



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:33 PM UTC

PDB ID : 1CGI / pdb_00001cgi
Title : THREE-DIMENSIONAL STRUCTURE OF THE COMPLEXES BETWEEN BOVINE CHYMOTRYPSINOGEN*A AND TWO RECOMBINANT VARIANTS OF HUMAN PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL-TYPE)
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Deposited on : 1991-10-08
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

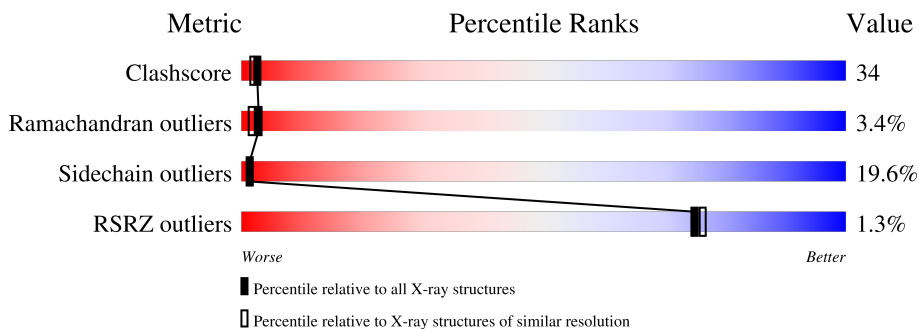
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	E	245	<p>1% 21% 42% 31% 5%</p>
2	I	56	<p>2% 20% 41% 34% 5%</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2291 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 ALPHA-CHYMOTRYPSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	245	1799	1127	307	353	12	20	0	0

- Molecule 2 is a protein called PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL TYPE) VARIANT 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	56	440	267	77	90	6	24	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	18	TYR	LYS	conflict	UNP P00995
I	19	GLU	ILE	conflict	UNP P00995
I	21	ARG	ASP	conflict	UNP P00995
I	29	ASP	ASN	conflict	UNP P00995

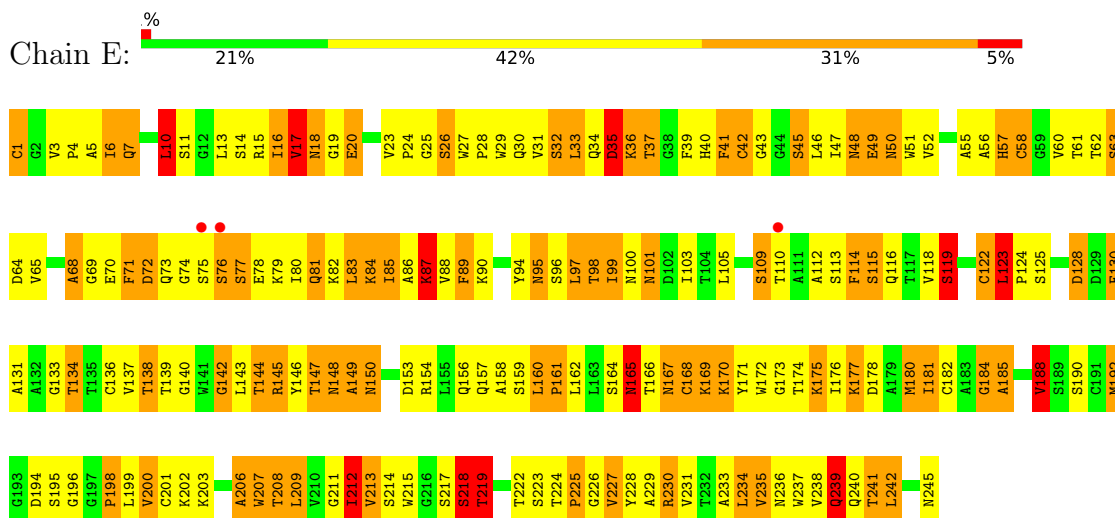
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	48	Total	O	0	0
			48	48		
3	I	4	Total	O	0	0
			4	4		

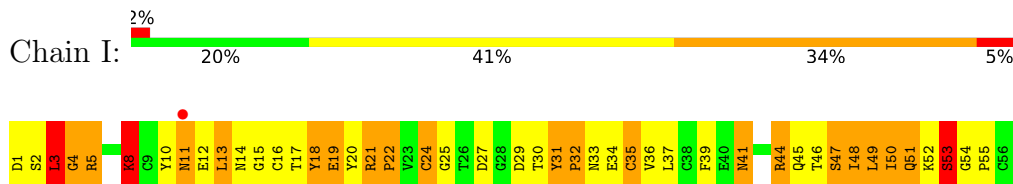
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ALPHA-CHYMOTRYPSINOGEN



- Molecule 2: PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL TYPE) VARIANT



4 Data and refinement statistics i

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.40Å 84.40Å 86.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 8.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.30) 69.2 (8.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.30Å)	Xtrriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.195 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtrriage
Anisotropy	0.427	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.042 for -h,l,k 0.031 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2291	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	1.33	5/1835 (0.3%)	3.03	235/2502 (9.4%)
2	I	1.39	3/447 (0.7%)	3.54	68/601 (11.3%)
All	All	1.34	8/2282 (0.4%)	3.13	303/3103 (9.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	LEU	C-N	8.55	1.46	1.32
2	I	8	LYS	CD-CE	-8.52	1.26	1.52
1	E	71	PHE	CA-C	7.23	1.56	1.52
1	E	36	LYS	CA-CB	-5.91	1.43	1.53
1	E	18	ASN	CG-OD1	5.37	1.33	1.23
1	E	77	SER	CA-CB	5.33	1.60	1.53
2	I	14	ASN	N-CA	5.22	1.52	1.46
1	E	175	LYS	CG-CD	-5.07	1.37	1.52

