



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:09 PM UTC

PDB ID : 1SBN / pdb_00001sbn
Title : REFINED CRYSTAL STRUCTURES OF SUBTILISIN NOVO IN COM-
PLEX WITH WILD-TYPE AND TWO MUTANT EGLINS. COMPARISON
WITH OTHER SERINE PROTEINASE INHIBITOR COMPLEXES
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Deposited on : 1991-12-20
Resolution : 2.10 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)	:	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

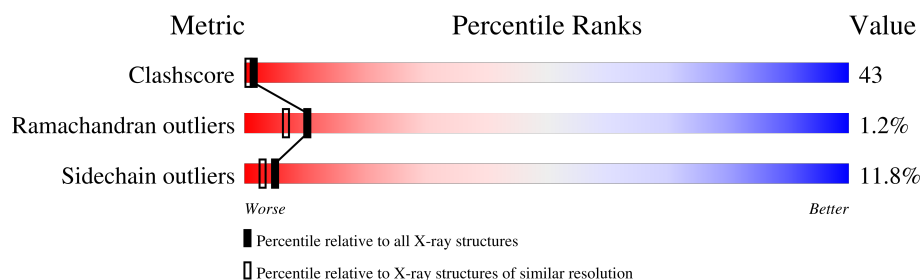
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	E	275	
2	I	70	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2781 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 SUBTILISIN NOVO BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	275	Total	C	N	O	S	0	0	0
			1938	1204	335	394	5			

- Molecule 2 is a protein called EGLIN C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	63	Total	C	N	O	0	0	0
			525	339	93	93			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	33	ASN	ASP	conflict	UNP P01051
I	45	ARG	LEU	conflict	UNP P01051

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

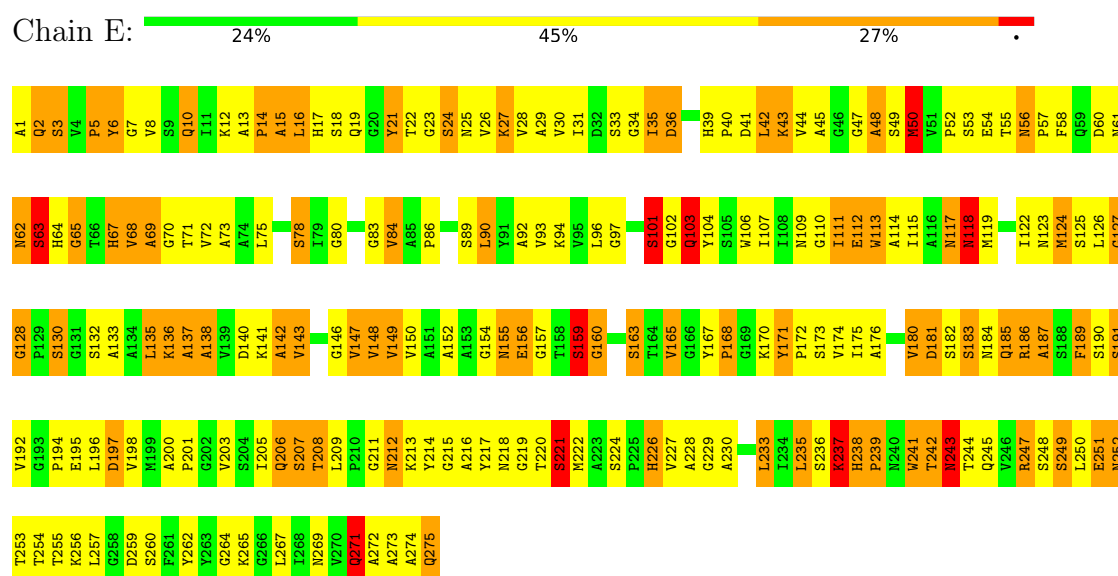
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	255	Total	O	0	0
			255	255		
4	I	61	Total	O	0	0
			61	61		

3 Residue-property plots

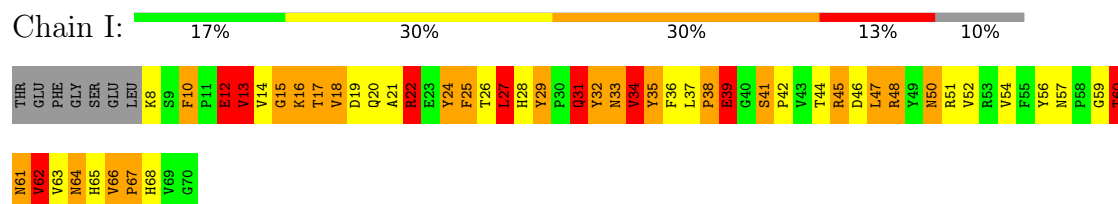
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: EGLIN C



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.90Å 84.90Å 89.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2781	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	E	1.28	0/1976	3.14	284/2697 (10.5%)
2	I	1.14	0/543	2.92	65/741 (8.8%)
All	All	1.25	0/2519	3.09	349/3438 (10.2%)

There are no bond length outliers.

