Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 06:16 am BST

PDB ID	:	1RLD
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)

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

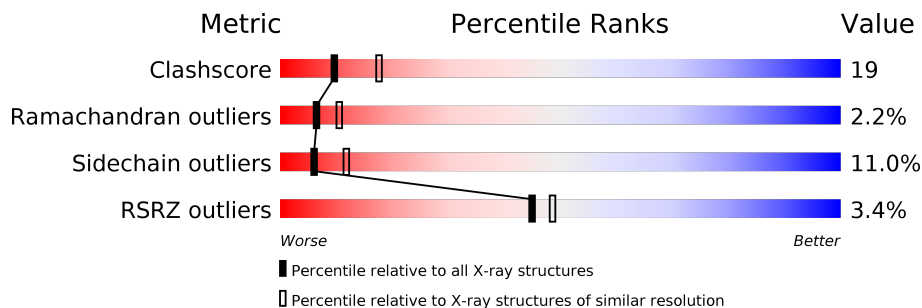|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	Percentile Ranks	Value
Clashscore		19
Ramachandran outliers		2.2%
Sidechain outliers		11.0%
RSRZ outliers		3.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	446	3% 51% · 36% · 10% · ·
1	B	446	4% 50% · 37% · 10% · ·
2	S	123	% 49% · 35% · 13% ·
2	T	123	2% 49% · 37% · 11% ·

2 Entry composition (i)

