



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:36 PM UTC

PDB ID : 3RUB / pdb_00003rub
Title : CRYSTAL STRUCTURE OF THE UNACTIVATED FORM OF RIBULOS
E-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE FROM
TOBACCO REFINED AT 2.0-ANGSTROMS RESOLUTION
Authors : Schreuder, H.; Cascio, D.; Curmi, P.M.G.; Chapman, M.S.; Suh, S.W.; Eisen-
berg, D.S.
Deposited on : 1990-05-25
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

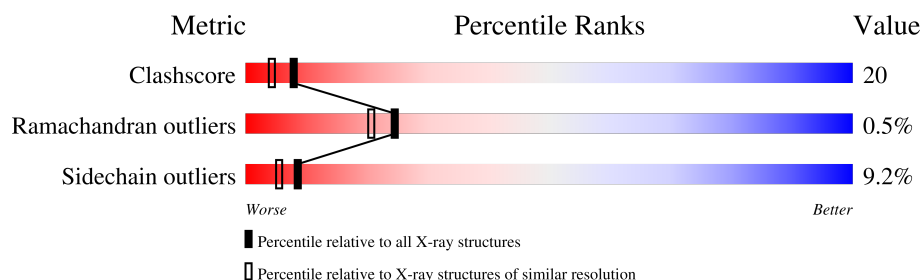
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	477	
2	S	123	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4716 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, FORM III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	441	Total	C	N	O	S	0	0	0
			3455	2194	612	633	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	377	VAL	GLU	conflict	UNP P00876
L	405	MET	GLY	conflict	UNP P00876

- Molecule 2 is a protein called RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE, FORM III.

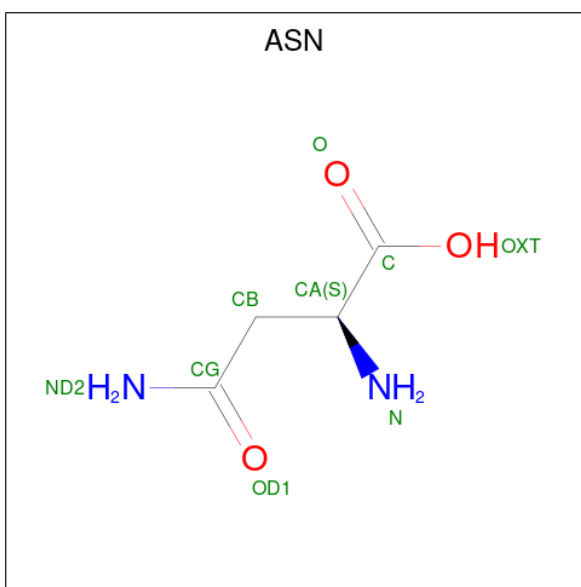
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	123	Total	C	N	O	S	0	0	0
			1029	672	163	188	6			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	N	0	0
			1	1		

- Molecule 5 is water.

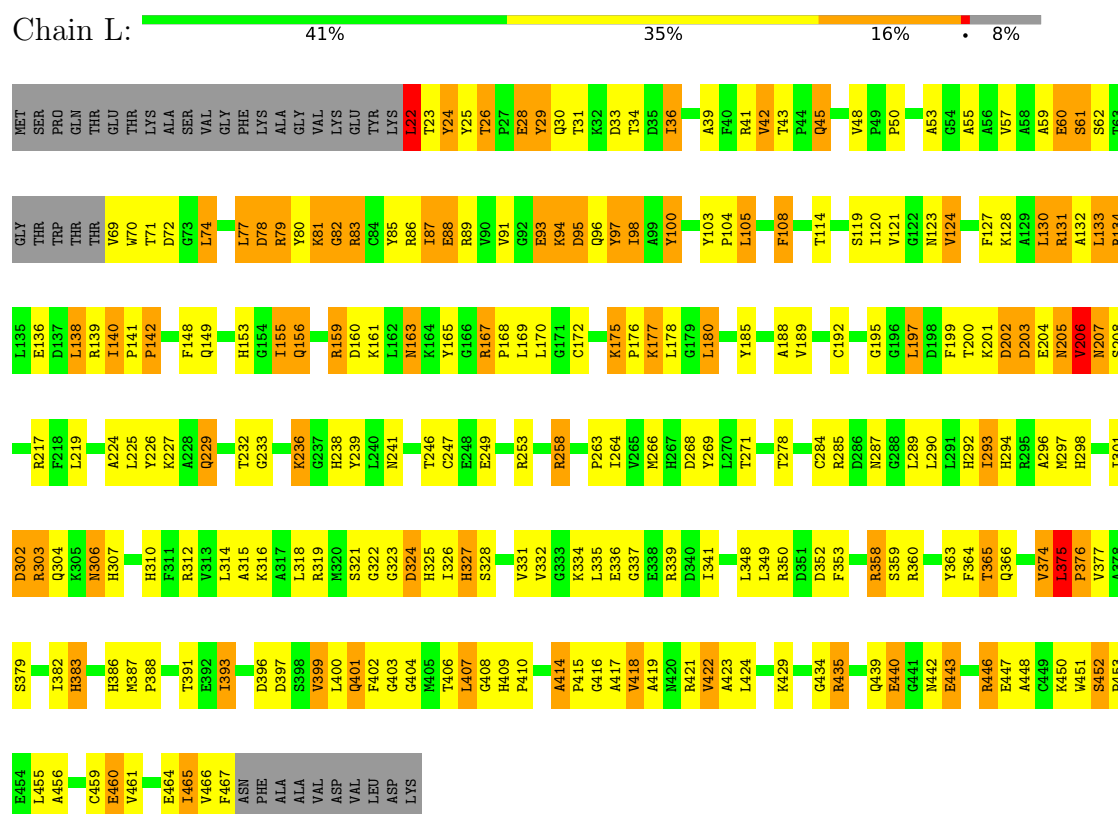
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	179	Total 179	O 179	0	0
5	S	37	Total 37	O 37	0	0

