



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:56 AM UTC

PDB ID : 1SIB / pdb_00001sib
Title : REFINED CRYSTAL STRUCTURES OF SUBTILISIN NOVO IN COM-
PLEX WITH WILD-TYPE AND TWO MUTANT EGLINS. COMPARISON
WITH OTHER SERINE PROTEINASE INHIBITOR COMPLEXES
Authors : Gruetter, M.G.; Heinz, D.W.; Priestle, J.P.
Deposited on : 1993-08-02
Resolution : 2.40 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

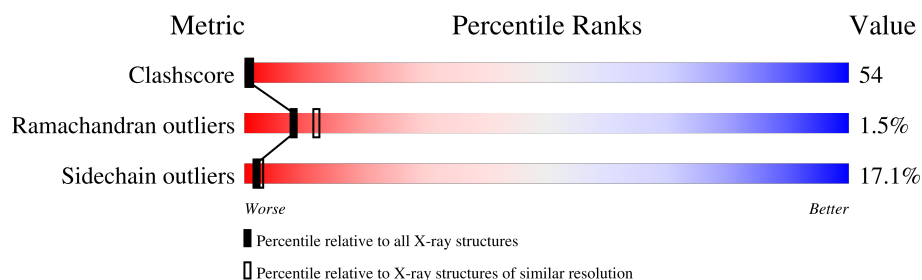
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 2655 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
			520	339	87	94			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	53	LYS	ARG	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.

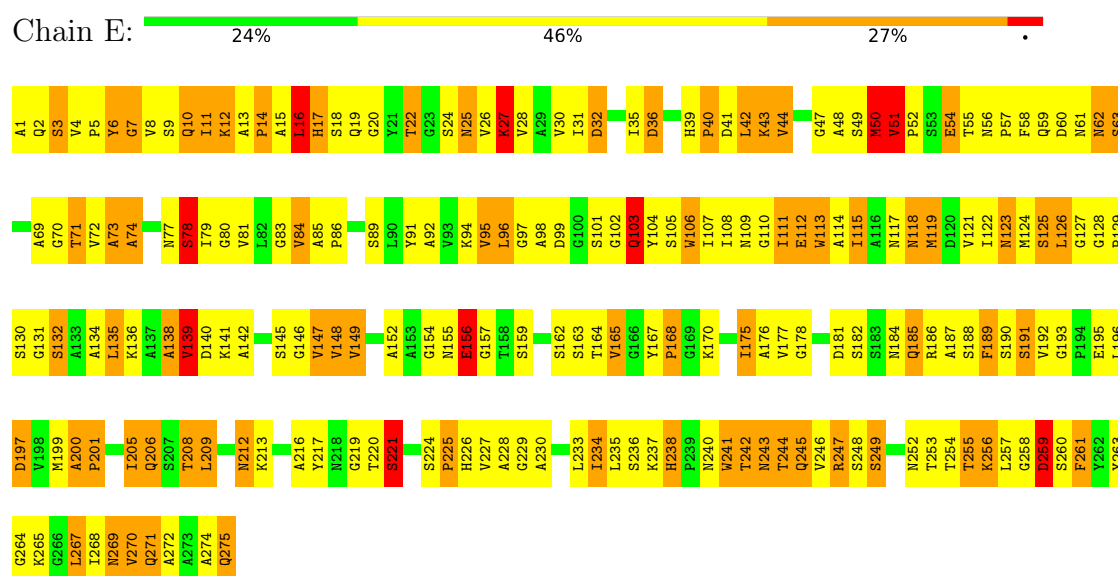
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	155	Total	O	0	0
			155	155		
4	I	40	Total	O	0	0
			40	40		

3 Residue-property plots

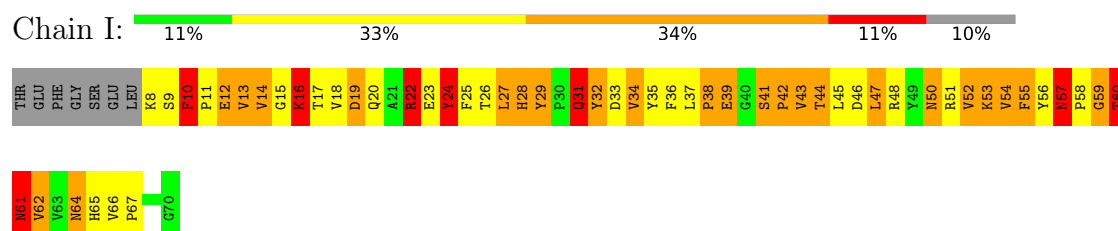
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2655	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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	1.19	2/1976 (0.1%)	2.85	222/2697 (8.2%)
2	I	1.05	0/538	2.76	61/735 (8.3%)
All	All	1.16	2/2514 (0.1%)	2.83	283/3432 (8.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	127	GLY	N-CA	5.05	1.51	1.45
1	E	178	GLY	N-CA	5.00	1.50	1.44

All (283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	212	ASN	CA-CB-CG	14.97	127.57	112.60
1	E	118	ASN	CA-CB-CG	14.74	127.34	112.60
1	E	77	ASN	CA-CB-CG	14.09	126.69	112.60
1	E	73	ALA	N-CA-C	12.44	125.09	110.41
2	I	61	ASN	CA-CB-CG	12.43	125.03	112.60
1	E	110	GLY	CA-C-N	12.25	136.24	120.56
1	E	110	GLY	C-N-CA	12.25	136.24	120.56
1	E	200	ALA	N-CA-CB	11.60	123.24	111.29
1	E	200	ALA	N-CA-C	-10.63	98.61	108.07
2	I	57	ASN	OD1-CG-ND2	-10.57	112.03	122.60
2	I	33	ASP	CA-CB-CG	10.11	122.71	112.60
1	E	209	LEU	O-C-N	9.94	129.30	121.55
1	E	269	ASN	CA-C-O	-9.91	106.75	120.52
1	E	36	ASP	CA-CB-CG	-9.86	102.74	112.60
2	I	10	PHE	CA-CB-CG	9.69	123.48	113.80
1	E	123	ASN	CA-CB-CG	-9.20	103.40	112.60
2	I	54	VAL	CA-C-N	9.16	134.67	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	54	VAL	C-N-CA	9.16	134.67	122.30
1	E	191	SER	CA-C-O	-9.16	111.00	121.81
2	I	12	GLU	CA-C-N	9.16	132.19	121.84
2	I	12	GLU	C-N-CA	9.16	132.19	121.84
1	E	139	VAL	CA-C-O	-9.15	110.37	120.25
1	E	229	GLY	CA-C-N	9.12	132.30	120.44
1	E	229	GLY	C-N-CA	9.12	132.30	120.44
1	E	56	ASN	CB-CA-C	-9.09	102.26	110.44
1	E	40	PRO	CA-C-N	9.04	137.28	122.73
1	E	40	PRO	C-N-CA	9.04	137.28	122.73
1	E	219	GLY	CA-C-O	-8.66	113.05	122.14
1	E	249	SER	O-C-N	8.60	130.98	122.03
1	E	84	VAL	O-C-N	8.48	130.22	121.91
1	E	14	PRO	CA-C-N	8.47	132.32	120.29
1	E	14	PRO	C-N-CA	8.47	132.32	120.29
2	I	28	HIS	CA-CB-CG	-8.42	105.38	113.80
1	E	56	ASN	CA-CB-CG	-8.39	104.21	112.60
1	E	73	ALA	N-CA-CB	-8.34	101.78	111.79
1	E	197	ASP	N-CA-C	8.30	123.72	112.68
1	E	4	VAL	O-C-N	8.28	126.59	121.37
1	E	58	PHE	CA-CB-CG	-8.28	105.52	113.80
2	I	42	PRO	CB-CA-C	-8.26	101.45	111.11
2	I	22	ARG	CA-C-N	8.23	131.64	120.44
2	I	22	ARG	C-N-CA	8.23	131.64	120.44
1	E	182	SER	CA-C-O	-8.23	109.32	119.28
1	E	71	THR	CA-C-N	8.20	131.06	120.56
1	E	71	THR	C-N-CA	8.20	131.06	120.56
1	E	31	ILE	CA-C-O	8.15	130.97	120.78
2	I	41	SER	CA-C-N	8.12	129.31	120.13
