Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:31 PM GMT

PDB ID	:	1B65
Title	:	Structure of l-aminopeptidase d-ala-esterase/amidase from ochrobactrum anthropi, a prototype for the serine aminopeptidases, reveals a new variant among the ntn hydrolase fold
Authors	:	Bompard-Gilles, C.; Villeret, V.; Davies, G.J.; Fanuel, L.; Joris, B.; Frere, J.M.; Van Beeumen, J.
Deposited on	:	1999-01-20
Resolution	:	1.82 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

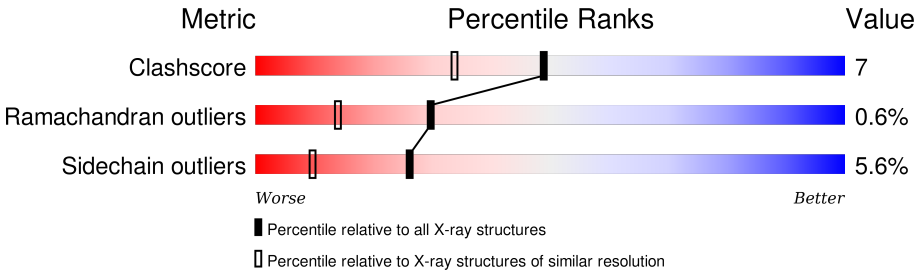
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)

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 >=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 <=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	A	375	80% 13%
1	B	375	80% 13%
1	C	375	80% 14%
1	D	375	78% 14%
1	E	375	80% 13%
1	F	375	79% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17786 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 PROTEIN (AMINOPEPTIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2747	1719	499	516	13			
1	B	363	Total	C	N	O	S	0	0	0
			2747	1719	499	516	13			
1	C	363	Total	C	N	O	S	0	0	0
			2747	1719	499	516	13			
1	D	363	Total	C	N	O	S	0	0	0
			2747	1719	499	516	13			
1	E	363	Total	C	N	O	S	0	0	0
			2747	1719	499	516	13			
1	F	363	Total	C	N	O	S	0	0	0
			2747	1719	499	516	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	220	Total	O	0	0
			220	220		
2	B	220	Total	O	0	0
			220	220		
2	C	230	Total	O	0	0
			230	230		
2	D	216	Total	O	0	0
			216	216		
2	E	207	Total	O	0	0
			207	207		
2	F	211	Total	O	0	0
			211	211		

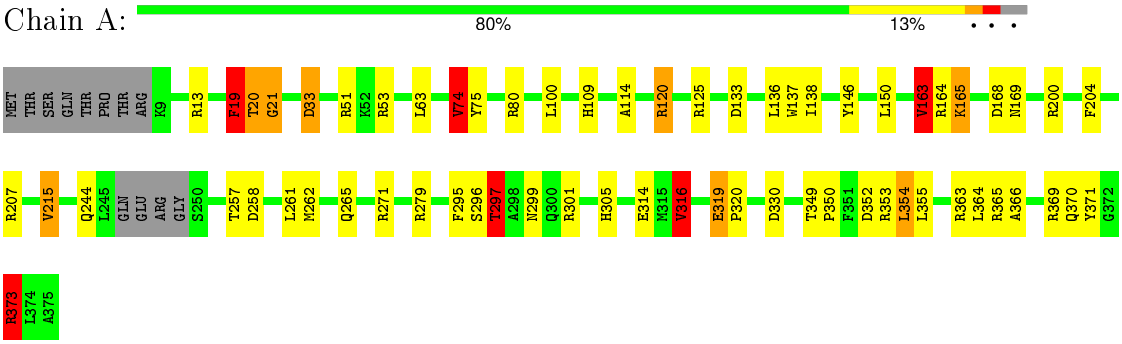
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

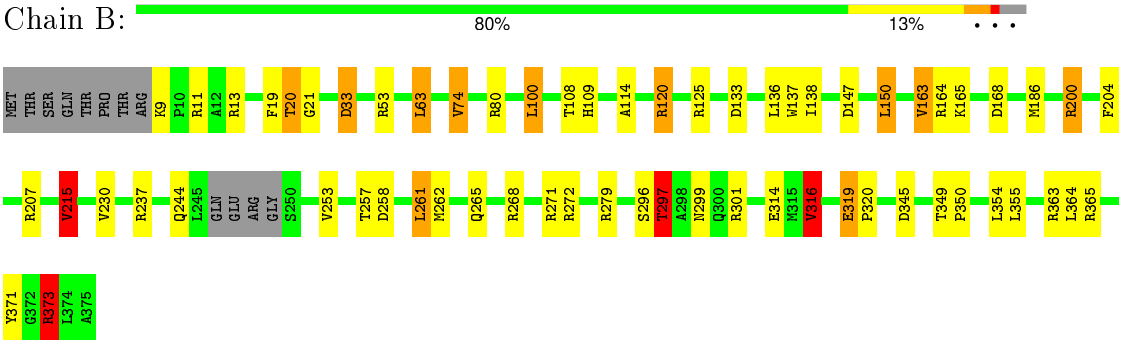
- Molecule 1: PROTEIN (AMINOPEPTIDASE)

Chain A:



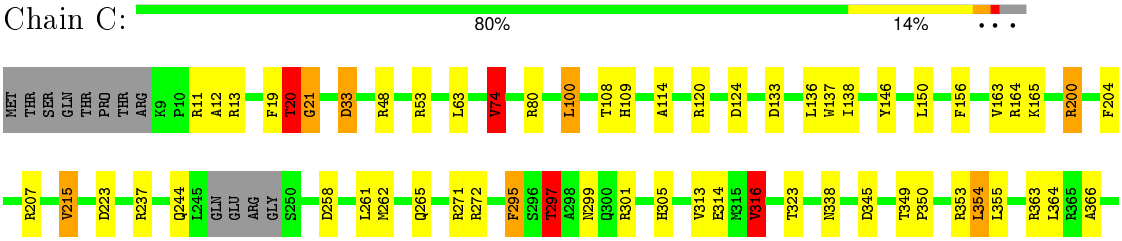
- Molecule 1: PROTEIN (AMINOPEPTIDASE)

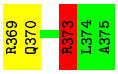
Chain B:



- Molecule 1: PROTEIN (AMINOPEPTIDASE)

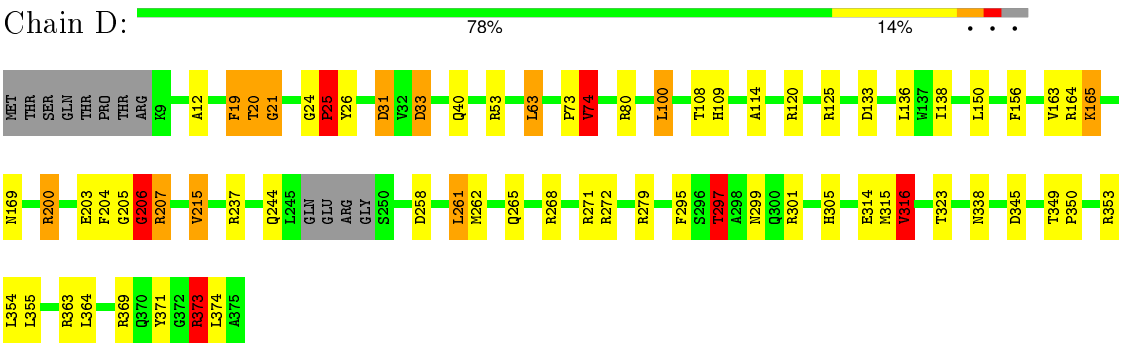
Chain C:





