



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:36 PM UTC

PDB ID : 1PFG / pdb_00001pfg
Title : Strategy to design inhibitors: Structure of a complex of Proteinase K with a designed octapeptide inhibitor N-Ac-Pro-Ala-Pro-Phe-DAla-Ala-Ala-Ala-NH₂ at 2.5Å resolution
Authors : Saxena, A.K.; Singh, T.P.; Peters, K.; Fittkau, S.; Betzel, C.
Deposited on : 2003-05-27
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

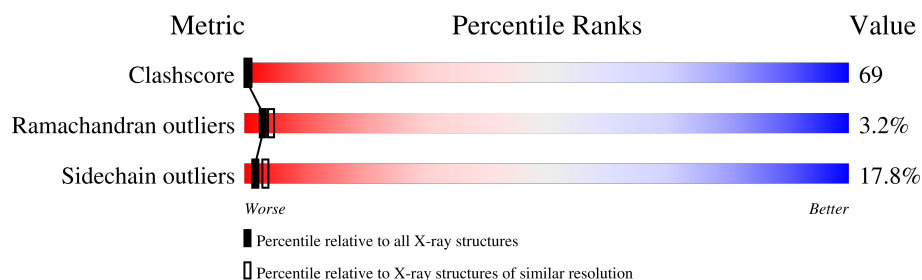
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	A	279	30% 41% 22% 6%
2	B	10	20% 30% 40% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2277 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	A	279	Total	C	N	O	S	0	0	0
			2017	1242	352	413	10			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called N-Ac-PAPFAAAA-NH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	1
			54	36	9	9			

- Molecule 3 is water.

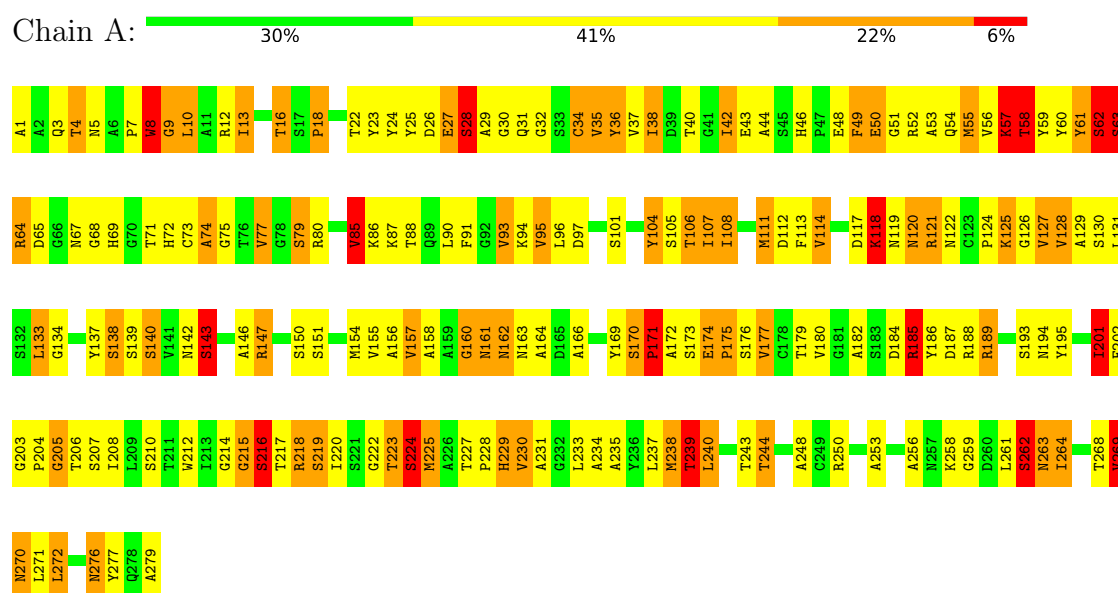
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total	O	0	0
			196	196		
3	B	10	Total	O	0	0
			10	10		

3 Residue-property plots

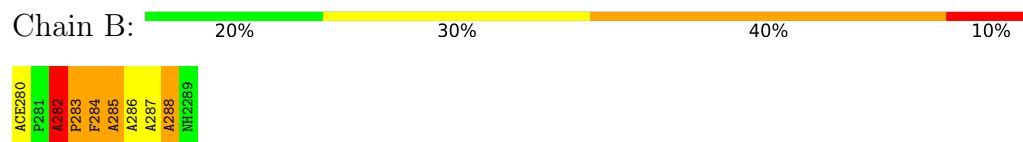
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: N-Ac-PAPFAAAA-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, α , β , γ	68.00Å 68.00Å 107.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2277	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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	A	1.67	27/2056 (1.3%)	2.42	91/2796 (3.3%)
2	B	3.36	3/52 (5.8%)	2.95	10/71 (14.1%)
All	All	1.73	30/2108 (1.4%)	2.43	101/2867 (3.5%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	285	ALA	N-CA	-17.95	1.12	1.46
1	A	127	VAL	CA-C	-9.83	1.40	1.52
1	A	268	THR	C-N	-8.84	1.22	1.33
2	B	280	ACE	C-N	-8.27	1.35	1.43
1	A	35	VAL	CA-CB	-7.94	1.44	1.54
1	A	244	THR	CA-C	-7.11	1.44	1.52
1	A	264	ILE	CA-C	-6.99	1.47	1.53
1	A	121	ARG	CA-C	-6.91	1.44	1.52
1	A	142	ASN	CA-C	-6.67	1.43	1.52
1	A	125	LYS	CA-C	-6.45	1.43	1.52
1	A	63	SER	N-CA	-6.32	1.37	1.45
1	A	238	MET	CG-SD	-6.21	1.65	1.80
1	A	38	ILE	N-CA	-6.05	1.39	1.46
1	A	127	VAL	CA-CB	-6.05	1.46	1.54
1	A	62	SER	CA-C	-6.04	1.44	1.53
1	A	34	CYS	CA-C	-6.02	1.45	1.52
1	A	106	THR	CA-CB	5.91	1.63	1.53
1	A	263	ASN	CA-C	5.90	1.61	1.52
1	A	272	LEU	C-O	-5.88	1.17	1.24
1	A	229	HIS	C-O	-5.84	1.17	1.24
1	A	85	VAL	CA-CB	-5.72	1.46	1.54
1	A	113	PHE	C-N	5.70	1.40	1.34