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	ASN	CA-CB-CG	19.57	132.17	112.60
1	E	186	ARG	CD-NE-CZ	13.75	143.65	124.40
1	E	221	SER	CA-CB-OG	13.67	138.43	111.10
1	E	200	ALA	O-C-N	13.30	131.36	121.65
2	I	33	ASN	CA-CB-CG	12.39	124.99	112.60
1	E	25	ASN	CA-CB-CG	-12.21	100.39	112.60
1	E	19	GLN	OE1-CD-NE2	-12.18	110.42	122.60
2	I	22	ARG	CD-NE-CZ	11.85	140.99	124.40
1	E	140	ASP	CA-C-N	11.82	135.81	120.44
1	E	140	ASP	C-N-CA	11.82	135.81	120.44
1	E	186	ARG	NE-CZ-NH2	11.76	129.78	119.20
1	E	73	ALA	N-CA-C	11.57	125.08	110.61
2	I	16	LYS	CA-C-O	11.38	133.73	121.44
2	I	35	TYR	CA-C-O	-11.29	107.68	120.66
1	E	259	ASP	CA-C-N	10.72	135.01	120.54
1	E	259	ASP	C-N-CA	10.72	135.01	120.54
1	E	101	SER	O-C-N	10.55	135.93	123.17
1	E	128	GLY	O-C-N	10.54	132.31	121.77
1	E	200	ALA	CA-C-O	-10.40	110.77	120.34
1	E	64	HIS	CA-C-N	10.37	131.64	120.03
1	E	64	HIS	C-N-CA	10.37	131.64	120.03
1	E	143	VAL	CA-C-O	-10.35	109.56	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	110	GLY	CA-C-N	10.32	133.61	120.70
1	E	110	GLY	C-N-CA	10.32	133.61	120.70
1	E	123	ASN	CA-C-O	-10.31	109.14	120.38
1	E	73	ALA	N-CA-CB	-10.26	97.28	111.65
1	E	65	GLY	CA-C-N	10.25	134.84	120.29
1	E	65	GLY	C-N-CA	10.25	134.84	120.29
1	E	243	ASN	CA-C-O	-10.07	108.72	120.10
2	I	34	VAL	CB-CA-C	10.00	125.08	110.98
1	E	233	LEU	O-C-N	9.99	132.71	122.12
1	E	123	ASN	OD1-CG-ND2	9.86	132.46	122.60
1	E	48	ALA	CA-C-O	-9.86	110.26	121.40
1	E	155	ASN	CA-CB-CG	9.84	122.44	112.60
1	E	14	PRO	CA-C-N	9.78	133.38	120.28
1	E	14	PRO	C-N-CA	9.78	133.38	120.28
1	E	219	GLY	CA-C-O	-9.59	112.46	122.05
1	E	249	SER	O-C-N	9.43	131.78	122.07
1	E	229	GLY	CA-C-N	9.39	132.65	120.44
1	E	229	GLY	C-N-CA	9.39	132.65	120.44
1	E	10	GLN	OE1-CD-NE2	-9.39	113.21	122.60
1	E	269	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	E	84	VAL	CA-C-O	-9.09	111.82	121.27
2	I	27	LEU	O-C-N	9.02	132.57	122.11
1	E	213	LYS	CA-C-N	8.88	136.94	122.29
1	E	213	LYS	C-N-CA	8.88	136.94	122.29
1	E	15	ALA	O-C-N	8.80	131.45	122.12
1	E	208	THR	CA-CB-OG1	-8.75	96.47	109.60
2	I	35	TYR	O-C-N	8.73	133.92	123.27
1	E	71	THR	CA-CB-OG1	-8.71	96.54	109.60
1	E	136	LYS	CA-C-O	-8.59	109.10	119.49
1	E	237	LYS	N-CA-CB	8.46	123.03	110.33
1	E	24	SER	N-CA-CB	8.40	122.55	109.69
1	E	198	VAL	CA-C-O	-8.35	112.67	121.44
1	E	192	VAL	CA-C-O	-8.34	112.91	121.67
2	I	22	ARG	N-CA-C	-8.34	101.88	110.97
1	E	187	ALA	CA-C-O	-8.32	111.84	121.16
1	E	5	PRO	CB-CA-C	8.28	121.83	111.23
1	E	135	LEU	N-CA-C	-8.27	101.86	111.03
1	E	42	LEU	CA-C-O	-8.16	111.59	121.06
1	E	253	THR	N-CA-C	8.15	123.02	112.26
1	E	33	SER	O-C-N	8.12	132.77	122.37
1	E	6	TYR	N-CA-C	8.07	120.99	111.71
2	I	29	TYR	N-CA-C	8.02	123.56	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	19	ASP	CA-CB-CG	-8.00	104.60	112.60
1	E	22	THR	CA-C-N	7.98	132.59	121.26
1	E	22	THR	C-N-CA	7.98	132.59	121.26
2	I	60	THR	N-CA-C	-7.98	101.96	112.34
1	E	114	ALA	O-C-N	7.97	130.70	122.09
1	E	19	GLN	N-CA-C	-7.92	103.07	112.89
1	E	238	HIS	O-C-N	7.91	128.52	121.32
1	E	68	VAL	CA-C-O	-7.88	113.21	121.41
1	E	227	VAL	CA-C-O	-7.82	112.56	120.85
1	E	203	VAL	CA-C-N	7.73	134.04	122.68
1	E	203	VAL	C-N-CA	7.73	134.04	122.68
1	E	156	GLU	CG-CD-OE2	-7.73	100.63	118.40
1	E	101	SER	CA-C-O	-7.72	112.68	121.40
1	E	109	ASN	CA-C-N	7.72	128.49	120.00
1	E	109	ASN	C-N-CA	7.72	128.49	120.00
2	I	33	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	E	48	ALA	N-CA-CB	-7.64	98.39	111.69
1	E	65	GLY	O-C-N	-7.62	114.77	122.17
1	E	143	VAL	N-CA-C	-7.60	103.38	110.53
1	E	271	GLN	OE1-CD-NE2	7.58	130.18	122.60
1	E	118	ASN	CA-C-O	-7.58	111.47	120.57
