



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:14 PM UTC

PDB ID : 1E8F / pdb_00001e8f
Title : STRUCTURE OF THE H61T MUTANT OF THE FLAVOENZYME
VANILLYL-ALCOHOL OXIDASE IN THE APO FORM
Authors : Mattevi, A.; Fraaije, M.W.
Deposited on : 2000-09-20
Resolution : 2.90 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

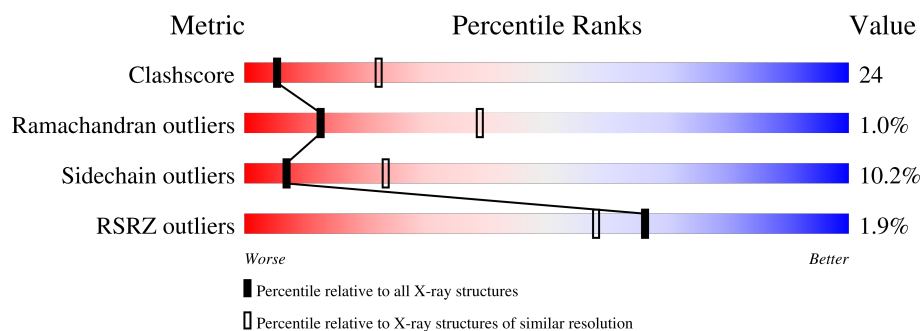
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	560	2% 37% 41% 17% • •
1	B	560	2% 41% 37% 17% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8642 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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	136	0	0
			4311	2768	737	782	24			
1	B	545	Total	C	N	O	S	136	0	0
			4311	2768	737	782	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	HIS	engineered mutation	UNP P56216
B	61	THR	HIS	engineered mutation	UNP P56216

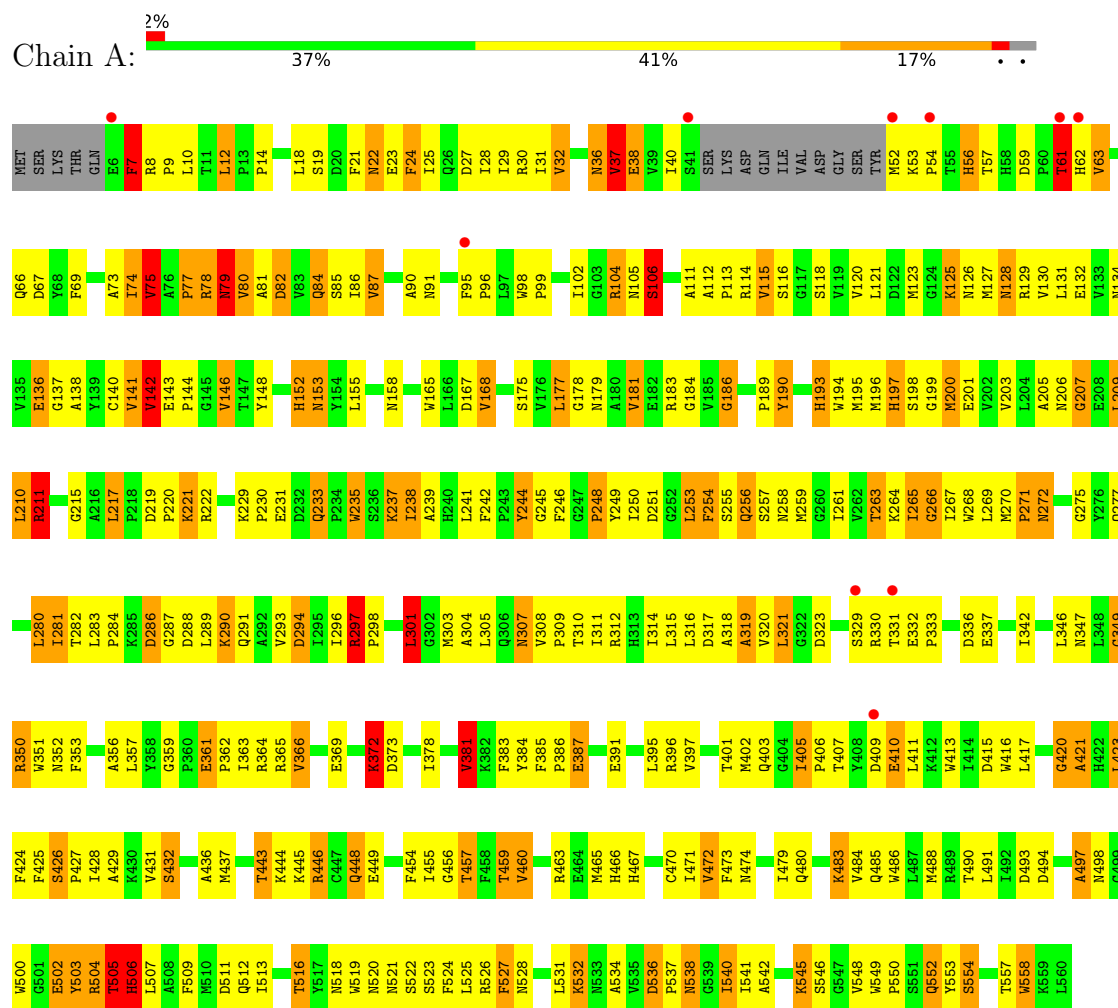
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	8	Total	O	0	0
			8	8		

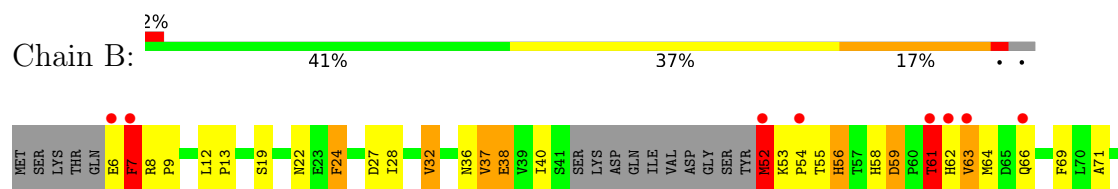
3 Residue-property plots

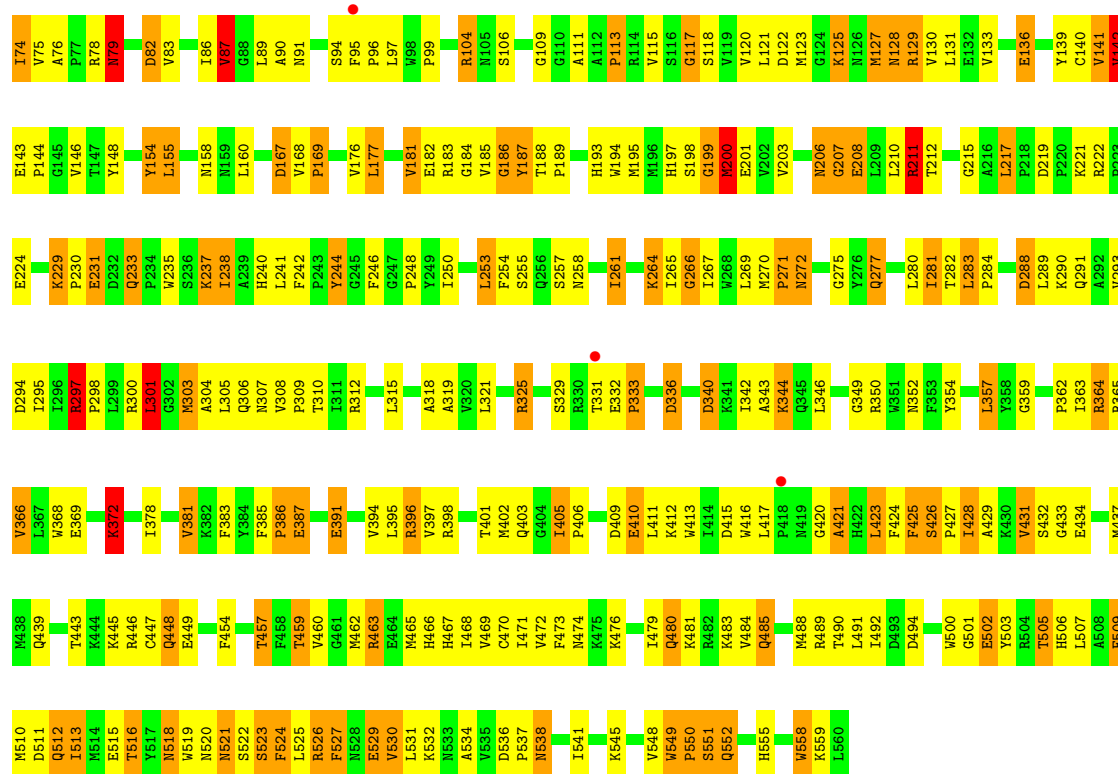
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	129.28Å 129.28Å 130.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.90) 97.8 (20.00-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.312 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 18.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.005 for -l,-k,-h 0.015 for -h,-l,-k 0.000 for -h,l,k 0.039 for -h,k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.95	5/4428 (0.1%)	2.30	244/6018 (4.1%)
1	B	0.96	9/4428 (0.2%)	2.26	218/6018 (3.6%)
All	All	0.96	14/8856 (0.2%)	2.28	462/12036 (3.8%)

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

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	LYS	CG-CD	-28.05	0.68	1.52
1	B	52	MET	CA-CB	17.74	1.89	1.53
1	B	53	LYS	CB-CG	16.24	2.01	1.52
1	B	476	LYS	CG-CD	14.61	1.96	1.52
1	B	53	LYS	CA-CB	13.21	1.74	1.53
1	B	221	LYS	CG-CD	-9.87	1.22	1.52
1	B	325	ARG	CB-CG	-8.81	1.26	1.52
1	A	66	GLN	CA-CB	-6.92	1.42	1.53
1	A	372	LYS	CG-CD	6.86	1.73	1.52
1	B	52	MET	CB-CG	5.94	1.70	1.52
1	B	229	LYS	CG-CD	-5.84	1.34	1.52
1	A	483	LYS	CG-CD	-5.41	1.36	1.52
1	A	37	VAL	C-O	5.17	1.30	1.24
1	B	372	LYS	CG-CD	5.05	1.67	1.52