1	A	128	VAL	CA-C	-5.31	1.46	1.52
1	A	111	MET	SD-CE	-5.27	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	LYS	CB-CG	-5.22	1.36	1.52
1	A	36	TYR	C-O	5.20	1.30	1.24
2	B	282	ALA	N-CA	5.13	1.53	1.46
1	A	55	MET	C-N	-5.08	1.27	1.33
1	A	54	GLN	CA-C	-5.06	1.46	1.52
1	A	158	ALA	CA-CB	-5.01	1.45	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	SER	CA-C-N	40.88	170.94	119.84
1	A	170	SER	C-N-CA	40.88	170.94	119.84
1	A	171	PRO	CA-N-CD	-17.72	87.19	112.00
1	A	171	PRO	N-CA-CB	14.17	118.12	103.25
1	A	171	PRO	N-CD-CG	11.99	121.19	103.20
1	A	71	THR	N-CA-C	-11.15	99.20	111.36
1	A	80	ARG	NE-CZ-NH1	-10.71	110.80	121.50
1	A	157	VAL	N-CA-CB	-10.69	97.29	111.82
1	A	61	TYR	N-CA-C	10.47	122.69	111.28
1	A	58	THR	CB-CA-C	-10.32	91.99	110.36
1	A	170	SER	C-N-CD	-9.89	84.45	125.00
1	A	118	LYS	N-CA-C	-9.85	100.39	111.71
2	B	285	ALA	N-CA-CB	-9.67	95.89	110.40
1	A	63	SER	N-CA-C	-9.37	102.22	114.31
1	A	93	VAL	N-CA-C	-9.34	93.95	107.77
1	A	80	ARG	NE-CZ-NH2	8.25	126.63	119.20
1	A	174	GLU	N-CA-C	-8.21	91.66	109.81
1	A	63	SER	CB-CA-C	8.14	122.70	109.02
1	A	106	THR	N-CA-CB	8.09	122.82	110.28
1	A	233	LEU	N-CA-C	-7.93	102.57	111.14
1	A	223	THR	N-CA-C	-7.92	103.50	113.01
1	A	175	PRO	N-CD-CG	-7.83	91.46	103.20
1	A	121	ARG	NE-CZ-NH2	-7.82	112.16	119.20
1	A	121	ARG	NE-CZ-NH1	7.75	129.25	121.50
1	A	85	VAL	CB-CA-C	-7.55	98.91	111.29
1	A	80	ARG	CB-CA-C	-7.53	98.24	110.74
1	A	230	VAL	CB-CA-C	-7.48	99.96	112.16
1	A	157	VAL	CB-CA-C	7.47	120.51	110.42
2	B	284	PHE	CB-CA-C	-7.45	100.91	111.85
1	A	79	SER	N-CA-C	-7.43	98.51	110.32
1	A	125	LYS	CB-CA-C	-7.33	95.64	109.72
1	A	264	ILE	CB-CA-C	-7.23	104.21	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	SER	N-CA-C	-7.01	103.65	111.71
1	A	140	SER	N-CA-C	-6.82	103.97	112.90
1	A	185	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	A	224	SER	N-CA-CB	6.67	120.58	110.30
1	A	128	VAL	N-CA-CB	-6.59	101.40	112.47
1	A	63	SER	N-CA-CB	-6.59	102.14	110.90
1	A	147	ARG	NE-CZ-NH2	6.58	125.12	119.20
1	A	205	GLY	CA-C-N	-6.44	113.84	122.72
1	A	205	GLY	C-N-CA	-6.44	113.84	122.72
1	A	219	SER	CB-CA-C	-6.39	98.98	109.53
1	A	125	LYS	N-CA-C	6.37	121.05	113.28
1	A	264	ILE	N-CA-C	6.32	114.06	108.63
1	A	9	GLY	N-CA-C	-6.29	104.71	112.77
2	B	282	ALA	N-CA-C	6.27	123.67	109.81
1	A	214	GLY	N-CA-C	-6.26	106.69	115.32
1	A	16	THR	CB-CA-C	6.25	121.29	110.72
1	A	117	ASP	CB-CA-C	-6.22	98.38	110.46
1	A	215	GLY	N-CA-C	-6.17	104.23	114.48