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	33	ASN	CA-CB-CG	17.36	129.96	112.60
2	I	8	LYS	CG-CD-CE	17.06	150.53	111.30
2	I	3	LEU	O-C-N	-16.72	100.35	122.59
2	I	14	ASN	CA-C-N	15.89	136.31	122.17
2	I	14	ASN	C-N-CA	15.89	136.31	122.17
1	E	30	GLN	OE1-CD-NE2	-14.34	108.27	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	VAL	CA-C-N	13.66	147.64	121.54
1	E	17	VAL	C-N-CA	13.66	147.64	121.54
1	E	225	PRO	CA-C-N	13.19	134.37	121.57
1	E	225	PRO	C-N-CA	13.19	134.37	121.57
1	E	226	GLY	CA-C-O	-12.83	109.89	121.18
1	E	128	ASP	CA-CB-CG	-12.78	99.82	112.60
1	E	52	VAL	O-C-N	12.47	136.44	123.10
1	E	236	ASN	CB-CA-C	12.27	130.28	110.90
1	E	17	VAL	CA-C-O	11.95	135.72	120.78
1	E	212	ILE	CA-C-O	-11.84	107.81	120.36
1	E	35	ASP	CA-C-O	-11.75	109.67	122.01
2	I	14	ASN	OD1-CG-ND2	-11.64	110.95	122.60
2	I	44	ARG	CA-CB-CG	11.32	136.74	114.10
1	E	214	SER	CA-C-O	11.17	127.61	119.68
2	I	18	TYR	N-CA-C	10.96	125.20	112.93
1	E	146	TYR	CA-C-O	10.87	132.37	120.20
2	I	33	ASN	OD1-CG-ND2	-10.85	111.75	122.60
2	I	2	SER	O-C-N	10.84	135.19	122.72
2	I	14	ASN	CB-CA-C	10.67	128.15	111.28
2	I	15	GLY	O-C-N	-10.51	115.86	123.95
2	I	51	GLN	CA-C-O	10.31	135.25	120.51
2	I	36	VAL	O-C-N	10.21	131.77	121.87
1	E	190	SER	CA-C-O	-10.19	109.44	121.05
1	E	219	THR	OG1-CB-CG2	9.96	129.21	109.30
1	E	153	ASP	CA-CB-CG	9.94	122.54	112.60
2	I	10	TYR	N-CA-C	-9.88	92.42	108.52
1	E	217	SER	CA-CB-OG	9.77	130.64	111.10
2	I	39	PHE	CA-CB-CG	-9.67	104.13	113.80
1	E	23	VAL	N-CA-C	-9.65	100.33	108.63
2	I	19	GLU	CB-CG-CD	9.57	128.88	112.60
1	E	123	LEU	CA-C-O	-9.34	112.35	120.19
1	E	42	CYS	O-C-N	-9.29	114.00	123.29
1	E	71	PHE	O-C-N	9.28	131.07	120.58
1	E	200	VAL	CA-C-O	9.26	130.02	120.39
1	E	18	ASN	CA-CB-CG	-9.25	103.35	112.60
2	I	10	TYR	CA-C-O	-9.16	110.24	120.32
1	E	130	PHE	CA-CB-CG	9.13	122.93	113.80
1	E	5	ALA	N-CA-C	-9.12	101.33	111.28
2	I	36	VAL	CA-C-O	-9.04	111.55	120.95
1	E	109	SER	CA-C-O	8.93	130.10	120.55
1	E	150	ASN	CA-CB-CG	8.91	121.51	112.60
1	E	47	ILE	CA-C-N	8.87	137.45	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	ILE	C-N-CA	8.87	137.45	122.20
1	E	35	ASP	O-C-N	8.82	134.17	122.36
1	E	219	THR	N-CA-CB	-8.70	96.84	111.20
1	E	97	LEU	O-C-N	8.67	133.50	122.23
1	E	36	LYS	N-CA-C	-8.66	102.16	112.89
2	I	48	ILE	CA-C-O	-8.57	111.25	121.28
1	E	222	THR	CA-C-N	8.51	135.68	122.49
1	E	222	THR	C-N-CA	8.51	135.68	122.49
1	E	134	THR	O-C-N	8.43	132.90	123.04
1	E	236	ASN	CA-C-O	-8.34	112.11	120.70
1	E	48	ASN	CB-CA-C	-8.32	93.96	113.02
2	I	33	ASN	CA-C-N	8.32	134.81	120.58
2	I	33	ASN	C-N-CA	8.32	134.81	120.58
1	E	34	GLN	CA-C-N	8.30	135.73	121.29
1	E	34	GLN	C-N-CA	8.30	135.73	121.29
1	E	58	CYS	CA-CB-SG	8.19	133.23	114.40
1	E	219	THR	N-CA-C	8.15	123.01	112.41
1	E	145	ARG	NE-CZ-NH2	-8.14	111.88	119.20
1	E	219	THR	CA-CB-OG1	-8.11	97.44	109.60
1	E	35	ASP	CB-CA-C	-8.11	93.22	111.30
1	E	87	LYS	CA-C-N	7.99	133.12	122.90
1	E	87	LYS	C-N-CA	7.99	133.12	122.90
1	E	6	ILE	CA-C-O	7.97	129.10	120.57
1	E	174	THR	CA-C-O	-7.91	110.28	119.61
2	I	22	PRO	CB-CA-C	7.88	121.47	111.39
1	E	149	ALA	CA-C-O	7.88	131.77	120.51
1	E	192	MET	CA-C-O	7.71	128.12	120.88