All (462) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LYS	CG-CD-CE	-25.09	53.59	111.30
1	B	325	ARG	CB-CG-CD	21.66	161.11	111.30
1	A	291	GLN	OE1-CD-NE2	20.76	143.36	122.60
1	B	291	GLN	OE1-CD-NE2	19.55	142.15	122.60
1	A	221	LYS	CB-CG-CD	19.29	155.67	111.30
1	B	53	LYS	CB-CA-C	18.56	146.73	110.17
1	B	325	ARG	CA-CB-CG	18.02	150.15	114.10
1	B	211	ARG	CD-NE-CZ	14.31	144.44	124.40
1	B	476	LYS	CB-CG-CD	14.28	144.14	111.30
1	A	242	PHE	CA-CB-CG	13.21	127.01	113.80
1	A	211	ARG	CD-NE-CZ	13.03	142.65	124.40
1	B	304	ALA	CA-C-O	12.49	133.35	119.24
1	B	485	GLN	OE1-CD-NE2	-12.44	110.16	122.60
1	B	221	LYS	CB-CG-CD	12.31	139.62	111.30
1	B	272	ASN	OD1-CG-ND2	12.01	134.61	122.60
1	B	242	PHE	CA-CB-CG	11.93	125.73	113.80
1	B	52	MET	N-CA-CB	11.62	130.26	110.50
1	A	307	ASN	CA-C-N	-11.42	114.83	122.60
1	A	307	ASN	C-N-CA	-11.42	114.83	122.60
1	B	185	VAL	CA-C-N	11.40	132.31	122.17
1	B	185	VAL	C-N-CA	11.40	132.31	122.17
1	A	528	ASN	O-C-N	-10.80	110.67	122.12
1	B	476	LYS	CG-CD-CE	10.78	136.10	111.30
1	B	207	GLY	CA-C-O	10.76	128.97	119.83
1	A	37	VAL	O-C-N	-10.55	109.38	122.57
1	A	37	VAL	CA-C-O	-10.19	108.05	120.78
1	B	66	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	A	36	ASN	CA-C-O	-9.91	107.49	119.18
1	B	203	VAL	CA-C-O	-9.87	109.23	120.97
1	A	136	GLU	CA-CB-CG	9.86	133.82	114.10
1	A	498	ASN	OD1-CG-ND2	9.86	132.46	122.60
1	B	420	GLY	CA-C-O	9.82	132.90	121.71
1	B	448	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	66	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	448	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	244	TYR	CA-C-O	-9.67	107.79	119.49
1	A	128	ASN	N-CA-C	9.61	125.32	113.50
1	A	219	ASP	CA-CB-CG	9.48	122.08	112.60
1	A	142	VAL	N-CA-CB	-9.33	94.67	111.93
1	A	10	LEU	CA-C-O	9.19	130.16	120.42
1	B	480	GLN	OE1-CD-NE2	9.18	131.78	122.60
1	A	474	ASN	OD1-CG-ND2	9.15	131.75	122.60
1	A	485	GLN	OE1-CD-NE2	-9.15	113.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	GLU	CA-C-O	-9.13	110.31	120.81
1	A	498	ASN	CA-CB-CG	-9.11	103.49	112.60
1	A	62	HIS	CA-C-O	-9.06	111.22	121.19
1	B	463	ARG	NE-CZ-NH1	9.06	130.56	121.50
1	B	558	TRP	N-CA-C	9.05	124.45	113.41
1	A	190	TYR	CB-CG-CD1	8.74	133.91	120.80
1	A	304	ALA	CA-C-O	8.73	129.27	119.41
1	A	304	ALA	N-CA-C	-8.71	102.79	113.41
1	A	446	ARG	NH1-CZ-NH2	8.70	130.61	119.30
1	A	558	TRP	N-CA-C	8.67	123.99	113.41
1	B	429	ALA	CA-C-O	-8.66	111.01	121.06
1	A	106	SER	CA-C-O	-8.65	112.09	121.44
1	B	307	ASN	OD1-CG-ND2	-8.62	113.98	122.60
1	A	272	ASN	OD1-CG-ND2	8.55	131.15	122.60
1	A	125	LYS	CA-C-O	-8.52	111.78	120.90
1	B	128	ASN	N-CA-C	8.47	123.92	113.50
1	B	336	ASP	CA-CB-CG	-8.40	104.20	112.60
1	B	521	ASN	OD1-CG-ND2	8.34	130.94	122.60
1	A	249	TYR	O-C-N	-8.34	112.53	122.46
1	B	7	PHE	N-CA-C	8.29	128.46	110.80
1	A	24	PHE	CA-CB-CG	8.28	122.08	113.80
1	B	293	VAL	CA-C-O	-8.26	112.36	120.95
1	A	349	GLY	CA-C-O	8.24	130.52	122.28
1	A	281	ILE	CA-C-O	-8.19	111.77	120.53
1	B	53	LYS	N-CA-CB	-8.17	95.83	110.37
1	B	215	GLY	N-CA-C	-8.13	104.57	114.66
1	B	136	GLU	CA-CB-CG	8.10	130.31	114.10
1	A	207	GLY	CA-C-O	8.02	127.37	119.27
1	A	7	PHE	N-CA-C	7.99	127.81	110.80
1	A	265	ILE	O-C-N	7.95	129.89	122.97
1	A	421	ALA	N-CA-C	-7.91	97.36	109.14
1	B	129	ARG	N-CA-C	7.90	121.98	110.28
1	B	424	PHE	CA-C-O	-7.90	111.90	120.36
1	A	538	ASN	OD1-CG-ND2	7.87	130.47	122.60
1	A	168	VAL	O-C-N	7.85	127.92	121.40
1	A	12	LEU	CA-C-O	7.77	127.42	120.19
1	A	129	ARG	N-CA-C	7.74	121.73	110.28
1	B	78	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	B	305	LEU	CA-C-O	7.67	129.98	121.39
1	A	193	HIS	N-CA-C	7.66	119.27	111.07
1	A	287	GLY	CA-C-O	7.62	125.98	119.04
1	B	184	GLY	CA-C-O	-7.62	112.09	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ASN	CB-CA-C	-7.59	95.47	109.29
1	A	38	GLU	N-CA-C	7.59	121.34	109.96
1	A	251	ASP	CA-CB-CG	-7.59	105.01	112.60
1	B	281	ILE	CA-C-O	-7.58	112.50	120.39
1	A	266	GLY	O-C-N	-7.56	117.79	123.61
1	B	37	VAL	CA-C-O	-7.49	112.64	120.51
1	B	193	HIS	N-CA-C	7.41	119.00	111.07
1	B	423	LEU	CA-C-O	-7.38	112.50	121.06
1	B	235	TRP	CA-C-O	-7.35	112.66	121.56
1	B	489	ARG	NE-CZ-NH1	-7.33	114.17	121.50
1	A	511	ASP	CA-CB-CG	-7.31	105.29	112.60
1	B	142	VAL	N-CA-CB	-7.31	98.41	111.93
1	A	78	ARG	NE-CZ-NH1	-7.29	114.21	121.50
1	B	428	ILE	CA-C-O	-7.28	112.15	121.40
1	A	268	TRP	O-C-N	-7.27	114.02	122.89
1	A	518	ASN	N-CA-C	7.24	120.64	112.97
1	B	344	LYS	CB-CG-CD	-7.21	94.72	111.30
1	A	128	ASN	CB-CA-C	-7.19	96.21	109.29
1	A	184	GLY	CA-C-O	-7.18	112.69	122.31
1	A	405	ILE	CA-C-O	7.18	123.39	119.15
1	A	423	LEU	CA-C-O	-7.18	112.73	121.06
1	B	210	LEU	CA-C-O	-7.17	111.72	120.54
1	A	259	MET	CA-C-O	-7.16	109.74	119.05
1	A	130	VAL	N-CA-C	-7.15	96.20	107.15
1	B	457	THR	CB-CA-C	-7.13	93.73	109.56
1	B	198	SER	O-C-N	7.12	132.06	122.59
1	B	454	PHE	CA-CB-CG	-7.12	106.69	113.80
1	B	141	VAL	CA-C-O	7.10	127.77	120.39
1	A	61	THR	CB-CA-C	7.09	123.08	112.03
1	B	6	GLU	CA-C-N	7.08	135.06	121.54
1	B	6	GLU	C-N-CA	7.08	135.06	121.54
1	A	301	LEU	CA-C-O	-7.07	112.11	120.10
1	A	235	TRP	CA-C-O	-7.06	113.02	121.56
1	B	62	HIS	CA-C-O	-7.06	113.43	121.19
1	B	127	MET	CA-C-N	7.06	134.13	121.92
1	B	127	MET	C-N-CA	7.06	134.13	121.92
1	A	206	ASN	CA-CB-CG	7.01	119.61	112.60
1	B	468	ILE	N-CA-C	7.00	117.31	107.37
1	B	272	ASN	CB-CG-ND2	-6.99	105.92	116.40
1	B	271	PRO	CA-C-O	-6.98	113.76	121.23
1	B	538	ASN	OD1-CG-ND2	6.95	129.55	122.60
1	B	211	ARG	CA-CB-CG	6.95	128.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CA-C-O	-6.94	113.27	121.11
1	A	106	SER	N-CA-C	-6.88	101.30	110.24
1	A	141	VAL	CA-C-O	6.86	127.20	120.27
1	B	303	MET	O-C-N	-6.85	114.36	122.58
1	B	421	ALA	N-CA-C	-6.84	98.95	109.14
1	A	118	SER	O-C-N	6.82	130.97	122.65
1	A	61	THR	N-CA-C	-6.81	96.71	108.56
1	B	304	ALA	N-CA-C	-6.80	105.51	113.88
1	B	66	GLN	CG-CD-NE2	6.79	126.58	116.40
1	A	272	ASN	CB-CG-ND2	-6.75	106.27	116.40
1	B	283	LEU	CB-CA-C	6.73	117.89	110.15
1	B	501	GLY	CA-C-O	6.72	129.50	121.77
1	A	211	ARG	CA-CB-CG	6.70	127.49	114.10
1	A	291	GLN	CG-CD-NE2	-6.69	106.36	116.40
1	B	536	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	545	LYS	CB-CA-C	6.68	120.81	109.72
1	B	211	ARG	N-CA-CB	6.68	122.51	111.08
1	B	448	GLN	CG-CD-NE2	6.68	126.42	116.40
1	A	420	GLY	CA-C-O	6.66	129.09	121.90
1	A	66	GLN	CG-CD-NE2	6.65	126.37	116.40
1	A	211	ARG	CG-CD-NE	6.65	126.62	112.00
1	B	297	ARG	CD-NE-CZ	6.65	133.71	124.40
1	A	505	THR	CB-CA-C	-6.62	96.18	111.95
1	A	448	GLN	CG-CD-NE2	6.62	126.33	116.40
1	B	125	LYS	CA-C-O	-6.59	113.85	120.90
1	A	253	LEU	N-CA-C	-6.58	104.19	111.82
1	A	503	TYR	CA-C-O	-6.56	111.92	119.14