2	B	288	ALA	N-CA-C	6.15	128.21	111.00
1	A	224	SER	CB-CA-C	-6.08	97.98	110.38
1	A	119	ASN	CA-C-N	-6.03	113.05	123.25
1	A	119	ASN	C-N-CA	-6.03	113.05	123.25
1	A	65	ASP	N-CA-C	-6.03	99.38	108.96
1	A	18	PRO	N-CA-C	-6.00	102.40	111.41
1	A	269	VAL	CB-CA-C	5.95	119.49	111.28
1	A	239	THR	N-CA-C	-5.93	104.94	111.82
2	B	285	ALA	CA-C-N	5.91	131.91	122.10
2	B	285	ALA	C-N-CA	5.91	131.91	122.10
2	B	283	PRO	CA-C-N	-5.90	115.13	123.03
2	B	283	PRO	C-N-CA	-5.90	115.13	123.03
1	A	129	ALA	N-CA-C	-5.88	99.07	109.06
1	A	173	SER	N-CA-C	5.88	119.51	112.93
1	A	74	ALA	N-CA-C	-5.84	104.10	111.11
1	A	80	ARG	CD-NE-CZ	-5.81	116.26	124.40
1	A	185	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	A	143	SER	N-CA-C	-5.77	104.90	111.07
1	A	27	GLU	N-CA-C	5.76	119.56	112.54
1	A	160	GLY	N-CA-C	-5.73	106.20	112.04
1	A	61	TYR	CB-CA-C	-5.56	101.57	110.79
1	A	189	ARG	N-CA-C	-5.54	102.20	110.23
1	A	147	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	A	37	VAL	N-CA-C	-5.51	99.03	106.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	SER	CB-CA-C	-5.50	104.52	113.37
1	A	52	ARG	N-CA-C	5.50	119.08	112.93
1	A	263	ASN	N-CA-CB	-5.41	105.40	114.27
1	A	95	VAL	N-CA-C	-5.41	107.09	113.42
1	A	108	ILE	N-CA-C	-5.33	105.30	110.42
1	A	133	LEU	CA-CB-CG	5.33	134.95	116.30
1	A	49	PHE	N-CA-C	-5.24	106.57	113.17
1	A	175	PRO	N-CA-C	-5.22	105.97	113.75
1	A	127	VAL	N-CA-C	-5.22	101.12	108.27
1	A	120	ASN	CB-CA-C	5.21	120.36	111.46
1	A	188	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	57	LYS	N-CA-CB	-5.16	101.77	110.49
1	A	161	ASN	CA-C-N	-5.16	114.43	122.73
1	A	161	ASN	C-N-CA	-5.16	114.43	122.73
1	A	85	VAL	N-CA-CB	-5.14	102.75	111.23
1	A	8	TRP	N-CA-CB	-5.13	102.31	110.22
2	B	284	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	55	MET	N-CA-CB	-5.10	102.25	109.85
2	B	284	PHE	N-CA-C	5.08	116.87	108.49
1	A	276	ASN	CA-C-N	-5.08	113.93	121.24
1	A	276	ASN	C-N-CA	-5.08	113.93	121.24
1	A	9	GLY	CA-C-O	5.07	126.03	120.66
1	A	262	SER	N-CA-C	-5.04	102.73	110.14
1	A	157	VAL	N-CA-C	5.03	115.22	107.77
1	A	170	SER	CA-CB-OG	-5.03	101.04	111.10
1	A	121	ARG	CD-NE-CZ	5.03	131.44	124.40
1	A	37	VAL	N-CA-CB	5.00	117.98	111.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2017	0	1916	268	3
2	B	54	0	50	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	196	0	0	36	5
3	B	10	0	0	1	0
All	All	2277	0	1966	277	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 69.