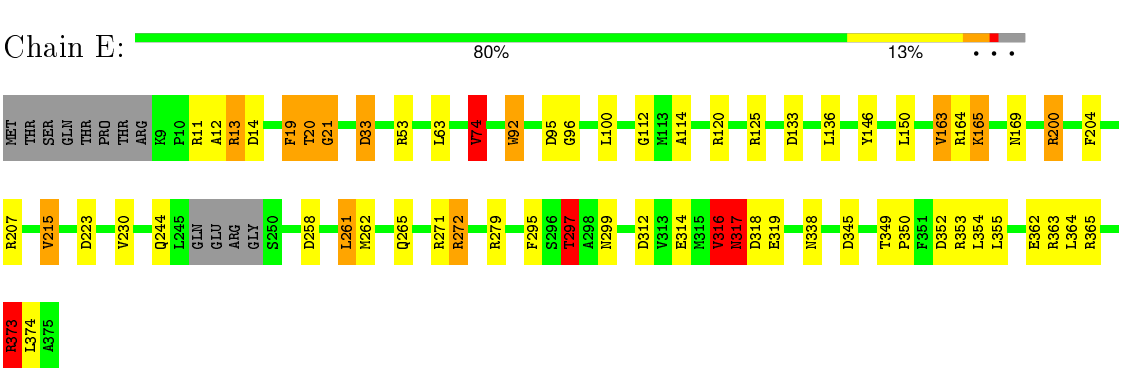
• Molecule 1: PROTEIN (AMINOPEPTIDASE)

Chain D:



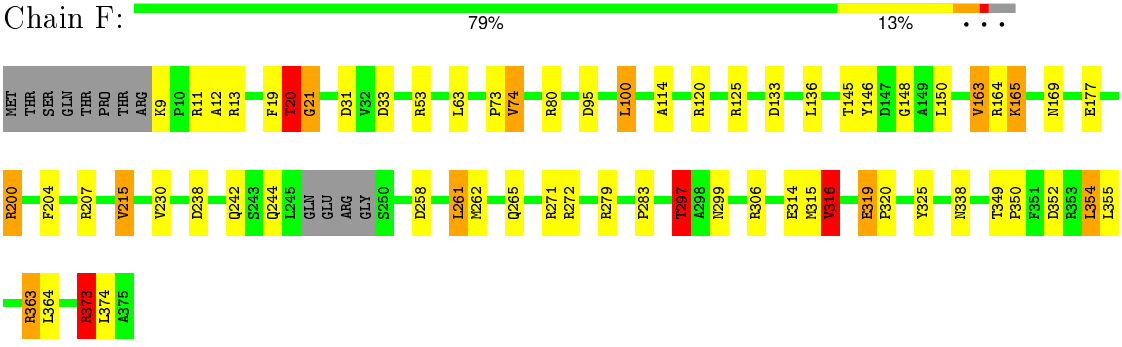
• Molecule 1: PROTEIN (AMINOPEPTIDASE)

Chain E:



• Molecule 1: PROTEIN (AMINOPEPTIDASE)

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	156.97Å 96.22Å 154.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.50 – 1.82	Depositor
% Data completeness (in resolution range)	95.8 (12.50-1.82)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17786	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.64	0/2808	1.65	53/3820 (1.4%)
1	B	0.64	0/2808	1.73	59/3820 (1.5%)
1	C	0.63	0/2808	1.73	52/3820 (1.4%)
1	D	0.66	1/2808 (0.0%)	1.74	58/3820 (1.5%)
1	E	0.68	3/2808 (0.1%)	1.74	55/3820 (1.4%)
1	F	0.64	0/2808	1.68	48/3820 (1.3%)
All	All	0.65	4/16848 (0.0%)	1.71	325/22920 (1.4%)

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	A	0	1
1	D	0	2
1	E	0	3
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	317	ASN	CA-CB	9.04	1.76	1.53
1	E	92	TRP	CZ3-CH2	8.86	1.54	1.40
1	D	25	PRO	CA-CB	6.79	1.67	1.53
1	E	92	TRP	CZ2-CH2	6.29	1.49	1.37

