



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:50 PM UTC

PDB ID : 1RLD / pdb_00001rld
Title : SOLID-STATE PHASE TRANSITION IN THE CRYSTAL STRUCTURE OF
RIBULOSE 1,5-BIPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE
Authors : Zhang, K.Y.J.; Eisenberg, D.
Deposited on : 1993-12-10
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	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

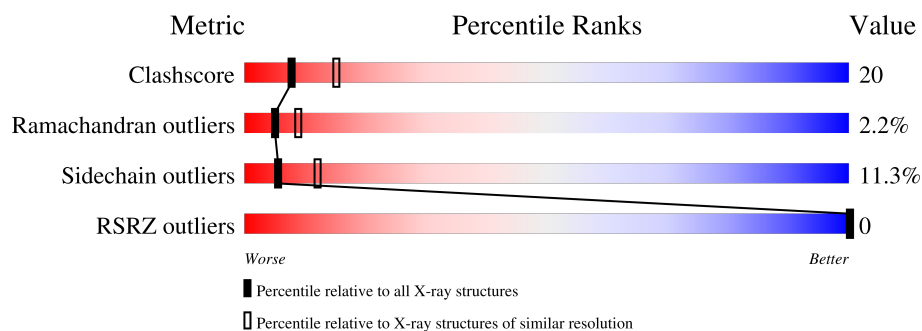
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

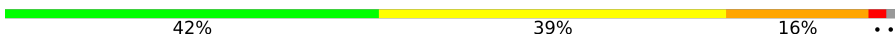
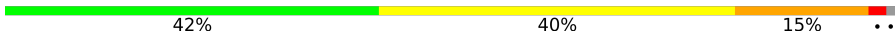
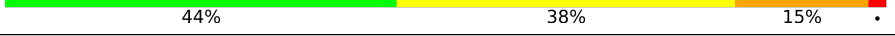
The reported resolution of this entry is 2.50 Å.

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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	446	
1	B	446	
2	S	123	
2	T	123	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8970 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 RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3456	2194	611	635	16			
1	B	441	Total	C	N	O	S	0	0	0
			3456	2194	611	635	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	GLU	GLN	conflict	UNP P00876
A	377	VAL	GLU	conflict	UNP P00876
B	229	GLU	GLN	conflict	UNP P00876
B	377	VAL	GLU	conflict	UNP P00876

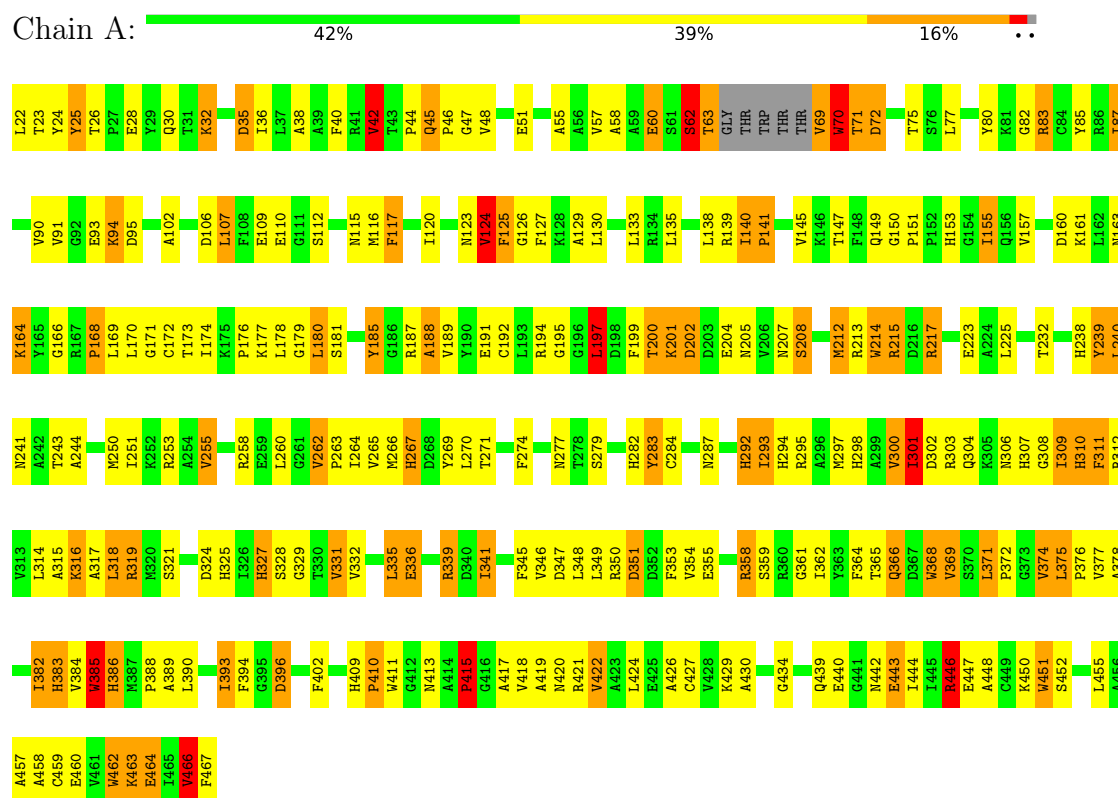
- Molecule 2 is a protein called RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1029	672	163	188	6			
2	T	123	Total	C	N	O	S	0	0	0
			1029	672	163	188	6			

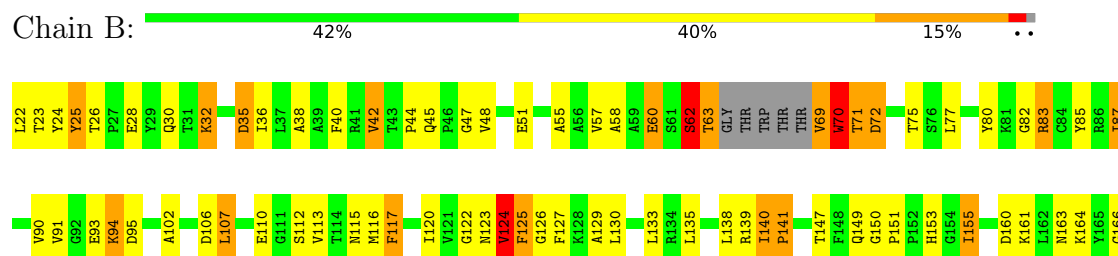
3 Residue-property plots

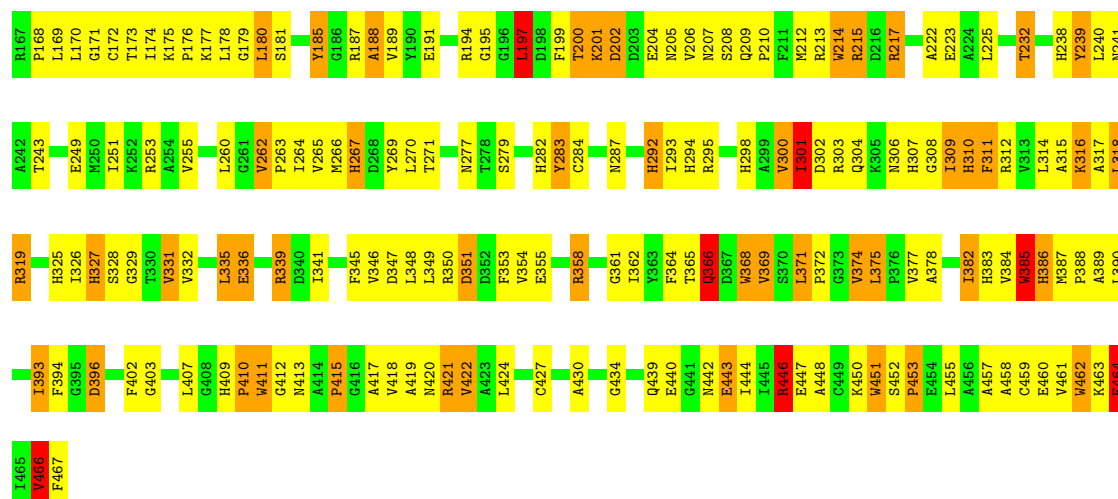
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



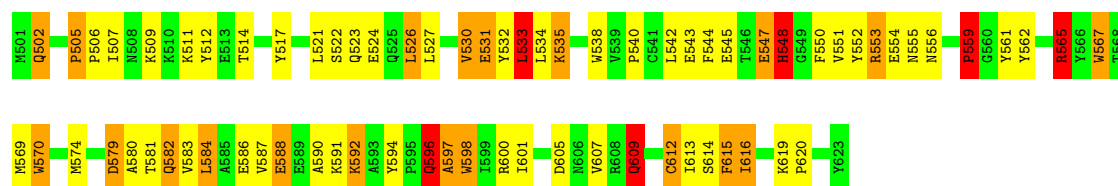
- Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)





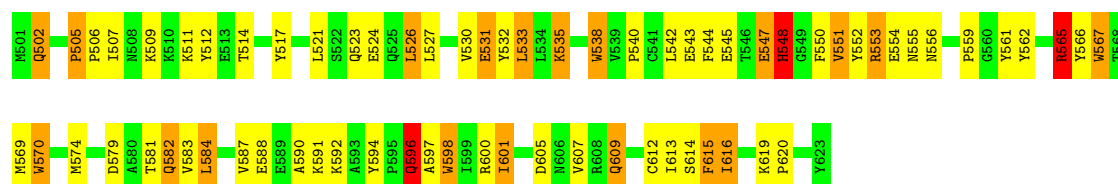
- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain S: 41% 37% 16% 5%



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain T: 44% 38% 15% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	153.01Å 153.01Å 113.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 76.2 (8.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.50Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.211 , (Not available) 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.266 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8970	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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	1.44	35/3539 (1.0%)	2.26	166/4796 (3.5%)
1	B	1.40	29/3539 (0.8%)	2.25	168/4796 (3.5%)
2	S	1.27	4/1062 (0.4%)	2.22	57/1442 (4.0%)
2	T	1.24	3/1062 (0.3%)	2.24	56/1442 (3.9%)
All	All	1.38	71/9202 (0.8%)	2.25	447/12476 (3.6%)