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/OXYG ENASE (LARGE CHAIN).

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

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/OXYG ENASE (SMALL CHAIN).

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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)
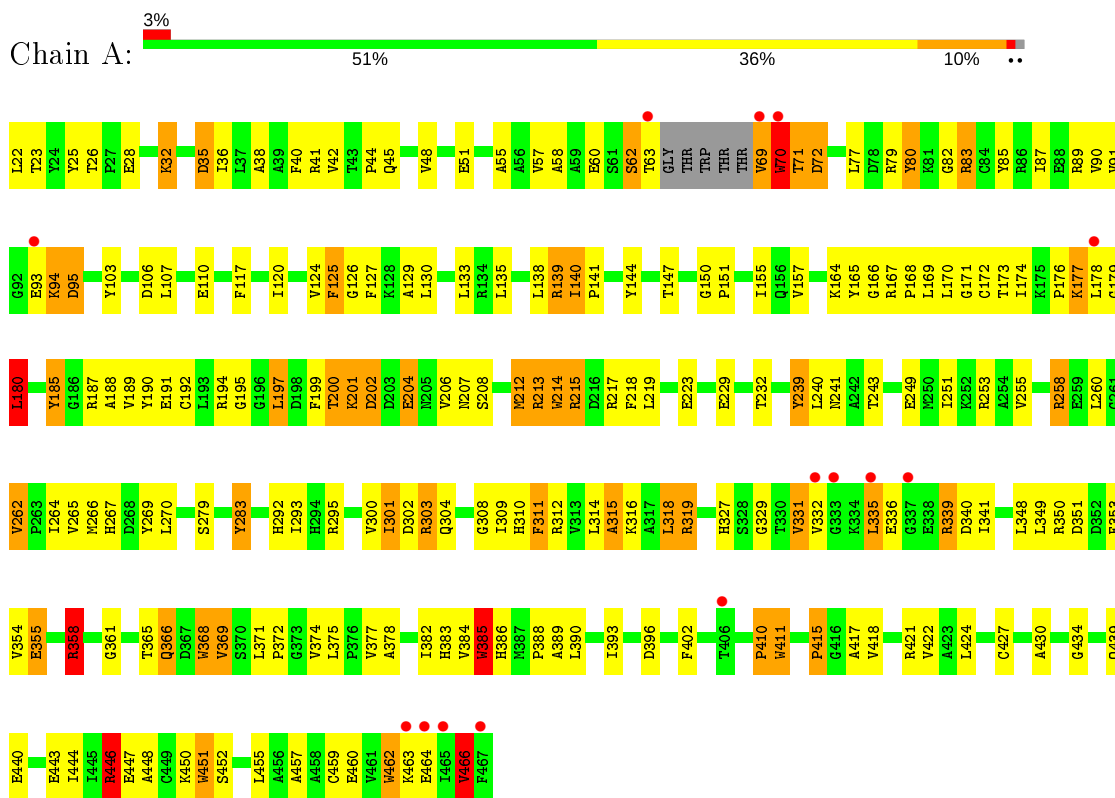
- Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)
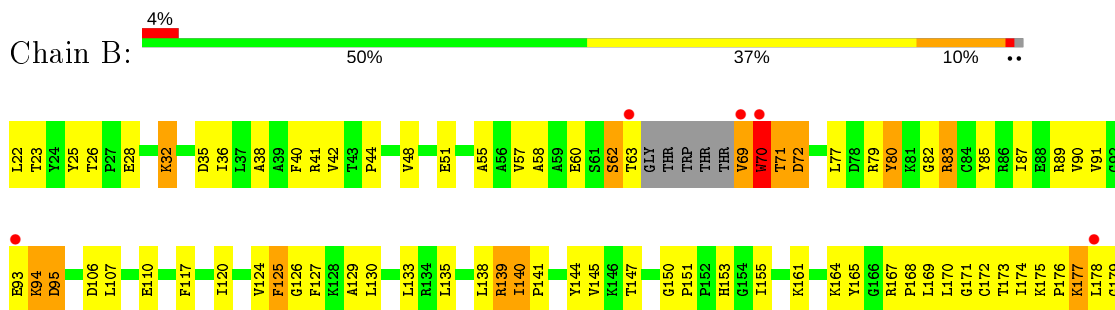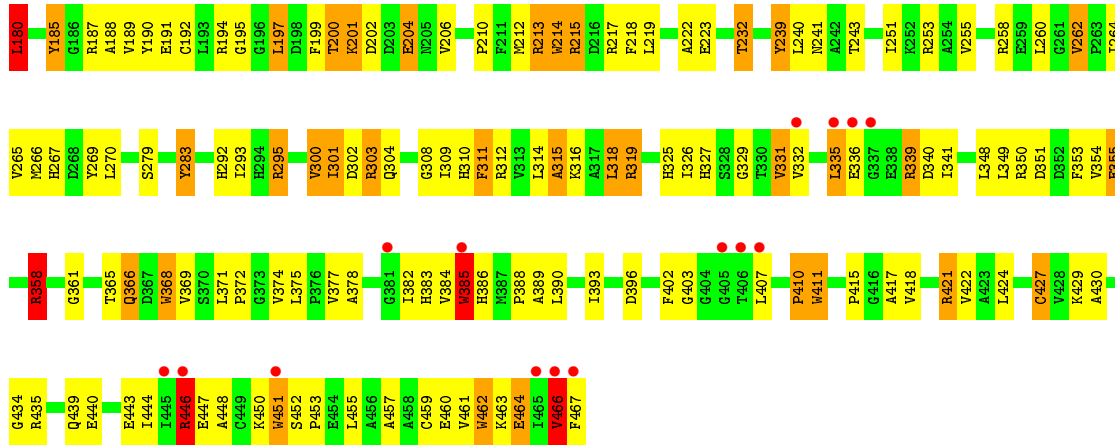
● Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)
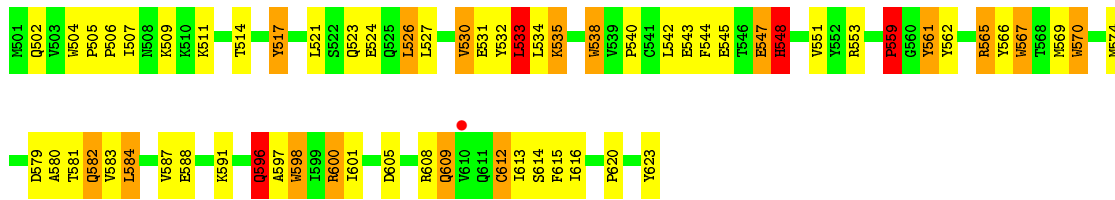
Chain S:

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

Chain T:
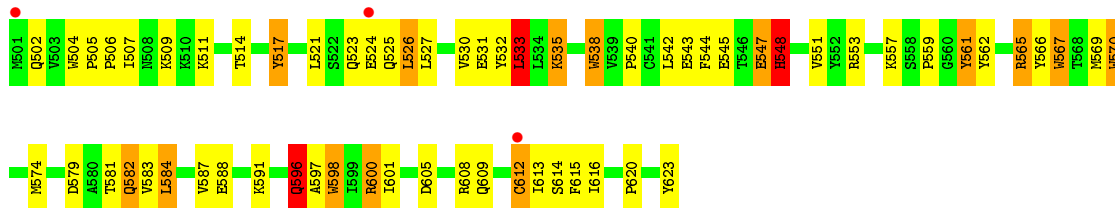
4   Data and refinement statistics (i)

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 19.53 – 2.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 76.0 (19.53-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.30 , 57.0	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.266 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	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.*

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

5 Model quality ⓘ

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	1.08	3/3539 (0.1%)	1.93	97/4796 (2.0%)
1	B	1.06	2/3539 (0.1%)	1.93	102/4796 (2.1%)
2	S	1.09	1/1062 (0.1%)	2.02	40/1442 (2.8%)
2	T	1.06	2/1062 (0.2%)	2.04	40/1442 (2.8%)
All	All	1.07	8/9202 (0.1%)	1.95	279/12476 (2.2%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	TRP	CB-CG	5.58	1.60	1.50
1	A	70	TRP	CB-CG	5.54	1.60	1.50
1	B	368	TRP	CD1-NE1	-5.53	1.28	1.38
2	T	538	TRP	CG-CD2	-5.51	1.34	1.43
1	A	229	GLU	CD-OE1	-5.34	1.19	1.25
1	A	70	TRP	CA-CB	5.30	1.65	1.53
2	S	567	TRP	NE1-CE2	-5.29	1.30	1.37
2	T	557	LYS	CD-CE	5.22	1.64	1.51