1	A	209	LEU	CA-C-O	-6.56	113.57	121.05
1	B	364	ARG	NE-CZ-NH2	6.56	125.10	119.20
1	B	551	SER	N-CA-C	6.51	119.19	111.71
1	B	136	GLU	CB-CG-CD	6.50	123.65	112.60
1	B	425	PHE	CA-C-N	-6.50	114.69	123.46
1	B	425	PHE	C-N-CA	-6.50	114.69	123.46
1	A	198	SER	N-CA-C	-6.49	96.99	110.80
1	B	113	PRO	CA-C-O	-6.46	114.11	122.12
1	B	38	GLU	CB-CA-C	-6.45	99.23	109.80
1	B	233	GLN	CA-C-O	6.45	127.72	120.70
1	A	165	TRP	CA-CB-CG	6.43	125.82	113.60
1	A	557	THR	CA-C-O	-6.42	113.61	120.42
1	A	74	ILE	CA-C-O	-6.40	113.42	120.84
1	A	127	MET	CA-C-N	6.39	132.98	121.92
1	A	127	MET	C-N-CA	6.39	132.98	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	CA-C-O	-6.39	113.82	120.27
1	B	129	ARG	CA-C-O	6.38	128.30	121.16
1	A	8	ARG	CA-C-O	6.37	124.87	119.71
1	B	32	VAL	N-CA-C	6.36	118.27	112.29
1	B	130	VAL	N-CA-C	-6.31	98.41	107.37
1	A	206	ASN	N-CA-C	-6.30	105.56	113.18
1	A	521	ASN	N-CA-CB	-6.30	102.38	111.70
1	A	56	HIS	CA-CB-CG	6.30	120.10	113.80
1	B	463	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	B	426	SER	N-CA-C	6.29	120.80	108.21
1	A	512	GLN	OE1-CD-NE2	6.28	128.88	122.60
1	A	305	LEU	CA-C-N	6.26	128.92	120.65
1	A	305	LEU	C-N-CA	6.26	128.92	120.65
1	A	527	PHE	CA-C-O	-6.25	113.88	120.63
1	A	78	ARG	NH1-CZ-NH2	6.23	127.39	119.30
1	B	142	VAL	N-CA-C	6.23	119.01	108.86
1	B	221	LYS	CG-CD-CE	6.22	125.62	111.30
1	A	446	ARG	NE-CZ-NH1	-6.22	115.28	121.50
1	B	545	LYS	CB-CA-C	6.22	120.04	109.72
1	A	305	LEU	CA-C-O	6.21	128.35	121.39
1	A	536	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	200	MET	O-C-N	6.20	130.83	123.27
1	B	424	PHE	O-C-N	6.20	130.28	123.22
1	A	84	GLN	OE1-CD-NE2	6.20	128.79	122.60
1	A	466	HIS	CA-C-O	-6.18	113.71	120.81
1	A	22	ASN	CA-CB-CG	-6.17	106.43	112.60
1	B	198	SER	CA-C-O	-6.17	111.69	120.51
1	B	211	ARG	CG-CD-NE	6.14	125.52	112.00
1	A	128	ASN	N-CA-CB	-6.14	101.50	110.53
1	B	169	PRO	N-CA-C	-6.14	102.23	111.57
1	A	132	GLU	O-C-N	-6.13	116.50	123.48
1	A	242	PHE	CA-C-O	6.12	124.36	119.59
1	A	8	ARG	N-CA-C	6.12	120.58	108.59
1	B	264	LYS	CA-C-O	-6.12	114.16	120.89
1	A	548	VAL	N-CA-CB	6.11	119.59	111.64
1	A	265	ILE	CA-C-O	-6.11	115.83	120.96
1	A	429	ALA	CA-C-O	-6.10	113.99	121.06
1	A	283	LEU	CB-CA-C	6.09	117.15	110.15
1	A	199	GLY	CA-C-O	-6.08	110.00	120.57
1	B	186	GLY	O-C-N	-6.07	119.27	123.95
1	A	186	GLY	O-C-N	-6.07	119.28	123.95
1	B	466	HIS	CA-C-O	-6.06	113.55	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	VAL	N-CA-C	6.06	118.83	112.83
1	B	405	ILE	CA-C-O	6.05	122.72	119.15
1	B	301	LEU	N-CA-C	-6.04	105.17	112.54
1	B	122	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	96	PRO	CA-C-O	6.04	128.72	121.48
1	A	23	GLU	CA-C-O	6.03	126.91	120.70
1	B	396	ARG	CA-C-O	-6.01	114.18	120.55
1	B	526	ARG	CA-C-O	6.01	127.31	121.00
1	B	128	ASN	N-CA-CB	-6.00	101.72	110.53
1	A	211	ARG	NH1-CZ-NH2	5.99	127.08	119.30
1	B	160	LEU	CA-C-O	5.97	125.95	119.15
1	B	106	SER	CA-C-O	-5.96	114.63	121.19
1	A	249	TYR	CA-C-O	5.96	129.22	122.37
1	A	490	THR	N-CA-C	-5.96	104.36	111.69
1	A	215	GLY	N-CA-C	-5.95	107.52	115.32
1	A	457	THR	CB-CA-C	-5.95	96.35	109.56
1	A	244	TYR	N-CA-C	5.93	119.61	112.38
1	A	356	ALA	CA-C-N	5.93	130.90	122.72
1	A	356	ALA	C-N-CA	5.93	130.90	122.72
1	A	518	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	424	PHE	CA-C-N	-5.91	115.16	122.84
1	A	424	PHE	C-N-CA	-5.91	115.16	122.84
1	B	501	GLY	O-C-N	-5.91	118.15	123.29
1	B	148	TYR	CA-C-O	-5.90	114.62	120.70
1	A	95	PHE	CB-CA-C	5.90	116.44	109.47
1	A	256	GLN	CB-CA-C	-5.90	103.10	111.95
1	A	526	ARG	NH1-CZ-NH2	-5.89	111.64	119.30
1	A	118	SER	CA-C-O	-5.89	115.28	121.99
1	A	294	ASP	CA-C-N	5.89	128.10	120.56
1	A	294	ASP	C-N-CA	5.89	128.10	120.56
1	B	229	LYS	CB-CG-CD	5.88	124.84	111.30
1	B	397	VAL	N-CA-CB	5.88	118.10	110.57
1	B	118	SER	O-C-N	5.87	129.62	122.75
1	B	529	GLU	CA-C-O	-5.87	114.33	120.55
1	B	515	GLU	CA-C-N	5.86	128.61	120.29
1	B	515	GLU	C-N-CA	5.86	128.61	120.29
1	A	471	ILE	CA-C-N	-5.86	115.54	123.10
1	A	471	ILE	C-N-CA	-5.86	115.54	123.10
1	B	485	GLN	CG-CD-NE2	5.86	125.18	116.40
1	B	474	ASN	OD1-CG-ND2	5.85	128.45	122.60
1	B	56	HIS	CA-CB-CG	5.85	119.65	113.80
1	B	530	VAL	CA-C-O	-5.85	115.03	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	B	207	GLY	N-CA-C	-5.84	107.33	113.58
1	A	321	LEU	CA-C-O	-5.83	113.26	119.97
1	B	261	ILE	CA-CB-CG1	-5.83	100.48	110.40
1	A	381	VAL	CA-C-O	-5.83	114.99	121.23
1	A	372	LYS	CG-CD-CE	5.83	124.70	111.30
1	B	206	ASN	CA-CB-CG	5.82	118.42	112.60
1	B	365	ARG	CA-C-O	-5.82	114.67	120.90
1	B	372	LYS	CA-C-N	5.82	128.40	120.54
1	B	372	LYS	C-N-CA	5.82	128.40	120.54
1	B	291	GLN	CG-CD-OE1	-5.82	109.16	120.80
1	A	431	VAL	N-CA-CB	5.82	120.83	111.23
1	A	142	VAL	N-CA-C	5.79	118.31	108.86
1	B	509	PHE	CA-C-O	5.79	126.22	119.32
1	B	253	LEU	CA-C-O	-5.79	113.31	119.97
1	A	24	PHE	N-CA-CB	-5.79	101.32	109.94
1	A	233	GLN	CA-C-O	5.78	126.59	120.64
1	A	153	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	104	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	A	460	VAL	CA-C-N	5.76	128.91	121.13
1	A	460	VAL	C-N-CA	5.76	128.91	121.13
1	A	459	THR	CA-CB-OG1	5.76	118.25	109.60
1	B	167	ASP	CA-CB-CG	-5.76	106.84	112.60
1	A	505	THR	N-CA-CB	5.74	120.79	111.21
1	B	38	GLU	CA-C-O	-5.74	114.06	120.54
1	A	500	TRP	CA-CB-CG	5.72	124.47	113.60
1	B	524	PHE	CA-C-O	-5.72	114.49	120.55
1	B	521	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	504	ARG	CA-C-O	-5.70	115.17	121.33
1	A	129	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	190	TYR	CB-CG-CD2	-5.69	112.27	120.80
1	B	266	GLY	O-C-N	-5.68	119.23	123.61
1	A	238	ILE	CA-C-N	5.67	128.15	120.38
1	A	238	ILE	C-N-CA	5.67	128.15	120.38
1	A	446	ARG	NE-CZ-NH2	-5.66	114.11	119.20
1	B	61	THR	CB-CA-C	5.66	120.65	112.05
1	B	439	GLN	OE1-CD-NE2	5.66	128.26	122.60
1	A	104	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	A	397	VAL	N-CA-CB	5.65	117.80	110.57
1	B	169	PRO	CB-CA-C	5.65	118.39	110.60
1	A	540	ILE	CB-CA-C	5.65	121.16	110.94
1	B	253	LEU	N-CA-CB	5.64	119.02	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	NE-CZ-NH2	-5.63	114.13	119.20
1	B	237	LYS	CA-C-O	-5.63	114.88	121.07
1	A	314	ILE	N-CA-C	5.62	116.26	110.36
1	B	253	LEU	N-CA-C	-5.62	105.30	111.82
1	A	308	VAL	N-CA-C	-5.62	102.44	107.56
1	A	211	ARG	N-CA-C	-5.62	100.24	109.40
1	A	246	PHE	CA-C-O	-5.62	114.20	120.66
1	B	61	THR	N-CA-C	-5.61	98.08	108.24
1	A	248	PRO	CB-CA-C	-5.60	102.32	111.56
1	B	350	ARG	CA-C-N	5.60	131.36	122.62
1	B	350	ARG	C-N-CA	5.60	131.36	122.62
1	A	426	SER	N-CA-C	5.60	120.75	108.66
1	A	459	THR	N-CA-CB	5.59	119.33	110.55
1	A	197	HIS	CB-CG-CD2	5.56	138.43	131.20