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	2
1	B	0	2
All	All	0	4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	HIS	CD2-NE2	-9.39	1.27	1.37
2	S	616	ILE	CA-CB	8.64	1.64	1.53
1	A	238	HIS	CD2-NE2	-8.47	1.28	1.37
2	T	616	ILE	CA-CB	8.09	1.63	1.53
1	A	298	HIS	CD2-NE2	-7.89	1.29	1.37
1	B	69	VAL	CA-C	7.77	1.62	1.52
1	B	63	THR	CA-C	7.76	1.62	1.52
1	A	386	HIS	CD2-NE2	-7.36	1.29	1.37
1	B	287	ASN	CA-CB	-7.28	1.43	1.53
1	A	70	TRP	CA-CB	7.19	1.65	1.53
1	B	69	VAL	CA-CB	7.17	1.64	1.54
1	A	69	VAL	CA-C	7.11	1.61	1.52
1	A	63	THR	CA-C	7.08	1.61	1.52
1	A	69	VAL	CA-CB	6.94	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	327	HIS	CG-ND1	-6.91	1.30	1.38
1	B	327	HIS	CD2-NE2	-6.87	1.30	1.37
1	B	206	VAL	CA-CB	6.85	1.61	1.53
1	B	327	HIS	CG-ND1	-6.73	1.30	1.38
2	T	548	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	292	HIS	CG-ND1	-6.69	1.30	1.38
1	B	70	TRP	CA-CB	6.66	1.64	1.53
2	S	548	HIS	CD2-NE2	-6.63	1.30	1.37
1	B	310	HIS	CG-ND1	-6.55	1.31	1.38
1	B	113	VAL	CA-CB	6.51	1.62	1.54
1	A	287	ASN	CA-CB	-6.51	1.45	1.54
1	B	310	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	212	MET	CA-CB	-6.47	1.44	1.52
1	B	409	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	267	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	294	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	292	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	325	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	298	HIS	CG-ND1	-6.23	1.31	1.38
1	B	325	HIS	CD2-NE2	-6.17	1.31	1.37
2	S	567	TRP	NE1-CE2	-6.16	1.30	1.37
1	A	153	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	310	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	307	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	385	TRP	CA-CB	6.03	1.62	1.53
1	A	409	HIS	CD2-NE2	-6.02	1.31	1.37
1	B	238	HIS	CG-ND1	-6.01	1.31	1.38
1	A	238	HIS	CG-ND1	-5.99	1.31	1.38
1	B	386	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	298	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	282	HIS	CD2-NE2	-5.90	1.31	1.37
2	S	555	ASN	CA-C	-5.78	1.44	1.52
1	B	153	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	462	TRP	CA-CB	5.72	1.63	1.53
1	B	387	MET	CA-CB	-5.67	1.47	1.53
1	A	327	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	346	VAL	CA-CB	-5.66	1.47	1.54
1	A	376	PRO	CA-CB	-5.63	1.46	1.53
1	B	292	HIS	CG-ND1	-5.53	1.32	1.38
1	B	294	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	346	VAL	CA-CB	-5.45	1.48	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	HIS	CG-ND1	-5.42	1.32	1.38
1	B	462	TRP	CA-CB	5.38	1.62	1.53
1	B	282	HIS	CD2-NE2	-5.37	1.31	1.37
1	A	217	ARG	CA-CB	-5.36	1.45	1.53
1	A	383	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	267	HIS	CD2-NE2	-5.33	1.31	1.37
2	T	538	TRP	CG-CD2	-5.25	1.34	1.43
1	A	386	HIS	CG-ND1	-5.25	1.32	1.38
1	A	164	LYS	CA-C	-5.21	1.46	1.52
1	A	42	VAL	CA-CB	5.19	1.61	1.54
1	A	141	PRO	CA-C	5.13	1.54	1.51
1	A	69	VAL	N-CA	5.10	1.52	1.46
1	B	69	VAL	N-CA	5.09	1.52	1.46
1	B	328	SER	CA-CB	-5.04	1.45	1.53
1	B	292	HIS	CA-CB	-5.03	1.46	1.53

