



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 12:35 PM EST

PDB ID : 1PEK  
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 : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

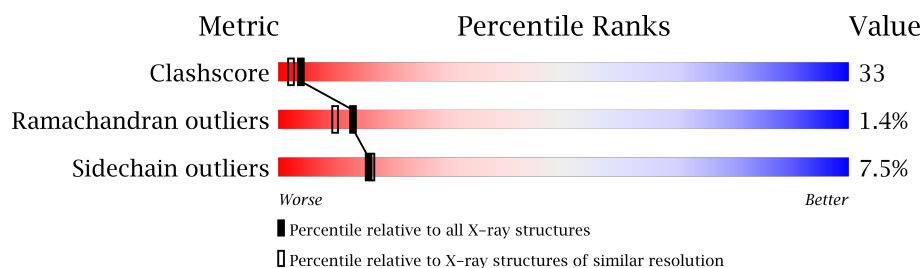
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

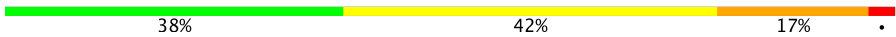


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

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	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.

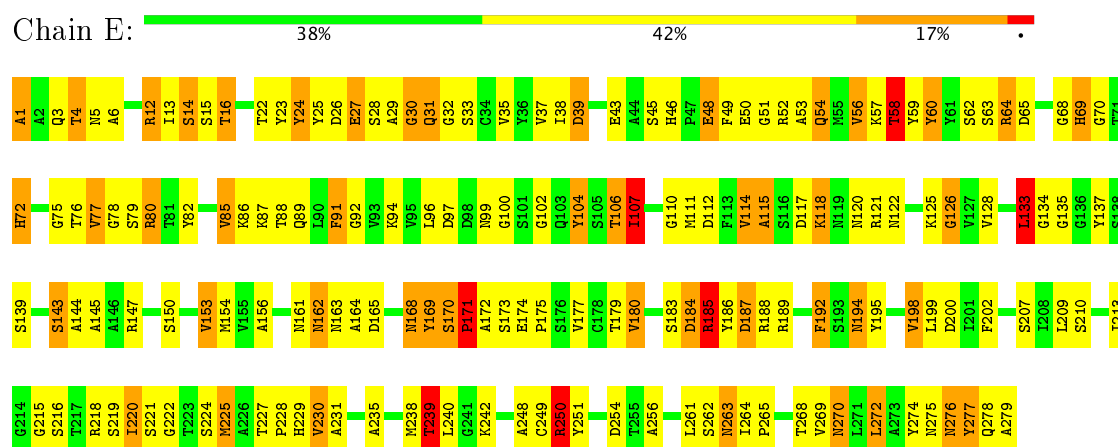
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	183	Total	O	0	0
			183	183		
4	C	1	Total	O	0	0
			1	1		
4	D	4	Total	O	0	0
			4	4		

### 3 Residue-property plots [i](#)

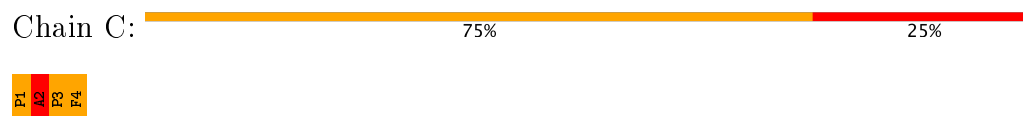
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