2	I	41	SER	C-N-CA	8.12	129.31	120.13
1	E	19	GLN	N-CA-C	-8.11	102.95	113.17
1	E	226	HIS	CA-CB-CG	8.08	121.88	113.80
1	E	238	HIS	O-C-N	8.08	128.77	121.42
1	E	84	VAL	CA-C-O	-8.01	112.68	121.17
2	I	46	ASP	CA-C-O	-8.01	111.71	121.89
1	E	17	HIS	O-C-N	8.00	130.59	122.12
1	E	92	ALA	CA-C-N	7.92	131.31	122.59
1	E	92	ALA	C-N-CA	7.92	131.31	122.59
1	E	70	GLY	N-CA-C	-7.92	103.86	113.99
1	E	192	VAL	CA-C-O	-7.91	113.80	121.63
1	E	10	GLN	OE1-CD-NE2	-7.89	114.71	122.60
1	E	200	ALA	O-C-N	7.89	129.37	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	220	THR	N-CA-C	-7.88	103.64	113.18
2	I	41	SER	O-C-N	7.81	128.84	121.27
1	E	8	VAL	CA-C-N	7.70	130.91	120.44
1	E	8	VAL	C-N-CA	7.70	130.91	120.44
1	E	112	GLU	N-CA-C	-7.69	102.90	111.28
1	E	182	SER	O-C-N	7.68	132.96	122.37
1	E	105	SER	N-CA-CB	7.66	121.62	110.20
1	E	74	ALA	N-CA-C	-7.66	98.98	110.24
1	E	261	PHE	CA-CB-CG	7.65	121.45	113.80
1	E	205	ILE	N-CA-C	7.50	118.03	107.37
1	E	186	ARG	NE-CZ-NH1	-7.46	114.04	121.50
1	E	128	GLY	O-C-N	7.43	129.20	121.77
1	E	245	GLN	OE1-CD-NE2	7.42	130.02	122.60
1	E	32	ASP	CA-CB-CG	7.40	120.00	112.60
2	I	14	VAL	N-CA-C	-7.37	98.99	108.93
2	I	38	PRO	CB-CA-C	7.29	120.72	111.39
1	E	267	LEU	CA-C-O	-7.28	112.55	120.92
1	E	26	VAL	CB-CA-C	7.28	121.18	111.21
1	E	51	VAL	CB-CA-C	7.26	119.53	111.18
1	E	47	GLY	CA-C-O	7.20	129.30	121.96
1	E	25	ASN	CA-C-O	-7.17	111.83	119.00
1	E	219	GLY	O-C-N	7.12	131.87	122.47
1	E	254	THR	CA-C-O	-7.06	113.94	121.99
2	I	55	PHE	CA-CB-CG	-7.04	106.76	113.80
1	E	9	SER	CA-C-O	-7.00	113.49	120.70
1	E	134	ALA	O-C-N	6.97	130.09	122.15
1	E	103	GLN	OE1-CD-NE2	6.96	129.56	122.60
1	E	259	ASP	CA-C-N	6.96	130.30	120.28
1	E	259	ASP	C-N-CA	6.96	130.30	120.28
2	I	42	PRO	O-C-N	6.90	130.82	123.03
1	E	206	GLN	OE1-CD-NE2	6.89	129.49	122.60
1	E	134	ALA	N-CA-C	-6.87	103.88	111.36
1	E	132	SER	CB-CA-C	-6.85	98.96	109.99
1	E	7	GLY	CA-C-N	6.83	129.30	120.56
1	E	7	GLY	C-N-CA	6.83	129.30	120.56
1	E	6	TYR	CA-C-N	6.81	128.66	120.14
1	E	6	TYR	C-N-CA	6.81	128.66	120.14
1	E	177	VAL	CA-C-O	-6.79	113.02	120.43
1	E	181	ASP	N-CA-C	-6.77	99.69	109.31
1	E	165	VAL	CB-CA-C	6.75	118.52	111.23
2	I	48	ARG	N-CA-CB	6.73	122.45	110.80
1	E	112	GLU	CA-CB-CG	6.73	127.56	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	HIS	CA-C-O	-6.72	113.42	120.55
1	E	111	ILE	N-CA-C	6.71	116.83	110.53
2	I	61	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	E	9	SER	N-CA-C	-6.67	103.94	111.14
1	E	175	ILE	CB-CA-C	-6.66	103.28	111.88
2	I	34	VAL	O-C-N	6.63	130.25	122.69
1	E	42	LEU	CA-C-O	-6.61	112.41	120.54
2	I	27	LEU	N-CA-CB	-6.61	100.36	110.07
2	I	25	PHE	CA-CB-CG	-6.60	107.20	113.80
1	E	209	LEU	CA-C-O	-6.58	114.13	120.64
1	E	189	PHE	CB-CA-C	6.55	121.21	109.29
2	I	16	LYS	CA-C-O	6.55	129.87	120.51
1	E	188	SER	CA-C-O	6.53	127.54	119.05
2	I	26	THR	O-C-N	6.51	129.83	122.22
1	E	105	SER	N-CA-C	-6.50	103.69	111.69
1	E	17	HIS	CA-CB-CG	6.50	120.30	113.80
1	E	119	MET	CA-C-O	-6.50	113.64	121.05
1	E	96	LEU	CA-CB-CG	6.48	138.99	116.30
1	E	247	ARG	NE-CZ-NH2	6.47	125.03	119.20
2	I	57	ASN	CB-CG-ND2	6.43	126.05	116.40
1	E	123	ASN	OD1-CG-ND2	6.43	129.03	122.60
1	E	96	LEU	CA-C-O	-6.38	113.84	120.99
2	I	39	GLU	CA-CB-CG	6.37	126.84	114.10
1	E	175	ILE	CA-C-N	6.35	129.89	120.87
1	E	175	ILE	C-N-CA	6.35	129.89	120.87
1	E	84	VAL	CG1-CB-CG2	6.34	124.75	110.80