All (447) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	VAL	N-CA-C	15.30	130.18	111.05
1	A	384	VAL	N-CA-C	14.76	129.50	111.05
1	A	384	VAL	CA-C-O	-14.28	105.29	120.57
1	B	384	VAL	CA-C-O	-14.11	105.47	120.57
1	A	385	TRP	CA-CB-CG	14.01	140.21	113.60
1	B	385	TRP	CA-CB-CG	13.76	139.75	113.60
2	T	547	GLU	N-CA-C	13.56	128.12	112.93
2	S	547	GLU	N-CA-C	13.41	127.95	112.93
1	A	69	VAL	N-CA-C	12.05	134.41	109.34
1	B	69	VAL	N-CA-C	11.88	134.06	109.34
1	B	35	ASP	CA-CB-CG	10.89	123.49	112.60
1	B	117	PHE	CA-C-O	-10.80	109.57	120.70
1	A	413	ASN	N-CA-C	10.44	123.63	111.11
1	B	385	TRP	CB-CG-CD1	-9.97	111.95	126.90
1	A	335	LEU	N-CA-C	9.87	125.16	109.86
1	A	35	ASP	CA-CB-CG	9.68	122.28	112.60
1	B	214	TRP	N-CA-C	9.67	121.41	111.07
1	B	413	ASN	N-CA-C	9.62	122.66	111.11
1	A	214	TRP	N-CA-C	9.51	121.24	111.07
1	B	335	LEU	N-CA-C	9.24	124.69	110.36
1	A	160	ASP	CA-CB-CG	9.23	121.83	112.60
2	S	615	PHE	CA-CB-CG	9.19	122.99	113.80
1	A	385	TRP	CB-CG-CD1	-9.17	113.14	126.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	PHE	CA-C-O	-8.94	111.49	120.70
1	B	153	HIS	CA-CB-CG	-8.78	105.02	113.80
1	B	140	ILE	N-CA-CB	-8.73	98.99	111.21
2	T	615	PHE	CA-CB-CG	8.71	122.51	113.80
1	B	325	HIS	CA-CB-CG	8.66	122.46	113.80
1	A	140	ILE	N-CA-CB	-8.64	99.11	111.21
1	B	63	THR	O-C-N	-8.60	114.94	123.46
2	S	548	HIS	CA-CB-CG	8.59	122.39	113.80
1	B	204	GLU	CA-CB-CG	8.54	131.17	114.10
1	A	283	TYR	N-CA-C	-8.51	101.97	111.07
1	B	36	ILE	N-CA-C	-8.45	96.27	108.36
1	A	36	ILE	N-CA-C	-8.37	96.39	108.36
1	A	63	THR	O-C-N	-8.28	115.26	123.46
1	B	462	TRP	CA-CB-CG	8.28	129.32	113.60
2	T	548	HIS	CA-CB-CG	8.16	121.96	113.80
1	A	462	TRP	CA-CB-CG	8.15	129.08	113.60
1	A	284	CYS	CA-C-O	-8.09	110.67	119.97
1	A	204	GLU	CA-CB-CG	8.05	130.20	114.10
1	B	69	VAL	CA-C-N	8.00	136.81	121.54
1	B	69	VAL	C-N-CA	8.00	136.81	121.54
1	B	263	PRO	N-CA-C	7.98	123.83	113.86
1	B	385	TRP	CG-CD2-CE3	7.93	141.83	133.90
2	T	553	ARG	N-CA-C	-7.93	94.49	108.13
1	B	302	ASP	N-CA-C	7.92	123.09	112.88
1	A	30	GLN	OE1-CD-NE2	-7.90	114.70	122.60
1	A	69	VAL	CA-C-N	7.87	136.56	121.54
1	A	69	VAL	C-N-CA	7.87	136.56	121.54
1	A	458	ALA	N-CA-C	-7.86	101.81	111.40
2	S	609	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	B	124	VAL	N-CA-C	7.83	117.89	110.53
2	T	550	PHE	CA-CB-CG	-7.82	105.98	113.80
1	A	302	ASP	N-CA-C	7.80	122.95	112.88
2	T	555	ASN	CA-CB-CG	-7.73	104.87	112.60
2	S	550	PHE	CA-CB-CG	-7.72	106.08	113.80
1	B	160	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	345	PHE	CA-CB-CG	7.69	121.49	113.80
1	A	153	HIS	CA-CB-CG	-7.66	106.14	113.80
1	A	70	TRP	CB-CG-CD1	-7.64	115.44	126.90
1	A	345	PHE	CA-CB-CG	7.62	121.42	113.80
1	A	336	GLU	N-CA-C	7.61	121.42	110.24
1	B	317	ALA	N-CA-C	-7.60	102.93	111.14
2	T	555	ASN	N-CA-C	7.59	120.44	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	553	ARG	N-CA-C	-7.58	95.10	108.13
1	B	458	ALA	N-CA-C	-7.57	102.38	111.69
1	B	364	PHE	CA-CB-CG	7.55	121.35	113.80
1	B	70	TRP	CB-CG-CD1	-7.53	115.61	126.90
1	B	70	TRP	CG-CD2-CE3	7.52	141.42	133.90
1	B	351	ASP	N-CA-C	7.52	122.28	110.17
2	T	512	TYR	CA-C-O	7.51	130.20	121.34
1	A	325	HIS	CA-CB-CG	7.49	121.29	113.80
1	B	283	TYR	N-CA-C	-7.49	103.06	111.07
1	A	70	TRP	CG-CD2-CE3	7.45	141.35	133.90
1	B	30	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	A	442	ASN	CA-CB-CG	7.41	120.01	112.60
1	B	262	VAL	CA-C-N	7.41	127.05	119.56
1	B	262	VAL	C-N-CA	7.41	127.05	119.56
1	A	318	LEU	CA-C-O	-7.35	112.76	120.55
2	S	512	TYR	CA-C-O	7.35	130.01	121.34
1	B	336	GLU	N-CA-C	7.35	121.15	110.42
1	B	467	PHE	CA-CB-CG	7.34	121.14	113.80
1	B	141	PRO	CA-C-O	-7.31	115.63	120.90
1	B	292	HIS	CB-CG-CD2	-7.26	121.76	131.20
1	B	294	HIS	CB-CG-CD2	-7.24	121.79	131.20
1	B	123	ASN	CA-CB-CG	7.19	119.79	112.60
1	B	362	ILE	N-CA-CB	-7.18	102.48	111.31
1	A	319	ARG	CB-CG-CD	7.17	127.80	111.30
2	S	570	TRP	CA-C-O	7.12	127.95	120.54
1	B	279	SER	O-C-N	-7.10	114.59	122.12
2	T	514	THR	CA-C-O	7.08	128.99	120.92
1	A	385	TRP	CG-CD2-CE3	7.08	140.98	133.90
1	A	263	PRO	N-CA-C	7.07	122.70	113.86
1	A	310	HIS	CA-CB-CG	-7.07	106.73	113.80
2	T	570	TRP	CG-CD2-CE3	7.06	140.96	133.90
1	A	309	ILE	N-CA-C	-7.03	97.98	108.46
2	S	555	ASN	CA-CB-CG	-7.03	105.57	112.60
1	A	396	ASP	N-CA-C	7.02	118.93	111.28
2	S	569	MET	CA-CB-CG	7.00	128.09	114.10
1	B	24	TYR	N-CA-C	-6.98	104.41	114.12
1	A	301	ILE	N-CA-C	6.98	118.60	111.00
1	A	420	ASN	CA-CB-CG	-6.97	105.63	112.60
1	B	309	ILE	N-CA-C	-6.97	98.07	108.46
2	T	569	MET	CA-CB-CG	6.93	127.96	114.10
1	B	385	TRP	CB-CG-CD2	6.92	136.49	126.80
1	A	225	LEU	N-CA-C	6.91	119.83	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	565	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	B	300	VAL	N-CA-C	-6.88	104.07	110.53
1	A	141	PRO	CA-C-O	-6.87	115.95	120.90
1	B	420	ASN	CA-CB-CG	-6.86	105.75	112.60
1	A	200	THR	O-C-N	-6.83	114.27	123.15
1	A	351	ASP	N-CA-C	6.83	121.16	110.17
1	B	319	ARG	NE-CZ-NH1	6.83	128.33	121.50
2	T	548	HIS	CB-CG-CD2	-6.82	122.34	131.20
1	A	24	TYR	N-CA-C	-6.78	104.69	114.12
1	A	362	ILE	N-CA-CB	-6.78	102.97	111.31
2	T	570	TRP	CA-C-O	6.78	127.59	120.54
1	B	200	THR	O-C-N	-6.76	114.36	123.15
2	T	609	GLN	OE1-CD-NE2	-6.76	115.83	122.60
1	A	279	SER	O-C-N	-6.75	114.96	122.12
2	S	514	THR	CA-C-O	6.74	128.61	120.92
2	T	548	HIS	N-CA-CB	6.74	121.88	110.49
1	A	157	VAL	N-CA-C	-6.72	103.76	110.62
1	B	318	LEU	CA-C-O	-6.70	113.78	120.82
1	B	301	ILE	N-CA-C	6.69	118.29	111.00
1	B	310	HIS	CA-CB-CG	-6.69	107.11	113.80
1	B	253	ARG	CG-CD-NE	-6.67	97.33	112.00
1	B	319	ARG	CB-CG-CD	6.66	126.62	111.30
1	A	294	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	A	364	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	385	TRP	CB-CG-CD2	6.65	136.10	126.80
2	S	514	THR	O-C-N	6.64	131.19	122.95
1	B	284	CYS	CA-C-O	-6.62	112.36	119.97
1	A	300	VAL	N-CA-C	-6.60	104.32	110.53
1	A	253	ARG	CG-CD-NE	-6.60	97.47	112.00
1	A	47	GLY	CA-C-O	-6.60	113.82	119.56
1	A	215	ARG	NE-CZ-NH1	6.59	128.09	121.50
1	A	306	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	62	SER	N-CA-C	6.58	117.26	108.38
1	A	262	VAL	CA-C-N	6.58	126.20	119.56
1	A	262	VAL	C-N-CA	6.58	126.20	119.56
2	S	548	HIS	CB-CG-CD2	-6.57	122.66	131.20
2	T	526	LEU	CB-CA-C	-6.57	99.88	110.79
1	A	393	ILE	N-CA-C	-6.57	104.36	110.53
1	A	208	SER	N-CA-C	-6.56	98.21	108.90
1	A	321	SER	N-CA-C	-6.55	104.06	111.14
1	B	32	LYS	CA-CB-CG	6.55	127.20	114.10
1	B	225	LEU	N-CA-C	6.54	119.40	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	555	ASN	N-CA-C	6.53	119.22	111.71
2	S	548	HIS	N-CA-CB	6.53	121.53	110.49
1	B	442	ASN	CA-CB-CG	6.50	119.10	112.60
1	B	316	LYS	N-CA-C	-6.50	104.04	112.23
1	A	255	VAL	CA-C-O	-6.49	114.30	121.05
1	A	332	VAL	CA-C-O	6.49	128.89	120.78
2	T	531	GLU	CB-CG-CD	6.48	123.61	112.60
1	A	70	TRP	CA-CB-CG	6.46	125.88	113.60
1	A	369	VAL	N-CA-C	6.46	122.77	109.34
1	A	123	ASN	CA-CB-CG	6.46	119.06	112.60
2	S	531	GLU	CB-CG-CD	6.44	123.55	112.60
1	A	124	VAL	N-CA-C	6.44	116.58	110.53
2	T	565	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	B	62	SER	N-CA-C	6.43	117.06	108.38
1	B	375	LEU	CA-C-N	6.40	126.74	119.83
1	B	375	LEU	C-N-CA	6.40	126.74	119.83
1	A	362	ILE	N-CA-C	-6.39	97.77	107.73
1	A	244	ALA	O-C-N	6.38	129.81	122.99
2	S	526	LEU	CB-CA-C	-6.38	100.21	110.79
1	B	332	VAL	CA-C-O	6.38	128.75	120.78
1	B	215	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	B	70	TRP	CA-CB-CG	6.33	125.64	113.60
1	A	141	PRO	CA-C-N	6.33	126.25	119.28
1	A	141	PRO	C-N-CA	6.33	126.25	119.28
1	A	166	GLY	O-C-N	-6.32	114.12	122.28
1	A	32	LYS	CA-CB-CG	6.30	126.70	114.10
1	A	292	HIS	CB-CG-CD2	-6.30	123.02	131.20
2	S	570	TRP	CG-CD2-CE3	6.27	140.17	133.90
2	T	502	GLN	N-CA-C	6.27	120.14	110.42
1	A	316	LYS	N-CA-C	-6.26	104.34	112.23
1	B	306	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	B	310	HIS	CA-C-O	-6.24	113.58	120.69
1	A	140	ILE	CA-C-N	6.24	124.21	119.66
1	A	140	ILE	C-N-CA	6.24	124.21	119.66
1	B	141	PRO	CA-C-N	6.24	126.14	119.28
1	B	141	PRO	C-N-CA	6.24	126.14	119.28
2	T	514	THR	CA-CB-OG1	-6.23	100.26	109.60
1	B	70	TRP	CB-CG-CD2	6.22	135.50	126.80
1	A	70	TRP	CB-CG-CD2	6.21	135.49	126.80
1	B	212	MET	O-C-N	6.20	129.95	123.62
1	A	375	LEU	CA-C-N	6.20	126.53	119.83
1	A	375	LEU	C-N-CA	6.20	126.53	119.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	A	350	ARG	CB-CG-CD	-6.18	97.09	111.30
1	B	153	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	B	187	ARG	CB-CG-CD	-6.17	97.11	111.30
1	B	369	VAL	N-CA-C	6.17	122.17	109.34
1	A	271	THR	N-CA-CB	-6.15	101.09	110.01
2	T	514	THR	O-C-N	6.15	130.58	122.95
1	B	350	ARG	CB-CG-CD	-6.15	97.16	111.30
2	S	570	TRP	CB-CG-CD1	-6.15	117.68	126.90
1	A	207	ASN	O-C-N	-6.14	114.42	122.59
1	A	304	GLN	O-C-N	6.13	130.25	123.01
1	A	45	GLN	CA-C-O	-6.12	113.98	120.23
2	S	552	TYR	O-C-N	-6.12	115.65	122.75