All (277) 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:A:126:GLY:HA3	1:A:238:MET:CE	1.60	1.28
1:A:85:VAL:O	1:A:85:VAL:CG1	1.73	1.23
1:A:220:ILE:HD12	2:B:286:ALA:HB2	1.23	1.18
1:A:269:VAL:CG1	1:A:271:LEU:HD12	1.75	1.16
1:A:126:GLY:HA3	1:A:238:MET:HE3	1.18	1.16
1:A:224:SER:HB3	1:A:225:MET:CE	1.76	1.15
1:A:85:VAL:HG11	1:A:88:THR:HB	1.29	1.13
1:A:224:SER:CB	1:A:225:MET:CE	2.34	1.05
1:A:224:SER:CB	1:A:225:MET:HE3	1.85	1.05
1:A:269:VAL:HG11	1:A:271:LEU:HD12	1.37	1.04
1:A:164:ALA:H	1:A:194:ASN:ND2	1.54	1.03
1:A:13:ILE:CD1	1:A:204:PRO:HG2	1.88	1.02
1:A:230:VAL:HB	3:A:359:HOH:O	1.58	1.02
1:A:137:TYR:HA	1:A:170:SER:OG	1.59	1.02
2:B:283:PRO:O	2:B:284:PHE:HD1	1.43	1.01
1:A:224:SER:HB3	1:A:225:MET:HE3	1.38	0.99
1:A:9:GLY:O	1:A:13:ILE:HD12	1.61	0.99
1:A:180:VAL:HG21	1:A:230:VAL:HG21	1.44	0.99
1:A:220:ILE:HD12	2:B:286:ALA:CB	1.92	0.98
1:A:107:ILE:HD13	1:A:111:MET:HE2	1.46	0.97
1:A:225:MET:HE2	3:A:517:HOH:O	1.65	0.96
1:A:13:ILE:HD11	1:A:204:PRO:HG2	1.48	0.95
1:A:176:SER:HA	3:A:415:HOH:O	1.66	0.95
1:A:126:GLY:CA	1:A:238:MET:CE	2.44	0.95
1:A:125:LYS:HG3	1:A:239:THR:HB	1.50	0.94
1:A:85:VAL:HG11	1:A:88:THR:CB	1.96	0.94
1:A:29:ALA:HB3	1:A:87:LYS:HD2	1.50	0.94
1:A:16:THR:HG22	3:A:421:HOH:O	1.70	0.92
1:A:55:MET:HE2	1:A:63:SER:O	1.68	0.92
1:A:224:SER:C	1:A:225:MET:HE3	1.95	0.91
1:A:261:LEU:H	1:A:270:ASN:HD21	1.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:HG13	1:A:271:LEU:HD12	1.48	0.91
1:A:164:ALA:H	1:A:194:ASN:HD22	1.20	0.89
2:B:283:PRO:C	2:B:284:PHE:HD1	1.80	0.89
1:A:220:ILE:CD1	2:B:286:ALA:HB2	2.02	0.88
1:A:13:ILE:HD11	1:A:204:PRO:CG	2.06	0.85
1:A:225:MET:O	1:A:229:HIS:HD2	1.59	0.85
1:A:207:SER:HB2	3:A:376:HOH:O	1.77	0.84
2:B:283:PRO:C	2:B:284:PHE:CD1	2.56	0.84
1:A:85:VAL:CG1	1:A:88:THR:HB	2.08	0.83
1:A:175:PRO:HG2	1:A:176:SER:N	1.92	0.83
1:A:207:SER:HB3	3:A:405:HOH:O	1.76	0.83
2:B:283:PRO:O	2:B:284:PHE:CD1	2.32	0.83
1:A:85:VAL:O	1:A:85:VAL:HG12	0.96	0.82
1:A:13:ILE:HD11	1:A:204:PRO:CD	2.09	0.82
1:A:163:ASN:HA	1:A:193:SER:O	1.79	0.82
3:A:601:HOH:O	2:B:282:ALA:HB2	1.79	0.81
1:A:220:ILE:CD1	2:B:286:ALA:CB	2.58	0.81
1:A:127:VAL:N	1:A:238:MET:HE1	1.96	0.80
1:A:225:MET:HE3	1:A:225:MET:N	1.96	0.79
1:A:73:CYS:SG	3:A:516:HOH:O	2.41	0.78
1:A:13:ILE:HD11	1:A:204:PRO:HD2	1.65	0.78
1:A:95:VAL:HB	1:A:107:ILE:HG22	1.64	0.78
1:A:32:GLY:HA3	1:A:125:LYS:HG2	1.66	0.78
1:A:9:GLY:O	1:A:13:ILE:CD1	2.32	0.77
1:A:224:SER:CB	1:A:225:MET:HE1	2.12	0.77
1:A:85:VAL:HG11	1:A:88:THR:CG2	2.14	0.77
1:A:13:ILE:HD12	1:A:204:PRO:HG2	1.67	0.77
1:A:107:ILE:C	1:A:107:ILE:HD12	2.10	0.76
1:A:225:MET:O	1:A:229:HIS:CD2	2.38	0.76
1:A:224:SER:HB2	1:A:225:MET:CE	2.14	0.76