1	E	62	ASN	CA-CB-CG	-6.33	106.27	112.60
1	E	20	GLY	N-CA-C	6.32	124.05	115.32
1	E	238	HIS	CA-CB-CG	6.32	120.12	113.80
1	E	3	SER	CA-C-O	-6.30	113.75	121.06
1	E	30	VAL	CA-CB-CG1	6.30	121.11	110.40
1	E	35	ILE	N-CA-C	6.29	117.18	108.12
1	E	177	VAL	O-C-N	6.25	129.82	123.07
1	E	44	VAL	CA-C-O	-6.24	113.69	121.11
1	E	200	ALA	CA-C-O	-6.24	114.88	120.56
1	E	146	GLY	N-CA-C	6.20	124.01	115.27
2	I	10	PHE	O-C-N	6.19	126.94	121.37
1	E	74	ALA	CB-CA-C	6.19	119.12	109.84
1	E	267	LEU	O-C-N	6.18	130.33	123.16
2	I	33	ASP	CB-CA-C	6.17	121.79	111.30
2	I	53	LYS	N-CA-CB	6.15	120.21	110.55
1	E	127	GLY	O-C-N	6.14	130.68	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	SER	N-CA-C	6.14	120.93	113.38
1	E	112	GLU	CA-C-O	-6.13	114.05	120.55
1	E	147	VAL	CA-C-N	6.13	130.03	122.37
1	E	147	VAL	C-N-CA	6.13	130.03	122.37
2	I	47	LEU	CA-C-O	-6.12	113.59	120.32
1	E	259	ASP	CA-CB-CG	-6.11	106.49	112.60
1	E	22	THR	CA-C-N	6.11	130.81	120.91
1	E	22	THR	C-N-CA	6.11	130.81	120.91
1	E	247	ARG	NH1-CZ-NH2	-6.10	111.37	119.30
1	E	69	ALA	O-C-N	6.09	129.54	122.17
1	E	78	SER	N-CA-CB	-6.07	101.48	110.53
2	I	9	SER	O-C-N	6.06	131.07	123.19
1	E	109	ASN	CA-CB-CG	6.06	118.66	112.60
1	E	40	PRO	O-C-N	-6.05	114.85	122.17
1	E	91	TYR	N-CA-C	6.03	118.66	107.99
1	E	234	ILE	CB-CA-C	-6.01	102.52	112.26
1	E	135	LEU	O-C-N	5.98	128.55	122.09
2	I	29	TYR	N-CA-C	5.98	123.03	109.81
1	E	228	ALA	CA-C-N	5.96	126.60	119.98
1	E	228	ALA	C-N-CA	5.96	126.60	119.98
2	I	31	GLN	N-CA-C	5.95	119.73	112.23
1	E	69	ALA	CA-C-O	-5.95	114.18	120.55
1	E	189	PHE	N-CA-C	-5.95	106.18	113.50
1	E	72	VAL	O-C-N	5.95	128.08	121.90
2	I	60	THR	CA-C-N	5.95	132.89	121.54
2	I	60	THR	C-N-CA	5.95	132.89	121.54
1	E	168	PRO	CA-C-N	5.92	126.66	120.03
1	E	168	PRO	C-N-CA	5.92	126.66	120.03
1	E	11	ILE	O-C-N	5.89	128.95	122.12
1	E	3	SER	N-CA-C	-5.89	100.10	109.23
1	E	39	HIS	O-C-N	5.82	126.37	121.31
1	E	149	VAL	O-C-N	5.81	129.36	123.20
1	E	114	ALA	CA-C-O	-5.81	114.92	120.90
1	E	6	TYR	CA-C-O	-5.79	114.41	120.55
1	E	16	LEU	CA-C-N	5.79	128.04	120.28
1	E	16	LEU	C-N-CA	5.79	128.04	120.28
1	E	201	PRO	CA-C-O	-5.79	114.43	121.03
1	E	60	ASP	CA-CB-CG	5.78	118.38	112.60
1	E	19	GLN	CA-C-O	5.78	126.11	119.35
1	E	72	VAL	CA-CB-CG2	5.78	120.22	110.40
1	E	265	LYS	O-C-N	5.77	130.34	122.37
1	E	225	PRO	O-C-N	-5.76	114.86	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	95	VAL	CA-C-O	-5.75	113.60	120.78
1	E	126	LEU	CA-C-N	-5.73	112.04	121.04
1	E	126	LEU	C-N-CA	-5.73	112.04	121.04
1	E	253	THR	N-CA-CB	-5.71	103.26	111.54
2	I	48	ARG	N-CA-C	-5.70	99.12	108.76
1	E	187	ALA	CA-C-O	-5.70	114.78	121.16
1	E	259	ASP	CA-C-O	5.70	128.66	120.51
1	E	31	ILE	CB-CA-C	5.68	120.61	111.29
1	E	105	SER	CA-CB-OG	5.68	122.46	111.10
2	I	56	TYR	CA-C-O	-5.68	114.82	121.46
2	I	32	TYR	N-CA-C	5.66	119.14	110.20
1	E	255	THR	CA-CB-OG1	-5.64	101.14	109.60
1	E	109	ASN	CB-CG-ND2	5.63	124.85	116.40
2	I	12	GLU	CA-CB-CG	5.61	125.31	114.10
1	E	190	SER	CA-C-O	-5.59	115.04	121.19
1	E	111	ILE	CB-CA-C	-5.58	104.71	112.02
1	E	206	GLN	N-CA-CB	5.58	118.20	110.17
1	E	81	VAL	CA-C-N	5.58	131.96	122.37
1	E	81	VAL	C-N-CA	5.58	131.96	122.37
1	E	165	VAL	CA-CB-CG1	5.57	119.87	110.40
1	E	185	GLN	CB-CA-C	-5.56	100.14	109.53
1	E	51	VAL	N-CA-C	-5.55	101.67	107.60
2	I	9	SER	CA-C-N	-5.53	116.36	123.16