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	373	ARG	NE-CZ-NH2	-29.83	105.39	120.30
1	E	373	ARG	NE-CZ-NH2	-28.43	106.08	120.30
1	D	373	ARG	NE-CZ-NH2	-28.11	106.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	373	ARG	NE-CZ-NH2	-26.91	106.84	120.30
1	C	373	ARG	NE-CZ-NH2	-26.02	107.29	120.30
1	C	164	ARG	CD-NE-CZ	24.05	157.27	123.60
1	E	164	ARG	CD-NE-CZ	23.68	156.75	123.60
1	B	373	ARG	NE-CZ-NH2	-23.05	108.77	120.30
1	B	33	ASP	CB-CG-OD1	-22.97	97.63	118.30
1	F	207	ARG	CD-NE-CZ	21.74	154.04	123.60
1	B	33	ASP	CB-CG-OD2	21.72	137.85	118.30
1	D	33	ASP	CB-CG-OD1	-21.05	99.36	118.30
1	A	207	ARG	NE-CZ-NH2	-21.01	109.80	120.30
1	C	33	ASP	CB-CG-OD1	-20.50	99.85	118.30
1	E	317	ASN	CB-CA-C	-19.97	70.46	110.40
1	E	33	ASP	CB-CG-OD1	-19.77	100.50	118.30
1	F	164	ARG	NE-CZ-NH2	-18.88	110.86	120.30
1	B	207	ARG	NE-CZ-NH1	17.68	129.14	120.30
1	C	200	ARG	NE-CZ-NH1	17.44	129.02	120.30
1	B	120	ARG	NE-CZ-NH1	17.39	129.00	120.30
1	C	271	ARG	NE-CZ-NH2	-16.74	111.93	120.30
1	A	120	ARG	NE-CZ-NH1	16.45	128.52	120.30
1	A	164	ARG	CD-NE-CZ	16.40	146.56	123.60
1	C	207	ARG	NE-CZ-NH2	-15.88	112.36	120.30
1	E	33	ASP	CB-CG-OD2	15.88	132.59	118.30
1	D	33	ASP	CB-CG-OD2	15.78	132.50	118.30
1	C	33	ASP	CB-CG-OD2	15.68	132.42	118.30
1	A	19	PHE	C-N-CA	15.53	160.52	121.70
1	D	164	ARG	NE-CZ-NH2	-15.13	112.74	120.30
1	F	164	ARG	NE-CZ-NH1	15.01	127.81	120.30
1	A	207	ARG	CD-NE-CZ	14.62	144.07	123.60
1	D	19	PHE	C-N-CA	14.44	157.80	121.70
1	E	279	ARG	NE-CZ-NH2	-14.32	113.14	120.30
1	D	164	ARG	CD-NE-CZ	14.31	143.63	123.60
1	F	200	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	E	271	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	C	164	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	D	279	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	A	164	ARG	NE-CZ-NH2	-13.91	113.35	120.30
1	E	19	PHE	C-N-CA	13.71	155.97	121.70
1	F	207	ARG	NE-CZ-NH1	-13.52	113.54	120.30
1	B	164	ARG	CD-NE-CZ	13.33	142.26	123.60
1	F	80	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	F	164	ARG	CD-NE-CZ	13.22	142.10	123.60
1	E	207	ARG	NE-CZ-NH2	-13.20	113.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ARG	CD-NE-CZ	13.18	142.05	123.60
1	D	207	ARG	NE-CZ-NH1	13.09	126.84	120.30
1	B	164	ARG	NE-CZ-NH2	-12.95	113.83	120.30
1	C	120	ARG	NE-CZ-NH1	12.94	126.77	120.30
1	D	120	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	C	19	PHE	C-N-CA	12.84	153.80	121.70
1	A	373	ARG	NH1-CZ-NH2	12.84	133.52	119.40
1	A	207	ARG	NE-CZ-NH1	12.79	126.69	120.30
1	F	19	PHE	C-N-CA	12.71	153.49	121.70
1	F	373	ARG	NH1-CZ-NH2	12.71	133.38	119.40
1	B	19	PHE	C-N-CA	12.60	153.19	121.70
1	E	164	ARG	NE-CZ-NH2	-12.53	114.04	120.30
1	B	125	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	F	207	ARG	NE-CZ-NH2	12.01	126.31	120.30
1	D	25	PRO	N-CA-C	11.96	143.19	112.10
1	D	200	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	E	279	ARG	NE-CZ-NH1	11.79	126.19	120.30
1	A	363	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	D	25	PRO	N-CA-CB	-11.62	89.36	103.30
1	B	125	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	D	207	ARG	CD-NE-CZ	11.53	139.74	123.60
1	B	207	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	E	373	ARG	NH1-CZ-NH2	11.34	131.88	119.40
1	C	80	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	C	207	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	B	53	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	E	207	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	E	317	ASN	O-C-N	10.97	140.25	122.70
1	C	373	ARG	NH1-CZ-NH2	10.80	131.28	119.40
1	A	297	THR	N-CA-CB	-10.73	89.92	110.30
1	B	80	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	F	120	ARG	NE-CZ-NH1	10.59	125.60	120.30
1	E	297	THR	N-CA-CB	-10.51	90.33	110.30
1	D	205	GLY	C-N-CA	10.43	144.21	122.30
1	E	317	ASN	N-CA-CB	10.36	129.25	110.60
1	F	297	THR	N-CA-CB	-10.36	90.62	110.30
1	C	237	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	B	207	ARG	CD-NE-CZ	10.27	137.98	123.60
1	A	279	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	C	297	THR	N-CA-CB	-10.26	90.80	110.30
1	E	200	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	D	297	THR	N-CA-CB	-10.12	91.08	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	301	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	A	164	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	C	53	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	B	297	THR	N-CA-CB	-10.09	91.13	110.30
1	E	125	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	F	125	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	E	271	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	120	ARG	CD-NE-CZ	9.64	137.09	123.60
1	D	373	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	A	80	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	E	125	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	271	ARG	CD-NE-CZ	9.48	136.87	123.60
1	B	271	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	D	363	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	B	363	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	C	237	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	F	11	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	D	31	ASP	CB-CG-OD2	9.17	126.55	118.30
1	D	200	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	B	13	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	F	279	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	D	271	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	363	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	F	271	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	F	271	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	D	19	PHE	CA-C-O	8.62	138.21	120.10
1	A	271	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	E	19	PHE	CA-C-O	8.56	138.08	120.10
1	D	80	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	E	53	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	F	53	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	D	373	ARG	NH1-CZ-NH2	8.36	128.60	119.40
1	F	120	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	271	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	C	120	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	19	PHE	CA-C-O	8.21	137.34	120.10
1	D	316	VAL	N-CA-CB	-8.18	93.51	111.50
1	F	74	VAL	N-CA-CB	-8.16	93.55	111.50
1	D	345	ASP	CB-CG-OD1	8.14	125.63	118.30
1	D	19	PHE	O-C-N	-8.11	109.72	122.70
1	C	237	ARG	CD-NE-CZ	8.06	134.88	123.60
1	E	120	ARG	NE-CZ-NH1	8.02	124.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	373	ARG	NH1-CZ-NH2	8.01	128.21	119.40
1	F	271	ARG	CD-NE-CZ	8.00	134.80	123.60
1	A	125	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	D	215	VAL	N-CA-CB	-7.97	93.96	111.50
1	E	317	ASN	CA-C-N	-7.97	99.66	117.20
1	E	316	VAL	N-CA-CB	-7.96	93.99	111.50
1	D	271	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	E	19	PHE	O-C-N	-7.88	110.10	122.70
1	E	353	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	223	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	D	316	VAL	CG1-CB-CG2	7.86	123.47	110.90
1	A	215	VAL	CG1-CB-CG2	7.80	123.39	110.90
1	E	164	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	268	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	C	200	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	120	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	C	316	VAL	N-CA-CB	-7.65	94.67	111.50
1	E	365	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	E	215	VAL	N-CA-CB	-7.61	94.76	111.50
1	E	363	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	371	TYR	CB-CG-CD1	7.51	125.50	121.00
1	F	31	ASP	CB-CG-OD1	7.48	125.03	118.30
1	E	13	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	F	316	VAL	N-CA-CB	-7.38	95.26	111.50
1	C	297	THR	OG1-CB-CG2	7.33	126.85	110.00
1	C	215	VAL	N-CA-CB	-7.31	95.43	111.50
1	B	120	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	E	200	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	272	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	E	297	THR	OG1-CB-CG2	7.24	126.66	110.00
1	F	297	THR	OG1-CB-CG2	7.23	126.64	110.00
1	B	74	VAL	N-CA-CB	-7.21	95.64	111.50
1	D	25	PRO	CA-C-N	-7.17	101.43	117.20
