Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 02:10 PM EDT

PDB ID	:	1T1U
Title	:	Structural Insights and Functional Implications of Choline Acetyltransferase
Authors	:	Govindasamy, L.; Pedersen, B.; Lian, W.; Kukar, T.; Gu, Y.; Jin, S.; Agbandje-McKenna, M.; Wu, D.
Deposited on	:	2004-04-18
Resolution	:	1.55 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 (i) 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 (1)) were used in the production of this report:

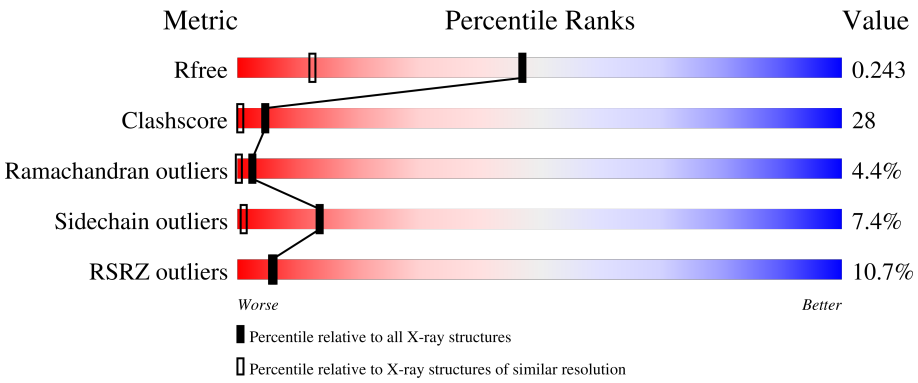
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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))
R_{free}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	639	10%, 29%, 43%, 13%, 8%, 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5119 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 Choline O-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	597	4711	2975	817	880	39	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	TRP	LEU	see Remark 999	UNP P32738
A	499	GLN	HIS	see Remark 999	UNP P32738
A	500	THR	LYS	see Remark 999	UNP P32738
A	501	GLU	GLN	see Remark 999	UNP P32738
A	570	TYR	ASN	see Remark 999	UNP P32738

- Molecule 2 is water.

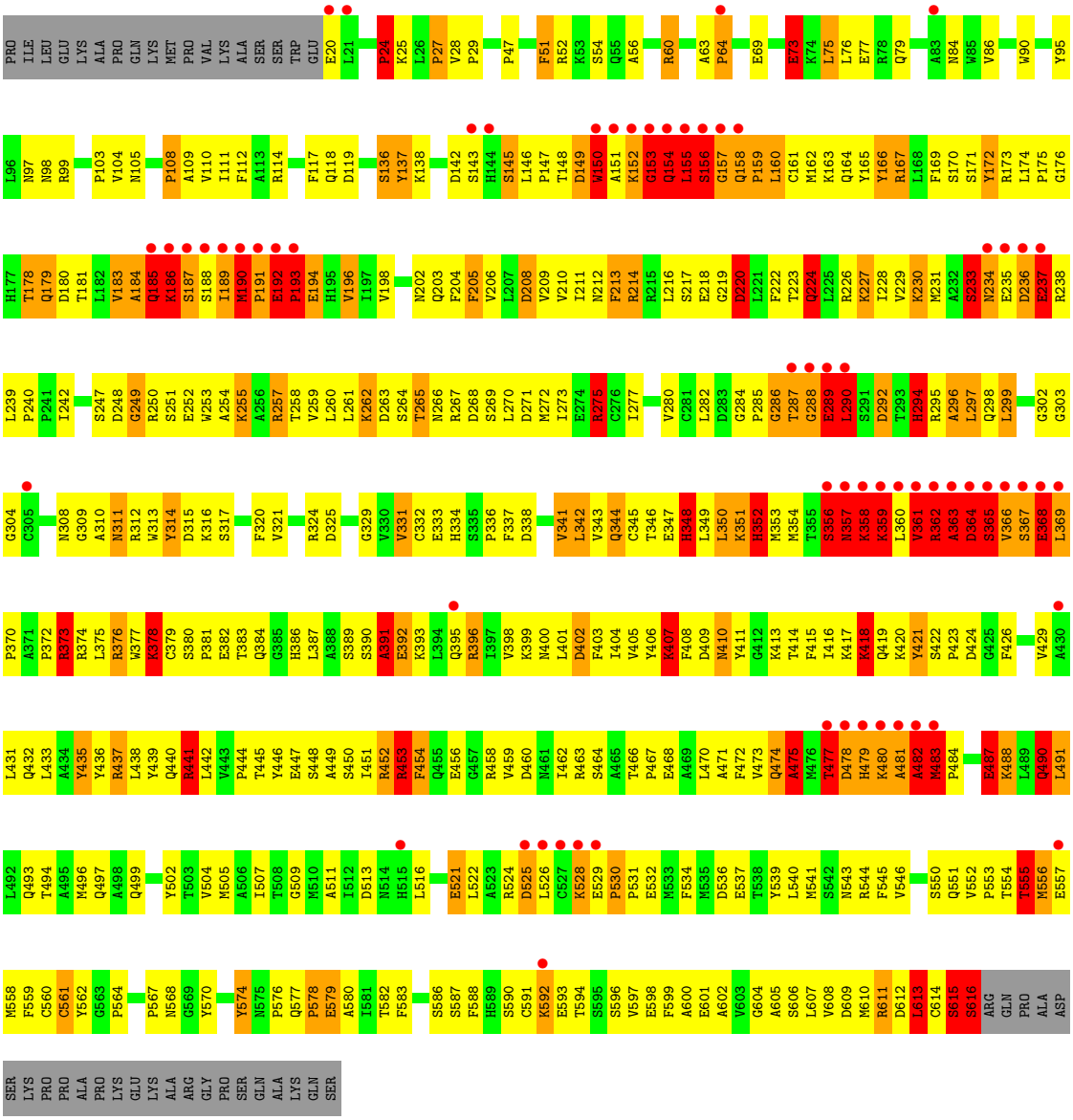
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	408	408	408	0	0

3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

- Molecule 1: Choline O-acetyltransferase

Chain A: 10% 29% 43% 13% 8% 7%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.95Å 77.50Å 59.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.55 19.88 – 1.55	Depositor EDS
% Data completeness (in resolution range)	5.0 (30.00-1.55) 77.5 (19.88-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.55Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.171 , 0.227 0.208 , 0.243	Depositor DCC
R_{free} test set	3646 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5119	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	3.30	524/4811 (10.9%)	3.27	542/6516 (8.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	53