1	B	446	ARG	CA-CB-CG	6.12	126.33	114.10
1	A	70	TRP	N-CA-CB	6.11	120.81	110.49
2	T	619	LYS	CA-C-N	6.10	126.06	119.78
2	T	619	LYS	C-N-CA	6.10	126.06	119.78
1	B	208	SER	O-C-N	-6.09	116.05	123.30
1	B	393	ILE	N-CA-C	-6.08	104.81	110.53
1	B	409	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	A	419	ALA	CA-C-O	-6.05	114.47	120.82
2	S	514	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	277	ASN	CA-CB-CG	-6.02	106.58	112.60
1	B	368	TRP	CE2-CD2-CG	-6.02	99.98	107.20
2	S	619	LYS	CA-C-N	6.01	125.98	119.78
2	S	619	LYS	C-N-CA	6.01	125.98	119.78
2	S	547	GLU	CA-C-N	6.01	133.01	121.54
2	S	547	GLU	C-N-CA	6.01	133.01	121.54
1	A	383	HIS	CA-C-O	-6.00	114.71	121.25
1	B	309	ILE	CB-CG1-CD1	-6.00	101.21	113.80
1	B	396	ASP	N-CA-C	6.00	117.81	111.28
1	A	466	VAL	CG1-CB-CG2	-5.99	97.62	110.80
2	T	570	TRP	O-C-N	5.99	130.18	123.05
1	A	197	LEU	N-CA-C	-5.99	102.80	110.53
1	B	70	TRP	N-CA-CB	5.99	120.61	110.49
2	S	596	GLN	CA-CB-CG	5.98	126.06	114.10
1	A	462	TRP	CG-CD2-CE3	5.96	139.86	133.90
1	A	262	VAL	CA-CB-CG2	5.96	120.54	110.40
1	B	371	LEU	N-CA-C	-5.96	102.54	109.93
1	B	107	LEU	N-CA-C	-5.96	105.84	113.23
1	A	102	ALA	CA-C-O	5.95	126.54	120.24
2	T	570	TRP	CB-CG-CD1	-5.94	117.99	126.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ALA	N-CA-C	-5.94	104.73	111.14
1	A	446	ARG	CA-CB-CG	5.92	125.94	114.10
2	T	535	LYS	CA-CB-CG	5.92	125.93	114.10
1	B	466	VAL	CG1-CB-CG2	-5.92	97.79	110.80
1	B	462	TRP	CB-CG-CD1	-5.91	118.04	126.90
1	B	45	GLN	CA-C-O	-5.90	114.21	120.23
1	B	277	ASN	CA-CB-CG	-5.90	106.70	112.60
1	B	209	GLN	CA-C-O	-5.89	114.92	120.34
1	B	304	GLN	O-C-N	5.87	129.94	123.01
2	S	502	GLN	N-CA-C	5.87	119.51	110.42
1	A	293	ILE	N-CA-CB	-5.86	104.33	110.72
1	A	309	ILE	CB-CG1-CD1	-5.85	101.51	113.80
2	T	598	TRP	N-CA-C	-5.85	99.71	109.24
1	A	347	ASP	CB-CA-C	-5.83	101.72	110.88
1	B	232	THR	CA-CB-OG1	-5.82	100.87	109.60
1	B	394	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	374	VAL	CA-C-N	5.82	129.34	121.20
1	A	374	VAL	C-N-CA	5.82	129.34	121.20
1	B	102	ALA	CA-C-O	5.82	126.40	120.24
1	A	382	ILE	N-CA-C	5.81	118.31	109.12
1	A	297	MET	CB-CA-C	-5.81	101.69	110.06
2	T	530	VAL	CG1-CB-CG2	-5.81	98.02	110.80
1	B	409	HIS	CA-C-N	5.78	127.07	119.84
1	B	409	HIS	C-N-CA	5.78	127.07	119.84
1	A	307	HIS	O-C-N	5.78	130.55	123.44
1	B	181	SER	N-CA-C	-5.78	103.08	110.53
1	A	409	HIS	CA-C-N	5.77	127.06	119.84
1	A	409	HIS	C-N-CA	5.77	127.06	119.84
2	S	591	LYS	CB-CG-CD	-5.77	98.04	111.30
1	B	347	ASP	CB-CA-C	-5.77	101.83	110.88
2	S	598	TRP	N-CA-C	-5.76	99.84	109.24
1	B	205	ASN	OD1-CG-ND2	-5.76	116.83	122.60
2	T	591	LYS	CB-CG-CD	-5.76	98.05	111.30
2	T	596	GLN	CA-CB-CG	5.74	125.58	114.10
2	S	535	LYS	CA-CB-CG	5.73	125.56	114.10
2	S	591	LYS	CA-CB-CG	5.73	125.56	114.10
2	S	514	THR	CB-CA-C	5.72	118.83	109.90
2	S	505	PRO	CA-C-N	5.71	125.25	119.19
2	S	505	PRO	C-N-CA	5.71	125.25	119.19
1	B	197	LEU	N-CA-C	-5.71	103.16	110.53
1	A	217	ARG	N-CA-C	-5.71	104.96	111.07
1	B	161	LYS	O-C-N	5.70	128.65	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASN	CA-CB-CG	5.70	118.30	112.60
1	B	374	VAL	CA-C-N	5.70	129.18	121.20
1	B	374	VAL	C-N-CA	5.70	129.18	121.20
1	A	161	LYS	O-C-N	5.70	128.65	122.15
1	A	212	MET	O-C-N	5.69	129.83	123.40
1	A	188	ALA	O-C-N	5.69	128.00	122.09
1	B	188	ALA	O-C-N	5.68	128.00	122.09
2	T	556	ASN	CB-CG-ND2	5.68	124.92	116.40
1	B	382	ILE	N-CA-C	5.67	118.08	109.12
1	B	271	THR	N-CA-C	5.67	117.26	111.14
1	A	301	ILE	CB-CA-C	-5.66	104.65	112.24
1	B	60	GLU	CA-C-N	5.66	132.35	121.54
1	B	60	GLU	C-N-CA	5.66	132.35	121.54
1	A	185	TYR	CA-C-N	5.65	126.22	120.00
1	A	185	TYR	C-N-CA	5.65	126.22	120.00
1	A	25	TYR	N-CA-C	-5.64	98.55	108.20
1	A	451	TRP	CE2-CD2-CG	-5.64	100.44	107.20
1	A	155	ILE	N-CA-C	5.63	121.04	109.34
1	B	294	HIS	O-C-N	-5.63	116.91	123.27
2	T	547	GLU	CA-C-N	5.62	132.28	121.54
2	T	547	GLU	C-N-CA	5.62	132.28	121.54
2	T	590	ALA	O-C-N	5.62	128.07	122.12
2	S	554	GLU	N-CA-C	-5.61	98.85	110.80
1	B	262	VAL	CA-CB-CG2	5.60	119.92	110.40
1	B	464	GLU	N-CA-C	-5.59	105.55	112.38
1	B	451	TRP	CE2-CD2-CG	-5.59	100.49	107.20
1	B	115	ASN	CA-CB-CG	-5.59	107.01	112.60
1	A	60	GLU	CA-C-N	5.59	132.21	121.54
1	A	60	GLU	C-N-CA	5.59	132.21	121.54
1	B	83	ARG	CB-CA-C	-5.59	101.69	110.79
1	A	368	TRP	CB-CG-CD1	-5.58	118.53	126.90
1	A	467	PHE	CA-CB-CG	5.56	119.36	113.80
2	S	514	THR	N-CA-CB	-5.55	101.19	109.69
1	A	70	TRP	NE1-CE2-CZ2	-5.53	121.81	130.10
1	B	140	ILE	CA-C-N	5.53	123.69	119.66
1	B	140	ILE	C-N-CA	5.53	123.69	119.66
1	B	70	TRP	NE1-CE2-CZ2	-5.52	121.81	130.10
1	B	462	TRP	CE2-CD2-CG	-5.52	100.57	107.20
1	A	253	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	B	215	ARG	CA-CB-CG	5.51	125.13	114.10
1	A	464	GLU	N-CA-C	-5.51	105.82	112.54
1	B	253	ARG	NE-CZ-NH1	5.51	127.01	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	554	GLU	N-CA-C	-5.50	99.08	110.80
1	A	112	SER	CA-CB-OG	-5.50	100.10	111.10
1	A	274	PHE	CA-CB-CG	-5.50	108.30	113.80
1	B	287	ASN	CA-CB-CG	-5.50	107.11	112.60
1	B	75	THR	N-CA-C	-5.49	100.97	108.38
1	B	124	VAL	CB-CA-C	-5.48	104.84	112.02
1	A	328	SER	CA-CB-OG	-5.48	100.14	111.10
1	A	462	TRP	CB-CG-CD1	-5.48	118.69	126.90
1	A	168	PRO	CB-CA-C	5.47	118.24	111.23
1	B	217	ARG	N-CA-C	-5.47	105.31	111.28
2	T	514	THR	CB-CA-C	5.47	118.43	109.90
1	B	25	TYR	N-CA-C	-5.47	98.85	108.20
2	T	526	LEU	N-CA-CB	5.47	118.16	110.12
1	A	124	VAL	CB-CA-C	-5.46	104.87	112.02
1	A	332	VAL	CB-CA-C	5.45	120.23	111.29
1	B	419	ALA	CA-C-O	-5.45	115.09	120.82
2	S	530	VAL	CG1-CB-CG2	-5.45	98.81	110.80
1	B	366	GLN	CA-CB-CG	-5.45	103.20	114.10
2	T	566	TYR	CB-CA-C	-5.45	102.09	110.26
2	T	570	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	A	240	LEU	O-C-N	-5.44	116.33	123.02
1	B	318	LEU	O-C-N	-5.44	116.47	122.07
1	B	368	TRP	CB-CG-CD1	-5.44	118.74	126.90
2	S	556	ASN	CB-CG-ND2	5.43	124.55	116.40
1	A	181	SER	N-CA-C	-5.42	103.54	110.53
1	A	205	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	371	LEU	N-CA-C	-5.42	102.82	109.65
1	B	294	HIS	CB-CG-ND1	5.42	130.83	122.70
1	A	187	ARG	CB-CG-CD	-5.38	98.92	111.30
1	B	375	LEU	CD1-CG-CD2	-5.38	98.97	110.80
2	S	556	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	385	TRP	CE2-CD2-CG	-5.37	100.75	107.20
1	A	153	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	B	87	ILE	O-C-N	-5.35	117.48	123.26
2	T	601	ILE	O-C-N	5.35	128.80	123.18
1	A	306	ASN	CB-CG-ND2	5.35	124.42	116.40
2	S	592	LYS	CA-C-O	5.35	126.27	120.55
2	S	594	TYR	N-CA-CB	-5.35	103.66	111.20
1	A	75	THR	N-CA-C	-5.34	101.17	108.38
1	B	282	HIS	N-CA-C	-5.33	105.92	112.90
1	B	374	VAL	N-CA-C	-5.33	100.80	108.53
1	B	385	TRP	CE2-CD2-CG	-5.33	100.81	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ILE	O-C-N	-5.31	117.53	123.26
2	T	548	HIS	CB-CG-ND1	5.29	130.64	122.70
2	T	591	LYS	CA-CB-CG	5.29	124.67	114.10
1	A	145	VAL	O-C-N	5.28	127.07	121.89
1	B	185	TYR	CA-C-N	5.28	125.81	120.00
1	B	185	TYR	C-N-CA	5.28	125.81	120.00
1	B	212	MET	CA-C-O	5.28	125.42	120.09
2	T	570	TRP	N-CA-C	-5.28	99.18	108.20
2	T	505	PRO	CA-C-N	5.28	124.78	119.19
2	T	505	PRO	C-N-CA	5.28	124.78	119.19
1	B	362	ILE	N-CA-C	-5.27	99.50	107.73
1	B	207	ASN	O-C-N	-5.27	115.58	122.59
1	B	306	ASN	CB-CG-ND2	5.27	124.30	116.40
1	A	197	LEU	O-C-N	-5.27	116.17	122.65
1	B	149	GLN	O-C-N	-5.26	116.41	122.09
1	A	202	ASP	N-CA-C	-5.26	101.40	109.76
1	A	394	PHE	CA-CB-CG	-5.25	108.55	113.80
2	T	569	MET	N-CA-CB	5.25	117.99	110.06
2	S	526	LEU	N-CA-CB	5.25	117.83	110.12
1	B	232	THR	CA-CB-CG2	5.25	119.42	110.50
1	A	341	ILE	CA-C-O	-5.24	115.10	120.71
1	B	123	ASN	N-CA-C	5.24	121.06	114.31
1	B	421	ARG	N-CA-CB	-5.23	102.27	109.91
2	T	551	VAL	O-C-N	-5.23	118.05	122.65
1	B	22	LEU	N-CA-C	-5.23	96.36	111.00
1	B	166	GLY	O-C-N	-5.23	115.54	122.28
2	T	567	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	A	429	LYS	N-CA-C	-5.22	105.28	110.97
1	A	109	GLU	CA-CB-CG	-5.21	103.67	114.10
2	S	533	LEU	CA-C-O	5.21	126.80	121.07
1	B	301	ILE	CB-CA-C	-5.21	105.26	112.24
1	B	47	GLY	CA-C-O	-5.21	114.01	119.27
2	T	590	ALA	CA-C-N	5.20	127.76	120.28
2	T	590	ALA	C-N-CA	5.20	127.76	120.28
1	A	115	ASN	CA-CB-CG	-5.19	107.41	112.60
1	A	123	ASN	N-CA-C	5.19	121.00	114.31
1	B	249	GLU	CA-C-O	-5.18	114.93	120.42
1	B	332	VAL	CB-CA-C	5.17	119.78	111.29
1	A	149	GLN	O-C-N	-5.17	116.51	122.09
2	T	514	THR	CA-CB-CG2	5.16	119.28	110.50
2	T	552	TYR	O-C-N	-5.16	116.78	122.72
2	T	598	TRP	O-C-N	-5.16	117.44	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	594	TYR	N-CA-CB	-5.16	103.93	111.20
2	S	590	ALA	CA-C-N	5.16	128.85	120.60
2	S	590	ALA	C-N-CA	5.16	128.85	120.60
1	B	307	HIS	O-C-N	5.15	129.78	123.44
1	A	426	ALA	N-CA-C	-5.15	105.56	111.07
2	S	586	GLU	CA-C-O	-5.14	115.41	120.70
1	A	83	ARG	CB-CA-C	-5.13	102.57	110.78
1	A	415	PRO	CA-N-CD	-5.13	104.82	112.00
2	T	548	HIS	N-CA-C	-5.13	99.87	110.80