1	B	468	ILE	CB-CA-C	-5.56	105.91	111.80
1	A	361	GLU	CG-CD-OE1	5.55	131.17	118.40
1	B	306	GLN	CB-CG-CD	5.54	122.03	112.60
1	A	436	ALA	O-C-N	5.53	127.99	122.12
1	B	24	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	254	PHE	CA-C-O	-5.52	112.75	119.43
1	B	264	LYS	O-C-N	5.52	129.66	123.48
1	B	386	PRO	CA-C-N	5.52	132.08	121.54
1	B	386	PRO	C-N-CA	5.52	132.08	121.54
1	B	200	MET	CA-CB-CG	5.50	125.09	114.10
1	B	82	ASP	CA-CB-CG	5.50	118.09	112.60
1	A	245	GLY	CA-C-O	5.49	128.42	121.56
1	A	505	THR	O-C-N	5.49	129.34	122.92
1	B	244	TYR	CA-C-O	-5.49	113.66	119.97
1	B	340	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	244	TYR	O-C-N	-5.48	115.27	122.39
1	A	459	THR	OG1-CB-CG2	-5.47	98.36	109.30
1	A	554	SER	CA-C-O	5.47	126.42	120.95
1	A	548	VAL	O-C-N	5.46	128.99	123.20
1	A	365	ARG	CA-C-O	-5.46	114.63	121.02
1	A	525	LEU	CA-C-O	-5.46	114.64	120.42
1	A	203	VAL	CB-CA-C	-5.44	104.46	111.53
1	A	466	HIS	CA-C-N	5.44	132.25	123.33
1	A	466	HIS	C-N-CA	5.44	132.25	123.33
1	B	333	PRO	N-CA-C	5.44	119.01	110.80
1	A	134	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	B	527	PHE	CA-C-N	5.43	127.83	120.44
1	B	527	PHE	C-N-CA	5.43	127.83	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	210	LEU	CA-C-O	-5.42	113.61	120.28
1	B	176	VAL	CA-C-O	-5.42	115.42	121.05
1	A	350	ARG	CA-C-N	5.42	131.31	122.81
1	A	350	ARG	C-N-CA	5.42	131.31	122.81
1	A	301	LEU	N-CA-CB	5.39	118.53	110.22
1	A	77	PRO	N-CA-CB	5.39	108.11	103.31
1	B	158	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	76	ALA	CB-CA-C	-5.38	104.84	110.33
1	B	222	ARG	CB-CA-C	5.38	117.23	109.92
1	A	129	ARG	CA-C-O	5.37	127.18	121.16
1	A	486	TRP	CA-C-O	5.36	126.11	120.42
1	A	82	ASP	CA-C-O	-5.36	115.16	120.90
1	B	24	PHE	N-CA-CB	-5.35	102.10	109.91
1	B	219	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	79	ASN	CA-C-O	-5.35	115.38	120.94
1	B	512	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	B	369	GLU	N-CA-C	-5.34	105.36	111.07
1	B	288	ASP	CA-C-O	5.33	125.92	119.31
1	A	90	ALA	CB-CA-C	-5.32	101.80	110.85
1	B	96	PRO	CA-C-O	5.32	127.87	121.48
1	B	208	GLU	CA-C-N	5.32	129.29	120.94
1	B	208	GLU	C-N-CA	5.32	129.29	120.94
1	B	211	ARG	NE-CZ-NH1	-5.32	116.19	121.50
1	A	239	ALA	N-CA-C	5.31	117.75	111.33
1	B	188	THR	O-C-N	-5.30	115.22	121.32
1	B	106	SER	N-CA-C	-5.30	102.55	110.23
1	B	549	TRP	O-C-N	5.30	126.11	121.39
1	A	286	ASP	O-C-N	-5.29	115.51	122.39
1	A	307	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	455	ILE	CA-C-O	-5.29	114.67	120.43
1	B	396	ARG	O-C-N	5.28	127.72	122.12
1	A	291	GLN	CG-CD-OE1	-5.28	110.24	120.80
1	A	319	ALA	CA-C-O	5.28	126.36	120.82
1	B	431	VAL	O-C-N	5.27	129.16	122.57
1	A	203	VAL	CA-C-O	-5.27	113.85	120.86
1	A	460	VAL	N-CA-C	5.27	115.94	107.98
1	B	182	GLU	CG-CD-OE2	-5.26	106.30	118.40
1	A	80	VAL	CA-C-O	-5.25	115.49	120.95
1	A	457	THR	CA-C-O	-5.25	114.97	121.06
1	B	397	VAL	CB-CA-C	-5.24	105.15	112.02
1	A	158	ASN	CA-CB-CG	5.24	117.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	GLN	O-C-N	-5.23	116.44	122.09
1	A	366	VAL	N-CA-CB	5.23	117.66	110.54
1	A	432	SER	CA-C-N	5.23	125.75	119.94
1	A	432	SER	C-N-CA	5.23	125.75	119.94
1	A	178	GLY	N-CA-C	-5.23	106.44	112.50
1	A	465	MET	CA-CB-CG	5.22	124.55	114.10
1	A	263	THR	CA-C-O	5.21	125.30	119.41
1	B	368	TRP	N-CA-C	5.21	116.95	111.28
1	A	61	THR	CA-C-O	-5.21	116.38	122.37
1	A	136	GLU	CB-CG-CD	5.21	121.45	112.60
1	B	277	GLN	N-CA-CB	5.20	119.55	110.81
1	A	471	ILE	CA-C-O	-5.20	114.36	120.76
1	B	212	THR	N-CA-C	5.20	118.16	110.46
1	B	154	TYR	CA-C-O	-5.20	115.54	121.00
1	B	109	GLY	CA-C-O	5.20	124.78	119.01
1	B	59	ASP	CA-C-N	5.19	124.88	119.64
1	B	59	ASP	C-N-CA	5.19	124.88	119.64
1	A	524	PHE	N-CA-CB	-5.18	102.51	110.12
1	A	506	HIS	O-C-N	-5.18	117.14	122.94
1	B	89	LEU	CA-C-O	-5.17	115.04	120.63
1	B	117	GLY	N-CA-C	-5.17	108.54	114.69
1	B	357	LEU	N-CA-CB	-5.17	102.46	110.57
1	A	222	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	8	ARG	N-CA-C	5.16	118.70	108.59
1	B	208	GLU	N-CA-C	5.16	117.79	110.10
1	B	459	THR	N-CA-CB	5.16	118.84	110.43
1	A	443	THR	N-CA-C	5.16	117.57	111.33
1	A	456	GLY	N-CA-C	5.16	119.12	110.56
1	A	198	SER	CA-C-N	5.16	131.52	121.41
1	A	198	SER	C-N-CA	5.16	131.52	121.41
1	B	8	ARG	CA-C-O	5.15	123.88	119.71
1	B	155	LEU	N-CA-C	5.15	117.56	111.33
1	A	271	PRO	CA-C-O	-5.15	111.23	120.60
1	B	129	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	B	291	GLN	CG-CD-NE2	-5.14	108.69	116.40
1	A	152	HIS	CA-CB-CG	5.14	118.94	113.80
1	B	104	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	143	GLU	O-C-N	-5.13	116.11	120.99
1	A	311	ILE	CA-C-O	-5.13	114.03	120.86
1	A	127	MET	CA-C-O	5.13	129.38	122.51
1	B	471	ILE	CA-C-N	-5.13	114.99	122.68
1	B	471	ILE	C-N-CA	-5.13	114.99	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	VAL	N-CA-CB	5.12	116.55	110.55
1	B	513	ILE	CA-C-N	-5.12	112.52	120.31
1	B	513	ILE	C-N-CA	-5.12	112.52	120.31
1	A	90	ALA	N-CA-CB	5.12	117.73	110.16
1	B	237	LYS	CA-CB-CG	5.11	124.32	114.10
1	B	421	ALA	CA-C-N	-5.11	113.49	121.87
1	B	421	ALA	C-N-CA	-5.11	113.49	121.87
1	A	259	MET	CA-CB-CG	-5.11	103.88	114.10
1	B	510	MET	O-C-N	5.10	127.39	122.09
1	A	384	TYR	CB-CA-C	-5.10	99.03	109.38
1	A	423	LEU	O-C-N	5.09	129.17	123.27
1	A	407	THR	N-CA-C	5.08	116.71	109.14
1	A	460	VAL	CA-C-O	5.08	127.00	120.76
1	B	490	THR	CA-C-O	5.08	125.78	119.79
1	A	115	VAL	CA-CB-CG2	5.07	119.03	110.40
1	B	187	TYR	O-C-N	-5.07	115.41	122.20
1	A	136	GLU	N-CA-CB	5.07	118.13	110.28
1	A	211	ARG	CB-CA-C	-5.07	99.69	109.37
1	A	114	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	B	104	ARG	CD-NE-CZ	5.06	131.48	124.40
1	B	83	VAL	O-C-N	-5.06	116.96	121.87
1	B	344	LYS	CA-CB-CG	-5.05	103.99	114.10
1	A	271	PRO	O-C-N	5.05	129.46	122.64
1	A	296	ILE	N-CA-C	5.05	115.77	110.62
1	B	246	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	37	VAL	N-CA-CB	-5.03	102.92	111.23
1	A	528	ASN	CA-C-O	5.03	125.88	120.55
1	B	87	VAL	CA-CB-CG1	5.03	118.95	110.40
1	B	550	PRO	CB-CA-C	5.03	117.57	110.98
1	B	74	ILE	CA-C-O	-5.03	115.19	120.57
1	A	361	GLU	CB-CG-CD	5.02	121.14	112.60
1	B	199	GLY	O-C-N	-5.02	116.18	122.70
1	B	396	ARG	CA-C-N	5.01	126.97	120.56
1	B	396	ARG	C-N-CA	5.01	126.97	120.56
1	A	128	ASN	OD1-CG-ND2	5.01	127.61	122.60
1	A	421	ALA	CA-C-O	-5.01	115.90	121.51
1	A	497	ALA	O-C-N	-5.01	116.81	122.12
1	B	537	PRO	CB-CA-C	-5.00	103.93	112.64
1	A	79	ASN	CA-C-O	-5.00	115.80	121.05
1	A	61	THR	CA-CB-CG2	5.00	119.00	110.50
1	B	300	ARG	NH1-CZ-NH2	5.00	125.80	119.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	VAL	Mainchain