2	I	9	SER	C-N-CA	-5.53	116.36	123.16
1	E	138	ALA	O-C-N	5.52	127.98	122.12
1	E	186	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	E	148	VAL	N-CA-C	-5.50	99.81	108.23
2	I	9	SER	CA-CB-OG	-5.50	100.10	111.10
2	I	53	LYS	CB-CA-C	-5.49	101.18	110.19
1	E	126	LEU	CA-C-O	-5.49	115.58	121.45
1	E	128	GLY	CA-C-O	-5.48	113.68	121.52
1	E	126	LEU	O-C-N	5.46	129.38	123.10
1	E	17	HIS	N-CA-CB	5.46	118.15	110.12
2	I	33	ASP	N-CA-CB	-5.46	102.21	110.35
1	E	27	LYS	CA-C-O	5.46	126.32	120.32
1	E	221	SER	N-CA-C	-5.45	105.50	111.82
1	E	125	SER	CA-C-O	-5.44	115.15	122.44
1	E	265	LYS	CA-C-O	-5.43	112.71	119.28
1	E	25	ASN	O-C-N	5.43	126.72	121.56
1	E	208	THR	N-CA-CB	-5.43	101.44	110.23
2	I	22	ARG	CD-NE-CZ	5.42	131.99	124.40
2	I	19	ASP	CA-CB-CG	-5.42	107.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	50	MET	CA-CB-CG	-5.39	103.31	114.10
2	I	46	ASP	N-CA-C	-5.39	102.48	110.46
1	E	112	GLU	CB-CG-CD	5.37	121.73	112.60
1	E	165	VAL	CA-C-O	5.36	127.35	120.76
1	E	242	THR	CA-CB-OG1	-5.36	101.57	109.60
1	E	197	ASP	CB-CA-C	-5.34	101.31	110.24
2	I	51	ARG	NH1-CZ-NH2	5.33	126.23	119.30
1	E	140	ASP	CA-C-N	5.33	127.68	120.65
1	E	140	ASP	C-N-CA	5.33	127.68	120.65
1	E	106	TRP	CA-C-N	5.32	127.26	120.56
1	E	106	TRP	C-N-CA	5.32	127.26	120.56
1	E	163	SER	N-CA-CB	5.30	118.34	110.29
1	E	225	PRO	CA-C-N	5.26	127.33	120.28
1	E	225	PRO	C-N-CA	5.26	127.33	120.28
2	I	27	LEU	CA-C-N	5.25	127.59	120.44
2	I	27	LEU	C-N-CA	5.25	127.59	120.44
1	E	249	SER	CA-C-O	-5.25	115.49	121.00
1	E	148	VAL	O-C-N	5.25	129.34	122.94
1	E	85	ALA	O-C-N	5.24	127.35	121.32
1	E	165	VAL	CA-C-N	5.24	129.04	121.54
1	E	165	VAL	C-N-CA	5.24	129.04	121.54
1	E	165	VAL	CG1-CB-CG2	-5.22	99.31	110.80
1	E	19	GLN	N-CA-CB	5.22	118.22	110.49
1	E	233	LEU	O-C-N	5.22	129.95	122.28
1	E	89	SER	CA-C-O	-5.20	115.52	120.92
2	I	22	ARG	O-C-N	-5.19	116.69	122.09
2	I	51	ARG	N-CA-C	5.19	117.91	109.24
1	E	212	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	E	92	ALA	CA-C-O	-5.19	113.09	120.51
1	E	42	LEU	O-C-N	5.16	129.45	123.41
1	E	156	GLU	CB-CG-CD	5.15	121.36	112.60
1	E	217	TYR	CA-C-N	5.15	130.65	122.62
1	E	217	TYR	C-N-CA	5.15	130.65	122.62
1	E	51	VAL	O-C-N	5.12	125.63	120.92
2	I	28	HIS	N-CA-C	5.11	116.66	111.14
1	E	44	VAL	CA-C-N	5.11	130.92	121.52
1	E	44	VAL	C-N-CA	5.11	130.92	121.52
1	E	164	THR	O-C-N	5.09	128.35	122.19
1	E	129	PRO	N-CA-C	5.08	121.14	114.27
1	E	181	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	115	ILE	CB-CA-C	-5.06	105.40	111.88
1	E	56	ASN	O-C-N	5.06	125.96	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	256	LYS	CA-C-N	5.05	130.39	122.11
1	E	256	LYS	C-N-CA	5.05	130.39	122.11
2	I	44	THR	CA-C-N	5.05	131.45	122.31
2	I	44	THR	C-N-CA	5.05	131.45	122.31
1	E	61	ASN	N-CA-C	-5.05	106.63	112.89
1	E	208	THR	CA-C-O	5.05	126.72	120.92
1	E	269	ASN	N-CA-C	-5.04	97.16	107.70
1	E	84	VAL	N-CA-CB	-5.04	104.65	110.55
1	E	91	TYR	CA-C-O	-5.04	115.07	120.46
1	E	113	TRP	CB-CA-C	-5.03	102.43	110.79
1	E	240	ASN	N-CA-C	-5.01	107.01	113.02
2	I	59	GLY	N-CA-C	-5.01	101.30	113.18
2	I	52	VAL	CA-C-N	5.00	130.06	123.05
2	I	52	VAL	C-N-CA	5.00	130.06	123.05

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	183	0
2	I	520	0	498	91	0
3	E	2	0	0	0	0
4	E	155	0	0	26	1
4	I	40	0	0	8	0
All	All	2655	0	2397	261	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 54.

