.83	113.80
1	A	369	GLY	O-C-N	9.62	129.33	123.08
1	A	412	GLN	OE1-CD-NE2	9.56	132.16	122.60
1	A	288	ARG	N-CA-C	9.52	124.44	113.02
1	B	337	ARG	N-CA-C	-9.51	101.60	113.01
1	A	393	GLY	N-CA-C	-9.46	101.92	112.33
1	B	445	ASP	CA-CB-CG	9.32	121.92	112.60
1	B	139	PRO	CB-CA-C	9.31	123.18	110.98
1	A	164	ILE	CA-C-O	-9.26	110.67	120.39
1	A	92	ARG	NE-CZ-NH2	9.25	127.53	119.20
1	B	450	GLY	CA-C-N	9.18	132.58	120.28
1	B	450	GLY	C-N-CA	9.18	132.58	120.28
1	B	429	GLU	CA-CB-CG	9.17	132.44	114.10
1	A	284	LEU	CA-C-O	9.12	130.03	120.54
1	B	423	VAL	CA-C-O	-9.11	110.82	120.57
1	A	453	LYS	CA-CB-CG	9.10	132.29	114.10
1	B	99	ALA	O-C-N	-9.05	112.47	122.79
1	B	219	GLN	OE1-CD-NE2	-9.03	113.58	122.60
1	B	137	ASP	CA-C-O	-9.01	111.55	121.00
1	A	445	ASP	CA-CB-CG	8.99	121.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	THR	N-CA-CB	-8.87	97.49	110.53
1	A	182	ALA	CA-C-O	-8.85	111.52	120.82
1	B	430	HIS	CA-CB-CG	-8.83	104.97	113.80
1	A	422	PRO	CB-CA-C	8.64	122.61	111.46
1	B	282	ASN	OD1-CG-ND2	8.64	131.24	122.60
1	B	117	ASP	CA-CB-CG	8.48	121.08	112.60
1	B	277	ARG	CA-C-O	-8.45	109.82	119.79
1	A	76	GLU	CA-C-N	8.40	131.37	120.44
1	A	76	GLU	C-N-CA	8.40	131.37	120.44
1	B	304	THR	CA-CB-OG1	-8.36	97.07	109.60
1	A	298	GLN	CB-CG-CD	8.35	126.79	112.60
1	A	152	ARG	NE-CZ-NH2	-8.32	111.71	119.20
1	A	396	ALA	N-CA-C	-8.32	103.03	113.01
1	B	371	MET	CA-C-O	-8.26	111.27	120.60
1	B	315	GLN	CA-C-O	8.25	129.42	120.10
1	A	205	ARG	CD-NE-CZ	-8.25	112.86	124.40
1	A	67	VAL	CA-C-O	8.24	126.39	118.98
1	B	67	VAL	CB-CA-C	8.19	124.73	111.29
1	B	68	ASP	CA-CB-CG	8.07	120.67	112.60
1	A	232	ILE	CA-C-O	-8.04	112.66	119.97
1	A	447	ILE	N-CA-C	8.03	117.97	110.42
1	A	155	VAL	CA-C-O	-8.02	111.97	120.39
1	A	79	GLU	CB-CG-CD	8.01	126.21	112.60
1	A	133	ARG	NE-CZ-NH2	-8.01	112.00	119.20
1	A	198	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	A	298	GLN	N-CA-C	-7.98	103.53	113.18
1	B	283	PHE	CA-CB-CG	7.96	121.76	113.80
1	B	236	ASP	CB-CG-OD1	7.96	136.70	118.40
1	A	220	ASP	CA-CB-CG	-7.93	104.67	112.60
1	B	66	GLY	N-CA-C	-7.92	94.41	113.18
1	A	3	GLN	CA-C-O	7.89	131.79	120.51
1	B	14	GLU	CG-CD-OE1	7.89	136.55	118.40
1	B	119	GLU	CA-CB-CG	-7.87	98.36	114.10
1	A	316	GLY	CA-C-O	-7.83	111.41	118.77
1	A	239	GLU	N-CA-CB	7.83	121.72	110.13
1	B	236	ASP	O-C-N	7.82	127.96	121.31
1	B	382	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	194	GLU	CA-CB-CG	7.78	129.66	114.10
1	A	162	GLY	CA-C-O	7.77	129.78	121.31
1	A	190	ILE	O-C-N	7.72	131.36	123.10
1	A	221	GLU	N-CA-C	7.71	120.58	111.71
1	A	437	PHE	CA-C-N	7.70	133.77	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	PHE	C-N-CA	7.70	133.77	120.68
1	A	117	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	288	ARG	N-CA-CB	-7.70	99.31	110.47
1	B	399	HIS	CA-CB-CG	7.70	121.50	113.80
1	A	96	ASP	CA-C-O	-7.69	110.95	119.34
1	A	213	ASP	CA-C-O	-7.64	112.83	120.70
1	A	147	TRP	CA-C-N	7.56	130.75	120.54
1	A	147	TRP	C-N-CA	7.56	130.75	120.54
1	A	193	ASP	N-CA-C	-7.55	99.31	110.48
1	A	128	VAL	CA-C-O	7.55	126.47	119.98
1	A	195	PRO	N-CA-C	7.54	124.46	114.27
1	B	236	ASP	CA-C-O	-7.53	113.66	119.46
1	A	391	THR	CA-C-N	7.53	131.56	120.87
1	A	391	THR	C-N-CA	7.53	131.56	120.87
1	B	45	PHE	CA-C-O	-7.52	112.92	120.82
1	A	130	GLU	CB-CG-CD	7.51	125.36	112.60
1	B	194	GLU	CG-CD-OE1	7.50	135.64	118.40
1	A	152	ARG	O-C-N	7.48	128.09	120.99
1	B	39	VAL	CA-C-N	7.44	130.11	120.44
1	B	39	VAL	C-N-CA	7.44	130.11	120.44
1	A	214	ALA	CA-C-N	7.43	130.55	120.44
1	A	214	ALA	C-N-CA	7.43	130.55	120.44
1	B	193	ASP	N-CA-C	-7.42	100.04	110.50
1	A	44	HIS	CA-CB-CG	-7.40	106.40	113.80
1	A	141	VAL	N-CA-CB	-7.38	96.87	112.00
1	B	276	ARG	O-C-N	-7.38	114.42	122.09
1	B	364	THR	N-CA-C	7.35	118.91	109.65
1	B	144	SER	CB-CA-C	7.34	125.82	110.32
1	A	159	LEU	N-CA-C	7.34	121.14	110.28
1	A	271	ALA	O-C-N	7.34	130.01	122.09
1	B	172	ARG	NE-CZ-NH1	7.31	128.81	121.50
1	B	316	GLY	O-C-N	7.29	130.09	122.51
1	A	216	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	A	196	GLN	OE1-CD-NE2	7.24	129.84	122.60
1	B	451	TRP	CA-CB-CG	7.24	127.35	113.60
1	A	288	ARG	CD-NE-CZ	-7.21	114.31	124.40
1	A	265	TYR	CA-C-O	-7.19	113.25	120.80
1	A	364	THR	N-CA-C	7.18	120.06	109.50
1	B	318	SER	CA-C-O	7.17	128.20	120.24
1	A	194	GLU	CG-CD-OE1	7.13	134.80	118.40
1	B	218	ALA	N-CA-CB	7.12	120.74	110.06
1	A	273	THR	CA-C-O	-7.11	112.07	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	HIS	CA-CB-CG	-7.11	106.69	113.80
1	A	224	GLU	CA-C-O	-7.08	113.11	121.11
1	A	408	ARG	CD-NE-CZ	-7.08	114.48	124.40
1	B	363	CYS	N-CA-C	-7.06	97.39	108.90
1	A	76	GLU	CB-CG-CD	7.04	124.57	112.60
1	A	278	ARG	NE-CZ-NH1	7.04	128.54	121.50
1	B	68	ASP	O-C-N	7.02	131.30	123.01
1	B	236	ASP	OD1-CG-OD2	-7.01	106.07	122.90
1	B	347	GLU	CA-C-O	-7.00	111.65	120.20
1	B	395	GLY	N-CA-C	-6.98	96.64	113.18
1	A	261	LEU	O-C-N	6.97	131.15	123.27
1	B	141	VAL	N-CA-CB	-6.96	97.72	112.00
1	A	239	GLU	N-CA-C	-6.95	102.92	111.40
1	A	206	ASP	O-C-N	6.93	129.57	122.09
1	A	119	GLU	N-CA-CB	6.91	120.35	110.13
1	A	298	GLN	N-CA-CB	6.91	122.02	110.41
1	A	430	HIS	CA-C-N	6.90	129.86	120.54
