Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 11:02 AM EDT

PDB ID	:	2AAA
Title	:	CALCIUM BINDING IN ALPHA-AMYLASES: AN X-RAY DIFFRACTION STUDY AT 2.1 ANGSTROMS RESOLUTION OF TWO ENZYMES FROM ASPERGILLUS
Authors	:	Brady, L.; Brzozowski, A.M.; Derewenda, Z.; Dodson, E.J.; Dodson, G.G.
Deposited on	:	1991-02-27
Resolution	:	2.12 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:

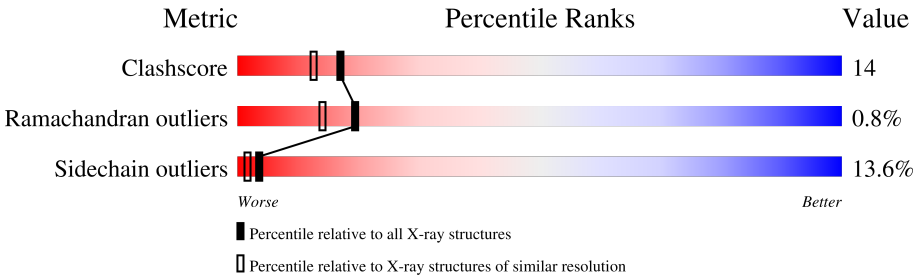
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.12 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	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	484	47% 34% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4021 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	3669	2321	580	751	17	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	2	2	2	0	0

- Molecule 3 is water.

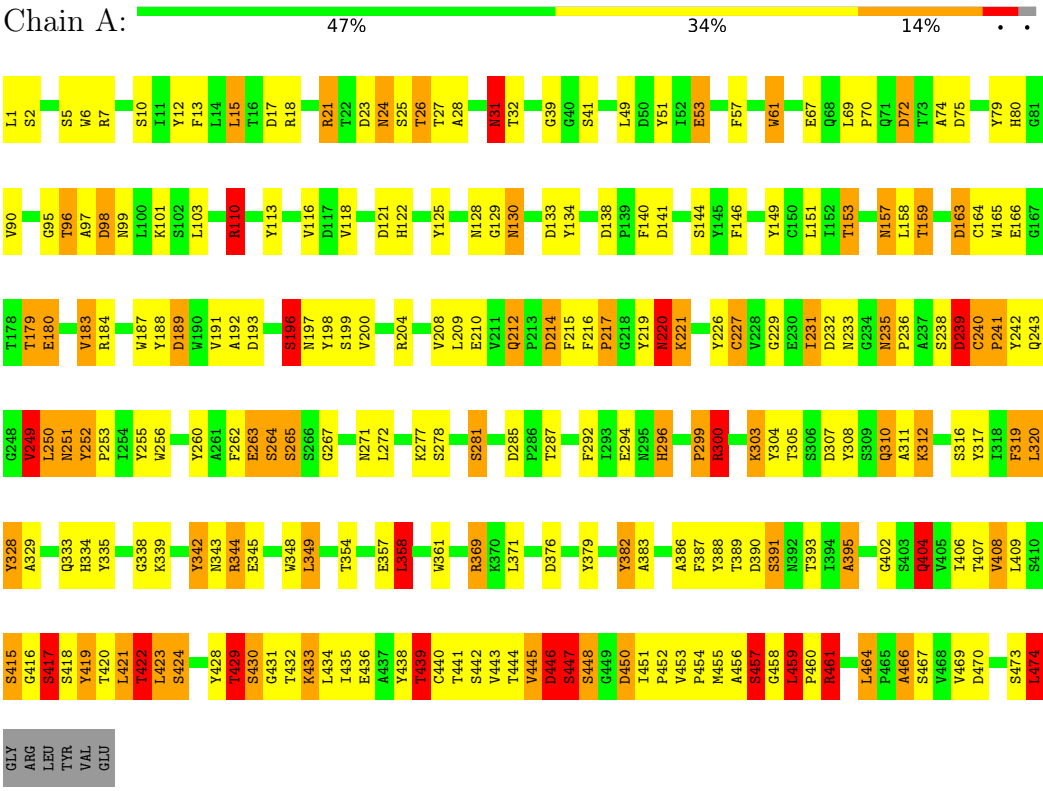
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	350	350	350	0	0

3 Residue-property plots (i)

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

- Molecule 1: ALPHA-AMYLASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	81.10Å 98.30Å 138.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.12 24.57 – 2.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.12) 97.7 (24.57-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	19.71 (at 2.11Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available) 0.361 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 95.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.68	EDS
Total number of atoms	4021	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.28	6/3764 (0.2%)	2.71	307/5149 (6.0%)

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	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	ASP	N-CA	8.42	1.63	1.46
1	A	2	SER	CB-OG	6.81	1.51	1.42
1	A	476	GLY	C-O	6.75	1.34	1.23
1	A	238	SER	CB-OG	5.87	1.49	1.42
1	A	180	GLU	CD-OE1	-5.50	1.19	1.25
1	A	391	SER	CA-CB	5.09	1.60	1.52

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	ASN	CA-CB-CG	23.12	164.27	113.40
1	A	110	ARG	NE-CZ-NH1	20.86	130.73	120.30
1	A	247	ASP	N-CA-CB	20.38	147.28	110.60
1	A	239	ASP	CB-CA-C	19.24	148.88	110.40
1	A	304	TYR	CB-CG-CD2	-18.73	109.76	121.00
1	A	461	ARG	NE-CZ-NH2	16.28	128.44	120.30
1	A	450	ASP	CB-CG-OD2	-15.70	104.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	ARG	NE-CZ-NH1	-15.27	112.67	120.30