All (261) 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:242:THR:H	1:E:245:GLN:NE2	1.15	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:60:THR:O	2:I:62:VAL:HG12	1.41	1.18
2:I:60:THR:HG22	2:I:62:VAL:CG1	1.76	1.16
1:E:242:THR:N	1:E:245:GLN:HE21	1.48	1.10
1:E:242:THR:N	1:E:245:GLN:NE2	2.00	1.08
1:E:196:LEU:HD13	4:E:342:HOH:O	1.59	1.03
1:E:102:GLY:O	2:I:42:PRO:HD2	1.59	1.02
1:E:196:LEU:HD22	4:E:342:HOH:O	1.61	0.99
1:E:170:LYS:HG3	1:E:195:GLU:HG2	1.48	0.96
1:E:221:SER:OG	2:I:45:LEU:C	2.10	0.95
2:I:31:GLN:H	2:I:31:GLN:NE2	1.66	0.93
1:E:49:SER:C	1:E:50:MET:HG2	1.97	0.88
1:E:170:LYS:CG	1:E:195:GLU:HG2	2.03	0.88
2:I:22:ARG:HA	2:I:22:ARG:HH11	1.40	0.87
2:I:50:ASN:HD22	2:I:50:ASN:H	1.23	0.86
1:E:108:ILE:HG23	1:E:138:ALA:HB2	1.59	0.85
1:E:49:SER:O	1:E:50:MET:HG2	1.76	0.84
1:E:40:PRO:O	4:E:337:HOH:O	1.94	0.84
2:I:11:PRO:HA	2:I:66:VAL:HG13	1.57	0.84
2:I:31:GLN:H	2:I:31:GLN:HE21	1.26	0.83
2:I:60:THR:HG22	2:I:62:VAL:HG12	1.60	0.83
1:E:165:VAL:O	1:E:170:LYS:HD2	1.79	0.83
2:I:31:GLN:HE21	2:I:31:GLN:N	1.76	0.83
1:E:235:LEU:HD21	1:E:246:VAL:HG21	1.62	0.82
1:E:15:ALA:CB	1:E:271:GLN:HG3	2.10	0.81
1:E:11:ILE:O	1:E:12:LYS:HB2	1.81	0.79
1:E:206:GLN:OE1	1:E:216:ALA:HB2	1.84	0.78
2:I:64:ASN:H	2:I:64:ASN:HD22	1.32	0.77
1:E:230:ALA:HB1	1:E:270:VAL:HG13	1.65	0.77
1:E:108:ILE:HG23	1:E:138:ALA:CB	2.13	0.77
1:E:196:LEU:CD2	4:E:342:HOH:O	2.26	0.77
2:I:57:ASN:O	2:I:61:ASN:HA	1.84	0.77
1:E:104:TYR:CE1	2:I:42:PRO:HG3	2.20	0.77
1:E:148:VAL:HG22	1:E:243:ASN:HB2	1.68	0.76
1:E:238:HIS:O	1:E:241:TRP:HB2	1.85	0.76
2:I:11:PRO:CA	2:I:66:VAL:HG13	2.14	0.75
1:E:123:ASN:ND2	1:E:224:SER:OG	2.19	0.75
1:E:139:VAL:HA	4:E:412:HOH:O	1.86	0.75
1:E:230:ALA:HB1	1:E:270:VAL:CG1	2.16	0.75
2:I:14:VAL:HG21	2:I:66:VAL:HG22	1.67	0.75
1:E:221:SER:OG	2:I:45:LEU:O	2.01	0.74
1:E:196:LEU:CD1	4:E:342:HOH:O	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:GLN:HA	4:I:92:HOH:O	1.87	0.73
2:I:22:ARG:HD3	2:I:22:ARG:C	2.12	0.72
1:E:200:ALA:HB1	1:E:201:PRO:CD	2.19	0.72
1:E:189:PHE:HA	4:E:315:HOH:O	1.91	0.71
1:E:136:LYS:O	1:E:136:LYS:HG2	1.91	0.70
1:E:36:ASP:C	1:E:36:ASP:OD1	2.32	0.70
2:I:11:PRO:HB3	2:I:66:VAL:HG11	1.74	0.70
2:I:60:THR:HG22	2:I:62:VAL:HG13	1.71	0.70
1:E:96:LEU:CD1	2:I:44:THR:HG22	2.20	0.70
1:E:62:ASN:O	1:E:63:SER:HB3	1.91	0.70
2:I:50:ASN:H	2:I:50:ASN:ND2	1.90	0.70
2:I:59:GLY:C	2:I:61:ASN:H	1.98	0.70
1:E:17:HIS:NE2	1:E:84:VAL:O	2.25	0.69
2:I:64:ASN:HD22	2:I:64:ASN:N	1.89	0.69
2:I:43:VAL:HG11	2:I:53:LYS:HD3	1.75	0.69
1:E:152:ALA:HB3	2:I:45:LEU:HD12	1.75	0.69
1:E:18:SER:HB3	4:E:413:HOH:O	1.93	0.69
2:I:50:ASN:HD22	2:I:50:ASN:N	1.89	0.68
1:E:242:THR:H	1:E:245:GLN:HE21	0.71	0.67
1:E:243:ASN:HD22	1:E:244:THR:N	1.93	0.67
1:E:10:GLN:HE21	1:E:184:ASN:HD21	1.43	0.67
1:E:108:ILE:HG22	1:E:108:ILE:O	1.94	0.66
1:E:1:ALA:HA	1:E:78:SER:O	1.95	0.66
2:I:11:PRO:HB3	2:I:66:VAL:CG1	2.25	0.66
1:E:275:GLN:CG	4:E:305:HOH:O	2.44	0.66
1:E:22:THR:HB	1:E:86:PRO:HG2	1.78	0.66
1:E:236:SER:HB2	4:E:410:HOH:O	1.96	0.66
1:E:15:ALA:HB3	1:E:271:GLN:HG3	1.78	0.66
1:E:200:ALA:HB1	1:E:201:PRO:HD2	1.79	0.65
2:I:24:TYR:CE1	2:I:28:HIS:ND1	2.65	0.65
1:E:10:GLN:HE21	1:E:184:ASN:ND2	1.95	0.65