1	A	430	HIS	C-N-CA	6.90	129.86	120.54
1	B	113	GLN	OE1-CD-NE2	6.87	129.47	122.60
1	A	318	SER	CA-C-N	6.86	130.33	121.27
1	A	318	SER	C-N-CA	6.86	130.33	121.27
1	A	291	HIS	CA-CB-CG	-6.85	106.95	113.80
1	B	232	ILE	O-C-N	6.85	129.55	122.09
1	B	146	LEU	O-C-N	6.82	129.45	122.09
1	A	226	LYS	CA-C-O	-6.81	113.49	121.46
1	A	161	VAL	O-C-N	6.81	131.25	122.94
1	A	98	LYS	CA-CB-CG	-6.80	100.49	114.10
1	A	14	GLU	CG-CD-OE1	6.80	134.04	118.40
1	B	40	ALA	O-C-N	6.80	129.07	122.07
1	B	361	LYS	CB-CA-C	6.79	121.77	109.62
1	A	222	THR	N-CA-CB	-6.78	100.58	110.47
1	B	169	LEU	CA-C-O	-6.77	114.02	121.33
1	B	295	THR	CA-CB-OG1	-6.77	99.45	109.60
1	A	113	GLN	O-C-N	6.76	130.79	122.34
1	B	164	ILE	CA-C-O	-6.75	113.30	120.39
1	A	298	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	A	408	ARG	NH1-CZ-NH2	6.74	128.06	119.30
1	B	190	ILE	O-C-N	6.72	130.29	123.10
1	B	423	VAL	O-C-N	6.71	128.65	121.87
1	A	98	LYS	N-CA-C	6.71	119.96	110.50
1	A	432	GLU	CB-CG-CD	6.69	123.98	112.60
1	B	291	HIS	CA-CB-CG	-6.69	107.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ALA	N-CA-C	6.66	120.14	110.28
1	B	68	ASP	CA-C-O	-6.65	113.47	121.05
1	A	404	VAL	O-C-N	6.64	128.81	121.90
1	A	345	GLN	OE1-CD-NE2	-6.62	115.98	122.60
1	A	321	HIS	CA-CB-CG	-6.62	107.18	113.80
1	A	443	ASP	CA-CB-CG	-6.62	105.98	112.60
1	B	426	TYR	O-C-N	6.60	129.22	122.09
1	B	385	ASN	CA-C-O	-6.60	114.25	121.31
1	B	145	ALA	CA-C-N	6.60	129.41	120.44
1	B	145	ALA	C-N-CA	6.60	129.41	120.44
1	B	391	THR	CA-CB-OG1	-6.60	99.70	109.60
1	A	112	ASN	CA-CB-CG	6.59	119.19	112.60
1	A	452	ARG	CA-C-O	6.57	127.93	120.90
1	A	291	HIS	CA-C-N	6.57	127.10	119.94
1	A	291	HIS	C-N-CA	6.57	127.10	119.94
1	B	276	ARG	NE-CZ-NH1	6.57	128.07	121.50
1	B	254	ASN	OD1-CG-ND2	6.56	129.16	122.60
1	A	221	GLU	CA-C-O	6.54	127.49	120.10
1	B	387	ASN	OD1-CG-ND2	6.53	129.13	122.60
1	B	298	GLN	N-CA-C	-6.53	105.94	114.04
1	A	67	VAL	N-CA-C	-6.53	106.88	113.47
1	B	65	ARG	CB-CA-C	-6.53	102.98	111.40
1	A	455	LEU	CB-CA-C	6.53	119.45	109.34
1	B	46	ALA	CA-C-N	6.51	129.25	120.65
1	B	46	ALA	C-N-CA	6.51	129.25	120.65
1	B	276	ARG	CA-C-O	6.51	127.87	120.90
1	A	452	ARG	CA-C-N	6.51	129.84	120.79
1	A	452	ARG	C-N-CA	6.51	129.84	120.79
1	B	130	GLU	N-CA-C	6.50	118.02	111.07
1	A	125	ASP	O-C-N	6.50	129.89	123.46
1	B	119	GLU	N-CA-C	6.49	119.67	111.69
1	B	164	ILE	CA-C-N	-6.48	111.90	120.91
1	B	164	ILE	C-N-CA	-6.48	111.90	120.91
1	B	44	HIS	CA-CB-CG	6.47	120.27	113.80
1	B	274	THR	O-C-N	6.47	128.74	122.07
1	B	190	ILE	CA-C-O	-6.47	113.43	120.67
1	A	361	LYS	CG-CD-CE	6.47	126.17	111.30
1	B	199	GLN	CA-CB-CG	6.47	127.03	114.10
1	A	185	LEU	N-CA-C	-6.46	104.09	112.23
1	A	408	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	B	159	LEU	N-CA-C	6.45	119.63	109.96
1	B	250	THR	CA-C-O	-6.44	112.56	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	A	249	GLU	CA-C-N	6.40	128.75	120.44
1	A	249	GLU	C-N-CA	6.40	128.75	120.44
1	A	381	GLU	CG-CD-OE2	-6.39	103.69	118.40
1	B	189	PHE	N-CA-CB	-6.39	99.43	111.00
1	A	347	GLU	N-CA-CB	-6.38	100.06	110.59
1	B	319	GLY	CA-C-O	-6.38	115.39	121.19
1	A	198	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	276	ARG	CA-C-O	6.38	127.72	120.90
1	B	92	ARG	CB-CA-C	6.37	124.14	110.45
1	A	380	PHE	CA-CB-CG	6.36	120.16	113.80
1	A	240	ILE	O-C-N	-6.35	115.69	121.91
1	A	404	VAL	N-CA-C	-6.33	104.58	110.53
1	A	65	ARG	CA-C-N	6.33	133.81	121.41
1	A	65	ARG	C-N-CA	6.33	133.81	121.41
1	B	29	ILE	N-CA-CB	6.31	119.59	111.83
1	A	218	ALA	CA-C-O	-6.30	112.72	119.97
1	A	22	GLU	CB-CG-CD	6.30	123.31	112.60
1	A	236	ASP	O-C-N	6.29	127.14	121.35
1	B	322	THR	CA-CB-OG1	-6.28	100.19	109.60
1	B	109	MET	N-CA-CB	-6.27	99.08	110.88
1	B	278	ARG	NE-CZ-NH2	6.26	124.84	119.20
1	B	437	PHE	CA-CB-CG	6.26	120.06	113.80
1	B	271	ALA	O-C-N	6.25	128.84	122.09
1	A	94	ILE	CA-C-O	6.25	127.00	120.25
1	A	194	GLU	OE1-CD-OE2	-6.25	107.91	122.90
1	B	277	ARG	CD-NE-CZ	-6.25	115.66	124.40
1	A	356	SER	CA-CB-OG	-6.24	98.62	111.10
1	A	387	ASN	OD1-CG-ND2	6.24	128.84	122.60
1	A	133	ARG	NE-CZ-NH1	6.24	127.74	121.50
1	A	166	LYS	CA-C-O	-6.23	112.99	120.41
1	A	105	LEU	O-C-N	6.22	128.81	122.09
1	A	336	ASP	N-CA-CB	6.22	119.81	110.22
1	B	288	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	B	247	VAL	CA-C-O	-6.21	114.59	121.17
1	A	218	ALA	N-CA-C	-6.20	104.62	111.82
1	A	189	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	291	HIS	N-CA-C	-6.20	105.77	113.15
1	B	224	GLU	CA-C-O	-6.19	113.87	121.11
1	B	222	THR	OG1-CB-CG2	6.19	121.67	109.30
1	A	65	ARG	O-C-N	6.18	132.90	123.00
1	B	2	ASP	CA-CB-CG	6.18	118.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	VAL	O-C-N	6.18	127.23	121.61
1	B	119	GLU	CG-CD-OE2	-6.17	104.21	118.40
1	B	356	SER	CA-CB-OG	-6.17	98.77	111.10
1	A	440	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	428	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	A	433	LEU	O-C-N	6.16	129.17	122.15
1	B	105	LEU	O-C-N	6.16	129.17	122.15
1	B	288	ARG	N-CA-CB	-6.15	101.54	110.70
1	A	125	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	354	ARG	CB-CA-C	6.14	119.87	109.80
