



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:07 AM UTC

PDB ID : 1PEK / pdb_00001pek
Title : STRUCTURE OF THE COMPLEX OF PROTEINASE K WITH
A SUBSTRATE-ANALOGUE HEXA-PEPTIDE INHIBITOR AT 2.2
ANGSTROMS RESOLUTION
Authors : Betzel, C.; Singh, T.P.; Visanji, M.; Peters, K.; Fittkau, S.; Saenger, W.;
Wilson, K.S.
Deposited on : 1993-01-19
Resolution : 2.20 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

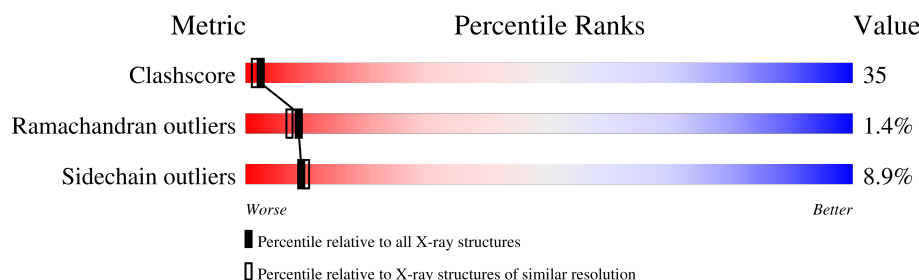
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	279	
2	C	4	
3	D	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DAL	D	5	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2246 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 PROTEINASE K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	279	Total	C	N	O	S	0	0	0
			2018	1243	352	413	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	85	VAL	ALA	conflict	UNP P06873

- Molecule 2 is a protein called PEPTIDE PRO-ALA-PRO-PHE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	1	0	0
			30	22	4	4			

- Molecule 3 is a protein called D-DAL-ALA-NH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			10	6	2	2			

- Molecule 4 is water.

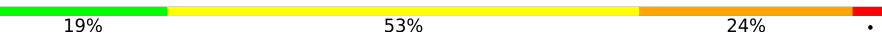
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	183	Total	O	0	0
			183	183		
4	C	1	Total	O	0	0
			1	1		
4	D	4	Total	O	0	0
			4	4		

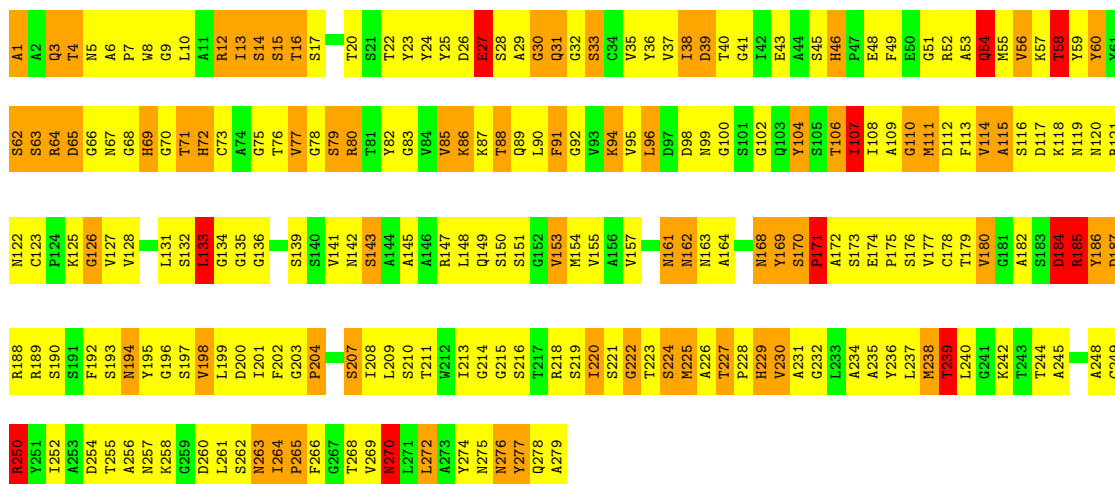
3 Residue-property plots

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: PROTEINASE K

Chain E: 



• Molecule 2: PEPTIDE PRO-ALA-PRO-PHE

Chain C: 



• Molecule 3: D-DAL-ALA-NH2

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.28Å 68.28Å 107.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	95.0 (8.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2246	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: DAL

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	2.02	39/2057 (1.9%)	4.00	440/2797 (15.7%)
2	C	1.80	0/32	9.25	23/43 (53.5%)
3	D	31.35	4/4 (100.0%)	20.14	4/4 (100.0%)
All	All	2.43	43/2093 (2.1%)	4.19	467/2844 (16.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	1	4
2	C	1	2
3	D	0	1
All	All	2	7

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	ALA	C-O	51.72	2.27	1.23
3	D	6	ALA	N-CA	28.35	2.00	1.46
3	D	6	ALA	CA-C	20.35	1.95	1.52
1	E	168	ASN	C-O	16.17	1.42	1.24
1	E	185	ARG	NE-CZ	11.12	1.45	1.33
1	E	168	ASN	CA-C	-9.97	1.40	1.52
1	E	185	ARG	CZ-NH2	8.66	1.44	1.33
1	E	185	ARG	CZ-NH1	8.23	1.44	1.32
1	E	83	GLY	CA-C	-6.47	1.45	1.52
3	D	6	ALA	CA-CB	6.22	1.73	1.52
1	E	277	TYR	C-N	-6.21	1.25	1.33
1	E	14	SER	N-CA	-6.14	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	91	PHE	C-N	-6.06	1.28	1.33
1	E	237	LEU	C-O	-6.02	1.17	1.24
1	E	141	VAL	C-O	-5.96	1.17	1.24
1	E	108	ILE	C-O	-5.95	1.17	1.24
1	E	170	SER	C-O	-5.89	1.17	1.24
1	E	13	ILE	CA-C	-5.84	1.44	1.52
1	E	57	LYS	CA-C	-5.75	1.45	1.52
1	E	244	THR	CA-C	-5.75	1.45	1.52
1	E	270	ASN	CA-C	-5.71	1.47	1.53
1	E	68	GLY	C-O	-5.67	1.16	1.24
1	E	141	VAL	CA-C	-5.66	1.45	1.52
1	E	142	ASN	C-O	-5.64	1.17	1.24
1	E	161	ASN	CA-C	-5.48	1.46	1.53
1	E	72	HIS	C-O	-5.47	1.17	1.24
1	E	197	SER	C-N	-5.27	1.27	1.34
1	E	179	THR	N-CA	-5.26	1.40	1.46
1	E	229	HIS	CE1-NE2	-5.25	1.27	1.32
1	E	108	ILE	C-N	-5.25	1.26	1.34
1	E	78	GLY	N-CA	-5.25	1.37	1.45
1	E	73	CYS	C-O	-5.24	1.18	1.24
1	E	157	VAL	N-CA	-5.22	1.40	1.46
1	E	62	SER	C-N	-5.18	1.26	1.33
1	E	237	LEU	C-N	-5.16	1.26	1.33
1	E	229	HIS	C-O	-5.15	1.18	1.24
1	E	214	GLY	C-N	-5.15	1.27	1.33
1	E	108	ILE	N-CA	-5.10	1.40	1.46
1	E	211	THR	CA-C	-5.10	1.46	1.52
1	E	46	HIS	CE1-NE2	-5.07	1.27	1.32
1	E	66	GLY	C-O	-5.06	1.19	1.24
1	E	170	SER	N-CA	-5.04	1.38	1.46
1	E	263	ASN	C-N	-5.02	1.28	1.33