2:I:19:ASP:N	4:I:108:HOH:O	2.29	0.64
1:E:272:ALA:O	1:E:275:GLN:NE2	2.30	0.64
1:E:95:VAL:HG23	1:E:95:VAL:O	1.97	0.64
1:E:142:ALA:O	1:E:147:VAL:HB	1.97	0.64
1:E:275:GLN:HG2	4:E:305:HOH:O	1.97	0.64
2:I:64:ASN:H	2:I:64:ASN:ND2	1.94	0.64
1:E:48:ALA:HB1	1:E:50:MET:HE2	1.80	0.63
1:E:44:VAL:N	4:E:336:HOH:O	2.29	0.63
2:I:60:THR:O	2:I:62:VAL:N	2.32	0.63
2:I:18:VAL:O	2:I:22:ARG:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:16:LYS:HB3	2:I:20:GLN:HB2	1.81	0.62
2:I:10:PHE:CA	2:I:12:GLU:OE1	2.47	0.62
1:E:51:VAL:HG12	1:E:54:GLU:HB2	1.81	0.62
1:E:107:ILE:CD1	1:E:126:LEU:HD13	2.30	0.62
1:E:132:SER:HB2	1:E:135:LEU:H	1.65	0.61
2:I:10:PHE:HA	2:I:12:GLU:OE1	2.00	0.61
1:E:104:TYR:CE1	2:I:42:PRO:CG	2.83	0.61
2:I:10:PHE:C	2:I:12:GLU:OE1	2.44	0.60
1:E:49:SER:N	1:E:57:PRO:HG3	2.16	0.60
2:I:29:TYR:HB3	2:I:32:TYR:HD2	1.67	0.60
2:I:24:TYR:HE1	2:I:28:HIS:ND1	2.00	0.59
1:E:205:ILE:HD12	4:E:429:HOH:O	2.01	0.59
1:E:10:GLN:NE2	1:E:184:ASN:ND2	2.51	0.59
1:E:107:ILE:HD13	1:E:126:LEU:CD1	2.33	0.58
2:I:22:ARG:HD3	2:I:22:ARG:O	2.04	0.58
2:I:64:ASN:ND2	2:I:65:HIS:ND1	2.51	0.58
1:E:43:LYS:NZ	4:E:348:HOH:O	2.36	0.58
1:E:154:GLY:C	1:E:191:SER:OG	2.47	0.58
1:E:115:ILE:HD11	1:E:142:ALA:HB2	1.86	0.58
1:E:107:ILE:HD13	1:E:126:LEU:HD11	1.85	0.57
1:E:107:ILE:HD11	1:E:126:LEU:HD13	1.86	0.57
1:E:2:GLN:HA	1:E:80:GLY:O	2.05	0.57
1:E:96:LEU:HD21	1:E:126:LEU:HD22	1.87	0.57
1:E:108:ILE:CG2	1:E:138:ALA:HB2	2.34	0.57
1:E:130:SER:HA	1:E:167:TYR:CE1	2.40	0.56
1:E:51:VAL:CG1	1:E:54:GLU:HB2	2.36	0.56
1:E:208:THR:O	1:E:209:LEU:HD23	2.05	0.56
2:I:60:THR:HG22	2:I:62:VAL:HG11	1.81	0.56
1:E:57:PRO:C	1:E:59:GLN:H	2.13	0.56
1:E:115:ILE:HD11	1:E:142:ALA:CA	2.36	0.56
2:I:24:TYR:CD1	2:I:24:TYR:C	2.84	0.56
1:E:242:THR:H	1:E:245:GLN:HE22	1.39	0.55
1:E:234:ILE:CG2	1:E:241:TRP:CZ3	2.88	0.55
2:I:24:TYR:HE1	2:I:28:HIS:HD1	1.51	0.55
2:I:27:LEU:HD22	2:I:28:HIS:CD2	2.41	0.55
1:E:96:LEU:HD12	2:I:44:THR:HG22	1.87	0.55
2:I:35:TYR:OH	4:I:106:HOH:O	2.18	0.54
1:E:258:GLY:O	1:E:259:ASP:C	2.49	0.54
1:E:267:LEU:HG	1:E:268:ILE:O	2.07	0.54
1:E:184:ASN:O	1:E:257:LEU:HD13	2.07	0.54
1:E:132:SER:HB2	1:E:135:LEU:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ALA:O	1:E:197:ASP:HB2	2.09	0.53
1:E:48:ALA:HB2	1:E:113:TRP:NE1	2.23	0.53
1:E:170:LYS:HG2	1:E:195:GLU:HG2	1.88	0.53
1:E:108:ILE:O	1:E:108:ILE:CG2	2.56	0.53
2:I:13:VAL:HG23	2:I:24:TYR:CE2	2.43	0.53
2:I:59:GLY:O	2:I:61:ASN:N	2.42	0.52
1:E:111:ILE:HG21	4:E:412:HOH:O	2.10	0.52
1:E:141:LYS:HB2	1:E:141:LYS:NZ	2.25	0.51
1:E:7:GLY:CA	1:E:201:PRO:HG2	2.40	0.51
1:E:49:SER:C	1:E:50:MET:CG	2.76	0.51
1:E:11:ILE:O	1:E:12:LYS:CB	2.57	0.51
1:E:55:THR:O	1:E:57:PRO:HD3	2.10	0.51
1:E:101:SER:OG	2:I:37:LEU:HD22	2.10	0.51
2:I:15:GLY:O	2:I:62:VAL:HG23	2.10	0.51
2:I:31:GLN:NE2	2:I:31:GLN:N	2.39	0.51
2:I:59:GLY:C	2:I:61:ASN:N	2.63	0.51
1:E:275:GLN:HG3	4:E:305:HOH:O	2.08	0.50
1:E:234:ILE:HG21	1:E:241:TRP:HZ3	1.77	0.50
1:E:62:ASN:ND2	1:E:98:ALA:O	2.34	0.50
1:E:124:MET:CE	1:E:149:VAL:HG13	2.42	0.50
1:E:243:ASN:HD22	1:E:243:ASN:C	2.19	0.50
1:E:62:ASN:O	1:E:63:SER:CB	2.59	0.50
1:E:107:ILE:CD1	1:E:126:LEU:CD1	2.90	0.50
1:E:248:SER:O	1:E:252:ASN:HB2	2.12	0.50