1	B	451	TRP	CD1-CG-CD2	5.13	114.50	106.30
2	S	548	HIS	N-CA-C	-5.12	99.89	110.80
1	A	451	TRP	CD1-CG-CD2	5.11	114.48	106.30
1	B	122	GLY	CA-C-O	-5.11	115.18	120.90
1	B	453	PRO	CA-C-N	5.10	127.89	120.79
1	B	453	PRO	C-N-CA	5.10	127.89	120.79
1	A	463	LYS	N-CA-C	5.10	119.26	113.19
1	A	22	LEU	N-CA-C	-5.09	96.75	111.00
2	S	547	GLU	CA-C-O	-5.09	113.33	119.59
2	S	514	THR	CA-CB-CG2	5.09	119.15	110.50
1	B	155	ILE	N-CA-C	5.09	119.92	109.34
1	A	284	CYS	N-CA-C	-5.08	105.93	111.82
2	S	502	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	S	597	ALA	N-CA-C	5.07	121.60	110.80
1	B	112	SER	CA-CB-OG	-5.07	100.96	111.10
2	T	566	TYR	N-CA-C	5.07	117.04	109.59
1	A	208	SER	O-C-N	-5.07	117.27	123.30
2	S	588	GLU	CB-CG-CD	5.07	121.21	112.60
1	B	346	VAL	N-CA-CB	-5.07	104.89	110.51
1	A	46	PRO	CA-C-N	-5.06	117.42	123.44
1	A	46	PRO	C-N-CA	-5.06	117.42	123.44
1	B	384	VAL	CB-CA-C	-5.06	104.31	112.16
1	B	202	ASP	N-CA-C	-5.06	101.71	109.76
2	S	522	SER	N-CA-C	-5.06	103.72	110.55
2	S	579	ASP	CA-C-O	5.06	125.71	120.40
1	A	107	LEU	N-CA-C	-5.06	106.96	113.23
1	B	462	TRP	CG-CD2-CE3	5.06	138.96	133.90
1	B	412	GLY	O-C-N	5.06	127.71	122.91
1	A	204	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	163	ASN	CA-CB-CG	5.04	117.64	112.60
1	A	324	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	415	PRO	CA-N-CD	-5.03	104.96	112.00
1	A	319	ARG	NE-CZ-NH1	5.03	126.53	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	548	HIS	CB-CG-ND1	5.02	130.23	122.70
1	B	328	SER	CA-CB-OG	-5.01	101.08	111.10
2	S	570	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	B	411	TRP	CG-CD2-CE3	5.00	138.90	133.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	TYR	Sidechain
1	A	283	TYR	Sidechain
1	B	239	TYR	Sidechain
1	B	283	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3456	0	3387	148	0
1	B	3456	0	3387	148	0
2	S	1029	0	991	39	0
2	T	1029	0	991	37	0
All	All	8970	0	8756	352	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (352) 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:463:LYS:HG2	1:B:466:VAL:HB	1.53	0.90
1:A:463:LYS:HG2	1:A:466:VAL:HB	1.51	0.90
2:T:521:LEU:HB2	2:T:526:LEU:HD12	1.51	0.90
1:B:151:PRO:HD2	1:B:372:PRO:HG2	1.54	0.89
2:S:521:LEU:HB2	2:S:526:LEU:HD12	1.53	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:CYS:HB2	1:B:197:LEU:HD23	1.57	0.84
1:A:151:PRO:HD2	1:A:372:PRO:HG2	1.63	0.80
1:A:172:CYS:HB2	1:A:197:LEU:HD23	1.62	0.79
1:A:316:LYS:HZ3	1:A:366:GLN:HG3	1.50	0.76
1:B:463:LYS:HA	1:B:466:VAL:HB	1.68	0.75
2:T:523:GLN:HG3	2:T:584:LEU:HD21	1.69	0.74
2:S:523:GLN:HG3	2:S:584:LEU:HD21	1.70	0.74
1:A:168:PRO:HG2	1:A:424:LEU:HD11	1.69	0.74
1:A:463:LYS:HA	1:A:466:VAL:HB	1.72	0.71
1:B:25:TYR:HB2	1:B:55:ALA:HB2	1.71	0.71
1:A:25:TYR:HB2	1:A:55:ALA:HB2	1.73	0.71
1:B:168:PRO:HG2	1:B:424:LEU:HD11	1.71	0.70
1:A:459:CYS:O	1:A:462:TRP:HB3	1.92	0.69
1:A:300:VAL:HG12	1:B:301:ILE:HG22	1.72	0.69
1:B:295:ARG:HD3	1:B:311:PHE:CE1	2.29	0.68
1:B:459:CYS:O	1:B:462:TRP:HB3	1.94	0.67
1:A:301:ILE:HG22	1:B:300:VAL:HG12	1.74	0.67
1:A:295:ARG:HD3	1:A:311:PHE:CE1	2.30	0.66
1:A:135:LEU:HB3	1:A:309:ILE:HG23	1.76	0.65
1:A:315:ALA:HB1	1:A:349:LEU:HD21	1.78	0.65
1:B:201:LYS:HB2	1:B:239:TYR:HD2	1.62	0.65
1:B:385:TRP:N	1:B:462:TRP:HE1	1.95	0.64
1:A:355:GLU:HA	1:A:365:THR:HG23	1.79	0.64
1:B:422:VAL:HG12	2:T:517:TYR:HB3	1.80	0.64
1:A:185:TYR:O	1:A:189:VAL:HG23	1.98	0.63
1:B:385:TRP:CZ2	1:B:466:VAL:HG22	2.34	0.63
1:A:443:GLU:O	1:A:446:ARG:HB3	1.98	0.63
1:A:385:TRP:CZ2	1:A:466:VAL:HG22	2.33	0.63
1:B:355:GLU:HA	1:B:365:THR:HG23	1.81	0.63
1:A:195:GLY:HA3	1:A:417:ALA:HB3	1.81	0.62
1:B:315:ALA:HB1	1:B:349:LEU:HD21	1.81	0.62
1:A:463:LYS:HA	1:A:466:VAL:H	1.63	0.62
1:B:168:PRO:HD3	1:B:396:ASP:HA	1.82	0.62
1:B:172:CYS:HB3	1:B:200:THR:HG22	1.82	0.62
1:B:443:GLU:O	1:B:446:ARG:HB3	2.00	0.61
1:B:462:TRP:O	1:B:466:VAL:HG23	2.00	0.61
1:B:452:SER:HB3	1:B:455:LEU:HB3	1.82	0.61
1:A:176:PRO:HD2	1:A:180:LEU:HD11	1.82	0.61
2:T:598:TRP:CD1	2:T:620:PRO:HD2	2.36	0.61
1:B:316:LYS:HZ3	1:B:366:GLN:HG3	1.64	0.61
1:B:176:PRO:HD2	1:B:180:LEU:HD11	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:545:GLU:HB2	2:S:567:TRP:CD2	2.35	0.61
2:T:545:GLU:HB2	2:T:567:TRP:CD2	2.36	0.61
1:A:452:SER:HB3	1:A:455:LEU:HB3	1.83	0.61
1:B:140:ILE:HB	1:B:366:GLN:HE22	1.65	0.60
1:B:463:LYS:HA	1:B:466:VAL:H	1.66	0.60
1:A:140:ILE:HB	1:A:366:GLN:HE22	1.66	0.60
1:B:202:ASP:OD2	1:B:240:LEU:HA	2.02	0.60
1:A:385:TRP:N	1:A:462:TRP:HE1	1.99	0.60
1:B:185:TYR:O	1:B:189:VAL:HG23	2.02	0.60
1:A:462:TRP:O	1:A:466:VAL:HG23	2.00	0.60
1:A:62:SER:HB2	1:A:77:LEU:HD21	1.84	0.59
1:A:385:TRP:HB3	1:A:462:TRP:CZ2	2.36	0.59
1:A:168:PRO:HD3	1:A:396:ASP:HA	1.84	0.59
1:B:358:ARG:HH11	1:B:358:ARG:HB3	1.67	0.59
1:B:385:TRP:HB3	1:B:462:TRP:CZ2	2.37	0.59
1:B:62:SER:HB2	1:B:77:LEU:HD21	1.85	0.59
1:B:135:LEU:HB3	1:B:309:ILE:HG23	1.83	0.59
1:B:170:LEU:HD21	1:B:424:LEU:HD22	1.84	0.59
1:B:418:VAL:O	1:B:422:VAL:HG13	2.02	0.59
2:S:598:TRP:CD1	2:S:620:PRO:HD2	2.37	0.59
1:B:319:ARG:HD3	1:B:372:PRO:O	2.02	0.59
1:B:38:ALA:HB1	1:B:135:LEU:HD11	1.84	0.58
1:A:172:CYS:HB3	1:A:200:THR:HG22	1.83	0.58
1:B:120:ILE:HD13	1:B:138:LEU:HD21	1.85	0.58
2:S:543:GLU:HB3	2:S:567:TRP:HB2	1.85	0.58
1:A:312:ARG:HH21	1:A:341:ILE:HG23	1.69	0.58
2:T:543:GLU:HB3	2:T:567:TRP:HB2	1.85	0.58
1:A:38:ALA:HB1	1:A:135:LEU:HD11	1.85	0.58
1:A:358:ARG:HB3	1:A:358:ARG:HH11	1.68	0.58
1:A:388:PRO:HG3	1:A:427:CYS:SG	2.44	0.58
1:B:51:GLU:HA	1:B:87:ILE:CD1	2.33	0.58
2:S:596:GLN:O	2:S:620:PRO:HB3	2.04	0.57
1:B:353:PHE:CE1	1:B:355:GLU:HB3	2.39	0.57
1:A:80:TYR:CD2	1:B:179:GLY:HA2	2.39	0.57
1:B:331:VAL:HB	1:B:339:ARG:HH11	1.68	0.57
1:A:319:ARG:HD3	1:A:372:PRO:O	2.04	0.57
1:A:331:VAL:HB	1:A:339:ARG:HH11	1.68	0.57
1:B:336:GLU:HA	1:B:339:ARG:HB2	1.86	0.57
1:A:51:GLU:HA	1:A:87:ILE:CD1	2.35	0.57
1:B:195:GLY:HA3	1:B:417:ALA:HB3	1.86	0.57
2:T:596:GLN:O	2:T:620:PRO:HB3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:533:LEU:HD13	2:T:540:PRO:HB3	1.87	0.57
1:A:202:ASP:OD2	1:A:240:LEU:HA	2.04	0.57
1:A:309:ILE:HD11	1:B:300:VAL:HG11	1.87	0.57
1:A:201:LYS:HB2	1:A:239:TYR:HD2	1.67	0.57
2:T:532:TYR:HA	2:T:535:LYS:HG2	1.87	0.57
1:A:336:GLU:HA	1:A:339:ARG:HB2	1.87	0.56
1:A:385:TRP:HB3	1:A:462:TRP:HZ2	1.70	0.56
1:A:422:VAL:HG12	2:S:517:TYR:HB3	1.87	0.56
1:A:57:VAL:HG13	1:A:124:VAL:HG11	1.88	0.56
1:B:164:LYS:HD2	1:B:169:LEU:HD23	1.86	0.56
1:B:385:TRP:H	1:B:462:TRP:HE1	1.52	0.56
1:A:331:VAL:HB	1:A:339:ARG:HD2	1.86	0.56
1:A:179:GLY:HA2	1:B:80:TYR:CD2	2.41	0.55
1:B:312:ARG:HH21	1:B:341:ILE:HG23	1.69	0.55
1:A:120:ILE:HD13	1:A:138:LEU:HD21	1.88	0.55
2:S:562:TYR:HB2	2:S:565:ARG:HD2	1.87	0.55
1:A:170:LEU:HD21	1:A:424:LEU:HD22	1.88	0.55
1:A:300:VAL:HG11	1:B:309:ILE:HD11	1.88	0.55
1:B:40:PHE:CD1	1:B:133:LEU:HD11	2.41	0.55
1:B:385:TRP:HB3	1:B:462:TRP:HZ2	1.69	0.55
1:B:150:GLY:HA3	1:B:371:LEU:HD11	1.89	0.54
2:T:562:TYR:HB2	2:T:565:ARG:HD2	1.88	0.54
1:A:353:PHE:CE1	1:A:355:GLU:HB3	2.42	0.54
1:B:382:ILE:HG21	1:B:390:LEU:HD11	1.89	0.54
1:A:385:TRP:CH2	1:A:466:VAL:HG22	2.43	0.54
1:B:331:VAL:HB	1:B:339:ARG:HD2	1.89	0.54
1:A:35:ASP:O	1:A:141:PRO:HD3	2.08	0.54
1:B:411:TRP:CZ3	2:T:502:GLN:HB2	2.42	0.54
1:A:312:ARG:NH2	1:A:361:GLY:HA3	2.23	0.54
2:S:532:TYR:HA	2:S:535:LYS:HG2	1.90	0.54
2:S:543:GLU:HB2	2:S:600:ARG:HG3	1.90	0.54
1:B:57:VAL:HG13	1:B:124:VAL:HG11	1.90	0.54
1:B:251:ILE:O	1:B:255:VAL:HG23	2.08	0.53
1:B:310:HIS:ND1	1:B:312:ARG:HG2	2.24	0.53
1:A:26:THR:OG1	1:A:83:ARG:HB3	2.09	0.53
1:A:418:VAL:O	1:A:422:VAL:HG13	2.09	0.53
2:S:533:LEU:HD13	2:S:540:PRO:HB3	1.90	0.53
1:B:312:ARG:NH2	1:B:361:GLY:HA3	2.24	0.53
1:A:389:ALA:O	1:A:393:ILE:HG12	2.08	0.53
1:A:42:VAL:HG23	1:A:44:PRO:HD3	1.91	0.53
1:A:170:LEU:HD12	1:A:421:ARG:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ALA:HB1	1:A:444:ILE:HD13	1.90	0.53
1:A:447:GLU:O	1:A:450:LYS:HB2	2.09	0.53
1:B:42:VAL:HG23	1:B:44:PRO:HD3	1.90	0.53
1:A:310:HIS:ND1	1:A:312:ARG:HG2	2.23	0.52
1:B:69:VAL:HA	1:B:72:ASP:CG	2.34	0.52
1:B:430:ALA:HB1	1:B:444:ILE:HD13	1.91	0.52
1:B:69:VAL:HA	1:B:72:ASP:OD1	2.10	0.52
2:T:505:PRO:HG2	2:T:509:LYS:HE2	1.91	0.52
1:B:26:THR:HG21	1:B:83:ARG:HH11	1.74	0.52
2:T:543:GLU:HB2	2:T:600:ARG:HG3	1.92	0.52
1:A:171:GLY:HA2	1:A:199:PHE:O	2.10	0.52
1:B:26:THR:OG1	1:B:83:ARG:HB3	2.09	0.52
1:B:201:LYS:HB2	1:B:239:TYR:CD2	2.43	0.52
1:A:40:PHE:CD1	1:A:133:LEU:HD11	2.46	0.51
1:A:172:CYS:O	1:A:200:THR:HA	2.09	0.51
1:B:447:GLU:O	1:B:450:LYS:HB2	2.10	0.51
1:A:164:LYS:HD2	1:A:169:LEU:HD23	1.91	0.51
1:A:382:ILE:HG21	1:A:390:LEU:HD11	1.92	0.51
1:A:385:TRP:CB	1:A:462:TRP:HE1	2.24	0.51
1:A:385:TRP:H	1:A:462:TRP:HE1	1.57	0.51
1:B:35:ASP:O	1:B:141:PRO:HD3	2.10	0.51
1:A:69:VAL:HA	1:A:72:ASP:CG	2.35	0.51
2:T:579:ASP:HB3	2:T:582:GLN:OE1	2.11	0.51