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	565	ARG	NE-CZ-NH1	16.15	128.38	120.30
1	B	319	ARG	NE-CZ-NH1	16.05	128.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	ARG	NE-CZ-NH1	15.58	128.09	120.30
2	T	565	ARG	NE-CZ-NH1	15.26	127.93	120.30
1	B	215	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	A	385	TRP	CA-CB-CG	13.95	140.21	113.70
1	B	385	TRP	CA-CB-CG	13.71	139.75	113.70
1	A	253	ARG	NE-CZ-NH1	13.43	127.01	120.30
1	B	253	ARG	NE-CZ-NH1	13.42	127.01	120.30
1	A	319	ARG	NE-CZ-NH1	12.45	126.53	120.30
1	B	385	TRP	CB-CG-CD1	-11.58	111.95	127.00
1	A	385	TRP	CB-CG-CD1	-10.66	113.14	127.00
2	S	600	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	B	451	TRP	CD1-CG-CD2	10.26	114.50	106.30
1	A	451	TRP	CD1-CG-CD2	10.23	114.48	106.30
1	B	253	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	B	167	ARG	NE-CZ-NH2	-10.11	115.24	120.30
2	S	553	ARG	NE-CZ-NH2	-10.10	115.25	120.30
2	T	553	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	A	167	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	B	303	ARG	NE-CZ-NH1	9.60	125.10	120.30
2	T	561	TYR	CB-CG-CD2	-9.55	115.27	121.00
1	B	368	TRP	CD1-CG-CD2	9.48	113.89	106.30
1	B	384	VAL	CA-C-N	9.28	137.62	117.20
1	A	384	VAL	CA-C-N	9.26	137.58	117.20
2	T	600	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	B	368	TRP	CE2-CD2-CG	-9.15	99.98	107.30
1	B	185	TYR	CB-CG-CD1	-9.07	115.56	121.00
1	A	215	ARG	NE-CZ-NH2	-9.05	115.78	120.30
2	T	570	TRP	CD1-CG-CD2	8.98	113.48	106.30
1	A	303	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	190	TYR	CB-CG-CD2	-8.95	115.63	121.00
2	S	538	TRP	CD1-CG-CD2	8.89	113.42	106.30
1	A	70	TRP	CB-CG-CD1	-8.89	115.44	127.00
1	A	253	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	B	385	TRP	CG-CD2-CE3	8.82	141.83	133.90
1	B	70	TRP	CB-CG-CD1	-8.77	115.61	127.00
1	A	187	ARG	NE-CZ-NH2	-8.71	115.94	120.30
2	S	569	MET	CA-CB-CG	8.70	128.09	113.30
2	T	538	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	A	69	VAL	N-CA-C	8.67	134.41	111.00
2	T	569	MET	CA-CB-CG	8.63	127.96	113.30
1	A	451	TRP	CE2-CD2-CG	-8.58	100.44	107.30
2	S	570	TRP	CD1-CG-CD2	8.57	113.15	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	VAL	N-CA-C	8.54	134.06	111.00
1	B	451	TRP	CE2-CD2-CG	-8.52	100.49	107.30
1	A	185	TYR	CB-CG-CD1	-8.42	115.95	121.00
1	B	462	TRP	CE2-CD2-CG	-8.41	100.57	107.30
2	S	514	THR	CA-C-N	-8.41	98.70	117.20
2	T	514	THR	CA-C-N	-8.41	98.71	117.20
1	B	70	TRP	CG-CD2-CE3	8.35	141.42	133.90
1	A	466	VAL	CG1-CB-CG2	-8.30	97.62	110.90
2	T	570	TRP	CE2-CD2-CG	-8.29	100.67	107.30
1	A	70	TRP	CG-CD2-CE3	8.27	141.35	133.90
2	S	504	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	B	462	TRP	CA-CB-CG	8.22	129.32	113.70
1	B	466	VAL	CG1-CB-CG2	-8.20	97.79	110.90
1	A	385	TRP	CE2-CD2-CG	-8.18	100.75	107.30
1	B	385	TRP	CE2-CD2-CG	-8.11	100.81	107.30
1	A	462	TRP	CA-CB-CG	8.10	129.08	113.70
1	B	204	GLU	CA-CB-CG	8.08	131.17	113.40
2	T	504	TRP	CD1-CG-CD2	8.07	112.75	106.30
2	T	530	VAL	CG1-CB-CG2	-8.05	98.02	110.90
1	B	215	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	385	TRP	CG-CD2-CE3	7.86	140.98	133.90
2	T	570	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	A	70	TRP	NE1-CE2-CZ2	-7.81	121.81	130.40
1	B	70	TRP	NE1-CE2-CZ2	-7.81	121.81	130.40
1	B	187	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	204	GLU	CA-CB-CG	7.64	130.20	113.40
1	A	368	TRP	CD1-CG-CD2	7.64	112.41	106.30
2	S	570	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	B	385	TRP	CB-CG-CD2	7.61	136.49	126.60
2	S	530	VAL	CG1-CB-CG2	-7.55	98.81	110.90
2	S	504	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	A	41	ARG	NE-CZ-NH2	-7.53	116.54	120.30
2	T	517	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	A	462	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	A	368	TRP	CE2-CD2-CG	-7.48	101.31	107.30
2	T	565	ARG	NE-CZ-NH2	-7.43	116.59	120.30
2	S	561	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	A	83	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	385	TRP	CB-CG-CD2	7.31	136.10	126.60
2	S	538	TRP	CE2-CD2-CG	-7.30	101.46	107.30
2	S	570	TRP	CB-CG-CD1	-7.17	117.68	127.00
2	T	538	TRP	CE2-CD2-CG	-7.15	101.58	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	TYR	CB-CG-CD2	-7.14	116.72	121.00
1	A	165	TYR	CB-CG-CD1	-7.11	116.73	121.00
1	B	384	VAL	N-CA-C	7.10	130.18	111.00
2	S	517	TYR	CB-CG-CD1	-7.09	116.74	121.00
1	A	384	VAL	CA-C-O	-7.05	105.29	120.10