All (524) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	TYR	CE2-CZ	24.47	1.70	1.38
1	A	437	ARG	CZ-NH1	23.57	1.63	1.33
1	A	218	GLU	CD-OE2	20.20	1.47	1.25
1	A	189	ILE	C-O	-20.18	0.85	1.23
1	A	267	ARG	NE-CZ	19.43	1.58	1.33
1	A	252	GLU	CD-OE2	18.55	1.46	1.25
1	A	441	ARG	CZ-NH1	17.68	1.56	1.33
1	A	189	ILE	C-N	-16.67	0.95	1.34
1	A	167	ARG	CD-NE	-16.39	1.18	1.46
1	A	456	GLU	CD-OE1	16.36	1.43	1.25
1	A	579	GLU	CD-OE1	15.93	1.43	1.25
1	A	437	ARG	CZ-NH2	15.41	1.53	1.33
1	A	194	GLU	CD-OE1	15.39	1.42	1.25
1	A	521	GLU	CD-OE2	15.34	1.42	1.25
1	A	289	GLU	C-N	-15.03	0.99	1.34
1	A	226	ARG	NE-CZ	-14.87	1.13	1.33
1	A	456	GLU	CD-OE2	14.86	1.42	1.25
1	A	421	TYR	CZ-OH	14.86	1.63	1.37
1	A	373	ARG	CG-CD	14.82	1.89	1.51
1	A	532	GLU	CG-CD	14.79	1.74	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	562	TYR	CE2-CZ	-14.71	1.19	1.38
1	A	204	PHE	CE1-CZ	-14.70	1.09	1.37
1	A	255	LYS	CD-CE	14.34	1.87	1.51
1	A	453	ARG	CD-NE	14.27	1.70	1.46
1	A	598	GLU	CD-OE2	-14.24	1.09	1.25
1	A	452	ARG	CD-NE	-14.22	1.22	1.46
1	A	379	CYS	CA-CB	-14.18	1.22	1.53
1	A	453	ARG	CA-CB	13.95	1.84	1.53
1	A	418	LYS	CD-CE	13.87	1.85	1.51
1	A	235	GLU	CD-OE2	13.81	1.40	1.25
1	A	422	SER	CB-OG	13.78	1.60	1.42
1	A	421	TYR	CD1-CE1	13.61	1.59	1.39
1	A	376	ARG	NE-CZ	13.61	1.50	1.33
1	A	294	HIS	CB-CG	13.44	1.74	1.50
1	A	615	SER	C-O	13.18	1.48	1.23
1	A	378	LYS	CE-NZ	13.11	1.81	1.49
1	A	218	GLU	CD-OE1	12.50	1.39	1.25
1	A	344	GLN	CD-OE1	12.47	1.51	1.24
1	A	586	SER	CA-CB	-12.37	1.34	1.52
1	A	172	TYR	CE2-CZ	12.32	1.54	1.38
1	A	190	MET	C-N	12.31	1.57	1.34
1	A	226	ARG	CZ-NH1	12.23	1.49	1.33
1	A	190	MET	N-CA	-12.20	1.22	1.46
1	A	446	TYR	CD2-CE2	-11.76	1.21	1.39
1	A	470	LEU	C-O	11.70	1.45	1.23
1	A	537	GLU	CD-OE2	11.66	1.38	1.25
1	A	531	PRO	N-CD	-11.59	1.31	1.47
1	A	611	ARG	NE-CZ	11.53	1.48	1.33
1	A	396	ARG	CG-CD	11.47	1.80	1.51
1	A	230	LYS	CD-CE	11.42	1.79	1.51
1	A	262	LYS	CE-NZ	11.19	1.77	1.49
1	A	331	VAL	CB-CG1	-11.15	1.29	1.52
1	A	220	ASP	CB-CG	11.12	1.75	1.51
1	A	213	PHE	CE1-CZ	11.03	1.58	1.37
1	A	570	TYR	CG-CD2	-11.02	1.24	1.39
1	A	337	PHE	CE2-CZ	10.99	1.58	1.37
1	A	267	ARG	CZ-NH2	-10.99	1.18	1.33
1	A	475	ALA	N-CA	10.97	1.68	1.46
1	A	166	TYR	CE1-CZ	-10.80	1.24	1.38
1	A	240	PRO	CA-C	10.79	1.74	1.52
1	A	613	LEU	CG-CD1	10.79	1.91	1.51
1	A	448	SER	CA-CB	10.79	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	PRO	N-CD	10.78	1.62	1.47
1	A	441	ARG	NE-CZ	10.75	1.47	1.33
1	A	179	GLN	CG-CD	10.73	1.75	1.51
1	A	406	TYR	CG-CD2	-10.73	1.25	1.39
1	A	521	GLU	CD-OE1	10.71	1.37	1.25
1	A	537	GLU	CD-OE1	10.71	1.37	1.25
1	A	593	GLU	CD-OE2	10.69	1.37	1.25
1	A	415	PHE	CD2-CE2	10.69	1.60	1.39
1	A	452	ARG	CB-CG	-10.68	1.23	1.52
1	A	257	ARG	CZ-NH1	10.62	1.46	1.33
1	A	217	SER	CB-OG	-10.60	1.28	1.42
1	A	237	GLU	N-CA	10.60	1.67	1.46
1	A	550	SER	CA-CB	-10.59	1.37	1.52
1	A	437	ARG	CB-CG	-10.47	1.24	1.52
1	A	255	LYS	CE-NZ	10.39	1.75	1.49
1	A	570	TYR	CD2-CE2	10.27	1.54	1.39
1	A	271	ASP	CB-CG	-10.22	1.30	1.51
1	A	166	TYR	CZ-OH	10.13	1.55	1.37
1	A	344	GLN	CD-NE2	10.07	1.58	1.32
1	A	348	HIS	C-O	10.05	1.42	1.23
1	A	373	ARG	CZ-NH2	10.04	1.46	1.33
1	A	436	TYR	CZ-OH	10.03	1.54	1.37
1	A	263	ASP	CA-CB	-9.97	1.32	1.53
1	A	386	HIS	CA-CB	-9.97	1.32	1.53
1	A	165	TYR	CG-CD2	-9.89	1.26	1.39
1	A	436	TYR	CE2-CZ	-9.87	1.25	1.38
1	A	613	LEU	CB-CG	-9.80	1.24	1.52
1	A	522	LEU	C-O	9.79	1.42	1.23
1	A	579	GLU	CD-OE2	-9.78	1.14	1.25
1	A	466	THR	CB-OG1	-9.76	1.23	1.43
1	A	351	LYS	CG-CD	9.75	1.85	1.52
1	A	396	ARG	NE-CZ	9.75	1.45	1.33
1	A	376	ARG	CZ-NH1	9.75	1.45	1.33
1	A	426	PHE	CD1-CE1	9.74	1.58	1.39
1	A	303	GLY	C-O	9.71	1.39	1.23
1	A	380	SER	CA-CB	-9.70	1.38	1.52
1	A	446	TYR	CE1-CZ	-9.63	1.26	1.38
1	A	411	TYR	CG-CD2	-9.58	1.26	1.39
1	A	373	ARG	CD-NE	9.56	1.62	1.46
1	A	615	SER	CB-OG	9.54	1.54	1.42
1	A	214	ARG	CA-CB	-9.52	1.33	1.53
1	A	351	LYS	CD-CE	9.51	1.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	GLY	C-O	9.50	1.38	1.23
1	A	497	GLN	CG-CD	9.47	1.72	1.51
1	A	267	ARG	N-CA	-9.46	1.27	1.46
1	A	418	LYS	CE-NZ	9.37	1.72	1.49
1	A	555	THR	C-O	9.36	1.41	1.23
1	A	216	LEU	N-CA	-9.33	1.27	1.46
1	A	209	VAL	CA-CB	-9.29	1.35	1.54
1	A	604	GLY	N-CA	9.26	1.59	1.46
1	A	166	TYR	CD2-CE2	9.24	1.53	1.39
1	A	410	ASN	C-O	9.23	1.40	1.23
1	A	173	ARG	NE-CZ	-9.23	1.21	1.33
1	A	415	PHE	CA-C	-9.17	1.29	1.52
1	A	226	ARG	N-CA	-9.15	1.28	1.46
1	A	409	ASP	CB-CG	-9.13	1.32	1.51
1	A	384	GLN	CG-CD	9.10	1.72	1.51
1	A	219	GLY	N-CA	-9.09	1.32	1.46
1	A	448	SER	C-O	9.06	1.40	1.23
1	A	179	GLN	CD-OE1	-9.05	1.04	1.24
1	A	382	GLU	CA-CB	-9.02	1.34	1.53
1	A	611	ARG	CZ-NH1	8.98	1.44	1.33
1	A	593	GLU	CG-CD	-8.97	1.38	1.51
1	A	344	GLN	C-O	8.89	1.40	1.23
1	A	579	GLU	CG-CD	8.87	1.65	1.51
1	A	258	THR	C-O	8.85	1.40	1.23
1	A	562	TYR	CB-CG	-8.83	1.38	1.51
1	A	259	VAL	CA-CB	-8.82	1.36	1.54
1	A	269	SER	CA-CB	-8.80	1.39	1.52
1	A	172	TYR	CE1-CZ	-8.78	1.27	1.38
1	A	464	SER	CB-OG	8.76	1.53	1.42
1	A	586	SER	CB-OG	8.75	1.53	1.42
1	A	178	THR	CA-CB	8.74	1.76	1.53
1	A	295	ARG	CZ-NH2	8.73	1.44	1.33
1	A	450	SER	CB-OG	8.72	1.53	1.42
1	A	260	LEU	C-O	8.71	1.39	1.23
1	A	415	PHE	CD1-CE1	8.71	1.56	1.39
1	A	591	CYS	CB-SG	8.70	1.97	1.82
1	A	475	ALA	CA-CB	8.70	1.70	1.52
1	A	474	GLN	CB-CG	-8.69	1.29	1.52
1	A	440	GLN	CD-OE1	8.63	1.43	1.24
1	A	230	LYS	CA-C	-8.63	1.30	1.52
1	A	308	ASN	CB-CG	-8.61	1.31	1.51
1	A	317	SER	CB-OG	-8.61	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ASN	C-O	8.60	1.39	1.23
1	A	415	PHE	CG-CD2	-8.60	1.25	1.38
1	A	390	SER	CB-OG	8.59	1.53	1.42
1	A	490	GLN	CD-NE2	8.59	1.54	1.32
1	A	494	THR	C-O	-8.58	1.07	1.23
1	A	266	ASN	C-O	8.58	1.39	1.23
1	A	226	ARG	CG-CD	8.57	1.73	1.51
1	A	437	ARG	C-O	8.57	1.39	1.23
1	A	164	GLN	CG-CD	8.56	1.70	1.51
1	A	559	PHE	CB-CG	-8.53	1.36	1.51
1	A	224	GLN	CD-OE1	8.52	1.42	1.24
1	A	173	ARG	CD-NE	8.51	1.60	1.46
1	A	615	SER	CA-C	-8.50	1.30	1.52
1	A	578	PRO	C-O	8.47	1.40	1.23
1	A	598	GLU	CG-CD	8.44	1.64	1.51
1	A	588	PHE	CB-CG	8.43	1.65	1.51
1	A	406	TYR	CE1-CZ	-8.40	1.27	1.38
1	A	491	LEU	C-O	8.34	1.39	1.23
1	A	303	GLY	CA-C	-8.32	1.38	1.51
1	A	352	HIS	C-O	8.30	1.39	1.23
1	A	234	ASN	C-O	8.26	1.39	1.23
1	A	497	GLN	CD-OE1	8.22	1.42	1.24
1	A	408	PHE	CG-CD1	8.21	1.51	1.38
1	A	539	TYR	CG-CD1	8.19	1.49	1.39
1	A	324	ARG	CD-NE	8.19	1.60	1.46
1	A	213	PHE	CE2-CZ	8.18	1.52	1.37
1	A	214	ARG	NE-CZ	8.15	1.43	1.33
1	A	165	TYR	CE1-CZ	-8.14	1.27	1.38
1	A	166	TYR	CG-CD1	-8.14	1.28	1.39
1	A	439	TYR	CD1-CE1	-8.11	1.27	1.39
1	A	601	GLU	CD-OE1	-8.11	1.16	1.25
1	A	415	PHE	C-N	8.08	1.52	1.34
1	A	216	LEU	CG-CD2	-8.08	1.22	1.51
1	A	615	SER	CA-CB	8.05	1.65	1.52
1	A	437	ARG	NE-CZ	8.01	1.43	1.33
1	A	553	PRO	N-CD	-8.00	1.36	1.47
1	A	362	ARG	N-CA	7.99	1.62	1.46
1	A	324	ARG	CZ-NH2	7.98	1.43	1.33
1	A	257	ARG	NE-CZ	-7.98	1.22	1.33
1	A	440	GLN	CD-NE2	7.97	1.52	1.32
1	A	258	THR	CB-OG1	7.95	1.59	1.43
1	A	600	ALA	CA-C	7.90	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	609	ASP	CB-CG	-7.88	1.35	1.51
1	A	334	HIS	CE1-NE2	7.88	1.50	1.32
1	A	494	THR	CA-C	7.88	1.73	1.52
1	A	210	VAL	CB-CG1	7.88	1.69	1.52
1	A	365	SER	N-CA	7.78	1.61	1.46
1	A	172	TYR	CB-CG	-7.77	1.40	1.51
1	A	484	PRO	N-CD	-7.76	1.36	1.47
1	A	253	TRP	CZ2-CH2	-7.75	1.22	1.37
1	A	456	GLU	CA-CB	-7.71	1.36	1.53
1	A	415	PHE	N-CA	-7.68	1.30	1.46
1	A	350	LEU	C-O	7.68	1.38	1.23
1	A	435	TYR	CE2-CZ	-7.64	1.28	1.38
1	A	198	VAL	CB-CG1	7.62	1.68	1.52
1	A	414	THR	CB-OG1	7.56	1.58	1.43
1	A	213	PHE	CG-CD2	7.53	1.50	1.38
1	A	324	ARG	CZ-NH1	-7.53	1.23	1.33
1	A	205	PHE	CD2-CE2	7.52	1.54	1.39
1	A	233	SER	CB-OG	7.52	1.52	1.42
1	A	447	GLU	CD-OE2	7.52	1.33	1.25
1	A	440	GLN	CB-CG	-7.51	1.32	1.52
1	A	496	MET	CB-CG	-7.51	1.27	1.51
1	A	266	ASN	CA-C	-7.50	1.33	1.52
1	A	463	ARG	CA-CB	-7.50	1.37	1.53
1	A	218	GLU	C-N	7.48	1.46	1.33
1	A	304	GLY	CA-C	7.45	1.63	1.51
1	A	250	ARG	CZ-NH1	7.44	1.42	1.33
1	A	231	MET	CA-CB	-7.42	1.37	1.53
1	A	544	ARG	CZ-NH1	7.41	1.42	1.33
1	A	344	GLN	CG-CD	-7.40	1.34	1.51
1	A	161	CYS	CB-SG	-7.38	1.69	1.82
1	A	570	TYR	CZ-OH	7.37	1.50	1.37
1	A	454	PHE	CG-CD1	7.34	1.49	1.38
1	A	424	ASP	C-O	7.33	1.37	1.23
1	A	564	PRO	N-CD	7.33	1.58	1.47
1	A	421	TYR	CE1-CZ	-7.32	1.29	1.38
1	A	390	SER	CA-CB	-7.32	1.42	1.52
1	A	218	GLU	CB-CG	-7.31	1.38	1.52
1	A	187	SER	C-O	7.29	1.37	1.23
1	A	396	ARG	CD-NE	-7.29	1.34	1.46
1	A	608	VAL	C-O	7.27	1.37	1.23
1	A	474	GLN	N-CA	7.25	1.60	1.46
1	A	601	GLU	CG-CD	7.25	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	ALA	C-O	-7.22	1.09	1.23
1	A	482	ALA	CA-CB	7.22	1.67	1.52
1	A	349	LEU	CA-CB	7.18	1.70	1.53
1	A	488	LYS	CA-CB	-7.18	1.38	1.53
1	A	298	GLN	CG-CD	7.16	1.67	1.51
1	A	487	GLU	CA-C	7.15	1.71	1.52
1	A	343	VAL	C-O	7.15	1.36	1.23
1	A	196	VAL	CA-CB	-7.13	1.39	1.54
1	A	265	THR	CB-OG1	7.13	1.57	1.43
1	A	292	ASP	C-O	-7.12	1.09	1.23
1	A	180	ASP	C-O	7.12	1.36	1.23
1	A	387	LEU	N-CA	7.11	1.60	1.46
1	A	429	VAL	C-O	7.10	1.36	1.23
1	A	616	SER	C-O	7.05	1.36	1.23
1	A	544	ARG	NE-CZ	7.02	1.42	1.33
1	A	280	VAL	CB-CG1	7.02	1.67	1.52
1	A	320	PHE	CD1-CE1	7.02	1.53	1.39
1	A	381	PRO	CA-CB	7.01	1.67	1.53
1	A	537	GLU	CB-CG	-7.00	1.38	1.52
1	A	418	LYS	N-CA	6.99	1.60	1.46
1	A	262	LYS	CD-CE	6.98	1.68	1.51
1	A	481	ALA	N-CA	-6.94	1.32	1.46
1	A	275	ARG	NE-CZ	6.89	1.42	1.33
1	A	483	MET	C-O	-6.86	1.10	1.23
1	A	444	PRO	N-CD	6.84	1.57	1.47
1	A	275	ARG	CD-NE	-6.84	1.34	1.46
1	A	299	LEU	CG-CD1	-6.83	1.26	1.51
1	A	417	LYS	CA-C	6.82	1.70	1.52
1	A	235	GLU	CD-OE1	6.81	1.33	1.25
1	A	604	GLY	CA-C	-6.81	1.41	1.51
1	A	435	TYR	CD1-CE1	6.81	1.49	1.39
1	A	439	TYR	CG-CD2	6.81	1.48	1.39
1	A	423	PRO	C-O	6.81	1.36	1.23
1	A	309	GLY	CA-C	-6.80	1.41	1.51
1	A	351	LYS	C-O	6.78	1.36	1.23
1	A	453	ARG	C-O	6.78	1.36	1.23
1	A	313	TRP	CA-CB	6.77	1.68	1.53
1	A	169	PHE	CD1-CE1	6.75	1.52	1.39
1	A	504	VAL	CA-CB	6.74	1.69	1.54
1	A	257	ARG	CZ-NH2	6.73	1.41	1.33
1	A	554	THR	CA-CB	6.72	1.70	1.53
1	A	235	GLU	CB-CG	6.71	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	TYR	N-CA	6.70	1.59	1.46
1	A	439	TYR	CD2-CE2	-6.70	1.29	1.39
1	A	551	GLN	CD-OE1	6.69	1.38	1.24
1	A	579	GLU	C-N	6.67	1.49	1.34
1	A	167	ARG	NE-CZ	-6.66	1.24	1.33
1	A	344	GLN	CA-CB	-6.66	1.39	1.53
1	A	285	PRO	CA-CB	6.66	1.66	1.53
1	A	596	SER	CB-OG	-6.65	1.33	1.42
1	A	223	THR	CB-OG1	6.63	1.56	1.43
1	A	576	PRO	C-N	-6.63	1.18	1.34
1	A	546	VAL	CB-CG2	-6.62	1.39	1.52
1	A	496	MET	CG-SD	-6.62	1.64	1.81
1	A	325	ASP	CB-CG	-6.61	1.37	1.51
1	A	577	GLN	CG-CD	-6.60	1.35	1.51
1	A	373	ARG	CZ-NH1	6.59	1.41	1.33
1	A	353	MET	C-O	6.58	1.35	1.23
1	A	541	MET	CG-SD	6.56	1.98	1.81
1	A	594	THR	C-O	6.53	1.35	1.23
1	A	444	PRO	N-CA	6.52	1.58	1.47
1	A	277	ILE	CA-CB	6.51	1.69	1.54
1	A	426	PHE	CE1-CZ	-6.50	1.25	1.37
1	A	233	SER	N-CA	-6.50	1.33	1.46
1	A	436	TYR	CG-CD2	-6.50	1.30	1.39
1	A	562	TYR	CA-CB	-6.49	1.39	1.53
1	A	337	PHE	CG-CD1	6.49	1.48	1.38
1	A	407	LYS	CG-CD	6.48	1.74	1.52
1	A	268	ASP	CG-OD2	6.47	1.40	1.25
1	A	269	SER	C-O	6.47	1.35	1.23
1	A	605	ALA	C-O	6.46	1.35	1.23
1	A	616	SER	CA-CB	-6.45	1.43	1.52
1	A	261	LEU	C-O	-6.44	1.11	1.23
1	A	407	LYS	CD-CE	-6.44	1.35	1.51
1	A	159	PRO	C-O	-6.44	1.10	1.23
1	A	389	SER	CB-OG	-6.43	1.33	1.42
1	A	166	TYR	CG-CD2	-6.42	1.30	1.39
1	A	435	TYR	CG-CD2	-6.42	1.30	1.39
1	A	169	PHE	CG-CD2	-6.41	1.29	1.38
1	A	570	TYR	CG-CD1	-6.39	1.30	1.39
1	A	468	GLU	CD-OE1	-6.37	1.18	1.25
1	A	444	PRO	CG-CD	-6.37	1.29	1.50
1	A	426	PHE	CB-CG	-6.37	1.40	1.51
1	A	583	PHE	CG-CD2	-6.34	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	LEU	C-O	6.34	1.35	1.23
1	A	285	PRO	CG-CD	6.31	1.71	1.50
1	A	411	TYR	CD2-CE2	6.31	1.48	1.39
1	A	422	SER	CA-CB	6.28	1.62	1.52
1	A	267	ARG	CG-CD	6.27	1.67	1.51
1	A	472	PHE	CG-CD1	6.27	1.48	1.38
1	A	275	ARG	CG-CD	6.26	1.67	1.51
1	A	286	GLY	CA-C	6.26	1.61	1.51
1	A	264	SER	CA-CB	6.24	1.62	1.52
1	A	483	MET	CA-CB	-6.22	1.40	1.53
1	A	209	VAL	CB-CG2	-6.21	1.39	1.52
1	A	593	GLU	C-O	-6.21	1.11	1.23
1	A	321	VAL	CA-CB	-6.20	1.41	1.54
1	A	426	PHE	CE2-CZ	-6.17	1.25	1.37
1	A	270	LEU	C-O	6.17	1.35	1.23
1	A	392	GLU	CB-CG	-6.16	1.40	1.52
1	A	203	GLN	CD-OE1	6.16	1.37	1.24
1	A	350	LEU	CG-CD1	6.14	1.74	1.51
1	A	179	GLN	CD-NE2	-6.13	1.17	1.32
1	A	502	TYR	CG-CD2	-6.13	1.31	1.39
1	A	29	PRO	C-N	-6.12	1.22	1.34
1	A	164	GLN	CA-CB	-6.12	1.40	1.53
1	A	507	ILE	C-O	6.11	1.34	1.23
1	A	423	PRO	CG-CD	-6.09	1.30	1.50
1	A	174	LEU	N-CA	6.09	1.58	1.46
1	A	378	LYS	N-CA	6.09	1.58	1.46
1	A	267	ARG	CD-NE	-6.08	1.36	1.46
1	A	376	ARG	CD-NE	6.07	1.56	1.46
1	A	176	GLY	N-CA	6.06	1.55	1.46
1	A	226	ARG	CA-CB	6.05	1.67	1.53
1	A	478	ASP	CA-C	-6.04	1.37	1.52
1	A	399	LYS	CG-CD	6.03	1.73	1.52
1	A	610	MET	CG-SD	6.02	1.96	1.81
1	A	497	GLN	CB-CG	-6.02	1.36	1.52
1	A	588	PHE	CE2-CZ	-6.01	1.25	1.37
1	A	475	ALA	C-O	-6.01	1.11	1.23
1	A	218	GLU	N-CA	6.00	1.58	1.46
1	A	472	PHE	CE1-CZ	-5.99	1.25	1.37
1	A	545	PHE	CE1-CZ	-5.98	1.25	1.37
1	A	493	GLN	C-O	5.98	1.34	1.23
1	A	407	LYS	N-CA	-5.97	1.34	1.46
1	A	416	ILE	CA-CB	5.96	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	CYS	CA-C	5.96	1.68	1.52
1	A	484	PRO	CG-CD	5.96	1.70	1.50
1	A	467	PRO	CA-CB	5.96	1.65	1.53
1	A	162	MET	C-O	5.95	1.34	1.23
1	A	235	GLU	CG-CD	5.93	1.60	1.51
1	A	433	LEU	C-O	5.93	1.34	1.23
1	A	509	GLY	CA-C	-5.93	1.42	1.51
1	A	205	PHE	CA-C	-5.91	1.37	1.52
1	A	612	ASP	C-O	5.91	1.34	1.23
1	A	592	LYS	C-N	-5.90	1.20	1.34
1	A	570	TYR	CE1-CZ	-5.90	1.30	1.38
1	A	418	LYS	CA-C	-5.87	1.37	1.52
1	A	496	MET	CA-C	-5.86	1.37	1.52
1	A	172	TYR	C-O	5.86	1.34	1.23
1	A	314	TYR	CE1-CZ	-5.86	1.30	1.38
1	A	435	TYR	CD2-CE2	-5.85	1.30	1.39
1	A	504	VAL	CB-CG2	-5.85	1.40	1.52
1	A	490	GLN	N-CA	5.85	1.58	1.46
1	A	343	VAL	CB-CG1	5.84	1.65	1.52
1	A	378	LYS	CD-CE	5.84	1.65	1.51
1	A	540	LEU	CG-CD1	5.84	1.73	1.51
1	A	324	ARG	NE-CZ	-5.83	1.25	1.33
1	A	370	PRO	CA-C	5.83	1.64	1.52
1	A	374	ARG	NE-CZ	-5.83	1.25	1.33
1	A	444	PRO	CA-CB	-5.81	1.42	1.53
1	A	491	LEU	N-CA	5.81	1.57	1.46
1	A	499	GLN	C-O	5.81	1.34	1.23
1	A	616	SER	CB-OG	5.81	1.49	1.42
1	A	304	GLY	N-CA	-5.80	1.37	1.46
1	A	311	ASN	CG-OD1	5.80	1.36	1.24
1	A	499	GLN	CA-CB	-5.80	1.41	1.53
1	A	539	TYR	CE2-CZ	-5.80	1.31	1.38
1	A	236	ASP	N-CA	5.79	1.57	1.46
1	A	396	ARG	N-CA	-5.79	1.34	1.46
1	A	206	VAL	CA-CB	-5.78	1.42	1.54
1	A	296	ALA	C-O	5.77	1.34	1.23
1	A	159	PRO	CA-C	5.76	1.64	1.52
1	A	487	GLU	CG-CD	5.76	1.60	1.51
1	A	213	PHE	CA-CB	5.75	1.66	1.53
1	A	474	GLN	C-O	5.75	1.34	1.23
1	A	382	GLU	CD-OE1	5.74	1.31	1.25
1	A	263	ASP	CA-C	-5.73	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	534	PHE	CE2-CZ	5.72	1.48	1.37
1	A	452	ARG	C-O	5.71	1.34	1.23
1	A	392	GLU	CG-CD	5.70	1.60	1.51
1	A	558	MET	N-CA	5.70	1.57	1.46
1	A	475	ALA	CA-C	-5.69	1.38	1.52
1	A	467	PRO	N-CA	5.69	1.56	1.47
1	A	414	THR	N-CA	5.68	1.57	1.46
1	A	450	SER	C-O	5.66	1.34	1.23
1	A	551	GLN	CD-NE2	-5.66	1.18	1.32
1	A	460	ASP	CB-CG	-5.66	1.39	1.51
1	A	169	PHE	CB-CG	-5.66	1.41	1.51
1	A	252	GLU	CA-CB	-5.65	1.41	1.53
1	A	574	TYR	CD1-CE1	-5.65	1.30	1.39
1	A	284	GLY	CA-C	-5.64	1.42	1.51
1	A	298	GLN	CB-CG	-5.63	1.37	1.52
1	A	251	SER	C-O	5.63	1.34	1.23
1	A	576	PRO	CA-C	5.63	1.64	1.52
1	A	158	GLN	N-CA	-5.62	1.35	1.46
1	A	169	PHE	CA-C	-5.61	1.38	1.52
1	A	439	TYR	C-O	5.60	1.33	1.23
1	A	172	TYR	CG-CD1	5.60	1.46	1.39
1	A	472	PHE	N-CA	5.59	1.57	1.46
1	A	532	GLU	CD-OE1	5.59	1.31	1.25
1	A	530	PRO	CA-C	-5.58	1.41	1.52
1	A	214	ARG	CD-NE	-5.57	1.36	1.46
1	A	254	ALA	C-N	-5.56	1.21	1.34
1	A	231	MET	CB-CG	5.56	1.69	1.51
1	A	577	GLN	CA-CB	-5.56	1.41	1.53
1	A	249	GLY	N-CA	-5.56	1.37	1.46
1	A	374	ARG	C-O	5.55	1.33	1.23
1	A	439	TYR	CE1-CZ	-5.55	1.31	1.38
1	A	398	VAL	CB-CG2	-5.55	1.41	1.52
1	A	446	TYR	CD1-CE1	5.55	1.47	1.39
1	A	532	GLU	CD-OE2	-5.54	1.19	1.25
1	A	374	ARG	CZ-NH2	-5.53	1.25	1.33
1	A	600	ALA	N-CA	-5.53	1.35	1.46
1	A	554	THR	CB-OG1	-5.52	1.32	1.43
1	A	466	THR	C-O	-5.50	1.12	1.23
1	A	446	TYR	CA-CB	-5.50	1.41	1.53
1	A	550	SER	CB-OG	-5.50	1.35	1.42
1	A	316	LYS	CG-CD	5.50	1.71	1.52
1	A	432	GLN	C-O	5.49	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	LYS	CB-CG	-5.48	1.37	1.52
1	A	593	GLU	CD-OE1	5.47	1.31	1.25
1	A	418	LYS	C-O	5.46	1.33	1.23
1	A	459	VAL	CB-CG1	-5.46	1.41	1.52
1	A	160	LEU	CA-CB	5.46	1.66	1.53
1	A	574	TYR	C-O	5.43	1.33	1.23
1	A	511	ALA	CA-CB	-5.39	1.41	1.52
1	A	205	PHE	CG-CD2	5.38	1.46	1.38
1	A	423	PRO	N-CA	-5.37	1.38	1.47
1	A	612	ASP	CG-OD1	5.36	1.37	1.25
1	A	568	ASN	C-O	-5.35	1.13	1.23
1	A	502	TYR	CG-CD1	-5.34	1.32	1.39
1	A	580	ALA	C-O	-5.34	1.13	1.23
1	A	261	LEU	CA-C	5.33	1.66	1.52
1	A	471	ALA	CA-C	5.33	1.66	1.52
1	A	536	ASP	C-N	5.33	1.46	1.34
1	A	415	PHE	CE2-CZ	5.33	1.47	1.37
1	A	64	PRO	N-CD	5.33	1.55	1.47
1	A	521	GLU	N-CA	5.33	1.57	1.46
1	A	372	PRO	N-CD	5.33	1.55	1.47
1	A	295	ARG	CA-CB	-5.32	1.42	1.53
1	A	47	PRO	N-CD	5.32	1.55	1.47
1	A	108	PRO	N-CD	5.32	1.55	1.47
1	A	460	ASP	C-N	-5.32	1.21	1.34
1	A	29	PRO	N-CD	5.31	1.55	1.47
1	A	260	LEU	C-N	-5.31	1.21	1.34
1	A	210	VAL	C-N	5.31	1.46	1.34
1	A	488	LYS	CB-CG	5.31	1.66	1.52
1	A	493	GLN	C-N	-5.31	1.21	1.34
1	A	597	VAL	CB-CG2	-5.30	1.41	1.52
1	A	175	PRO	N-CD	5.29	1.55	1.47
1	A	435	TYR	C-O	5.28	1.33	1.23
1	A	532	GLU	CA-C	5.28	1.66	1.52
1	A	477	THR	C-N	-5.28	1.22	1.34
1	A	516	LEU	CG-CD2	5.28	1.71	1.51
1	A	445	THR	N-CA	5.28	1.56	1.46
1	A	521	GLU	C-N	-5.27	1.22	1.34
1	A	441	ARG	CB-CG	-5.27	1.38	1.52
1	A	171	SER	CA-CB	5.26	1.60	1.52
1	A	440	GLN	C-N	5.25	1.46	1.34
1	A	367	SER	N-CA	-5.25	1.35	1.46
1	A	536	ASP	CG-OD1	5.24	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	LEU	CA-CB	-5.23	1.41	1.53
1	A	463	ARG	CB-CG	5.23	1.66	1.52
1	A	346	THR	CB-OG1	5.23	1.53	1.43
1	A	261	LEU	CA-CB	-5.23	1.41	1.53
1	A	341	VAL	CA-C	-5.22	1.39	1.52
1	A	228	ILE	C-O	5.22	1.33	1.23
1	A	423	PRO	N-CD	5.22	1.55	1.47
1	A	413	LYS	CD-CE	-5.22	1.38	1.51
1	A	157	GLY	CA-C	5.20	1.60	1.51
1	A	426	PHE	CA-CB	5.20	1.65	1.53
1	A	454	PHE	C-N	5.20	1.46	1.34
1	A	302	GLY	C-N	-5.18	1.23	1.33
1	A	552	VAL	N-CA	5.18	1.56	1.46
1	A	174	LEU	CB-CG	-5.18	1.37	1.52
1	A	357	ASN	N-CA	-5.18	1.35	1.46
1	A	612	ASP	N-CA	5.18	1.56	1.46
1	A	259	VAL	N-CA	5.16	1.56	1.46
1	A	377	TRP	CD2-CE2	5.15	1.47	1.41
1	A	205	PHE	C-N	5.13	1.45	1.34
1	A	504	VAL	CA-C	-5.13	1.39	1.52
1	A	487	GLU	N-CA	-5.13	1.36	1.46
1	A	227	LYS	CB-CG	5.11	1.66	1.52
1	A	350	LEU	CG-CD2	-5.10	1.32	1.51
1	A	337	PHE	CA-CB	5.10	1.65	1.53
1	A	185	GLN	CA-C	-5.10	1.39	1.52
1	A	570	TYR	CE2-CZ	-5.09	1.31	1.38
1	A	446	TYR	N-CA	5.08	1.56	1.46
1	A	429	VAL	CB-CG1	5.08	1.63	1.52
1	A	555	THR	C-N	-5.08	1.22	1.34
1	A	386	HIS	N-CA	5.07	1.56	1.46
1	A	166	TYR	CA-C	-5.07	1.39	1.52
1	A	610	MET	N-CA	-5.05	1.36	1.46
1	A	308	ASN	CA-C	5.05	1.66	1.52
1	A	282	LEU	CG-CD1	5.05	1.70	1.51
1	A	353	MET	CG-SD	5.03	1.94	1.81
1	A	272	MET	CA-CB	-5.03	1.42	1.53
1	A	613	LEU	CA-CB	5.03	1.65	1.53
1	A	336	PRO	CA-CB	-5.02	1.43	1.53
1	A	505	MET	N-CA	-5.01	1.36	1.46
1	A	562	TYR	CG-CD2	5.01	1.45	1.39
1	A	578	PRO	N-CA	5.01	1.55	1.47
1	A	578	PRO	CB-CG	-5.00	1.25	1.50