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	80	ARG	CD-NE-CZ	36.74	175.84	124.40
1	E	168	ASN	O-C-N	-33.52	85.83	122.03
1	E	170	SER	CA-C-N	31.99	159.82	119.84
1	E	170	SER	C-N-CA	31.99	159.82	119.84
2	C	3	PRO	CA-C-N	27.85	171.84	121.70
2	C	3	PRO	C-N-CA	27.85	171.84	121.70
3	D	6	ALA	CA-C-O	-24.20	79.66	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	ALA	CB-CA-C	22.64	144.46	110.50
1	E	169	TYR	N-CA-CB	20.43	145.22	110.50
1	E	168	ASN	CA-C-O	-19.71	100.60	120.90
1	E	185	ARG	CD-NE-CZ	19.30	151.42	124.40
2	C	2	ALA	O-C-N	-19.18	99.26	121.32
3	D	6	ALA	N-CA-CB	18.36	137.94	110.40
1	E	170	SER	O-C-N	16.61	141.88	121.29
1	E	254	ASP	CA-CB-CG	16.26	128.86	112.60
1	E	168	ASN	CA-C-N	15.88	150.28	121.70
1	E	168	ASN	C-N-CA	15.88	150.28	121.70
1	E	75	GLY	CA-C-O	-15.85	103.86	120.66
1	E	272	LEU	CA-C-O	-15.41	103.37	120.32
1	E	126	GLY	CA-C-O	15.24	132.12	122.22
2	C	3	PRO	CB-CA-C	-15.03	95.17	111.56
1	E	85	VAL	N-CA-CB	-14.62	95.29	112.40
1	E	89	GLN	OE1-CD-NE2	-14.05	108.55	122.60
1	E	168	ASN	CB-CA-C	13.72	132.22	110.95
3	D	6	ALA	N-CA-C	-13.65	72.77	111.00
1	E	27	GLU	CB-CG-CD	13.39	135.37	112.60
1	E	68	GLY	CA-C-O	-13.06	106.08	119.27
1	E	231	ALA	CA-C-N	12.93	134.29	119.94
1	E	231	ALA	C-N-CA	12.93	134.29	119.94
1	E	169	TYR	CA-C-N	12.79	144.92	122.28
1	E	169	TYR	C-N-CA	12.79	144.92	122.28
2	C	4	PHE	CA-CB-CG	12.79	126.59	113.80
1	E	200	ASP	CA-CB-CG	-12.71	99.89	112.60
1	E	171	PRO	N-CA-CB	12.67	116.55	103.25
1	E	107	ILE	CA-CB-CG2	12.40	131.58	110.50
1	E	199	LEU	CA-C-O	-12.14	108.33	121.56
1	E	163	ASN	OD1-CG-ND2	-12.07	110.53	122.60
1	E	194	ASN	OD1-CG-ND2	12.05	134.65	122.60
1	E	68	GLY	O-C-N	12.03	135.55	122.56
2	C	2	ALA	N-CA-C	12.00	136.33	109.81
1	E	70	GLY	O-C-N	11.94	133.65	122.19
1	E	171	PRO	CA-N-CD	-11.92	95.31	112.00
1	E	162	ASN	CA-CB-CG	11.74	124.34	112.60
1	E	250	ARG	NE-CZ-NH2	11.64	129.68	119.20
1	E	263	ASN	CA-CB-CG	11.63	124.23	112.60
1	E	185	ARG	NE-CZ-NH2	-11.61	108.75	119.20
1	E	64	ARG	CD-NE-CZ	-11.60	108.17	124.40
1	E	254	ASP	CA-C-O	-11.46	106.79	119.97
1	E	89	GLN	CB-CG-CD	11.44	132.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	276	ASN	OD1-CG-ND2	11.35	133.95	122.60
2	C	2	ALA	CA-C-N	11.33	134.17	120.23
2	C	2	ALA	C-N-CA	11.33	134.17	120.23
1	E	39	ASP	CA-CB-CG	11.27	123.87	112.60
1	E	219	SER	CA-C-O	-11.26	108.16	120.43
1	E	64	ARG	NE-CZ-NH1	-11.08	110.42	121.50
1	E	209	LEU	CA-C-O	-11.01	107.72	120.49
1	E	80	ARG	CA-CB-CG	11.00	136.10	114.10
1	E	14	SER	CA-C-N	11.00	140.55	122.73
1	E	14	SER	C-N-CA	11.00	140.55	122.73
1	E	171	PRO	N-CD-CG	10.95	119.62	103.20
1	E	163	ASN	CB-CG-ND2	10.90	132.75	116.40
1	E	95	VAL	N-CA-C	-10.83	101.62	113.43
1	E	199	LEU	O-C-N	10.83	135.64	122.86
1	E	221	SER	CA-C-O	-10.74	108.55	121.11
2	C	4	PHE	CB-CA-C	-10.70	89.77	110.10
1	E	58	THR	CA-C-N	-10.61	105.68	122.65
1	E	58	THR	C-N-CA	-10.61	105.68	122.65
1	E	184	ASP	CA-C-N	10.53	135.76	120.38
1	E	184	ASP	C-N-CA	10.53	135.76	120.38
1	E	220	ILE	CA-CB-CG2	10.49	128.33	110.50
1	E	143	SER	O-C-N	10.46	132.84	122.07
1	E	53	ALA	CA-C-O	-10.38	109.38	121.11
1	E	107	ILE	CB-CA-C	10.37	125.60	112.02
1	E	72	HIS	CA-C-N	10.33	134.49	120.44
1	E	72	HIS	C-N-CA	10.33	134.49	120.44
1	E	256	ALA	O-C-N	10.29	135.20	122.65
1	E	17	SER	O-C-N	10.28	129.18	121.88
1	E	115	ALA	CA-C-O	-10.26	109.55	120.63
1	E	169	TYR	CA-C-O	-10.23	103.41	120.80
1	E	106	THR	CA-CB-CG2	10.21	127.85	110.50
1	E	149	GLN	OE1-CD-NE2	-10.16	112.44	122.60
2	C	2	ALA	CA-C-O	-10.07	106.37	120.16
1	E	219	SER	O-C-N	9.87	134.42	123.27
1	E	223	THR	N-CA-C	-9.87	101.24	113.18
1	E	179	THR	CA-CB-OG1	-9.79	94.91	109.60
1	E	256	ALA	CA-C-O	-9.79	110.83	121.99
1	E	171	PRO	O-C-N	-9.74	109.49	122.64
2	C	4	PHE	N-CA-CB	9.63	126.87	110.50
1	E	58	THR	CB-CA-C	-9.63	89.26	109.38
1	E	117	ASP	CA-C-O	-9.62	109.22	120.10
1	E	162	ASN	CB-CG-ND2	9.60	130.81	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	PRO	CB-CA-C	9.60	128.34	110.10
1	E	13	ILE	CA-C-O	-9.57	110.33	120.57