1	A	439	THR	CA-CB-CG2	15.04	133.46	112.40
1	A	239	ASP	CB-CG-OD1	-14.94	104.85	118.30
1	A	216	PHE	CB-CG-CD1	-14.92	110.36	120.80
1	A	450	ASP	CB-CG-OD1	14.82	131.64	118.30
1	A	189	ASP	CB-CG-OD2	14.70	131.53	118.30
1	A	369	ARG	NE-CZ-NH1	13.78	127.19	120.30
1	A	239	ASP	N-CA-CB	-13.66	86.00	110.60
1	A	138	ASP	CB-CG-OD2	13.22	130.19	118.30
1	A	357	GLU	OE1-CD-OE2	12.59	138.41	123.30
1	A	246	LEU	CA-C-N	12.45	144.59	117.20
1	A	439	THR	N-CA-CB	-12.18	87.16	110.30
1	A	307	ASP	CB-CG-OD2	12.15	129.24	118.30
1	A	388	TYR	CB-CG-CD1	-11.86	113.89	121.00
1	A	308	TYR	CB-CG-CD2	11.81	128.09	121.00
1	A	304	TYR	CB-CG-CD1	11.81	128.09	121.00
1	A	464	LEU	CA-CB-CG	11.70	142.21	115.30
1	A	344	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	A	110	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	A	300	ARG	CA-CB-CG	11.41	138.51	113.40
1	A	220	ASN	OD1-CG-ND2	-11.37	95.75	121.90
1	A	7	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	A	210	GLU	OE1-CD-OE2	-11.18	109.89	123.30
1	A	18	ARG	NE-CZ-NH2	11.13	125.86	120.30
1	A	177	ASP	CB-CG-OD2	-10.96	108.43	118.30
1	A	252	TYR	CB-CG-CD1	-10.85	114.49	121.00
1	A	134	TYR	CB-CG-CD2	-10.83	114.50	121.00
1	A	246	LEU	O-C-N	-10.78	105.45	122.70
1	A	446	ASP	CB-CG-OD2	10.76	127.98	118.30
1	A	189	ASP	CB-CG-OD1	-10.64	108.72	118.30
1	A	476	GLY	CA-C-O	-10.62	101.47	120.60
1	A	308	TYR	CB-CG-CD1	-10.61	114.63	121.00
1	A	239	ASP	O-C-N	-10.55	105.83	122.70
1	A	17	ASP	CB-CG-OD2	10.18	127.46	118.30
1	A	168	ASP	CB-CG-OD1	9.99	127.29	118.30
1	A	445	VAL	C-N-CA	9.78	146.14	121.70
1	A	122	HIS	C-N-CA	9.73	146.03	121.70
1	A	312	LYS	CB-CG-CD	9.71	136.85	111.60
1	A	198	TYR	CB-CG-CD1	-9.66	115.20	121.00
1	A	210	GLU	CG-CD-OE1	9.62	137.54	118.30
1	A	121	ASP	CB-CG-OD2	9.51	126.86	118.30
1	A	188	TYR	CB-CG-CD1	9.44	126.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	PHE	CB-CG-CD1	9.42	127.39	120.80
1	A	188	TYR	CB-CG-CD2	-9.41	115.35	121.00
1	A	292	PHE	CB-CG-CD2	9.33	127.33	120.80
1	A	90	VAL	CA-CB-CG2	9.29	124.84	110.90
1	A	163	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	262	PHE	CB-CG-CD2	9.14	127.20	120.80
1	A	39	GLY	N-CA-C	9.08	135.80	113.10
1	A	423	LEU	CA-C-O	8.86	138.71	120.10
1	A	376	ASP	CB-CG-OD1	-8.70	110.47	118.30
1	A	184	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	A	212	GLN	OE1-CD-NE2	-8.57	102.19	121.90