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	4311	0	4260	228	18
1	B	4311	0	4260	205	10
2	A	12	0	0	2	0
2	B	8	0	0	1	0
All	All	8642	0	8520	394	18

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 24.

All (394) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG11	1:B:423:LEU:HD11	1.44	1.00
1:B:310:THR:HG22	1:B:459:THR:HG22	1.45	0.96
1:A:357:LEU:HB3	1:A:364:ARG:HG2	1.55	0.89
1:A:310:THR:HG22	1:A:459:THR:HG22	1.55	0.88
1:B:79:ASN:ND2	1:B:82:ASP:H	1.74	0.86
1:A:79:ASN:ND2	1:A:82:ASP:H	1.73	0.86
1:A:200:MET:HB3	1:A:265:ILE:HG13	1.56	0.86
1:A:552:GLN:H	1:A:552:GLN:NE2	1.76	0.83
1:A:63:VAL:HG11	1:A:423:LEU:HD11	1.59	0.83
1:B:357:LEU:HB3	1:B:364:ARG:HG2	1.61	0.82
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.60	0.82
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.63	0.80
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.63	0.80
1:B:552:GLN:H	1:B:552:GLN:NE2	1.80	0.79
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.65	0.79
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.13	0.78
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD11	1:B:74:ILE:HD11	1.65	0.77
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.64	0.77
1:A:168:VAL:HG11	1:A:406:PRO:HB3	1.69	0.75
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.69	0.74
1:A:238:ILE:HG21	1:B:428:ILE:HG21	1.70	0.73
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.17	0.72
1:B:280:LEU:HB3	1:B:395:LEU:HD22	1.72	0.72
1:A:310:THR:CG2	1:A:459:THR:HG22	2.20	0.71
1:B:79:ASN:HD21	1:B:82:ASP:H	1.38	0.71
1:A:40:ILE:HD11	1:A:74:ILE:HD11	1.71	0.70
1:B:250:ILE:HD12	1:B:254:PHE:HE2	1.56	0.70
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.73	0.70
1:A:183:ARG:HD2	1:B:244:TYR:CD2	2.26	0.70
1:A:463:ARG:O	1:B:241:LEU:HB3	1.91	0.70
1:A:502:GLU:HB2	1:A:513:ILE:HD13	1.73	0.70
1:A:552:GLN:H	1:A:552:GLN:HE21	1.37	0.69
1:A:319:ALA:HB1	1:A:413:TRP:HB2	1.75	0.68
1:B:290:LYS:HB2	1:B:437:MET:HG3	1.75	0.68
1:A:238:ILE:HG21	1:B:428:ILE:CG2	2.24	0.68
1:B:52:MET:O	1:B:54:PRO:HD3	1.94	0.68
1:A:277:GLN:HB3	1:A:357:LEU:HD12	1.77	0.67
1:A:56:HIS:HA	1:A:111:ALA:HB3	1.76	0.67
1:B:277:GLN:HB3	1:B:357:LEU:HD12	1.76	0.66
1:B:297:ARG:HH11	1:B:298:PRO:HD3	1.60	0.66
1:B:168:VAL:HG11	1:B:406:PRO:HB3	1.78	0.66
1:A:52:MET:O	1:A:54:PRO:HD3	1.96	0.65
1:A:38:GLU:HB3	1:A:74:ILE:CD1	2.27	0.65
1:A:258:ASN:OD1	1:A:532:LYS:HE2	1.97	0.65
1:B:513:ILE:O	1:B:516:THR:HB	1.96	0.65
1:B:275:GLY:HA3	1:B:359:GLY:O	1.95	0.65
1:A:261:ILE:HD11	1:A:541:ILE:HD12	1.79	0.65
1:A:362:PRO:HB2	1:B:366:VAL:HG21	1.78	0.65
1:A:38:GLU:HB3	1:A:74:ILE:HD12	1.78	0.65
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.79	0.65
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.28	0.64
1:B:123:MET:O	1:B:127:MET:HB2	1.97	0.64
1:B:427:PRO:HD2	1:B:467:HIS:O	1.98	0.63
1:B:201:GLU:HG3	1:B:211:ARG:HD3	1.80	0.63
1:A:250:ILE:HD12	1:A:254:PHE:HE2	1.63	0.63
1:B:79:ASN:C	1:B:79:ASN:HD22	2.07	0.63
1:A:99:PRO:HA	1:A:121:LEU:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:THR:CG2	1:B:459:THR:HG22	2.26	0.63
1:A:297:ARG:NH1	1:A:298:PRO:HD3	2.13	0.62
1:A:427:PRO:HD2	1:A:467:HIS:O	1.98	0.62
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.81	0.62
1:A:315:LEU:HA	1:A:318:ALA:HB3	1.80	0.62
1:B:177:LEU:O	1:B:181:VAL:HG13	1.99	0.62
1:B:56:HIS:HA	1:B:111:ALA:HB3	1.81	0.62
1:B:290:LYS:HE3	1:B:294:ASP:OD2	2.00	0.61
1:A:37:VAL:HG13	1:A:75:VAL:HG22	1.82	0.61
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.82	0.61
1:A:79:ASN:HD22	1:A:82:ASP:H	1.48	0.60
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.83	0.60
1:B:297:ARG:NH1	1:B:298:PRO:HD3	2.15	0.60
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.17	0.60
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.36	0.60
1:A:349:GLY:H	1:A:352:ASN:HD21	1.49	0.60
1:B:258:ASN:CG	1:B:532:LYS:HE2	2.27	0.60
1:A:131:LEU:HD12	1:A:141:VAL:HG12	1.84	0.60
1:B:289:LEU:HD23	1:B:437:MET:SD	2.41	0.60
1:B:280:LEU:HD12	1:B:281:ILE:N	2.17	0.59
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.17	0.59
1:A:312:ARG:NH2	1:A:410:GLU:OE1	2.35	0.59
1:B:502:GLU:HB2	1:B:513:ILE:HD13	1.85	0.59
1:A:513:ILE:O	1:A:516:THR:HB	2.03	0.59
1:B:183:ARG:NH1	1:B:255:SER:HB3	2.17	0.59
1:B:258:ASN:OD1	1:B:532:LYS:HE2	2.03	0.58
1:B:183:ARG:HH11	1:B:255:SER:HB3	1.68	0.58
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.83	0.58
1:A:183:ARG:NH1	1:A:255:SER:HB3	2.18	0.58
1:B:425:PHE:HA	1:B:488:MET:HE1	1.86	0.58
1:B:200:MET:HB3	1:B:265:ILE:HG13	1.85	0.58
1:A:36:ASN:OD1	1:A:125:LYS:HE2	2.04	0.58
1:A:290:LYS:HE3	1:A:294:ASP:OD2	2.02	0.58
1:B:555:HIS:HB3	1:B:559:LYS:HD2	1.86	0.58
1:A:479:ILE:O	1:A:483:LYS:HG3	2.04	0.58
1:B:38:GLU:HB3	1:B:74:ILE:HD12	1.86	0.57
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.34	0.57
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.86	0.57
1:A:91:ASN:OD1	1:A:538:ASN:ND2	2.36	0.57
1:A:275:GLY:HA3	1:A:359:GLY:O	2.04	0.57
1:A:425:PHE:HA	1:A:488:MET:HE1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ASN:OD1	1:B:538:ASN:ND2	2.36	0.57
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.87	0.56
1:B:140:CYS:SG	1:B:269:LEU:HD21	2.45	0.56
1:B:297:ARG:HB3	1:B:297:ARG:HH11	1.71	0.56
1:A:505:THR:OG1	1:A:513:ILE:HD12	2.06	0.56
1:B:69:PHE:O	1:B:113:PRO:HD2	2.05	0.56
1:B:261:ILE:HD11	1:B:541:ILE:HD12	1.88	0.56
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.40	0.56
1:A:123:MET:HE3	1:A:144:PRO:HG2	1.88	0.56
1:A:183:ARG:HH11	1:A:255:SER:HB3	1.71	0.56
1:A:54:PRO:HG3	1:A:104:ARG:HG3	1.89	0.55
1:B:36:ASN:OD1	1:B:125:LYS:HE2	2.06	0.55
1:A:79:ASN:HD22	1:A:79:ASN:C	2.15	0.55
1:A:443:THR:HA	1:A:491:LEU:HD21	1.89	0.55
1:B:7:PHE:HA	1:B:22:ASN:OD1	2.07	0.55
1:A:79:ASN:HD21	1:A:82:ASP:H	1.53	0.55
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.20	0.55
1:B:63:VAL:CG1	1:B:423:LEU:HD11	2.27	0.55
1:B:75:VAL:HG11	1:B:86:ILE:HD13	1.89	0.55
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.42	0.55
1:A:284:PRO:HD2	1:A:288:ASP:OD2	2.07	0.54
1:A:420:GLY:HA2	1:A:473:PHE:O	2.06	0.54
1:A:75:VAL:HG11	1:A:86:ILE:HD13	1.88	0.54
1:A:271:PRO:O	1:A:272:ASN:C	2.50	0.54
1:B:99:PRO:HA	1:B:121:LEU:HB3	1.89	0.54
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.35	0.54
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.43	0.54
1:A:257:SER:HB2	1:B:248:PRO:HG3	1.90	0.54
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.37	0.53
1:A:194:TRP:O	1:A:197:HIS:HD2	1.91	0.53
1:A:290:LYS:HB2	1:A:437:MET:HG3	1.89	0.53
1:A:309:PRO:HD2	1:A:460:VAL:HB	1.88	0.53
1:B:194:TRP:O	1:B:197:HIS:HD2	1.91	0.53
1:B:230:PRO:HA	1:B:233:GLN:CD	2.33	0.53
1:B:332:GLU:HB3	1:B:333:PRO:CD	2.37	0.53
1:B:511:ASP:O	1:B:512:GLN:C	2.50	0.53
1:A:280:LEU:HD12	1:A:281:ILE:N	2.23	0.53
1:A:315:LEU:HD22	1:A:416:TRP:CH2	2.44	0.53
1:A:488:MET:HG2	1:A:509:PHE:CE2	2.44	0.52
1:B:54:PRO:HG3	1:B:104:ARG:HG3	1.90	0.52
1:B:38:GLU:HB3	1:B:74:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:MET:SD	1:B:485:GLN:OE1	2.67	0.52
1:B:309:PRO:HG2	1:B:460:VAL:CG2	2.39	0.52
1:A:31:ILE:HD13	1:A:85:SER:HB3	1.92	0.52
1:A:241:LEU:HB3	1:B:463:ARG:O	2.09	0.52
1:B:443:THR:HA	1:B:491:LEU:HD21	1.90	0.52
1:B:312:ARG:NH2	1:B:410:GLU:OE1	2.43	0.52
1:A:38:GLU:O	1:A:73:ALA:HA	2.10	0.52
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.38	0.52
1:A:195:MET:SD	1:B:195:MET:SD	3.08	0.52
1:A:297:ARG:HH11	1:A:298:PRO:HD3	1.75	0.52
1:A:448:GLN:O	1:A:449:GLU:C	2.52	0.52
1:A:217:LEU:HD13	1:A:217:LEU:C	2.35	0.52
1:A:237:LYS:HD2	1:B:500:TRP:CD1	2.45	0.52
1:A:142:VAL:HG22	1:A:146:VAL:CG2	2.38	0.51
1:A:332:GLU:CB	1:A:333:PRO:HD2	2.37	0.51
1:A:257:SER:CB	1:B:248:PRO:HG3	2.41	0.51
1:A:258:ASN:CG	1:A:532:LYS:HE2	2.35	0.51
1:A:280:LEU:HB3	1:A:395:LEU:HD22	1.92	0.51
1:A:195:MET:O	1:A:196:MET:HE2	2.11	0.51
1:B:505:THR:OG1	1:B:513:ILE:HD12	2.11	0.51
1:A:473:PHE:CG	1:A:484:VAL:HG21	2.46	0.51
1:A:183:ARG:HD2	1:B:244:TYR:CE2	2.46	0.51
1:B:387:GLU:HA	1:B:396:ARG:NH2	2.26	0.51
1:A:31:ILE:HD13	1:A:85:SER:CB	2.41	0.50
1:A:426:SER:O	1:A:502:GLU:HA	2.12	0.50
1:A:550:PRO:HG2	1:A:553:TYR:HD1	1.77	0.50
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.27	0.50
1:A:253:LEU:CG	1:B:253:LEU:HD21	2.41	0.50
1:A:280:LEU:CB	1:A:395:LEU:HD22	2.42	0.50
1:A:494:ASP:O	1:A:497:ALA:HB3	2.11	0.50
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.46	0.50
1:B:552:GLN:H	1:B:552:GLN:HE21	1.52	0.50
1:B:319:ALA:HB1	1:B:413:TRP:HB2	1.93	0.50
1:A:229:LYS:O	1:A:233:GLN:HG3	2.12	0.50
1:A:366:VAL:HG21	1:B:362:PRO:HB2	1.93	0.50
1:A:63:VAL:HG12	1:A:473:PHE:CZ	2.46	0.50
1:A:24:PHE:O	1:A:27:ASP:HB2	2.12	0.50
1:A:179:ASN:OD1	1:A:193:HIS:ND1	2.43	0.49
1:A:413:TRP:CH2	1:A:470:CYS:HB3	2.47	0.49
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.47	0.49
1:A:480:GLN:O	1:A:483:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:MET:HG2	1:B:509:PHE:CE2	2.47	0.49
1:A:536:ASP:N	1:A:537:PRO:CD	2.76	0.49
1:B:315:LEU:HD22	1:B:416:TRP:CH2	2.47	0.49
1:A:69:PHE:O	1:A:113:PRO:HD2	2.13	0.49
1:B:199:GLY:HA3	1:B:240:HIS:CD2	2.48	0.49
1:A:37:VAL:HG13	1:A:75:VAL:CG2	2.42	0.49
1:A:369:GLU:O	1:A:373:ASP:HB2	2.12	0.49
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.48	0.49