1	E	160	GLY	CA-C-O	-7.42	112.45	122.39
1	E	219	GLY	O-C-N	7.39	131.36	123.23
1	E	247	ARG	CA-C-N	7.36	130.48	120.54
1	E	247	ARG	C-N-CA	7.36	130.48	120.54
1	E	149	VAL	O-C-N	7.36	131.00	123.20
1	E	140	ASP	CA-C-O	7.35	128.41	120.10
1	E	127	GLY	O-C-N	7.33	132.24	122.70
1	E	220	THR	CA-C-O	7.31	128.38	119.38
1	E	226	HIS	N-CA-C	-7.30	103.40	111.36
1	E	235	LEU	CA-C-N	7.30	131.41	120.31
1	E	235	LEU	C-N-CA	7.30	131.41	120.31
2	I	18	VAL	CA-C-O	-7.30	113.36	120.95
1	E	58	PHE	CA-CB-CG	-7.28	106.52	113.80
1	E	103	GLN	CA-C-O	-7.27	112.77	121.56
1	E	42	LEU	O-C-N	7.20	131.62	123.27
1	E	67	HIS	O-C-N	-7.17	114.28	122.03
2	I	15	GLY	CA-C-N	7.15	131.33	120.82
2	I	15	GLY	C-N-CA	7.15	131.33	120.82
1	E	2	GLN	OE1-CD-NE2	-7.12	115.48	122.60
2	I	25	PHE	CA-C-O	7.10	128.87	120.92
1	E	84	VAL	O-C-N	7.09	129.03	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	135	LEU	O-C-N	7.08	129.68	122.03
2	I	68	HIS	CA-CB-CG	7.04	120.84	113.80
1	E	221	SER	CA-C-N	7.01	132.59	120.68
1	E	221	SER	C-N-CA	7.01	132.59	120.68
2	I	48	ARG	NE-CZ-NH1	6.98	128.48	121.50
1	E	69	ALA	CA-C-O	-6.98	112.38	120.20
1	E	243	ASN	N-CA-C	-6.94	103.73	111.71
2	I	33	ASN	CB-CA-C	6.93	122.25	110.81
1	E	75	LEU	N-CA-C	6.92	119.75	110.35
1	E	191	SER	CA-C-O	-6.91	114.02	121.56
1	E	123	ASN	CA-CB-CG	-6.90	105.70	112.60
1	E	148	VAL	N-CA-C	-6.86	97.74	108.23
1	E	26	VAL	CA-C-N	6.85	131.75	122.84
1	E	26	VAL	C-N-CA	6.85	131.75	122.84
1	E	31	ILE	CB-CA-C	6.84	120.70	111.88
1	E	103	GLN	N-CA-C	-6.83	99.55	110.14
1	E	26	VAL	CB-CA-C	6.80	119.99	111.15
1	E	69	ALA	O-C-N	6.80	129.95	122.20
1	E	24	SER	CA-C-O	6.78	128.65	120.92
1	E	209	LEU	CB-CA-C	6.76	119.49	109.22
1	E	68	VAL	N-CA-C	-6.75	103.20	110.23
1	E	142	ALA	CA-C-N	6.75	129.20	120.56
1	E	142	ALA	C-N-CA	6.75	129.20	120.56
1	E	180	VAL	CA-C-O	-6.75	113.78	121.75
1	E	143	VAL	O-C-N	6.75	128.92	121.90
1	E	114	ALA	CA-C-O	-6.73	113.76	120.70
1	E	64	HIS	CA-CB-CG	6.73	120.53	113.80
1	E	35	ILE	N-CA-C	6.73	117.81	107.78
1	E	269	ASN	O-C-N	6.73	131.75	123.14
1	E	203	VAL	O-C-N	-6.70	116.10	123.20
1	E	3	SER	CA-C-O	-6.70	113.27	121.11
1	E	186	ARG	CA-C-N	6.69	130.37	120.87
1	E	186	ARG	C-N-CA	6.69	130.37	120.87
1	E	103	GLN	O-C-N	6.66	131.69	123.10
1	E	262	TYR	CA-C-N	6.65	132.67	122.29
1	E	262	TYR	C-N-CA	6.65	132.67	122.29
1	E	44	VAL	CA-C-N	6.64	133.35	121.66
1	E	44	VAL	C-N-CA	6.64	133.35	121.66
1	E	190	SER	CB-CA-C	6.63	120.73	109.72
2	I	51	ARG	N-CA-C	6.61	119.72	109.07
2	I	51	ARG	NE-CZ-NH1	-6.61	114.89	121.50
1	E	217	TYR	CA-C-O	-6.59	113.72	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	175	ILE	CA-CB-CG2	6.58	121.69	110.50
1	E	128	GLY	CA-C-O	-6.57	112.13	121.52
1	E	163	SER	N-CA-C	-6.56	100.77	110.48
1	E	212	ASN	CA-CB-CG	-6.56	106.04	112.60
1	E	125	SER	N-CA-C	-6.55	101.57	110.68
1	E	272	ALA	N-CA-CB	6.51	119.80	110.16
1	E	124	MET	CA-C-N	6.48	131.80	122.08
1	E	124	MET	C-N-CA	6.48	131.80	122.08
1	E	269	ASN	CA-C-O	-6.48	111.72	120.47
2	I	60	THR	CA-CB-CG2	6.47	121.50	110.50
1	E	220	THR	CA-CB-OG1	-6.45	99.93	109.60
1	E	63	SER	CA-C-N	6.44	133.84	121.54
1	E	63	SER	C-N-CA	6.44	133.84	121.54
2	I	47	LEU	CA-C-O	-6.43	113.37	120.38
1	E	259	ASP	CA-CB-CG	-6.42	106.18	112.60
2	I	29	TYR	O-C-N	6.41	127.25	121.42
2	I	60	THR	CA-CB-OG1	-6.41	99.98	109.60
1	E	252	ASN	CA-CB-CG	-6.40	106.20	112.60
2	I	13	VAL	CA-C-O	-6.39	113.22	119.92
1	E	197	ASP	N-CA-C	6.38	121.17	112.68
1	E	90	LEU	N-CA-C	6.38	119.10	108.96
1	E	200	ALA	N-CA-C	-6.37	100.86	108.25
2	I	34	VAL	N-CA-CB	-6.37	100.67	110.86
1	E	90	LEU	N-CA-CB	-6.32	99.55	110.17
1	E	196	LEU	CA-C-O	-6.31	113.56	120.81