1	A	446	ASP	OD1-CG-OD2	-8.55	107.05	123.30
1	A	212	GLN	CG-CD-OE1	8.54	138.68	121.60
1	A	382	TYR	CB-CG-CD1	-8.54	115.88	121.00
1	A	339	LYS	CB-CA-C	-8.52	93.36	110.40
1	A	220	ASN	CB-CG-ND2	8.47	137.04	116.70
1	A	307	ASP	OD1-CG-OD2	-8.44	107.27	123.30
1	A	220	ASN	N-CA-CB	8.36	125.64	110.60
1	A	153	THR	CA-CB-OG1	-8.27	91.63	109.00
1	A	247	ASP	CB-CG-OD2	8.23	125.71	118.30
1	A	129	GLY	CA-C-O	-8.22	105.80	120.60
1	A	200	VAL	CA-CB-CG2	-7.91	99.04	110.90
1	A	379	TYR	CB-CG-CD1	7.88	125.73	121.00
1	A	319	PHE	CB-CG-CD2	-7.88	115.29	120.80
1	A	386	ALA	N-CA-CB	7.87	121.12	110.10
1	A	169	THR	N-CA-CB	-7.85	95.39	110.30
1	A	357	GLU	CG-CD-OE2	-7.85	102.61	118.30
1	A	461	ARG	NH1-CZ-NH2	-7.83	110.79	119.40
1	A	12	TYR	CZ-CE2-CD2	-7.77	112.81	119.80
1	A	247	ASP	O-C-N	7.75	136.37	123.20
1	A	216	PHE	CB-CG-CD2	7.72	126.20	120.80
1	A	15	LEU	CA-CB-CG	7.69	133.00	115.30
1	A	82	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	A	183	VAL	CA-CB-CG1	7.64	122.36	110.90
1	A	422	THR	O-C-N	7.62	134.89	122.70
1	A	467	SER	N-CA-CB	-7.60	99.09	110.50
1	A	316	SER	O-C-N	-7.55	110.62	122.70
1	A	345	GLU	OE1-CD-OE2	7.54	132.35	123.30
1	A	263	GLU	CA-CB-CG	7.48	129.85	113.40
1	A	1	LEU	CA-CB-CG	7.47	132.49	115.30
1	A	226	TYR	CB-CG-CD2	-7.46	116.52	121.00
1	A	134	TYR	CB-CG-CD1	7.44	125.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	198	TYR	CB-CG-CD2	7.43	125.46	121.00
1	A	369	ARG	NH1-CZ-NH2	-7.41	111.25	119.40
1	A	417	SER	N-CA-CB	7.40	121.60	110.50
1	A	304	TYR	CG-CD2-CE2	-7.39	115.38	121.30
1	A	75	ASP	CB-CG-OD2	7.37	124.93	118.30
1	A	446	ASP	CB-CA-C	-7.35	95.70	110.40
1	A	88	TYR	CG-CD1-CE1	7.31	127.15	121.30
1	A	110	ARG	CD-NE-CZ	7.30	133.82	123.60
1	A	130	ASN	CA-CB-CG	-7.29	97.37	113.40
1	A	446	ASP	CB-CG-OD1	7.28	124.86	118.30
1	A	12	TYR	CG-CD1-CE1	-7.25	115.50	121.30
1	A	26	THR	N-CA-CB	-7.23	96.56	110.30
1	A	74	ALA	N-CA-CB	7.23	120.22	110.10
1	A	214	ASP	N-CA-CB	7.21	123.58	110.60
1	A	61	TRP	CA-CB-CG	7.21	127.39	113.70
1	A	264	SER	N-CA-CB	7.19	121.28	110.50
1	A	226	TYR	CG-CD1-CE1	-7.10	115.62	121.30
1	A	27	THR	CA-C-N	7.09	132.80	117.20
1	A	292	PHE	CB-CG-CD1	-7.08	115.85	120.80
1	A	28	ALA	CB-CA-C	7.07	120.70	110.10
1	A	25	SER	C-N-CA	7.06	139.36	121.70
1	A	424	SER	N-CA-CB	-7.04	99.94	110.50
1	A	474	LEU	CA-CB-CG	7.03	131.46	115.30
1	A	41	SER	O-C-N	7.01	133.91	122.70
1	A	196	SER	CB-CA-C	6.87	123.15	110.10