1:A:177:VAL:HG23	3:A:513:HOH:O	1.87	0.74
1:A:67:ASN:HD21	2:B:288:ALA:HB3	1.52	0.74
1:A:161:ASN:HD22	2:B:285:ALA:HB2	1.53	0.73
1:A:262:SER:HB3	3:A:436:HOH:O	1.89	0.72
1:A:175:PRO:HG2	1:A:176:SER:H	1.51	0.72
1:A:13:ILE:CD1	1:A:204:PRO:CG	2.61	0.72
1:A:147:ARG:HG3	3:A:423:HOH:O	1.88	0.72
1:A:224:SER:HB2	1:A:225:MET:HE1	1.69	0.72
1:A:134:GLY:C	2:B:284:PHE:CE2	2.68	0.71
1:A:95:VAL:HG23	1:A:96:LEU:HG	1.72	0.71
1:A:46:HIS:CD2	1:A:48:GLU:HB2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASN:CG	3:A:420:HOH:O	2.34	0.70
1:A:30:GLY:C	1:A:239:THR:HG21	2.18	0.69
1:A:269:VAL:HG13	1:A:271:LEU:CD1	2.20	0.69
1:A:73:CYS:O	1:A:77:VAL:HG12	1.92	0.68
2:B:282:ALA:HB3	2:B:283:PRO:HD3	1.75	0.68
1:A:107:ILE:HG12	3:A:531:HOH:O	1.92	0.67
1:A:126:GLY:C	1:A:127:VAL:HG23	2.18	0.67
1:A:126:GLY:CA	1:A:238:MET:HE1	2.25	0.67
1:A:262:SER:O	1:A:263:ASN:CB	2.43	0.67
1:A:126:GLY:HA3	1:A:238:MET:HE1	1.73	0.67
1:A:180:VAL:CG2	1:A:230:VAL:HG21	2.24	0.66
1:A:69:HIS:CD2	3:A:516:HOH:O	2.49	0.66
1:A:107:ILE:HD13	1:A:111:MET:CE	2.23	0.66
1:A:227:THR:O	1:A:230:VAL:HG22	1.95	0.66
1:A:169:TYR:HB3	3:A:532:HOH:O	1.95	0.65
1:A:155:VAL:HG12	1:A:157:VAL:HG23	1.79	0.65
1:A:157:VAL:HG21	1:A:177:VAL:HG21	1.79	0.64
1:A:216:SER:O	1:A:217:THR:HG22	1.98	0.64
1:A:243:THR:HG21	1:A:248:ALA:HA	1.79	0.64
1:A:25:TYR:HD1	1:A:26:ASP:O	1.80	0.64
1:A:32:GLY:CA	1:A:125:LYS:HG2	2.28	0.63
1:A:164:ALA:N	1:A:194:ASN:HD22	1.95	0.63
1:A:180:VAL:HG21	1:A:230:VAL:CG2	2.23	0.63
1:A:49:PHE:O	1:A:51:GLY:N	2.31	0.63
1:A:155:VAL:HG12	1:A:157:VAL:CG2	2.30	0.62
1:A:67:ASN:ND2	2:B:288:ALA:HB3	2.14	0.62
1:A:201:ILE:HD11	1:A:256:ALA:HB2	1.81	0.62
1:A:224:SER:N	2:B:284:PHE:O	2.33	0.62
1:A:137:TYR:CA	1:A:170:SER:OG	2.43	0.62
1:A:127:VAL:H	1:A:238:MET:HE1	1.64	0.61
1:A:227:THR:O	1:A:230:VAL:CG2	2.47	0.61
1:A:163:ASN:CG	1:A:163:ASN:O	2.43	0.61
1:A:57:LYS:HD2	1:A:59:TYR:CE2	2.36	0.60
1:A:126:GLY:CA	1:A:238:MET:HE3	2.12	0.60
1:A:277:TYR:CZ	1:A:279:ALA:HA	2.36	0.60
1:A:126:GLY:C	1:A:238:MET:HE1	2.25	0.60
1:A:29:ALA:HB3	1:A:87:LYS:CD	2.29	0.60
1:A:60:TYR:N	1:A:60:TYR:CD2	2.69	0.60
1:A:185:ARG:HB2	3:A:400:HOH:O	2.01	0.60
1:A:208:ILE:HD13	3:A:320:HOH:O	2.04	0.58
1:A:220:ILE:CD1	2:B:286:ALA:HB1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ILE:CD1	1:A:111:MET:HE2	2.26	0.58
1:A:154:MET:HE3	1:A:234:ALA:HB2	1.85	0.58
1:A:261:LEU:HD21	1:A:272:LEU:HD13	1.86	0.57
1:A:49:PHE:O	1:A:50:GLU:C	2.48	0.57
1:A:74:ALA:O	1:A:77:VAL:HG13	2.03	0.57
1:A:107:ILE:CD1	1:A:111:MET:CE	2.82	0.57
1:A:227:THR:HB	1:A:228:PRO:CD	2.35	0.57
1:A:4:THR:O	1:A:5:ASN:C	2.46	0.57
1:A:35:VAL:HG11	1:A:77:VAL:HG21	1.86	0.57
1:A:59:TYR:C	1:A:60:TYR:CD2	2.82	0.57
1:A:46:HIS:HD2	1:A:48:GLU:H	1.53	0.57