1	A	293	ALA	CA-C-N	-6.11	116.91	123.08
1	A	293	ALA	C-N-CA	-6.11	116.91	123.08
1	B	435	ARG	CD-NE-CZ	-6.11	115.85	124.40
1	A	2	ASP	CA-C-O	-6.10	110.43	120.80
1	A	415	GLN	CA-C-O	-6.10	114.38	120.90
1	B	236	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	399	HIS	CA-CB-CG	6.08	119.88	113.80
1	A	226	LYS	O-C-N	6.07	131.25	123.11
1	A	83	ILE	N-CA-C	6.06	116.60	108.11
1	A	322	THR	CA-CB-OG1	-6.06	100.51	109.60
1	B	137	ASP	O-C-N	6.05	128.32	122.03
1	B	361	LYS	O-C-N	-6.04	115.38	122.81
1	B	96	ASP	CB-CG-OD1	6.04	132.29	118.40
1	B	99	ALA	CA-C-N	6.02	132.45	122.33
1	B	99	ALA	C-N-CA	6.02	132.45	122.33
1	B	282	ASN	CA-C-N	6.02	129.91	121.24
1	B	282	ASN	C-N-CA	6.02	129.91	121.24
1	A	215	MET	CA-C-O	-6.00	114.52	120.70
1	A	399	HIS	CA-C-O	-5.99	113.54	120.31
1	B	336	ASP	CA-CB-CG	-5.99	106.61	112.60
1	A	46	ALA	CA-C-O	5.98	127.10	120.82
1	A	41	THR	O-C-N	5.98	129.62	122.27
1	B	289	ALA	O-C-N	5.98	129.81	123.11
1	B	355	GLN	CA-C-O	-5.97	114.25	120.70
1	A	92	ARG	CA-C-N	5.97	129.19	120.71
1	A	92	ARG	C-N-CA	5.97	129.19	120.71
1	A	301	ARG	CA-C-O	-5.97	114.46	121.44
1	A	152	ARG	NE-CZ-NH1	-5.96	115.54	121.50
1	A	92	ARG	NE-CZ-NH1	-5.95	115.56	121.50
1	A	276	ARG	O-C-N	-5.94	115.91	122.09
1	B	347	GLU	CB-CG-CD	-5.94	102.50	112.60
1	A	336	ASP	N-CA-C	-5.94	104.88	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	LYS	CA-C-O	5.93	127.84	121.55
1	B	411	ARG	CG-CD-NE	5.93	125.04	112.00
1	B	65	ARG	N-CA-CB	5.92	118.54	110.42
1	A	7	TYR	CA-C-O	-5.92	112.63	119.56
1	A	124	HIS	CA-CB-CG	-5.90	107.90	113.80
1	B	299	SER	CA-C-N	-5.89	113.24	122.73
1	B	299	SER	C-N-CA	-5.89	113.24	122.73
1	B	149	VAL	CA-C-O	-5.89	114.93	121.17
1	B	232	ILE	CA-C-O	-5.89	114.61	119.97
1	A	41	THR	CA-CB-OG1	-5.88	100.78	109.60
1	A	208	ILE	CA-C-O	-5.86	114.85	120.95
1	A	152	ARG	CD-NE-CZ	-5.86	116.20	124.40
1	B	298	GLN	CA-C-O	5.85	126.38	119.06
1	B	226	LYS	CA-C-O	-5.85	114.50	121.11
1	B	298	GLN	OE1-CD-NE2	5.85	128.45	122.60
1	B	151	GLY	O-C-N	-5.84	115.49	122.33
1	A	180	CYS	O-C-N	5.83	128.38	122.09
1	B	108	THR	CA-C-O	-5.83	112.25	119.18
1	A	232	ILE	O-C-N	5.82	128.43	122.09
1	A	205	ARG	NH1-CZ-NH2	5.81	126.86	119.30
1	A	36	TYR	CA-C-N	5.81	126.24	120.31
1	A	36	TYR	C-N-CA	5.81	126.24	120.31
1	B	431	LYS	N-CA-C	5.81	117.61	111.28
1	A	213	ASP	CA-C-N	5.80	128.85	120.38
1	A	213	ASP	C-N-CA	5.80	128.85	120.38
1	B	401	ASP	CA-CB-CG	-5.80	106.80	112.60
1	A	45	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	278	ARG	NH1-CZ-NH2	-5.79	111.78	119.30
1	A	266	VAL	CA-C-O	-5.78	114.22	120.47
1	A	451	TRP	CA-C-N	5.78	128.34	120.54
1	A	451	TRP	C-N-CA	5.78	128.34	120.54
1	B	290	GLY	N-CA-C	5.77	122.75	115.42
1	A	292	GLY	O-C-N	5.77	127.73	122.19
1	B	274	THR	CA-CB-OG1	-5.77	100.95	109.60
1	B	276	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	A	235	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	101	ILE	O-C-N	5.76	128.31	121.80
1	A	381	GLU	CB-CG-CD	-5.75	102.82	112.60
1	B	393	GLY	O-C-N	5.75	130.18	122.70
1	A	275	ALA	CA-C-O	-5.74	114.80	120.82
1	B	107	LEU	N-CA-C	5.74	117.40	111.03
1	A	202	ALA	O-C-N	5.73	125.37	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	209	ALA	CA-C-O	-5.73	114.81	120.82
1	B	397	PHE	CA-CB-CG	-5.73	108.07	113.80
1	B	338	ALA	N-CA-CB	5.73	118.61	110.13
1	A	205	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	B	457	VAL	CA-C-O	-5.72	111.08	120.80
1	B	361	LYS	N-CA-CB	-5.71	101.65	110.04
1	B	160	VAL	CB-CA-C	5.71	119.29	110.96
1	B	215	MET	CA-C-N	5.70	127.85	120.44
1	B	215	MET	C-N-CA	5.70	127.85	120.44
1	B	354	ARG	CD-NE-CZ	-5.69	116.43	124.40
1	A	133	ARG	CA-CB-CG	-5.69	102.72	114.10
1	A	236	ASP	CA-C-O	-5.69	115.11	119.32
1	A	24	VAL	CA-C-O	-5.68	114.29	120.71
1	A	211	VAL	CA-C-N	5.68	127.89	120.28
1	A	211	VAL	C-N-CA	5.68	127.89	120.28
1	B	194	GLU	CG-CD-OE2	-5.68	105.33	118.40
1	B	179	ALA	N-CA-C	-5.67	105.10	111.28
1	B	381	GLU	CA-C-O	-5.67	114.87	120.82
1	A	14	GLU	CG-CD-OE2	-5.66	105.37	118.40
1	A	8	VAL	CA-CB-CG2	5.65	120.01	110.40
1	B	257	HIS	N-CA-CB	5.65	118.86	110.49
1	A	367	ILE	CB-CG1-CD1	5.64	125.64	113.80
1	B	445	ASP	CA-C-O	5.62	127.60	121.02
1	B	442	GLY	CA-C-O	5.61	126.53	120.75
1	A	34	ALA	N-CA-CB	-5.61	101.01	110.49
1	B	146	LEU	N-CA-C	-5.60	105.09	111.14
1	A	76	GLU	CA-C-O	5.59	127.18	120.92
1	A	335	SER	N-CA-C	5.59	122.70	110.80
1	A	149	VAL	CA-C-O	-5.59	115.14	120.95
1	A	249	GLU	CB-CG-CD	5.56	122.06	112.60
1	B	347	GLU	CG-CD-OE2	-5.56	105.61	118.40
1	A	178	GLU	O-C-N	-5.55	115.82	122.15
1	B	396	ALA	CA-C-N	5.55	128.27	120.28
1	B	396	ALA	C-N-CA	5.55	128.27	120.28
1	A	238	PHE	CA-C-O	-5.54	112.56	119.38
1	A	386	ALA	N-CA-CB	-5.54	103.50	111.54
1	B	364	THR	CA-C-N	5.54	125.72	119.90
1	B	364	THR	C-N-CA	5.54	125.72	119.90
1	A	172	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	B	337	ARG	N-CA-CB	5.53	120.07	110.39
1	B	405	ALA	N-CA-C	-5.53	105.33	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	THR	CA-C-N	5.53	132.24	121.41
1	A	322	THR	C-N-CA	5.53	132.24	121.41
1	B	196	GLN	O-C-N	-5.53	116.10	122.95
1	B	86	PRO	CB-CA-C	5.52	118.58	111.46
1	A	74	VAL	CA-CB-CG1	5.52	119.78	110.40