3 Residue-property plots

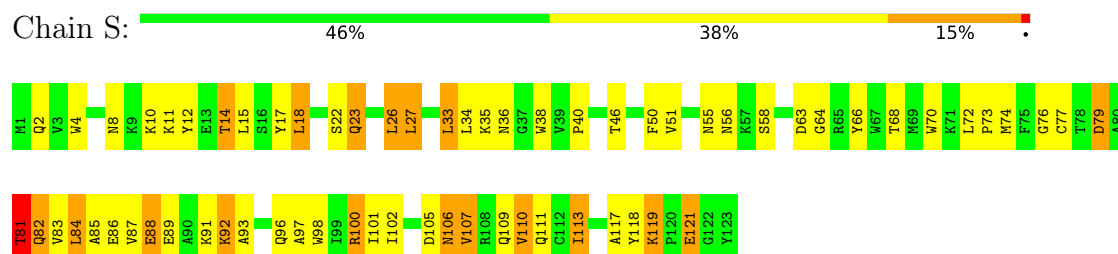
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE, FORM III



- Molecule 2: RIBULOSE 1,5-BISPHOSPHATE CARBOXYLASE/OXYGENASE, FORM III



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	148.70 Å 148.70 Å 137.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4716	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	L	1.42	8/3537 (0.2%)	2.39	221/4793 (4.6%)
2	S	1.30	2/1062 (0.2%)	2.26	61/1442 (4.2%)
All	All	1.39	10/4599 (0.2%)	2.36	282/6235 (4.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	72	LEU	N-CA	6.71	1.50	1.46
1	L	140	ILE	N-CA	5.98	1.50	1.46
2	S	100	ARG	CD-NE	-5.94	1.38	1.46
1	L	322	GLY	N-CA	-5.82	1.36	1.45
1	L	82	GLY	CA-C	5.34	1.58	1.52
1	L	258	ARG	N-CA	5.30	1.52	1.46
1	L	353	PHE	N-CA	5.30	1.52	1.46
1	L	414	ALA	N-CA	5.24	1.50	1.46
1	L	460	GLU	C-O	5.10	1.29	1.24
1	L	142	PRO	C-N	-5.09	1.27	1.33