1:E:106:TRP:HA	4:E:432:HOH:O	2.11	0.50
2:I:22:ARG:HD2	4:I:89:HOH:O	2.12	0.49
1:E:28:VAL:HG22	1:E:121:VAL:HB	1.94	0.49
1:E:96:LEU:CD1	2:I:44:THR:CG2	2.88	0.49
1:E:13:ALA:N	1:E:14:PRO:CD	2.75	0.49
1:E:71:THR:CG2	1:E:225:PRO:HB2	2.43	0.49
1:E:113:TRP:O	1:E:117:ASN:ND2	2.46	0.49
2:I:17:THR:OG1	4:I:108:HOH:O	2.20	0.48
1:E:55:THR:HG23	4:E:403:HOH:O	2.13	0.48
2:I:34:VAL:HA	2:I:52:VAL:O	2.12	0.48
2:I:60:THR:C	2:I:62:VAL:H	2.22	0.48
1:E:10:GLN:NE2	1:E:184:ASN:HD21	2.08	0.48
2:I:37:LEU:O	2:I:38:PRO:C	2.54	0.48
1:E:115:ILE:CD1	1:E:142:ALA:HA	2.44	0.48
1:E:242:THR:CA	1:E:245:GLN:HE21	2.25	0.48
1:E:49:SER:OG	1:E:54:GLU:O	2.25	0.48
1:E:104:TYR:CE2	1:E:131:GLY:HA2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:MET:HE3	1:E:199:MET:HB3	1.75	0.48
1:E:234:ILE:HG21	1:E:241:TRP:CZ3	2.49	0.47
1:E:24:SER:O	1:E:25:ASN:HB2	2.12	0.47
1:E:59:GLN:O	1:E:94:LYS:CE	2.62	0.47
1:E:104:TYR:O	1:E:108:ILE:HG13	2.14	0.47
2:I:36:PHE:C	2:I:37:LEU:HG	2.39	0.47
1:E:148:VAL:CG2	1:E:243:ASN:HB2	2.42	0.47
1:E:255:THR:OG1	4:E:285:HOH:O	2.18	0.47
1:E:16:LEU:HD11	1:E:274:ALA:CB	2.43	0.47
1:E:99:ASP:HB3	4:E:319:HOH:O	2.13	0.47
1:E:122:ILE:CG2	1:E:124:MET:HE2	2.45	0.47
1:E:102:GLY:O	2:I:42:PRO:CD	2.48	0.47
1:E:155:ASN:ND2	2:I:47:LEU:HD22	2.29	0.47
1:E:138:ALA:C	4:E:412:HOH:O	2.58	0.46
1:E:15:ALA:HB1	1:E:271:GLN:HG3	1.92	0.46
1:E:209:LEU:HB2	1:E:213:LYS:HB2	1.97	0.46
2:I:11:PRO:CB	2:I:66:VAL:HG13	2.45	0.46
1:E:1:ALA:CA	1:E:78:SER:O	2.62	0.46
2:I:10:PHE:HD1	2:I:67:PRO:O	1.99	0.46
1:E:73:ALA:O	1:E:74:ALA:C	2.59	0.46
2:I:16:LYS:HB3	2:I:20:GLN:CB	2.44	0.46
2:I:12:GLU:HG2	2:I:24:TYR:CE2	2.51	0.45
1:E:7:GLY:HA2	1:E:201:PRO:HG2	1.97	0.45
2:I:23:GLU:O	2:I:27:LEU:HB2	2.16	0.45
1:E:115:ILE:HD11	1:E:142:ALA:N	2.31	0.45
1:E:108:ILE:HG23	1:E:138:ALA:HB1	1.98	0.45
2:I:60:THR:O	2:I:62:VAL:CG1	2.35	0.45
1:E:175:ILE:HG12	1:E:247:ARG:NE	2.31	0.44
1:E:25:ASN:HA	4:E:431:HOH:O	2.16	0.44
1:E:103:GLN:HG3	1:E:106:TRP:CE2	2.53	0.44
1:E:227:VAL:HG22	1:E:268:ILE:HD13	1.99	0.44
1:E:124:MET:HE3	1:E:124:MET:HB2	1.85	0.44
1:E:275:GLN:OXT	4:E:305:HOH:O	2.21	0.44
1:E:230:ALA:HA	1:E:270:VAL:HG11	1.99	0.44
1:E:256:LYS:HE3	4:E:423:HOH:O	2.16	0.44
1:E:83:GLY:O	1:E:86:PRO:HD3	2.18	0.43
1:E:12:LYS:HD3	1:E:269:ASN:OD1	2.17	0.43
1:E:260:SER:HB2	4:E:419:HOH:O	2.18	0.43
2:I:13:VAL:HG11	2:I:67:PRO:HG3	2.00	0.43
2:I:37:LEU:O	2:I:55:PHE:HA	2.18	0.43
1:E:119:MET:O	1:E:147:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:38:PRO:HB3	2:I:58:PRO:HG3	2.01	0.43
1:E:97:GLY:O	1:E:98:ALA:C	2.60	0.43
2:I:60:THR:C	2:I:62:VAL:N	2.76	0.43
1:E:48:ALA:HB2	1:E:113:TRP:CE2	2.54	0.43
1:E:104:TYR:CD1	2:I:42:PRO:CG	3.02	0.42
2:I:17:THR:OG1	2:I:20:GLN:HG3	2.19	0.42
1:E:6:TYR:CD1	1:E:6:TYR:C	2.97	0.42
1:E:175:ILE:HG21	1:E:175:ILE:HD13	1.65	0.42
1:E:235:LEU:CD2	1:E:246:VAL:HG21	2.40	0.42
2:I:23:GLU:O	2:I:24:TYR:C	2.60	0.42
1:E:104:TYR:HD1	1:E:107:ILE:HD12	1.84	0.42
1:E:115:ILE:HD11	1:E:142:ALA:CB	2.47	0.42
2:I:24:TYR:C	2:I:24:TYR:HD1	2.27	0.42
1:E:79:ILE:HD13	1:E:79:ILE:HG21	1.87	0.42
1:E:130:SER:O	1:E:167:TYR:CE1	2.72	0.42
1:E:230:ALA:HB1	1:E:270:VAL:HG11	2.01	0.42
1:E:263:TYR:O	1:E:264:GLY:C	2.61	0.42