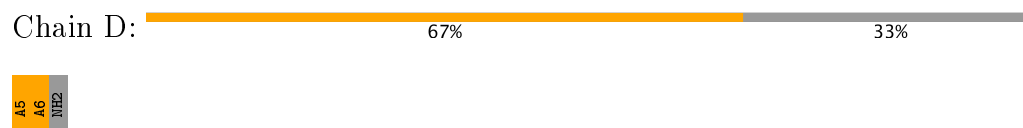
#### • Molecule 1: PROTEINASE K



#### • Molecule 2: PEPTIDE PRO-ALA-PRO-PHE



#### • Molecule 3: D-DAL-ALA-NH2



## 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, $\alpha$ , $\beta$ , $\gamma$	68.28 Å 68.28 Å 107.87 Å 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 <sup>2</sup> )	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	1.53	11/2057 (0.5%)	3.20	228/2797 (8.2%)
2	C	1.72	0/32	6.50	19/43 (44.2%)
3	D	31.88	4/4 (100.0%)	19.31	4/4 (100.0%)
All	All	2.07	15/2093 (0.7%)	3.35	251/2844 (8.8%)

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
1	E	1	4
2	C	1	2
3	D	0	1
All	All	2	7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	6	ALA	C-O	54.54	2.27	1.23
3	D	6	ALA	N-CA	26.88	2.00	1.46
3	D	6	ALA	CA-C	16.43	1.95	1.52
1	E	168	ASN	C-O	10.27	1.42	1.23
3	D	6	ALA	CA-CB	9.83	1.73	1.52
1	E	185	ARG	NE-CZ	9.41	1.45	1.33
1	E	185	ARG	CZ-NH2	8.96	1.44	1.33
1	E	185	ARG	CZ-NH1	8.63	1.44	1.33
1	E	43	GLU	CD-OE1	-5.87	1.19	1.25
1	E	43	GLU	CD-OE2	-5.66	1.19	1.25
1	E	174	GLU	CD-OE2	-5.58	1.19	1.25
1	E	78	GLY	N-CA	-5.53	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	91	PHE	CB-CG	-5.31	1.42	1.51
1	E	137	TYR	CG-CD1	-5.25	1.32	1.39
1	E	48	GLU	CD-OE1	-5.12	1.20	1.25