1	E	86	ALA	CA-C-O	7.68	128.51	119.67
1	E	85	ILE	CA-C-O	-7.68	111.96	120.72
1	E	146	TYR	CA-C-N	7.67	137.66	122.31
1	E	146	TYR	C-N-CA	7.67	137.66	122.31
2	I	2	SER	N-CA-C	7.61	118.28	108.24
1	E	52	VAL	CA-C-N	-7.60	113.76	123.19
1	E	52	VAL	C-N-CA	-7.60	113.76	123.19
2	I	35	CYS	N-CA-C	-7.58	103.03	111.82
1	E	234	LEU	N-CA-CB	-7.57	100.99	110.98
2	I	31	TYR	CA-C-O	7.53	127.38	119.69
2	I	48	ILE	O-C-N	7.53	130.80	122.75
2	I	24	CYS	CA-C-O	-7.49	112.57	120.58
1	E	213	VAL	O-C-N	7.47	130.28	122.67
1	E	55	ALA	O-C-N	7.44	131.79	123.16
1	E	213	VAL	CA-C-O	-7.40	112.55	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	PRO	CB-CA-C	7.38	121.18	110.63
1	E	32	SER	CA-C-O	-7.37	112.34	120.38
1	E	144	THR	CB-CA-C	7.37	124.19	110.70
1	E	154	ARG	CA-C-O	-7.37	112.58	121.28
1	E	180	MET	CA-C-N	7.37	133.32	122.71
1	E	180	MET	C-N-CA	7.37	133.32	122.71
1	E	50	ASN	CB-CA-C	-7.29	96.17	109.15
1	E	149	ALA	CA-C-N	7.27	135.43	121.54
1	E	149	ALA	C-N-CA	7.27	135.43	121.54
1	E	242	LEU	CA-C-N	7.21	132.75	120.71
1	E	242	LEU	C-N-CA	7.21	132.75	120.71
2	I	29	ASP	CA-C-N	7.19	132.32	122.19
2	I	29	ASP	C-N-CA	7.19	132.32	122.19
1	E	207	TRP	N-CA-C	-7.14	97.60	108.96
1	E	98	THR	N-CA-CB	-7.12	100.06	110.53
1	E	83	LEU	CA-C-O	-7.11	112.75	120.92
2	I	47	SER	CA-CB-OG	-7.10	96.89	111.10
1	E	169	LYS	CA-CB-CG	-7.10	99.90	114.10
1	E	30	GLN	CA-C-O	-6.99	112.39	120.49
1	E	240	GLN	N-CA-C	6.96	118.52	111.07
2	I	5	ARG	NE-CZ-NH2	-6.96	112.93	119.20
2	I	22	PRO	CA-C-N	6.96	132.73	122.71
2	I	22	PRO	C-N-CA	6.96	132.73	122.71
2	I	41	ASN	CA-C-O	6.93	127.84	120.70
1	E	3	VAL	O-C-N	6.93	129.00	121.10
1	E	140	GLY	N-CA-C	6.92	121.13	110.88
2	I	15	GLY	CA-C-O	6.92	127.77	121.47
1	E	224	THR	CA-CB-CG2	6.91	122.24	110.50
1	E	217	SER	O-C-N	6.91	131.35	123.06
1	E	230	ARG	CA-C-O	-6.90	113.53	120.98
1	E	70	GLU	CG-CD-OE1	-6.89	102.55	118.40
2	I	24	CYS	O-C-N	6.87	131.18	122.93
1	E	226	GLY	O-C-N	6.87	130.22	123.35
1	E	178	ASP	CB-CA-C	6.86	123.26	110.70
2	I	19	GLU	CA-C-N	-6.86	113.32	122.85
2	I	19	GLU	C-N-CA	-6.86	113.32	122.85
1	E	137	VAL	N-CA-C	6.86	118.67	108.46
1	E	134	THR	CA-C-N	-6.85	112.53	122.19
1	E	134	THR	C-N-CA	-6.85	112.53	122.19
2	I	21	ARG	O-C-N	6.83	126.76	121.23
1	E	119	SER	N-CA-CB	6.80	123.46	111.49
1	E	37	THR	CA-CB-OG1	-6.80	99.41	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	212	ILE	O-C-N	6.79	130.53	123.20
1	E	114	PHE	CA-CB-CG	-6.77	107.03	113.80
1	E	72	ASP	O-C-N	6.77	131.06	122.93
1	E	236	ASN	N-CA-C	-6.75	103.85	111.14
1	E	1	CYS	CA-C-N	6.75	134.63	121.41
1	E	1	CYS	C-N-CA	6.75	134.63	121.41
1	E	217	SER	CA-C-N	6.70	129.93	120.28
1	E	217	SER	C-N-CA	6.70	129.93	120.28
1	E	84	LYS	CB-CG-CD	6.69	126.69	111.30
1	E	20	GLU	CA-CB-CG	6.66	127.42	114.10
1	E	145	ARG	CD-NE-CZ	6.64	133.70	124.40
1	E	43	GLY	N-CA-C	-6.62	101.07	112.06
1	E	222	THR	O-C-N	-6.62	113.33	122.46
2	I	19	GLU	O-C-N	6.59	130.41	122.96
1	E	7	GLN	OE1-CD-NE2	6.58	129.18	122.60
1	E	190	SER	N-CA-C	-6.58	99.81	110.20
1	E	160	LEU	O-C-N	6.57	126.45	121.85
1	E	194	ASP	CA-CB-CG	6.54	119.14	112.60
1	E	26	SER	CA-C-O	-6.50	110.79	119.11
2	I	2	SER	CA-C-N	6.50	133.96	121.54
2	I	2	SER	C-N-CA	6.50	133.96	121.54