2:I:13:VAL:HG23	2:I:24:TYR:HE2	1.84	0.42
1:E:108:ILE:O	1:E:112:GLU:HG2	2.19	0.42
2:I:24:TYR:CE1	2:I:28:HIS:CG	3.08	0.42
1:E:115:ILE:CD1	1:E:142:ALA:CA	2.96	0.42
1:E:243:ASN:HD22	1:E:244:THR:H	1.67	0.42
2:I:57:ASN:ND2	2:I:58:PRO:HD2	2.35	0.41
1:E:224:SER:N	1:E:225:PRO:HD2	2.34	0.41
2:I:24:TYR:HE1	2:I:28:HIS:CG	2.37	0.41
1:E:59:GLN:O	1:E:94:LYS:HE3	2.20	0.41
1:E:71:THR:HG22	1:E:225:PRO:HB2	2.00	0.41
1:E:230:ALA:CB	1:E:270:VAL:CG1	2.94	0.41
2:I:50:ASN:ND2	2:I:50:ASN:N	2.54	0.41
1:E:41:ASP:CG	1:E:41:ASP:O	2.62	0.41
1:E:184:ASN:HD22	1:E:184:ASN:HA	1.72	0.41
1:E:230:ALA:CA	1:E:270:VAL:HG11	2.51	0.41
1:E:234:ILE:CG2	1:E:241:TRP:HZ3	2.30	0.41
1:E:235:LEU:HD21	1:E:246:VAL:CG2	2.42	0.41
2:I:19:ASP:HA	4:I:109:HOH:O	2.20	0.41
2:I:17:THR:C	4:I:108:HOH:O	2.63	0.41
2:I:22:ARG:CD	4:I:89:HOH:O	2.69	0.41
1:E:27:LYS:HZ2	1:E:27:LYS:HG2	1.47	0.41
1:E:130:SER:C	1:E:167:TYR:CD1	2.98	0.41
1:E:51:VAL:O	1:E:54:GLU:O	2.39	0.41
1:E:122:ILE:HG13	1:E:147:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:GLY:N	1:E:261:PHE:O	2.50	0.41
2:I:10:PHE:N	2:I:10:PHE:CD1	2.88	0.41
2:I:66:VAL:HA	2:I:67:PRO:HD2	1.89	0.41
1:E:57:PRO:C	1:E:59:GLN:N	2.78	0.41
1:E:221:SER:O	1:E:225:PRO:CD	2.69	0.41
2:I:28:HIS:CD2	2:I:28:HIS:N	2.89	0.41
1:E:156:GLU:O	1:E:157:GLY:C	2.64	0.40
2:I:11:PRO:HB3	2:I:66:VAL:HG13	2.01	0.40
1:E:48:ALA:HB1	1:E:50:MET:CE	2.47	0.40
1:E:49:SER:HA	1:E:94:LYS:HB3	2.03	0.40
1:E:167:TYR:HB3	1:E:168:PRO:HA	2.03	0.40
1:E:52:PRO:HA	4:E:347:HOH:O	2.21	0.40
1:E:122:ILE:HD13	1:E:122:ILE:HG21	1.82	0.40
2:I:41:SER:HA	2:I:42:PRO:HD3	1.66	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)
4:E:365:HOH:O	4:E:365:HOH:O[4_556]	1.85	0.35

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%)	246 (90%)	25 (9%)	2 (1%)	18	28
2	I	61/70 (87%)	48 (79%)	10 (16%)	3 (5%)	1	1
All	All	334/345 (97%)	294 (88%)	35 (10%)	5 (2%)	8	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	61	ASN
1	E	63	SER
1	E	259	ASP
2	I	60	THR
2	I	24	TYR

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%)	174 (85%)	31 (15%)	3	3
2	I	58/64 (91%)	44 (76%)	14 (24%)	1	1
All	All	263/269 (98%)	218 (83%)	45 (17%)	2	2

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	SER
1	E	5	PRO
1	E	12	LYS
1	E	16	LEU
1	E	27	LYS
1	E	32	ASP
1	E	42	LEU
1	E	43	LYS
1	E	50	MET
1	E	51	VAL
1	E	54	GLU
1	E	78	SER
1	E	103	GLN
1	E	118	ASN
1	E	125	SER
1	E	139	VAL
1	E	145	SER
1	E	156	GLU
1	E	159	SER

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Mol	Chain	Res	Type
1	E	162	SER
1	E	185	GLN
1	E	212	ASN
1	E	221	SER
1	E	237	LYS
1	E	241	TRP
1	E	243	ASN
1	E	244	THR
1	E	249	SER
1	E	270	VAL
1	E	271	GLN
1	E	275	GLN
2	I	8	LYS
2	I	10	PHE
2	I	13	VAL
2	I	16	LYS
2	I	22	ARG
2	I	24	TYR
2	I	31	GLN
2	I	39	GLU
2	I	43	VAL
2	I	50	ASN
2	I	54	VAL
2	I	57	ASN
2	I	62	VAL
2	I	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	56	ASN
1	E	59	GLN
1	E	61	ASN
1	E	76	ASN
1	E	77	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

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Mol	Chain	Res	Type
1	E	252	ASN
1	E	271	GLN
1	E	275	GLN
2	I	31	GLN
2	I	50	ASN
2	I	57	ASN
2	I	64	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.