2:S:505:PRO:HG2	2:S:509:LYS:HE2	1.92	0.51
2:T:545:GLU:O	2:T:597:ALA:HA	2.11	0.51
2:T:561:TYR:CD1	2:T:561:TYR:C	2.89	0.51
1:B:382:ILE:HA	1:B:386:HIS:ND1	2.26	0.50
1:B:382:ILE:HG22	1:B:402:PHE:HE1	1.75	0.50
1:B:172:CYS:O	1:B:200:THR:HA	2.10	0.50
2:T:523:GLN:O	2:T:527:LEU:HB2	2.11	0.50
2:T:542:LEU:HD22	2:T:570:TRP:CD1	2.46	0.50
1:A:110:GLU:HB3	1:A:147:THR:HB	1.93	0.50
1:A:335:LEU:HD22	1:A:339:ARG:NH2	2.26	0.50
1:B:385:TRP:CH2	1:B:466:VAL:HG22	2.46	0.50
2:T:574:MET:SD	2:T:583:VAL:HG22	2.50	0.50
2:S:567:TRP:CZ3	2:S:600:ARG:HG2	2.47	0.50
1:B:389:ALA:O	1:B:393:ILE:HG12	2.12	0.50
1:B:58:ALA:HB1	1:B:82:GLY:O	2.11	0.50
2:S:579:ASP:HB3	2:S:582:GLN:OE1	2.12	0.50
1:B:385:TRP:CE2	1:B:466:VAL:HG13	2.46	0.50
1:A:241:ASN:HA	1:A:266:MET:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:NH1	1:B:141:PRO:HB3	2.27	0.49
1:A:38:ALA:HB1	1:A:135:LEU:CD1	2.42	0.49
1:A:150:GLY:HA3	1:A:371:LEU:HD11	1.94	0.49
1:A:69:VAL:HA	1:A:72:ASP:OD1	2.12	0.49
1:B:110:GLU:HB3	1:B:147:THR:HB	1.93	0.49
1:B:138:LEU:O	1:B:316:LYS:NZ	2.45	0.49
1:B:385:TRP:N	1:B:462:TRP:NE1	2.59	0.49
2:S:561:TYR:CD1	2:S:561:TYR:C	2.90	0.49
1:B:155:ILE:HG12	1:B:375:LEU:HD13	1.94	0.49
1:B:351:ASP:O	1:B:368:TRP:HD1	1.95	0.49
1:A:382:ILE:HA	1:A:386:HIS:ND1	2.27	0.49
2:S:533:LEU:HD23	2:S:538:TRP:HB2	1.94	0.49
1:A:26:THR:HG21	1:A:83:ARG:HH11	1.77	0.49
1:A:251:ILE:O	1:A:255:VAL:HG23	2.13	0.49
1:A:385:TRP:CE2	1:A:466:VAL:HG13	2.47	0.49
2:S:523:GLN:O	2:S:527:LEU:HB2	2.12	0.49
1:B:42:VAL:HG12	1:B:133:LEU:HD13	1.95	0.49
1:A:42:VAL:HG12	1:A:133:LEU:HD13	1.95	0.49
2:S:574:MET:SD	2:S:583:VAL:HG22	2.52	0.49
2:T:567:TRP:CZ3	2:T:600:ARG:HG2	2.48	0.49
1:B:388:PRO:HG3	1:B:427:CYS:SG	2.52	0.48
1:A:58:ALA:HB1	1:A:82:GLY:O	2.13	0.48
1:A:138:LEU:O	1:A:316:LYS:NZ	2.44	0.48
1:B:170:LEU:HD12	1:B:421:ARG:HD3	1.93	0.48
1:B:312:ARG:HH21	1:B:341:ILE:CG2	2.27	0.48
1:B:329:GLY:O	1:B:378:ALA:HA	2.14	0.48
1:B:125:PHE:HA	1:B:133:LEU:HD23	1.95	0.48
1:B:171:GLY:HA2	1:B:199:PHE:O	2.13	0.48
1:B:385:TRP:CB	1:B:462:TRP:HE1	2.25	0.48
2:T:533:LEU:HD23	2:T:538:TRP:HB2	1.94	0.48
1:A:312:ARG:HH21	1:A:341:ILE:CG2	2.27	0.48
1:A:329:GLY:O	1:A:378:ALA:HA	2.13	0.48
2:S:545:GLU:O	2:S:597:ALA:HA	2.13	0.48
1:A:42:VAL:HG12	1:A:133:LEU:CD1	2.44	0.48
1:B:42:VAL:HG12	1:B:133:LEU:CD1	2.43	0.48
1:A:139:ARG:NH1	1:A:141:PRO:HB3	2.29	0.48
1:A:303:ARG:HD2	1:B:126:GLY:HA2	1.96	0.48
1:B:180:LEU:HD22	1:B:180:LEU:H	1.79	0.48
1:B:327:HIS:HA	1:B:377:VAL:HB	1.94	0.48
1:B:174:ILE:HD12	1:B:188:ALA:CB	2.44	0.48
1:A:292:HIS:HE1	1:A:377:VAL:HG21	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD22	1:B:339:ARG:NH2	2.28	0.47
1:B:140:ILE:HB	1:B:366:GLN:NE2	2.28	0.47
1:B:292:HIS:HE1	1:B:377:VAL:HG21	1.78	0.47
1:B:38:ALA:HB1	1:B:135:LEU:CD1	2.44	0.47
1:A:191:GLU:O	1:A:194:ARG:HG2	2.14	0.47
2:S:505:PRO:HA	2:S:506:PRO:HD2	1.73	0.47
1:A:177:LYS:HG3	1:A:178:LEU:H	1.78	0.47
1:A:140:ILE:HB	1:A:366:GLN:NE2	2.30	0.47
1:B:191:GLU:O	1:B:194:ARG:HG2	2.14	0.47
2:T:542:LEU:HG	2:T:601:ILE:CD1	2.45	0.47
1:A:201:LYS:HB2	1:A:239:TYR:CD2	2.47	0.47
1:B:457:ALA:HA	1:B:460:GLU:HG2	1.97	0.47
1:A:125:PHE:HE2	1:A:308:GLY:O	1.97	0.47
1:A:126:GLY:HA2	1:B:303:ARG:HD2	1.96	0.47
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.74	0.47
1:A:382:ILE:HG22	1:A:402:PHE:HE1	1.79	0.47
1:A:430:ALA:CB	1:A:444:ILE:HD13	2.45	0.47
1:B:42:VAL:HG11	1:B:57:VAL:HG21	1.97	0.47
1:B:177:LYS:HG3	1:B:178:LEU:H	1.80	0.46
2:T:544:PHE:HD1	2:T:570:TRP:HB2	1.80	0.46
1:A:42:VAL:HG11	1:A:57:VAL:HG21	1.98	0.46
1:A:44:PRO:HB2	1:A:48:VAL:HB	1.97	0.46
1:A:90:VAL:HG12	1:A:93:GLU:HB2	1.98	0.46
1:A:174:ILE:HD12	1:A:188:ALA:CB	2.45	0.46
1:A:243:THR:OG1	1:A:267:HIS:HD2	1.98	0.46
2:S:544:PHE:HD1	2:S:570:TRP:HB2	1.80	0.46
2:T:547:GLU:O	2:T:548:HIS:CG	2.69	0.46
1:A:348:LEU:HA	1:A:354:VAL:HG21	1.97	0.46
2:S:542:LEU:HD22	2:S:570:TRP:CD1	2.51	0.46
1:A:180:LEU:H	1:A:180:LEU:HD22	1.81	0.46
1:B:385:TRP:H	1:B:462:TRP:NE1	2.11	0.46
1:A:127:PHE:CE2	1:A:129:ALA:HB3	2.51	0.46
1:B:355:GLU:HA	1:B:365:THR:HA	1.97	0.46
1:B:385:TRP:CE2	1:B:466:VAL:HG22	2.51	0.46
2:T:509:LYS:O	2:T:511:LYS:HG2	2.15	0.46
1:A:107:LEU:HD22	1:B:178:LEU:HD13	1.97	0.45
1:A:351:ASP:O	1:A:368:TRP:HD1	1.98	0.45
1:B:90:VAL:HG12	1:B:93:GLU:HB2	1.99	0.45
1:A:385:TRP:N	1:A:462:TRP:NE1	2.64	0.45
1:A:457:ALA:HA	1:A:460:GLU:HG2	1.99	0.45
1:B:241:ASN:HA	1:B:266:MET:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.66	0.45
2:S:601:ILE:HB	2:S:615:PHE:CE1	2.52	0.45
1:B:169:LEU:HD12	1:B:169:LEU:H	1.82	0.45
2:T:598:TRP:HB3	2:T:616:ILE:HD11	1.98	0.45
1:A:125:PHE:HA	1:A:133:LEU:HD23	1.98	0.45
1:A:208:SER:HB2	1:A:214:TRP:HB3	1.98	0.45
1:B:44:PRO:HB2	1:B:48:VAL:HB	1.98	0.45
1:A:155:ILE:HG12	1:A:375:LEU:HD13	1.97	0.45
1:B:125:PHE:HE2	1:B:308:GLY:O	1.99	0.45
2:S:547:GLU:O	2:S:548:HIS:CG	2.70	0.44
1:A:173:THR:HG23	1:A:201:LYS:HG2	1.98	0.44
2:T:587:VAL:HG22	2:T:601:ILE:HD11	2.00	0.44
1:A:353:PHE:HA	1:A:366:GLN:O	2.17	0.44
2:S:567:TRP:CE3	2:S:600:ARG:HG2	2.53	0.44
2:T:567:TRP:CE3	2:T:600:ARG:HG2	2.53	0.44
2:S:598:TRP:HB3	2:S:616:ILE:HD11	1.99	0.44
1:B:448:ALA:HA	1:B:451:TRP:NE1	2.31	0.44
1:B:461:VAL:O	1:B:464:GLU:HB3	2.18	0.44
2:T:601:ILE:HB	2:T:615:PHE:CE1	2.52	0.44
1:A:178:LEU:HD13	1:B:107:LEU:HD22	1.99	0.44
1:B:383:HIS:HE2	1:B:385:TRP:HZ3	1.64	0.44
2:T:511:LYS:HG3	2:T:517:TYR:CZ	2.52	0.44
2:S:542:LEU:HG	2:S:601:ILE:CD1	2.47	0.44
2:T:587:VAL:CG2	2:T:601:ILE:HD11	2.48	0.44
1:A:214:TRP:HA	1:A:217:ARG:NH1	2.33	0.43
1:A:335:LEU:HD22	1:A:339:ARG:HH21	1.81	0.43
1:A:355:GLU:HA	1:A:365:THR:HA	1.99	0.43
1:B:70:TRP:CG	1:B:71:THR:N	2.85	0.43
1:A:448:ALA:HA	1:A:451:TRP:NE1	2.33	0.43
1:B:243:THR:OG1	1:B:267:HIS:HD2	2.01	0.43
1:A:130:LEU:O	1:B:303:ARG:NH2	2.50	0.43
1:B:430:ALA:CB	1:B:444:ILE:HD13	2.48	0.43
1:B:222:ALA:HB2	1:B:260:LEU:HD13	2.00	0.43
1:A:201:LYS:HG3	1:A:202:ASP:O	2.18	0.43
2:S:587:VAL:CG2	2:S:601:ILE:HD11	2.48	0.43
1:B:127:PHE:CE2	1:B:129:ALA:HB3	2.53	0.43
1:B:348:LEU:HA	1:B:354:VAL:HG21	2.01	0.43
1:B:353:PHE:HA	1:B:366:GLN:O	2.18	0.43
2:T:605:ASP:HB2	2:T:612:CYS:SG	2.59	0.43
2:S:509:LYS:O	2:S:511:LYS:HG2	2.17	0.43
1:B:260:LEU:HB2	1:B:262:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TRP:CE2	1:A:466:VAL:HG22	2.54	0.43
1:B:175:LYS:HB2	1:B:407:LEU:HD22	2.00	0.43
1:B:335:LEU:HD22	1:B:339:ARG:HH21	1.84	0.43
1:A:327:HIS:HA	1:A:377:VAL:HB	2.01	0.43
1:A:383:HIS:HE2	1:A:385:TRP:HZ3	1.65	0.43
1:A:411:TRP:HB2	1:A:415:PRO:CB	2.49	0.43
2:T:538:TRP:CZ3	2:T:613:ILE:HD11	2.54	0.43
1:A:45:GLN:O	1:A:48:VAL:HG23	2.19	0.42
1:A:258:ARG:HG2	2:S:559:PRO:HG2	1.99	0.42
2:S:511:LYS:HG3	2:S:517:TYR:CZ	2.54	0.42
1:B:173:THR:HG23	1:B:201:LYS:HG2	2.02	0.42
1:A:293:ILE:HG13	1:A:318:LEU:HD21	2.01	0.42
2:T:505:PRO:HD2	2:T:509:LYS:HG3	2.00	0.42
1:A:309:ILE:CD1	1:B:300:VAL:HG11	2.49	0.42
1:B:403:GLY:O	1:B:407:LEU:HB2	2.19	0.42
1:A:300:VAL:HG11	1:B:309:ILE:CD1	2.49	0.42
2:S:538:TRP:CZ3	2:S:613:ILE:HD11	2.54	0.42
2:T:579:ASP:O	2:T:582:GLN:HB2	2.19	0.42
1:B:459:CYS:HB3	1:B:462:TRP:CE3	2.54	0.42
1:A:319:ARG:HG3	1:A:374:VAL:HG23	2.01	0.42
2:S:609:GLN:O	2:S:609:GLN:HG2	2.20	0.42
1:B:214:TRP:HA	1:B:217:ARG:NH1	2.35	0.42
1:B:440:GLU:O	1:B:444:ILE:HG13	2.18	0.42
1:A:70:TRP:CG	1:A:71:THR:N	2.87	0.42
1:A:116:MET:HE3	1:A:117:PHE:CD1	2.55	0.42
1:B:292:HIS:CE1	1:B:377:VAL:HG21	2.54	0.42
1:A:446:ARG:NH1	1:A:450:LYS:HZ2	2.18	0.41
2:T:505:PRO:HA	2:T:506:PRO:HD2	1.76	0.41
1:B:116:MET:HE3	1:B:117:PHE:CD1	2.55	0.41
1:A:194:ARG:HH11	1:A:194:ARG:HD2	1.63	0.41
1:A:260:LEU:HB2	1:A:262:VAL:HG22	2.02	0.41
1:B:463:LYS:HA	1:B:466:VAL:CB	2.43	0.41
1:B:463:LYS:CA	1:B:466:VAL:HB	2.46	0.41
1:A:26:THR:O	1:A:85:TYR:HA	2.20	0.41
1:A:185:TYR:CD1	1:A:212:MET:HE1	2.56	0.41
1:A:250:MET:HE2	1:A:250:MET:HB3	1.92	0.41
1:A:411:TRP:CZ3	2:S:502:GLN:HB2	2.56	0.41
1:B:385:TRP:CA	1:B:462:TRP:HE1	2.33	0.41
1:A:264:ILE:HD11	1:A:292:HIS:HB2	2.02	0.41
2:S:526:LEU:O	2:S:530:VAL:HG23	2.21	0.41
1:B:26:THR:O	1:B:85:TYR:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:SER:HA	1:B:453:PRO:HD2	1.94	0.41
1:A:292:HIS:CE1	1:A:377:VAL:HG21	2.56	0.41
1:A:463:LYS:CA	1:A:466:VAL:HB	2.48	0.41
2:S:534:LEU:HD12	2:S:580:ALA:HB2	2.02	0.41
2:S:544:PHE:CD1	2:S:570:TRP:HB2	2.56	0.41
2:S:605:ASP:HB2	2:S:612:CYS:SG	2.61	0.41
1:B:264:ILE:HD11	1:B:292:HIS:HB2	2.03	0.41
1:A:106:ASP:HA	1:B:210:PRO:HG2	2.03	0.41
1:A:303:ARG:NH2	1:B:130:LEU:O	2.53	0.40
1:B:293:ILE:HG13	1:B:318:LEU:HD21	2.02	0.40
1:B:462:TRP:C	1:B:466:VAL:HG23	2.47	0.40
1:A:446:ARG:HH11	1:A:446:ARG:HD3	1.78	0.40
2:T:544:PHE:CD1	2:T:570:TRP:HB2	2.56	0.40
1:A:385:TRP:H	1:A:462:TRP:NE1	2.17	0.40
1:A:116:MET:HE2	1:A:116:MET:HB3	1.94	0.40
1:A:440:GLU:O	1:A:444:ILE:HG13	2.21	0.40
2:S:587:VAL:HG22	2:S:601:ILE:HD11	2.03	0.40
1:B:326:ILE:HG22	1:B:374:VAL:CG1	2.51	0.40
1:B:459:CYS:C	1:B:462:TRP:HB3	2.47	0.40