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	383	HIS	CA-CB-CG	-11.99	101.81	113.80
2	S	100	ARG	CG-CD-NE	10.86	135.89	112.00
2	S	100	ARG	NE-CZ-NH1	10.45	131.95	121.50
1	L	464	GLU	CA-CB-CG	10.32	134.74	114.10
2	S	100	ARG	CB-CG-CD	10.25	134.88	111.30
1	L	29	TYR	CA-C-N	10.20	137.02	122.85
1	L	29	TYR	C-N-CA	10.20	137.02	122.85
1	L	93	GLU	CA-C-O	10.15	132.31	121.55
1	L	33	ASP	CA-CB-CG	-10.08	102.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	82	GLY	N-CA-C	-10.06	98.29	112.37
2	S	33	LEU	O-C-N	9.81	132.29	122.09
1	L	139	ARG	CA-C-N	-9.60	116.07	122.60
1	L	139	ARG	C-N-CA	-9.60	116.07	122.60
1	L	401	GLN	CA-CB-CG	9.54	133.18	114.10
1	L	258	ARG	CA-CB-CG	9.44	132.97	114.10
1	L	134	ARG	CD-NE-CZ	-9.42	111.21	124.40
1	L	400	LEU	CA-C-O	-9.14	110.41	120.38
1	L	310	HIS	CA-CB-CG	-9.03	104.77	113.80
1	L	156	GLN	O-C-N	8.99	131.32	122.07
1	L	465	ILE	N-CA-C	8.84	119.65	110.72
1	L	383	HIS	CA-C-O	-8.76	111.19	121.44
1	L	29	TYR	CA-C-O	8.67	130.80	120.92
1	L	156	GLN	CA-C-O	-8.62	111.77	120.82
1	L	203	ASP	CA-CB-CG	-8.56	104.04	112.60
1	L	26	THR	O-C-N	8.52	128.41	121.17
1	L	339	ARG	CD-NE-CZ	8.50	136.30	124.40
1	L	328	SER	CA-C-O	-8.35	109.62	119.48
1	L	325	HIS	CA-CB-CG	8.32	122.12	113.80
1	L	464	GLU	CB-CG-CD	8.30	126.72	112.60
1	L	127	PHE	CA-CB-CG	-8.26	105.54	113.80
1	L	180	LEU	N-CA-CB	-8.10	97.21	110.41
1	L	133	LEU	O-C-N	8.09	133.12	123.33
1	L	22	LEU	CB-CA-C	8.03	125.35	110.10
2	S	38	TRP	O-C-N	7.93	131.99	123.03
1	L	450	LYS	CA-C-O	-7.81	112.27	120.55
1	L	360	ARG	NE-CZ-NH1	-7.78	113.72	121.50
1	L	153	HIS	CA-CB-CG	-7.77	106.03	113.80
2	S	106	ASN	OD1-CG-ND2	7.74	130.34	122.60
2	S	36	ASN	OD1-CG-ND2	7.73	130.33	122.60
1	L	459	CYS	N-CA-C	7.71	122.69	113.28
1	L	79	ARG	N-CA-CB	7.69	121.54	110.16
1	L	36	ILE	CA-C-O	-7.67	112.36	120.57
1	L	421	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	L	226	TYR	CA-C-O	7.50	128.37	120.42
2	S	101	ILE	CA-C-O	-7.47	112.21	120.72
2	S	100	ARG	NE-CZ-NH2	-7.46	112.48	119.20
1	L	401	GLN	N-CA-CB	-7.43	98.90	110.57
1	L	79	ARG	CA-CB-CG	7.42	128.95	114.10
1	L	165	TYR	CA-C-O	-7.38	112.50	121.06
2	S	100	ARG	CD-NE-CZ	7.29	134.60	124.40
1	L	269	TYR	CA-C-O	-7.13	112.04	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	450	LYS	N-CA-CB	7.12	120.59	110.12
1	L	100	TYR	O-C-N	7.07	131.28	123.22
2	S	55	ASN	CA-CB-CG	-6.99	105.61	112.60
1	L	167	ARG	O-C-N	6.98	129.34	121.32
1	L	206	VAL	CA-CB-CG2	6.90	122.13	110.40
1	L	246	THR	CA-CB-OG1	-6.89	99.26	109.60
2	S	109	GLN	OE1-CD-NE2	6.88	129.48	122.60
1	L	205	ASN	CA-C-O	-6.85	111.25	119.27
1	L	36	ILE	N-CA-C	-6.84	98.58	108.36
1	L	375	LEU	O-C-N	6.84	127.12	121.31
1	L	79	ARG	CA-C-O	-6.83	113.18	120.42
1	L	180	LEU	CB-CA-C	6.82	121.18	109.51
1	L	23	THR	N-CA-C	-6.81	104.55	112.92
1	L	327	HIS	CA-C-O	6.79	128.46	120.58
2	S	38	TRP	CA-C-O	-6.76	113.42	121.66
1	L	399	VAL	CA-C-O	-6.75	112.77	120.67
1	L	396	ASP	N-CA-C	6.74	119.46	111.71
1	L	80	TYR	N-CA-C	6.73	120.39	112.72
2	S	102	ILE	CA-C-O	-6.68	114.66	121.67
1	L	375	LEU	CA-C-O	-6.61	114.37	119.46
2	S	92	LYS	N-CA-CB	6.60	119.64	110.07
2	S	22	SER	O-C-N	6.58	130.31	122.94
1	L	119	SER	CA-C-O	-6.55	113.95	120.70
1	L	464	GLU	N-CA-CB	6.53	119.48	110.01
2	S	98	TRP	N-CA-C	-6.51	99.02	109.96
2	S	107	VAL	N-CA-C	-6.48	104.18	110.72
1	L	233	GLY	N-CA-C	-6.47	106.31	115.43
1	L	287	ASN	CA-CB-CG	-6.47	106.13	112.60
1	L	88	GLU	CB-CA-C	6.45	121.46	109.86
1	L	120	ILE	CB-CG1-CD1	-6.43	100.31	113.80
1	L	264	ILE	N-CA-CB	-6.36	100.93	111.36
2	S	107	VAL	CB-CA-C	6.36	120.99	112.22
1	L	423	ALA	N-CA-C	-6.32	104.31	111.07
1	L	253	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	L	114	THR	CA-CB-OG1	-6.30	100.15	109.60
1	L	93	GLU	N-CA-C	6.29	118.91	110.35
1	L	130	LEU	CA-C-O	-6.29	113.90	120.70
2	S	64	GLY	CA-C-O	-6.29	111.45	119.13
2	S	119	LYS	O-C-N	6.28	127.66	121.57
1	L	304	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	L	241	ASN	CB-CG-OD1	6.25	133.31	120.80