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	80	ARG	CD-NE-CZ	37.31	175.84	123.60
1	E	185	ARG	NE-CZ-NH2	-23.10	108.75	120.30
1	E	168	ASN	O-C-N	-23.04	85.83	122.70
3	D	6	ALA	CB-CA-C	22.91	144.46	110.10
2	C	3	PRO	C-N-CA	20.05	171.84	121.70
3	D	6	ALA	N-CA-CB	19.89	137.94	110.10
1	E	185	ARG	CD-NE-CZ	19.87	151.42	123.60
1	E	39	ASP	CB-CG-OD2	19.79	136.11	118.30
1	E	64	ARG	NE-CZ-NH1	-19.75	110.42	120.30
3	D	6	ALA	CA-C-O	-19.26	79.66	120.10
1	E	169	TYR	N-CA-CB	19.24	145.22	110.60
1	E	250	ARG	NE-CZ-NH2	18.75	129.68	120.30
1	E	195	TYR	CB-CG-CD2	-17.50	110.50	121.00
1	E	168	ASN	CA-C-N	16.67	153.87	117.20
1	E	112	ASP	CB-CG-OD1	14.29	131.16	118.30
3	D	6	ALA	N-CA-C	-14.16	72.77	111.00
1	E	52	ARG	NE-CZ-NH2	-13.75	113.43	120.30
1	E	170	SER	C-N-CD	-13.33	91.27	120.60
2	C	2	ALA	CA-C-N	13.05	153.64	117.10
1	E	64	ARG	NE-CZ-NH2	12.39	126.49	120.30
1	E	26	ASP	CB-CG-OD1	12.38	129.44	118.30
1	E	104	TYR	CB-CG-CD2	-12.20	113.68	121.00
2	C	1	PRO	CA-C-N	11.72	142.99	117.20
1	E	25	TYR	CB-CG-CD1	-11.70	113.98	121.00
1	E	171	PRO	CA-N-CD	-11.57	95.31	111.50
2	C	2	ALA	O-C-N	-11.49	99.26	121.10
1	E	168	ASN	C-N-CA	11.43	150.28	121.70
1	E	184	ASP	CB-CG-OD1	11.40	128.56	118.30
1	E	185	ARG	NE-CZ-NH1	-11.30	114.65	120.30
1	E	175	PRO	CA-C-N	11.20	141.84	117.20
1	E	171	PRO	N-CA-CB	11.04	116.55	103.30
1	E	106	THR	CA-CB-CG2	11.04	127.85	112.40
1	E	64	ARG	CD-NE-CZ	-11.03	108.17	123.60
1	E	171	PRO	N-CD-CG	10.95	119.62	103.20
1	E	170	SER	O-C-N	10.94	141.88	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	168	ASN	CB-CA-C	10.91	132.22	110.40
1	E	24	TYR	CB-CG-CD1	10.86	127.52	121.00
1	E	195	TYR	CB-CG-CD1	10.73	127.44	121.00
1	E	250	ARG	NH1-CZ-NH2	-10.52	107.82	119.40
1	E	107	ILE	CA-CB-CG2	10.34	131.58	110.90
1	E	80	ARG	CA-CB-CG	10.32	136.10	113.40
2	C	4	PHE	CB-CA-C	-10.32	89.77	110.40
1	E	147	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	E	25	TYR	CB-CG-CD2	9.86	126.92	121.00
2	C	1	PRO	CA-C-O	-9.79	96.72	120.20
1	E	60	TYR	CB-CG-CD1	9.71	126.83	121.00
2	C	2	ALA	N-CA-C	9.38	136.33	111.00
1	E	169	TYR	CZ-CE2-CD2	-9.32	111.41	119.80
1	E	80	ARG	CG-CD-NE	-9.31	92.24	111.80
1	E	75	GLY	CA-C-O	-9.30	103.86	120.60
1	E	168	ASN	CA-C-O	-9.29	100.60	120.10
1	E	169	TYR	C-N-CA	9.29	144.92	121.70
1	E	169	TYR	CA-C-N	9.26	137.58	117.20
1	E	59	TYR	CB-CG-CD2	-9.15	115.51	121.00
1	E	165	ASP	CB-CG-OD2	9.12	126.51	118.30
2	C	4	PHE	N-CA-CB	9.04	126.87	110.60
1	E	170	SER	C-N-CA	9.01	159.82	122.00
1	E	65	ASP	CB-CG-OD2	8.73	126.16	118.30
1	E	220	ILE	CA-CB-CG2	8.72	128.33	110.90
1	E	133	LEU	CA-CB-CG	8.69	135.29	115.30
1	E	121	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	E	97	ASP	CB-CG-OD1	8.65	126.08	118.30
1	E	128	VAL	CA-CB-CG1	8.62	123.82	110.90