1	D	363	ARG	CD-NE-CZ	7.16	133.62	123.60
1	E	207	ARG	CD-NE-CZ	7.06	133.49	123.60
1	C	48	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	124	ASP	CB-CG-OD1	7.05	124.65	118.30
1	B	279	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	215	VAL	N-CA-CB	-7.03	96.03	111.50
1	B	316	VAL	N-CA-CB	-7.03	96.03	111.50
1	D	125	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	F	215	VAL	N-CA-CB	-6.95	96.21	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	200	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	F	363	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	352	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	371	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	C	19	PHE	CA-C-O	6.86	134.51	120.10
1	D	371	TYR	CB-CG-CD1	6.84	125.11	121.00
1	F	279	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	215	VAL	N-CA-CB	-6.82	96.50	111.50
1	C	207	ARG	CD-NE-CZ	6.78	133.09	123.60
1	A	19	PHE	CA-C-O	6.77	134.32	120.10
1	A	369	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	206	GLY	CA-C-N	-6.76	102.33	117.20
1	A	316	VAL	N-CA-CB	-6.74	96.68	111.50
1	A	74	VAL	N-CA-CB	-6.72	96.71	111.50
1	B	268	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	D	301	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	19	PHE	O-C-N	-6.67	112.02	122.70
1	C	13	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	271	ARG	CD-NE-CZ	6.66	132.92	123.60
1	B	297	THR	OG1-CB-CG2	6.65	125.29	110.00
1	B	365	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	E	272	ARG	CD-NE-CZ	6.61	132.85	123.60
1	B	345	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	D	371	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	F	363	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	316	VAL	CG1-CB-CG2	6.57	121.41	110.90
1	F	74	VAL	CB-CA-C	6.57	123.87	111.40
1	A	369	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	168	ASP	CB-CG-OD1	6.56	124.20	118.30
1	C	48	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	345	ASP	CB-CG-OD1	6.54	124.19	118.30
1	B	271	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	D	297	THR	OG1-CB-CG2	6.48	124.91	110.00
1	E	146	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	297	THR	OG1-CB-CG2	6.45	124.84	110.00
1	C	271	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	215	VAL	CG1-CB-CG2	6.43	121.19	110.90
1	C	353	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	74	VAL	CA-CB-CG1	6.40	120.49	110.90
1	A	316	VAL	CA-CB-CG1	6.38	120.47	110.90
1	D	215	VAL	CA-CB-CG1	6.37	120.46	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	373	ARG	CG-CD-NE	-6.37	98.43	111.80
1	A	353	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	371	TYR	CB-CG-CD2	6.32	124.79	121.00
1	F	352	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	E	74	VAL	CA-CB-CG1	6.31	120.36	110.90
1	B	164	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	279	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	F	19	PHE	CA-C-O	6.25	133.22	120.10
1	B	19	PHE	O-C-N	-6.24	112.72	122.70
1	D	207	ARG	CA-C-O	-6.23	107.03	120.10
1	E	120	ARG	CG-CD-NE	6.20	124.83	111.80
1	C	11	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	C	369	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	215	VAL	CA-CB-CG1	6.16	120.14	110.90
1	D	74	VAL	N-CA-CB	-6.15	97.96	111.50
1	B	20	THR	N-CA-CB	-6.15	98.61	110.30
1	C	53	ARG	NH1-CZ-NH2	6.15	126.17	119.40
1	F	316	VAL	CG1-CB-CG2	6.15	120.73	110.90
1	F	215	VAL	CA-CB-CG1	6.12	120.09	110.90
1	D	237	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	369	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	295	PHE	CB-CG-CD2	-6.09	116.54	120.80
1	D	207	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	C	74	VAL	N-CA-CB	-6.06	98.16	111.50
1	D	25	PRO	CA-N-CD	6.06	120.18	111.70
1	F	21	GLY	N-CA-C	6.05	128.22	113.10
1	C	21	GLY	N-CA-C	6.00	128.10	113.10
1	C	345	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	E	352	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	301	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	237	ARG	CD-NE-CZ	5.95	131.93	123.60
1	D	25	PRO	CA-C-O	5.90	134.35	120.20
1	B	63	LEU	CB-CG-CD2	5.89	121.01	111.00
1	D	268	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	271	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	21	GLY	N-CA-C	5.86	127.75	113.10
1	A	365	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	E	261	LEU	CA-CB-CG	5.84	128.74	115.30
1	F	74	VAL	CG1-CB-CG2	5.83	120.23	110.90
1	E	74	VAL	N-CA-CB	-5.82	98.69	111.50
1	B	371	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	163	VAL	CG1-CB-CG2	5.81	120.19	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	353	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	E	312	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	D	279	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	146	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	C	301	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	316	VAL	CG1-CB-CG2	5.73	120.07	110.90
1	A	373	ARG	CG-CD-NE	-5.72	99.79	111.80
1	F	95	ASP	CB-CG-OD1	5.71	123.44	118.30
1	F	145	THR	N-CA-CB	5.71	121.14	110.30
1	E	215	VAL	CA-CB-CG1	5.69	119.44	110.90
1	D	53	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	E	223	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	74	VAL	CB-CA-C	5.66	122.15	111.40
1	A	215	VAL	CA-CB-CG1	5.65	119.38	110.90
1	F	31	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	D	261	LEU	CA-CB-CG	5.62	128.22	115.30
1	C	363	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	11	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	E	316	VAL	CG1-CB-CG2	5.58	119.82	110.90
1	E	373	ARG	CG-CD-NE	-5.58	100.09	111.80
1	C	301	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	120	ARG	CG-CD-NE	5.56	123.48	111.80
1	E	345	ASP	CB-CG-OD1	5.55	123.29	118.30
1	E	362	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	75	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	E	120	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	373	ARG	CG-CD-NE	-5.51	100.23	111.80
1	D	164	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	E	21	GLY	N-CA-C	5.50	126.86	113.10
1	D	21	GLY	N-CA-C	5.49	126.83	113.10
1	E	14	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	125	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	F	177	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	A	330	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	363	ARG	CD-NE-CZ	5.42	131.19	123.60
1	B	74	VAL	CB-CA-C	5.41	121.68	111.40
1	B	150	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	74	VAL	CB-CA-C	5.38	121.62	111.40
1	F	272	ARG	CG-CD-NE	5.37	123.07	111.80
1	C	146	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	D	24	GLY	N-CA-C	-5.35	99.73	113.10
1	B	373	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	237	ARG	CD-NE-CZ	5.31	131.03	123.60
1	B	53	ARG	NH1-CZ-NH2	5.28	125.21	119.40
1	A	316	VAL	CG1-CB-CG2	5.25	119.31	110.90
1	D	63	LEU	CA-CB-CG	5.25	127.38	115.30
1	F	325	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	C	100	LEU	CA-CB-CG	5.24	127.34	115.30
1	F	261	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	20	THR	N-CA-CB	-5.20	100.42	110.30
1	E	363	ARG	CD-NE-CZ	5.20	130.88	123.60
1	B	168	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	F	20	THR	N-CA-CB	-5.15	100.52	110.30
1	E	11	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	272	ARG	CG-CD-NE	5.14	122.59	111.80
1	E	74	VAL	CB-CA-C	5.13	121.16	111.40
1	B	272	ARG	CG-CD-NE	5.12	122.56	111.80
1	D	272	ARG	CG-CD-NE	5.12	122.54	111.80
1	C	80	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	316	VAL	CA-CB-CG1	5.09	118.53	110.90
1	F	80	ARG	NH1-CZ-NH2	5.08	124.99	119.40
1	A	301	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	74	VAL	CG1-CB-CG2	5.07	119.02	110.90
1	B	261	LEU	CA-CB-CG	5.04	126.90	115.30
1	F	352	ASP	CB-CG-OD2	5.04	122.83	118.30
1	F	200	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	A	363	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	100	LEU	CB-CA-C	-5.01	100.69	110.20
1	D	206	GLY	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	PHE	Peptide
1	D	19	PHE	Peptide
1	D	206	GLY	Mainchain
1	E	19	PHE	Peptide
1	E	317	ASN	Sidechain,Mainchain