1	A	278	ARG	CB-CG-CD	5.51	123.98	111.30
1	A	422	PRO	CA-C-O	-5.51	115.06	121.34
1	B	146	LEU	CA-C-O	-5.50	115.03	120.70
1	A	240	ILE	CA-C-N	5.50	127.49	120.56
1	A	240	ILE	C-N-CA	5.50	127.49	120.56
1	A	173	PRO	O-C-N	5.49	128.11	122.18
1	A	440	PHE	CA-C-N	5.47	124.99	119.19
1	A	440	PHE	C-N-CA	5.47	124.99	119.19
1	B	356	SER	N-CA-CB	5.47	119.54	110.52
1	A	428	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	B	64	THR	CA-CB-OG1	-5.45	101.42	109.60
1	B	375	ARG	CD-NE-CZ	5.45	132.03	124.40
1	A	18	ILE	CA-C-O	5.45	127.12	121.29
1	A	215	MET	N-CA-C	-5.45	105.26	111.14
1	B	442	GLY	CA-C-N	5.44	127.84	120.44
1	B	442	GLY	C-N-CA	5.44	127.84	120.44
1	A	284	LEU	CB-CA-C	5.44	119.49	110.78
1	B	65	ARG	O-C-N	5.44	130.32	121.89
1	A	83	ILE	N-CA-CB	-5.44	103.90	111.41
1	A	94	ILE	CB-CG1-CD1	5.43	125.21	113.80
1	B	190	ILE	CA-C-N	-5.43	114.28	122.81
1	B	190	ILE	C-N-CA	-5.43	114.28	122.81
1	B	344	THR	CA-CB-OG1	-5.43	101.46	109.60
1	B	76	GLU	CB-CG-CD	5.42	121.81	112.60
1	B	315	GLN	OE1-CD-NE2	5.42	128.02	122.60
1	B	140	SER	CA-CB-OG	-5.41	100.27	111.10
1	A	438	GLU	CA-CB-CG	5.41	124.91	114.10
1	B	163	THR	CA-CB-OG1	-5.40	101.49	109.60
1	B	202	ALA	O-C-N	5.40	127.53	121.32
1	B	318	SER	CA-C-N	5.40	127.97	121.38
1	B	318	SER	C-N-CA	5.40	127.97	121.38
1	A	181	HIS	CA-CB-CG	-5.40	108.40	113.80
1	A	273	THR	CA-CB-OG1	-5.39	101.51	109.60
1	B	412	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	308	HIS	CA-C-O	5.39	126.48	120.82
1	B	110	GLY	CA-C-O	5.39	129.94	120.57
1	A	371	MET	N-CA-C	-5.38	99.91	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	283	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	337	ARG	O-C-N	5.36	127.80	122.12
1	A	189	PHE	N-CA-CB	-5.36	101.30	111.00
1	B	288	ARG	CG-CD-NE	5.35	123.77	112.00
1	A	171	LEU	N-CA-C	5.35	118.20	110.28
1	B	75	ASP	N-CA-C	-5.34	98.31	107.23
1	A	315	GLN	CA-C-N	-5.34	115.26	122.63
1	A	315	GLN	C-N-CA	-5.34	115.26	122.63
1	B	24	VAL	N-CA-CB	5.34	116.54	110.72
1	A	381	GLU	CG-CD-OE1	5.33	130.66	118.40
1	A	151	GLY	N-CA-C	-5.33	105.70	114.76
1	A	146	LEU	O-C-N	5.30	127.82	122.09
1	B	152	ARG	CD-NE-CZ	-5.30	116.97	124.40
1	B	211	VAL	CA-C-N	5.30	127.39	120.28
1	B	211	VAL	C-N-CA	5.30	127.39	120.28
1	A	444	ALA	N-CA-C	-5.28	105.21	110.97
1	A	227	LEU	N-CA-CB	-5.28	101.76	111.37
1	A	190	ILE	CA-C-N	-5.27	115.04	122.94
1	A	190	ILE	C-N-CA	-5.27	115.04	122.94
1	A	288	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	B	166	LYS	O-C-N	-5.26	116.88	121.35
1	A	6	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	B	176	PHE	CA-C-O	-5.24	115.30	120.70
1	A	104	PHE	O-C-N	-5.24	116.64	122.09
1	A	130	GLU	CA-C-N	5.24	127.30	120.28
1	A	130	GLU	C-N-CA	5.24	127.30	120.28
1	A	131	ALA	CA-C-O	5.24	126.11	120.55
1	B	391	THR	N-CA-C	-5.24	96.83	107.41
1	B	7	TYR	N-CA-CB	-5.24	103.33	110.56
1	A	29	ILE	N-CA-C	-5.23	99.42	106.85
1	B	448	TYR	O-C-N	5.23	126.00	121.34
1	A	47	ALA	CA-C-N	5.23	127.81	120.28
1	A	47	ALA	C-N-CA	5.23	127.81	120.28
1	A	386	ALA	N-CA-C	-5.22	104.35	111.56
1	A	152	ARG	CA-C-O	-5.22	115.84	121.27
1	A	374	LEU	CA-C-O	-5.22	114.89	120.42
1	B	194	GLU	CB-CG-CD	5.21	121.46	112.60
1	A	51	THR	CA-C-O	5.21	126.11	120.43
1	A	79	GLU	CA-CB-CG	5.20	124.50	114.10
1	B	29	ILE	N-CA-C	-5.19	99.48	106.85
1	A	253	GLU	CA-CB-CG	5.18	124.47	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	VAL	N-CA-C	5.18	115.77	108.36
1	A	389	ILE	N-CA-CB	5.18	117.27	111.21
1	A	354	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	45	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	78	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	B	425	ASP	CA-CB-CG	-5.17	107.43	112.60
1	A	51	THR	CB-CA-C	5.17	118.27	109.75
1	A	74	VAL	N-CA-CB	-5.17	101.81	111.62
1	A	273	THR	OG1-CB-CG2	5.16	119.63	109.30
1	A	222	THR	OG1-CB-CG2	5.16	119.62	109.30
1	A	360	MET	CA-C-O	-5.16	115.38	121.16
1	B	99	ALA	CA-C-O	5.16	127.85	121.87
1	B	81	THR	CA-CB-OG1	-5.16	101.87	109.60
1	A	3	GLN	CA-C-N	5.15	131.64	122.31
1	A	3	GLN	C-N-CA	5.15	131.64	122.31
1	B	176	PHE	O-C-N	5.15	127.65	122.09
1	B	268	GLY	N-CA-C	5.15	121.85	112.58
1	B	31	LYS	CG-CD-CE	5.15	123.14	111.30
1	B	361	LYS	N-CA-C	5.14	117.34	110.35
1	B	263	ASP	CA-C-O	-5.14	115.43	120.98
1	B	166	LYS	CB-CA-C	5.13	116.94	109.08
1	A	294	VAL	N-CA-C	5.13	115.97	111.56
1	A	42	ALA	N-CA-C	-5.12	105.78	111.36
1	A	434	ALA	CA-C-N	5.12	127.65	120.28
1	A	434	ALA	C-N-CA	5.12	127.65	120.28
1	A	404	VAL	N-CA-CB	5.12	117.12	110.57
1	B	152	ARG	NH1-CZ-NH2	5.12	125.95	119.30
1	B	454	ALA	N-CA-C	5.12	117.25	111.11
1	B	338	ALA	O-C-N	5.11	128.36	122.17
1	A	144	SER	CB-CA-C	5.11	120.09	110.63
1	B	229	SER	CA-C-O	-5.10	114.89	120.70
1	A	121	ALA	CA-C-N	-5.09	113.77	122.33
1	A	121	ALA	C-N-CA	-5.09	113.77	122.33
1	B	130	GLU	CG-CD-OE1	5.09	130.12	118.40
1	B	188	ASP	CB-CG-OD2	-5.09	106.68	118.40
1	A	188	ASP	O-C-N	5.09	129.64	122.20
1	A	51	THR	O-C-N	-5.09	117.52	123.27
1	A	247	VAL	CA-C-N	5.09	127.10	120.28
1	A	247	VAL	C-N-CA	5.09	127.10	120.28
1	B	419	ASP	CA-CB-CG	-5.09	107.51	112.60
1	B	157	GLY	CA-C-N	5.08	130.46	121.01