1	E	30	GLY	CA-C-N	-9.54	107.16	120.71
1	E	30	GLY	C-N-CA	-9.54	107.16	120.71
1	E	22	THR	CA-CB-OG1	-9.47	95.39	109.60
1	E	219	SER	CB-CA-C	-9.47	94.13	109.75
1	E	49	PHE	CA-C-O	-9.45	108.38	119.15
1	E	249	CYS	CA-C-N	9.44	133.31	120.38
1	E	249	CYS	C-N-CA	9.44	133.31	120.38
1	E	29	ALA	O-C-N	-9.42	110.79	122.57
1	E	236	TYR	CA-C-N	9.34	133.55	120.29
1	E	236	TYR	C-N-CA	9.34	133.55	120.29
1	E	202	PHE	CA-C-O	-9.32	110.63	120.70
1	E	122	ASN	OD1-CG-ND2	9.30	131.90	122.60
1	E	41	GLY	CA-C-O	-9.27	113.08	122.26
1	E	260	ASP	CA-CB-CG	9.16	121.76	112.60
1	E	76	THR	CA-CB-OG1	-9.10	95.95	109.60
1	E	175	PRO	CA-C-O	-9.05	105.74	119.86
1	E	13	ILE	CA-CB-CG2	9.04	125.86	110.50
1	E	102	GLY	CA-C-O	-9.02	112.78	121.62
1	E	108	ILE	CA-C-O	-8.99	111.07	121.05
1	E	80	ARG	CG-CD-NE	-8.98	92.24	112.00
1	E	70	GLY	CA-C-O	-8.95	111.53	120.75
1	E	69	HIS	CA-CB-CG	8.86	122.66	113.80
1	E	49	PHE	O-C-N	8.85	134.02	122.42
1	E	92	GLY	O-C-N	8.85	131.94	123.80
1	E	250	ARG	NH1-CZ-NH2	-8.83	107.82	119.30
1	E	56	VAL	CB-CA-C	8.77	118.87	110.63
1	E	122	ASN	CA-C-O	8.66	130.57	120.70
2	C	4	PHE	CA-C-O	-8.63	106.13	120.80
1	E	69	HIS	CA-C-N	8.62	129.54	119.98
1	E	69	HIS	C-N-CA	8.62	129.54	119.98
1	E	218	ARG	CA-C-O	-8.61	111.42	120.89
1	E	120	ASN	CB-CA-C	8.58	124.92	111.02
1	E	178	CYS	CA-C-N	8.57	133.82	122.42
1	E	178	CYS	C-N-CA	8.57	133.82	122.42
1	E	143	SER	CA-C-O	-8.55	111.85	120.82
1	E	89	GLN	CG-CD-NE2	8.52	129.17	116.40
1	E	196	GLY	CA-C-O	8.50	128.57	122.45
1	E	107	ILE	CA-C-N	8.40	131.31	120.56
1	E	107	ILE	C-N-CA	8.40	131.31	120.56
1	E	15	SER	CA-C-O	8.40	130.32	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	262	SER	CB-CA-C	8.40	125.95	109.66
1	E	276	ASN	CA-CB-CG	-8.35	104.25	112.60
1	E	175	PRO	O-C-N	-8.30	112.27	122.23
2	C	4	PHE	N-CA-C	8.28	134.17	111.00
1	E	198	VAL	CA-C-O	-8.25	109.20	119.43
1	E	184	ASP	O-C-N	-8.23	113.29	122.84
1	E	90	LEU	CA-C-O	-8.23	111.41	120.38
1	E	170	SER	C-N-CD	-8.23	91.27	125.00
1	E	219	SER	CA-C-N	-8.20	112.23	123.46
1	E	219	SER	C-N-CA	-8.20	112.23	123.46
1	E	5	ASN	CB-CG-ND2	8.19	128.69	116.40
1	E	106	THR	CB-CA-C	8.12	125.57	110.70
1	E	64	ARG	NE-CZ-NH2	8.10	126.49	119.20
1	E	278	GLN	CA-C-O	-8.10	111.58	120.33
1	E	43	GLU	CA-C-O	-8.08	112.63	122.41
1	E	95	VAL	O-C-N	8.07	130.40	122.25
1	E	141	VAL	N-CA-C	-8.06	103.01	110.82
1	E	29	ALA	N-CA-CB	-8.04	100.13	111.62
1	E	4	THR	N-CA-CB	-7.97	98.69	110.17
1	E	170	SER	N-CA-C	7.95	122.43	109.15
1	E	16	THR	N-CA-CB	-7.95	98.69	110.53
1	E	119	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	E	128	VAL	CA-CB-CG1	7.90	123.82	110.40
1	E	109	ALA	CA-C-N	7.89	128.68	120.00
1	E	109	ALA	C-N-CA	7.89	128.68	120.00
1	E	255	THR	CA-C-O	7.81	128.69	119.56
1	E	6	ALA	N-CA-CB	-7.77	99.45	109.55
1	E	56	VAL	N-CA-CB	-7.73	99.67	111.57
1	E	49	PHE	N-CA-C	-7.73	103.88	113.38
1	E	39	ASP	CB-CG-OD2	7.70	136.11	118.40
1	E	135	GLY	N-CA-C	-7.70	100.03	111.19
1	E	188	ARG	CA-C-O	-7.68	112.22	121.28
1	E	185	ARG	CG-CD-NE	-7.64	95.19	112.00
1	E	108	ILE	N-CA-C	-7.64	103.35	110.53
1	E	219	SER	CA-CB-OG	-7.63	95.83	111.10
1	E	204	PRO	CB-CA-C	-7.61	102.06	111.64
1	E	276	ASN	CA-C-O	-7.51	112.34	121.28
1	E	115	ALA	N-CA-C	-7.51	102.25	111.33
1	E	270	ASN	CA-C-O	-7.48	111.46	121.86
1	E	31	GLN	CB-CG-CD	-7.48	99.89	112.60
1	E	255	THR	N-CA-C	7.46	122.10	112.92
1	E	258	LYS	CA-C-O	7.45	128.61	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	278	GLN	CA-C-N	7.45	135.11	121.70
1	E	278	GLN	C-N-CA	7.45	135.11	121.70
1	E	227	THR	CA-C-O	-7.43	109.97	120.16
2	C	1	PRO	CA-C-O	-7.43	96.72	119.00
1	E	60	TYR	CA-C-N	7.40	131.56	120.31
1	E	60	TYR	C-N-CA	7.40	131.56	120.31
1	E	80	ARG	CB-CG-CD	-7.33	94.43	111.30
1	E	221	SER	O-C-N	7.32	132.25	123.24
1	E	122	ASN	CB-CA-C	7.31	123.80	111.22
1	E	180	VAL	N-CA-C	7.30	118.39	107.51
1	E	263	ASN	CB-CA-C	7.29	122.69	111.39
1	E	98	ASP	CA-CB-CG	-7.28	105.32	112.60
1	E	266	PHE	CA-CB-CG	7.24	121.04	113.80
1	E	131	LEU	CA-C-N	7.23	132.93	122.08