1	A	113	TYR	CB-CG-CD2	6.86	125.11	121.00
1	A	166	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	A	179	THR	CA-CB-OG1	-6.85	94.62	109.00
1	A	199	SER	CB-CA-C	-6.84	97.10	110.10
1	A	249	VAL	CA-CB-CG1	6.84	121.16	110.90
1	A	255	TYR	CG-CD2-CE2	6.83	126.77	121.30
1	A	149	TYR	CG-CD1-CE1	6.77	126.72	121.30
1	A	12	TYR	CG-CD2-CE2	6.77	126.72	121.30
1	A	214	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	A	445	VAL	CA-C-N	6.74	132.03	117.20
1	A	79	TYR	CG-CD1-CE1	-6.73	115.92	121.30
1	A	163	ASP	N-CA-CB	-6.72	98.50	110.60
1	A	445	VAL	N-CA-CB	-6.69	96.79	111.50
1	A	187	TRP	CB-CG-CD2	6.63	135.22	126.60
1	A	469	VAL	CA-CB-CG2	6.62	120.84	110.90
1	A	285	ASP	CB-CG-OD1	6.59	124.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	SER	O-C-N	-6.58	112.18	122.70
1	A	247	ASP	C-N-CA	-6.57	108.50	122.30
1	A	89	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	328	TYR	CB-CG-CD1	6.54	124.93	121.00
1	A	214	ASP	O-C-N	6.54	133.16	122.70
1	A	255	TYR	CZ-CE2-CD2	-6.54	113.91	119.80
1	A	379	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	A	88	TYR	CB-CG-CD2	6.53	124.92	121.00
1	A	247	ASP	N-CA-C	-6.53	93.38	111.00
1	A	79	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	A	199	SER	N-CA-CB	6.51	120.26	110.50
1	A	429	THR	O-C-N	6.51	133.11	122.70
1	A	382	TYR	CD1-CE1-CZ	-6.48	113.97	119.80
1	A	57	PHE	CG-CD2-CE2	-6.45	113.71	120.80
1	A	294	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	A	141	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	232	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	316	SER	CA-C-O	6.42	133.58	120.10
1	A	214	ASP	CA-C-O	-6.42	106.62	120.10
1	A	389	THR	N-CA-CB	6.41	122.47	110.30
1	A	344	ARG	CD-NE-CZ	-6.40	114.65	123.60
1	A	32	THR	CA-CB-CG2	-6.38	103.47	112.40
1	A	163	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	23	ASP	CA-C-O	-6.35	106.76	120.10
1	A	67	GLU	CG-CD-OE2	6.29	130.88	118.30
1	A	387	PHE	CB-CG-CD2	-6.28	116.40	120.80
1	A	247	ASP	CB-CA-C	-6.27	97.85	110.40
1	A	333	GLN	O-C-N	-6.27	112.67	122.70
1	A	474	LEU	C-N-CA	-6.23	106.13	121.70
1	A	404	GLN	CB-CG-CD	6.21	127.74	111.60
1	A	18	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
1	A	294	GLU	CA-CB-CG	6.19	127.01	113.40
1	A	294	GLU	CG-CD-OE2	6.18	130.67	118.30
1	A	256	TRP	CE3-CZ3-CH2	-6.16	114.42	121.20
1	A	245	VAL	N-CA-CB	-6.15	97.96	111.50
1	A	382	TYR	N-CA-CB	-6.10	99.61	110.60