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	A	2747	0	2683	40	0
1	B	2747	0	2683	38	0
1	C	2747	0	2683	41	0
1	D	2747	0	2682	54	5
1	E	2747	0	2683	65	3
1	F	2747	0	2683	37	0
2	A	220	0	0	2	0
2	B	220	0	0	4	0
2	C	230	0	0	8	5
2	D	216	0	0	10	0
2	E	207	0	0	9	4
2	F	211	0	0	5	1
All	All	17786	0	16097	235	9

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 7.

All (235) 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:317:ASN:CA	1:E:317:ASN:CB	1.76	1.55
1:E:317:ASN:C	1:E:317:ASN:CB	1.90	1.39
1:E:317:ASN:HB3	1:E:318:ASP:N	1.42	1.31
1:D:25:PRO:HB2	1:D:31:ASP:OD1	1.43	1.18
1:E:317:ASN:CB	1:E:318:ASP:N	2.01	1.17
1:E:92:TRP:CH2	2:E:798:HOH:O	2.03	1.10
1:A:373:ARG:NH2	1:C:373:ARG:HH22	1.50	1.09
1:B:373:ARG:NH2	1:D:373:ARG:HH22	1.51	1.08
1:A:373:ARG:HH22	1:C:373:ARG:NH2	1.52	1.06
1:E:373:ARG:NH2	1:F:373:ARG:HH22	1.56	1.03
1:B:373:ARG:HH22	1:D:373:ARG:NH2	1.57	1.01
1:E:92:TRP:CH2	1:E:96:GLY:HA2	1.94	1.01
1:E:373:ARG:HH22	1:F:373:ARG:NH2	1.58	1.01
1:E:92:TRP:CZ3	2:E:798:HOH:O	2.16	0.99
1:F:244:GLN:HE22	1:F:355:LEU:H	1.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:MET:HB3	2:D:459:HOH:O	1.69	0.93
1:D:25:PRO:CB	1:D:31:ASP:OD1	2.19	0.91
1:E:317:ASN:C	1:E:317:ASN:HB3	1.73	0.90
1:A:109:HIS:HE1	1:D:138:ILE:H	1.18	0.88
1:A:299:ASN:HD21	1:A:314:GLU:H	1.18	0.88
1:F:20:THR:OG1	1:F:200:ARG:NH2	2.07	0.88
1:E:299:ASN:HD21	1:E:314:GLU:H	1.21	0.87
1:E:373:ARG:HH22	1:F:373:ARG:HH22	0.86	0.86
1:B:33:ASP:OD1	2:B:422:HOH:O	1.94	0.85
1:B:138:ILE:H	1:C:109:HIS:HE1	1.20	0.85
1:A:138:ILE:H	1:D:109:HIS:HE1	1.23	0.85
1:B:109:HIS:HE1	1:C:138:ILE:H	1.22	0.84
1:E:92:TRP:CH2	1:E:96:GLY:CA	2.60	0.83
1:D:33:ASP:OD1	2:D:427:HOH:O	1.95	0.83
1:E:112:GLY:N	2:E:868:HOH:O	2.06	0.83
1:B:349:THR:HB	1:B:350:PRO:HD2	1.60	0.83
1:E:92:TRP:CZ2	2:E:798:HOH:O	2.24	0.82
1:B:299:ASN:HD21	1:B:314:GLU:H	1.26	0.82
1:C:299:ASN:HD21	1:C:314:GLU:H	1.27	0.82
1:B:244:GLN:HE22	1:B:355:LEU:H	1.25	0.81
1:C:244:GLN:HE22	1:C:355:LEU:H	1.28	0.81
1:D:258:ASP:HA	1:D:297:THR:HG22	1.63	0.81
1:A:244:GLN:HE22	1:A:355:LEU:H	1.29	0.80
1:D:244:GLN:HE22	1:D:355:LEU:H	1.31	0.79
1:C:33:ASP:OD1	2:C:425:HOH:O	2.00	0.79
1:E:317:ASN:HB3	1:E:318:ASP:CA	2.12	0.78
1:F:262:MET:H	1:F:265:GLN:HE21	1.30	0.78
1:D:299:ASN:HD21	1:D:314:GLU:H	1.28	0.78
1:E:244:GLN:HE22	1:E:355:LEU:H	1.32	0.77
1:E:262:MET:H	1:E:265:GLN:HE21	1.33	0.77
1:B:20:THR:OG1	1:B:200:ARG:NH2	2.17	0.77
1:E:33:ASP:OD1	2:E:788:HOH:O	2.02	0.77
1:F:299:ASN:HD21	1:F:314:GLU:H	1.31	0.76
1:C:20:THR:OG1	1:C:200:ARG:NH2	2.18	0.76
1:A:373:ARG:NH1	1:C:373:ARG:NH1	2.33	0.76
1:D:20:THR:OG1	1:D:200:ARG:NH2	2.20	0.75
1:E:317:ASN:HB3	1:E:319:GLU:N	2.01	0.75
1:E:92:TRP:CZ3	1:E:96:GLY:N	2.56	0.74
1:C:258:ASP:HA	1:C:297:THR:HG22	1.71	0.73
1:E:317:ASN:O	1:E:317:ASN:CB	2.36	0.73
1:C:297:THR:HG21	2:C:425:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:MET:H	1:A:265:GLN:HE21	1.35	0.73
1:B:262:MET:H	1:B:265:GLN:HE21	1.36	0.73
1:E:258:ASP:HA	1:E:297:THR:HG22	1.71	0.73
1:C:33:ASP:OD1	2:C:538:HOH:O	2.07	0.72
1:C:262:MET:H	1:C:265:GLN:HE21	1.36	0.72
1:A:373:ARG:NH1	1:C:373:ARG:HH12	1.87	0.72
1:B:297:THR:HG21	2:B:422:HOH:O	1.90	0.71
1:A:258:ASP:HA	1:A:297:THR:HG22	1.71	0.71
1:A:373:ARG:HH12	1:C:373:ARG:NH1	1.89	0.70
1:A:373:ARG:HH22	1:C:373:ARG:HH22	0.75	0.70
1:B:258:ASP:HA	1:B:297:THR:HG22	1.74	0.70
1:B:33:ASP:OD1	2:B:532:HOH:O	2.09	0.70
1:E:20:THR:OG1	1:E:200:ARG:NH2	2.25	0.69
1:E:33:ASP:OD1	2:E:906:HOH:O	2.10	0.69
1:A:20:THR:OG1	1:A:200:ARG:NH2	2.26	0.68