2	C	4	PHE	N-CA-C	8.58	134.17	111.00
1	E	274	TYR	CD1-CE1-CZ	-8.50	112.15	119.80
1	E	169	TYR	CB-CG-CD2	-8.43	115.94	121.00
1	E	219	SER	CB-CA-C	-8.41	94.13	110.10
1	E	262	SER	CB-CA-C	8.34	125.95	110.10
1	E	58	THR	CB-CA-C	-8.27	89.26	111.60
1	E	117	ASP	CB-CG-OD1	-8.26	110.87	118.30
1	E	171	PRO	O-C-N	-8.25	109.49	122.70
1	E	137	TYR	CB-CG-CD2	-8.21	116.08	121.00
1	E	170	SER	CA-C-N	-8.11	94.39	117.10
1	E	199	LEU	O-C-N	8.09	135.64	122.70
1	E	68	GLY	CA-C-O	-8.07	106.08	120.60
1	E	184	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	E	68	GLY	O-C-N	8.03	135.55	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	LEU	CA-C-O	-7.97	103.37	120.10
1	E	169	TYR	CA-C-O	-7.95	103.41	120.10
1	E	185	ARG	CG-CD-NE	-7.91	95.19	111.80
1	E	89	GLN	CB-CG-CD	7.86	132.05	111.60
1	E	27	GLU	CB-CG-CD	7.84	135.37	114.20
1	E	256	ALA	O-C-N	7.81	135.20	122.70
1	E	85	VAL	CA-CB-CG2	7.78	122.58	110.90
1	E	218	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	E	60	TYR	CG-CD2-CE2	7.63	127.41	121.30
1	E	6	ALA	N-CA-CB	-7.61	99.45	110.10
1	E	56	VAL	CG1-CB-CG2	7.56	122.99	110.90
1	E	23	TYR	CB-CG-CD2	7.54	125.53	121.00
1	E	14	SER	C-N-CA	7.54	140.55	121.70
1	E	169	TYR	CG-CD1-CE1	-7.51	115.30	121.30
1	E	13	ILE	CA-CB-CG2	7.48	125.86	110.90
1	E	85	VAL	N-CA-CB	-7.37	95.29	111.50
1	E	219	SER	O-C-N	7.33	134.42	122.70
1	E	80	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	E	29	ALA	O-C-N	-7.30	110.79	123.20
1	E	230	VAL	CA-CB-CG1	7.28	121.83	110.90
1	E	120	ASN	CB-CA-C	7.26	124.92	110.40
1	E	188	ARG	CD-NE-CZ	7.24	133.73	123.60
1	E	37	VAL	CG1-CB-CG2	-7.18	99.42	110.90
1	E	29	ALA	N-CA-CB	-7.12	100.13	110.10
1	E	187	ASP	CB-CG-OD1	7.11	124.69	118.30
1	E	202	PHE	CA-C-N	7.10	130.41	116.20
1	E	49	PHE	O-C-N	7.07	134.02	122.70
1	E	39	ASP	OD1-CG-OD2	-7.07	109.86	123.30
1	E	254	ASP	CA-CB-CG	7.03	128.86	113.40
1	E	107	ILE	CB-CA-C	7.00	125.60	111.60
1	E	254	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	E	58	THR	N-CA-CB	6.94	123.48	110.30
1	E	49	PHE	CG-CD2-CE2	-6.92	113.18	120.80
1	E	70	GLY	O-C-N	6.85	133.65	122.70
1	E	188	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	E	77	VAL	CA-CB-CG2	6.81	121.11	110.90
1	E	87	LYS	CD-CE-NZ	-6.78	96.10	111.70
1	E	268	THR	CA-CB-CG2	6.78	121.89	112.40
2	C	3	PRO	CB-CA-C	-6.73	95.17	112.00
1	E	179	THR	CA-CB-OG1	-6.71	94.91	109.00
1	E	122	ASN	CB-CA-C	6.70	123.80	110.40
1	E	163	ASN	CB-CG-ND2	6.69	132.75	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	PHE	CA-C-O	-6.65	106.13	120.10
1	E	180	VAL	CA-CB-CG1	-6.65	100.93	110.90
1	E	239	THR	CA-CB-CG2	6.62	121.66	112.40
1	E	80	ARG	CB-CG-CD	-6.60	94.43	111.60
2	C	1	PRO	N-CA-CB	-6.59	95.36	102.60
1	E	147	ARG	CD-NE-CZ	-6.58	114.39	123.60
2	C	2	ALA	CA-C-O	-6.54	106.37	120.10