1	A	116	VAL	CG1-CB-CG2	-6.10	101.14	110.90
1	A	82	TYR	CG-CD1-CE1	-6.08	116.43	121.30
1	A	342	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	21	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	459	LEU	N-CA-CB	-6.04	98.32	110.40
1	A	382	TYR	CD1-CG-CD2	6.03	124.53	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	474	LEU	N-CA-C	-6.03	94.73	111.00
1	A	82	TYR	C-N-CA	6.02	136.75	121.70
1	A	90	VAL	CA-CB-CG1	-6.00	101.90	110.90
1	A	13	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	A	165	TRP	CB-CG-CD1	5.97	134.77	127.00
1	A	197	ASN	O-C-N	5.96	132.24	122.70
1	A	21	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	A	72	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	390	ASP	N-CA-CB	5.92	121.25	110.60
1	A	243	GLN	O-C-N	-5.91	113.24	122.70
1	A	67	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	256	TRP	CB-CG-CD2	-5.90	118.93	126.60
1	A	10	SER	N-CA-CB	5.88	119.31	110.50
1	A	473	SER	N-CA-CB	5.87	119.30	110.50
1	A	241	PRO	O-C-N	-5.87	113.31	122.70
1	A	391	SER	N-CA-CB	-5.83	101.76	110.50
1	A	219	TYR	CG-CD2-CE2	-5.83	116.64	121.30
1	A	98	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	159	THR	O-C-N	5.81	132.00	122.70
1	A	24	ASN	CB-CG-OD1	-5.81	109.98	121.60
1	A	239	ASP	OD1-CG-OD2	5.79	134.30	123.30
1	A	300	ARG	CB-CG-CD	5.77	126.60	111.60
1	A	129	GLY	CA-C-N	5.76	129.87	117.20
1	A	382	TYR	CA-CB-CG	-5.74	102.50	113.40
1	A	391	SER	CA-CB-OG	-5.72	95.74	111.20
1	A	342	TYR	CZ-CE2-CD2	-5.72	114.65	119.80
1	A	113	TYR	CB-CG-CD1	-5.71	117.58	121.00
1	A	242	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	A	419	TYR	CG-CD1-CE1	-5.67	116.76	121.30
1	A	461	ARG	N-CA-CB	5.67	120.81	110.60
1	A	388	TYR	CB-CG-CD2	5.67	124.40	121.00
1	A	307	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	214	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	252	TYR	CB-CG-CD2	5.65	124.39	121.00
1	A	256	TRP	CB-CG-CD1	5.65	134.35	127.00
1	A	335	TYR	C-N-CA	5.64	135.80	121.70
1	A	382	TYR	CG-CD2-CE2	-5.62	116.80	121.30
1	A	39	GLY	C-N-CA	5.61	134.08	122.30
1	A	281	SER	O-C-N	-5.61	113.72	122.70
1	A	423	LEU	CA-C-N	-5.61	104.86	117.20
1	A	383	ALA	CB-CA-C	-5.61	101.69	110.10
1	A	433	LYS	CA-CB-CG	5.60	125.73	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	TYR	CB-CG-CD1	5.60	124.36	121.00
1	A	419	TYR	CZ-CE2-CD2	-5.59	114.77	119.80
1	A	79	TYR	CD1-CG-CD2	5.59	124.05	117.90