There are no symmetry-related clashes.

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	439/446 (98%)	393 (90%)	36 (8%)	10 (2%)	5	8
1	B	439/446 (98%)	393 (90%)	35 (8%)	11 (2%)	4	7
2	S	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	7	13
2	T	121/123 (98%)	108 (89%)	11 (9%)	2 (2%)	7	13
All	All	1120/1138 (98%)	1000 (89%)	95 (8%)	25 (2%)	5	9

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	TRP
1	A	72	ASP
1	A	94	LYS
1	A	466	VAL
2	S	548	HIS
1	B	70	TRP
1	B	72	ASP
1	B	94	LYS
1	B	466	VAL
2	T	548	HIS
1	A	125	PHE
1	A	311	PHE
1	A	434	GLY
1	B	125	PHE
1	B	311	PHE
1	A	410	PRO
1	B	410	PRO
1	B	434	GLY
1	A	223	GLU
1	B	223	GLU
1	B	106	ASP
2	T	559	PRO
1	A	369	VAL
1	B	369	VAL
2	S	559	PRO

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	357/361 (99%)	320 (90%)	37 (10%)	7	14
1	B	357/361 (99%)	322 (90%)	35 (10%)	7	16
2	S	110/110 (100%)	92 (84%)	18 (16%)	2	4
2	T	110/110 (100%)	94 (86%)	16 (14%)	3	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	934/942 (99%)	828 (89%)	106 (11%)	5 12