1	B	157	GLY	C-N-CA	5.08	130.46	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	GLU	OE1-CD-OE2	5.07	135.08	122.90
1	B	300	LYS	N-CA-C	-5.07	106.94	112.72
1	A	73	GLU	CA-CB-CG	5.07	124.24	114.10
1	B	304	THR	N-CA-CB	-5.07	103.19	110.44
1	B	13	LYS	O-C-N	5.07	129.00	123.27
1	B	352	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	278	ARG	CB-CG-CD	5.06	122.94	111.30
1	B	310	LYS	O-C-N	-5.06	116.83	122.09
1	A	193	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	49	SER	O-C-N	5.04	129.02	122.42
1	A	204	LEU	CA-C-N	5.04	127.34	120.54
1	A	204	LEU	C-N-CA	5.04	127.34	120.54
1	A	435	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	A	449	PRO	CB-CA-C	5.04	115.99	111.40
1	A	322	THR	CA-CB-CG2	5.04	119.06	110.50
1	A	180	CYS	N-CA-CB	5.03	117.36	110.07
1	A	369	GLY	N-CA-C	-5.03	105.27	111.45
1	B	16	ASP	O-C-N	5.03	127.45	122.12
1	B	142	ASN	OD1-CG-ND2	5.03	127.62	122.60
1	A	281	ASP	CA-CB-CG	-5.02	107.58	112.60
1	A	393	GLY	CA-C-O	-5.02	115.71	122.24
1	A	238	PHE	O-C-N	5.02	129.15	122.43
1	B	164	ILE	O-C-N	5.02	128.68	123.26
1	A	189	PHE	N-CA-C	5.01	117.61	109.24
1	A	320	ILE	CA-C-O	-5.00	115.98	121.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	277	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3233	194	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3311	0	3216	217	0
2	A	342	0	0	30	0
2	B	394	0	0	30	0
All	All	7377	0	6449	392	1

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 (392) 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:2:ASP:O	1:A:3:GLN:HG3	1.36	1.24
1:B:337:ARG:HD2	1:B:341:TYR:CZ	1.79	1.18
1:A:194:GLU:HG3	1:A:195:PRO:HD3	1.31	1.11
1:A:371:MET:HE2	1:A:375:ARG:HD3	1.29	1.08
1:B:456:GLY:O	1:B:457:VAL:HG23	1.54	1.07
1:A:3:GLN:HB3	1:A:6:ARG:HB3	1.35	1.07
1:B:194:GLU:OE1	1:B:195:PRO:HG3	1.59	1.01
1:B:263:ASP:OD2	1:B:289:ALA:HB3	1.60	0.99
1:B:299:SER:HA	1:B:301:ARG:NH1	1.76	0.99
1:B:112:ASN:ND2	1:B:112:ASN:H	1.56	0.98
1:B:64:THR:HG22	1:B:65:ARG:H	1.29	0.98
1:A:2:ASP:O	1:A:3:GLN:CG	2.11	0.98
1:B:299:SER:HA	1:B:301:ARG:HH12	1.26	0.97
1:B:65:ARG:HD2	1:B:86:PRO:HB3	1.45	0.97
1:A:194:GLU:CG	1:A:195:PRO:HD3	1.94	0.96
1:A:263:ASP:OD1	1:A:289:ALA:HB3	1.64	0.96
1:A:371:MET:HE1	2:A:743:HOH:O	1.65	0.95
1:B:337:ARG:O	1:B:337:ARG:HG2	1.68	0.93
1:B:111:ASN:O	1:B:113:GLN:N	2.00	0.93
1:A:385:ASN:HD22	1:A:387:ASN:H	1.17	0.92
1:B:112:ASN:H	1:B:112:ASN:HD22	1.19	0.91
1:A:48:GLU:HG3	1:A:115:MET:HE3	1.53	0.91
1:B:44:HIS:CE1	1:B:115:MET:HE2	2.05	0.90
1:B:411:ARG:NH1	2:B:815:HOH:O	2.05	0.89
1:B:65:ARG:CD	1:B:86:PRO:HB3	2.01	0.89
1:B:41:THR:CG2	1:B:118:VAL:HG22	2.03	0.88
1:B:15:GLU:HG2	2:B:809:HOH:O	1.74	0.87
1:B:213:ASP:HB3	2:B:777:HOH:O	1.75	0.87
1:B:111:ASN:C	1:B:113:GLN:H	1.81	0.87
1:A:52:GLY:H	1:B:168:LYS:H	1.19	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:HG22	1:B:65:ARG:N	1.89	0.86
1:A:371:MET:SD	1:A:375:ARG:HB3	2.16	0.85
1:B:65:ARG:HD3	1:B:86:PRO:HA	1.56	0.85
1:A:253:GLU:HG2	2:A:687:HOH:O	1.74	0.84
1:A:65:ARG:N	2:A:506:HOH:O	2.11	0.83
1:A:222:THR:HG23	1:A:224:GLU:HB2	1.61	0.83
1:A:105:LEU:HD23	1:A:109:MET:CE	2.08	0.83
1:A:424:LEU:HD21	1:A:448:TYR:HB3	1.62	0.82
1:A:424:LEU:HD22	1:A:448:TYR:CD1	2.13	0.82
1:B:376:MET:HB3	1:B:377:PRO:HD3	1.59	0.82
1:B:222:THR:HG22	1:B:224:GLU:H	1.42	0.81
1:B:194:GLU:CD	1:B:195:PRO:HD3	2.05	0.81
1:B:52:GLY:HA3	2:B:845:HOH:O	1.80	0.81
1:A:370:GLY:HA3	1:A:396:ALA:HB2	1.63	0.81
1:B:41:THR:HG22	1:B:118:VAL:HG22	1.63	0.80
1:A:450:GLY:O	1:A:453:LYS:HB3	1.81	0.80
1:A:222:THR:CG2	1:A:224:GLU:HB2	2.11	0.80
1:B:456:GLY:O	1:B:457:VAL:CG2	2.30	0.80
1:A:52:GLY:N	1:B:168:LYS:H	1.79	0.79
1:A:222:THR:HG22	1:A:224:GLU:H	1.47	0.79
1:A:33:LYS:HG3	1:A:117:ASP:HA	1.63	0.79
1:A:65:ARG:HA	1:A:70:LEU:HD11	1.65	0.79
1:B:194:GLU:OE1	1:B:195:PRO:CG	2.31	0.79
1:B:222:THR:CG2	1:B:224:GLU:H	1.96	0.79
1:B:65:ARG:NH1	1:B:88:ALA:H	1.81	0.78
1:B:52:GLY:CA	2:B:845:HOH:O	2.32	0.78
1:A:2:ASP:C	1:A:3:GLN:HG3	2.09	0.77
1:B:222:THR:HG23	1:B:224:GLU:HB2	1.66	0.77
1:A:194:GLU:HG3	1:A:195:PRO:CD	2.13	0.77
1:A:438:GLU:O	1:A:441:PRO:HD3	1.83	0.77
1:B:76:GLU:O	2:B:591:HOH:O	2.02	0.77
1:B:105:LEU:O	1:B:109:MET:HB3	1.84	0.77
1:B:337:ARG:HD2	1:B:341:TYR:OH	1.84	0.77
1:B:65:ARG:HH11	1:B:86:PRO:CB	1.98	0.76
1:B:23:HIS:NE2	1:B:65:ARG:HG2	2.00	0.76
1:B:431:LYS:HB2	1:B:431:LYS:NZ	1.99	0.76
1:A:107:LEU:CD1	1:B:195:PRO:HB3	2.16	0.76
1:A:52:GLY:H	1:B:168:LYS:N	1.83	0.75
1:B:424:LEU:O	1:B:428:ARG:HG3	1.86	0.75
1:A:119:GLU:O	1:A:301:ARG:NH2	2.20	0.75
1:B:337:ARG:CD	1:B:341:TYR:CZ	2.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:HG23	1:A:367:ILE:HG21	1.69	0.74
1:A:452:ARG:HG2	1:A:457:VAL:HG23	1.68	0.74
1:B:205:ARG:HD2	2:B:829:HOH:O	1.87	0.74
1:B:399:HIS:CE1	1:B:401:ASP:HB2	2.22	0.74
1:A:425:ASP:HA	1:A:428:ARG:HD3	1.70	0.73
1:A:48:GLU:CG	1:A:115:MET:HE3	2.18	0.73
1:A:105:LEU:CD2	1:A:109:MET:HE3	2.18	0.73
1:A:33:LYS:HE3	1:A:116:GLY:O	1.88	0.73
1:A:376:MET:HB3	1:A:377:PRO:HD3	1.71	0.73
1:A:218:ALA:O	1:A:222:THR:HB	1.90	0.72
1:B:130:GLU:CD	1:B:130:GLU:H	1.95	0.72
1:A:290:GLY:C	1:A:292:GLY:H	1.96	0.72
1:B:231:ASN:ND2	2:B:537:HOH:O	2.23	0.71