2	C	1	PRO	CB-CA-C	6.54	128.34	112.00
1	E	175	PRO	O-C-N	-6.52	112.27	122.70
1	E	22	THR	CA-CB-OG1	-6.48	95.39	109.00
1	E	104	TYR	CB-CG-CD1	6.43	124.86	121.00
1	E	58	THR	C-N-CA	-6.41	105.68	121.70
2	C	4	PHE	CZ-CE2-CD2	-6.41	112.41	120.10
1	E	126	GLY	CA-C-O	6.40	132.12	120.60
1	E	43	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	E	250	ARG	CG-CD-NE	6.34	125.12	111.80
1	E	254	ASP	CA-C-O	-6.34	106.79	120.10
1	E	143	SER	O-C-N	6.34	132.84	122.70
1	E	115	ALA	N-CA-CB	6.26	118.87	110.10
1	E	12	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	E	76	THR	CA-CB-OG1	-6.21	95.95	109.00
1	E	80	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	E	215	GLY	CA-C-N	6.16	130.74	117.20
1	E	274	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	E	263	ASN	CB-CA-C	6.15	122.69	110.40
1	E	200	ASP	CA-CB-CG	-6.14	99.89	113.40
1	E	200	ASP	CB-CG-OD2	6.14	123.83	118.30
1	E	169	TYR	CG-CD2-CE2	6.13	126.20	121.30
1	E	4	THR	N-CA-CB	-6.11	98.69	110.30
1	E	16	THR	N-CA-CB	-6.11	98.69	110.30
1	E	53	ALA	O-C-N	6.07	132.41	122.70
1	E	82	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	E	175	PRO	CA-C-O	-6.03	105.74	120.20
1	E	80	ARG	NH1-CZ-NH2	5.97	125.97	119.40
1	E	239	THR	N-CA-CB	5.94	121.59	110.30
1	E	50	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	E	121	ARG	CD-NE-CZ	5.91	131.87	123.60
1	E	209	LEU	CA-C-O	-5.89	107.72	120.10
1	E	24	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	E	184	ASP	O-C-N	-5.88	113.29	122.70
1	E	162	ASN	CB-CG-ND2	5.88	130.81	116.70
1	E	49	PHE	CB-CG-CD2	-5.87	116.69	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	114	VAL	CA-CB-CG2	5.87	119.70	110.90
1	E	156	ALA	N-CA-CB	5.82	118.25	110.10
1	E	43	GLU	CG-CD-OE1	5.82	129.94	118.30
1	E	30	GLY	C-N-CA	-5.82	107.16	121.70
1	E	89	GLN	OE1-CD-NE2	-5.81	108.55	121.90
1	E	39	ASP	N-CA-CB	-5.79	100.17	110.60
1	E	162	ASN	N-CA-CB	-5.79	100.18	110.60
1	E	92	GLY	O-C-N	5.78	131.94	122.70
1	E	187	ASP	OD1-CG-OD2	-5.76	112.36	123.30
1	E	219	SER	N-CA-CB	5.73	119.09	110.50
1	E	274	TYR	CG-CD2-CE2	-5.72	116.73	121.30
1	E	231	ALA	C-N-CA	5.71	134.29	122.30
1	E	263	ASN	O-C-N	-5.71	113.57	122.70
1	E	153	VAL	CA-CB-CG2	5.69	119.44	110.90
1	E	219	SER	CA-CB-OG	-5.69	95.83	111.20
1	E	219	SER	CA-C-O	-5.68	108.16	120.10
1	E	112	ASP	OD1-CG-OD2	-5.66	112.55	123.30
1	E	60	TYR	CD1-CG-CD2	-5.66	111.68	117.90
1	E	25	TYR	CG-CD2-CE2	-5.64	116.78	121.30
1	E	118	LYS	CD-CE-NZ	-5.62	98.77	111.70
1	E	184	ASP	C-N-CA	5.62	135.76	121.70
1	E	14	SER	O-C-N	-5.62	113.71	122.70
1	E	162	ASN	O-C-N	-5.61	113.72	122.70
2	C	1	PRO	C-N-CA	5.61	135.72	121.70
1	E	199	LEU	CA-C-O	-5.61	108.33	120.10
1	E	242	LYS	CA-CB-CG	5.61	125.73	113.40
1	E	49	PHE	CA-C-O	-5.58	108.38	120.10