All (542) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ARG	NE-CZ-NH2	-52.05	94.27	120.30
1	A	267	ARG	NE-CZ-NH1	38.59	139.59	120.30
1	A	376	ARG	NE-CZ-NH1	38.55	139.57	120.30
1	A	226	ARG	NE-CZ-NH1	-35.44	102.58	120.30
1	A	452	ARG	NE-CZ-NH2	30.42	135.51	120.30
1	A	544	ARG	NE-CZ-NH2	-26.98	106.81	120.30
1	A	532	GLU	OE1-CD-OE2	25.75	154.20	123.30
1	A	214	ARG	NE-CZ-NH2	-22.53	109.04	120.30
1	A	544	ARG	NE-CZ-NH1	22.25	131.43	120.30
1	A	376	ARG	NE-CZ-NH2	-22.00	109.30	120.30
1	A	275	ARG	NE-CZ-NH2	-21.10	109.75	120.30
1	A	267	ARG	NH1-CZ-NH2	-20.58	96.77	119.40
1	A	373	ARG	NE-CZ-NH1	-20.30	110.15	120.30
1	A	289	GLU	O-C-N	-20.07	90.59	122.70
1	A	275	ARG	NE-CZ-NH1	19.30	129.95	120.30
1	A	437	ARG	NE-CZ-NH1	-19.08	110.76	120.30
1	A	295	ARG	NE-CZ-NH2	-18.90	110.85	120.30
1	A	396	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	A	454	PHE	CB-CG-CD2	18.01	133.41	120.80
1	A	611	ARG	NE-CZ-NH2	-17.43	111.58	120.30
1	A	496	MET	CG-SD-CE	-17.19	72.70	100.20
1	A	295	ARG	NE-CZ-NH1	16.81	128.70	120.30
1	A	189	ILE	O-C-N	16.44	149.01	122.70
1	A	452	ARG	NE-CZ-NH1	-16.37	112.12	120.30
1	A	190	MET	O-C-N	-16.32	90.09	121.10
1	A	441	ARG	NE-CZ-NH2	-16.18	112.21	120.30
1	A	166	TYR	CG-CD1-CE1	15.99	134.09	121.30
1	A	612	ASP	CB-CG-OD2	15.84	132.56	118.30
1	A	220	ASP	CB-CG-OD1	-15.70	104.17	118.30
1	A	367	SER	N-CA-CB	-15.61	87.08	110.50
1	A	189	ILE	CA-C-O	-15.33	87.90	120.10
1	A	409	ASP	CB-CG-OD1	15.23	132.01	118.30
1	A	532	GLU	CG-CD-OE2	-15.08	88.14	118.30
1	A	190	MET	N-CA-CB	14.85	137.33	110.60
1	A	218	GLU	OE1-CD-OE2	14.82	141.08	123.30
1	A	226	ARG	NH1-CZ-NH2	14.71	135.58	119.40
1	A	360	LEU	C-N-CA	14.30	157.45	121.70
1	A	267	ARG	CA-CB-CG	14.21	144.66	113.40
1	A	271	ASP	CB-CG-OD1	14.20	131.08	118.30
1	A	237	GLU	N-CA-CB	13.96	135.74	110.60
1	A	365	SER	N-CA-CB	-13.64	90.04	110.50
1	A	374	ARG	NE-CZ-NH2	-13.63	113.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	GLY	O-C-N	-13.60	100.94	122.70
1	A	456	GLU	OE1-CD-OE2	-13.56	107.02	123.30
1	A	315	ASP	CB-CG-OD1	13.45	130.41	118.30
1	A	437	ARG	NH1-CZ-NH2	13.32	134.05	119.40
1	A	286	GLY	CA-C-N	-13.29	87.96	117.20
1	A	222	PHE	CB-CG-CD2	12.89	129.83	120.80
1	A	312	ARG	NE-CZ-NH2	-12.65	113.97	120.30
1	A	167	ARG	CD-NE-CZ	12.55	141.17	123.60
1	A	588	PHE	CG-CD1-CE1	-12.50	107.05	120.80
1	A	437	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	A	286	GLY	C-N-CA	12.27	152.37	121.70
1	A	257	ARG	NE-CZ-NH2	12.25	126.43	120.30
1	A	178	THR	CA-CB-CG2	-12.00	95.60	112.40
1	A	570	TYR	CB-CG-CD1	-11.98	113.81	121.00
1	A	337	PHE	CB-CG-CD2	11.96	129.17	120.80
1	A	526	LEU	N-CA-CB	-11.77	86.85	110.40
1	A	411	TYR	CZ-CE2-CD2	-11.71	109.26	119.80
1	A	570	TYR	CZ-CE2-CD2	-11.57	109.38	119.80
1	A	612	ASP	CB-CG-OD1	-11.53	107.93	118.30
1	A	421	TYR	CG-CD2-CE2	-11.43	112.16	121.30
1	A	609	ASP	CB-CG-OD1	11.40	128.56	118.30
1	A	559	PHE	CB-CG-CD2	11.39	128.77	120.80
1	A	403	PHE	CB-CG-CD2	11.38	128.77	120.80
1	A	209	VAL	CA-CB-CG2	11.30	127.84	110.90
1	A	331	VAL	CA-CB-CG1	11.29	127.83	110.90
1	A	204	PHE	CG-CD2-CE2	-11.23	108.44	120.80
1	A	521	GLU	CG-CD-OE1	11.21	140.73	118.30
1	A	436	TYR	CB-CG-CD1	-11.15	114.31	121.00
1	A	263	ASP	CB-CG-OD2	11.13	128.32	118.30
1	A	154	GLN	C-N-CA	-11.10	93.96	121.70
1	A	324	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	A	539	TYR	CZ-CE2-CD2	11.08	129.77	119.80
1	A	289	GLU	CA-C-N	11.06	141.54	117.20
1	A	167	ARG	NH1-CZ-NH2	11.06	131.56	119.40
1	A	312	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	A	172	TYR	CG-CD1-CE1	11.03	130.12	121.30
1	A	267	ARG	CG-CD-NE	-11.00	88.71	111.80
1	A	599	PHE	CB-CG-CD2	10.95	128.46	120.80
1	A	216	LEU	CB-CG-CD2	10.92	129.57	111.00
1	A	458	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	A	613	LEU	CB-CG-CD2	10.80	129.37	111.00
1	A	583	PHE	CG-CD2-CE2	10.76	132.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	SER	CA-C-N	10.73	140.81	117.20
1	A	381	PRO	N-CD-CG	-10.71	87.14	103.20
1	A	237	GLU	N-CA-C	-10.69	82.15	111.00
1	A	435	TYR	CB-CG-CD1	-10.64	114.62	121.00
1	A	166	TYR	CG-CD2-CE2	-10.59	112.83	121.30
1	A	411	TYR	CB-CG-CD1	-10.57	114.66	121.00
1	A	583	PHE	CB-CG-CD2	10.48	128.14	120.80
1	A	172	TYR	CB-CG-CD2	10.41	127.25	121.00
1	A	417	LYS	O-C-N	10.37	139.29	122.70
1	A	453	ARG	CA-CB-CG	10.33	136.13	113.40
1	A	616	SER	CA-C-O	-10.22	98.63	120.10
1	A	383	THR	O-C-N	-10.21	106.36	122.70
1	A	373	ARG	NE-CZ-NH2	10.16	125.38	120.30
1	A	190	MET	CA-C-N	10.16	145.55	117.10
1	A	426	PHE	CB-CG-CD1	-10.10	113.73	120.80
1	A	453	ARG	CG-CD-NE	10.07	132.94	111.80
1	A	376	ARG	CD-NE-CZ	10.04	137.66	123.60
1	A	609	ASP	OD1-CG-OD2	-10.04	104.23	123.30
1	A	189	ILE	CA-C-N	-9.94	95.33	117.20
1	A	194	GLU	OE1-CD-OE2	9.89	135.17	123.30
1	A	178	THR	OG1-CB-CG2	-9.87	87.31	110.00
1	A	513	ASP	CB-CG-OD2	9.82	127.13	118.30
1	A	454	PHE	CD1-CG-CD2	-9.81	105.55	118.30
1	A	426	PHE	CB-CG-CD2	9.78	127.65	120.80
1	A	490	GLN	CB-CG-CD	9.77	136.99	111.60
1	A	218	GLU	CG-CD-OE1	-9.73	98.83	118.30
1	A	460	ASP	CB-CG-OD1	9.70	127.03	118.30
1	A	598	GLU	N-CA-CB	9.68	128.02	110.60
1	A	415	PHE	CA-C-O	9.67	140.41	120.10
1	A	488	LYS	CD-CE-NZ	9.65	133.89	111.70
1	A	545	PHE	CB-CG-CD1	-9.62	114.06	120.80
1	A	436	TYR	CG-CD1-CE1	-9.59	113.63	121.30
1	A	393	LYS	CD-CE-NZ	9.57	133.72	111.70
1	A	539	TYR	CB-CG-CD1	-9.56	115.26	121.00
1	A	185	GLN	C-N-CA	-9.56	97.81	121.70
1	A	415	PHE	O-C-N	-9.54	107.44	122.70
1	A	454	PHE	CG-CD2-CE2	9.51	131.26	120.80
1	A	261	LEU	O-C-N	9.42	137.78	122.70
1	A	288	GLY	CA-C-N	9.42	137.91	117.20
1	A	559	PHE	CD1-CG-CD2	-9.40	106.08	118.30
1	A	411	TYR	CG-CD2-CE2	9.39	128.81	121.30
1	A	437	ARG	CD-NE-CZ	-9.38	110.47	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	435	TYR	CG-CD1-CE1	-9.32	113.85	121.30
1	A	452	ARG	CD-NE-CZ	9.24	136.53	123.60
1	A	379	CYS	CA-CB-SG	-9.16	97.52	114.00
1	A	612	ASP	O-C-N	-9.09	108.16	122.70
1	A	605	ALA	O-C-N	-9.06	108.21	122.70
1	A	521	GLU	OE1-CD-OE2	-9.04	112.45	123.30
1	A	275	ARG	CD-NE-CZ	9.01	136.22	123.60
1	A	192	GLU	N-CA-C	8.97	135.23	111.00
1	A	190	MET	N-CA-C	-8.97	86.78	111.00
1	A	483	MET	N-CA-CB	8.97	126.74	110.60
1	A	409	ASP	CB-CG-OD2	-8.92	110.28	118.30
1	A	220	ASP	O-C-N	8.91	136.95	122.70
1	A	378	LYS	CB-CG-CD	8.90	134.74	111.60
1	A	348	HIS	O-C-N	-8.90	108.46	122.70
1	A	189	ILE	N-CA-C	8.89	135.00	111.00
1	A	570	TYR	CD1-CG-CD2	8.84	127.62	117.90
1	A	439	TYR	CD1-CE1-CZ	8.79	127.71	119.80
1	A	593	GLU	OE1-CD-OE2	-8.79	112.76	123.30
1	A	266	ASN	O-C-N	-8.72	108.75	122.70
1	A	466	THR	CA-CB-CG2	-8.68	100.26	112.40
1	A	213	PHE	CG-CD1-CE1	8.67	130.33	120.80
1	A	219	GLY	CA-C-O	8.67	136.20	120.60
1	A	173	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	261	LEU	CB-CG-CD1	-8.63	96.32	111.00
1	A	436	TYR	CB-CG-CD2	8.58	126.15	121.00
1	A	222	PHE	CB-CG-CD1	-8.55	114.82	120.80
1	A	233	SER	N-CA-CB	-8.54	97.68	110.50
1	A	494	THR	O-C-N	8.54	136.36	122.70
1	A	252	GLU	OE1-CD-OE2	-8.52	113.07	123.30
1	A	172	TYR	CD1-CG-CD2	-8.48	108.57	117.90
1	A	337	PHE	CB-CG-CD1	-8.41	114.91	120.80
1	A	446	TYR	CB-CG-CD1	-8.40	115.96	121.00
1	A	271	ASP	OD1-CG-OD2	-8.39	107.36	123.30
1	A	223	THR	CA-CB-CG2	-8.35	100.71	112.40
1	A	213	PHE	CD1-CE1-CZ	-8.27	110.17	120.10
1	A	396	ARG	CD-NE-CZ	-8.27	112.03	123.60
1	A	236	ASP	CB-CA-C	-8.26	93.88	110.40
1	A	333	GLU	OE1-CD-OE2	-8.26	113.39	123.30
1	A	483	MET	CA-CB-CG	-8.25	99.28	113.30
1	A	607	LEU	O-C-N	8.25	135.90	122.70
1	A	396	ARG	NH1-CZ-NH2	8.21	128.44	119.40
1	A	374	ARG	NE-CZ-NH1	8.16	124.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	337	PHE	CZ-CE2-CD2	-8.13	110.35	120.10
1	A	484	PRO	N-CA-CB	8.11	113.04	103.30
1	A	418	LYS	CD-CE-NZ	8.11	130.35	111.70
1	A	609	ASP	O-C-N	-8.11	109.73	122.70
1	A	450	SER	N-CA-CB	-8.10	98.35	110.50
1	A	487	GLU	CA-C-N	-8.08	99.43	117.20
1	A	423	PRO	CA-CB-CG	-8.06	88.68	104.00
1	A	376	ARG	CG-CD-NE	-8.04	94.92	111.80
1	A	487	GLU	CG-CD-OE2	-8.04	102.23	118.30
1	A	288	GLY	C-N-CA	8.02	141.75	121.70
1	A	373	ARG	N-CA-CB	-8.01	96.18	110.60
1	A	588	PHE	CB-CG-CD1	-7.99	115.21	120.80
1	A	347	GLU	OE1-CD-OE2	7.98	132.88	123.30
1	A	379	CYS	CB-CA-C	-7.98	94.44	110.40
1	A	380	SER	CA-CB-OG	7.98	132.74	111.20
1	A	292	ASP	CB-CG-OD1	7.96	125.47	118.30
1	A	453	ARG	CD-NE-CZ	-7.96	112.45	123.60
1	A	377	TRP	O-C-N	7.90	135.34	122.70
1	A	446	TYR	CG-CD1-CE1	-7.89	114.98	121.30
1	A	437	ARG	CG-CD-NE	-7.88	95.25	111.80
1	A	611	ARG	CB-CA-C	-7.88	94.64	110.40
1	A	399	LYS	CD-CE-NZ	-7.80	93.75	111.70
1	A	257	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	A	186	LYS	C-N-CA	7.78	141.15	121.70
1	A	391	ALA	O-C-N	-7.76	110.28	122.70
1	A	479	HIS	CA-C-N	-7.75	100.14	117.20
1	A	154	GLN	O-C-N	-7.74	110.32	122.70
1	A	252	GLU	CG-CD-OE1	7.67	133.65	118.30
1	A	456	GLU	CG-CD-OE1	7.64	133.58	118.30
1	A	567	PRO	O-C-N	7.64	134.92	122.70
1	A	208	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	204	PHE	CB-CG-CD1	-7.61	115.47	120.80
1	A	437	ARG	O-C-N	-7.60	110.54	122.70
1	A	381	PRO	CA-CB-CG	-7.59	89.58	104.00
1	A	235	GLU	CA-C-N	7.58	133.88	117.20
1	A	382	GLU	OE1-CD-OE2	7.57	132.38	123.30
1	A	187	SER	O-C-N	-7.56	110.60	122.70
1	A	613	LEU	CA-CB-CG	7.55	132.66	115.30
1	A	410	ASN	O-C-N	-7.53	110.65	122.70
1	A	191	PRO	C-N-CA	7.53	140.52	121.70
1	A	376	ARG	NH1-CZ-NH2	-7.52	111.13	119.40
1	A	308	ASN	N-CA-CB	-7.49	97.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	478	ASP	CA-C-N	-7.49	100.73	117.20
1	A	611	ARG	NH1-CZ-NH2	7.47	127.62	119.40
1	A	588	PHE	CD1-CE1-CZ	7.42	129.01	120.10
1	A	543	ASN	O-C-N	7.40	134.55	122.70
1	A	365	SER	N-CA-C	7.39	130.96	111.00
1	A	235	GLU	O-C-N	-7.35	110.94	122.70
1	A	574	TYR	CG-CD2-CE2	7.32	127.15	121.30
1	A	349	LEU	CB-CG-CD2	7.30	123.42	111.00
1	A	539	TYR	CB-CG-CD2	7.28	125.37	121.00
1	A	601	GLU	OE1-CD-OE2	7.28	132.03	123.30
1	A	411	TYR	CG-CD1-CE1	-7.27	115.48	121.30
1	A	446	TYR	CZ-CE2-CD2	7.27	126.34	119.80
1	A	376	ARG	N-CA-CB	-7.26	97.54	110.60
1	A	137	TYR	CB-CG-CD1	7.25	125.35	121.00
1	A	599	PHE	CD1-CG-CD2	-7.24	108.89	118.30
1	A	599	PHE	CG-CD2-CE2	7.23	128.75	120.80
1	A	219	GLY	N-CA-C	7.22	131.16	113.10
1	A	189	ILE	C-N-CA	7.20	139.71	121.70
1	A	350	LEU	CB-CG-CD1	-7.20	98.76	111.00
1	A	363	ALA	CA-C-N	-7.20	101.37	117.20
1	A	29	PRO	C-N-CD	-7.17	104.83	120.60
1	A	487	GLU	N-CA-CB	7.16	123.48	110.60
1	A	349	LEU	CB-CG-CD1	-7.14	98.86	111.00
1	A	356	SER	CA-C-N	-7.13	101.51	117.20
1	A	191	PRO	CA-C-N	-7.13	101.52	117.20
1	A	536	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	458	ARG	NH1-CZ-NH2	7.12	127.23	119.40
1	A	377	TRP	CD1-CG-CD2	7.11	111.99	106.30
1	A	254	ALA	O-C-N	7.10	134.06	122.70
1	A	231	MET	CA-CB-CG	7.08	125.34	113.30
1	A	460	ASP	OD1-CG-OD2	-7.08	109.84	123.30
1	A	51	PHE	CB-CG-CD1	7.07	125.75	120.80
1	A	610	MET	CA-CB-CG	-7.04	101.32	113.30
1	A	258	THR	CA-C-O	-7.04	105.31	120.10
1	A	155	LEU	CB-CA-C	7.03	123.55	110.20
1	A	196	VAL	CG1-CB-CG2	-7.01	99.68	110.90
1	A	166	TYR	CD1-CE1-CZ	-7.01	113.49	119.80
1	A	314	TYR	CZ-CE2-CD2	-6.98	113.52	119.80
1	A	358	LYS	N-CA-CB	-6.97	98.05	110.60
1	A	472	PHE	CB-CG-CD2	6.96	125.67	120.80
1	A	551	GLN	CG-CD-OE1	-6.94	107.72	121.60
1	A	315	ASP	CB-CA-C	-6.93	96.54	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	PRO	N-CD-CG	-6.92	92.82	103.20
1	A	456	GLU	N-CA-CB	6.92	123.06	110.60
1	A	452	ARG	NH1-CZ-NH2	-6.92	111.79	119.40
1	A	614	CYS	O-C-N	6.91	133.76	122.70
1	A	424	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	570	TYR	CE1-CZ-CE2	6.90	130.83	119.80
1	A	314	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	A	448	SER	N-CA-CB	6.87	120.81	110.50
1	A	361	VAL	O-C-N	-6.86	111.72	122.70
1	A	608	VAL	O-C-N	-6.83	111.78	122.70
1	A	257	ARG	CD-NE-CZ	6.82	133.15	123.60
1	A	578	PRO	N-CA-CB	-6.82	95.10	102.60
1	A	242	ILE	CA-CB-CG1	-6.81	98.05	111.00
1	A	479	HIS	C-N-CA	6.81	138.72	121.70
1	A	483	MET	CG-SD-CE	-6.80	89.33	100.20
1	A	370	PRO	N-CD-CG	-6.79	93.01	103.20