1	E	142	GLY	CA-C-O	-6.47	110.75	122.14
1	E	13	LEU	N-CA-C	-6.43	105.25	113.23
1	E	34	GLN	CB-CG-CD	6.43	123.53	112.60
1	E	154	ARG	CD-NE-CZ	-6.43	115.40	124.40
1	E	50	ASN	OD1-CG-ND2	6.42	129.03	122.60
1	E	128	ASP	N-CA-C	6.42	119.29	110.24
1	E	199	LEU	CA-C-N	6.41	131.63	123.10
1	E	199	LEU	C-N-CA	6.41	131.63	123.10
1	E	101	ASN	N-CA-CB	-6.39	102.19	111.91
1	E	150	ASN	CB-CG-ND2	-6.39	106.81	116.40
1	E	68	ALA	CA-C-N	6.37	134.05	121.06
1	E	68	ALA	C-N-CA	6.37	134.05	121.06
1	E	219	THR	CA-C-N	6.33	131.12	122.19
1	E	219	THR	C-N-CA	6.33	131.12	122.19
1	E	41	PHE	CA-C-O	6.32	125.85	118.90
1	E	130	PHE	CA-C-N	6.32	129.69	120.71
1	E	130	PHE	C-N-CA	6.32	129.69	120.71
1	E	119	SER	O-C-N	6.32	129.61	123.04
2	I	5	ARG	N-CA-CB	6.30	121.13	110.49
1	E	144	THR	CA-C-O	6.28	127.21	120.24
1	E	55	ALA	CA-C-O	-6.28	113.70	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	235	VAL	O-C-N	6.26	128.19	121.87
1	E	177	LYS	CA-C-O	6.23	129.40	121.55
1	E	198	PRO	N-CA-C	6.21	123.44	112.01
1	E	31	VAL	O-C-N	6.20	129.92	123.04
1	E	50	ASN	N-CA-C	6.20	121.73	114.04
1	E	48	ASN	CA-CB-CG	6.18	118.78	112.60
1	E	101	ASN	CA-C-N	6.17	131.33	122.08
1	E	101	ASN	C-N-CA	6.17	131.33	122.08
2	I	24	CYS	N-CA-CB	6.15	119.99	110.21
2	I	37	LEU	CA-C-O	-6.15	114.03	120.55
1	E	168	CYS	CA-CB-SG	6.14	128.53	114.40
1	E	128	ASP	CA-C-O	6.12	127.89	121.15
1	E	73	GLN	N-CA-C	-6.12	105.30	112.89
1	E	62	THR	CA-C-N	6.12	130.93	120.72
1	E	62	THR	C-N-CA	6.12	130.93	120.72
1	E	73	GLN	CB-CG-CD	6.11	122.99	112.60
1	E	234	LEU	CA-CB-CG	6.10	137.65	116.30
1	E	72	ASP	CA-C-O	-6.08	114.07	120.58
1	E	23	VAL	CA-C-O	6.08	124.45	119.47
1	E	20	GLU	CA-C-O	6.08	128.63	121.58
1	E	105	LEU	O-C-N	6.05	130.43	123.29
1	E	167	ASN	CB-CA-C	6.05	121.34	109.72
1	E	98	THR	N-CA-C	6.04	120.93	113.50
1	E	68	ALA	CA-C-O	6.03	127.97	121.16
1	E	201	CYS	CB-CA-C	6.02	120.14	109.72
1	E	77	SER	N-CA-C	5.98	119.81	111.56
2	I	3	LEU	CA-C-N	-5.95	108.40	122.07
2	I	3	LEU	C-N-CA	-5.95	108.40	122.07
1	E	35	ASP	N-CA-CB	-5.94	102.18	110.25
2	I	5	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	E	7	GLN	O-C-N	5.92	130.12	121.54
1	E	194	ASP	O-C-N	5.92	130.42	122.49
1	E	26	SER	N-CA-CB	5.88	120.29	110.41
1	E	166	THR	CA-CB-OG1	-5.88	100.78	109.60
2	I	17	THR	N-CA-C	-5.88	101.79	110.48
1	E	182	CYS	CA-CB-SG	5.82	127.78	114.40
1	E	185	ALA	N-CA-C	-5.80	106.16	113.23
1	E	154	ARG	N-CA-C	5.80	119.50	110.17
1	E	78	GLU	CB-CG-CD	5.79	122.45	112.60
1	E	80	ILE	CA-C-O	5.79	128.58	121.75
1	E	199	LEU	N-CA-C	-5.77	95.64	107.70
1	E	227	VAL	CA-C-N	5.77	132.08	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	227	VAL	C-N-CA	5.77	132.08	122.73
1	E	123	LEU	N-CA-C	-5.77	102.80	110.07
1	E	88	VAL	O-C-N	5.75	130.57	122.97
2	I	32	PRO	O-C-N	5.75	129.12	122.17
2	I	31	TYR	CB-CA-C	5.74	117.17	109.42
1	E	30	GLN	O-C-N	5.73	130.07	123.02
1	E	1	CYS	CB-CA-C	5.73	120.98	110.10
1	E	133	GLY	N-CA-C	-5.69	107.25	115.27
1	E	30	GLN	N-CA-CB	5.68	119.12	109.87
1	E	42	CYS	CA-CB-SG	5.67	127.44	114.40
1	E	63	SER	CA-C-O	5.65	126.33	119.38
1	E	82	LYS	CA-C-O	-5.64	115.08	121.39
1	E	146	TYR	N-CA-CB	-5.63	101.24	110.14