1	E	250	LEU	O-C-N	6.30	128.80	122.12
1	E	27	LYS	CB-CA-C	-6.29	100.71	110.78
1	E	23	GLY	CA-C-O	-6.29	112.04	119.46
1	E	227	VAL	O-C-N	6.29	128.31	121.83
1	E	113	TRP	CA-C-O	6.27	127.20	120.55
1	E	146	GLY	N-CA-C	6.27	124.11	115.27
2	I	22	ARG	CB-CG-CD	6.27	125.72	111.30
1	E	259	ASP	CA-C-O	6.26	127.21	120.95
1	E	152	ALA	N-CA-CB	-6.26	99.91	109.92
1	E	18	SER	CA-C-N	6.23	132.04	121.14
1	E	18	SER	C-N-CA	6.23	132.04	121.14
1	E	137	ALA	CA-C-N	6.22	128.61	120.28
1	E	137	ALA	C-N-CA	6.22	128.61	120.28
1	E	159	SER	O-C-N	6.21	130.84	122.59
1	E	117	ASN	CA-CB-CG	6.20	118.80	112.60
1	E	6	TYR	O-C-N	-6.19	114.98	122.22
1	E	255	THR	N-CA-C	-6.17	99.15	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	VAL	N-CA-C	-6.17	104.73	110.53
1	E	19	GLN	CA-CB-CG	6.16	126.42	114.10
1	E	132	SER	CB-CA-C	-6.14	99.20	110.62
1	E	50	MET	CA-C-N	6.13	127.01	122.59
1	E	50	MET	C-N-CA	6.13	127.01	122.59
2	I	51	ARG	CD-NE-CZ	6.11	132.95	124.40
2	I	47	LEU	O-C-N	6.10	130.49	123.29
1	E	181	ASP	N-CA-C	-6.09	100.55	109.63
2	I	44	THR	CA-CB-CG2	6.07	120.83	110.50
1	E	191	SER	O-C-N	6.05	130.00	122.86
1	E	7	GLY	CA-C-O	-6.05	113.65	120.30
1	E	132	SER	N-CA-C	6.03	118.01	108.79
2	I	31	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	E	103	GLN	N-CA-CB	6.02	120.12	110.85
1	E	18	SER	CA-C-O	-6.00	112.00	119.38
1	E	56	ASN	O-C-N	5.99	128.20	121.32
2	I	67	PRO	CB-CA-C	-5.95	103.30	111.21
1	E	96	LEU	CA-C-O	-5.94	114.17	121.06
2	I	54	VAL	O-C-N	5.92	130.64	122.88
2	I	62	VAL	N-CA-C	5.90	117.08	108.58
1	E	165	VAL	CB-CA-C	5.89	118.81	111.15
1	E	189	PHE	CA-C-O	5.89	126.62	119.31
1	E	201	PRO	CB-CA-C	5.89	119.06	111.64
2	I	32	TYR	CA-CB-CG	5.89	124.50	113.90
1	E	197	ASP	CA-C-O	-5.88	111.89	120.13
1	E	19	GLN	N-CA-CB	5.84	119.93	110.40
1	E	228	ALA	CA-C-N	-5.84	113.49	119.98
1	E	228	ALA	C-N-CA	-5.84	113.49	119.98
2	I	66	VAL	CA-C-N	5.84	125.60	119.76
2	I	66	VAL	C-N-CA	5.84	125.60	119.76
2	I	22	ARG	CA-C-N	5.83	128.41	120.54
2	I	22	ARG	C-N-CA	5.83	128.41	120.54
1	E	127	GLY	CA-C-N	-5.82	112.74	121.87
1	E	127	GLY	C-N-CA	-5.82	112.74	121.87
1	E	22	THR	O-C-N	-5.78	115.20	122.19
1	E	185	GLN	CA-C-O	-5.77	114.28	120.92
2	I	39	GLU	O-C-N	-5.77	116.14	123.06
1	E	174	VAL	CA-C-N	5.75	129.67	122.48
1	E	174	VAL	C-N-CA	5.75	129.67	122.48
2	I	39	GLU	CA-C-O	5.75	127.23	120.96
1	E	93	VAL	CB-CA-C	5.75	119.00	111.53
1	E	243	ASN	CA-CB-CG	5.75	118.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	176	ALA	CB-CA-C	5.74	119.20	109.84
1	E	243	ASN	N-CA-CB	5.74	119.06	110.22
2	I	48	ARG	N-CA-CB	5.73	120.71	110.80
1	E	251	GLU	CB-CG-CD	-5.72	102.87	112.60
1	E	150	VAL	N-CA-CB	-5.71	101.45	111.39
1	E	254	THR	N-CA-CB	-5.68	102.60	110.38
1	E	189	PHE	O-C-N	-5.67	114.63	122.46
1	E	194	PRO	CB-CA-C	5.66	120.42	111.31
1	E	206	GLN	CB-CG-CD	5.66	122.22	112.60
2	I	32	TYR	N-CA-C	5.65	118.93	109.95
1	E	219	GLY	N-CA-C	5.65	117.68	110.96
1	E	43	LYS	CB-CA-C	5.65	118.86	110.62
1	E	73	ALA	O-C-N	-5.64	115.00	121.99
1	E	224	SER	CA-C-N	5.62	125.30	119.56
1	E	224	SER	C-N-CA	5.62	125.30	119.56
1	E	163	SER	N-CA-CB	5.62	118.83	110.29
1	E	226	HIS	O-C-N	-5.61	115.76	122.15
1	E	243	ASN	O-C-N	5.58	128.75	122.22
2	I	17	THR	N-CA-C	-5.58	102.64	110.35
1	E	15	ALA	N-CA-C	-5.58	105.20	111.28
1	E	148	VAL	CA-CB-CG2	5.58	119.88	110.40
1	E	269	ASN	CA-CB-CG	5.57	118.17	112.60
1	E	221	SER	O-C-N	-5.56	115.71	122.22
1	E	159	SER	N-CA-CB	5.55	119.87	110.49
1	E	239	PRO	CA-C-O	5.54	127.49	119.34
1	E	73	ALA	CA-C-N	5.54	128.63	120.82
1	E	73	ALA	C-N-CA	5.54	128.63	120.82
1	E	182	SER	CA-C-N	5.53	131.06	122.49
1	E	182	SER	C-N-CA	5.53	131.06	122.49