2	S	565	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	A	411	TRP	CE2-CD2-CG	-7.00	101.70	107.30
2	S	570	TRP	CG-CD2-CE3	6.97	140.17	133.90
1	B	384	VAL	CA-C-O	-6.96	105.47	120.10
1	B	283	TYR	CB-CG-CD1	-6.94	116.83	121.00
2	T	570	TRP	CB-CG-CD1	-6.93	117.99	127.00
1	A	258	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	462	TRP	CD1-CG-CD2	6.93	111.84	106.30
1	B	258	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	462	TRP	CB-CG-CD1	-6.89	118.04	127.00
1	B	253	ARG	CG-CD-NE	-6.89	97.33	111.80
1	A	206	VAL	CG1-CB-CG2	-6.88	99.89	110.90
1	A	384	VAL	N-CA-C	6.85	129.50	111.00
1	B	70	TRP	CB-CG-CD2	6.85	135.50	126.60
1	A	70	TRP	CB-CG-CD2	6.84	135.49	126.60
1	A	253	ARG	CG-CD-NE	-6.82	97.47	111.80
2	T	570	TRP	CA-C-N	-6.81	102.21	117.20
1	A	70	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	185	TYR	CB-CG-CD2	6.78	125.07	121.00
1	A	190	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	B	41	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	T	566	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	A	462	TRP	CD1-CG-CD2	6.64	111.62	106.30
1	A	462	TRP	CG-CD2-CE3	6.63	139.86	133.90
1	B	70	TRP	CE2-CD2-CG	-6.60	102.02	107.30
2	T	504	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	B	83	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	206	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	A	368	TRP	CB-CG-CD1	-6.51	118.53	127.00
1	B	185	TYR	CB-CG-CD2	6.50	124.90	121.00
1	B	411	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	B	213	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	262	VAL	CA-CB-CG2	6.42	120.54	110.90
1	A	70	TRP	CA-CB-CG	6.41	125.88	113.70
1	B	219	LEU	CA-CB-CG	6.40	130.03	115.30
1	A	462	TRP	CB-CG-CD1	-6.40	118.69	127.00
2	S	566	TYR	CB-CG-CD1	-6.37	117.18	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LEU	CA-CB-CG	6.37	129.95	115.30
1	A	144	TYR	CB-CG-CD1	-6.37	117.18	121.00
2	T	567	TRP	CE2-CD2-CG	-6.37	102.21	107.30
1	B	368	TRP	CB-CG-CD1	-6.35	118.74	127.00
1	B	451	TRP	CG-CD1-NE1	-6.35	103.75	110.10
2	T	547	GLU	N-CA-C	6.34	128.12	111.00
1	A	79	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	358	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	214	TRP	CD1-CG-CD2	6.29	111.33	106.30
1	B	70	TRP	CA-CB-CG	6.28	125.64	113.70
2	S	547	GLU	N-CA-C	6.28	127.95	111.00
1	B	32	LYS	CA-CB-CG	6.27	127.20	113.40
2	T	548	HIS	N-CA-CB	6.27	121.88	110.60
1	A	202	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	319	ARG	CB-CG-CD	6.23	127.80	111.60
1	A	213	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	B	80	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	B	421	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	411	TRP	CD1-CG-CD2	6.22	111.27	106.30
2	S	570	TRP	CA-C-N	-6.20	103.55	117.20
1	A	180	LEU	CA-CB-CG	6.19	129.53	115.30
1	B	218	PHE	CB-CG-CD2	-6.16	116.49	120.80
1	A	451	TRP	CG-CD1-NE1	-6.15	103.95	110.10
2	T	553	ARG	N-CA-C	-6.11	94.49	111.00
1	B	427	CYS	CA-CB-SG	-6.10	103.02	114.00
1	A	218	PHE	CB-CG-CD2	-6.09	116.54	120.80
1	B	79	ARG	NE-CZ-NH1	6.09	123.34	120.30
2	S	548	HIS	N-CA-CB	6.07	121.53	110.60
1	A	32	LYS	CA-CB-CG	6.05	126.70	113.40
1	B	69	VAL	C-N-CA	6.04	136.81	121.70
1	B	283	TYR	CB-CG-CD2	6.02	124.61	121.00
2	S	570	TRP	CG-CD1-NE1	-6.02	104.08	110.10
1	B	262	VAL	CA-CB-CG2	6.01	119.92	110.90
1	B	262	VAL	CA-CB-CG1	-6.00	101.91	110.90
1	A	262	VAL	CA-CB-CG1	-5.99	101.92	110.90
2	T	598	TRP	CE2-CD2-CG	-5.98	102.52	107.30
2	S	567	TRP	CE2-CD2-CG	-5.96	102.54	107.30
1	A	69	VAL	C-N-CA	5.95	136.56	121.70
2	S	547	GLU	CA-C-N	5.94	130.26	117.20
1	A	214	TRP	CE2-CD2-CG	-5.93	102.55	107.30
2	T	598	TRP	CD1-CG-CD2	5.93	111.04	106.30
1	B	180	LEU	CA-CB-CG	5.93	128.93	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	533	LEU	CA-CB-CG	5.92	128.93	115.30
1	B	304	GLN	CA-C-N	-5.91	104.20	117.20
2	T	623	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	A	304	GLN	CA-C-N	-5.90	104.22	117.20
1	A	318	LEU	CA-C-N	5.89	130.16	117.20
2	S	553	ARG	N-CA-C	-5.89	95.10	111.00
1	B	446	ARG	CA-CB-CG	5.88	126.33	113.40
2	T	570	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	A	103	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	B	385	TRP	CD1-CG-CD2	5.85	110.98	106.30
2	T	533	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	212	MET	CA-C-N	-5.85	104.34	117.20
1	A	411	TRP	CD1-CG-CD2	5.84	110.97	106.30
2	T	567	TRP	CG-CD2-CE3	5.81	139.13	133.90
1	B	358	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	315	ALA	CB-CA-C	-5.78	101.43	110.10