2	I	47	SER	O-C-N	5.62	129.18	122.21
1	E	18	ASN	O-C-N	5.60	130.04	122.59
2	I	30	THR	O-C-N	-5.59	116.84	123.22
1	E	218	SER	CA-C-O	5.59	126.41	120.10
1	E	49	GLU	N-CA-C	-5.58	106.24	113.16
1	E	119	SER	N-CA-C	-5.58	100.02	107.88
1	E	200	VAL	CA-CB-CG2	5.57	119.86	110.40
2	I	44	ARG	N-CA-CB	5.56	119.19	110.46
1	E	89	PHE	CA-CB-CG	5.53	119.33	113.80
1	E	130	PHE	CB-CA-C	5.52	119.79	110.79
1	E	10	LEU	N-CA-CB	-5.50	101.46	110.21
1	E	147	THR	CA-CB-CG2	5.49	119.83	110.50
1	E	73	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	E	192	MET	CB-CA-C	5.48	116.53	109.80
2	I	50	ILE	O-C-N	5.46	130.79	122.76
1	E	227	VAL	CA-CB-CG1	5.45	119.67	110.40
2	I	44	ARG	NE-CZ-NH1	-5.43	116.07	121.50
2	I	4	GLY	CA-C-N	5.42	131.90	121.54
2	I	4	GLY	C-N-CA	5.42	131.90	121.54
1	E	17	VAL	N-CA-CB	5.42	120.17	111.23
1	E	145	ARG	NH1-CZ-NH2	5.42	126.35	119.30
1	E	138	THR	CB-CA-C	5.42	119.71	109.37
1	E	201	CYS	CA-C-O	5.42	126.28	120.38
1	E	181	ILE	CA-C-O	5.39	126.69	120.76
1	E	118	VAL	CB-CA-C	5.39	118.20	110.33
1	E	185	ALA	O-C-N	5.38	130.70	122.03
1	E	122	CYS	O-C-N	-5.37	116.33	122.89
2	I	10	TYR	N-CA-CB	5.37	118.99	110.55
1	E	48	ASN	O-C-N	5.36	129.65	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	13	LEU	CA-C-N	-5.34	114.09	122.79
2	I	13	LEU	C-N-CA	-5.34	114.09	122.79
1	E	208	THR	N-CA-C	5.32	117.57	108.90
1	E	148	ASN	CA-CB-CG	-5.31	107.29	112.60
1	E	31	VAL	N-CA-CB	5.31	121.36	112.44
1	E	184	GLY	N-CA-C	5.30	116.92	111.56
1	E	145	ARG	CA-C-N	5.29	128.10	120.38
1	E	145	ARG	C-N-CA	5.29	128.10	120.38
1	E	136	CYS	N-CA-C	5.29	116.69	109.18
1	E	230	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	E	188	VAL	CA-C-O	-5.28	115.68	121.28
2	I	53	SER	CA-C-N	-5.28	113.58	121.87
2	I	53	SER	C-N-CA	-5.28	113.58	121.87
1	E	241	THR	CA-C-N	5.26	128.31	120.31
1	E	241	THR	C-N-CA	5.26	128.31	120.31
1	E	165	ASN	CA-C-O	5.25	126.30	120.63
1	E	14	SER	CA-C-O	5.24	125.86	119.05
2	I	14	ASN	CA-C-O	5.22	127.07	120.65
1	E	20	GLU	CB-CG-CD	5.20	121.44	112.60
1	E	181	ILE	CA-C-N	-5.17	114.11	122.81
1	E	181	ILE	C-N-CA	-5.17	114.11	122.81
1	E	235	VAL	N-CA-C	5.13	117.46	111.05
1	E	239	GLN	CA-C-N	5.12	127.10	120.44
1	E	239	GLN	C-N-CA	5.12	127.10	120.44
1	E	206	ALA	O-C-N	5.12	129.05	123.01
1	E	47	ILE	CB-CG1-CD1	-5.11	103.06	113.80
1	E	147	THR	N-CA-CB	-5.11	102.58	110.46
1	E	13	LEU	O-C-N	5.10	129.45	122.46
1	E	69	GLY	CA-C-O	-5.10	114.01	119.82
2	I	33	ASN	CB-CA-C	5.09	121.86	111.78
1	E	148	ASN	OD1-CG-ND2	5.08	127.68	122.60
1	E	98	THR	CA-C-O	5.08	124.73	119.14
1	E	65	VAL	N-CA-C	5.07	115.78	108.48
1	E	138	THR	N-CA-CB	5.06	119.64	110.83
1	E	206	ALA	CB-CA-C	-5.06	100.98	109.53
1	E	140	GLY	CA-C-O	5.04	126.97	121.83
1	E	46	LEU	CA-C-O	-5.04	114.79	120.43
2	I	35	CYS	CA-CB-SG	5.04	125.98	114.40
2	I	10	TYR	O-C-N	5.03	129.21	123.27
1	E	230	ARG	O-C-N	5.02	129.30	122.57
1	E	81	GLN	CB-CG-CD	5.02	121.13	112.60
1	E	233	ALA	O-C-N	5.02	129.29	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	168	CYS	N-CA-C	-5.01	105.52	111.69
1	E	57	HIS	CA-C-O	5.01	125.14	119.18
1	E	25	GLY	N-CA-C	5.00	122.01	115.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	3	LEU	Peptide,Mainchain