1	E	75	LEU	O-C-N	5.51	129.58	122.81
2	I	33	ASN	CA-C-O	5.50	126.47	120.58
1	E	152	ALA	CA-C-N	5.49	130.01	120.68
1	E	152	ALA	C-N-CA	5.49	130.01	120.68
2	I	33	ASN	CB-CG-ND2	5.48	124.62	116.40
1	E	233	LEU	N-CA-CB	5.46	118.15	110.12
2	I	48	ARG	N-CA-C	-5.46	99.53	108.76
1	E	30	VAL	CA-C-N	5.46	129.30	122.48
1	E	30	VAL	C-N-CA	5.46	129.30	122.48
1	E	111	ILE	O-C-N	5.45	127.56	121.94
1	E	157	GLY	CA-C-N	5.45	131.64	122.87
1	E	157	GLY	C-N-CA	5.45	131.64	122.87
1	E	112	GLU	CA-CB-CG	5.44	124.98	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	128	GLY	N-CA-C	-5.44	101.25	112.34
2	I	12	GLU	CB-CG-CD	5.43	121.84	112.60
1	E	218	ASN	CB-CG-ND2	5.43	124.54	116.40
1	E	272	ALA	CA-C-N	5.41	127.47	120.44
1	E	272	ALA	C-N-CA	5.41	127.47	120.44
1	E	112	GLU	N-CA-C	-5.38	105.58	111.82
1	E	211	GLY	CA-C-O	-5.36	113.61	119.88
1	E	147	VAL	CA-C-N	5.36	129.07	122.37
1	E	147	VAL	C-N-CA	5.36	129.07	122.37
1	E	201	PRO	O-C-N	-5.35	116.86	123.01
1	E	207	SER	CA-CB-OG	-5.35	100.41	111.10
1	E	171	TYR	CA-C-O	-5.34	112.85	120.16
1	E	208	THR	CA-CB-CG2	5.33	119.56	110.50
2	I	62	VAL	CA-CB-CG1	-5.33	101.34	110.40
1	E	8	VAL	CA-C-N	-5.32	113.52	120.44
1	E	8	VAL	C-N-CA	-5.32	113.52	120.44
2	I	46	ASP	CA-C-O	-5.32	115.13	121.89
1	E	171	TYR	CA-C-N	5.32	124.95	119.05
1	E	171	TYR	O-C-N	5.32	127.44	121.32
1	E	171	TYR	C-N-CA	5.32	124.95	119.05
1	E	211	GLY	O-C-N	5.32	128.56	122.34
1	E	70	GLY	N-CA-C	-5.27	107.78	114.16
2	I	50	ASN	CA-C-N	5.27	130.27	123.00
2	I	50	ASN	C-N-CA	5.27	130.27	123.00
1	E	255	THR	CA-C-N	5.26	128.31	120.95
1	E	255	THR	C-N-CA	5.26	128.31	120.95
1	E	143	VAL	CB-CA-C	5.25	118.90	112.02
2	I	25	PHE	CA-CB-CG	-5.25	108.56	113.80
1	E	168	PRO	CA-C-N	5.22	125.88	120.03
1	E	168	PRO	C-N-CA	5.22	125.88	120.03
2	I	31	GLN	CA-C-N	-5.20	114.49	122.87
2	I	31	GLN	C-N-CA	-5.20	114.49	122.87
1	E	132	SER	O-C-N	5.20	128.99	123.42
1	E	259	ASP	O-C-N	-5.20	117.29	123.11
2	I	46	ASP	CA-CB-CG	5.20	117.80	112.60
1	E	255	THR	CA-CB-CG2	5.19	119.32	110.50
1	E	242	THR	N-CA-CB	5.18	118.74	110.46
1	E	138	ALA	O-C-N	5.17	127.61	122.12
2	I	26	THR	CA-CB-OG1	-5.17	101.85	109.60
2	I	41	SER	CA-CB-OG	-5.16	100.78	111.10
1	E	78	SER	N-CA-CB	-5.16	102.82	110.61
1	E	101	SER	N-CA-CB	5.15	120.66	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	206	GLN	CG-CD-OE1	5.15	131.10	120.80
1	E	192	VAL	O-C-N	5.15	128.75	123.04
1	E	19	GLN	CG-CD-OE1	5.14	131.08	120.80
1	E	62	ASN	CA-CB-CG	-5.14	107.46	112.60
1	E	271	GLN	CA-CB-CG	-5.13	103.84	114.10
1	E	186	ARG	NH1-CZ-NH2	-5.12	112.64	119.30
1	E	254	THR	CA-C-O	-5.11	116.16	121.99
1	E	21	TYR	CA-CB-CG	-5.11	104.70	113.90
2	I	31	GLN	CA-C-O	-5.11	113.31	119.49
2	I	16	LYS	N-CA-C	5.10	116.87	110.24
1	E	36	ASP	O-C-N	5.10	129.37	122.59
1	E	187	ALA	O-C-N	5.10	129.11	122.89
1	E	130	SER	CA-C-N	-5.09	114.06	121.44
1	E	130	SER	C-N-CA	-5.09	114.06	121.44
1	E	89	SER	O-C-N	5.09	129.13	122.87
1	E	215	GLY	CA-C-N	5.09	129.74	122.72
1	E	215	GLY	C-N-CA	5.09	129.74	122.72
1	E	30	VAL	CA-C-O	-5.08	114.56	120.75
1	E	67	HIS	CA-C-O	5.06	126.11	120.90
1	E	249	SER	CA-C-O	-5.05	115.52	120.82
1	E	228	ALA	N-CA-C	-5.04	105.86	111.36
1	E	230	ALA	O-C-N	5.04	127.26	122.07
1	E	41	ASP	O-C-N	-5.04	115.89	122.39
2	I	62	VAL	N-CA-CB	5.04	116.21	110.72
1	E	24	SER	CB-CA-C	-5.04	102.04	109.90
2	I	37	LEU	N-CA-C	5.04	117.33	108.82
1	E	156	GLU	N-CA-C	5.03	119.40	113.16
1	E	185	GLN	CB-CA-C	-5.03	101.23	109.53
2	I	38	PRO	CA-C-O	5.03	126.55	121.27
1	E	183	SER	CA-C-O	5.03	125.30	119.32
1	E	67	HIS	CA-C-N	5.01	127.33	120.77
1	E	67	HIS	C-N-CA	5.01	127.33	120.77
2	I	45	ARG	CA-CB-CG	5.01	124.12	114.10