1:A:109:HIS:CE1	1:D:138:ILE:H	2.08	0.68
1:D:297:THR:HG21	2:D:427:HOH:O	1.94	0.68
1:D:262:MET:H	1:D:265:GLN:HE21	1.39	0.67
1:E:297:THR:HG21	2:E:788:HOH:O	1.95	0.67
1:D:203:GLU:OE2	1:D:206:GLY:HA2	1.95	0.67
1:E:317:ASN:HB3	1:E:319:GLU:H	1.61	0.66
1:F:258:ASP:HA	1:F:297:THR:HG22	1.78	0.66
1:B:109:HIS:CE1	1:C:138:ILE:H	2.11	0.66
1:C:20:THR:CB	1:C:200:ARG:HH21	2.09	0.66
1:B:297:THR:CG2	2:B:422:HOH:O	2.44	0.65
1:E:373:ARG:NH1	1:F:373:ARG:NH1	2.45	0.65
1:A:20:THR:CB	1:A:200:ARG:HH21	2.09	0.65
1:D:297:THR:CG2	2:D:427:HOH:O	2.46	0.64
1:C:323:THR:HG23	2:C:603:HOH:O	1.98	0.63
1:F:242:GLN:HB2	2:F:581:HOH:O	1.99	0.63
1:D:25:PRO:CG	1:D:31:ASP:OD1	2.47	0.62
1:D:25:PRO:HG2	1:D:31:ASP:OD1	2.00	0.62
1:C:204:PHE:CE1	1:C:316:VAL:HG22	2.35	0.61
1:E:317:ASN:HB3	1:E:318:ASP:C	2.21	0.60
1:C:349:THR:HB	1:C:350:PRO:HD2	1.83	0.60
1:B:138:ILE:H	1:C:109:HIS:CE1	2.12	0.59
1:B:349:THR:HB	1:B:350:PRO:CD	2.29	0.59
1:E:297:THR:CG2	2:E:788:HOH:O	2.51	0.59
1:D:20:THR:CB	1:D:200:ARG:HH21	2.16	0.59
1:E:92:TRP:CE2	1:E:96:GLY:HA3	2.38	0.58
1:E:20:THR:CB	1:E:200:ARG:HH21	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ARG:NH2	1:F:373:ARG:NH2	2.32	0.58
1:E:92:TRP:HZ3	1:E:95:ASP:HB3	1.68	0.58
1:E:92:TRP:CZ2	1:E:96:GLY:CA	2.87	0.58
1:B:204:PHE:CE1	1:B:316:VAL:HG22	2.38	0.58
1:D:204:PHE:CE1	1:D:316:VAL:HG22	2.39	0.58
1:C:262:MET:H	1:C:265:GLN:NE2	2.01	0.57
1:E:204:PHE:CE1	1:E:316:VAL:HG22	2.39	0.57
1:C:297:THR:CG2	2:C:425:HOH:O	2.47	0.57
1:E:92:TRP:HA	1:E:92:TRP:CE3	2.41	0.56
1:A:138:ILE:H	1:D:109:HIS:CE1	2.13	0.56
1:F:204:PHE:CE1	1:F:316:VAL:HG22	2.40	0.56
1:A:19:PHE:HD1	1:A:20:THR:HG1	1.54	0.56
1:D:25:PRO:HG3	2:D:490:HOH:O	2.04	0.56
1:E:317:ASN:CB	1:E:319:GLU:H	2.18	0.56
1:D:25:PRO:CG	2:D:490:HOH:O	2.53	0.55
1:A:319:GLU:HB3	1:A:320:PRO:HD3	1.88	0.55
1:D:323:THR:HG23	2:D:590:HOH:O	2.05	0.55
1:C:20:THR:HG1	1:C:200:ARG:NH2	2.04	0.55
1:E:92:TRP:CE2	2:E:798:HOH:O	2.57	0.55
1:E:272:ARG:HD2	1:F:283:PRO:O	2.07	0.54
1:D:114:ALA:HA	1:D:163:VAL:HG11	1.90	0.54
1:B:373:ARG:HH22	1:D:373:ARG:HH22	0.71	0.54
1:F:319:GLU:HB3	1:F:320:PRO:HD3	1.90	0.54
1:B:20:THR:HG1	1:B:200:ARG:NH2	2.05	0.54
1:E:165:LYS:HD3	1:E:169:ASN:HD21	1.73	0.54
1:D:349:THR:HB	1:D:350:PRO:CD	2.37	0.54
1:F:20:THR:CB	1:F:200:ARG:HH21	2.21	0.53
1:E:92:TRP:CZ2	1:E:96:GLY:HA3	2.44	0.53
1:C:349:THR:HB	1:C:350:PRO:CD	2.38	0.53
1:B:137:TRP:HB2	1:C:108:THR:HG21	1.90	0.53
1:D:349:THR:HB	1:D:350:PRO:HD2	1.89	0.53
1:D:262:MET:H	1:D:265:GLN:NE2	2.07	0.52
1:A:204:PHE:CE1	1:A:316:VAL:HG22	2.45	0.52
1:F:262:MET:H	1:F:265:GLN:NE2	2.01	0.52
1:A:262:MET:H	1:A:265:GLN:NE2	2.05	0.52
1:D:20:THR:HG21	2:D:419:HOH:O	2.08	0.52
1:C:366:ALA:O	1:C:370:GLN:HG3	2.10	0.52
1:E:317:ASN:CB	1:E:318:ASP:H	2.16	0.52
1:A:33:ASP:HB2	2:F:572:HOH:O	2.09	0.51
1:E:92:TRP:CZ3	1:E:96:GLY:CA	2.93	0.51
1:D:33:ASP:N	1:D:33:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLU:HB3	1:B:320:PRO:HD3	1.93	0.51
1:B:230:VAL:HG22	1:B:373:ARG:NH1	2.26	0.51
1:A:299:ASN:ND2	1:A:314:GLU:H	1.96	0.51
1:F:20:THR:HG21	2:F:420:HOH:O	2.10	0.50
1:E:92:TRP:CZ2	1:E:96:GLY:HA2	2.41	0.50
1:E:114:ALA:HA	1:E:163:VAL:HG11	1.94	0.50
1:A:373:ARG:NH2	1:C:373:ARG:NH2	2.30	0.50
1:F:20:THR:HG1	1:F:200:ARG:NH2	2.06	0.50
1:A:137:TRP:HB2	1:D:108:THR:HG21	1.94	0.50
1:A:305:HIS:HE1	2:A:436:HOH:O	1.95	0.50
1:D:73:PRO:HA	1:D:100:LEU:HD13	1.94	0.50
1:E:262:MET:H	1:E:265:GLN:NE2	2.04	0.49
1:B:20:THR:CB	1:B:200:ARG:HH21	2.25	0.49
1:E:349:THR:HB	1:E:350:PRO:CD	2.42	0.49
1:B:373:ARG:NH2	1:D:373:ARG:NH2	2.34	0.49
1:D:262:MET:CB	2:D:459:HOH:O	2.42	0.49