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	1799	0	1777	122	0
2	I	440	0	412	36	0
3	E	48	0	0	1	0
3	I	4	0	0	0	0
All	All	2291	0	2189	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (147) 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:35:ASP:OD2	1:E:37:THR:HB	1.58	1.04
1:E:180:MET:O	1:E:230:ARG:NH1	1.92	1.01
1:E:4:PRO:HB2	1:E:6:ILE:O	1.74	0.87
2:I:27:ASP:HB3	2:I:48:ILE:HD12	1.60	0.82
2:I:44:ARG:HB2	2:I:46:THR:HG23	1.63	0.81
1:E:158:ALA:HB1	1:E:188:VAL:HG11	1.63	0.80
1:E:33:LEU:HD23	1:E:33:LEU:N	1.96	0.80
1:E:95:ASN:ND2	1:E:97:LEU:H	1.80	0.79
1:E:95:ASN:HD22	1:E:97:LEU:H	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:THR:O	1:E:245:ASN:HB2	1.85	0.77
1:E:158:ALA:HB1	1:E:188:VAL:CG1	2.16	0.76
1:E:94:TYR:HB2	1:E:101:ASN:O	1.86	0.74
2:I:27:ASP:HB3	2:I:48:ILE:CD1	2.17	0.74
1:E:33:LEU:CD1	1:E:60:VAL:HG21	2.17	0.74
1:E:81:GLN:HE22	1:E:113:SER:H	1.35	0.73
2:I:22:PRO:HA	2:I:31:TYR:O	1.88	0.72
1:E:4:PRO:CB	1:E:6:ILE:O	2.40	0.69
1:E:123:LEU:HD11	1:E:238:VAL:HG11	1.75	0.69
1:E:198:PRO:HB2	1:E:200:VAL:HG13	1.72	0.69
1:E:99:ILE:HG13	2:I:13:LEU:HD22	1.75	0.69
2:I:11:ASN:C	2:I:11:ASN:HD22	1.98	0.68
1:E:35:ASP:HB3	1:E:37:THR:H	1.58	0.68
1:E:35:ASP:HB3	1:E:37:THR:N	2.08	0.68
1:E:64:ASP:O	1:E:85:ILE:HD12	1.93	0.68
1:E:35:ASP:HB2	1:E:39:PHE:H	1.57	0.67
1:E:35:ASP:OD2	1:E:37:THR:CB	2.41	0.65
1:E:192:MET:HG2	2:I:32:PRO:HB2	1.77	0.65
1:E:239:GLN:HA	1:E:239:GLN:OE1	1.97	0.64
1:E:165:ASN:O	1:E:169:LYS:HG3	1.98	0.63
1:E:172:TRP:CB	1:E:176:ILE:HD11	2.27	0.63
1:E:219:THR:HG23	1:E:219:THR:O	1.99	0.61
1:E:177:LYS:HG2	1:E:180:MET:HE3	1.82	0.61
1:E:198:PRO:HB2	1:E:200:VAL:CG1	2.30	0.61
2:I:8:LYS:HG3	2:I:34:GLU:OE2	2.00	0.61
1:E:97:LEU:O	2:I:12:GLU:HB2	2.01	0.60
1:E:98:THR:HG22	1:E:100:ASN:HB2	1.82	0.60
1:E:215:TRP:CD2	2:I:13:LEU:HD11	2.36	0.60
1:E:184:GLY:O	1:E:185:ALA:HB3	2.01	0.59
1:E:68:ALA:HB3	1:E:81:GLN:HB2	1.84	0.59
1:E:215:TRP:CE2	2:I:13:LEU:HD11	2.39	0.58
1:E:29:TRP:O	1:E:45:SER:HA	2.04	0.58
1:E:99:ILE:HG13	2:I:13:LEU:CD2	2.34	0.58
2:I:52:LYS:NZ	2:I:55:PRO:O	2.36	0.58
1:E:161:PRO:O	1:E:161:PRO:HG2	2.03	0.58
1:E:171:TYR:CD2	1:E:225:PRO:HD3	2.38	0.57
1:E:1:CYS:C	1:E:122:CYS:SG	2.87	0.57
2:I:27:ASP:CB	2:I:48:ILE:HD12	2.34	0.57
1:E:125:SER:O	1:E:128:ASP:HB2	2.04	0.57
1:E:131:ALA:O	1:E:134:THR:OG1	2.09	0.57
1:E:32:SER:OG	1:E:40:HIS:ND1	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:24:CYS:HB3	2:I:52:LYS:HG2	1.85	0.56
1:E:134:THR:O	1:E:161:PRO:HA	2.06	0.56
1:E:97:LEU:HB3	2:I:12:GLU:HG3	1.88	0.56
1:E:181:ILE:HG13	1:E:230:ARG:NH2	2.20	0.56
1:E:32:SER:C	1:E:33:LEU:HD23	2.30	0.55
1:E:11:SER:OG	1:E:20:GLU:OE1	2.22	0.55
1:E:27:TRP:CD1	1:E:139:THR:HG21	2.42	0.55
1:E:95:ASN:HD22	1:E:95:ASN:C	2.14	0.55
1:E:103:ILE:HG23	1:E:237:TRP:CZ3	2.42	0.55
1:E:81:GLN:NE2	1:E:113:SER:H	2.02	0.54
1:E:35:ASP:CG	1:E:37:THR:HB	2.29	0.54
1:E:72:ASP:OD1	1:E:74:GLY:N	2.41	0.53
1:E:113:SER:O	1:E:114:PHE:C	2.52	0.53
1:E:41:PHE:O	1:E:42:CYS:SG	2.66	0.53
2:I:4:GLY:O	2:I:50:ILE:O	2.26	0.53
1:E:138:THR:HA	1:E:198:PRO:O	2.09	0.53
1:E:16:ILE:O	1:E:17:VAL:C	2.52	0.53
1:E:33:LEU:HD12	1:E:60:VAL:CG2	2.39	0.53
1:E:94:TYR:HA	1:E:100:ASN:O	2.08	0.53
1:E:124:PRO:CG	1:E:231:VAL:HG12	2.39	0.52
1:E:48:ASN:HB2	1:E:50:ASN:H	1.74	0.52
1:E:81:GLN:HE22	1:E:113:SER:N	2.03	0.52
1:E:130:PHE:CZ	1:E:203:LYS:CE	2.93	0.52
1:E:114:PHE:HD1	1:E:114:PHE:N	2.08	0.51