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	E	1938	0	1899	151	1
2	I	525	0	502	63	0
3	E	2	0	0	0	0
4	E	255	0	0	33	5
4	I	61	0	0	7	0
All	All	2781	0	2401	210	5

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 43.

All (210) 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:E:130:SER:HB3	4:E:523:HOH:O	1.31	1.25
1:E:103:GLN:HG3	4:E:395:HOH:O	1.51	1.09
1:E:133:ALA:HA	4:E:416:HOH:O	1.68	0.92
1:E:52:PRO:HD2	4:E:457:HOH:O	1.68	0.92
2:I:27:LEU:HD23	4:I:587:HOH:O	1.69	0.91
1:E:165:VAL:O	1:E:170:LYS:HD2	1.71	0.91
1:E:1:ALA:HA	1:E:78:SER:O	1.72	0.89
1:E:40:PRO:HD3	1:E:212:ASN:OD1	1.74	0.87
1:E:138:ALA:HA	1:E:141:LYS:HE2	1.55	0.86
1:E:13:ALA:N	1:E:14:PRO:HD2	1.89	0.86
1:E:62:ASN:O	1:E:63:SER:HB3	1.75	0.84
1:E:136:LYS:O	1:E:136:LYS:HG3	1.78	0.83
2:I:31:GLN:H	2:I:31:GLN:NE2	1.77	0.82
1:E:136:LYS:O	1:E:136:LYS:CG	2.27	0.82
1:E:12:LYS:C	1:E:14:PRO:HD2	2.03	0.82
2:I:8:LYS:N	4:I:325:HOH:O	2.13	0.80
2:I:60:THR:O	2:I:62:VAL:HG22	1.82	0.80
1:E:242:THR:H	1:E:245:GLN:HE21	1.29	0.78
2:I:29:TYR:HD1	2:I:31:GLN:OE1	1.66	0.78
1:E:13:ALA:N	1:E:14:PRO:CD	2.45	0.77
1:E:242:THR:H	1:E:245:GLN:NE2	1.84	0.75
1:E:275:GLN:HE21	1:E:275:GLN:N	1.83	0.75
1:E:10:GLN:HE21	1:E:184:ASN:ND2	1.84	0.74
2:I:16:LYS:HB3	2:I:20:GLN:HB2	1.69	0.74
1:E:133:ALA:CA	4:E:416:HOH:O	2.32	0.72
1:E:62:ASN:O	1:E:63:SER:CB	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ALA:CB	1:E:271:GLN:HG3	2.22	0.70
2:I:39:GLU:OE1	2:I:64:ASN:OD1	2.11	0.69
1:E:238:HIS:HD2	1:E:241:TRP:CZ3	2.11	0.68
1:E:271:GLN:NE2	4:E:407:HOH:O	2.27	0.67
1:E:10:GLN:HE21	1:E:184:ASN:HD21	1.40	0.67
1:E:102:GLY:O	2:I:42:PRO:HD2	1.95	0.66
1:E:248:SER:O	1:E:252:ASN:N	2.29	0.66
2:I:60:THR:C	2:I:62:VAL:N	2.54	0.66
1:E:239:PRO:HG2	4:E:555:HOH:O	1.97	0.64
1:E:275:GLN:HE21	1:E:275:GLN:CA	2.10	0.64
1:E:16:LEU:HD13	1:E:21:TYR:HB2	1.80	0.64
1:E:195:GLU:OE2	4:E:441:HOH:O	2.15	0.64
1:E:16:LEU:HD13	1:E:21:TYR:CB	2.27	0.64
1:E:83:GLY:O	1:E:86:PRO:HD3	1.98	0.63
1:E:181:ASP:OD2	4:E:359:HOH:O	2.16	0.63
2:I:60:THR:HB	2:I:62:VAL:HG23	1.81	0.62
2:I:16:LYS:HB3	2:I:20:GLN:CB	2.28	0.62
2:I:48:ARG:HD3	4:I:410:HOH:O	2.00	0.62
1:E:103:GLN:HA	4:E:436:HOH:O	2.00	0.62
1:E:10:GLN:NE2	1:E:184:ASN:ND2	2.47	0.62
2:I:50:ASN:H	2:I:50:ASN:HD22	1.46	0.62
2:I:60:THR:C	2:I:62:VAL:H	2.08	0.62
1:E:243:ASN:HD22	1:E:244:THR:N	1.99	0.61
1:E:54:GLU:HB2	1:E:94:LYS:HE2	1.83	0.61
1:E:29:ALA:HB2	1:E:119:MET:HG3	1.82	0.60
1:E:43:LYS:HG2	4:E:482:HOH:O	2.01	0.60
1:E:195:GLU:OE2	4:E:439:HOH:O	2.16	0.60
1:E:103:GLN:HG2	1:E:106:TRP:CE2	2.37	0.60
1:E:43:LYS:NZ	4:E:496:HOH:O	2.35	0.59
1:E:127:GLY:HA2	1:E:167:TYR:O	2.03	0.59
1:E:247:ARG:HD3	4:E:564:HOH:O	2.03	0.59
1:E:221:SER:HB2	2:I:45:ARG:O	2.03	0.59
1:E:102:GLY:HA2	1:E:106:TRP:CZ3	2.38	0.58
1:E:137:ALA:O	1:E:141:LYS:HB2	2.04	0.58
2:I:60:THR:O	2:I:62:VAL:N	2.36	0.57
1:E:148:VAL:HG22	1:E:243:ASN:HB2	1.87	0.57
2:I:59:GLY:C	2:I:61:ASN:N	2.57	0.57
2:I:60:THR:HG22	2:I:62:VAL:CG2	2.34	0.57
1:E:56:ASN:C	1:E:56:ASN:HD22	2.13	0.56
2:I:60:THR:CB	2:I:62:VAL:HG23	2.36	0.56
1:E:130:SER:CB	4:E:523:HOH:O	2.11	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:59:GLY:HA2	4:I:593:HOH:O	2.05	0.55
2:I:64:ASN:ND2	2:I:65:HIS:ND1	2.54	0.55
1:E:136:LYS:HB2	1:E:171:TYR:CZ	2.42	0.55
1:E:56:ASN:C	1:E:56:ASN:ND2	2.64	0.54
1:E:112:GLU:HG3	4:E:540:HOH:O	2.06	0.54
1:E:205:ILE:O	1:E:216:ALA:HA	2.07	0.54
1:E:238:HIS:CD2	1:E:241:TRP:CZ3	2.96	0.54
2:I:59:GLY:C	2:I:61:ASN:H	2.14	0.54
2:I:12:GLU:OE1	2:I:24:TYR:OH	2.16	0.54
2:I:31:GLN:H	2:I:31:GLN:HE21	1.54	0.54
2:I:60:THR:O	2:I:62:VAL:CG2	2.54	0.54
1:E:103:GLN:NE2	4:E:481:HOH:O	2.40	0.54
1:E:138:ALA:CA	1:E:141:LYS:HE2	2.36	0.54
1:E:239:PRO:HD2	4:E:555:HOH:O	2.07	0.54
1:E:15:ALA:HB3	1:E:271:GLN:HG3	1.90	0.54
2:I:57:ASN:O	2:I:61:ASN:HA	2.07	0.54
1:E:40:PRO:CD	1:E:212:ASN:OD1	2.52	0.53
1:E:55:THR:O	1:E:57:PRO:HD3	2.08	0.53
1:E:97:GLY:HA3	4:E:332:HOH:O	2.07	0.53
1:E:17:HIS:NE2	1:E:84:VAL:O	2.40	0.53
1:E:186:ARG:HG2	1:E:187:ALA:O	2.09	0.53
1:E:107:ILE:O	1:E:111:ILE:HG13	2.10	0.52
1:E:5:PRO:HA	4:E:342:HOH:O	2.10	0.52
2:I:31:GLN:NE2	2:I:31:GLN:N	2.55	0.52
1:E:238:HIS:HD2	1:E:241:TRP:CE3	2.27	0.52
2:I:21:ALA:O	2:I:22:ARG:C	2.53	0.52
1:E:28:VAL:HG11	1:E:72:VAL:HG11	1.91	0.52
1:E:170:LYS:HE3	4:E:439:HOH:O	2.10	0.52
1:E:36:ASP:OD1	1:E:36:ASP:C	2.53	0.52
1:E:275:GLN:NE2	1:E:275:GLN:OXT	2.43	0.52
1:E:21:TYR:CZ	1:E:237:LYS:HG3	2.46	0.51
1:E:48:ALA:C	1:E:57:PRO:HG3	2.36	0.51
1:E:155:ASN:HA	1:E:189:PHE:O	2.11	0.51
2:I:33:ASN:ND2	4:I:445:HOH:O	2.44	0.51
1:E:60:ASP:OD2	1:E:63:SER:HA	2.11	0.51