1:A:363:ILE:HD13	1:B:363:ILE:HG23	1.94	0.49
1:B:224:GLU:CD	1:B:224:GLU:H	2.20	0.49
1:A:197:HIS:HA	1:A:266:GLY:O	2.14	0.48
1:B:309:PRO:HG2	1:B:460:VAL:CB	2.42	0.48
1:A:74:ILE:HG23	1:A:120:VAL:HG12	1.96	0.48
1:A:177:LEU:O	1:A:181:VAL:HG13	2.13	0.48
1:A:280:LEU:HD12	1:A:280:LEU:C	2.38	0.48
1:A:312:ARG:HD3	1:A:317:ASP:OD1	2.14	0.48
1:B:479:ILE:O	1:B:483:LYS:HG3	2.12	0.48
1:A:7:PHE:HA	1:A:22:ASN:OD1	2.13	0.48
1:A:201:GLU:HB3	1:A:264:LYS:HB2	1.96	0.48
1:A:319:ALA:CB	1:A:413:TRP:HB2	2.42	0.48
1:B:40:ILE:HD11	1:B:74:ILE:CD1	2.40	0.48
1:B:187:TYR:O	1:B:402:MET:HG2	2.14	0.48
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.48	0.48
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.49	0.48
1:A:253:LEU:HD21	1:B:253:LEU:CG	2.44	0.48
1:A:332:GLU:HB3	1:A:333:PRO:CD	2.39	0.48
1:A:289:LEU:HD23	1:A:437:MET:SD	2.54	0.47
1:B:354:TYR:CE2	1:B:394:VAL:HG12	2.49	0.47
1:A:32:VAL:HG12	1:A:82:ASP:OD2	2.14	0.47
1:B:443:THR:HG21	1:B:469:VAL:CG2	2.44	0.47
1:A:248:PRO:HG3	1:B:257:SER:HB2	1.96	0.47
1:A:363:ILE:CD1	1:B:363:ILE:HG23	2.43	0.47
1:A:387:GLU:HA	1:A:396:ARG:NH2	2.29	0.47
1:B:71:ALA:HB2	1:B:120:VAL:HG23	1.96	0.47
1:B:229:LYS:O	1:B:233:GLN:HG3	2.14	0.47
1:B:526:ARG:HH21	1:B:529:GLU:CD	2.21	0.47
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.15	0.47
1:A:77:PRO:O	1:A:126:ASN:HB2	2.14	0.47
1:A:363:ILE:HG23	1:B:363:ILE:HD13	1.97	0.47
1:A:553:TYR:O	1:A:554:SER:C	2.57	0.47
1:B:492:ILE:HG23	1:B:502:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:NH2	1:B:269:LEU:O	2.48	0.47
1:A:506:HIS:O	1:A:507:LEU:C	2.56	0.47
1:B:217:LEU:CD1	1:B:217:LEU:C	2.88	0.47
1:B:403:GLN:HG3	1:B:405:ILE:HG13	1.96	0.47
1:A:534:ALA:HB1	1:B:530:VAL:HG12	1.97	0.47
1:B:61:THR:OG1	1:B:421:ALA:HB1	2.14	0.47
1:B:518:ASN:O	1:B:519:TRP:C	2.56	0.47
1:A:210:LEU:HD11	1:B:524:PHE:HA	1.97	0.47
1:A:217:LEU:C	1:A:217:LEU:CD1	2.88	0.46
1:B:197:HIS:HA	1:B:266:GLY:O	2.15	0.46
1:B:61:THR:HA	1:B:421:ALA:HB1	1.98	0.46
1:B:398:ARG:NH1	1:B:410:GLU:OE2	2.48	0.46
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.51	0.46
1:A:286:ASP:HB2	1:A:350:ARG:HG2	1.97	0.46
1:A:264:LYS:HG3	2:A:2008:HOH:O	2.16	0.46
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.81	0.46
1:B:131:LEU:HD12	1:B:141:VAL:HG12	1.97	0.46
1:B:378:ILE:O	1:B:381:VAL:HB	2.16	0.46
1:A:167:ASP:OD1	1:A:193:HIS:NE2	2.49	0.45
1:A:237:LYS:HD2	1:B:500:TRP:NE1	2.32	0.45
1:A:372:LYS:HG2	1:A:383:PHE:CZ	2.51	0.45
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.99	0.45
1:B:97:LEU:HD12	1:B:541:ILE:HD13	1.98	0.45
1:A:534:ALA:HB2	1:B:534:ALA:HB2	1.97	0.45
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.51	0.45
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.51	0.45
1:A:361:GLU:O	1:A:362:PRO:C	2.60	0.45
1:A:443:THR:O	1:A:443:THR:HG22	2.17	0.45
1:B:217:LEU:C	1:B:217:LEU:HD13	2.42	0.45
1:B:520:ASN:O	1:B:521:ASN:HB2	2.15	0.45
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.97	0.45
1:A:253:LEU:CD2	1:B:253:LEU:HD21	2.47	0.45
1:B:230:PRO:HA	1:B:233:GLN:NE2	2.32	0.45
1:A:315:LEU:HD22	1:A:416:TRP:CZ2	2.51	0.45
1:B:413:TRP:CH2	1:B:470:CYS:HB3	2.52	0.45
1:A:61:THR:OG1	1:A:421:ALA:HB1	2.16	0.45
1:B:168:VAL:HB	1:B:169:PRO:HD2	1.99	0.45
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.99	0.45
1:B:559:LYS:HE2	2:B:2007:HOH:O	2.15	0.45
1:B:258:ASN:HB2	1:B:541:ILE:O	2.17	0.44
1:A:444:LYS:O	1:A:445:LYS:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:VAL:HG22	1:A:146:VAL:CB	2.48	0.44
1:A:244:TYR:CG	1:B:183:ARG:HD2	2.52	0.44
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.52	0.44
1:A:61:THR:HA	1:A:421:ALA:HB1	1.99	0.44
1:A:319:ALA:O	1:A:320:VAL:C	2.60	0.44
1:B:79:ASN:ND2	1:B:79:ASN:C	2.75	0.44
1:A:38:GLU:HB3	1:A:74:ILE:HD13	1.99	0.44
1:B:177:LEU:HD12	1:B:177:LEU:C	2.42	0.44
1:B:549:TRP:HA	1:B:550:PRO:HD3	1.85	0.44
1:A:137:GLY:O	1:A:138:ALA:HB3	2.17	0.44
1:A:253:LEU:HD21	1:B:253:LEU:CD2	2.47	0.44
1:A:378:ILE:O	1:A:381:VAL:HB	2.18	0.44
1:B:63:VAL:HG11	1:B:423:LEU:CD1	2.32	0.44
1:B:448:GLN:O	1:B:449:GLU:C	2.61	0.44
1:A:105:ASN:O	1:A:106:SER:C	2.58	0.44
1:A:428:ILE:HG21	1:B:238:ILE:HG21	1.99	0.44
1:A:144:PRO:HD3	1:A:263:THR:O	2.18	0.44
1:A:211:ARG:HD2	1:A:235:TRP:CH2	2.53	0.44
1:A:255:SER:O	1:A:256:GLN:C	2.59	0.44
1:B:295:ILE:O	1:B:298:PRO:HD2	2.18	0.44
1:A:80:VAL:O	1:A:81:ALA:C	2.60	0.44
1:A:301:LEU:HD22	2:A:2010:HOH:O	2.17	0.43
1:A:346:LEU:O	1:A:347:ASN:HB2	2.18	0.43
1:A:553:TYR:HD2	1:A:558:TRP:NE1	2.16	0.43
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.18	0.43
1:B:349:GLY:H	1:B:352:ASN:HD21	1.65	0.43
1:B:480:GLN:O	1:B:483:LYS:HB2	2.17	0.43
1:A:84:GLN:NE2	1:A:207:GLY:O	2.32	0.43
1:A:402:MET:HE3	1:A:402:MET:HB2	1.91	0.43
1:A:195:MET:HE2	1:B:244:TYR:OH	2.18	0.43
1:A:473:PHE:CE2	1:A:484:VAL:HG11	2.53	0.43
1:A:372:LYS:HG2	1:A:383:PHE:CE2	2.53	0.43
1:B:386:PRO:HD2	1:B:387:GLU:OE2	2.17	0.43
1:A:112:ALA:O	1:A:507:LEU:HD11	2.19	0.43
1:A:230:PRO:HA	1:A:233:GLN:CD	2.43	0.43
1:A:415:ASP:O	1:A:416:TRP:C	2.58	0.43
1:B:308:VAL:HG13	1:B:460:VAL:O	2.18	0.43
1:A:111:ALA:O	1:A:112:ALA:C	2.61	0.43
1:B:28:ILE:O	1:B:32:VAL:HG22	2.18	0.43
1:B:271:PRO:O	1:B:272:ASN:C	2.61	0.43
1:A:271:PRO:HG3	1:B:301:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:THR:HG21	1:A:509:PHE:HB2	2.01	0.43
1:B:321:LEU:HD13	1:B:346:LEU:HD22	2.01	0.43
1:B:445:LYS:O	1:B:446:ARG:C	2.61	0.43
1:A:131:LEU:HD11	1:A:264:LYS:HG2	2.01	0.43
1:A:307:ASN:O	1:A:309:PRO:HD3	2.19	0.43
1:B:79:ASN:HD22	1:B:82:ASP:H	1.63	0.43
1:B:527:PHE:CZ	1:B:531:LEU:HD11	2.54	0.43
1:A:9:PRO:HG2	1:A:12:LEU:HD23	2.00	0.43
1:A:253:LEU:HD21	1:B:253:LEU:HG	2.00	0.43
1:A:78:ARG:HH11	1:A:78:ARG:HD2	1.52	0.42
1:B:201:GLU:HB3	1:B:264:LYS:HB2	2.00	0.42
1:A:205:ALA:HB2	1:A:541:ILE:HG12	2.00	0.42
1:A:493:ASP:O	1:A:494:ASP:C	2.61	0.42
1:A:545:LYS:HD2	1:A:546:SER:N	2.34	0.42
1:A:140:CYS:SG	1:A:269:LEU:HD21	2.59	0.42
1:A:403:GLN:HG3	1:A:405:ILE:HG13	2.01	0.42
1:A:454:PHE:CD2	1:A:454:PHE:C	2.98	0.42
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.99	0.42
1:B:417:LEU:HD12	1:B:473:PHE:HA	2.01	0.42
1:B:506:HIS:O	1:B:507:LEU:C	2.59	0.42
1:B:309:PRO:HD2	1:B:460:VAL:HB	2.00	0.42
1:B:387:GLU:HA	1:B:396:ARG:HH22	1.82	0.42
1:B:206:ASN:OD1	1:B:208:GLU:HB2	2.19	0.42
1:B:340:ASP:O	1:B:343:ALA:HB3	2.19	0.42
1:B:519:TRP:O	1:B:520:ASN:C	2.59	0.42
1:A:209:LEU:HD13	1:B:519:TRP:HH2	1.85	0.42
1:A:289:LEU:O	1:A:293:VAL:HG23	2.20	0.42
1:B:143:GLU:HB3	1:B:144:PRO:CD	2.50	0.42
1:A:372:LYS:HA	1:A:383:PHE:CE1	2.55	0.42
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.19	0.42
1:A:152:HIS:O	1:A:153:ASN:C	2.62	0.42
1:A:519:TRP:O	1:A:520:ASN:C	2.63	0.42
1:B:433:GLY:O	1:B:434:GLU:C	2.63	0.42
1:A:502:GLU:CB	1:A:513:ILE:HD13	2.46	0.42
1:B:90:ALA:O	1:B:94:SER:N	2.53	0.42
1:B:129:ARG:HH21	1:B:143:GLU:CD	2.26	0.42
1:B:315:LEU:HA	1:B:318:ALA:HB3	2.01	0.42
1:B:372:LYS:HG2	1:B:383:PHE:CE2	2.55	0.42
1:A:28:ILE:O	1:A:32:VAL:HG22	2.20	0.42
1:B:9:PRO:HG2	1:B:12:LEU:CD2	2.50	0.42
1:A:63:VAL:CG1	1:A:423:LEU:HD11	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:C	1:A:177:LEU:HD12	2.44	0.41
1:A:258:ASN:HB2	1:A:542:ALA:HB3	2.02	0.41
1:A:473:PHE:CD2	1:A:484:VAL:HG21	2.55	0.41
1:B:59:ASP:CG	1:B:506:HIS:HE2	2.28	0.41
1:B:129:ARG:NH2	1:B:143:GLU:OE2	2.36	0.41
1:B:315:LEU:HD22	1:B:416:TRP:CZ2	2.55	0.41
1:A:25:ILE:HG22	1:A:29:ILE:HD12	2.02	0.41
1:A:87:VAL:HG11	1:A:207:GLY:HA2	2.01	0.41
1:A:364:ARG:HH11	1:A:364:ARG:HD2	1.59	0.41
1:B:284:PRO:HD2	1:B:288:ASP:OD2	2.20	0.41
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.54	0.41
1:A:321:LEU:HD13	1:A:346:LEU:HD22	2.02	0.41
1:B:231:GLU:H	1:B:231:GLU:HG3	1.15	0.41
1:B:250:ILE:HD12	1:B:254:PHE:CE2	2.46	0.41
1:B:473:PHE:CD2	1:B:484:VAL:HG21	2.55	0.41
1:A:250:ILE:HD12	1:A:254:PHE:CE2	2.51	0.41
1:A:256:GLN:NE2	1:A:504:ARG:HG3	2.34	0.41
1:A:309:PRO:HB2	1:A:353:PHE:CZ	2.56	0.41
1:B:90:ALA:HB1	1:B:95:PHE:O	2.20	0.41
1:B:201:GLU:CB	1:B:264:LYS:HB2	2.50	0.41
1:B:139:TYR:CD1	1:B:139:TYR:C	2.99	0.41
1:B:525:LEU:CD1	1:B:548:VAL:HG22	2.50	0.41
1:A:38:GLU:N	1:A:74:ILE:O	2.53	0.41
1:A:316:LEU:O	1:A:319:ALA:HB3	2.20	0.41
1:B:9:PRO:HG2	1:B:12:LEU:HD23	2.02	0.41
1:B:24:PHE:O	1:B:27:ASP:HB2	2.20	0.41
1:B:481:LYS:O	1:B:484:VAL:HB	2.21	0.41
1:B:530:VAL:O	1:B:531:LEU:C	2.64	0.41
1:A:148:TYR:CD1	1:A:168:VAL:HG12	2.56	0.41
1:A:297:ARG:HB3	1:A:297:ARG:HH11	1.86	0.41
1:A:522:SER:O	1:A:523:SER:C	2.63	0.41
1:B:87:VAL:HG11	1:B:207:GLY:HA2	2.02	0.41
1:B:522:SER:O	1:B:523:SER:C	2.63	0.41
1:B:13:PRO:HA	1:B:117:GLY:HA3	2.03	0.41
1:B:177:LEU:HB2	1:B:265:ILE:CG2	2.51	0.41
1:A:59:ASP:CG	1:A:506:HIS:HE2	2.28	0.40
1:A:319:ALA:HB1	1:A:413:TRP:CB	2.49	0.40
1:A:82:ASP:O	1:A:86:ILE:HG13	2.20	0.40
1:A:417:LEU:HD12	1:A:473:PHE:HA	2.03	0.40
1:A:428:ILE:CG2	1:B:238:ILE:HG21	2.51	0.40
1:A:540:ILE:H	1:A:540:ILE:HG13	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:PRO:O	1:B:460:VAL:HG23	2.22	0.40
1:A:9:PRO:HG2	1:A:12:LEU:CD2	2.52	0.40
1:B:37:VAL:HG13	1:B:75:VAL:HG22	2.03	0.40
1:B:133:VAL:HG21	1:B:154:TYR:CE1	2.56	0.40
1:B:177:LEU:HB2	1:B:265:ILE:HG21	2.03	0.40
1:B:431:VAL:HG22	1:B:465:MET:CG	2.52	0.40
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.57	0.40
1:B:446:ARG:O	1:B:447:CYS:C	2.65	0.40