1:E:172:TRP:HB2	1:E:176:ILE:CG1	2.41	0.51
1:E:56:ALA:HB1	1:E:90:LYS:HD2	1.93	0.51
1:E:238:VAL:O	1:E:242:LEU:HB2	2.11	0.51
2:I:52:LYS:HG3	2:I:53:SER:O	2.12	0.50
1:E:24:PRO:HG3	1:E:71:PHE:CE2	2.46	0.50
1:E:33:LEU:CD1	1:E:60:VAL:CG2	2.88	0.50
1:E:27:TRP:HE3	1:E:29:TRP:CZ2	2.29	0.50
1:E:124:PRO:HG3	1:E:231:VAL:HG12	1.93	0.49
1:E:172:TRP:CG	1:E:176:ILE:HD11	2.47	0.49
1:E:169:LYS:O	1:E:173:GLY:N	2.45	0.49
1:E:95:ASN:HD22	1:E:96:SER:N	2.11	0.49
1:E:167:ASN:HA	1:E:170:LYS:HD2	1.94	0.49
1:E:20:GLU:O	1:E:156:GLN:HA	2.13	0.48
1:E:130:PHE:CZ	1:E:203:LYS:HE2	2.48	0.48
2:I:41:ASN:OD1	2:I:46:THR:OG1	2.31	0.48
1:E:200:VAL:HG23	1:E:207:TRP:CE3	2.49	0.48
1:E:49:GLU:HB3	1:E:112:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:TYR:CE2	2:I:22:PRO:HG3	2.49	0.48
1:E:57:HIS:C	1:E:57:HIS:CD2	2.91	0.48
1:E:148:ASN:O	1:E:149:ALA:C	2.55	0.48
1:E:114:PHE:N	1:E:114:PHE:CD1	2.80	0.47
1:E:20:GLU:O	1:E:157:GLN:N	2.44	0.47
1:E:20:GLU:HG3	1:E:157:GLN:HE21	1.79	0.47
2:I:52:LYS:HG2	2:I:52:LYS:O	2.14	0.47
1:E:87:LYS:HB3	1:E:89:PHE:CE1	2.50	0.47
1:E:130:PHE:HZ	1:E:203:LYS:CE	2.28	0.46
1:E:168:CYS:SG	1:E:172:TRP:HD1	2.37	0.46
1:E:158:ALA:HB1	1:E:188:VAL:HG13	1.95	0.46
2:I:11:ASN:O	2:I:11:ASN:ND2	2.31	0.46
1:E:33:LEU:HD12	1:E:60:VAL:HG21	1.92	0.46
1:E:51:TRP:CE2	1:E:242:LEU:HD12	2.50	0.46
1:E:195:SER:OG	2:I:18:TYR:C	2.59	0.46
1:E:142:GLY:HA2	1:E:192:MET:O	2.15	0.45
2:I:52:LYS:O	2:I:52:LYS:CG	2.60	0.45
1:E:160:LEU:HD23	1:E:160:LEU:N	2.31	0.45
1:E:99:ILE:CG1	2:I:13:LEU:HD22	2.46	0.45
1:E:181:ILE:CG1	1:E:230:ARG:NH2	2.79	0.45
1:E:156:GLN:HG3	3:E:252:HOH:O	2.17	0.44
1:E:218:SER:HA	2:I:16:CYS:HB2	2.00	0.44
1:E:27:TRP:CE3	1:E:29:TRP:CZ2	3.06	0.44
1:E:177:LYS:HG2	1:E:180:MET:CE	2.47	0.44
1:E:203:LYS:NZ	1:E:208:THR:HG21	2.32	0.44
2:I:11:ASN:C	2:I:11:ASN:ND2	2.73	0.44
1:E:124:PRO:HD3	1:E:209:LEU:O	2.18	0.43
1:E:196:GLY:HA2	1:E:212:ILE:HG23	2.01	0.43
1:E:172:TRP:HB2	1:E:176:ILE:HD11	1.98	0.43
2:I:25:GLY:HA2	2:I:49:LEU:O	2.18	0.43
1:E:10:LEU:HD12	1:E:10:LEU:HA	1.84	0.43
1:E:211:GLY:HA2	1:E:229:ALA:O	2.19	0.43
2:I:41:ASN:O	2:I:45:GLN:N	2.52	0.43
2:I:44:ARG:HH11	2:I:44:ARG:HD3	1.56	0.43
1:E:28:PRO:HB2	1:E:119:SER:N	2.34	0.43
1:E:123:LEU:HD11	1:E:238:VAL:CG1	2.46	0.43
1:E:95:ASN:O	1:E:99:ILE:N	2.51	0.42
1:E:115:SER:HB2	1:E:116:GLN:H	1.53	0.42
1:E:202:LYS:HA	1:E:206:ALA:O	2.18	0.42
2:I:27:ASP:HB3	2:I:48:ILE:HD11	2.01	0.42
1:E:203:LYS:HB2	1:E:203:LYS:HE3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:VAL:HG22	1:E:228:TYR:HE2	1.85	0.42
2:I:44:ARG:HB2	2:I:46:THR:CG2	2.42	0.42
1:E:124:PRO:O	1:E:235:VAL:HG21	2.19	0.42
1:E:15:ARG:HG2	1:E:159:SER:HB2	2.01	0.42
2:I:53:SER:OG	2:I:54:GLY:N	2.52	0.41
2:I:44:ARG:NE	2:I:46:THR:HG21	2.35	0.41
1:E:56:ALA:HB1	1:E:90:LYS:CD	2.50	0.41
1:E:83:LEU:CD1	1:E:112:ALA:HB2	2.51	0.41
1:E:209:LEU:HD12	1:E:209:LEU:HA	1.80	0.41
2:I:4:GLY:HA2	2:I:49:LEU:HD13	2.03	0.41
1:E:58:CYS:O	2:I:21:ARG:NH2	2.31	0.41
1:E:35:ASP:CB	1:E:37:THR:HB	2.51	0.41
1:E:172:TRP:HB2	1:E:176:ILE:HG12	2.03	0.41
1:E:95:ASN:HD22	1:E:97:LEU:N	2.08	0.40
1:E:169:LYS:O	1:E:173:GLY:HA2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	243/245 (99%)	224 (92%)	11 (4%)	8 (3%)	3	2
2	I	54/56 (96%)	51 (94%)	1 (2%)	2 (4%)	2	1
All	All	297/301 (99%)	275 (93%)	12 (4%)	10 (3%)	3	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	VAL
1	E	19	GLY
1	E	75	SER