1:A:224:SER:CA	2:B:284:PHE:O	2.52	0.57
1:A:58:THR:HG21	1:A:62:SER:O	2.06	0.56
1:A:68:GLY:HA3	1:A:212:TRP:CZ2	2.41	0.56
1:A:126:GLY:C	1:A:127:VAL:CG2	2.78	0.56
1:A:32:GLY:C	1:A:125:LYS:HG2	2.30	0.56
1:A:67:ASN:O	2:B:288:ALA:HB1	2.06	0.56
1:A:161:ASN:ND2	2:B:285:ALA:HB2	2.20	0.55
1:A:4:THR:HG22	1:A:5:ASN:OD1	2.07	0.55
1:A:67:ASN:ND2	2:B:288:ALA:CB	2.70	0.55
1:A:118:LYS:NZ	1:A:151:SER:O	2.40	0.55
1:A:58:THR:HG22	1:A:59:TYR:H	1.72	0.55
1:A:58:THR:HG23	1:A:94:LYS:HB3	1.89	0.54
1:A:1:ALA:O	1:A:24:TYR:HA	2.07	0.54
1:A:224:SER:CA	1:A:225:MET:HE3	2.36	0.54
1:A:186:TYR:O	1:A:187:ASP:HB2	2.06	0.54
1:A:216:SER:C	1:A:217:THR:CG2	2.82	0.54
1:A:75:GLY:HA2	1:A:79:SER:HB3	1.90	0.53
1:A:126:GLY:C	1:A:238:MET:CE	2.81	0.53
1:A:25:TYR:CD1	1:A:26:ASP:O	2.61	0.53
1:A:77:VAL:O	1:A:85:VAL:HB	2.08	0.53
1:A:139:SER:O	1:A:143:SER:HB2	2.08	0.53
1:A:230:VAL:HG23	1:A:231:ALA:N	2.22	0.53
1:A:56:VAL:HG21	1:A:91:PHE:CD2	2.44	0.53
1:A:57:LYS:HG3	1:A:93:VAL:HG13	1.90	0.53
1:A:228:PRO:HA	1:A:231:ALA:HB3	1.91	0.52
1:A:262:SER:O	1:A:263:ASN:HB2	2.09	0.52
1:A:61:TYR:CE1	3:A:345:HOH:O	2.53	0.52
1:A:69:HIS:O	1:A:72:HIS:HB3	2.10	0.52
1:A:171:PRO:O	1:A:172:ALA:C	2.52	0.52
1:A:131:LEU:HD12	1:A:131:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:C	1:A:124:PRO:HD3	2.35	0.51
1:A:86:LYS:C	1:A:87:LYS:HG3	2.35	0.51
1:A:3:GLN:HE22	1:A:86:LYS:HZ1	1.57	0.51
1:A:139:SER:HB2	3:A:474:HOH:O	2.11	0.51
1:A:161:ASN:HD21	2:B:285:ALA:N	2.07	0.51
1:A:73:CYS:O	1:A:74:ALA:C	2.50	0.51
1:A:120:ASN:C	1:A:121:ARG:HG2	2.34	0.51
1:A:46:HIS:HE1	1:A:216:SER:O	1.94	0.50
1:A:138:SER:N	1:A:170:SER:OG	2.44	0.50
1:A:3:GLN:O	1:A:22:THR:HA	2.12	0.50
1:A:201:ILE:HD11	1:A:256:ALA:CB	2.41	0.50
1:A:208:ILE:O	1:A:219:SER:HA	2.10	0.50
1:A:237:LEU:HA	1:A:240:LEU:HB2	1.93	0.50
1:A:269:VAL:HG13	1:A:271:LEU:CG	2.42	0.50
1:A:8:TRP:CE3	1:A:8:TRP:C	2.89	0.50
1:A:38:ILE:HD11	1:A:114:VAL:HG11	1.93	0.50
1:A:270:ASN:HD22	1:A:270:ASN:C	2.19	0.50
1:A:28:SER:O	1:A:31:GLN:HG2	2.12	0.50
1:A:107:ILE:HD12	1:A:108:ILE:N	2.27	0.50
1:A:42:ILE:O	1:A:44:ALA:N	2.45	0.50
1:A:13:ILE:HD12	1:A:204:PRO:CG	2.35	0.49
1:A:220:ILE:HD13	2:B:286:ALA:HB1	1.95	0.49
1:A:69:HIS:CG	3:A:516:HOH:O	2.65	0.49
1:A:164:ALA:N	1:A:194:ASN:ND2	2.39	0.49
1:A:185:ARG:NH1	3:A:380:HOH:O	2.44	0.49
1:A:224:SER:OG	2:B:284:PHE:C	2.56	0.49
1:A:57:LYS:HD3	1:A:57:LYS:C	2.38	0.49
1:A:216:SER:O	1:A:217:THR:CG2	2.61	0.48
1:A:107:ILE:O	1:A:108:ILE:C	2.56	0.48
1:A:138:SER:H	1:A:170:SER:CB	2.26	0.48
1:A:185:ARG:NH2	3:A:380:HOH:O	2.46	0.48
1:A:64:ARG:CD	3:A:327:HOH:O	2.62	0.48
1:A:243:THR:CG2	1:A:248:ALA:HA	2.42	0.48
1:A:7:PRO:O	1:A:10:LEU:HB2	2.14	0.48