1	A	205	PHE	CZ-CE2-CD2	-6.79	111.95	120.10
1	A	320	PHE	CB-CG-CD1	6.76	125.53	120.80
1	A	364	ASP	C-N-CA	-6.75	104.84	121.70
1	A	267	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	258	THR	O-C-N	6.67	133.37	122.70
1	A	441	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	401	LEU	O-C-N	-6.65	112.06	122.70
1	A	112	PHE	CB-CG-CD2	-6.65	116.15	120.80
1	A	616	SER	N-CA-CB	6.63	120.45	110.50
1	A	562	TYR	CA-CB-CG	6.62	125.98	113.40
1	A	170	SER	N-CA-CB	-6.61	100.58	110.50
1	A	254	ALA	CA-C-O	-6.61	106.22	120.10
1	A	181	THR	OG1-CB-CG2	-6.59	94.83	110.00
1	A	308	ASN	N-CA-C	6.59	128.78	111.00
1	A	226	ARG	CG-CD-NE	-6.58	97.99	111.80
1	A	477	THR	C-N-CA	-6.58	105.26	121.70
1	A	411	TYR	O-C-N	6.57	134.37	123.20
1	A	230	LYS	CG-CD-CE	-6.56	92.21	111.90
1	A	190	MET	C-N-CD	-6.55	106.19	120.60
1	A	438	LEU	CB-CG-CD2	6.55	122.14	111.00
1	A	152	LYS	CB-CA-C	6.55	123.49	110.40
1	A	230	LYS	CB-CA-C	6.54	123.47	110.40
1	A	325	ASP	N-CA-CB	6.51	122.32	110.60
1	A	419	GLN	CG-CD-OE1	-6.50	108.61	121.60
1	A	240	PRO	O-C-N	6.49	133.43	121.10
1	A	161	CYS	O-C-N	-6.49	112.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	539	TYR	CG-CD1-CE1	-6.46	116.13	121.30
1	A	255	LYS	O-C-N	-6.46	112.37	122.70
1	A	559	PHE	CG-CD1-CE1	6.44	127.89	120.80
1	A	530	PRO	N-CD-CG	-6.43	93.55	103.20
1	A	399	LYS	CA-CB-CG	-6.43	99.25	113.40
1	A	173	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	218	GLU	CA-C-O	6.42	133.59	120.10
1	A	437	ARG	CA-C-N	6.41	131.30	117.20
1	A	73	GLU	CB-CA-C	6.41	123.21	110.40
1	A	444	PRO	CA-N-CD	-6.39	102.55	111.50
1	A	436	TYR	CZ-CE2-CD2	-6.39	114.05	119.80
1	A	419	GLN	CB-CA-C	-6.39	97.63	110.40
1	A	526	LEU	N-CA-C	-6.39	93.76	111.00
1	A	193	PRO	C-N-CA	-6.38	105.74	121.70
1	A	580	ALA	CB-CA-C	-6.38	100.54	110.10
1	A	260	LEU	C-N-CA	6.37	137.62	121.70
1	A	286	GLY	O-C-N	6.37	132.89	122.70
1	A	436	TYR	CG-CD2-CE2	6.35	126.38	121.30
1	A	178	THR	CA-CB-OG1	-6.34	95.69	109.00
1	A	222	PHE	CA-C-O	6.31	133.36	120.10
1	A	258	THR	OG1-CB-CG2	-6.31	95.49	110.00
1	A	253	TRP	CD1-CG-CD2	-6.30	101.26	106.30
1	A	204	PHE	CZ-CE2-CD2	6.30	127.66	120.10
1	A	487	GLU	OE1-CD-OE2	6.29	130.85	123.30
1	A	429	VAL	O-C-N	-6.29	112.64	122.70
1	A	24	PRO	CA-N-CD	-6.27	102.72	111.50
1	A	587	SER	N-CA-CB	6.26	119.89	110.50
1	A	608	VAL	CA-C-O	6.26	133.24	120.10
1	A	196	VAL	CB-CA-C	6.25	123.28	111.40
1	A	154	GLN	CA-C-N	6.25	130.94	117.20
1	A	226	ARG	N-CA-C	6.25	127.86	111.00
1	A	452	ARG	CB-CG-CD	6.22	127.78	111.60
1	A	365	SER	C-N-CA	-6.22	106.14	121.70
1	A	51	PHE	CB-CG-CD2	-6.22	116.45	120.80
1	A	166	TYR	O-C-N	-6.22	112.75	122.70
1	A	165	TYR	CZ-CE2-CD2	-6.19	114.22	119.80
1	A	402	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	A	370	PRO	O-C-N	6.18	132.59	122.70
1	A	156	SER	N-CA-C	6.17	127.67	111.00
1	A	392	GLU	N-CA-CB	6.17	121.71	110.60
1	A	418	LYS	CB-CA-C	-6.17	98.07	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	534	PHE	CB-CG-CD2	-6.16	116.49	120.80
1	A	367	SER	N-CA-C	6.15	127.61	111.00
1	A	559	PHE	CB-CG-CD1	6.15	125.10	120.80
1	A	559	PHE	CG-CD2-CE2	6.15	127.56	120.80
1	A	193	PRO	CA-C-N	6.14	130.71	117.20
1	A	224	GLN	O-C-N	-6.14	112.88	122.70
1	A	166	TYR	CZ-CE2-CD2	6.13	125.32	119.80
1	A	545	PHE	CG-CD1-CE1	-6.12	114.06	120.80
1	A	616	SER	N-CA-C	-6.12	94.48	111.00
1	A	337	PHE	CG-CD2-CE2	6.11	127.52	120.80
1	A	180	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	A	494	THR	CA-C-N	-6.08	103.82	117.20
1	A	478	ASP	CA-CB-CG	-6.08	100.03	113.40
1	A	273	ILE	O-C-N	-6.07	112.98	122.70
1	A	433	LEU	CA-C-N	6.06	130.54	117.20
1	A	406	TYR	CG-CD2-CE2	6.06	126.15	121.30
1	A	564	PRO	N-CD-CG	-6.04	94.14	103.20
1	A	297	LEU	O-C-N	-6.04	113.04	122.70
1	A	378	LYS	N-CA-CB	-6.02	99.76	110.60
1	A	349	LEU	CA-CB-CG	-6.01	101.48	115.30
1	A	473	VAL	O-C-N	6.00	132.31	122.70
1	A	511	ALA	O-C-N	-6.00	113.09	122.70
1	A	76	LEU	CB-CA-C	6.00	121.59	110.20
1	A	270	LEU	O-C-N	-5.98	113.13	122.70
1	A	502	TYR	OH-CZ-CE2	-5.98	103.96	120.10
1	A	451	ILE	CA-CB-CG2	-5.97	98.96	110.90
1	A	153	GLY	C-N-CA	-5.97	106.78	121.70
1	A	178	THR	N-CA-CB	5.96	121.63	110.30
1	A	303	GLY	O-C-N	-5.96	113.07	123.20
1	A	372	PRO	CA-N-CD	-5.96	103.16	111.50
1	A	165	TYR	CD1-CE1-CZ	-5.95	114.44	119.80
1	A	166	TYR	CB-CG-CD1	5.94	124.57	121.00
1	A	363	ALA	C-N-CA	5.94	136.56	121.70
1	A	209	VAL	O-C-N	5.94	132.20	122.70
1	A	315	ASP	OD1-CG-OD2	-5.92	112.06	123.30
1	A	570	TYR	CG-CD2-CE2	-5.92	116.57	121.30
1	A	260	LEU	CA-C-N	5.91	130.21	117.20
1	A	214	ARG	CG-CD-NE	-5.90	99.41	111.80
1	A	439	TYR	CB-CG-CD1	5.90	124.54	121.00
1	A	536	ASP	OD1-CG-OD2	-5.89	112.10	123.30
1	A	433	LEU	O-C-N	-5.89	113.27	122.70
1	A	334	HIS	CG-ND1-CE1	5.89	116.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	LYS	CA-C-O	-5.89	107.73	120.10
1	A	267	ARG	CA-C-O	5.88	132.45	120.10
1	A	491	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	A	504	VAL	N-CA-CB	-5.85	98.63	111.50
1	A	383	THR	C-N-CA	5.84	136.29	121.70
1	A	203	GLN	CG-CD-OE1	-5.83	109.93	121.60
1	A	389	SER	CB-CA-C	5.83	121.18	110.10
1	A	556	MET	O-C-N	-5.83	113.37	122.70
1	A	320	PHE	CB-CG-CD2	-5.82	116.72	120.80
1	A	273	ILE	CA-C-O	5.81	132.31	120.10
1	A	386	HIS	N-CA-CB	5.81	121.06	110.60
1	A	588	PHE	CD1-CG-CD2	5.80	125.84	118.30
1	A	211	ILE	O-C-N	5.78	131.95	122.70
1	A	600	ALA	O-C-N	5.78	131.95	122.70
1	A	176	GLY	CA-C-O	5.76	130.97	120.60
1	A	156	SER	C-N-CA	5.76	134.39	122.30
1	A	403	PHE	CB-CG-CD1	-5.75	116.78	120.80
1	A	521	GLU	CG-CD-OE2	-5.75	106.81	118.30
1	A	212	ASN	O-C-N	-5.74	113.52	122.70
1	A	95	TYR	CB-CG-CD1	5.73	124.44	121.00
1	A	561	CYS	CB-CA-C	5.72	121.85	110.40
1	A	173	ARG	O-C-N	-5.71	113.56	122.70
1	A	380	SER	CA-C-O	5.71	132.09	120.10
1	A	375	LEU	CB-CG-CD1	-5.71	101.30	111.00
1	A	214	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	448	SER	CA-CB-OG	-5.70	95.81	111.20
1	A	149	ASP	CA-C-N	-5.70	104.67	117.20
1	A	205	PHE	O-C-N	-5.69	113.59	122.70
1	A	453	ARG	CB-CA-C	5.69	121.78	110.40
1	A	574	TYR	CD1-CE1-CZ	5.69	124.92	119.80
1	A	208	ASP	OD1-CG-OD2	-5.69	112.49	123.30
1	A	424	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	A	223	THR	OG1-CB-CG2	-5.67	96.97	110.00
1	A	176	GLY	O-C-N	-5.65	113.66	122.70
1	A	220	ASP	C-N-CA	-5.65	107.57	121.70
1	A	472	PHE	O-C-N	-5.65	113.66	122.70
1	A	472	PHE	CZ-CE2-CD2	5.65	126.88	120.10
1	A	415	PHE	N-CA-C	5.64	126.23	111.00
1	A	321	VAL	CA-CB-CG1	-5.64	102.44	110.90
1	A	294	HIS	CA-CB-CG	-5.63	104.04	113.60
1	A	606	SER	N-CA-CB	5.62	118.93	110.50
1	A	219	GLY	O-C-N	-5.61	113.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	475	ALA	O-C-N	-5.60	113.73	122.70
1	A	421	TYR	OH-CZ-CE2	5.60	135.22	120.10
1	A	263	ASP	OD1-CG-OD2	-5.59	112.68	123.30
1	A	158	GLN	CA-C-N	-5.58	101.47	117.10
1	A	167	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	373	ARG	CA-CB-CG	-5.58	101.13	113.40
1	A	406	TYR	CB-CG-CD1	5.58	124.34	121.00
1	A	220	ASP	CA-C-O	-5.57	108.41	120.10
1	A	265	THR	OG1-CB-CG2	-5.57	97.19	110.00
1	A	615	SER	N-CA-CB	-5.55	102.18	110.50
1	A	260	LEU	CA-C-O	-5.54	108.47	120.10
1	A	479	HIS	CB-CA-C	5.54	121.47	110.40
1	A	435	TYR	CZ-CE2-CD2	5.53	124.78	119.80
1	A	90	TRP	CG-CD2-CE3	-5.53	128.92	133.90
1	A	224	GLN	CG-CD-OE1	-5.53	110.54	121.60
1	A	410	ASN	CB-CA-C	-5.53	99.34	110.40
1	A	431	LEU	CB-CG-CD1	5.52	120.39	111.00
1	A	605	ALA	C-N-CA	5.52	135.50	121.70
1	A	380	SER	N-CA-C	-5.51	96.12	111.00
1	A	413	LYS	CA-C-N	-5.50	105.09	117.20
1	A	369	LEU	N-CA-CB	-5.50	99.40	110.40
1	A	333	GLU	CB-CA-C	5.50	121.40	110.40
1	A	377	TRP	CB-CG-CD1	-5.50	119.86	127.00
1	A	187	SER	CA-C-O	-5.49	108.57	120.10
1	A	259	VAL	O-C-N	-5.49	113.92	122.70
1	A	413	LYS	O-C-N	5.48	131.47	122.70
1	A	226	ARG	CD-NE-CZ	-5.48	115.92	123.60
1	A	350	LEU	O-C-N	5.48	131.47	122.70
1	A	479	HIS	O-C-N	5.48	131.47	122.70
1	A	576	PRO	N-CA-CB	5.48	109.87	103.30
1	A	408	PHE	CB-CG-CD1	-5.48	116.97	120.80
1	A	380	SER	O-C-N	-5.47	110.70	121.10
1	A	253	TRP	NE1-CE2-CZ2	5.46	136.41	130.40
1	A	419	GLN	CB-CG-CD	5.46	125.80	111.60
1	A	562	TYR	CZ-CE2-CD2	5.46	124.72	119.80
1	A	431	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	277	ILE	CA-CB-CG1	-5.45	100.64	111.00
1	A	414	THR	OG1-CB-CG2	-5.45	97.46	110.00
1	A	429	VAL	CA-C-N	5.45	129.19	117.20
1	A	418	LYS	O-C-N	-5.45	113.99	122.70
1	A	253	TRP	CB-CA-C	5.44	121.28	110.40
1	A	268	ASP	CB-CG-OD2	-5.42	113.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	522	LEU	O-C-N	-5.42	114.03	122.70
1	A	606	SER	O-C-N	-5.42	114.03	122.70
1	A	484	PRO	O-C-N	5.41	131.36	122.70
1	A	536	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	454	PHE	CG-CD1-CE1	5.40	126.75	120.80
1	A	378	LYS	CD-CE-NZ	5.39	124.11	111.70
1	A	419	GLN	N-CA-CB	5.39	120.30	110.60
1	A	513	ASP	N-CA-CB	5.39	120.30	110.60
1	A	109	ALA	N-CA-CB	-5.38	102.57	110.10
1	A	363	ALA	O-C-N	5.38	131.31	122.70
1	A	180	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	615	SER	CA-CB-OG	5.36	125.66	111.20
1	A	310	ALA	CA-C-N	5.35	128.97	117.20
1	A	196	VAL	O-C-N	-5.35	114.14	122.70
1	A	344	GLN	CG-CD-NE2	-5.35	103.87	116.70
1	A	345	CYS	O-C-N	-5.35	114.14	122.70
1	A	157	GLY	O-C-N	5.34	131.24	122.70
1	A	292	ASP	N-CA-C	-5.31	96.66	111.00
1	A	407	LYS	C-N-CA	5.31	134.97	121.70
1	A	532	GLU	O-C-N	5.30	131.18	122.70
1	A	252	GLU	O-C-N	-5.29	114.23	122.70
1	A	491	LEU	CA-C-O	-5.29	108.99	120.10
1	A	350	LEU	CB-CA-C	5.29	120.24	110.20
1	A	528	LYS	N-CA-C	5.29	125.27	111.00
1	A	95	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	313	TRP	CE3-CZ3-CH2	-5.27	115.41	121.20
1	A	375	LEU	O-C-N	-5.27	114.27	122.70
1	A	419	GLN	N-CA-C	5.26	125.21	111.00
1	A	474	GLN	CA-CB-CG	5.26	124.98	113.40
1	A	391	ALA	CA-C-O	5.26	131.15	120.10
1	A	576	PRO	O-C-N	5.26	131.12	122.70
1	A	228	ILE	CA-CB-CG1	5.26	120.99	111.00
1	A	257	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	A	525	ASP	C-N-CA	-5.26	108.56	121.70
1	A	463	ARG	O-C-N	5.25	131.09	122.70
1	A	491	LEU	CA-CB-CG	-5.25	103.24	115.30
1	A	439	TYR	CD1-CG-CD2	-5.23	112.15	117.90
1	A	253	TRP	CG-CD2-CE3	-5.21	129.21	133.90
1	A	205	PHE	CD1-CE1-CZ	5.21	126.35	120.10
1	A	346	THR	O-C-N	5.21	131.03	122.70
1	A	609	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	261	LEU	CA-C-O	-5.19	109.19	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	GLY	O-C-N	-5.18	114.41	122.70
1	A	185	GLN	N-CA-C	5.17	124.95	111.00
1	A	487	GLU	C-N-CA	-5.14	108.84	121.70
1	A	502	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	541	MET	CG-SD-CE	-5.14	91.98	100.20
1	A	396	ARG	CB-CG-CD	-5.13	98.25	111.60
1	A	577	GLN	CA-C-O	5.13	130.88	120.10
1	A	384	GLN	N-CA-CB	5.13	119.83	110.60
1	A	441	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	192	GLU	CA-C-N	5.12	131.45	117.10
1	A	351	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	A	438	LEU	CA-CB-CG	-5.11	103.55	115.30
1	A	370	PRO	CA-C-O	-5.11	107.94	120.20
1	A	580	ALA	N-CA-CB	5.10	117.24	110.10
1	A	439	TYR	CA-CB-CG	-5.10	103.72	113.40
1	A	442	LEU	O-C-N	-5.10	114.55	122.70
1	A	169	PHE	CZ-CE2-CD2	5.10	126.22	120.10
1	A	248	ASP	CA-C-O	5.07	130.75	120.10
1	A	253	TRP	CH2-CZ2-CE2	5.07	122.47	117.40
1	A	338	ASP	CA-C-O	5.07	130.74	120.10
1	A	502	TYR	CE1-CZ-OH	5.07	133.78	120.10
1	A	184	ALA	CA-C-N	-5.06	106.06	117.20
1	A	472	PHE	CD1-CE1-CZ	5.06	126.17	120.10
1	A	421	TYR	CD1-CG-CD2	5.06	123.47	117.90
1	A	413	LYS	C-N-CA	-5.06	109.06	121.70
1	A	577	GLN	O-C-N	-5.05	111.50	121.10
1	A	220	ASP	CB-CA-C	-5.05	100.30	110.40
1	A	460	ASP	O-C-N	5.05	130.78	122.70
1	A	230	LYS	CD-CE-NZ	-5.05	100.09	111.70
1	A	382	GLU	CA-CB-CG	5.04	124.48	113.40
1	A	188	SER	N-CA-C	5.04	124.60	111.00
1	A	614	CYS	CA-C-O	-5.03	109.53	120.10
1	A	341	VAL	CA-CB-CG1	-5.03	103.36	110.90
1	A	474	GLN	CA-C-O	-5.03	109.53	120.10
1	A	593	GLU	CG-CD-OE2	5.03	128.36	118.30
1	A	209	VAL	CA-C-O	-5.03	109.55	120.10
1	A	493	GLN	CA-C-O	-5.01	109.58	120.10
1	A	158	GLN	O-C-N	5.01	130.61	121.10