All (18) 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:330:ARG:NH2	1:A:332:GLU:CB[2_765]	0.47	1.73
1:A:52:MET:SD	1:B:415:ASP:OD1[6_655]	0.77	1.43
1:A:18:LEU:CD2	1:A:30:ARG:NH1[3_655]	1.13	1.07
1:A:330:ARG:NH2	1:A:332:GLU:CA[2_765]	1.17	1.03
1:A:53:LYS:CA	1:B:412:LYS:NZ[6_655]	1.35	0.85
1:A:52:MET:SD	1:B:415:ASP:CG[6_655]	1.37	0.83
1:A:330:ARG:CZ	1:A:332:GLU:CB[2_765]	1.41	0.79
1:A:52:MET:CE	1:B:415:ASP:CB[6_655]	1.84	0.36
1:A:52:MET:CE	1:B:415:ASP:CG[6_655]	1.84	0.36
1:A:330:ARG:NH2	1:A:332:GLU:CG[2_765]	1.92	0.28
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	1.96	0.24
1:A:52:MET:CE	1:B:415:ASP:OD1[6_655]	2.01	0.19
1:A:52:MET:SD	1:B:415:ASP:OD2[6_655]	2.08	0.12
1:A:330:ARG:NH2	1:A:332:GLU:N[2_765]	2.10	0.10
1:A:337:GLU:OE2	1:A:448:GLN:O[2_765]	2.11	0.09
1:A:330:ARG:NH2	1:A:332:GLU:C[2_765]	2.13	0.07
1:A:53:LYS:C	1:B:412:LYS:NZ[6_655]	2.14	0.06
1:A:373:ASP:OD2	1:B:288:ASP:OD1[4_665]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	541/560 (97%)	494 (91%)	40 (7%)	7 (1%)	9	32
1	B	541/560 (97%)	490 (91%)	47 (9%)	4 (1%)	18	48
All	All	1082/1120 (97%)	984 (91%)	87 (8%)	11 (1%)	12	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	PHE
1	A	7	PHE
1	A	67	ASP
1	B	410	GLU
1	A	410	GLU
1	B	409	ASP
1	A	297	ARG
1	A	409	ASP
1	A	146	VAL
1	A	63	VAL
1	B	63	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	466/481 (97%)	418 (90%)	48 (10%)	7	23
1	B	466/481 (97%)	419 (90%)	47 (10%)	7	24
All	All	932/962 (97%)	837 (90%)	95 (10%)	7	23