1	B	319	ARG	CB-CG-CD	5.78	126.62	111.60
1	A	95	ASP	CA-C-N	-5.76	104.53	117.20
1	B	385	TRP	N-CA-CB	5.76	120.97	110.60
2	S	596	GLN	CA-CB-CG	5.75	126.06	113.40
2	T	567	TRP	CD1-CG-CD2	5.74	110.89	106.30
1	B	332	VAL	CA-C-N	-5.71	104.78	116.20
1	B	300	VAL	CG1-CB-CG2	-5.71	101.76	110.90
1	A	446	ARG	CA-CB-CG	5.70	125.94	113.40
2	T	535	LYS	CA-CB-CG	5.70	125.93	113.40
1	B	319	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	70	TRP	N-CA-CB	5.67	120.81	110.60
1	B	214	TRP	CE2-CD2-CG	-5.67	102.76	107.30
1	B	318	LEU	CA-C-N	5.66	129.65	117.20
1	B	165	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	A	303	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	S	598	TRP	CE2-CD2-CG	-5.63	102.79	107.30
1	B	95	ASP	CA-C-N	-5.62	104.83	117.20
1	B	462	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	A	80	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	A	332	VAL	CA-C-N	-5.58	105.03	116.20
1	A	350	ARG	CB-CG-CD	-5.58	97.09	111.60
1	B	187	ARG	CB-CG-CD	-5.57	97.11	111.60
2	S	623	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	B	70	TRP	N-CA-CB	5.56	120.61	110.60
1	A	315	ALA	CB-CA-C	-5.56	101.76	110.10
1	B	411	TRP	CG-CD2-CE3	5.56	138.90	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	350	ARG	CB-CG-CD	-5.55	97.16	111.60
1	A	302	ASP	CB-CG-OD1	5.54	123.29	118.30
2	T	596	GLN	CA-CB-CG	5.54	125.58	113.40
1	A	89	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	S	535	LYS	CA-CB-CG	5.53	125.56	113.40
2	S	591	LYS	CA-CB-CG	5.53	125.56	113.40
2	T	547	GLU	CA-C-N	5.51	129.33	117.20
1	B	89	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	451	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	A	279	SER	CA-C-N	5.48	129.26	117.20
1	A	411	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	B	36	ILE	N-CA-C	-5.45	96.27	111.00
1	A	451	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	A	167	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	T	567	TRP	NE1-CE2-CZ2	-5.43	124.42	130.40
1	B	303	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	T	526	LEU	CB-CA-C	-5.43	99.88	110.20
1	B	435	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	157	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	B	22	LEU	N-CA-C	-5.42	96.36	111.00
1	A	36	ILE	N-CA-C	-5.41	96.39	111.00
1	B	144	TYR	CB-CG-CD1	-5.41	117.75	121.00
2	S	504	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	A	35	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	S	538	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	B	161	LYS	CA-C-N	-5.38	105.36	117.20
2	T	504	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	A	166	GLY	O-C-N	-5.36	114.12	122.70
1	B	215	ARG	CA-CB-CG	5.33	125.13	113.40
2	S	514	THR	O-C-N	5.30	131.19	122.70
1	B	117	PHE	CA-C-N	5.30	128.86	117.20
1	A	22	LEU	N-CA-C	-5.28	96.75	111.00
1	B	302	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	200	THR	O-C-N	-5.27	114.27	122.70
1	B	145	VAL	CG1-CB-CG2	-5.26	102.48	110.90
2	S	526	LEU	CB-CA-C	-5.26	100.21	110.20
1	A	335	LEU	N-CA-C	5.24	125.16	111.00
1	A	187	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	S	567	TRP	CG-CD2-CE3	5.22	138.60	133.90
2	S	591	LYS	CB-CG-CD	-5.22	98.04	111.60
1	B	200	THR	O-C-N	-5.21	114.36	122.70
1	B	325	HIS	CA-CB-CG	5.21	122.46	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	591	LYS	CB-CG-CD	-5.21	98.05	111.60
1	A	139	ARG	CA-C-N	-5.20	105.75	117.20
1	A	117	PHE	CA-C-N	5.20	128.64	117.20
1	A	207	ASN	O-C-N	-5.17	114.42	122.70
2	S	548	HIS	CA-CB-CG	5.17	122.39	113.60
1	A	385	TRP	N-CA-CB	5.17	119.90	110.60
2	T	538	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	A	369	VAL	CA-CB-CG1	-5.14	103.18	110.90
2	S	608	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	140	ILE	N-CA-CB	-5.14	98.99	110.80
2	T	591	LYS	CA-CB-CG	5.12	124.67	113.40
1	B	139	ARG	CA-C-N	-5.09	105.99	117.20
2	T	608	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	140	ILE	N-CA-CB	-5.08	99.11	110.80
2	S	598	TRP	CD1-CG-CD2	5.07	110.36	106.30
1	B	335	LEU	N-CA-C	5.07	124.69	111.00
1	B	279	SER	O-C-N	-5.07	114.59	122.70
1	A	212	MET	CA-C-N	-5.05	106.08	117.20
1	B	153	HIS	CA-CB-CG	-5.05	105.02	113.60
1	B	462	TRP	NE1-CE2-CZ2	-5.05	124.85	130.40
1	A	36	ILE	CG1-CB-CG2	-5.02	100.35	111.40
1	B	295	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	283	TYR	CB-CG-CD1	5.02	124.01	121.00
1	B	232	THR	CA-CB-CG2	5.02	119.42	112.40
1	B	117	PHE	CA-C-O	-5.01	109.57	120.10