1	E	131	LEU	C-N-CA	7.23	132.93	122.08
1	E	75	GLY	O-C-N	7.23	129.21	122.19
1	E	120	ASN	CB-CG-ND2	7.22	127.22	116.40
1	E	227	THR	CA-CB-OG1	-7.21	98.78	109.60
1	E	67	ASN	CA-C-N	7.16	132.75	123.08
1	E	67	ASN	C-N-CA	7.16	132.75	123.08
1	E	85	VAL	CA-CB-CG2	7.16	122.58	110.40
1	E	142	ASN	OD1-CG-ND2	7.15	129.75	122.60
1	E	147	ARG	CD-NE-CZ	-7.15	114.39	124.40
1	E	142	ASN	CA-C-O	7.14	128.54	120.90
1	E	4	THR	CB-CA-C	7.13	122.66	109.54
1	E	80	ARG	N-CA-C	7.11	119.11	111.36
1	E	45	SER	CA-CB-OG	-7.11	96.89	111.10
1	E	53	ALA	O-C-N	7.10	132.41	123.19
1	E	189	ARG	CA-C-N	7.07	130.79	120.82
1	E	189	ARG	C-N-CA	7.07	130.79	120.82
1	E	162	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	E	204	PRO	CA-C-O	7.01	128.74	121.23
1	E	269	VAL	O-C-N	-7.00	115.41	122.62
1	E	122	ASN	O-C-N	-7.00	113.92	123.01
1	E	116	SER	CA-C-N	6.99	130.35	120.28
1	E	116	SER	C-N-CA	6.99	130.35	120.28
1	E	120	ASN	CA-C-O	6.99	128.40	119.95
1	E	269	VAL	CA-C-O	6.97	128.55	121.58
1	E	162	ASN	N-CA-CB	-6.97	100.18	110.49
1	E	14	SER	O-C-N	-6.95	113.71	122.26
2	C	1	PRO	N-CA-CB	-6.95	95.36	103.00
1	E	257	ASN	N-CA-C	-6.95	98.72	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	220	ILE	CB-CA-C	6.94	121.05	110.91
1	E	162	ASN	O-C-N	-6.89	113.72	122.34
1	E	221	SER	N-CA-C	6.88	120.36	109.50
1	E	245	ALA	CA-C-O	6.87	128.25	120.90
1	E	195	TYR	CB-CG-CD2	-6.87	110.50	120.80
1	E	178	CYS	CA-C-O	-6.86	113.12	120.46
1	E	185	ARG	NE-CZ-NH1	-6.85	114.65	121.50
1	E	82	TYR	N-CA-CB	-6.82	100.60	110.56
1	E	257	ASN	CB-CG-ND2	-6.81	106.18	116.40
1	E	279	ALA	CA-C-O	-6.81	109.22	120.80
1	E	207	SER	CA-C-N	6.80	130.87	122.37
1	E	207	SER	C-N-CA	6.80	130.87	122.37
1	E	31	GLN	N-CA-CB	6.80	120.10	109.83
1	E	234	ALA	CA-C-O	-6.80	113.86	121.00
1	E	87	LYS	O-C-N	6.78	130.75	122.20
1	E	122	ASN	CB-CG-ND2	-6.77	106.24	116.40
1	E	65	ASP	CA-C-N	-6.75	110.67	122.83
1	E	65	ASP	C-N-CA	-6.75	110.67	122.83
1	E	239	THR	N-CA-CB	6.75	121.59	110.39
1	E	3	GLN	CA-C-O	6.73	127.47	120.40
1	E	230	VAL	CA-CB-CG1	6.72	121.83	110.40
1	E	7	PRO	CA-C-N	6.71	130.89	120.82
1	E	7	PRO	C-N-CA	6.71	130.89	120.82
1	E	268	THR	CA-CB-CG2	6.70	121.89	110.50
1	E	102	GLY	O-C-N	6.69	131.43	123.67
1	E	265	PRO	CA-C-O	-6.69	113.51	121.67
1	E	108	ILE	CB-CA-C	-6.69	103.26	112.02
1	E	107	ILE	N-CA-C	-6.68	104.25	110.53
1	E	188	ARG	CD-NE-CZ	6.67	133.73	124.40
1	E	58	THR	N-CA-CB	6.65	123.48	111.37
1	E	16	THR	N-CA-C	-6.64	105.21	113.38
1	E	59	TYR	CA-C-O	-6.61	111.83	119.56
2	C	3	PRO	CA-C-O	-6.60	113.20	120.92
1	E	88	THR	CA-C-N	6.60	131.21	122.30
1	E	88	THR	C-N-CA	6.60	131.21	122.30
1	E	207	SER	CA-CB-OG	-6.59	97.93	111.10
1	E	110	GLY	CA-C-N	6.57	128.99	120.44
1	E	110	GLY	C-N-CA	6.57	128.99	120.44
1	E	207	SER	CA-C-O	6.57	129.91	120.51
1	E	194	ASN	CA-C-O	-6.57	114.25	121.87
1	E	239	THR	CA-CB-CG2	6.57	121.66	110.50
1	E	76	THR	CA-C-N	6.54	128.94	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	76	THR	C-N-CA	6.54	128.94	120.56
1	E	99	ASN	CA-C-N	6.52	133.32	121.85
1	E	99	ASN	C-N-CA	6.52	133.32	121.85
1	E	72	HIS	CA-CB-CG	-6.49	107.31	113.80
1	E	54	GLN	OE1-CD-NE2	-6.49	116.11	122.60
1	E	43	GLU	O-C-N	6.43	130.86	122.38
1	E	52	ARG	NE-CZ-NH2	-6.41	113.43	119.20
1	E	274	TYR	CB-CA-C	6.41	120.70	109.80
1	E	237	LEU	CA-C-O	-6.41	113.62	120.42
1	E	136	GLY	N-CA-C	-6.37	105.32	112.33
1	E	23	TYR	O-C-N	-6.34	116.11	123.27
1	E	148	LEU	CA-C-N	6.34	128.68	120.44
1	E	148	LEU	C-N-CA	6.34	128.68	120.44
1	E	175	PRO	N-CA-C	-6.33	104.73	113.53
1	E	249	CYS	O-C-N	-6.33	115.55	122.07
1	E	264	ILE	CA-C-O	6.33	123.82	119.20
1	E	5	ASN	CA-C-O	-6.32	114.63	122.03
1	E	119	ASN	N-CA-C	-6.32	105.42	113.01
1	E	229	HIS	N-CA-C	-6.32	104.47	111.36
1	E	86	LYS	N-CA-C	6.30	120.44	112.87
1	E	77	VAL	CA-CB-CG2	6.30	121.11	110.40
1	E	270	ASN	CA-CB-CG	-6.29	106.31	112.60
1	E	153	VAL	CA-C-O	-6.28	113.33	120.67
1	E	220	ILE	O-C-N	-6.25	116.12	122.75
1	E	198	VAL	N-CA-C	-6.24	104.59	113.07
1	E	5	ASN	CA-CB-CG	6.23	118.83	112.60