1	L	159	ARG	CA-C-O	6.25	127.17	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	38	TRP	CA-CB-CG	-6.24	101.74	113.60
1	L	224	ALA	CA-C-O	-6.22	114.28	120.82
2	S	84	LEU	CA-C-O	6.22	127.15	120.55
1	L	391	THR	CA-C-O	6.21	127.34	120.82
1	L	134	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	L	138	LEU	CA-C-N	-6.21	114.77	122.84
1	L	138	LEU	C-N-CA	-6.21	114.77	122.84
1	L	22	LEU	CA-CB-CG	6.20	137.98	116.30
1	L	360	ARG	CD-NE-CZ	-6.19	115.74	124.40
1	L	450	LYS	O-C-N	6.17	128.66	122.12
1	L	148	PHE	CA-CB-CG	-6.17	107.63	113.80
1	L	61	SER	CA-CB-OG	6.16	123.42	111.10
1	L	149	GLN	OE1-CD-NE2	6.15	128.75	122.60
1	L	163	ASN	OD1-CG-ND2	-6.14	116.45	122.60
2	S	2	GLN	OE1-CD-NE2	6.14	128.74	122.60
1	L	130	LEU	O-C-N	6.10	131.16	123.23
1	L	77	LEU	O-C-N	6.09	128.43	122.09
1	L	414	ALA	O-C-N	6.08	124.46	120.27
1	L	60	GLU	N-CA-CB	6.06	120.49	110.91
1	L	206	VAL	N-CA-CB	6.04	118.40	111.39
1	L	95	ASP	CB-CA-C	-5.98	103.87	111.22
2	S	106	ASN	CA-CB-CG	-5.96	106.64	112.60
1	L	229	GLN	CA-C-O	5.95	127.07	120.82
1	L	227	LYS	CA-C-O	-5.95	114.57	120.82
1	L	301	ILE	CA-CB-CG2	5.94	120.61	110.50
1	L	293	ILE	CA-C-O	-5.94	114.21	120.57
2	S	68	THR	CA-CB-OG1	-5.93	100.70	109.60
1	L	42	VAL	CA-C-N	5.92	131.09	122.98
1	L	42	VAL	C-N-CA	5.92	131.09	122.98
1	L	217	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	L	131	ARG	N-CA-C	-5.89	104.44	111.69
1	L	24	TYR	O-C-N	5.89	129.37	122.24
1	L	298	HIS	O-C-N	5.88	128.35	122.12
1	L	61	SER	N-CA-C	-5.87	105.43	113.30
1	L	238	HIS	CA-C-O	-5.86	114.03	120.24
1	L	440	GLU	N-CA-C	5.85	119.39	112.72
1	L	22	LEU	CA-C-N	5.85	132.00	122.65
1	L	22	LEU	C-N-CA	5.85	132.00	122.65
1	L	238	HIS	CA-CB-CG	-5.84	107.96	113.80
1	L	258	ARG	CB-CG-CD	5.84	124.73	111.30
1	L	219	LEU	N-CA-CB	-5.84	101.55	110.01
1	L	400	LEU	O-C-N	5.83	130.17	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	418	VAL	O-C-N	5.82	127.61	121.91
1	L	81	LYS	O-C-N	5.81	129.90	123.16
1	L	207	ASN	OD1-CG-ND2	5.79	128.40	122.60
1	L	285	ARG	O-C-N	5.77	128.02	122.07
1	L	264	ILE	N-CA-C	5.76	115.95	108.35
1	L	324	ASP	N-CA-C	-5.73	106.42	113.41
2	S	14	THR	N-CA-C	5.73	119.12	110.64
2	S	111	GLN	N-CA-C	-5.71	99.42	108.73
1	L	287	ASN	CB-CG-ND2	5.68	124.92	116.40
1	L	232	THR	CA-CB-CG2	5.68	120.15	110.50
1	L	439	GLN	CA-C-O	-5.67	113.08	120.00
1	L	59	ALA	CA-C-N	-5.66	114.12	122.83
1	L	59	ALA	C-N-CA	-5.66	114.12	122.83
2	S	92	LYS	O-C-N	5.66	128.20	122.09
1	L	374	VAL	CA-C-O	-5.65	114.27	120.72
2	S	113	ILE	CB-CA-C	5.65	120.55	111.29
2	S	8	ASN	N-CA-C	5.63	119.72	112.86
1	L	321	SER	CA-C-N	5.61	132.41	121.41
1	L	321	SER	C-N-CA	5.61	132.41	121.41
1	L	138	LEU	O-C-N	5.61	130.12	123.33
2	S	88	GLU	CA-C-N	5.61	127.73	120.44
2	S	88	GLU	C-N-CA	5.61	127.73	120.44
2	S	4	TRP	CA-C-N	5.60	126.15	120.38
2	S	4	TRP	C-N-CA	5.60	126.15	120.38
1	L	466	VAL	N-CA-CB	-5.59	102.31	111.98
2	S	110	VAL	O-C-N	5.58	128.91	122.82
1	L	177	LYS	N-CA-CB	5.57	118.41	110.16
2	S	26	LEU	CA-C-O	5.57	126.86	120.90
1	L	423	ALA	CA-C-O	-5.57	114.97	120.82
1	L	249	GLU	CA-CB-CG	5.57	125.24	114.10
1	L	200	THR	N-CA-C	-5.56	101.07	109.85
1	L	391	THR	CA-C-N	5.56	127.66	120.44
1	L	391	THR	C-N-CA	5.56	127.66	120.44
1	L	241	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	L	123	ASN	N-CA-C	5.54	120.91	114.04
1	L	263	PRO	N-CA-C	5.53	121.86	114.18
1	L	217	ARG	NH1-CZ-NH2	-5.52	112.12	119.30
1	L	364	PHE	CA-C-O	-5.52	114.66	121.11
1	L	236	LYS	CA-C-N	5.51	128.10	121.38
1	L	236	LYS	C-N-CA	5.51	128.10	121.38
1	L	301	ILE	N-CA-CB	-5.51	101.74	112.75
1	L	376	PRO	CB-CA-C	5.51	118.53	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	70	TRP	CA-C-O	-5.51	114.69	120.58
2	S	82	GLN	CA-CB-CG	-5.50	103.11	114.10
1	L	124	VAL	N-CA-C	5.49	117.92	111.05
1	L	93	GLU	CA-C-N	5.49	132.03	121.54
1	L	93	GLU	C-N-CA	5.49	132.03	121.54
1	L	208	SER	CA-C-O	-5.48	113.51	120.20
1	L	271	THR	CB-CA-C	5.48	120.73	110.70
1	L	365	THR	CA-CB-OG1	-5.46	101.41	109.60
1	L	421	ARG	NE-CZ-NH1	5.46	126.96	121.50
1	L	98	ILE	CB-CA-C	5.46	118.08	110.99