1:E:1:ALA:CA	1:E:78:SER:O	2.54	0.50
1:E:128:GLY:N	1:E:167:TYR:O	2.40	0.50
1:E:124:MET:CE	1:E:149:VAL:CG1	2.90	0.49
1:E:275:GLN:OXT	1:E:275:GLN:CD	2.56	0.49
2:I:17:THR:HG22	2:I:62:VAL:HG13	1.93	0.49
2:I:59:GLY:O	2:I:60:THR:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:ARG:O	1:E:251:GLU:HG3	2.12	0.49
2:I:57:ASN:O	2:I:61:ASN:N	2.46	0.48
1:E:35:ILE:HD13	1:E:69:ALA:HB2	1.96	0.48
1:E:69:ALA:HB1	1:E:90:LEU:HD21	1.95	0.48
1:E:122:ILE:HG21	1:E:124:MET:HE2	1.95	0.48
1:E:34:GLY:O	1:E:65:GLY:HA3	2.13	0.48
1:E:184:ASN:HD21	1:E:267:LEU:HD22	1.79	0.48
2:I:17:THR:HA	2:I:62:VAL:HA	1.94	0.48
1:E:136:LYS:O	1:E:136:LYS:HG2	2.13	0.48
1:E:21:TYR:O	1:E:233:LEU:HD22	2.13	0.48
2:I:24:TYR:O	2:I:27:LEU:N	2.46	0.48
1:E:133:ALA:CB	4:E:416:HOH:O	2.60	0.48
2:I:22:ARG:HH11	2:I:36:PHE:HE1	1.61	0.48
1:E:141:LYS:HG2	4:E:545:HOH:O	2.13	0.47
2:I:34:VAL:HG12	2:I:52:VAL:HB	1.96	0.47
1:E:2:GLN:HA	1:E:80:GLY:O	2.14	0.47
1:E:273:ALA:C	1:E:275:GLN:H	2.21	0.47
1:E:6:TYR:CD1	1:E:6:TYR:C	2.93	0.47
1:E:111:ILE:O	1:E:115:ILE:N	2.41	0.47
1:E:184:ASN:ND2	1:E:267:LEU:HD22	2.30	0.47
1:E:61:ASN:CG	4:E:345:HOH:O	2.57	0.47
1:E:107:ILE:HD13	1:E:126:LEU:CD1	2.44	0.47
2:I:38:PRO:O	2:I:39:GLU:C	2.58	0.47
1:E:12:LYS:CA	1:E:14:PRO:HD2	2.45	0.46
1:E:49:SER:C	1:E:50:MET:HG2	2.41	0.46
1:E:118:ASN:O	4:E:417:HOH:O	2.21	0.46
1:E:183:SER:HB2	1:E:185:GLN:HG2	1.98	0.46
2:I:17:THR:HA	2:I:61:ASN:O	2.15	0.46
1:E:35:ILE:HG13	1:E:92:ALA:HB2	1.98	0.46
1:E:165:VAL:O	1:E:170:LYS:CD	2.56	0.46
2:I:59:GLY:O	2:I:61:ASN:N	2.48	0.46
2:I:50:ASN:H	2:I:50:ASN:ND2	2.11	0.46
1:E:104:TYR:CE1	2:I:42:PRO:HG3	2.50	0.46
2:I:57:ASN:O	2:I:61:ASN:CA	2.64	0.45
1:E:15:ALA:HB1	1:E:271:GLN:HG3	1.99	0.45
2:I:60:THR:HG22	2:I:62:VAL:HG23	1.97	0.45
1:E:35:ILE:HG13	1:E:92:ALA:CB	2.47	0.45
2:I:33:ASN:ND2	2:I:35:TYR:CZ	2.85	0.45
2:I:32:TYR:O	2:I:34:VAL:HG22	2.17	0.45
2:I:31:GLN:HE21	2:I:31:GLN:N	2.13	0.44
1:E:101:SER:HB3	2:I:42:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:LEU:O	1:E:236:SER:OG	2.29	0.44
1:E:124:MET:CE	1:E:149:VAL:HG13	2.48	0.44
1:E:135:LEU:O	1:E:138:ALA:HB3	2.17	0.44
1:E:60:ASP:OD2	1:E:63:SER:CA	2.66	0.44
1:E:124:MET:HE3	1:E:149:VAL:CG1	2.46	0.44
1:E:275:GLN:CA	1:E:275:GLN:NE2	2.76	0.44
1:E:127:GLY:CA	1:E:167:TYR:O	2.66	0.44
1:E:163:SER:HB3	4:E:547:HOH:O	2.17	0.44
2:I:20:GLN:NE2	4:I:495:HOH:O	2.51	0.44
2:I:14:VAL:HG23	2:I:66:VAL:HA	2.00	0.44
2:I:57:ASN:ND2	2:I:60:THR:OG1	2.51	0.43
2:I:66:VAL:HA	2:I:67:PRO:HD3	1.82	0.43
1:E:207:SER:O	1:E:214:TYR:HA	2.18	0.43
1:E:249:SER:OG	1:E:273:ALA:O	2.36	0.43
1:E:159:SER:C	1:E:160:GLY:O	2.57	0.43
1:E:163:SER:CB	4:E:547:HOH:O	2.66	0.43
2:I:39:GLU:O	2:I:39:GLU:HG2	2.18	0.43
1:E:248:SER:O	1:E:252:ASN:HB2	2.19	0.43
2:I:13:VAL:HG12	2:I:63:VAL:HG11	2.01	0.43
1:E:67:HIS:CD2	1:E:207:SER:HB3	2.53	0.43
1:E:238:HIS:CD2	1:E:241:TRP:CE3	3.06	0.43
1:E:67:HIS:O	1:E:68:VAL:C	2.59	0.43
1:E:115:ILE:HG12	1:E:142:ALA:HA	2.01	0.43
1:E:113:TRP:O	1:E:117:ASN:ND2	2.49	0.42
1:E:207:SER:OG	1:E:208:THR:N	2.52	0.42
1:E:195:GLU:OE2	4:E:501:HOH:O	2.20	0.42
1:E:205:ILE:HG13	1:E:222:MET:HB3	2.00	0.42
1:E:154:GLY:HA3	4:E:550:HOH:O	2.19	0.42
1:E:170:LYS:NZ	4:E:430:HOH:O	2.43	0.42
1:E:156:GLU:HB2	1:E:191:SER:OG	2.19	0.42
1:E:107:ILE:HD13	1:E:126:LEU:HD11	2.01	0.42
1:E:260:SER:HA	1:E:264:GLY:O	2.19	0.42
2:I:10:PHE:CD1	2:I:10:PHE:N	2.87	0.42
1:E:117:ASN:O	1:E:118:ASN:CB	2.67	0.42
1:E:197:ASP:O	1:E:265:LYS:HG2	2.20	0.42
1:E:45:ALA:HA	4:E:541:HOH:O	2.19	0.42
1:E:257:LEU:HD11	1:E:267:LEU:HB2	2.02	0.42
1:E:274:ALA:O	1:E:275:GLN:C	2.63	0.42
2:I:60:THR:CG2	2:I:62:VAL:HG23	2.49	0.42
2:I:64:ASN:HD22	2:I:64:ASN:H	1.67	0.41
1:E:54:GLU:OE2	1:E:97:GLY:HA2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:HIS:HA	1:E:40:PRO:HD3	1.83	0.41
1:E:275:GLN:HB3	4:E:344:HOH:O	2.20	0.41
1:E:86:PRO:HG2	4:E:565:HOH:O	2.21	0.41
1:E:243:ASN:HD22	1:E:244:THR:H	1.66	0.41
1:E:248:SER:O	1:E:252:ASN:CB	2.68	0.41
2:I:24:TYR:CE1	2:I:28:HIS:ND1	2.89	0.41
1:E:27:LYS:HZ2	1:E:27:LYS:HG2	1.41	0.41
1:E:84:VAL:HG21	1:E:226:HIS:HA	2.02	0.41
1:E:143:VAL:HG22	1:E:147:VAL:O	2.20	0.41
1:E:171:TYR:HA	1:E:172:PRO:HD3	1.93	0.41
2:I:18:VAL:CG2	2:I:56:TYR:CD2	3.03	0.41
2:I:24:TYR:HB3	2:I:25:PHE:H	1.64	0.41
2:I:47:LEU:O	4:I:561:HOH:O	2.21	0.41
1:E:238:HIS:CD2	1:E:241:TRP:CH2	3.09	0.41
2:I:14:VAL:CG2	2:I:65:HIS:C	2.93	0.41
1:E:235:LEU:O	1:E:239:PRO:HA	2.20	0.40
2:I:10:PHE:O	2:I:67:PRO:HD2	2.20	0.40
1:E:167:TYR:HB3	1:E:168:PRO:HA	2.04	0.40
1:E:47:GLY:HA3	1:E:92:ALA:O	2.21	0.40
2:I:41:SER:HA	2:I:42:PRO:HD3	1.88	0.40