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3456	0	3387	143	0
1	B	3456	0	3387	145	0
2	S	1029	0	991	39	0
2	T	1029	0	991	38	0
All	All	8970	0	8756	344	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 19.

All (344) 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
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: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:316:LYS:HZ3	1:A:366:GLN:HG3	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:316:LYS:HZ3	1:B:366:GLN:HG3	1.63	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:176:PRO:HD2	1:B:180:LEU:HD11	1.81	0.61
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:385:TRP:HB3	1:A:462:TRP:CZ2	2.36	0.59
1:A:62:SER:HB2	1:A:77:LEU:HD21	1.84	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:135:LEU:HB3	1:B:309:ILE:HG23	1.83	0.59
1:B:62:SER:HB2	1:B:77:LEU:HD21	1.85	0.59
1:B:418:VAL:O	1:B:422:VAL:HG13	2.02	0.59
1:B:170:LEU:HD21	1:B:424:LEU:HD22	1.84	0.59
1:B:319:ARG:HD3	1:B:372:PRO:O	2.02	0.59
2:S:598:TRP:CD1	2:S:620:PRO:HD2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:358:ARG:HB3	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
1:B:353:PHE:CE1	1:B:355:GLU:HB3	2.39	0.57
2:S:596:GLN:O	2:S:620:PRO:HB3	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:312:ARG:NH2	1:B:361:GLY:HA3	2.24	0.53
2:S:533:LEU:HD13	2:S:540:PRO:HB3	1.90	0.53
1:A:389:ALA:O	1:A:393:ILE:HG12	2.08	0.53
1:A:170:LEU:HD12	1:A:421:ARG:HD3	1.91	0.53
1:A:42:VAL:HG23	1:A:44:PRO:HD3	1.91	0.53
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: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:172:CYS:O	1:A:200:THR:HA	2.09	0.51
1:A:40:PHE:CD1	1:A:133:LEU:HD11	2.46	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:389:ALA:O	1:B:393:ILE:HG12	2.12	0.50
2:S:567:TRP:CZ3	2:S:600:ARG:HG2	2.47	0.50
1:B:58:ALA:HB1	1:B:82:GLY:O	2.11	0.50
1:B:385:TRP:CE2	1:B:466:VAL:HG13	2.46	0.50
2:S:579:ASP:HB3	2:S:582:GLN:OE1	2.12	0.50
1:A:241:ASN:HA	1:A:266:MET:HB3	1.94	0.49
1:B:139:ARG:NH1	1:B:141:PRO:HB3	2.27	0.49
1:A:150:GLY:HA3	1:A:371:LEU:HD11	1.94	0.49
1:A:38:ALA:HB1	1:A:135:LEU:CD1	2.42	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
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: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
1:A:26:THR:HG21	1:A:83:ARG:HH11	1.77	0.49
1:B:42:VAL:HG12	1:B:133:LEU:HD13	1.95	0.49
2:S:523:GLN:O	2:S:527:LEU:HB2	2.12	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:138:LEU:O	1:A:316:LYS:NZ	2.44	0.48
1:A:58:ALA:HB1	1:A:82:GLY:O	2.13	0.48
1:B:170:LEU:HD12	1:B:421:ARG:HD3	1.93	0.48
1:B:329:GLY:O	1:B:378:ALA:HA	2.14	0.48
1:B:312:ARG:HH21	1:B:341:ILE:CG2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:69:VAL:HA	1:B:72:ASP:CG	2.34	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:B:191:GLU:O	1:B:194:ARG:HG2	2.14	0.47
1:A:140:ILE:HB	1:A:366:GLN:NE2	2.30	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:270:LEU:HA	1:A:270:LEU:HD23	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:A:126:GLY:HA2	1:B:303:ARG:HD2	1.96	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
1:A:69:VAL:HA	1:A:72:ASP:CG	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:T:561:TYR:C	2:T:561:TYR:CD1	2.89	0.46
1:A:180:LEU:HD22	1:A:180:LEU:H	1.81	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:457:ALA:HA	1:A:460:GLU:HG2	1.99	0.45
1:A:385:TRP:N	1:A:462:TRP:NE1	2.64	0.45
1:B:241:ASN:HA	1:B:266:MET:HB3	1.98	0.45
1:B:270:LEU:HA	1:B:270:LEU:HD23	1.66	0.45
1:B:169:LEU:H	1:B:169:LEU:HD12	1.82	0.45
2:S:601:ILE:HB	2:S:615:PHE:CE1	2.52	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
1:B:70:TRP:CG	1:B:71:THR:N	2.85	0.44
2:S:561:TYR:C	2:S:561:TYR:CD1	2.90	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
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:S:598:TRP:HB3	2:S:616:ILE:HD11	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:212:MET:HE2	1:A:212:MET:HB2	1.88	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:353:PHE:HA	1:B:366:GLN:O	2.18	0.43
1:B:348:LEU:HA	1:B:354:VAL:HG21	2.01	0.43
2:T:605:ASP:HB2	2:T:612:CYS:SG	2.59	0.43
1:B:260:LEU:HB2	1:B:262:VAL:HG22	2.00	0.43
2:S:509:LYS:O	2:S:511:LYS:HG2	2.17	0.43
1:A:385:TRP:CE2	1:A:466:VAL:HG22	2.54	0.43
1:B:335:LEU:HD22	1:B:339:ARG:HH21	1.84	0.43
1:B:175:LYS:HB2	1:B:407:LEU:HD22	2.00	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:B:173:THR:HG23	1:B:201:LYS:HG2	2.02	0.42
2:S:511:LYS:HG3	2:S:517:TYR:CZ	2.54	0.42
1:A:258:ARG:HG2	2:S:559:PRO:HG2	1.99	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
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
2:S:609:GLN:O	2:S:609:GLN:HG2	2.20	0.42
1:A:70:TRP:CG	1:A:71:THR:N	2.87	0.42
1:B:292:HIS:CE1	1:B:377:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:505:PRO:HA	2:T:506:PRO:HD2	1.76	0.41
1:A:194:ARG:HD2	1:A:194:ARG:HH11	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: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
1:B:429:LYS:HZ3	2:T:525:GLN:HG2	1.85	0.41
2:S:526:LEU:O	2:S:530:VAL:HG23	2.21	0.41
1:B:452:SER:HA	1:B:453:PRO:HD2	1.94	0.41
1:B:26:THR:O	1:B:85:TYR:HA	2.21	0.41
1:A:463:LYS:CA	1:A:466:VAL:HB	2.48	0.41
1:B:264:ILE:HD11	1:B:292:HIS:HB2	2.03	0.41
2:S:605:ASP:HB2	2:S:612:CYS:SG	2.61	0.41
1:A:292:HIS:CE1	1:A:377:VAL:HG21	2.56	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
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: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:440:GLU:O	1:A:444:ILE:HG13	2.21	0.40
1:B:326:ILE:HG22	1:B:374:VAL:CG1	2.51	0.40
2:S:587:VAL:HG22	2:S:601:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/446 (98%)	393 (90%)	36 (8%)	10 (2%)	6	10
1	B	439/446 (98%)	393 (90%)	35 (8%)	11 (2%)	5	8
2	S	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	9	16
2	T	121/123 (98%)	108 (89%)	11 (9%)	2 (2%)	9	16
All	All	1120/1138 (98%)	1000 (89%)	95 (8%)	25 (2%)	6	10