2	S	121	GLU	CB-CG-CD	5.46	121.88	112.60
1	L	278	THR	N-CA-C	-5.46	105.23	111.07
1	L	439	GLN	OE1-CD-NE2	5.43	128.03	122.60
2	S	66	TYR	CA-C-O	-5.43	114.86	121.05
1	L	227	LYS	O-C-N	5.43	127.66	122.07
2	S	117	ALA	CA-C-O	-5.43	113.16	118.97
1	L	95	ASP	O-C-N	5.42	130.21	121.53
2	S	14	THR	CA-CB-OG1	-5.42	101.48	109.60
1	L	160	ASP	CA-C-O	-5.41	115.13	120.70
1	L	453	PRO	O-C-N	5.41	128.46	122.24
1	L	94	LYS	CA-C-N	5.40	133.09	122.61
1	L	94	LYS	C-N-CA	5.40	133.09	122.61
1	L	247	CYS	CB-CA-C	-5.40	101.82	110.79
1	L	192	CYS	CB-CA-C	5.38	119.33	110.88
1	L	97	TYR	O-C-N	5.38	130.30	122.94
2	S	81	THR	O-C-N	5.38	129.53	122.33
1	L	205	ASN	O-C-N	5.37	129.82	122.46
1	L	39	ALA	CA-C-O	-5.37	114.58	120.70
2	S	73	PRO	CA-C-O	-5.35	115.35	121.56
2	S	92	LYS	N-CA-C	-5.34	105.37	111.14
2	S	18	LEU	O-C-N	5.34	128.28	121.34
2	S	12	TYR	CA-C-O	-5.34	114.88	120.32
1	L	312	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	L	188	ALA	N-CA-C	-5.32	105.65	111.82
1	L	124	VAL	CA-C-O	-5.32	114.88	120.57
2	S	81	THR	CA-CB-OG1	-5.31	101.63	109.60
1	L	287	ASN	CA-C-O	-5.30	113.23	119.48
1	L	26	THR	CA-CB-OG1	-5.29	101.66	109.60
2	S	22	SER	CA-C-O	-5.29	115.47	121.72
2	S	36	ASN	CA-CB-CG	-5.29	107.31	112.60
1	L	45	GLN	N-CA-C	-5.28	103.13	109.83
1	L	88	GLU	CA-CB-CG	5.27	124.64	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	34	LEU	CB-CA-C	5.27	119.16	110.88
1	L	108	PHE	N-CA-C	5.26	118.39	109.76
1	L	452	SER	N-CA-CB	5.26	120.33	111.39
1	L	301	ILE	CB-CA-C	-5.26	106.43	111.06
1	L	350	ARG	NE-CZ-NH1	5.26	126.76	121.50
2	S	79	ASP	CB-CA-C	5.25	119.19	110.74
2	S	119	LYS	CA-C-O	-5.25	114.17	120.41
1	L	202	ASP	N-CA-C	-5.25	102.52	110.28
1	L	83	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	L	323	GLY	N-CA-C	-5.24	100.77	113.18
1	L	226	TYR	O-C-N	-5.22	116.20	122.15
1	L	350	ARG	N-CA-C	5.21	119.70	112.45
1	L	393	ILE	N-CA-C	5.21	115.43	110.53
1	L	325	HIS	CA-C-O	-5.20	115.02	121.11
1	L	127	PHE	CA-C-N	5.18	128.59	120.82
1	L	127	PHE	C-N-CA	5.18	128.59	120.82
2	S	58	SER	CB-CA-C	5.18	118.82	109.45
1	L	149	GLN	N-CA-C	-5.17	105.33	111.69
1	L	460	GLU	CA-C-O	-5.16	115.38	120.90
1	L	302	ASP	N-CA-C	5.16	119.53	112.88
1	L	175	LYS	N-CA-C	-5.15	101.18	109.58
1	L	268	ASP	CA-C-O	-5.14	115.64	121.39
1	L	464	GLU	CA-C-O	-5.14	115.43	120.82
2	S	14	THR	O-C-N	5.13	129.25	122.89
2	S	56	ASN	N-CA-CB	-5.13	103.61	111.56
1	L	123	ASN	CA-CB-CG	-5.13	107.47	112.60
1	L	161	LYS	N-CA-C	-5.12	105.78	111.36
1	L	435	ARG	CB-CG-CD	-5.12	99.53	111.30
1	L	306	ASN	CA-C-N	-5.11	113.58	122.37
1	L	306	ASN	C-N-CA	-5.11	113.58	122.37
1	L	352	ASP	CA-CB-CG	-5.11	107.49	112.60
2	S	98	TRP	N-CA-CB	5.11	118.51	110.23
2	S	63	ASP	N-CA-C	-5.11	102.96	110.52
1	L	339	ARG	CA-C-N	5.10	127.53	120.29
1	L	339	ARG	C-N-CA	5.10	127.53	120.29
1	L	131	ARG	CA-C-O	5.09	125.89	120.24
2	S	73	PRO	N-CA-C	-5.09	103.11	111.21
2	S	118	TYR	CA-C-O	-5.09	114.56	120.31
1	L	301	ILE	CB-CG1-CD1	-5.09	103.11	113.80
1	L	83	ARG	NH1-CZ-NH2	5.08	125.90	119.30
1	L	285	ARG	CD-NE-CZ	5.06	131.49	124.40
1	L	119	SER	O-C-N	5.06	127.55	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	278	THR	N-CA-CB	5.06	117.34	110.01
1	L	399	VAL	O-C-N	5.05	128.64	123.18
1	L	105	LEU	O-C-N	5.05	127.47	122.12
1	L	303	ARG	CA-C-N	5.05	128.51	121.24
1	L	303	ARG	C-N-CA	5.05	128.51	121.24
1	L	365	THR	N-CA-C	-5.05	102.38	109.96
1	L	81	LYS	CA-C-N	-5.05	115.50	120.60
1	L	81	LYS	C-N-CA	-5.05	115.50	120.60
1	L	160	ASP	CA-CB-CG	5.04	117.64	112.60
1	L	60	GLU	CA-CB-CG	5.04	124.18	114.10
1	L	36	ILE	N-CA-CB	5.04	117.03	110.99
1	L	287	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	L	439	GLN	O-C-N	5.03	129.67	122.28
1	L	337	GLY	CA-C-N	5.02	129.10	120.71
1	L	337	GLY	C-N-CA	5.02	129.10	120.71
1	L	41	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	L	155	ILE	N-CA-C	5.02	119.78	109.34
1	L	416	GLY	CA-C-O	5.02	125.72	120.80
1	L	23	THR	CA-C-O	5.00	125.41	119.56
1	L	253	ARG	CD-NE-CZ	5.00	131.41	124.40
1	L	434	GLY	CA-C-O	-5.00	113.46	119.06