1	A	215	PHE	CG-CD1-CE1	5.59	126.94	120.80
1	A	140	PHE	CB-CG-CD1	5.57	124.70	120.80
1	A	422	THR	N-CA-CB	5.57	120.89	110.30
1	A	429	THR	CA-C-N	-5.57	104.95	117.20
1	A	204	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	317	TYR	CB-CG-CD1	5.56	124.34	121.00
1	A	28	ALA	CA-C-O	5.53	131.72	120.10
1	A	239	ASP	CA-C-N	5.52	129.34	117.20
1	A	27	THR	CA-C-O	-5.52	108.51	120.10
1	A	461	ARG	CB-CG-CD	5.52	125.94	111.60
1	A	358	LEU	CB-CA-C	5.51	120.67	110.20
1	A	31	ASN	OD1-CG-ND2	-5.51	109.23	121.90
1	A	408	VAL	O-C-N	5.50	131.51	122.70
1	A	447	SER	CA-C-O	5.50	131.66	120.10
1	A	21	ARG	CA-C-N	-5.49	105.13	117.20
1	A	153	THR	CA-CB-CG2	5.48	120.07	112.40
1	A	448	SER	CA-C-N	5.46	127.12	116.20
1	A	226	TYR	CZ-CE2-CD2	-5.46	114.89	119.80
1	A	349	LEU	CB-CG-CD2	5.44	120.25	111.00
1	A	125	TYR	CZ-CE2-CD2	-5.44	114.91	119.80
1	A	231	ILE	N-CA-CB	5.43	123.28	110.80
1	A	110	ARG	CA-C-N	5.42	127.04	116.20
1	A	244	LYS	CB-CA-C	-5.42	99.56	110.40
1	A	53	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	A	466	ALA	CA-C-O	5.38	131.40	120.10
1	A	419	TYR	C-N-CA	-5.38	108.25	121.70
1	A	457	SER	O-C-N	5.38	132.34	123.20
1	A	96	THR	N-CA-CB	-5.38	100.08	110.30
1	A	395	ALA	O-C-N	5.37	131.30	122.70
1	A	51	TYR	CG-CD1-CE1	5.37	125.60	121.30
1	A	354	THR	CA-CB-OG1	-5.37	97.72	109.00
1	A	242	TYR	CD1-CE1-CZ	-5.37	114.97	119.80
1	A	121	ASP	CB-CG-OD1	-5.36	113.47	118.30
1	A	80	HIS	CA-C-N	5.36	126.92	116.20
1	A	153	THR	C-N-CA	5.36	135.10	121.70
1	A	196	SER	N-CA-CB	-5.36	102.46	110.50
1	A	317	TYR	CG-CD1-CE1	5.36	125.59	121.30
1	A	249	VAL	N-CA-CB	-5.35	99.72	111.50
1	A	217	PRO	O-C-N	-5.34	114.12	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	SER	CB-CA-C	-5.34	99.96	110.10
1	A	238	SER	C-N-CA	-5.31	108.43	121.70
1	A	272	LEU	CB-CA-C	5.31	120.28	110.20
1	A	125	TYR	CG-CD2-CE2	5.29	125.53	121.30
1	A	198	TYR	C-N-CA	5.29	134.93	121.70
1	A	187	TRP	CB-CG-CD1	-5.28	120.13	127.00
1	A	242	TYR	CG-CD1-CE1	5.27	125.52	121.30
1	A	164	CYS	CA-CB-SG	-5.27	104.51	114.00
1	A	349	LEU	CB-CA-C	5.27	120.22	110.20
1	A	424	SER	CA-CB-OG	-5.27	96.97	111.20
1	A	179	THR	OG1-CB-CG2	-5.25	97.92	110.00
1	A	247	ASP	OD1-CG-OD2	-5.23	113.36	123.30
1	A	470	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	335	TYR	CZ-CE2-CD2	-5.23	115.09	119.80
1	A	382	TYR	CE1-CZ-CE2	5.23	128.16	119.80
1	A	99	ASN	CB-CG-OD1	-5.22	111.16	121.60
1	A	146	PHE	CA-C-O	5.21	131.03	120.10