1	E	91	PHE	CA-C-N	-6.22	116.95	122.73
1	E	91	PHE	C-N-CA	-6.22	116.95	122.73
1	E	40	THR	O-C-N	6.21	130.94	122.37
1	E	237	LEU	CA-C-N	6.21	129.10	120.29
1	E	237	LEU	C-N-CA	6.21	129.10	120.29
1	E	33	SER	O-C-N	6.18	130.02	123.03
1	E	5	ASN	CB-CA-C	-6.18	102.68	111.95
1	E	66	GLY	N-CA-C	-6.15	105.43	115.46
1	E	120	ASN	CA-C-N	6.15	132.47	122.81
1	E	120	ASN	C-N-CA	6.15	132.47	122.81
1	E	213	ILE	CA-C-N	-6.14	111.04	121.85
1	E	213	ILE	C-N-CA	-6.14	111.04	121.85
1	E	162	ASN	CB-CA-C	6.12	120.32	110.09
1	E	64	ARG	N-CA-CB	-6.12	101.05	110.04
1	E	39	ASP	N-CA-CB	-6.11	100.17	110.49
1	E	10	LEU	N-CA-C	-6.08	104.73	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	ASN	N-CA-CB	-6.08	101.17	111.20
1	E	170	SER	CA-C-O	-6.08	111.88	119.54
1	E	77	VAL	N-CA-CB	6.08	118.35	110.57
1	E	222	GLY	CA-C-O	-6.07	115.77	121.96
1	E	208	ILE	CA-C-N	6.06	130.51	121.72
1	E	208	ILE	C-N-CA	6.06	130.51	121.72
1	E	106	THR	CA-C-N	6.05	128.30	120.56
1	E	106	THR	C-N-CA	6.05	128.30	120.56
1	E	215	GLY	O-C-N	-6.04	115.89	122.41
1	E	142	ASN	CA-CB-CG	-6.03	106.57	112.60
1	E	189	ARG	N-CA-C	-6.03	101.48	110.23
1	E	108	ILE	N-CA-CB	6.03	118.28	110.57
1	E	113	PHE	CA-C-N	6.02	128.36	120.60
1	E	113	PHE	C-N-CA	6.02	128.36	120.60
1	E	266	PHE	N-CA-CB	6.01	118.88	109.69
1	E	174	GLU	CB-CG-CD	6.00	122.81	112.60
2	C	3	PRO	N-CA-C	6.00	119.92	110.50
1	E	106	THR	O-C-N	-6.00	114.43	122.23
1	E	250	ARG	CD-NE-CZ	-5.98	116.02	124.40
1	E	270	ASN	CB-CG-ND2	5.98	125.37	116.40
1	E	57	LYS	N-CA-CB	-5.97	100.85	110.77
1	E	7	PRO	CB-CA-C	-5.97	103.76	111.46
1	E	250	ARG	CG-CD-NE	5.96	125.12	112.00
1	E	272	LEU	O-C-N	5.96	130.31	123.27
1	E	113	PHE	N-CA-CB	5.95	118.87	109.82
1	E	232	GLY	N-CA-C	-5.94	105.61	112.50
1	E	73	CYS	N-CA-C	-5.94	104.73	111.14
1	E	215	GLY	N-CA-C	-5.88	104.72	114.48
1	E	115	ALA	N-CA-CB	5.87	118.87	110.06
1	E	226	ALA	CA-C-O	-5.87	113.72	120.24
1	E	8	TRP	CA-C-N	5.87	127.67	120.22
1	E	8	TRP	C-N-CA	5.87	127.67	120.22
1	E	147	ARG	O-C-N	-5.85	115.77	122.09
1	E	26	ASP	CA-C-O	5.85	127.72	121.05
1	E	135	GLY	CA-C-N	5.85	126.81	120.44
1	E	135	GLY	C-N-CA	5.85	126.81	120.44
1	E	82	TYR	N-CA-C	5.83	120.09	112.92
1	E	25	TYR	CA-C-O	-5.82	115.04	121.33
1	E	179	THR	O-C-N	5.82	129.91	122.93
1	E	242	LYS	CA-CB-CG	5.82	125.73	114.10
1	E	194	ASN	N-CA-C	-5.80	102.87	110.53
1	E	263	ASN	CA-C-O	5.80	127.53	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	131	LEU	CD1-CG-CD2	-5.80	98.05	110.80
1	E	31	GLN	CA-C-O	5.79	127.55	121.19
1	E	268	THR	O-C-N	5.78	129.95	123.19
1	E	112	ASP	N-CA-C	-5.77	104.99	111.28
1	E	201	ILE	N-CA-CB	-5.75	101.74	111.23
1	E	123	CYS	N-CA-CB	-5.74	102.77	111.21
1	E	211	THR	O-C-N	-5.73	116.49	122.96
2	C	1	PRO	CA-C-N	5.71	135.72	121.80
2	C	1	PRO	C-N-CA	5.71	135.72	121.80
1	E	96	LEU	CA-C-O	5.70	127.60	121.16
1	E	58	THR	O-C-N	5.69	130.24	123.24
1	E	94	LYS	CA-C-O	5.69	126.84	120.92
1	E	64	ARG	CA-C-N	5.68	131.43	122.34
1	E	64	ARG	C-N-CA	5.68	131.43	122.34
1	E	238	MET	CA-C-O	-5.68	114.40	120.42
1	E	13	ILE	CA-CB-CG1	-5.67	100.76	110.40
1	E	30	GLY	CA-C-O	-5.67	112.73	119.02
1	E	20	THR	CA-C-O	-5.65	115.28	121.89
1	E	116	SER	O-C-N	-5.64	115.34	122.17
1	E	174	GLU	N-CA-C	-5.63	97.36	109.81
1	E	111	MET	CA-C-N	5.63	127.83	120.28
1	E	111	MET	C-N-CA	5.63	127.83	120.28
1	E	268	THR	CA-CB-OG1	-5.63	101.16	109.60
1	E	79	SER	N-CA-C	-5.62	103.27	110.53
1	E	60	TYR	CA-CB-CG	-5.62	103.79	113.90
1	E	38	ILE	O-C-N	5.61	130.39	122.59
1	E	20	THR	CA-CB-OG1	-5.61	101.19	109.60
1	E	136	GLY	CA-C-N	5.60	129.05	121.05
1	E	136	GLY	C-N-CA	5.60	129.05	121.05
1	E	155	VAL	CA-C-O	-5.58	114.12	120.65
1	E	176	SER	N-CA-C	5.58	119.57	112.87
1	E	180	VAL	CA-CB-CG1	-5.57	100.93	110.40
1	E	64	ARG	N-CA-C	5.56	117.91	110.35
1	E	266	PHE	O-C-N	-5.55	116.06	122.95
1	E	112	ASP	CB-CG-OD1	5.55	131.16	118.40
1	E	83	GLY	CA-C-N	5.54	128.29	120.42
1	E	83	GLY	C-N-CA	5.54	128.29	120.42
1	E	58	THR	CA-C-O	-5.54	114.62	121.11
1	E	54	GLN	CG-CD-NE2	5.54	124.71	116.40