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	13
1	B	357/361 (99%)	320 (90%)	37 (10%)	7	13
2	S	110/110 (100%)	95 (86%)	15 (14%)	3	7
2	T	110/110 (100%)	96 (87%)	14 (13%)	4	8
All	All	934/942 (99%)	831 (89%)	103 (11%)	6	12

All (103) 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	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	177	LYS
1	A	180	LEU
1	A	192	CYS
1	A	197	LEU
1	A	201	LYS
1	A	204	GLU
1	A	213	ARG
1	A	215	ARG
1	A	232	THR
1	A	249	GLU
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	340	ASP
1	A	355	GLU
1	A	358	ARG
1	A	366	GLN

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Mol	Chain	Res	Type
1	A	385	TRP
1	A	410	PRO
1	A	415	PRO
1	A	439	GLN
1	A	446	ARG
1	A	464	GLU
2	S	507	ILE
2	S	524	GLU
2	S	531	GLU
2	S	533	LEU
2	S	548	HIS
2	S	551	VAL
2	S	559	PRO
2	S	581	THR
2	S	582	GLN
2	S	584	LEU
2	S	588	GLU
2	S	596	GLN
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	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	177	LYS
1	B	180	LEU
1	B	192	CYS
1	B	197	LEU
1	B	201	LYS
1	B	204	GLU
1	B	213	ARG
1	B	215	ARG
1	B	232	THR
1	B	265	VAL

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Mol	Chain	Res	Type
1	B	269	TYR
1	B	301	ILE
1	B	314	LEU
1	B	331	VAL
1	B	339	ARG
1	B	340	ASP
1	B	355	GLU
1	B	358	ARG
1	B	366	GLN
1	B	385	TRP
1	B	410	PRO
1	B	415	PRO
1	B	439	GLN
1	B	446	ARG
1	B	464	GLU
1	B	467	PHE
2	T	507	ILE
2	T	524	GLU
2	T	531	GLU
2	T	533	LEU
2	T	548	HIS
2	T	551	VAL
2	T	581	THR
2	T	582	GLN
2	T	584	LEU
2	T	588	GLU
2	T	596	GLN
2	T	609	GLN
2	T	612	CYS
2	T	614	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	GLN
1	A	420	ASN
2	S	536	ASN
1	B	366	GLN
1	B	420	ASN
2	T	536	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 carbohydrates 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%)	0.03	14 (3%)	47	51	11, 25, 72, 101	0
1	B	441/446 (98%)	-0.07	20 (4%)	33	36	11, 25, 72, 101	0
2	S	123/123 (100%)	-0.02	1 (0%)	86	87	14, 38, 69, 84	0
2	T	123/123 (100%)	0.08	3 (2%)	59	62	14, 38, 69, 84	0
All	All	1128/1138 (99%)	-0.01	38 (3%)	45	48	11, 28, 71, 101	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	VAL	11.9
1	A	467	PHE	11.4
1	A	63	THR	7.9
1	A	465	ILE	7.0
1	B	467	PHE	6.9
1	B	63	THR	6.4
1	A	178	LEU	5.8
1	B	466	VAL	5.1
1	B	178	LEU	4.7
1	A	463	LYS	4.1
1	B	465	ILE	4.0
1	B	70	TRP	3.9
1	B	69	VAL	3.9
1	A	70	TRP	3.9
1	A	93	GLU	3.8
1	B	406	THR	3.7
1	B	337	GLY	3.7
1	A	337	GLY	3.6
1	B	405	GLY	3.5
1	A	333	GLY	3.4
1	A	69	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	S	610	VAL	3.3
1	B	336	GLU	3.3
1	B	93	GLU	3.2
1	A	464	GLU	3.2
2	T	501	MET	2.9
1	B	332	VAL	2.9
1	B	385	TRP	2.8
1	B	407	LEU	2.6
1	A	406	THR	2.6
2	T	524	GLU	2.5
1	B	446	ARG	2.5
2	T	612	CYS	2.4
1	A	335	LEU	2.4
1	B	335	LEU	2.2
1	B	381	GLY	2.1
1	B	451	TRP	2.1
1	B	445	ILE	2.1

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

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

6.3　Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4　Ligands ⓘ

There are no ligands in this entry.

6.5　Other polymers ⓘ

There are no such residues in this entry.