There are no chirality outliers.

There are no planarity outliers.

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	L	3455	0	3389	143	1
2	S	1029	0	994	38	0
3	L	15	0	0	1	0
4	L	1	0	0	0	0
5	L	179	0	0	2	0
5	S	37	0	0	0	0
All	All	4716	0	4383	175	1

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

All (175) 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:L:172:CYS:HB2	1:L:197:LEU:HD23	1.34	1.07
2:S:40:PRO:HG2	2:S:74:MET:HE3	1.43	0.98
1:L:140:ILE:H	1:L:366:GLN:HE22	1.21	0.89
2:S:27:LEU:HD12	2:S:84:LEU:HD22	1.54	0.88
1:L:443:GLU:O	1:L:447:GLU:HG3	1.73	0.88
1:L:69:VAL:O	1:L:72:ASP:HB2	1.75	0.86
1:L:170:LEU:HD21	1:L:424:LEU:HD22	1.59	0.83
2:S:86:GLU:HA	2:S:86:GLU:OE1	1.81	0.80
2:S:11:LYS:HG3	2:S:17:TYR:CE1	2.16	0.80
1:L:172:CYS:HB2	1:L:197:LEU:CD2	2.12	0.79
1:L:156:GLN:HG2	2:S:110:VAL:HG12	1.65	0.78
1:L:156:GLN:HG2	2:S:110:VAL:CG1	2.14	0.78
1:L:30:GLN:O	1:L:30:GLN:HG2	1.86	0.76
1:L:132:ALA:CB	1:L:306:ASN:HD22	1.99	0.76
2:S:105:ASP:OD1	2:S:107:VAL:HG22	1.86	0.75
1:L:57:VAL:O	1:L:61:SER:CB	2.35	0.74
2:S:88:GLU:OE2	2:S:91:LYS:HE3	1.89	0.73
1:L:57:VAL:O	1:L:61:SER:HB3	1.90	0.72
2:S:33:LEU:CD1	2:S:113:ILE:HD13	2.18	0.72
1:L:406:THR:OG1	1:L:407:LEU:HD23	1.90	0.72
2:S:82:GLN:O	2:S:85:ALA:HB3	1.90	0.72
1:L:70:TRP:CZ3	1:L:74:LEU:HD21	2.24	0.71
1:L:98:ILE:HD13	1:L:363:TYR:CE2	2.26	0.70
1:L:70:TRP:HZ3	1:L:74:LEU:HD21	1.56	0.70
1:L:50:PRO:O	1:L:53:ALA:HB3	1.92	0.69
1:L:69:VAL:HG23	1:L:72:ASP:OD1	1.93	0.69
1:L:156:GLN:CG	2:S:110:VAL:HG12	2.23	0.68
1:L:446:ARG:HG3	1:L:467:PHE:CE2	2.29	0.68
1:L:22:LEU:HD23	1:L:25:TYR:HB3	1.76	0.67
2:S:33:LEU:HD12	2:S:113:ILE:HD13	1.77	0.67
1:L:36:ILE:HD13	1:L:108:PHE:CE2	2.30	0.66
2:S:27:LEU:HD12	2:S:84:LEU:CD2	2.27	0.65
1:L:71:THR:HA	1:L:74:LEU:HD22	1.80	0.64
1:L:69:VAL:CG2	1:L:72:ASP:OD1	2.46	0.63
1:L:156:GLN:CG	2:S:110:VAL:CG1	2.75	0.63
1:L:43:THR:HA	1:L:95:ASP:O	1.98	0.63
1:L:172:CYS:CB	1:L:197:LEU:HD23	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:316:LYS:NZ	1:L:366:GLN:HE21	1.98	0.62
1:L:43:THR:HG22	1:L:131:ARG:HB3	1.80	0.62
1:L:29:TYR:CE2	1:L:31:THR:HA	2.35	0.62
1:L:403:GLY:HA3	3:L:490:SO4:O2	2.00	0.61
1:L:98:ILE:HD13	1:L:363:TYR:HE2	1.63	0.61
2:S:92:LYS:HD2	2:S:93:ALA:N	2.14	0.61
1:L:138:LEU:O	1:L:316:LYS:NZ	2.33	0.61
1:L:57:VAL:O	1:L:61:SER:HB2	1.99	0.61
1:L:442:ASN:O	1:L:446:ARG:HB2	2.00	0.61
1:L:435:ARG:HH22	1:L:447:GLU:CD	2.09	0.61
1:L:132:ALA:HB1	1:L:306:ASN:HD22	1.65	0.60
1:L:414:ALA:HB3	1:L:415:PRO:HD3	1.82	0.60
2:S:106:ASN:OD1	2:S:106:ASN:C	2.40	0.60
1:L:88:GLU:OE2	1:L:358:ARG:NH1	2.32	0.60
1:L:422:VAL:CG2	1:L:455:LEU:HD22	2.32	0.60
1:L:61:SER:HB2	1:L:124:VAL:HG11	1.83	0.60
2:S:46:THR:HG22	2:S:97:ALA:HB2	1.84	0.59
2:S:79:ASP:OD1	2:S:81:THR:OG1	2.12	0.59
1:L:316:LYS:HZ1	1:L:366:GLN:HE21	1.49	0.59
1:L:167:ARG:HG3	1:L:168:PRO:O	2.02	0.59
1:L:203:ASP:HB3	1:L:206:VAL:HG13	1.84	0.59
1:L:155:ILE:HG12	1:L:375:LEU:HD13	1.84	0.59
2:S:33:LEU:HD11	2:S:113:ILE:HD13	1.85	0.57
1:L:86:ARG:HG2	1:L:100:TYR:CD1	2.39	0.57
2:S:40:PRO:HG2	2:S:74:MET:CE	2.28	0.57
1:L:201:LYS:HG2	1:L:202:ASP:O	2.05	0.56
1:L:42:VAL:HG23	1:L:130:LEU:HD22	1.88	0.56
1:L:85:TYR:O	1:L:86:ARG:HB2	2.04	0.56
1:L:318:LEU:C	1:L:318:LEU:HD13	2.30	0.56
1:L:379:SER:HB3	1:L:401:GLN:HB3	1.88	0.56
1:L:70:TRP:CZ3	1:L:74:LEU:CD2	2.90	0.55
1:L:382:ILE:HG21	1:L:402:PHE:HE1	1.71	0.54
2:S:14:THR:HG22	2:S:15:LEU:HG	1.89	0.54
1:L:42:VAL:HG23	1:L:130:LEU:CD2	2.37	0.54
2:S:79:ASP:C	2:S:81:THR:N	2.65	0.53
1:L:78:ASP:HA	1:L:81:LYS:HE3	1.91	0.53
1:L:404:GLY:O	1:L:408:GLY:HA3	2.09	0.53
1:L:414:ALA:N	1:L:415:PRO:CD	2.71	0.53
1:L:382:ILE:HG21	1:L:402:PHE:CE1	2.44	0.52
1:L:358:ARG:HD2	5:L:669:HOH:O	2.09	0.52
1:L:452:SER:O	1:L:456:ALA:N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:178:LEU:HD21	1:L:205:ASN:HB2	1.91	0.51
1:L:175:LYS:HA	1:L:176:PRO:C	2.34	0.51
2:S:35:LYS:O	2:S:35:LYS:HG3	2.11	0.51
1:L:442:ASN:ND2	5:L:552:HOH:O	2.29	0.51
2:S:79:ASP:C	2:S:81:THR:H	2.18	0.51
1:L:451:TRP:CE3	1:L:451:TRP:O	2.64	0.51