1	E	56	VAL	CG1-CB-CG2	5.54	122.99	110.80
2	C	3	PRO	N-CA-CB	5.53	107.72	103.30
1	E	186	TYR	CA-CB-CG	-5.53	103.95	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	127	VAL	O-C-N	5.52	129.16	123.20
1	E	36	TYR	N-CA-CB	5.51	119.43	110.17
1	E	6	ALA	CA-C-O	-5.51	113.34	121.27
1	E	161	ASN	N-CA-CB	-5.50	102.14	111.17
1	E	190	SER	N-CA-C	-5.49	101.92	110.10
1	E	193	SER	O-C-N	5.48	129.58	122.89
1	E	257	ASN	O-C-N	-5.48	116.63	123.04
1	E	187	ASP	CA-C-N	-5.47	113.34	122.64
1	E	187	ASP	C-N-CA	-5.47	113.34	122.64
1	E	114	VAL	CA-CB-CG2	5.47	119.70	110.40
1	E	4	THR	CA-C-N	5.46	130.17	122.46
1	E	4	THR	C-N-CA	5.46	130.17	122.46
1	E	12	ARG	CA-C-N	5.46	129.09	120.47
1	E	12	ARG	C-N-CA	5.46	129.09	120.47
1	E	231	ALA	N-CA-C	-5.46	105.33	111.28
1	E	232	GLY	CA-C-O	-5.45	115.11	121.00
1	E	77	VAL	N-CA-C	-5.44	105.42	110.53
1	E	39	ASP	OD1-CG-OD2	-5.43	109.86	122.90
1	E	133	LEU	CA-CB-CG	5.42	135.29	116.30
1	E	227	THR	O-C-N	5.42	127.55	121.32
1	E	157	VAL	O-C-N	5.41	129.06	123.05
1	E	180	VAL	N-CA-CB	-5.41	104.64	111.41
1	E	63	SER	N-CA-CB	5.41	118.59	110.53
1	E	148	LEU	N-CA-C	-5.41	105.28	111.07
1	E	250	ARG	CB-CG-CD	5.40	123.72	111.30
1	E	239	THR	N-CA-C	-5.39	105.97	112.54
1	E	53	ALA	CA-C-N	-5.38	111.31	121.63
1	E	53	ALA	C-N-CA	-5.38	111.31	121.63
1	E	104	TYR	CA-CB-CG	-5.37	104.23	113.90
1	E	151	SER	N-CA-C	-5.36	106.58	113.01
1	E	224	SER	CA-C-N	5.34	129.72	120.58
1	E	224	SER	C-N-CA	5.34	129.72	120.58
1	E	121	ARG	CD-NE-CZ	5.33	131.87	124.40
1	E	25	TYR	O-C-N	5.33	129.33	123.25
1	E	9	GLY	CA-C-O	-5.32	114.45	120.30
1	E	153	VAL	CA-CB-CG2	5.32	119.44	110.40
1	E	219	SER	N-CA-CB	5.32	119.09	110.43
1	E	54	GLN	CB-CG-CD	-5.31	103.58	112.60
1	E	254	ASP	N-CA-C	-5.31	105.66	111.82
1	E	1	ALA	CA-C-N	-5.30	112.61	121.94
1	E	1	ALA	C-N-CA	-5.30	112.61	121.94
1	E	174	GLU	CA-C-O	5.30	127.42	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	215	GLY	CA-C-O	-5.30	113.26	119.72
1	E	218	ARG	N-CA-CB	-5.29	102.13	111.39
2	C	1	PRO	N-CA-C	5.29	125.33	112.10
2	C	3	PRO	N-CD-CG	5.29	111.14	103.20
1	E	23	TYR	N-CA-C	-5.29	100.62	109.24
1	E	252	ILE	O-C-N	-5.27	116.40	121.83
1	E	263	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	E	106	THR	N-CA-CB	5.26	118.04	110.20
1	E	41	GLY	CA-C-N	5.21	130.22	122.71
1	E	41	GLY	C-N-CA	5.21	130.22	122.71
1	E	117	ASP	O-C-N	5.21	128.31	122.22
1	E	17	SER	CA-C-O	-5.20	114.92	120.28
1	E	23	TYR	CA-C-O	-5.19	114.77	120.43
1	E	59	TYR	CA-C-N	5.19	133.83	123.20
1	E	59	TYR	C-N-CA	5.19	133.83	123.20
1	E	132	SER	CA-C-O	-5.18	114.66	122.38
1	E	263	ASN	N-CA-CB	-5.18	104.60	112.47
1	E	69	HIS	O-C-N	-5.17	116.71	122.09
1	E	4	THR	CA-CB-CG2	5.17	119.29	110.50
1	E	37	VAL	CG1-CB-CG2	-5.17	99.42	110.80
1	E	263	ASN	O-C-N	-5.17	113.57	122.20
1	E	161	ASN	N-CA-C	5.15	119.06	112.26
1	E	269	VAL	CA-CB-CG2	5.14	119.14	110.40
1	E	80	ARG	NH1-CZ-NH2	5.13	125.97	119.30
1	E	5	ASN	N-CA-CB	5.12	118.95	111.62
1	E	171	PRO	CA-C-O	5.10	129.89	120.60
1	E	132	SER	CA-CB-OG	-5.10	100.90	111.10
1	E	182	ALA	CA-C-O	-5.09	115.36	121.11
1	E	59	TYR	N-CA-C	-5.05	106.70	112.92
1	E	76	THR	OG1-CB-CG2	5.04	119.39	109.30
1	E	244	THR	O-C-N	5.04	130.14	122.94
1	E	203	GLY	N-CA-C	-5.04	102.07	112.34
1	E	218	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	E	188	ARG	O-C-N	5.03	128.88	123.10
1	E	197	SER	CA-C-O	-5.02	113.20	119.38
1	E	225	MET	N-CA-CB	5.02	117.69	110.20
1	E	43	GLU	CG-CD-OE1	5.02	129.94	118.40
1	E	5	ASN	CB-CG-OD1	-5.01	110.78	120.80
1	E	71	THR	CA-CB-OG1	-5.01	102.09	109.60
1	E	224	SER	CA-CB-OG	5.00	121.10	111.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	169	TYR	CA
2	C	2	ALA	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1	PRO	Mainchain
2	C	2	ALA	Mainchain
3	D	5	DAL	Mainchain
1	E	168	ASN	Mainchain
1	E	170	SER	Peptide,Mainchain
1	E	185	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2018	0	1918	128	2
2	C	30	0	29	10	0
3	D	10	0	8	32	0
4	C	1	0	0	0	0
4	D	4	0	0	4	0
4	E	183	0	0	11	4
All	All	2246	0	1955	139	4