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Sidechain
1	A	167	ARG	Sidechain
1	A	185	GLN	Peptide
1	A	189	ILE	Mainchain
1	A	190	MET	Mainchain
1	A	196	VAL	Mainchain
1	A	205	PHE	Sidechain
1	A	208	ASP	Sidechain
1	A	213	PHE	Sidechain
1	A	220	ASP	Sidechain
1	A	224	GLN	Mainchain
1	A	239	LEU	Mainchain
1	A	249	GLY	Mainchain
1	A	257	ARG	Sidechain
1	A	265	THR	Mainchain
1	A	275	ARG	Mainchain
1	A	286	GLY	Mainchain
1	A	288	GLY	Peptide
1	A	289	GLU	Mainchain,Peptide
1	A	290	LEU	Mainchain
1	A	294	HIS	Sidechain
1	A	341	VAL	Mainchain
1	A	344	GLN	Sidechain
1	A	348	HIS	Sidechain
1	A	352	HIS	Sidechain
1	A	368	GLU	Peptide
1	A	373	ARG	Mainchain
1	A	376	ARG	Sidechain
1	A	378	LYS	Mainchain
1	A	391	ALA	Mainchain
1	A	402	ASP	Mainchain
1	A	410	ASN	Mainchain
1	A	418	LYS	Mainchain
1	A	420	LYS	Mainchain
1	A	421	TYR	Sidechain
1	A	435	TYR	Sidechain
1	A	437	ARG	Mainchain
1	A	441	ARG	Sidechain
1	A	452	ARG	Sidechain
1	A	453	ARG	Sidechain
1	A	475	ALA	Mainchain
1	A	477	THR	Mainchain
1	A	482	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	487	GLU	Mainchain,Sidechain
1	A	555	THR	Mainchain
1	A	560	CYS	Mainchain
1	A	561	CYS	Mainchain
1	A	579	GLU	Sidechain
1	A	602	ALA	Mainchain
1	A	611	ARG	Sidechain
1	A	615	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4711	0	4679	266	25
2	A	408	0	0	16	9
All	All	5119	0	4679	266	26