1:L:22:LEU:HD22	1:L:22:LEU:O	2.11	0.50
2:S:87:VAL:O	2:S:91:LYS:HG2	2.12	0.50
1:L:45:GLN:O	1:L:48:VAL:HG22	2.12	0.50
1:L:266:MET:HE3	1:L:294:HIS:HB2	1.94	0.50
1:L:451:TRP:O	1:L:451:TRP:HE3	1.95	0.50
2:S:11:LYS:HG3	2:S:17:TYR:CZ	2.47	0.50
2:S:33:LEU:HG	2:S:113:ILE:HG21	1.94	0.50
1:L:176:PRO:HD2	1:L:180:LEU:HD22	1.94	0.49
1:L:382:ILE:CG2	1:L:402:PHE:HE1	2.25	0.49
1:L:88:GLU:O	1:L:97:TYR:HA	2.12	0.49
1:L:387:MET:N	1:L:388:PRO:CD	2.75	0.49
1:L:169:LEU:HB2	1:L:399:VAL:HG22	1.95	0.49
1:L:409:HIS:CG	1:L:410:PRO:HD2	2.48	0.49
1:L:418:VAL:O	1:L:422:VAL:HG13	2.13	0.49
1:L:29:TYR:CD1	1:L:83:ARG:HD2	2.47	0.48
1:L:134:ARG:HD3	1:L:136:GLU:OE2	2.12	0.48
1:L:331:VAL:HG21	1:L:393:ILE:HG21	1.95	0.48
1:L:42:VAL:O	1:L:96:GLN:HA	2.13	0.48
2:S:23:GLN:HG3	2:S:84:LEU:HD21	1.95	0.48
1:L:302:ASP:C	1:L:302:ASP:OD1	2.55	0.48
2:S:35:LYS:O	2:S:35:LYS:CG	2.55	0.48
1:L:26:THR:HB	1:L:28:GLU:OE1	2.14	0.48
1:L:315:ALA:HB1	1:L:349:LEU:HD21	1.96	0.48
1:L:318:LEU:HG	1:L:326:ILE:HD12	1.94	0.48
1:L:62:SER:OG	1:L:82:GLY:N	2.35	0.48
1:L:414:ALA:O	1:L:418:VAL:HG23	2.15	0.47
1:L:422:VAL:HG23	1:L:455:LEU:HD22	1.96	0.47
1:L:159:ARG:O	1:L:163:ASN:N	2.48	0.47
1:L:382:ILE:CG2	1:L:402:PHE:CE1	2.98	0.47
1:L:376:PRO:HD2	1:L:397:ASP:O	2.14	0.46
1:L:383:HIS:N	1:L:386:HIS:ND1	2.63	0.46
1:L:239:TYR:HB3	1:L:266:MET:HB2	1.97	0.46
1:L:98:ILE:CD1	1:L:363:TYR:HE2	2.27	0.46
1:L:177:LYS:HE3	1:L:205:ASN:ND2	2.30	0.46
1:L:24:TYR:HB2	1:L:55:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:LEU:HA	1:L:180:LEU:HD12	1.56	0.46
1:L:42:VAL:CG1	1:L:97:TYR:HB2	2.46	0.46
1:L:296:ALA:O	1:L:297:MET:CB	2.64	0.45
2:S:79:ASP:O	2:S:81:THR:N	2.49	0.45
1:L:85:TYR:O	1:L:86:ARG:CB	2.63	0.45
1:L:169:LEU:O	1:L:399:VAL:HA	2.16	0.45
1:L:43:THR:HG22	1:L:131:ARG:CB	2.45	0.45
1:L:81:LYS:O	1:L:81:LYS:HG3	2.16	0.45
1:L:172:CYS:SG	1:L:407:LEU:HD21	2.57	0.45
1:L:199:PHE:HB3	1:L:239:TYR:CE1	2.52	0.45
1:L:316:LYS:HE3	1:L:348:LEU:HD13	1.99	0.45
1:L:87:ILE:HG22	1:L:88:GLU:N	2.33	0.44
1:L:435:ARG:NH1	1:L:440:GLU:OE1	2.34	0.44
1:L:206:VAL:C	1:L:207:ASN:HD22	2.26	0.44
2:S:26:LEU:HD12	2:S:26:LEU:HA	1.81	0.44
1:L:318:LEU:HD13	1:L:318:LEU:O	2.18	0.44
1:L:34:THR:HB	1:L:105:LEU:HD22	1.99	0.44
2:S:106:ASN:OD1	2:S:107:VAL:N	2.51	0.44
1:L:448:ALA:HA	1:L:451:TRP:NE1	2.33	0.43
1:L:197:LEU:HD21	1:L:406:THR:HG21	2.00	0.43
1:L:293:ILE:HG13	1:L:318:LEU:HD21	2.00	0.43
1:L:133:LEU:O	1:L:307:HIS:HA	2.19	0.42
2:S:74:MET:HE1	2:S:83:VAL:HG13	2.01	0.42
1:L:70:TRP:C	1:L:72:ASP:N	2.74	0.42
1:L:327:HIS:HA	1:L:377:VAL:HB	2.01	0.42
1:L:141:PRO:HA	1:L:142:PRO:HD3	1.87	0.42
1:L:103:TYR:HA	1:L:104:PRO:HD3	1.79	0.42
1:L:195:GLY:HA3	1:L:417:ALA:HB3	2.01	0.42
1:L:383:HIS:HB2	1:L:386:HIS:CE1	2.54	0.42
1:L:319:ARG:HG3	1:L:374:VAL:HG23	2.02	0.42
2:S:74:MET:HE3	2:S:74:MET:HB2	1.54	0.42
2:S:79:ASP:O	2:S:82:GLN:N	2.48	0.42
1:L:36:ILE:HD13	1:L:108:PHE:CD2	2.54	0.42
2:S:10:LYS:HB3	2:S:50:PHE:CZ	2.55	0.42
1:L:30:GLN:CD	1:L:30:GLN:H	2.28	0.41
1:L:89:ARG:HE	1:L:97:TYR:HE1	1.69	0.41
1:L:284:CYS:HB3	1:L:289:LEU:O	2.21	0.41
1:L:297:MET:O	1:L:297:MET:HG2	2.20	0.41
1:L:446:ARG:HH11	1:L:446:ARG:HD3	1.65	0.41
1:L:43:THR:CG2	1:L:131:ARG:HB3	2.48	0.41
1:L:387:MET:HG2	1:L:424:LEU:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:156:GLN:HG3	2:S:110:VAL:CG1	2.50	0.41
1:L:178:LEU:HD21	1:L:205:ASN:CB	2.50	0.41
1:L:290:LEU:HA	1:L:324:ASP:OD2	2.20	0.41
1:L:50:PRO:HG3	1:L:97:TYR:CZ	2.55	0.41
1:L:229:GLN:HE21	1:L:236:LYS:H	1.68	0.41
1:L:429:LYS:HD3	2:S:18:LEU:HD13	2.03	0.41
1:L:306:ASN:ND2	1:L:307:HIS:HB2	2.36	0.41
1:L:204:GLU:H	1:L:204:GLU:CD	2.28	0.40
1:L:239:TYR:CE2	1:L:292:HIS:CE1	3.09	0.40
1:L:89:ARG:HG3	1:L:97:TYR:CE1	2.55	0.40
1:L:98:ILE:HG22	1:L:100:TYR:CE1	2.57	0.40
1:L:178:LEU:HD23	1:L:206:VAL:HG12	2.04	0.40
1:L:185:TYR:O	1:L:189:VAL:HG23	2.22	0.40
1:L:418:VAL:O	1:L:419:ALA:C	2.64	0.40
1:L:358:ARG:HE	1:L:358:ARG:HB3	1.01	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:THR:OG1	1:L:175:LYS:O[7_556]	2.13	0.07