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 35.

All (139) 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:220:ILE:HB	3:D:6:ALA:CB	1.51	1.39
3:D:6:ALA:CA	3:D:6:ALA:C	1.95	1.37
1:E:220:ILE:CD1	3:D:6:ALA:HB3	1.60	1.30
3:D:6:ALA:CA	3:D:6:ALA:N	2.00	1.25
3:D:5:DAL:O	3:D:5:DAL:C	1.88	1.22
1:E:230:VAL:HB	4:E:359:HOH:O	1.07	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ILE:CB	3:D:6:ALA:CB	2.23	1.17
1:E:77:VAL:O	1:E:85:VAL:HG12	1.46	1.16
1:E:220:ILE:CB	3:D:6:ALA:HB3	1.75	1.15
1:E:100:GLY:O	2:C:3:PRO:HD3	1.50	1.12
1:E:220:ILE:HD12	3:D:6:ALA:HB3	1.26	1.12
1:E:64:ARG:NH1	1:E:64:ARG:HG2	1.63	1.11
1:E:207:SER:HB3	4:E:405:HOH:O	0.92	1.08
1:E:224:SER:OG	2:C:4:PHE:C	1.96	1.08
1:E:220:ILE:HB	3:D:6:ALA:HB2	1.33	1.07
1:E:230:VAL:CB	4:E:359:HOH:O	1.70	1.07
1:E:85:VAL:O	1:E:85:VAL:HG13	1.34	1.05
1:E:207:SER:HB2	4:E:376:HOH:O	1.56	1.01
1:E:85:VAL:O	1:E:85:VAL:CG1	2.06	1.01
1:E:220:ILE:CG1	3:D:6:ALA:HB3	1.91	1.00
1:E:180:VAL:HG21	1:E:230:VAL:HG21	1.42	1.00
1:E:161:ASN:ND2	3:D:5:DAL:HA	1.79	0.98
1:E:126:GLY:HA3	1:E:238:MET:HE2	1.47	0.97
1:E:263:ASN:HB2	4:E:379:HOH:O	1.64	0.94
1:E:220:ILE:HD12	3:D:6:ALA:CB	1.99	0.93
1:E:227:THR:O	1:E:230:VAL:HG22	1.69	0.93
1:E:54:GLN:NE2	1:E:91:PHE:HE1	1.67	0.92
1:E:224:SER:HB2	3:D:5:DAL:H	1.34	0.92
1:E:220:ILE:CD1	3:D:6:ALA:CB	2.48	0.91
1:E:100:GLY:O	2:C:3:PRO:CD	2.20	0.88
1:E:54:GLN:NE2	1:E:91:PHE:CE1	2.44	0.86
1:E:64:ARG:HG2	1:E:64:ARG:HH11	1.22	0.86
3:D:6:ALA:C	3:D:6:ALA:N	2.34	0.85
1:E:64:ARG:NH1	1:E:64:ARG:CG	2.20	0.84
1:E:261:LEU:H	1:E:270:ASN:HD21	1.25	0.84
1:E:224:SER:CB	3:D:5:DAL:H	1.91	0.83
1:E:161:ASN:HD21	3:D:5:DAL:HA	1.43	0.82
1:E:64:ARG:HH11	1:E:64:ARG:CG	1.71	0.82
1:E:58:THR:HG21	1:E:62:SER:O	1.80	0.81
1:E:30:GLY:HA3	1:E:85:VAL:HG22	1.61	0.81
3:D:6:ALA:C	3:D:6:ALA:O	2.27	0.78
1:E:180:VAL:CG2	1:E:230:VAL:HG21	2.16	0.76
3:D:6:ALA:HA	4:D:483:HOH:O	1.85	0.76
1:E:125:LYS:HG3	1:E:239:THR:HB	1.69	0.75
1:E:207:SER:CB	4:E:376:HOH:O	2.23	0.74
1:E:54:GLN:HE21	1:E:91:PHE:HE1	1.37	0.72
1:E:230:VAL:CG2	4:E:359:HOH:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:HIS:HD2	1:E:48:GLU:H	1.38	0.71
1:E:220:ILE:CG2	3:D:6:ALA:HB1	2.21	0.70
1:E:220:ILE:CG2	3:D:6:ALA:CB	2.69	0.70
1:E:30:GLY:C	1:E:239:THR:HG21	2.19	0.69
1:E:77:VAL:O	1:E:85:VAL:CG1	2.36	0.68
3:D:6:ALA:HB1	4:D:483:HOH:O	1.91	0.68
1:E:225:MET:O	1:E:229:HIS:HD2	1.77	0.68
1:E:164:ALA:H	1:E:194:ASN:ND2	1.90	0.68
1:E:227:THR:O	1:E:230:VAL:CG2	2.41	0.68
1:E:28:SER:O	1:E:31:GLN:HG2	1.95	0.65
1:E:48:GLU:HB3	1:E:79:SER:HB2	1.80	0.63
1:E:58:THR:CG2	1:E:94:LYS:HD3	2.29	0.63
1:E:110:GLY:O	1:E:114:VAL:HG23	1.99	0.62
1:E:126:GLY:HA3	1:E:238:MET:CE	2.27	0.61
1:E:107:ILE:CD1	1:E:111:MET:HE2	2.30	0.61
1:E:224:SER:HB2	3:D:5:DAL:N	2.13	0.60
1:E:33:SER:HB3	1:E:239:THR:HG22	1.84	0.60
1:E:38:ILE:HD11	1:E:114:VAL:HG21	1.83	0.60
1:E:46:HIS:CD2	1:E:48:GLU:H	2.20	0.59
1:E:107:ILE:HD11	1:E:111:MET:HE2	1.84	0.59
1:E:220:ILE:HB	3:D:6:ALA:HB1	1.74	0.59
1:E:115:ALA:O	1:E:118:LYS:HE3	2.03	0.58
1:E:134:GLY:HA3	2:C:4:PHE:CE2	2.38	0.57
1:E:207:SER:CB	4:E:405:HOH:O	1.77	0.57
1:E:207:SER:OG	1:E:207:SER:O	2.22	0.57
1:E:224:SER:CB	2:C:4:PHE:C	2.77	0.57
1:E:30:GLY:O	1:E:239:THR:HG21	2.06	0.56
1:E:96:LEU:HD13	2:C:3:PRO:HG3	1.89	0.55
1:E:220:ILE:HD12	3:D:6:ALA:CA	2.36	0.55
1:E:27:GLU:H	1:E:27:GLU:CD	2.14	0.55
1:E:30:GLY:HA2	1:E:239:THR:HG23	1.89	0.54
1:E:72:HIS:CD2	1:E:210:SER:HB3	2.42	0.54
3:D:6:ALA:CB	4:D:483:HOH:O	2.44	0.54
3:D:6:ALA:CA	4:D:483:HOH:O	2.49	0.54
1:E:139:SER:O	1:E:143:SER:HB2	2.08	0.54
1:E:85:VAL:HG13	1:E:88:THR:CG2	2.37	0.54
1:E:51:GLY:HA2	4:E:472:HOH:O	2.09	0.53
1:E:85:VAL:HG13	1:E:88:THR:HG22	1.89	0.53
1:E:30:GLY:HA3	1:E:85:VAL:CG2	2.36	0.53
1:E:261:LEU:HD21	1:E:272:LEU:HD22	1.91	0.53
1:E:275:ASN:O	1:E:276:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:PHE:N	3:D:5:DAL:CB	2.73	0.52
1:E:30:GLY:HA2	1:E:239:THR:CG2	2.40	0.52
1:E:58:THR:HG23	1:E:94:LYS:HD3	1.90	0.52
1:E:72:HIS:CE1	1:E:210:SER:HB3	2.45	0.51
1:E:55:MET:HE2	1:E:63:SER:O	2.11	0.51
1:E:65:ASP:OD2	1:E:71:THR:OG1	2.26	0.51
1:E:220:ILE:HG21	3:D:6:ALA:HB1	1.94	0.50
1:E:85:VAL:CG1	1:E:88:THR:CG2	2.89	0.50
1:E:46:HIS:HE1	1:E:216:SER:O	1.95	0.49
1:E:3:GLN:HE22	1:E:86:LYS:NZ	2.10	0.49
1:E:133:LEU:HA	2:C:3:PRO:HA	1.95	0.49
1:E:171:PRO:O	1:E:172:ALA:C	2.56	0.49
1:E:186:TYR:O	1:E:187:ASP:HB2	2.12	0.49
1:E:118:LYS:HD3	1:E:153:VAL:CG2	2.43	0.49
1:E:222:GLY:HA3	3:D:5:DAL:H2	1.77	0.48
2:C:4:PHE:C	3:D:5:DAL:N	2.71	0.48
1:E:58:THR:HG22	1:E:60:TYR:H	1.79	0.48
1:E:164:ALA:H	1:E:194:ASN:HD22	1.61	0.47
1:E:80:ARG:O	1:E:86:LYS:HD3	2.14	0.47
1:E:85:VAL:HG11	1:E:88:THR:HG21	1.96	0.47
1:E:14:SER:HA	1:E:275:ASN:OD1	2.15	0.46
1:E:1:ALA:N	1:E:27:GLU:OE2	2.41	0.46
1:E:145:ALA:HB1	1:E:177:VAL:HG11	1.97	0.45
1:E:72:HIS:NE2	1:E:210:SER:HB3	2.31	0.45
1:E:154:MET:HG3	1:E:248:ALA:HB3	1.99	0.45
1:E:225:MET:O	1:E:229:HIS:CD2	2.65	0.45
1:E:69:HIS:CE1	2:C:3:PRO:HB3	2.52	0.45
1:E:107:ILE:C	1:E:107:ILE:HD12	2.41	0.44
1:E:64:ARG:CZ	1:E:64:ARG:CB	2.82	0.44
1:E:125:LYS:HB3	1:E:239:THR:HA	1.99	0.44
1:E:24:TYR:HB3	1:E:277:TYR:CD1	2.53	0.44
1:E:235:ALA:O	1:E:239:THR:HG23	2.18	0.43
1:E:250:ARG:HA	4:E:467:HOH:O	2.18	0.43
1:E:54:GLN:NE2	1:E:91:PHE:CD1	2.87	0.43
1:E:32:GLY:HA3	1:E:125:LYS:HG2	2.00	0.43
1:E:184:ASP:OD1	1:E:184:ASP:C	2.61	0.43
1:E:12:ARG:NH1	1:E:15:SER:O	2.51	0.43
1:E:224:SER:O	1:E:228:PRO:CD	2.67	0.43
1:E:185:ARG:HB3	1:E:185:ARG:NH1	2.34	0.42
1:E:173:SER:HA	1:E:198:VAL:HG21	2.01	0.42
1:E:51:GLY:CA	4:E:472:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:VAL:HG11	1:E:77:VAL:HG11	2.01	0.42
1:E:275:ASN:O	1:E:276:ASN:CB	2.68	0.41
1:E:270:ASN:HD22	1:E:270:ASN:C	2.29	0.41
1:E:33:SER:CB	1:E:239:THR:HG22	2.51	0.41
1:E:222:GLY:HA3	3:D:5:DAL:N	2.35	0.41
1:E:107:ILE:HD11	1:E:111:MET:CE	2.48	0.41
1:E:192:PHE:CE1	1:E:222:GLY:HA2	2.56	0.40
1:E:85:VAL:CG1	1:E:88:THR:HG21	2.51	0.40
1:E:104:TYR:HD1	1:E:104:TYR:HA	1.65	0.40
1:E:264:ILE:HA	1:E:265:PRO:HD3	1.79	0.40