1:F:165:LYS:HD3	1:F:169:ASN:HD21	1.77	0.49
1:E:13:ARG:NH2	1:E:20:THR:O	2.46	0.48
1:C:12:ALA:H	1:C:338:ASN:ND2	2.11	0.48
1:F:12:ALA:H	1:F:338:ASN:ND2	2.11	0.48
1:E:230:VAL:HG22	1:E:373:ARG:NH1	2.28	0.48
1:E:74:VAL:HG13	1:E:295:PHE:HB2	1.95	0.48
1:B:262:MET:H	1:B:265:GLN:NE2	2.06	0.48
1:D:40:GLN:OE1	1:D:165:LYS:HD2	2.14	0.48
1:E:317:ASN:CB	1:E:319:GLU:N	2.75	0.48
1:E:165:LYS:HD3	1:E:169:ASN:ND2	2.28	0.47
1:F:354:LEU:N	1:F:354:LEU:HD12	2.29	0.47
1:E:92:TRP:CE3	1:E:96:GLY:N	2.81	0.47
1:D:12:ALA:H	1:D:338:ASN:ND2	2.12	0.47
1:A:354:LEU:HD12	1:A:354:LEU:N	2.30	0.47
1:C:114:ALA:HA	1:C:163:VAL:HG11	1.95	0.47
1:B:120:ARG:HG2	1:C:156:PHE:CZ	2.50	0.47
1:A:373:ARG:CZ	1:C:373:ARG:HH12	2.27	0.47
1:A:20:THR:HG21	2:A:409:HOH:O	2.15	0.47
1:E:299:ASN:ND2	1:E:314:GLU:H	2.00	0.46
1:E:20:THR:HG1	1:E:200:ARG:NH2	2.12	0.46
1:F:165:LYS:HD3	1:F:169:ASN:ND2	2.30	0.46
1:A:109:HIS:HE1	1:D:138:ILE:N	2.00	0.46
1:F:306:ARG:NH1	2:F:554:HOH:O	2.48	0.46
1:E:92:TRP:CZ3	1:E:95:ASP:HB3	2.50	0.46
1:B:138:ILE:N	1:C:109:HIS:HE1	2.01	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LYS:HD3	1:D:169:ASN:ND2	2.31	0.45
1:C:20:THR:HG21	2:C:417:HOH:O	2.16	0.45
1:B:108:THR:HG21	1:C:137:TRP:HB2	1.97	0.45
1:B:373:ARG:NH1	1:D:373:ARG:NH1	2.64	0.45
1:D:305:HIS:HE1	2:D:448:HOH:O	1.99	0.45
1:F:114:ALA:HA	1:F:163:VAL:HG11	1.99	0.45
1:B:373:ARG:HH12	1:D:373:ARG:CZ	2.30	0.45
1:A:349:THR:HB	1:A:350:PRO:CD	2.47	0.45
1:E:349:THR:HB	1:E:350:PRO:HD2	1.98	0.45
1:D:165:LYS:HD3	1:D:169:ASN:HD21	1.82	0.45
1:B:215:VAL:HG22	1:B:253:VAL:HG22	1.98	0.44
1:A:257:THR:O	1:A:296:SER:HA	2.17	0.44
1:F:146:TYR:CZ	1:F:148:GLY:HA3	2.52	0.44
1:F:73:PRO:HA	1:F:100:LEU:HD13	1.98	0.44
1:F:349:THR:HB	1:F:350:PRO:HD2	1.98	0.44
1:A:74:VAL:HG13	1:A:295:PHE:HB2	2.00	0.44
1:F:238:ASP:CG	1:F:363:ARG:HH22	2.21	0.44
1:A:373:ARG:HH12	1:C:373:ARG:CZ	2.31	0.44
1:D:73:PRO:HG3	1:D:100:LEU:HD11	1.99	0.44
1:C:354:LEU:HD12	1:C:354:LEU:N	2.33	0.43
1:E:20:THR:HB	1:E:200:ARG:HH21	1.83	0.43
1:E:373:ARG:NH1	1:F:373:ARG:HH12	2.16	0.43
1:F:374:LEU:HD12	1:F:374:LEU:HA	1.88	0.43
1:C:74:VAL:HG13	1:C:295:PHE:HB2	1.99	0.43
1:E:373:ARG:HH12	1:F:373:ARG:NH1	2.16	0.42
1:E:33:ASP:N	1:E:33:ASP:OD1	2.51	0.42
1:D:20:THR:HG1	1:D:200:ARG:NH2	2.17	0.42
1:A:13:ARG:NH2	1:A:20:THR:O	2.50	0.42
1:B:114:ALA:HA	1:B:163:VAL:HG11	2.01	0.42
1:E:374:LEU:HA	1:E:374:LEU:HD12	1.93	0.42
1:D:25:PRO:HB2	1:D:26:TYR:H	1.07	0.42
1:A:349:THR:HB	1:A:350:PRO:HD2	2.02	0.42
1:D:203:GLU:HG3	1:D:206:GLY:C	2.39	0.42
1:F:230:VAL:HG22	1:F:373:ARG:NH1	2.35	0.42
1:B:299:ASN:ND2	1:B:314:GLU:H	2.06	0.42
1:E:373:ARG:HH12	1:F:373:ARG:CZ	2.33	0.41
1:B:257:THR:O	1:B:296:SER:HA	2.20	0.41
1:E:12:ALA:H	1:E:338:ASN:ND2	2.17	0.41
1:D:374:LEU:HA	1:D:374:LEU:HD12	1.88	0.41
1:D:349:THR:CB	1:D:350:PRO:CD	2.99	0.41
1:C:305:HIS:HE1	2:C:446:HOH:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HG2	1:D:156:PHE:CZ	2.55	0.41
1:F:13:ARG:NH2	1:F:20:THR:O	2.46	0.41
1:D:315:MET:HB3	1:D:315:MET:HE2	1.95	0.41
1:A:165:LYS:HD3	1:A:169:ASN:HD21	1.86	0.41
1:A:114:ALA:HA	1:A:163:VAL:HG11	2.02	0.41
1:C:354:LEU:HD12	2:C:514:HOH:O	2.20	0.41
1:F:354:LEU:H	1:F:354:LEU:HD12	1.86	0.41
1:A:165:LYS:HD3	1:A:169:ASN:ND2	2.36	0.41
1:B:33:ASP:N	1:B:33:ASP:OD1	2.54	0.41
1:B:147:ASP:HB3	1:B:186:MET:CE	2.51	0.40
1:D:74:VAL:HG13	1:D:295:PHE:HB2	2.04	0.40
1:A:366:ALA:O	1:A:370:GLN:HG3	2.21	0.40
1:B:373:ARG:CZ	1:D:373:ARG:HH22	2.26	0.40
1:F:265:GLN:HE22	1:F:315:MET:HG3	1.86	0.40
1:F:33:ASP:HA	2:F:572:HOH:O	2.22	0.40