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	L	437/477 (92%)	413 (94%)	22 (5%)	2 (0%)	24	21
2	S	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	16	11
All	All	558/600 (93%)	525 (94%)	30 (5%)	3 (0%)	24	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	94	LYS
2	S	76	GLY
1	L	332	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	357/387 (92%)	324 (91%)	33 (9%)	8	5
2	S	110/110 (100%)	100 (91%)	10 (9%)	9	6
All	All	467/497 (94%)	424 (91%)	43 (9%)	8	5

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	22	LEU
1	L	28	GLU
1	L	60	GLU
1	L	74	LEU
1	L	77	LEU
1	L	78	ASP
1	L	79	ARG
1	L	87	ILE
1	L	91	VAL
1	L	93	GLU
1	L	121	VAL
1	L	128	LYS
1	L	197	LEU
1	L	206	VAL
1	L	225	LEU
1	L	258	ARG
1	L	303	ARG
1	L	314	LEU
1	L	334	LYS
1	L	335	LEU
1	L	336	GLU

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Mol	Chain	Res	Type
1	L	341	ILE
1	L	358	ARG
1	L	359	SER
1	L	365	THR
1	L	375	LEU
1	L	407	LEU
1	L	422	VAL
1	L	443	GLU
1	L	446	ARG
1	L	460	GLU
1	L	461	VAL
1	L	465	ILE
2	S	23	GLN
2	S	27	LEU
2	S	51	VAL
2	S	77	CYS
2	S	81	THR
2	S	89	GLU
2	S	96	GLN
2	S	100	ARG
2	S	119	LYS
2	S	121	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	30	GLN
1	L	45	GLN
1	L	205	ASN
1	L	207	ASN
1	L	229	GLN
1	L	306	ASN
1	L	366	GLN
1	L	401	GLN
1	L	420	ASN
2	S	8	ASN
2	S	36	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is modelled with single atom - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	L	490	-	4,4,4	0.73	0	6,6,6	0.43	0
3	SO4	L	492	-	4,4,4	0.80	0	6,6,6	0.94	0
3	SO4	L	491	-	4,4,4	0.77	0	6,6,6	1.20	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	491	SO4	O4-S-O1	2.31	121.66	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	490	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.