All (4) 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:457:HOH:O	4:E:457:HOH:O[7_465]	0.95	1.25
1:E:150:SER:CB	4:E:423:HOH:O[7_465]	1.41	0.79
1:E:150:SER:OG	4:E:423:HOH:O[7_465]	1.54	0.66
4:E:342:HOH:O	4:E:422:HOH:O[5_444]	2.07	0.13

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	277/279 (99%)	256 (92%)	18 (6%)	3 (1%)	11	10
2	C	2/4 (50%)	1 (50%)	0	1 (50%)	0	0
All	All	279/283 (99%)	257 (92%)	18 (6%)	4 (1%)	9	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	169	TYR
1	E	171	PRO
2	C	2	ALA
1	E	39	ASP

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	199/214 (93%)	181 (91%)	18 (9%)	9	9
2	C	3/3 (100%)	3 (100%)	0	100	100
All	All	202/217 (93%)	184 (91%)	18 (9%)	9	10

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	THR
1	E	13	ILE
1	E	16	THR
1	E	27	GLU
1	E	54	GLN
1	E	56	VAL
1	E	58	THR
1	E	106	THR
1	E	107	ILE
1	E	133	LEU
1	E	162	ASN
1	E	184	ASP
1	E	185	ARG
1	E	204	PRO
1	E	239	THR
1	E	240	LEU
1	E	250	ARG
1	E	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	GLN
1	E	89	GLN
1	E	119	ASN
1	E	162	ASN
1	E	194	ASN
1	E	229	HIS
1	E	257	ASN
1	E	263	ASN
1	E	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.