1	A	128	ASN	OD1-CG-ND2	5.20	133.85	121.90
1	A	57	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	A	391	SER	CB-CA-C	-5.19	100.24	110.10
1	A	227	CYS	O-C-N	5.18	130.98	122.70
1	A	193	ASP	O-C-N	5.17	130.98	122.70
1	A	118	VAL	CG1-CB-CG2	-5.16	102.64	110.90
1	A	250	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	345	GLU	CG-CD-OE1	-5.15	108.00	118.30
1	A	299	PRO	O-C-N	5.14	130.93	122.70
1	A	27	THR	C-N-CA	5.14	134.54	121.70
1	A	214	ASP	CB-CA-C	-5.13	100.14	110.40
1	A	287	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	461	ARG	CA-CB-CG	5.13	124.68	113.40
1	A	240	CYS	CA-CB-SG	-5.12	104.78	114.00
1	A	6	TRP	CG-CD2-CE3	-5.12	129.29	133.90
1	A	168	ASP	OD1-CG-OD2	-5.12	113.58	123.30
1	A	342	TYR	CG-CD2-CE2	5.12	125.39	121.30
1	A	334	HIS	CG-ND1-CE1	5.11	115.36	108.20
1	A	408	VAL	CA-CB-CG2	5.11	118.57	110.90
1	A	256	TRP	CD2-CE2-CZ2	-5.10	116.18	122.30
1	A	311	ALA	N-CA-CB	5.10	117.24	110.10
1	A	25	SER	CA-C-O	5.09	130.80	120.10
1	A	262	PHE	CB-CG-CD1	-5.09	117.24	120.80
1	A	110	ARG	CA-C-O	-5.09	109.42	120.10
1	A	80	HIS	CA-CB-CG	-5.08	104.95	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	HIS	CA-C-O	-5.05	109.49	120.10
1	A	23	ASP	CA-C-N	5.04	128.28	117.20
1	A	246	LEU	CA-C-O	-5.03	109.54	120.10
1	A	459	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	320	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	386	ALA	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	21	ARG	Sidechain
1	A	300	ARG	Sidechain
1	A	344	ARG	Sidechain
1	A	461	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3669	0	3423	99	246
2	A	2	0	0	0	0
3	A	350	0	0	15	41
All	All	4021	0	3423	99	249

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 14.

All (99) 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:422:THR:HG22	1:A:450:ASP:HB3	1.34	1.06
1:A:436:GLU:OE1	1:A:439:THR:HB	1.59	1.03
1:A:95:GLY:HA2	3:A:581:HOH:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLY:H	1:A:404:GLN:HE22	1.19	0.91
1:A:296:HIS:HD2	1:A:296:HIS:H	1.22	0.88
1:A:296:HIS:H	1:A:296:HIS:CD2	1.88	0.88
1:A:416:GLY:O	1:A:417:SER:HB3	1.75	0.86
1:A:95:GLY:CA	3:A:581:HOH:O	2.22	0.83
1:A:217:PRO:O	1:A:221:LYS:HG2	1.81	0.80
1:A:422:THR:HG22	1:A:450:ASP:CB	2.12	0.79
1:A:430:SER:OG	1:A:447:SER:HA	1.83	0.79
1:A:260:TYR:HE2	3:A:719:HOH:O	1.65	0.78
1:A:24:ASN:OD1	3:A:824:HOH:O	1.99	0.78
1:A:422:THR:CG2	1:A:450:ASP:HB3	2.14	0.78