1:B:375:ARG:NH1	1:B:443:ASP:OD1	2.23	0.71
1:A:194:GLU:OE1	1:B:111:ASN:HB2	1.90	0.71
1:B:52:GLY:C	2:B:845:HOH:O	2.33	0.71
1:B:337:ARG:O	1:B:337:ARG:CG	2.38	0.70
1:A:15:GLU:HG3	2:A:565:HOH:O	1.90	0.70
1:A:222:THR:CG2	1:A:224:GLU:H	2.04	0.70
1:B:23:HIS:CE1	1:B:65:ARG:HG2	2.26	0.70
1:B:372:ASN:HD21	1:B:375:ARG:HH11	1.40	0.70
1:B:452:ARG:NH1	2:B:860:HOH:O	2.15	0.70
1:A:13:LYS:O	1:A:16:ASP:HB2	1.92	0.69
1:A:2:ASP:O	1:A:3:GLN:CB	2.40	0.69
1:B:428:ARG:CB	1:B:428:ARG:HH11	2.04	0.69
1:B:112:ASN:ND2	1:B:112:ASN:N	2.35	0.69
1:A:112:ASN:C	1:A:112:ASN:HD22	1.99	0.69
1:B:65:ARG:HH12	1:B:88:ALA:CB	2.07	0.68
1:B:372:ASN:ND2	1:B:375:ARG:HH11	1.91	0.68
1:B:65:ARG:HH12	1:B:88:ALA:H	1.40	0.68
1:B:218:ALA:O	1:B:222:THR:HB	1.94	0.68
1:B:222:THR:CG2	1:B:224:GLU:HB2	2.24	0.67
1:B:424:LEU:HD12	1:B:455:LEU:CD1	2.25	0.67
1:A:52:GLY:CA	1:B:168:LYS:H	2.08	0.66
1:A:349:GLN:OE1	1:A:354:ARG:NE	2.23	0.66
1:A:105:LEU:HD23	1:A:109:MET:HE3	1.78	0.66
1:B:44:HIS:ND1	1:B:115:MET:HE2	2.10	0.66
1:B:112:ASN:HB2	2:B:858:HOH:O	1.95	0.65
1:B:64:THR:CG2	1:B:65:ARG:N	2.56	0.65
1:A:265:TYR:CZ	1:A:291:HIS:HA	2.31	0.65
1:A:452:ARG:HA	1:A:457:VAL:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LEU:HD12	1:B:455:LEU:HD11	1.79	0.65
1:B:75:ASP:OD1	1:B:78:ARG:HG3	1.96	0.65
1:B:65:ARG:HD3	1:B:86:PRO:CA	2.27	0.64
1:A:288:ARG:O	1:A:291:HIS:HD2	1.80	0.64
1:A:288:ARG:O	1:A:291:HIS:CD2	2.50	0.64
1:B:148:LYS:HD2	1:B:154:GLU:OE1	1.97	0.64
1:B:65:ARG:HH11	1:B:86:PRO:HB3	1.60	0.64
1:B:217:ARG:NH2	2:B:714:HOH:O	2.30	0.64
1:A:73:GLU:OE2	2:A:472:HOH:O	2.15	0.64
1:A:3:GLN:HB3	1:A:6:ARG:CB	2.21	0.63
1:A:194:GLU:CB	1:A:195:PRO:HD3	2.28	0.63
1:A:337:ARG:O	1:A:341:TYR:CD1	2.52	0.63
1:A:356:SER:HB3	2:A:494:HOH:O	1.98	0.63
1:A:107:LEU:HD11	1:B:195:PRO:CB	2.28	0.63
1:A:349:GLN:OE1	1:A:354:ARG:HB2	1.98	0.62
1:B:65:ARG:HH12	1:B:88:ALA:HB3	1.65	0.62
1:A:74:VAL:HA	1:A:80:LEU:O	1.99	0.62
1:A:105:LEU:HD23	1:A:109:MET:HE2	1.79	0.62
1:A:451:TRP:O	1:A:455:LEU:HD13	2.00	0.62
1:A:78:ARG:HE	1:A:80:LEU:HD22	1.64	0.62
1:A:107:LEU:HD11	1:B:195:PRO:HB3	1.80	0.61
1:A:111:ASN:ND2	1:B:194:GLU:HG2	2.15	0.61
1:B:287:HIS:CD2	2:B:750:HOH:O	2.52	0.61
1:B:288:ARG:NH2	1:B:291:HIS:NE2	2.48	0.61
1:B:376:MET:HA	1:B:376:MET:HE2	1.82	0.61
1:B:130:GLU:OE1	2:B:532:HOH:O	2.16	0.61
1:B:194:GLU:OE1	1:B:195:PRO:HD3	2.00	0.61
1:B:337:ARG:HG3	1:B:341:TYR:CE2	2.36	0.61
1:A:369:GLY:O	1:A:392:ALA:HA	2.01	0.60
1:B:288:ARG:O	1:B:289:ALA:C	2.45	0.60
1:A:424:LEU:HD22	1:A:448:TYR:HD1	1.63	0.60
1:A:133:ARG:NH2	2:A:510:HOH:O	2.06	0.59
1:A:443:ASP:O	1:A:447:ILE:HG12	2.02	0.59
1:A:18:ILE:HG22	2:A:598:HOH:O	2.01	0.59
1:A:424:LEU:CD2	1:A:448:TYR:HB3	2.31	0.59
1:B:194:GLU:OE1	1:B:195:PRO:CD	2.51	0.59
1:A:424:LEU:CD2	1:A:448:TYR:CD1	2.85	0.59
1:B:376:MET:HG3	1:B:380:PHE:CE2	2.37	0.59
1:A:422:PRO:HD2	2:A:586:HOH:O	2.02	0.59
1:A:424:LEU:CD2	1:A:448:TYR:HD1	2.16	0.59
1:A:65:ARG:N	1:A:68:ASP:HB2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASP:O	1:B:270:ALA:HA	2.03	0.59
1:A:288:ARG:NH2	1:A:291:HIS:CE1	2.71	0.59
1:A:67:VAL:O	1:A:89:LEU:HD11	2.04	0.58
1:B:321:HIS:CE1	1:B:323:GLY:HA2	2.38	0.58
1:A:105:LEU:CD2	1:A:109:MET:CE	2.79	0.58
1:A:288:ARG:HE	1:A:308:HIS:CD2	2.21	0.58
1:B:427:ALA:O	1:B:434:ALA:HB2	2.04	0.58
1:A:371:MET:CE	1:A:375:ARG:HD3	2.18	0.58
1:B:119:GLU:O	1:B:119:GLU:HG2	2.03	0.58
1:A:445:ASP:OD2	1:A:452:ARG:NH2	2.37	0.58
1:A:263:ASP:OD1	1:A:289:ALA:CB	2.46	0.58
1:B:65:ARG:HD3	1:B:86:PRO:HB3	1.81	0.58
1:A:324:THR:HG23	1:A:367:ILE:CG2	2.34	0.58
1:B:295:THR:HA	1:B:303:TYR:O	2.03	0.57
1:B:424:LEU:HD13	1:B:437:PHE:CZ	2.39	0.57
1:B:194:GLU:HB3	2:B:750:HOH:O	2.04	0.57
1:B:288:ARG:NH2	1:B:291:HIS:CD2	2.72	0.57
1:B:337:ARG:HD2	1:B:341:TYR:CE1	2.34	0.57
1:A:52:GLY:HA3	1:B:168:LYS:H	1.68	0.57
1:A:152:ARG:HB3	1:A:153:PRO:HD2	1.85	0.57
1:A:205:ARG:HD2	2:A:719:HOH:O	2.05	0.56
1:A:376:MET:HE2	1:A:376:MET:HA	1.87	0.56
1:A:265:TYR:CE2	1:A:291:HIS:HA	2.40	0.56
1:B:111:ASN:C	1:B:113:GLN:N	2.49	0.56
1:B:299:SER:CA	1:B:301:ARG:NH1	2.62	0.56
1:A:422:PRO:CD	2:A:586:HOH:O	2.54	0.56
1:B:44:HIS:CG	1:B:115:MET:HE2	2.40	0.56
1:B:23:HIS:HD2	2:B:604:HOH:O	1.88	0.56
1:B:446:GLN:C	1:B:446:GLN:HE21	2.13	0.56
1:B:166:LYS:HA	1:B:167:PRO:C	2.32	0.55
1:B:321:HIS:CE1	1:B:368:SER:OG	2.59	0.55
1:A:278:ARG:CD	2:A:760:HOH:O	2.53	0.55
1:B:41:THR:CG2	1:B:118:VAL:CG2	2.79	0.55
1:B:65:ARG:NH2	2:B:647:HOH:O	1.72	0.55
1:B:111:ASN:HB3	1:B:112:ASN:HD22	1.71	0.55
1:A:173:PRO:HG2	2:A:606:HOH:O	2.06	0.55
1:B:51:THR:OG1	1:B:68:ASP:OD1	2.24	0.54
1:A:66:GLY:HA3	2:A:605:HOH:O	2.06	0.54
1:A:222:THR:HG21	1:A:226:LYS:CE	2.37	0.54
1:A:370:GLY:CA	1:A:396:ALA:HB2	2.36	0.54
1:A:394:GLY:HA2	1:A:397:PHE:HD1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:OE2	1:B:354:ARG:NH1	2.40	0.54
1:A:421:VAL:HG13	1:A:422:PRO:HD2	1.89	0.54
1:B:65:ARG:HD3	1:B:86:PRO:CB	2.38	0.54
1:B:222:THR:HG23	1:B:224:GLU:CB	2.35	0.54
1:B:321:HIS:HE1	1:B:368:SER:OG	1.91	0.54
1:A:292:GLY:O	1:A:296:SER:HB2	2.08	0.54
1:A:404:VAL:O	1:A:408:ARG:HD2	2.08	0.54
1:B:67:VAL:O	1:B:89:LEU:HD21	2.08	0.53