1:A:182:ALA:HB1	1:A:205:GLY:HA3	1.96	0.48
1:A:224:SER:HA	2:B:284:PHE:O	2.13	0.48
1:A:222:GLY:C	1:A:224:SER:H	2.21	0.47
1:A:85:VAL:CG1	1:A:88:THR:H	2.27	0.47
1:A:134:GLY:O	2:B:284:PHE:CE2	2.67	0.47
1:A:157:VAL:CG1	3:A:513:HOH:O	2.62	0.47
1:A:49:PHE:C	1:A:51:GLY:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HE3	1:A:57:LYS:HB2	1.55	0.47
1:A:12:ARG:O	1:A:12:ARG:HG3	2.14	0.46
1:A:156:ALA:C	1:A:157:VAL:HG23	2.40	0.46
1:A:201:ILE:HG13	1:A:202:PHE:H	1.81	0.46
1:A:69:HIS:CE1	3:A:516:HOH:O	2.68	0.46
1:A:107:ILE:C	1:A:107:ILE:CD1	2.85	0.46
1:A:130:SER:HB2	1:A:231:ALA:HB1	1.96	0.46
1:A:195:TYR:C	1:A:195:TYR:CD2	2.93	0.46
2:B:282:ALA:HB3	2:B:283:PRO:CD	2.45	0.46
1:A:46:HIS:CE1	1:A:216:SER:O	2.68	0.46
1:A:184:ASP:C	1:A:184:ASP:OD1	2.58	0.46
1:A:64:ARG:HD2	3:A:327:HOH:O	2.15	0.45
1:A:189:ARG:NH2	3:A:386:HOH:O	2.45	0.45
1:A:154:MET:HE1	3:A:359:HOH:O	2.16	0.45
1:A:157:VAL:HG11	3:A:513:HOH:O	2.16	0.45
1:A:25:TYR:HE1	3:A:445:HOH:O	2.00	0.45
1:A:243:THR:HA	3:A:344:HOH:O	2.16	0.45
1:A:7:PRO:HD2	1:A:10:LEU:HD12	1.98	0.45
1:A:36:TYR:CD1	1:A:114:VAL:HB	2.52	0.45
1:A:164:ALA:O	1:A:194:ASN:HA	2.17	0.45
1:A:201:ILE:CD1	1:A:253:ALA:HA	2.47	0.45
1:A:222:GLY:C	1:A:224:SER:N	2.75	0.45
1:A:1:ALA:N	1:A:27:GLU:OE1	2.33	0.45
1:A:146:ALA:HB2	1:A:174:GLU:CD	2.41	0.45
1:A:46:HIS:HD2	1:A:48:GLU:HB2	1.80	0.44
1:A:264:ILE:HB	3:A:437:HOH:O	2.17	0.44
1:A:72:HIS:CD2	1:A:210:SER:HB3	2.52	0.44
1:A:30:GLY:HA3	1:A:85:VAL:HG22	2.00	0.44
1:A:157:VAL:O	1:A:180:VAL:N	2.47	0.43
1:A:161:ASN:ND2	2:B:285:ALA:CB	2.81	0.43
1:A:216:SER:HB2	1:A:217:THR:H	1.59	0.43
1:A:218:ARG:NH2	3:A:530:HOH:O	2.50	0.43
1:A:224:SER:O	1:A:228:PRO:CD	2.66	0.43
1:A:182:ALA:HA	1:A:203:GLY:O	2.18	0.43
1:A:157:VAL:O	1:A:179:THR:HA	2.18	0.43
1:A:187:ASP:O	1:A:261:LEU:HA	2.18	0.43
1:A:3:GLN:N	1:A:23:TYR:O	2.47	0.43
2:B:284:PHE:HZ	3:B:506:HOH:O	1.98	0.43
1:A:64:ARG:HH11	1:A:64:ARG:HG2	1.84	0.42
1:A:31:GLN:HB3	1:A:87:LYS:HB3	2.01	0.42
1:A:46:HIS:CE1	1:A:215:GLY:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HA	1:A:270:ASN:O	2.19	0.42
1:A:235:ALA:O	1:A:239:THR:HG23	2.18	0.42
1:A:224:SER:CB	2:B:284:PHE:C	2.92	0.42
1:A:3:GLN:NE2	1:A:86:LYS:HE3	2.35	0.42
1:A:85:VAL:CG1	1:A:88:THR:HG22	2.49	0.42
1:A:225:MET:CE	3:A:517:HOH:O	2.43	0.42
1:A:46:HIS:CE1	1:A:215:GLY:HA2	2.54	0.42
1:A:125:LYS:O	1:A:238:MET:HB3	2.19	0.42
1:A:127:VAL:C	1:A:128:VAL:HG23	2.44	0.42
1:A:189:ARG:NH1	1:A:193:SER:O	2.52	0.42
1:A:27:GLU:C	1:A:29:ALA:N	2.72	0.42
1:A:58:THR:CG2	1:A:94:LYS:HG2	2.49	0.42
1:A:56:VAL:CG2	1:A:91:PHE:CD2	3.03	0.41
1:A:202:PHE:HB2	1:A:271:LEU:O	2.20	0.41
1:A:227:THR:O	1:A:230:VAL:HG23	2.19	0.41
1:A:18:PRO:HD3	1:A:187:ASP:OD1	2.21	0.41