1	E	82	TYR	N-CA-CB	-5.56	100.60	110.60
1	E	249	CYS	CA-CB-SG	-5.55	104.00	114.00
1	E	194	ASN	OD1-CG-ND2	5.54	134.65	121.90
1	E	65	ASP	C-N-CA	-5.54	110.67	122.30
1	E	50	GLU	CG-CD-OE1	5.53	129.35	118.30
1	E	221	SER	CA-C-O	-5.50	108.55	120.10
1	E	122	ASN	O-C-N	-5.49	113.92	122.70
1	E	269	VAL	CA-CB-CG2	5.49	119.14	110.90
1	E	102	GLY	O-C-N	5.46	131.43	122.70
1	E	57	LYS	N-CA-CB	-5.42	100.85	110.60
1	E	277	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	E	250	ARG	CD-NE-CZ	-5.41	116.02	123.60
1	E	5	ASN	CB-CG-OD1	-5.41	110.78	121.60
1	E	52	ARG	NH1-CZ-NH2	5.41	125.35	119.40
1	E	63	SER	N-CA-CB	5.40	118.59	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	60	TYR	CG-CD1-CE1	5.39	125.62	121.30
1	E	13	ILE	CA-CB-CG1	-5.39	100.76	111.00
1	E	254	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	56	VAL	N-CA-CB	-5.38	99.67	111.50
1	E	278	GLN	C-N-CA	5.36	135.11	121.70
1	E	213	ILE	C-N-CA	-5.36	111.04	122.30
1	E	69	HIS	CA-CB-CG	5.33	122.66	113.60
1	E	221	SER	O-C-N	5.32	132.25	123.20
1	E	192	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	E	23	TYR	CA-C-N	5.31	128.88	117.20
1	E	64	ARG	N-CA-CB	-5.31	101.05	110.60
1	E	45	SER	CA-CB-OG	-5.30	96.89	111.20
2	C	3	PRO	N-CD-CG	5.29	111.14	103.20
2	C	4	PHE	CA-CB-CG	5.29	126.59	113.90
1	E	31	GLN	N-CA-CB	5.28	120.10	110.60
1	E	56	VAL	CA-CB-CG1	5.28	118.81	110.90
1	E	183	SER	N-CA-CB	5.26	118.39	110.50
1	E	99	ASN	C-N-CA	5.25	133.32	122.30
1	E	26	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	E	120	ASN	N-CA-CB	-5.24	101.17	110.60
1	E	25	TYR	CG-CD1-CE1	5.24	125.49	121.30
1	E	276	ASN	OD1-CG-ND2	5.24	133.95	121.90
1	E	135	GLY	N-CA-C	-5.23	100.03	113.10
1	E	1	ALA	N-CA-CB	5.22	117.41	110.10
1	E	189	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	E	144	ALA	N-CA-CB	5.21	117.39	110.10
1	E	89	GLN	CG-CD-NE2	5.20	129.17	116.70
1	E	198	VAL	CA-C-O	-5.19	109.20	120.10
1	E	272	LEU	CB-CG-CD1	5.18	119.81	111.00
1	E	279	ALA	CA-C-O	-5.18	109.22	120.10
1	E	29	ALA	CA-C-N	5.18	126.56	116.20
1	E	117	ASP	CA-C-O	-5.18	109.22	120.10
1	E	251	TYR	CD1-CE1-CZ	5.17	124.46	119.80
1	E	106	THR	CB-CA-C	5.17	125.57	111.60
1	E	106	THR	O-C-N	-5.17	114.43	122.70
1	E	137	TYR	CG-CD1-CE1	-5.17	117.17	121.30
1	E	194	ASN	CB-CG-OD1	-5.15	111.30	121.60
1	E	274	TYR	CB-CA-C	5.15	120.70	110.40
1	E	72	HIS	C-N-CA	5.12	134.49	121.70
1	E	53	ALA	CA-C-O	-5.10	109.38	120.10
1	E	43	GLU	O-C-N	5.10	130.86	122.70
1	E	49	PHE	CD1-CE1-CZ	-5.10	113.98	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	PRO	N-CA-C	5.09	125.33	112.10
1	E	60	TYR	CA-CB-CG	-5.06	103.79	113.40
1	E	174	GLU	N-CA-C	-5.05	97.36	111.00
1	E	70	GLY	CA-C-O	-5.04	111.53	120.60
1	E	87	LYS	O-C-N	5.03	130.75	122.70
1	E	115	ALA	CA-C-O	-5.03	109.55	120.10