1:A:335:SER:O	1:A:338:ALA:HB3	2.08	0.53
1:B:178:GLU:OE1	1:B:217:ARG:NH2	2.40	0.53
1:A:33:LYS:HB2	1:A:36:TYR:CD2	2.42	0.53
1:B:265:TYR:CZ	1:B:291:HIS:HA	2.43	0.53
1:A:431:LYS:HB2	2:A:662:HOH:O	2.07	0.53
1:A:290:GLY:C	1:A:292:GLY:N	2.67	0.53
1:B:337:ARG:CG	1:B:341:TYR:CE2	2.92	0.53
1:B:28:TYR:CE2	1:B:83:ILE:HD12	2.43	0.53
1:B:336:ASP:C	1:B:338:ALA:N	2.67	0.53
1:A:452:ARG:HA	1:A:457:VAL:HG23	1.89	0.52
1:B:23:HIS:HE1	1:B:64:THR:O	1.93	0.52
1:B:428:ARG:HH11	1:B:428:ARG:HB3	1.73	0.52
1:A:444:ALA:O	1:A:448:TYR:N	2.39	0.52
1:B:22:GLU:HB2	1:B:65:ARG:HE	1.73	0.52
1:A:222:THR:HG23	1:A:224:GLU:CB	2.38	0.52
1:B:51:THR:CG2	1:B:67:VAL:HG12	2.40	0.52
1:B:222:THR:CG2	1:B:224:GLU:N	2.70	0.52
1:A:174:LYS:HB3	1:A:175:PRO:HD3	1.92	0.52
1:B:65:ARG:CD	1:B:86:PRO:CB	2.83	0.52
1:B:6:ARG:HD3	1:B:7:TYR:CE2	2.45	0.52
1:A:401:ASP:OD2	1:A:435:ARG:HG3	2.11	0.51
1:B:194:GLU:CB	2:B:750:HOH:O	2.58	0.51
1:B:23:HIS:HE1	1:B:64:THR:C	2.19	0.51
1:B:148:LYS:HD2	1:B:154:GLU:CD	2.35	0.51
1:A:188:ASP:OD2	2:A:481:HOH:O	2.19	0.51
1:A:98:LYS:NZ	2:A:774:HOH:O	2.44	0.51
1:A:287:HIS:HD2	1:A:288:ARG:N	2.09	0.51
1:A:408:ARG:NH2	2:A:536:HOH:O	2.44	0.51
1:B:194:GLU:CG	1:B:195:PRO:HD3	2.41	0.51
1:A:37:GLY:O	1:A:41:THR:OG1	2.20	0.51
1:B:64:THR:CG2	1:B:65:ARG:H	2.01	0.51
1:B:371:MET:HB3	1:B:376:MET:HE1	1.92	0.51
1:A:13:LYS:HB2	1:A:16:ASP:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:THR:H	1:B:167:PRO:HA	1.76	0.51
1:A:113:GLN:NE2	2:A:747:HOH:O	2.43	0.50
1:A:278:ARG:HD3	2:A:760:HOH:O	2.11	0.50
1:B:291:HIS:O	1:B:293:ALA:N	2.44	0.50
1:B:372:ASN:HD21	1:B:375:ARG:NH1	2.04	0.50
1:A:48:GLU:CB	1:A:115:MET:HE3	2.42	0.50
1:A:372:ASN:OD1	1:A:374:LEU:HB2	2.12	0.50
1:B:261:LEU:HD11	1:B:287:HIS:HB2	1.93	0.50
1:A:73:GLU:O	1:A:74:VAL:HG23	2.11	0.50
1:A:79:GLU:OE2	1:A:120:TYR:OH	2.21	0.50
1:B:44:HIS:NE2	1:B:115:MET:HE2	2.27	0.50
1:A:278:ARG:HD2	2:A:760:HOH:O	2.10	0.50
1:B:75:ASP:CG	1:B:78:ARG:HG3	2.36	0.50
1:B:300:LYS:C	1:B:301:ARG:HG3	2.29	0.50
1:B:133:ARG:NH1	2:B:717:HOH:O	2.17	0.49
1:A:33:LYS:HG3	1:A:117:ASP:CA	2.38	0.49
1:A:162:GLY:HA2	1:A:189:PHE:O	2.12	0.49
1:A:200:PRO:HD2	1:B:88:ALA:O	2.12	0.49
1:B:168:LYS:HE2	1:B:194:GLU:OE2	2.12	0.49
1:A:65:ARG:O	1:A:68:ASP:O	2.31	0.49
1:A:444:ALA:O	1:A:445:ASP:C	2.55	0.49
1:A:337:ARG:HG2	1:A:341:TYR:CZ	2.48	0.49
1:B:424:LEU:HD12	1:B:455:LEU:HD13	1.95	0.49
1:A:33:LYS:HG2	1:A:117:ASP:C	2.38	0.49
1:B:174:LYS:HB3	1:B:175:PRO:HD3	1.95	0.49
1:A:261:LEU:HD11	1:A:287:HIS:HB2	1.95	0.48
1:A:442:GLY:O	1:A:446:GLN:HG2	2.13	0.48
1:A:94:ILE:HD12	1:B:205:ARG:NH1	2.28	0.48
1:B:122:LYS:NZ	2:B:603:HOH:O	2.47	0.48
1:B:215:MET:O	1:B:219:GLN:HG3	2.12	0.48
1:B:399:HIS:ND1	1:B:401:ASP:HB2	2.28	0.48
1:A:376:MET:N	1:A:377:PRO:CD	2.77	0.48
1:B:44:HIS:CD2	1:B:115:MET:HE2	2.49	0.48
1:A:222:THR:HG21	1:A:226:LYS:HE3	1.96	0.48
1:A:398:GLY:HA3	2:A:624:HOH:O	2.14	0.48
1:B:321:HIS:HB2	2:B:599:HOH:O	2.14	0.48
1:A:194:GLU:CB	1:A:195:PRO:CD	2.92	0.47
1:A:371:MET:SD	1:A:375:ARG:CB	2.96	0.47
1:A:165:ILE:O	1:A:166:LYS:HD3	2.14	0.47
1:B:448:TYR:O	1:B:451:TRP:HB3	2.14	0.47
1:B:428:ARG:CB	1:B:428:ARG:NH1	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LEU:HD11	1:A:451:TRP:HA	1.96	0.47
1:A:112:ASN:C	1:A:112:ASN:ND2	2.70	0.47
1:A:249:GLU:CD	2:A:721:HOH:O	2.57	0.47
1:A:270:ALA:HA	1:B:235:ASP:O	2.15	0.47
1:B:65:ARG:NH2	1:B:87:VAL:HG23	2.29	0.47
1:A:438:GLU:HG3	2:A:709:HOH:O	2.15	0.47
1:A:385:ASN:HD22	1:A:387:ASN:N	1.99	0.47
1:B:213:ASP:HB3	2:B:702:HOH:O	2.15	0.47
1:A:3:GLN:C	1:A:5:SER:H	2.23	0.47
1:A:435:ARG:NH1	1:A:438:GLU:OE1	2.48	0.46
1:B:222:THR:HG21	1:B:226:LYS:CE	2.45	0.46
1:B:222:THR:HG23	1:B:224:GLU:N	2.31	0.46
1:B:194:GLU:CG	2:B:750:HOH:O	2.64	0.46
1:B:397:PHE:CD1	1:B:403:PRO:HG3	2.51	0.46
1:A:33:LYS:CG	1:A:117:ASP:C	2.89	0.46
1:B:76:GLU:CD	1:B:76:GLU:H	2.22	0.46
1:B:336:ASP:C	1:B:338:ALA:H	2.21	0.46
1:B:222:THR:HG21	1:B:226:LYS:HE3	1.97	0.46
1:B:288:ARG:NH1	1:B:308:HIS:CD2	2.84	0.46
1:A:51:THR:HG22	1:B:169:LEU:O	2.15	0.45
1:A:3:GLN:NE2	1:A:6:ARG:HH11	2.14	0.45
1:A:7:TYR:CE1	1:A:47:ALA:HA	2.51	0.45
1:A:291:HIS:CD2	2:A:639:HOH:O	2.69	0.45
1:B:354:ARG:NH2	2:B:542:HOH:O	2.47	0.45
1:A:241:ILE:O	1:A:245:GLU:HG3	2.16	0.45
1:A:107:LEU:CD1	1:B:195:PRO:CB	2.88	0.45
1:B:51:THR:HG21	1:B:67:VAL:HG12	1.99	0.45
1:A:2:ASP:O	1:A:3:GLN:HB2	2.17	0.45
1:B:265:TYR:CE1	1:B:291:HIS:HA	2.51	0.45
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.99	0.45
1:B:202:ALA:N	1:B:203:PRO:HD3	2.32	0.45
1:A:23:HIS:HD2	2:A:528:HOH:O	1.99	0.45
1:A:422:PRO:HG2	1:A:425:ASP:HB2	1.98	0.45
1:B:6:ARG:NH2	1:B:68:ASP:OD1	2.47	0.45
1:A:301:ARG:HB3	2:A:747:HOH:O	2.16	0.44
1:B:120:TYR:CD1	1:B:120:TYR:C	2.95	0.44
1:A:107:LEU:HD11	1:B:195:PRO:HB2	1.99	0.44
1:A:288:ARG:HH21	1:A:291:HIS:CE1	2.34	0.44
1:A:398:GLY:O	1:A:399:HIS:HB2	2.16	0.44
1:B:411:ARG:HG3	2:B:566:HOH:O	2.17	0.44
1:B:307:VAL:HG12	1:B:311:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLU:OE2	1:B:178:GLU:HA	2.18	0.44
1:B:376:MET:HE2	1:B:376:MET:CA	2.45	0.44
1:A:159:LEU:HD22	1:A:380:PHE:HZ	1.83	0.44