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 28.

All (266) 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:178:THR:CB	1:A:178:THR:CA	1.76	1.61
1:A:351:LYS:CE	1:A:351:LYS:CD	1.75	1.59
1:A:230:LYS:CE	1:A:230:LYS:CD	1.79	1.59
1:A:407:LYS:CD	1:A:407:LYS:CG	1.74	1.59
1:A:214:ARG:CZ	1:A:365:SER:HB3	1.10	1.56
1:A:350:LEU:CG	1:A:350:LEU:CD1	1.74	1.55
1:A:351:LYS:CD	1:A:351:LYS:CG	1.85	1.55
1:A:237:GLU:N	1:A:237:GLU:CA	1.67	1.54
1:A:453:ARG:NE	1:A:453:ARG:CD	1.70	1.53
1:A:418:LYS:CE	1:A:418:LYS:CD	1.85	1.53
1:A:220:ASP:CG	1:A:220:ASP:CB	1.75	1.52
1:A:396:ARG:CD	1:A:396:ARG:CG	1.80	1.52
1:A:418:LYS:CE	1:A:418:LYS:NZ	1.72	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:CB	1:A:453:ARG:CA	1.84	1.51
1:A:255:LYS:CE	1:A:255:LYS:NZ	1.75	1.50
1:A:179:GLN:CD	1:A:179:GLN:CG	1.75	1.50
1:A:373:ARG:CD	1:A:373:ARG:CG	1.89	1.50
1:A:475:ALA:N	1:A:475:ALA:CA	1.68	1.49
1:A:613:LEU:CD1	1:A:613:LEU:CG	1.91	1.49
1:A:530:PRO:CG	1:A:530:PRO:CB	1.74	1.48
1:A:255:LYS:CE	1:A:255:LYS:CD	1.87	1.47
1:A:262:LYS:CE	1:A:262:LYS:NZ	1.77	1.47
1:A:378:LYS:NZ	1:A:378:LYS:CE	1.81	1.43
1:A:366:VAL:HG12	1:A:367:SER:N	1.52	1.22
1:A:365:SER:O	1:A:366:VAL:CG2	1.87	1.22
1:A:154:GLN:O	1:A:155:LEU:CD1	1.91	1.17
1:A:214:ARG:NH2	1:A:365:SER:OG	1.75	1.15
1:A:362:ARG:O	1:A:364:ASP:N	1.78	1.15
1:A:361:VAL:HG12	1:A:362:ARG:H	1.09	1.14
1:A:111:ILE:HG13	1:A:299:LEU:HD12	1.31	1.12
1:A:154:GLN:O	1:A:155:LEU:HD12	1.42	1.11
1:A:391:ALA:O	1:A:395:GLN:HG3	1.47	1.11
1:A:477:THR:HG21	2:A:993:HOH:O	1.50	1.11
1:A:366:VAL:CG1	1:A:367:SER:H	1.65	1.07
1:A:365:SER:O	1:A:366:VAL:HG23	1.54	1.06
1:A:359:LYS:O	1:A:359:LYS:HG2	1.54	1.06
1:A:477:THR:O	1:A:477:THR:HG22	1.52	1.04
1:A:362:ARG:C	1:A:364:ASP:H	1.57	1.04
1:A:480:LYS:H	1:A:480:LYS:HD3	0.89	1.03
1:A:237:GLU:N	1:A:237:GLU:C	2.11	1.02
1:A:237:GLU:H	1:A:238:ARG:N	1.57	1.00
1:A:150:TRP:HA	1:A:154:GLN:HA	1.40	1.00
1:A:480:LYS:HD3	1:A:480:LYS:N	1.74	1.00
1:A:230:LYS:CE	1:A:230:LYS:CG	2.40	0.99
1:A:214:ARG:NH2	1:A:365:SER:CB	0.84	0.99
1:A:178:THR:CA	1:A:178:THR:CG2	2.40	0.98
1:A:237:GLU:N	1:A:238:ARG:N	2.09	0.98
1:A:153:GLY:O	1:A:154:GLN:HB3	1.63	0.96
1:A:97:ASN:O	1:A:99:ARG:HD3	1.65	0.95
1:A:480:LYS:H	1:A:480:LYS:CD	1.79	0.95
1:A:56:ALA:HB1	1:A:60:ARG:HH12	1.30	0.95
1:A:214:ARG:NH2	1:A:365:SER:CA	2.29	0.95
1:A:214:ARG:NE	1:A:365:SER:OG	2.01	0.93
1:A:365:SER:O	1:A:366:VAL:HG22	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:HG12	1:A:362:ARG:N	1.83	0.93
1:A:237:GLU:H	1:A:238:ARG:H	1.13	0.93
1:A:214:ARG:CZ	1:A:365:SER:CB	1.90	0.92
1:A:150:TRP:CA	1:A:154:GLN:HA	1.99	0.92
1:A:342:LEU:C	1:A:342:LEU:HD23	1.91	0.91
1:A:366:VAL:HG12	1:A:367:SER:H	1.07	0.91
1:A:97:ASN:O	1:A:99:ARG:CD	2.20	0.90
1:A:150:TRP:CB	1:A:154:GLN:HA	2.02	0.90
1:A:396:ARG:CD	1:A:396:ARG:CB	2.53	0.86
1:A:453:ARG:CD	1:A:453:ARG:CZ	2.53	0.86
1:A:237:GLU:N	1:A:238:ARG:H	1.73	0.85
1:A:350:LEU:CD1	1:A:350:LEU:CB	2.55	0.85
1:A:361:VAL:CG1	1:A:362:ARG:H	1.89	0.84
1:A:56:ALA:HB1	1:A:60:ARG:NH1	1.93	0.83
1:A:214:ARG:NE	1:A:365:SER:CB	2.41	0.83
1:A:480:LYS:O	1:A:481:ALA:C	2.11	0.83
1:A:356:SER:O	1:A:358:LYS:N	2.12	0.83
1:A:154:GLN:O	1:A:155:LEU:HD13	1.76	0.82
1:A:365:SER:C	1:A:366:VAL:HG23	1.98	0.82
1:A:359:LYS:O	1:A:359:LYS:CG	2.26	0.82
1:A:150:TRP:HA	1:A:154:GLN:CA	2.08	0.82
1:A:362:ARG:O	1:A:364:ASP:HB2	1.80	0.82
1:A:407:LYS:CG	1:A:407:LYS:CE	2.55	0.81
1:A:28:VAL:CG1	1:A:75:LEU:HD13	2.11	0.80
1:A:351:LYS:CD	1:A:351:LYS:CB	2.59	0.80
1:A:98:ASN:C	1:A:99:ARG:HD2	2.02	0.79
1:A:152:LYS:O	1:A:153:GLY:O	2.00	0.79
1:A:184:ALA:O	1:A:185:GLN:HB2	1.79	0.79
1:A:236:ASP:C	1:A:237:GLU:CA	2.51	0.78
1:A:350:LEU:CD1	1:A:350:LEU:CD2	2.59	0.78
1:A:366:VAL:HG12	1:A:367:SER:CA	2.14	0.78
1:A:150:TRP:N	1:A:152:LYS:O	2.17	0.77
1:A:477:THR:O	1:A:477:THR:CG2	2.27	0.77
1:A:555:THR:HG23	2:A:864:HOH:O	1.84	0.77
1:A:148:THR:O	1:A:151:ALA:HB3	1.85	0.77
1:A:52:ARG:HG2	2:A:1008:HOH:O	1.86	0.76
1:A:289:GLU:CD	1:A:290:LEU:HD23	2.07	0.75
1:A:289:GLU:O	1:A:290:LEU:HG	1.85	0.75
1:A:557:GLU:HG2	2:A:754:HOH:O	1.86	0.74
1:A:172:TYR:O	1:A:183:VAL:HG12	1.86	0.74
1:A:289:GLU:OE2	1:A:290:LEU:HD23	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:HA	1:A:153:GLY:O	1.88	0.74
1:A:186:LYS:HG3	1:A:193:PRO:HG3	1.69	0.74
1:A:179:GLN:CG	1:A:179:GLN:NE2	2.47	0.73
1:A:143:SER:OG	1:A:145:SER:HB2	1.88	0.73
1:A:356:SER:C	1:A:358:LYS:N	2.41	0.73
1:A:474:GLN:C	1:A:475:ALA:CA	2.56	0.73
1:A:111:ILE:CG1	1:A:299:LEU:HD12	2.16	0.73
1:A:148:THR:O	1:A:151:ALA:CB	2.37	0.73
1:A:214:ARG:NH2	1:A:365:SER:HB2	1.06	0.72
1:A:172:TYR:O	1:A:183:VAL:CG1	2.37	0.72
1:A:178:THR:CA	1:A:178:THR:OG1	2.38	0.72
1:A:111:ILE:HG13	1:A:299:LEU:CD1	2.16	0.72
1:A:366:VAL:CG1	1:A:367:SER:N	2.23	0.72
1:A:28:VAL:HG11	1:A:75:LEU:HD13	1.71	0.72
1:A:351:LYS:CD	1:A:351:LYS:NZ	2.52	0.72
1:A:356:SER:OG	1:A:357:ASN:N	2.21	0.72
1:A:351:LYS:HG3	1:A:556:MET:CE	2.20	0.71
1:A:613:LEU:CD1	1:A:613:LEU:CB	2.64	0.71
1:A:396:ARG:CG	1:A:396:ARG:NE	2.53	0.71
1:A:178:THR:CB	1:A:178:THR:C	2.58	0.71
1:A:111:ILE:HD12	1:A:299:LEU:HD13	1.73	0.70
1:A:342:LEU:C	1:A:342:LEU:CD2	2.59	0.70
1:A:490:GLN:HG3	1:A:491:LEU:N	2.07	0.70
1:A:230:LYS:CD	1:A:230:LYS:NZ	2.55	0.69
1:A:110:VAL:C	1:A:111:ILE:HD12	2.11	0.69
1:A:352:HIS:HD2	2:A:937:HOH:O	1.75	0.69
1:A:407:LYS:CD	1:A:407:LYS:CB	2.70	0.69
1:A:111:ILE:CD1	1:A:299:LEU:HD13	2.23	0.68
1:A:214:ARG:NH2	1:A:365:SER:HB3	0.69	0.68
1:A:214:ARG:NH2	1:A:365:SER:HG	1.88	0.67
1:A:151:ALA:O	1:A:152:LYS:HG2	1.93	0.67
1:A:152:LYS:O	1:A:153:GLY:C	2.34	0.66
1:A:294:HIS:ND1	1:A:297:LEU:HD12	2.11	0.66
1:A:365:SER:C	1:A:366:VAL:CG2	2.58	0.66
1:A:362:ARG:O	1:A:364:ASP:CB	2.44	0.65
1:A:28:VAL:HG13	1:A:75:LEU:HD13	1.78	0.65
1:A:179:GLN:CD	1:A:179:GLN:CB	2.65	0.65
1:A:156:SER:OG	1:A:453:ARG:NH2	2.30	0.65
1:A:154:GLN:C	1:A:155:LEU:HD13	2.18	0.64
1:A:474:GLN:O	1:A:478:ASP:HB3	1.96	0.64
1:A:110:VAL:HG21	1:A:342:LEU:HD21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HD2	1:A:99:ARG:N	2.11	0.64
1:A:362:ARG:O	1:A:364:ASP:CA	2.45	0.64
1:A:342:LEU:HD23	1:A:342:LEU:O	1.99	0.63
1:A:366:VAL:O	1:A:367:SER:HB3	1.98	0.63
1:A:155:LEU:HD22	1:A:160:LEU:HD11	1.81	0.62
1:A:351:LYS:HG3	1:A:556:MET:HE1	1.81	0.62
1:A:220:ASP:CB	1:A:220:ASP:OD1	2.46	0.62
1:A:20:GLU:N	2:A:934:HOH:O	2.33	0.62
1:A:184:ALA:O	1:A:185:GLN:CB	2.48	0.62
1:A:97:ASN:O	1:A:99:ARG:HD2	2.00	0.61
1:A:28:VAL:HG13	1:A:75:LEU:CD1	2.31	0.61
1:A:51:PHE:O	1:A:54:SER:N	2.34	0.61
1:A:111:ILE:HD12	1:A:111:ILE:N	2.17	0.60
1:A:103:PRO:HG3	1:A:314:TYR:CZ	2.37	0.59
1:A:480:LYS:O	1:A:481:ALA:O	2.19	0.59
1:A:25:LYS:O	1:A:27:PRO:HD3	2.03	0.58
1:A:28:VAL:CG1	1:A:75:LEU:CD1	2.81	0.58
1:A:214:ARG:NH1	1:A:365:SER:HB3	1.97	0.58
1:A:152:LYS:C	1:A:153:GLY:O	2.38	0.58
1:A:362:ARG:C	1:A:364:ASP:N	2.38	0.58
1:A:153:GLY:O	1:A:154:GLN:CB	2.37	0.57
1:A:294:HIS:CG	2:A:925:HOH:O	2.58	0.57
1:A:111:ILE:CD1	1:A:299:LEU:CD1	2.83	0.57
1:A:149:ASP:O	1:A:150:TRP:CD1	2.58	0.56
1:A:158:GLN:CB	1:A:159:PRO:HD2	2.34	0.56
1:A:145:SER:O	1:A:147:PRO:HD3	2.06	0.56
1:A:56:ALA:O	1:A:60:ARG:CG	2.54	0.56
1:A:400:ASN:HD21	1:A:590:SER:H	1.54	0.56
1:A:192:GLU:O	1:A:194:GLU:N	2.39	0.55
1:A:56:ALA:O	1:A:60:ARG:HG2	2.06	0.55
1:A:361:VAL:CG1	1:A:362:ARG:N	2.55	0.55
1:A:111:ILE:CD1	1:A:111:ILE:N	2.70	0.54
1:A:224:GLN:HE22	1:A:227:LYS:NZ	2.04	0.54
1:A:289:GLU:C	1:A:290:LEU:HG	2.22	0.54
1:A:214:ARG:CZ	1:A:365:SER:OG	2.29	0.54
1:A:56:ALA:CB	1:A:60:ARG:HH12	2.14	0.54
1:A:356:SER:O	1:A:359:LYS:N	2.40	0.54
1:A:475:ALA:N	1:A:475:ALA:CB	2.69	0.54
1:A:150:TRP:HB2	1:A:154:GLN:HA	1.90	0.54
1:A:234:ASN:ND2	2:A:909:HOH:O	2.37	0.54
1:A:418:LYS:CE	1:A:418:LYS:CG	2.83	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LYS:CG	1:A:407:LYS:NZ	2.71	0.53
1:A:479:HIS:HA	1:A:480:LYS:HD3	1.90	0.53
1:A:108:PRO:HD2	1:A:332:CYS:O	2.09	0.52
1:A:150:TRP:CA	1:A:152:LYS:O	2.57	0.52
1:A:224:GLN:HE22	1:A:227:LYS:HZ2	1.58	0.52
1:A:84:ASN:OD1	1:A:86:VAL:HG12	2.11	0.51
1:A:299:LEU:HD11	1:A:329:GLY:HA3	1.93	0.51
1:A:238:ARG:NH1	2:A:1037:HOH:O	2.39	0.51
1:A:482:ALA:O	1:A:483:MET:CB	2.58	0.50
1:A:158:GLN:HB2	1:A:159:PRO:HD2	1.94	0.50
1:A:474:GLN:O	1:A:478:ASP:CB	2.59	0.50
1:A:407:LYS:NZ	1:A:407:LYS:HG2	2.27	0.49
1:A:136:SER:CB	1:A:352:HIS:HE1	2.25	0.49
1:A:172:TYR:O	1:A:183:VAL:HG13	2.11	0.49
1:A:351:LYS:HG3	1:A:556:MET:HE3	1.93	0.49
1:A:138:LYS:HE2	1:A:142:ASP:OD2	2.11	0.49
1:A:178:THR:CB	1:A:178:THR:HA	2.19	0.49
1:A:79:GLN:O	1:A:79:GLN:HG2	2.13	0.49
1:A:150:TRP:HA	1:A:154:GLN:CB	2.42	0.49
1:A:292:ASP:OD2	1:A:407:LYS:CE	2.61	0.48
1:A:178:THR:CG2	1:A:178:THR:N	2.76	0.48
1:A:172:TYR:HB3	1:A:183:VAL:HG13	1.96	0.48
1:A:202:ASN:H	1:A:311:ASN:ND2	2.12	0.48
1:A:111:ILE:CG1	1:A:299:LEU:CD1	2.85	0.48
1:A:224:GLN:HA	1:A:224:GLN:NE2	2.28	0.48
1:A:236:ASP:O	1:A:237:GLU:CA	2.62	0.48
1:A:152:LYS:HB2	2:A:785:HOH:O	2.14	0.48
1:A:373:ARG:CG	1:A:373:ARG:NE	2.73	0.47
1:A:289:GLU:HB2	1:A:290:LEU:HA	1.95	0.47
1:A:220:ASP:CB	1:A:220:ASP:OD2	2.46	0.47
1:A:69:GLU:O	1:A:73:GLU:OE1	2.32	0.47
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.67	0.47
1:A:220:ASP:CG	1:A:220:ASP:CA	2.75	0.47
1:A:477:THR:O	1:A:478:ASP:CB	2.60	0.47
1:A:616:SER:C	2:A:928:HOH:O	2.54	0.47
1:A:356:SER:O	1:A:357:ASN:C	2.52	0.46
1:A:487:GLU:O	1:A:490:GLN:CG	2.64	0.46
1:A:490:GLN:HG3	1:A:491:LEU:H	1.79	0.46
1:A:479:HIS:CA	1:A:480:LYS:HD3	2.46	0.45
1:A:230:LYS:CE	1:A:230:LYS:HG2	2.42	0.45
1:A:238:ARG:NH1	2:A:1019:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ILE:HD11	2:A:894:HOH:O	2.15	0.45
1:A:480:LYS:HA	1:A:488:LYS:NZ	2.31	0.45
1:A:136:SER:CB	1:A:352:HIS:CE1	2.99	0.45
1:A:158:GLN:HA	1:A:159:PRO:HD3	1.72	0.45
1:A:453:ARG:CB	1:A:453:ARG:N	2.69	0.45
1:A:103:PRO:O	1:A:105:ASN:N	2.45	0.45
1:A:63:ALA:HB1	1:A:64:PRO:CD	2.47	0.44
1:A:111:ILE:HG12	1:A:296:ALA:HA	1.99	0.44
1:A:24:PRO:HB2	1:A:454:PHE:HD2	1.82	0.44
1:A:289:GLU:OE2	1:A:290:LEU:CD2	2.61	0.44
1:A:400:ASN:HD21	1:A:590:SER:HB3	1.83	0.44
1:A:449:ALA:HB2	1:A:462:ILE:HG13	1.99	0.44
1:A:363:ALA:C	1:A:365:SER:N	2.71	0.44
1:A:229:VAL:O	1:A:233:SER:HB3	2.18	0.43
1:A:289:GLU:CG	1:A:290:LEU:HD23	2.48	0.43
1:A:400:ASN:HD21	1:A:590:SER:CB	2.31	0.43
1:A:56:ALA:O	1:A:60:ARG:HG3	2.18	0.43
1:A:578:PRO:HD2	2:A:1006:HOH:O	2.18	0.43
1:A:487:GLU:O	1:A:490:GLN:HG3	2.19	0.43
1:A:363:ALA:O	1:A:365:SER:N	2.52	0.43
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.84	0.43
1:A:186:LYS:HD2	1:A:186:LYS:O	2.19	0.43
1:A:86:VAL:HG22	1:A:86:VAL:O	2.18	0.42
1:A:117:PHE:O	1:A:118:GLN:C	2.57	0.42
1:A:172:TYR:HB3	1:A:183:VAL:CG1	2.49	0.42
1:A:192:GLU:O	1:A:193:PRO:C	2.57	0.42
1:A:137:TYR:HD1	1:A:348:HIS:CD2	2.38	0.42
1:A:151:ALA:C	1:A:152:LYS:HG2	2.39	0.42
1:A:186:LYS:NZ	1:A:190:MET:SD	2.92	0.42
1:A:368:GLU:O	1:A:369:LEU:O	2.38	0.42
1:A:405:VAL:HG12	1:A:407:LYS:HD2	2.01	0.42
1:A:453:ARG:CD	1:A:453:ARG:NH1	2.82	0.42
1:A:453:ARG:NH1	1:A:453:ARG:HD3	2.34	0.42
1:A:224:GLN:NE2	1:A:227:LYS:NZ	2.68	0.42
1:A:400:ASN:ND2	1:A:590:SER:H	2.17	0.42
1:A:441:ARG:NH2	2:A:890:HOH:O	2.37	0.41
1:A:20:GLU:HG3	1:A:163:LYS:NZ	2.35	0.41
1:A:294:HIS:CE1	1:A:297:LEU:HD12	2.56	0.41
1:A:186:LYS:HG3	1:A:193:PRO:CG	2.46	0.41
1:A:224:GLN:HA	1:A:224:GLN:HE21	1.86	0.41
1:A:521:GLU:O	1:A:524:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLN:O	1:A:154:GLN:HG3	2.21	0.40
1:A:574:TYR:HA	1:A:582:THR:O	2.21	0.40
1:A:186:LYS:O	1:A:193:PRO:HG2	2.22	0.40
1:A:149:ASP:O	1:A:150:TRP:HD1	2.03	0.40
1:A:613:LEU:CD1	1:A:613:LEU:CD2	2.82	0.40
1:A:247:SER:HB3	2:A:1025:HOH:O	2.20	0.40
1:A:351:LYS:CE	1:A:351:LYS:CG	2.95	0.40