All (9) 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)
1:E:317:ASN:CA	2:E:899:HOH:O[2_665]	1.71	0.49
1:D:25:PRO:CA	2:C:573:HOH:O[3_545]	1.88	0.32
1:E:317:ASN:CB	2:E:899:HOH:O[2_665]	1.94	0.26
1:D:33:ASP:OD1	2:C:589:HOH:O[3_545]	1.95	0.25
2:E:868:HOH:O	2:F:511:HOH:O[2_665]	1.95	0.25
1:D:25:PRO:CB	2:C:573:HOH:O[3_545]	2.03	0.17
1:D:207:ARG:N	2:C:566:HOH:O[3_545]	2.10	0.10
1:D:206:GLY:O	2:C:566:HOH:O[3_545]	2.15	0.05
1:E:317:ASN:CG	2:E:899:HOH:O[2_665]	2.15	0.05

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	A	359/375 (96%)	348 (97%)	9 (2%)	2 (1%)	30 14
1	B	359/375 (96%)	349 (97%)	9 (2%)	1 (0%)	46 29
1	C	359/375 (96%)	347 (97%)	10 (3%)	2 (1%)	30 14
1	D	359/375 (96%)	348 (97%)	8 (2%)	3 (1%)	24 8
1	E	359/375 (96%)	346 (96%)	11 (3%)	2 (1%)	30 14
1	F	359/375 (96%)	350 (98%)	7 (2%)	2 (1%)	30 14
All	All	2154/2250 (96%)	2088 (97%)	54 (2%)	12 (1%)	30 14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	25	PRO
1	A	21	GLY
1	B	21	GLY
1	C	21	GLY
1	D	20	THR
1	D	21	GLY
1	E	20	THR
1	E	21	GLY
1	F	21	GLY
1	A	20	THR
1	C	20	THR
1	F	20	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	286/297 (96%)	269 (94%)	17 (6%)	24 8
1	B	286/297 (96%)	269 (94%)	17 (6%)	24 8
1	C	286/297 (96%)	271 (95%)	15 (5%)	29 11
1	D	286/297 (96%)	272 (95%)	14 (5%)	31 13
1	E	286/297 (96%)	270 (94%)	16 (6%)	26 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	286/297 (96%)	269 (94%)	17 (6%)	24 8
All	All	1716/1782 (96%)	1620 (94%)	96 (6%)	26 10

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	63	LEU
1	A	74	VAL
1	A	100	LEU
1	A	133	ASP
1	A	136	LEU
1	A	150	LEU
1	A	163	VAL
1	A	165	LYS
1	A	215	VAL
1	A	261	LEU
1	A	297	THR
1	A	316	VAL
1	A	319	GLU
1	A	354	LEU
1	A	364	LEU
1	A	373	ARG
1	B	9	LYS
1	B	63	LEU
1	B	74	VAL
1	B	100	LEU
1	B	133	ASP
1	B	136	LEU
1	B	150	LEU
1	B	163	VAL
1	B	165	LYS
1	B	215	VAL
1	B	261	LEU
1	B	297	THR
1	B	316	VAL
1	B	319	GLU
1	B	354	LEU
1	B	364	LEU
1	B	373	ARG
1	C	63	LEU
1	C	74	VAL

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Mol	Chain	Res	Type
1	C	100	LEU
1	C	133	ASP
1	C	136	LEU
1	C	150	LEU
1	C	165	LYS
1	C	215	VAL
1	C	261	LEU
1	C	297	THR
1	C	313	VAL
1	C	316	VAL
1	C	354	LEU
1	C	364	LEU
1	C	373	ARG
1	D	63	LEU
1	D	74	VAL
1	D	100	LEU
1	D	133	ASP
1	D	136	LEU
1	D	150	LEU
1	D	165	LYS
1	D	215	VAL
1	D	261	LEU
1	D	297	THR
1	D	316	VAL
1	D	354	LEU
1	D	364	LEU
1	D	373	ARG
1	E	63	LEU
1	E	74	VAL
1	E	100	LEU
1	E	133	ASP
1	E	136	LEU
1	E	150	LEU
1	E	163	VAL
1	E	165	LYS
1	E	215	VAL
1	E	261	LEU
1	E	297	THR
1	E	316	VAL
1	E	317	ASN
1	E	354	LEU
1	E	364	LEU

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Mol	Chain	Res	Type
1	E	373	ARG
1	F	9	LYS
1	F	63	LEU
1	F	74	VAL
1	F	100	LEU
1	F	133	ASP
1	F	136	LEU
1	F	150	LEU
1	F	163	VAL
1	F	165	LYS
1	F	215	VAL
1	F	261	LEU
1	F	297	THR
1	F	316	VAL
1	F	319	GLU
1	F	354	LEU
1	F	364	LEU
1	F	373	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	82	ASN
1	A	109	HIS
1	A	131	GLN
1	A	221	GLN
1	A	244	GLN
1	A	265	GLN
1	A	280	ASN
1	A	299	ASN
1	A	305	HIS
1	A	317	ASN
1	A	338	ASN
1	B	79	HIS
1	B	82	ASN
1	B	109	HIS
1	B	131	GLN
1	B	221	GLN
1	B	234	GLN
1	B	244	GLN
1	B	265	GLN

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Mol	Chain	Res	Type
1	B	280	ASN
1	B	299	ASN
1	B	305	HIS
1	B	317	ASN
1	B	338	ASN
1	C	79	HIS
1	C	82	ASN
1	C	109	HIS
1	C	131	GLN
1	C	169	ASN
1	C	221	GLN
1	C	234	GLN
1	C	244	GLN
1	C	265	GLN
1	C	299	ASN
1	C	305	HIS
1	C	317	ASN
1	C	338	ASN
1	D	79	HIS
1	D	82	ASN
1	D	109	HIS
1	D	131	GLN
1	D	169	ASN
1	D	221	GLN
1	D	234	GLN
1	D	244	GLN
1	D	265	GLN
1	D	280	ASN
1	D	299	ASN
1	D	305	HIS
1	D	317	ASN
1	D	338	ASN
1	E	79	HIS
1	E	82	ASN
1	E	109	HIS
1	E	131	GLN
1	E	221	GLN
1	E	234	GLN
1	E	244	GLN
1	E	265	GLN
1	E	280	ASN
1	E	299	ASN

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Mol	Chain	Res	Type
1	E	300	GLN
1	E	305	HIS
1	E	338	ASN
1	F	79	HIS
1	F	82	ASN
1	F	109	HIS
1	F	131	GLN
1	F	169	ASN
1	F	221	GLN
1	F	234	GLN
1	F	244	GLN
1	F	265	GLN
1	F	280	ASN
1	F	299	ASN
1	F	305	HIS
1	F	317	ASN
1	F	338	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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 (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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.