1:A:337:ARG:HG2	1:A:341:TYR:OH	2.17	0.44
1:B:48:GLU:HB2	1:B:115:MET:HE3	2.00	0.44
1:A:168:LYS:HB2	1:A:168:LYS:HE2	1.56	0.44
1:A:424:LEU:O	1:A:428:ARG:HD2	2.18	0.44
1:B:136:PHE:O	2:B:613:HOH:O	2.21	0.44
1:B:310:LYS:N	2:B:738:HOH:O	2.50	0.44
1:A:147:TRP:CD2	1:A:157:GLY:HA3	2.53	0.44
1:A:217:ARG:HH11	1:A:217:ARG:HD2	1.70	0.44
1:B:33:LYS:N	1:B:117:ASP:O	2.42	0.44
1:B:65:ARG:HH12	1:B:88:ALA:N	2.10	0.44
1:B:424:LEU:CD1	1:B:437:PHE:CE2	3.01	0.44
1:A:288:ARG:HH11	1:A:288:ARG:HD3	1.46	0.43
1:B:294:VAL:HG13	1:B:302:GLY:HA3	2.00	0.43
1:A:376:MET:HE3	1:A:376:MET:HB2	1.68	0.43
1:B:3:GLN:HE21	1:B:3:GLN:HB3	1.56	0.43
1:A:205:ARG:O	1:A:246:TYR:OH	2.35	0.43
1:A:373:ALA:O	1:A:377:PRO:HD3	2.19	0.43
1:B:176:PHE:HE1	1:B:211:VAL:HG21	1.83	0.43
1:B:213:ASP:OD2	1:B:216:ARG:NH1	2.51	0.43
1:B:294:VAL:CG1	1:B:302:GLY:HA3	2.49	0.43
1:A:421:VAL:HG12	1:A:422:PRO:O	2.19	0.43
1:A:181:HIS:HB2	1:A:214:ALA:HB1	2.01	0.43
1:B:65:ARG:HH22	1:B:88:ALA:HB2	1.82	0.43
1:B:291:HIS:C	1:B:293:ALA:H	2.25	0.43
1:A:424:LEU:HD11	1:A:451:TRP:CB	2.48	0.43
1:B:23:HIS:CE1	1:B:65:ARG:HA	2.53	0.43
1:B:213:ASP:CB	2:B:702:HOH:O	2.67	0.43
1:B:291:HIS:C	1:B:293:ALA:N	2.75	0.43
1:B:376:MET:HE3	1:B:376:MET:HB2	1.54	0.43
1:A:205:ARG:HA	1:A:246:TYR:CE2	2.54	0.43
1:A:86:PRO:HB2	1:A:89:LEU:HD13	2.00	0.42
1:A:219:GLN:HB2	2:A:487:HOH:O	2.18	0.42
1:B:361:LYS:HE3	1:B:361:LYS:HB2	1.59	0.42
1:A:287:HIS:CD2	1:A:288:ARG:N	2.86	0.42
1:B:162:GLY:CA	1:B:189:PHE:O	2.67	0.42
1:B:265:TYR:HB3	1:B:289:ALA:O	2.18	0.42
1:B:374:LEU:HD11	1:B:437:PHE:HA	2.01	0.42
1:A:2:ASP:C	1:A:3:GLN:CG	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ALA:HB1	2:A:776:HOH:O	2.19	0.42
1:B:65:ARG:HH11	1:B:86:PRO:HB2	1.81	0.42
1:B:376:MET:CA	1:B:376:MET:CE	2.96	0.42
1:A:94:ILE:HD12	1:B:205:ARG:HH12	1.84	0.42
1:B:113:GLN:HE22	1:B:302:GLY:H	1.66	0.42
1:B:371:MET:HE1	1:B:379:PHE:CG	2.54	0.42
1:A:394:GLY:HA2	1:A:397:PHE:CD1	2.55	0.41
1:A:146:LEU:O	1:A:147:TRP:C	2.63	0.41
1:B:31:LYS:HG2	1:B:32:PRO:HD2	2.01	0.41
1:B:181:HIS:HB2	1:B:214:ALA:HB1	2.02	0.41
1:B:288:ARG:HB3	1:B:291:HIS:ND1	2.35	0.41
1:A:31:LYS:HA	1:A:32:PRO:HD3	1.90	0.41
1:B:44:HIS:O	1:B:115:MET:HE1	2.21	0.41
1:B:376:MET:HB3	1:B:377:PRO:CD	2.42	0.41
1:A:374:LEU:HD11	1:A:437:PHE:HA	2.03	0.41
1:A:40:ALA:O	1:A:43:ALA:HB3	2.20	0.41
1:A:369:GLY:O	1:A:393:GLY:N	2.49	0.41
1:B:347:GLU:HG2	1:B:354:ARG:NH1	2.35	0.41
1:B:288:ARG:HH11	1:B:288:ARG:HD2	1.49	0.41
1:B:309:CYS:HB2	2:B:738:HOH:O	2.21	0.41
1:A:354:ARG:HB2	1:A:354:ARG:HE	1.44	0.41
1:B:415:GLN:HE21	1:B:415:GLN:HB2	1.44	0.41
1:A:452:ARG:CG	1:A:457:VAL:HG23	2.45	0.41
1:B:424:LEU:HD13	1:B:437:PHE:CE2	2.55	0.41
1:B:278:ARG:NE	2:B:737:HOH:O	2.46	0.41
1:B:286:TYR:C	1:B:286:TYR:CD1	2.98	0.41
1:A:221:GLU:O	2:A:739:HOH:O	2.22	0.40
1:A:337:ARG:HE	1:A:337:ARG:HB3	1.64	0.40
1:A:400:ILE:HD11	1:A:435:ARG:CZ	2.51	0.40
1:B:65:ARG:CZ	1:B:88:ALA:H	2.31	0.40
1:B:263:ASP:OD2	1:B:289:ALA:CB	2.49	0.40
1:A:65:ARG:HB3	1:A:66:GLY:H	1.38	0.40
1:B:231:ASN:HD21	1:B:233:THR:CB	2.35	0.40
1:A:30:MET:O	1:A:79:GLU:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLY:O	1:A:431:LYS:NZ[2_646]	1.94	0.26

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	430/490 (88%)	404 (94%)	20 (5%)	6 (1%)	9	2
1	B	427/490 (87%)	404 (95%)	17 (4%)	6 (1%)	9	2
All	All	857/980 (87%)	808 (94%)	37 (4%)	12 (1%)	9	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	B	3	GLN
1	B	112	ASN
1	A	33	LYS
1	A	34	ALA
1	A	52	GLY
1	A	335	SER
1	B	292	GLY
1	B	456	GLY
1	A	5	SER
1	B	110	GLY
1	B	116	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	329/376 (88%)	302 (92%)	27 (8%)	10	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	326/376 (87%)	294 (90%)	32 (10%)	7	1
All	All	655/752 (87%)	596 (91%)	59 (9%)	9	2

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	65	ARG
1	A	74	VAL
1	A	76	GLU
1	A	107	LEU
1	A	109	MET
1	A	112	ASN
1	A	130	GLU
1	A	141	VAL
1	A	166	LYS
1	A	194	GLU
1	A	222	THR
1	A	284	LEU
1	A	298	GLN
1	A	301	ARG
1	A	324	THR
1	A	336	ASP
1	A	356	SER
1	A	371	MET
1	A	375	ARG
1	A	376	MET
1	A	408	ARG
1	A	424	LEU
1	A	431	LYS
1	A	443	ASP
1	A	446	GLN
1	A	453	LYS
1	B	3	GLN
1	B	5	SER
1	B	13	LYS
1	B	33	LYS
1	B	48	GLU
1	B	65	ARG
1	B	67	VAL
1	B	74	VAL
1	B	76	GLU

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Mol	Chain	Res	Type
1	B	78	ARG
1	B	109	MET
1	B	111	ASN
1	B	112	ASN
1	B	130	GLU
1	B	141	VAL
1	B	168	LYS
1	B	194	GLU
1	B	222	THR
1	B	284	LEU
1	B	286	TYR
1	B	298	GLN
1	B	301	ARG
1	B	347	GLU
1	B	371	MET
1	B	376	MET
1	B	411	ARG
1	B	424	LEU
1	B	428	ARG
1	B	429	GLU
1	B	431	LYS
1	B	446	GLN
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	ASN
1	A	23	HIS
1	A	93	ASN
1	A	111	ASN
1	A	112	ASN
1	A	113	GLN
1	A	287	HIS
1	A	291	HIS
1	A	308	HIS
1	A	345	GLN
1	A	382	ASN
1	A	385	ASN
1	A	415	GLN
1	B	3	GLN

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Mol	Chain	Res	Type
1	B	23	HIS
1	B	111	ASN
1	B	112	ASN
1	B	113	GLN
1	B	231	ASN
1	B	287	HIS
1	B	308	HIS
1	B	321	HIS
1	B	349	GLN
1	B	372	ASN
1	B	415	GLN
1	B	446	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.