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	61	THR

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Mol	Chain	Res	Type
1	A	75	VAL
1	A	79	ASN
1	A	87	VAL
1	A	106	SER
1	A	115	VAL
1	A	116	SER
1	A	128	ASN
1	A	136	GLU
1	A	142	VAL
1	A	155	LEU
1	A	177	LEU
1	A	181	VAL
1	A	211	ARG
1	A	217	LEU
1	A	220	PRO
1	A	221	LYS
1	A	231	GLU
1	A	237	LYS
1	A	267	ILE
1	A	280	LEU
1	A	290	LYS
1	A	297	ARG
1	A	301	LEU
1	A	303	MET
1	A	323	ASP
1	A	329	SER
1	A	331	THR
1	A	336	ASP
1	A	342	ILE
1	A	372	LYS
1	A	381	VAL
1	A	387	GLU
1	A	391	GLU
1	A	401	THR
1	A	411	LEU
1	A	432	SER
1	A	446	ARG
1	A	457	THR
1	A	472	VAL
1	A	502	GLU
1	A	503	TYR
1	A	505	THR

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Mol	Chain	Res	Type
1	A	506	HIS
1	A	516	THR
1	A	532	LYS
1	A	552	GLN
1	B	19	SER
1	B	52	MET
1	B	61	THR
1	B	79	ASN
1	B	87	VAL
1	B	115	VAL
1	B	128	ASN
1	B	136	GLU
1	B	142	VAL
1	B	155	LEU
1	B	177	LEU
1	B	181	VAL
1	B	200	MET
1	B	211	ARG
1	B	217	LEU
1	B	231	GLU
1	B	237	LYS
1	B	238	ILE
1	B	267	ILE
1	B	283	LEU
1	B	297	ARG
1	B	301	LEU
1	B	303	MET
1	B	325	ARG
1	B	329	SER
1	B	331	THR
1	B	336	ASP
1	B	342	ILE
1	B	344	LYS
1	B	372	LYS
1	B	381	VAL
1	B	387	GLU
1	B	391	GLU
1	B	401	THR
1	B	411	LEU
1	B	426	SER
1	B	432	SER
1	B	457	THR

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Mol	Chain	Res	Type
1	B	462	MET
1	B	472	VAL
1	B	502	GLU
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	523	SER
1	B	551	SER
1	B	552	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	79	ASN
1	A	128	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	403	GLN
1	A	439	GLN
1	A	467	HIS
1	A	520	ASN
1	A	552	GLN
1	B	62	HIS
1	B	79	ASN
1	B	128	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	467	HIS
1	B	520	ASN
1	B	552	GLN

5.3.3 RNA ⓘ

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

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	545/560 (97%)	-0.02	10 (1%) 67 59	3, 14, 34, 49	30 (5%)
1	B	545/560 (97%)	-0.01	11 (2%) 65 56	3, 14, 34, 49	30 (5%)
All	All	1090/1120 (97%)	-0.02	21 (1%) 66 58	3, 14, 34, 49	60 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	MET	3.4
1	A	95	PHE	2.8
1	B	61	THR	2.7
1	B	418	PRO	2.6
1	B	63	VAL	2.6
1	A	52	MET	2.5
1	B	62	HIS	2.5
1	B	6	GLU	2.4
1	B	7	PHE	2.4
1	B	54	PRO	2.4
1	A	54	PRO	2.3
1	A	62	HIS	2.2
1	A	6	GLU	2.2
1	A	409	ASP	2.1
1	A	331	THR	2.1
1	B	331	THR	2.1
1	A	61	THR	2.1
1	A	329	SER	2.1
1	A	41	SER	2.1
1	B	66	GLN	2.1
1	B	95	PHE	2.1

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 oligosaccharides 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.