All (26) 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)
2:A:773:HOH:O	2:A:898:HOH:O[2_544]	0.31	1.89
1:A:392:GLU:OE2	2:A:797:HOH:O[3_555]	0.70	1.50
1:A:192:GLU:C	2:A:687:HOH:O[2_544]	1.00	1.20
1:A:193:PRO:N	2:A:687:HOH:O[2_544]	1.33	0.87
1:A:392:GLU:CD	2:A:797:HOH:O[3_555]	1.47	0.73
1:A:192:GLU:OE2	1:A:354:MET:O[2_544]	1.49	0.71
1:A:214:ARG:CD	1:A:557:GLU:OE1[2_544]	1.55	0.65
1:A:192:GLU:CD	1:A:354:MET:O[2_544]	1.64	0.56
1:A:192:GLU:OE2	1:A:354:MET:CA[2_544]	1.66	0.54
1:A:192:GLU:OE2	1:A:354:MET:C[2_544]	1.70	0.50
1:A:192:GLU:CD	1:A:354:MET:C[2_544]	1.75	0.45
1:A:193:PRO:CD	2:A:687:HOH:O[2_544]	1.79	0.41
1:A:192:GLU:CA	2:A:687:HOH:O[2_544]	1.80	0.40
1:A:192:GLU:OE1	1:A:354:MET:C[2_544]	1.84	0.36
1:A:214:ARG:CG	1:A:557:GLU:OE1[2_544]	1.86	0.34
1:A:214:ARG:CD	1:A:557:GLU:OE2[2_544]	1.86	0.34
1:A:214:ARG:CD	1:A:557:GLU:CD[2_544]	1.87	0.33
1:A:592:LYS:NZ	1:A:615:SER:O[3_556]	1.87	0.33
1:A:214:ARG:CB	1:A:557:GLU:OE1[2_544]	1.89	0.31
1:A:192:GLU:OE2	1:A:354:MET:CB[2_544]	1.92	0.28
1:A:192:GLU:O	2:A:687:HOH:O[2_544]	1.92	0.28
1:A:275:ARG:NH2	1:A:357:ASN:ND2[2_544]	1.97	0.23
1:A:192:GLU:OE1	1:A:354:MET:CA[2_544]	1.98	0.22
1:A:192:GLU:CD	1:A:354:MET:CA[2_544]	2.05	0.15
1:A:592:LYS:NZ	1:A:615:SER:C[3_556]	2.14	0.06
1:A:392:GLU:CG	2:A:797:HOH:O[3_555]	2.15	0.05