All (5) 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)
4:E:351:HOH:O	4:E:351:HOH:O[4_556]	1.75	0.45
4:E:415:HOH:O	4:E:415:HOH:O[5_556]	1.95	0.25
1:E:160:GLY:N	4:E:351:HOH:O[4_556]	1.97	0.23
4:E:359:HOH:O	4:E:578:HOH:O[4_556]	2.06	0.14
4:E:446:HOH:O	4:E:511:HOH:O[3_664]	2.15	0.05

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	E	273/275 (99%)	255 (93%)	17 (6%)	1 (0%)	30	28
2	I	61/70 (87%)	51 (84%)	7 (12%)	3 (5%)	1	0
All	All	334/345 (97%)	306 (92%)	24 (7%)	4 (1%)	10	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	61	ASN
1	E	63	SER
2	I	24	TYR
2	I	15	GLY

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	E	205/205 (100%)	185 (90%)	20 (10%)	7	5
2	I	58/64 (91%)	47 (81%)	11 (19%)	1	1
All	All	263/269 (98%)	232 (88%)	31 (12%)	5	3

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	SER
1	E	16	LEU
1	E	24	SER
1	E	42	LEU
1	E	50	MET
1	E	53	SER
1	E	101	SER
1	E	103	GLN
1	E	118	ASN
1	E	159	SER

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Mol	Chain	Res	Type
1	E	173	SER
1	E	180	VAL
1	E	206	GLN
1	E	221	SER
1	E	237	LYS
1	E	241	TRP
1	E	243	ASN
1	E	256	LYS
1	E	271	GLN
1	E	275	GLN
2	I	10	PHE
2	I	12	GLU
2	I	13	VAL
2	I	22	ARG
2	I	27	LEU
2	I	31	GLN
2	I	34	VAL
2	I	39	GLU
2	I	60	THR
2	I	62	VAL
2	I	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	56	ASN
1	E	59	GLN
1	E	76	ASN
1	E	118	ASN
1	E	123	ASN
1	E	184	ASN
1	E	185	GLN
1	E	238	HIS
1	E	243	ASN
1	E	245	GLN
1	E	275	GLN
2	I	31	GLN
2	I	33	ASN
2	I	50	ASN
2	I	57	ASN
2	I	64	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.