1:A:25:TYR:CD2	1:A:25:TYR:N	2.86	0.41
1:A:161:ASN:ND2	2:B:285:ALA:N	2.68	0.41
1:A:189:ARG:HB3	1:A:263:ASN:HB3	2.02	0.41
1:A:8:TRP:HZ2	1:A:206:THR:O	2.03	0.41
1:A:227:THR:HB	1:A:228:PRO:HD3	2.01	0.41
1:A:34:CYS:C	1:A:35:VAL:HG23	2.45	0.41
1:A:162:ASN:ND2	1:A:162:ASN:N	2.68	0.41
1:A:104:TYR:O	1:A:108:ILE:N	2.47	0.41
1:A:32:GLY:HA3	1:A:125:LYS:CG	2.43	0.41
1:A:53:ALA:HA	1:A:90:LEU:O	2.21	0.41
1:A:130:SER:HB2	1:A:231:ALA:CB	2.51	0.41
1:A:258:LYS:HG2	1:A:271:LEU:HD23	2.02	0.41
1:A:261:LEU:N	1:A:270:ASN:HD21	2.00	0.41
1:A:40:THR:O	1:A:94:LYS:HD2	2.21	0.41
1:A:160:GLY:O	1:A:223:THR:HG21	2.20	0.41
1:A:162:ASN:H	1:A:162:ASN:HD22	1.69	0.41
3:A:530:HOH:O	2:B:287:ALA:HB3	2.21	0.41
1:A:210:SER:O	1:A:217:THR:HB	2.21	0.41
1:A:25:TYR:CZ	1:A:86:LYS:HD2	2.56	0.40
1:A:220:ILE:HD13	1:A:220:ILE:HG21	1.73	0.40
1:A:256:ALA:HB1	1:A:272:LEU:O	2.20	0.40
1:A:58:THR:HG22	1:A:59:TYR:N	2.34	0.40
1:A:216:SER:C	1:A:217:THR:HG23	2.46	0.40
1:A:97:ASP:OD2	1:A:97:ASP:C	2.65	0.40
1:A:29:ALA:HB1	3:A:459:HOH:O	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:457:HOH:O	3:A:457:HOH:O[7_465]	0.69	1.51
3:A:476:HOH:O	3:A:543:HOH:O[6_455]	0.81	1.39
1:A:112:ASP:OD1	3:A:339:HOH:O[7_465]	1.77	0.43
1:A:216:SER:CB	3:A:511:HOH:O[6_555]	1.80	0.40
1:A:150:SER:OG	3:A:423:HOH:O[7_465]	1.93	0.27

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/279 (99%)	244 (88%)	25 (9%)	8 (3%)	3	5
2	B	6/10 (60%)	4 (67%)	1 (17%)	1 (17%)	0	0
All	All	283/289 (98%)	248 (88%)	26 (9%)	9 (3%)	3	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	PRO
1	A	50	GLU
2	B	282	ALA
1	A	42	ILE
1	A	43	GLU
1	A	166	ALA
1	A	201	ILE
1	A	259	GLY
1	A	177	VAL

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	A	211/214 (99%)	173 (82%)	38 (18%)	2	3
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	214/217 (99%)	176 (82%)	38 (18%)	2	3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	TRP
1	A	10	LEU
1	A	13	ILE
1	A	28	SER
1	A	57	LYS
1	A	58	THR
1	A	62	SER
1	A	63	SER
1	A	64	ARG
1	A	77	VAL
1	A	85	VAL
1	A	101	SER
1	A	104	TYR
1	A	105	SER
1	A	106	THR
1	A	107	ILE
1	A	114	VAL
1	A	118	LYS
1	A	133	LEU
1	A	138	SER
1	A	140	SER
1	A	143	SER
1	A	162	ASN
1	A	171	PRO
1	A	185	ARG
1	A	201	ILE

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Mol	Chain	Res	Type
1	A	216	SER
1	A	218	ARG
1	A	224	SER
1	A	225	MET
1	A	239	THR
1	A	240	LEU
1	A	244	THR
1	A	250	ARG
1	A	262	SER
1	A	269	VAL
1	A	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	46	HIS
1	A	69	HIS
1	A	119	ASN
1	A	162	ASN
1	A	194	ASN
1	A	229	HIS
1	A	270	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	284:PHE	C	285:ALA	N	2.83

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.