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	595/639 (93%)	534 (90%)	35 (6%)	26 (4%)	2 0

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLY
1	A	156	SER
1	A	190	MET
1	A	192	GLU
1	A	237	GLU
1	A	287	THR
1	A	357	ASN
1	A	361	VAL
1	A	364	ASP
1	A	366	VAL
1	A	150	TRP
1	A	154	GLN
1	A	185	GLN
1	A	359	LYS
1	A	363	ALA
1	A	187	SER
1	A	368	GLU
1	A	157	GLY
1	A	290	LEU
1	A	525	ASP
1	A	104	VAL
1	A	193	PRO
1	A	356	SER
1	A	483	MET
1	A	191	PRO
1	A	477	THR

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	524/559 (94%)	485 (93%)	39 (7%)	13 1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	PRO
1	A	27	PRO
1	A	60	ARG
1	A	73	GLU
1	A	75	LEU
1	A	77	GLU
1	A	114	ARG
1	A	119	ASP
1	A	136	SER
1	A	145	SER
1	A	146	LEU
1	A	150	TRP
1	A	155	LEU
1	A	156	SER
1	A	183	VAL
1	A	185	GLN
1	A	186	LYS
1	A	192	GLU
1	A	233	SER
1	A	237	GLU
1	A	287	THR
1	A	289	GLU
1	A	290	LEU
1	A	294	HIS
1	A	331	VAL
1	A	342	LEU
1	A	358	LYS
1	A	359	LYS
1	A	362	ARG
1	A	365	SER

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Mol	Chain	Res	Type
1	A	407	LYS
1	A	453	ARG
1	A	480	LYS
1	A	490	GLN
1	A	528	LYS
1	A	529	GLU
1	A	613	LEU
1	A	615	SER
1	A	616	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	311	ASN
1	A	348	HIS
1	A	352	HIS
1	A	400	ASN
1	A	479	HIS
1	A	577	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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	576:PRO	C	577:GLN	N	1.18
1	A	289:GLU	C	290:LEU	N	0.99
1	A	189:ILE	C	190:MET	N	0.95

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	597/639 (93%)	0.79	64 (10%) 6 6	12, 18, 54, 91	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	PRO	21.9
1	A	360	LEU	19.8
1	A	151	ALA	16.3
1	A	153	GLY	15.3
1	A	361	VAL	13.4
1	A	188	SER	11.5
1	A	363	ALA	10.9
1	A	187	SER	10.6
1	A	362	ARG	10.2
1	A	189	ILE	9.8
1	A	358	LYS	9.7
1	A	366	VAL	9.6
1	A	481	ALA	9.3
1	A	357	ASN	8.9
1	A	478	ASP	8.8
1	A	365	SER	8.4
1	A	367	SER	8.2
1	A	154	GLN	8.1
1	A	193	PRO	7.4
1	A	290	LEU	7.3
1	A	186	LYS	7.0
1	A	364	ASP	7.0
1	A	526	LEU	7.0
1	A	479	HIS	6.7
1	A	192	GLU	6.7
1	A	152	LYS	6.6
1	A	150	TRP	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	356	SER	6.6
1	A	368	GLU	6.1
1	A	289	GLU	6.1
1	A	287	THR	5.9
1	A	529	GLU	5.8
1	A	190	MET	5.7
1	A	359	LYS	5.7
1	A	528	LYS	5.5
1	A	156	SER	5.4
1	A	288	GLY	5.3
1	A	155	LEU	5.2
1	A	527	CYS	5.2
1	A	236	ASP	5.2
1	A	157	GLY	3.9
1	A	234	ASN	3.9
1	A	237	GLU	3.9
1	A	515	HIS	3.6
1	A	185	GLN	3.6
1	A	480	LYS	3.5
1	A	21	LEU	3.3
1	A	143	SER	3.0
1	A	482	ALA	2.8
1	A	20	GLU	2.7
1	A	64	PRO	2.5
1	A	525	ASP	2.5
1	A	557	GLU	2.5
1	A	158	GLN	2.5
1	A	305	CYS	2.4
1	A	477	THR	2.4
1	A	395	GLN	2.2
1	A	430	ALA	2.2
1	A	369	LEU	2.2
1	A	592	LYS	2.1
1	A	235	GLU	2.1
1	A	483	MET	2.1
1	A	144	HIS	2.0
1	A	83	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.