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	Mainchain,Peptide
1	E	185	ARG	Sidechain

## 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	2018	0	1915	122	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	1952	133	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 33.

All (133) 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:C	3:D:6:ALA:CA	1.95	1.32
1:E:220:ILE:CD1	3:D:6:ALA:HB3	1.60	1.30
3:D:6:ALA:N	3:D:6:ALA:CA	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
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:HG2	1:E:64:ARG:NH1	1.63	1.11
1:E:207:SER:HB3	4:E:405:HOH:O	0.92	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:HG13	1:E:85:VAL:O	1.34	1.05
1:E:224:SER:OG	2:C:4:PHE:C	1.96	1.03
1:E:207:SER:HB2	4:E:376:HOH:O	1.56	1.01
1:E:85:VAL:CG1	1:E:85:VAL:O	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: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
1:E:64:ARG:CG	1:E:64:ARG:NH1	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:CG	1:E:64:ARG:HH11	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:N	2.34	0.80
3:D:6:ALA:HA	4:D:483:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:VAL:CG2	1:E:230:VAL:HG21	2.16	0.76
1:E:126:GLY:HA3	1:E:238:MET:HE2	1.68	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
3:D:6:ALA:C	3:D:6:ALA:O	2.27	0.73
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
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: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:126:GLY:HA3	1:E:238:MET:CE	2.27	0.64
1:E:30:GLY:C	1:E:239:THR:HG21	2.19	0.64
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:LEU:HD21	1:E:272:LEU:HD22	1.91	0.53
1:E:30:GLY:HA3	1:E:85:VAL:CG2	2.36	0.53
2:C:4:PHE:N	3:D:5:DAL:CB	2.73	0.52
1:E:275:ASN:O	1:E:276:ASN:HB2	2.09	0.52
1:E:224:SER:CB	2:C:4:PHE:C	2.77	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:27:GLU:H	1:E:27:GLU:CD	2.14	0.51
1:E:72:HIS:CE1	1:E:210:SER:HB3	2.45	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: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
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:171:PRO:O	1:E:172:ALA:C	2.56	0.45
1:E:125:LYS:HB3	1:E:239:THR:HA	1.99	0.44
1:E:64:ARG:CZ	1:E:64:ARG:CB	2.82	0.44
1:E:24:TYR:HB3	1:E:277:TYR:CD1	2.53	0.44
1:E:107:ILE:HD11	1:E:111:MET:CE	2.48	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
2:C:4:PHE:C	3:D:5:DAL:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C	1:E:107:ILE:HD12	2.41	0.40
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%)	17	13
2	C	2/4 (50%)	1 (50%)	0	1 (50%)	0	0
All	All	279/283 (99%)	257 (92%)	18 (6%)	4 (1%)	13	10

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	211/214 (99%)	195 (92%)	16 (8%)	15	16
2	C	3/3 (100%)	3 (100%)	0	100	100
All	All	214/217 (99%)	198 (92%)	16 (8%)	16	16

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	THR
1	E	16	THR
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	225	MET
1	E	239	THR
1	E	240	LEU
1	E	250	ARG
1	E	270	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	GLN
1	E	46	HIS
1	E	89	GLN
1	E	119	ASN
1	E	162	ASN
1	E	168	ASN
1	E	194	ASN
1	E	229	HIS
1	E	257	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.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	DAL	D	5	3	4,4,5	9.06	3 (75%)	1,4,6	7.19	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAL	D	5	3	-	0/0/2/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	DAL	CB-CA	-7.34	1.24	1.52
3	D	5	DAL	CA-C	3.84	1.55	1.50
3	D	5	DAL	O-C	16.11	1.88	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	DAL	CB-CA-N	7.19	133.10	109.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	DAL	10	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

### 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.