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	28	GLU
1	A	32	LYS
1	A	42	VAL
1	A	60	GLU
1	A	62	SER
1	A	63	THR
1	A	70	TRP
1	A	71	THR
1	A	91	VAL
1	A	94	LYS
1	A	95	ASP
1	A	124	VAL
1	A	180	LEU
1	A	192	CYS
1	A	197	LEU
1	A	201	LYS
1	A	213	ARG
1	A	215	ARG
1	A	232	THR
1	A	265	VAL
1	A	269	TYR
1	A	301	ILE
1	A	314	LEU
1	A	331	VAL
1	A	339	ARG
1	A	358	ARG
1	A	359	SER
1	A	366	GLN
1	A	385	TRP
1	A	410	PRO
1	A	415	PRO
1	A	422	VAL
1	A	439	GLN
1	A	443	GLU
1	A	446	ARG
1	A	464	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	507	ILE
2	S	524	GLU
2	S	531	GLU
2	S	533	LEU
2	S	551	VAL
2	S	553	ARG
2	S	559	PRO
2	S	565	ARG
2	S	581	THR
2	S	582	GLN
2	S	584	LEU
2	S	588	GLU
2	S	592	LYS
2	S	596	GLN
2	S	607	VAL
2	S	609	GLN
2	S	612	CYS
2	S	614	SER
1	B	23	THR
1	B	28	GLU
1	B	32	LYS
1	B	42	VAL
1	B	60	GLU
1	B	62	SER
1	B	63	THR
1	B	70	TRP
1	B	71	THR
1	B	91	VAL
1	B	94	LYS
1	B	95	ASP
1	B	124	VAL
1	B	180	LEU
1	B	197	LEU
1	B	201	LYS
1	B	213	ARG
1	B	215	ARG
1	B	232	THR
1	B	265	VAL
1	B	269	TYR
1	B	301	ILE
1	B	314	LEU
1	B	331	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	339	ARG
1	B	358	ARG
1	B	366	GLN
1	B	385	TRP
1	B	410	PRO
1	B	415	PRO
1	B	422	VAL
1	B	439	GLN
1	B	443	GLU
1	B	446	ARG
1	B	464	GLU
2	T	507	ILE
2	T	524	GLU
2	T	531	GLU
2	T	533	LEU
2	T	551	VAL
2	T	553	ARG
2	T	565	ARG
2	T	581	THR
2	T	582	GLN
2	T	584	LEU
2	T	588	GLU
2	T	592	LYS
2	T	596	GLN
2	T	607	VAL
2	T	609	GLN
2	T	614	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	163	ASN
1	A	207	ASN
1	A	366	GLN
2	S	536	ASN
2	S	606	ASN
1	B	45	GLN
1	B	163	ASN
1	B	207	ASN
1	B	366	GLN
2	T	508	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	T	525	GLN
2	T	536	ASN
2	T	555	ASN
2	T	606	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	441/446 (98%)	-1.56	0 100 100	11, 25, 72, 101	0
1	B	441/446 (98%)	-1.57	0 100 100	11, 25, 72, 101	0
2	S	123/123 (100%)	-1.56	0 100 100	14, 38, 69, 84	0
2	T	123/123 (100%)	-1.49	0 100 100	14, 38, 69, 84	0
All	All	1128/1138 (99%)	-1.56	0 100 100	11, 28, 71, 101	0

There are no RSRZ outliers to report.

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.