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Mol	Chain	Res	Type
1	E	76	SER
2	I	3	LEU
1	E	150	ASN
1	E	209	LEU
2	I	5	ARG
1	E	18	ASN
1	E	99	ILE

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	E	200/200 (100%)	161 (80%)	39 (20%)	1 1
2	I	50/50 (100%)	40 (80%)	10 (20%)	1 1
All	All	250/250 (100%)	201 (80%)	49 (20%)	1 1

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	7	GLN
1	E	10	LEU
1	E	16	ILE
1	E	26	SER
1	E	33	LEU
1	E	35	ASP
1	E	36	LYS
1	E	45	SER
1	E	61	THR
1	E	63	SER
1	E	76	SER
1	E	77	SER
1	E	79	LYS
1	E	84	LYS
1	E	87	LYS
1	E	95	ASN

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Mol	Chain	Res	Type
1	E	109	SER
1	E	110	THR
1	E	115	SER
1	E	119	SER
1	E	123	LEU
1	E	143	LEU
1	E	144	THR
1	E	145	ARG
1	E	147	THR
1	E	161	PRO
1	E	162	LEU
1	E	164	SER
1	E	165	ASN
1	E	170	LYS
1	E	175	LYS
1	E	188	VAL
1	E	212	ILE
1	E	218	SER
1	E	219	THR
1	E	223	SER
1	E	227	VAL
1	E	234	LEU
1	E	239	GLN
2	I	1	ASP
2	I	3	LEU
2	I	8	LYS
2	I	11	ASN
2	I	19	GLU
2	I	35	CYS
2	I	47	SER
2	I	49	LEU
2	I	51	GLN
2	I	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	81	GLN
1	E	95	ASN
1	E	116	GLN
1	E	165	ASN
1	E	167	ASN

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Mol	Chain	Res	Type
2	I	33	ASN
2	I	51	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	245/245 (100%)	-0.28	3 (1%) 76 77	2, 11, 32, 43	6 (2%)
2	I	53/56 (94%)	-0.15	1 (1%) 66 68	2, 8, 40, 47	1 (1%)
All	All	298/301 (99%)	-0.25	4 (1%) 75 76	2, 10, 35, 47	7 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	11	ASN	3.1
1	E	76	SER	2.8
1	E	110	THR	2.3
1	E	75	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.