1:A:231:ILE:HG21	1:A:239:ASP:HB2	1.68	0.76
1:A:263:GLU:HG3	3:A:609:HOH:O	1.85	0.76
1:A:233:ASN:HD22	1:A:235:ASN:H	1.33	0.76
1:A:402:GLY:H	1:A:404:GLN:NE2	1.88	0.72
1:A:233:ASN:ND2	1:A:235:ASN:H	1.87	0.71
1:A:231:ILE:CG2	1:A:239:ASP:HB2	2.21	0.71
1:A:209:LEU:HD13	1:A:231:ILE:HG23	1.72	0.71
1:A:439:THR:HG23	1:A:441:THR:OG1	1.91	0.70
1:A:271:ASN:OD1	3:A:615:HOH:O	2.10	0.69
1:A:436:GLU:OE1	1:A:439:THR:CB	2.41	0.67
1:A:263:GLU:CG	3:A:609:HOH:O	2.41	0.66
1:A:358:LEU:HB2	3:A:638:HOH:O	1.94	0.66
1:A:189:ASP:HB3	3:A:715:HOH:O	1.96	0.65
1:A:361:TRP:HZ2	1:A:460:PRO:HG2	1.60	0.65
1:A:446:ASP:HB2	1:A:450:ASP:H	1.61	0.65
1:A:406:ILE:CD1	1:A:428:TYR:HE2	2.10	0.64
1:A:157:ASN:C	1:A:157:ASN:HD22	2.02	0.63
1:A:371:LEU:HD22	1:A:474:LEU:HD23	1.81	0.63
1:A:439:THR:CG2	1:A:441:THR:OG1	2.48	0.62
1:A:296:HIS:CD2	1:A:296:HIS:N	2.57	0.62
1:A:416:GLY:HA3	1:A:457:SER:HA	1.82	0.61
1:A:404:GLN:HE21	1:A:404:GLN:H	1.50	0.60
1:A:435:ILE:HG13	1:A:466:ALA:HA	1.83	0.60
1:A:310:GLN:HE21	1:A:310:GLN:HA	1.67	0.59
1:A:180:GLU:HB2	1:A:183:VAL:HG13	1.84	0.59
1:A:361:TRP:CZ2	1:A:460:PRO:HG2	2.38	0.58
1:A:406:ILE:CD1	1:A:428:TYR:CE2	2.86	0.58
1:A:53:GLU:OE1	1:A:110:ARG:NH1	2.25	0.56
1:A:319:PHE:O	1:A:369:ARG:HD2	2.06	0.56
1:A:240:CYS:N	1:A:241:PRO:CD	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:THR:HG22	1:A:450:ASP:OD2	2.08	0.54
1:A:192:ALA:O	1:A:196:SER:HB3	2.09	0.53
1:A:267:GLY:HA2	3:A:723:HOH:O	2.09	0.52
1:A:236:PRO:O	1:A:240:CYS:HB2	2.10	0.52
1:A:402:GLY:N	1:A:404:GLN:NE2	2.57	0.52
1:A:395:ALA:HB1	1:A:423:LEU:HD21	1.92	0.51
1:A:395:ALA:CB	1:A:423:LEU:HD21	2.41	0.51
1:A:428:TYR:CD1	1:A:432:THR:HG21	2.45	0.51
1:A:406:ILE:HD11	1:A:428:TYR:CE2	2.46	0.50
1:A:418:SER:HA	1:A:455:MET:O	2.13	0.49
1:A:220:ASN:HD22	1:A:227:CYS:HB2	1.78	0.48
1:A:305:THR:O	1:A:305:THR:HG23	2.13	0.48
1:A:246:LEU:O	1:A:247:ASP:CB	2.56	0.48
1:A:446:ASP:HB3	1:A:448:SER:H	1.79	0.48
1:A:299:PRO:CB	1:A:303:LYS:HG2	2.44	0.47
1:A:231:ILE:HD12	1:A:249:VAL:HG22	1.96	0.47
1:A:251:ASN:HD22	1:A:253:PRO:HD2	1.78	0.47
1:A:382:TYR:CD1	1:A:382:TYR:C	2.88	0.47
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.34	0.47
1:A:231:ILE:CD1	1:A:249:VAL:HG22	2.43	0.47
1:A:312:LYS:HG2	1:A:361:TRP:CD2	2.49	0.47
1:A:265:SER:HA	1:A:411:ASN:O	2.15	0.47
1:A:348:TRP:CD1	1:A:349:LEU:HG	2.49	0.47
1:A:220:ASN:ND2	1:A:246:LEU:O	2.46	0.46
1:A:446:ASP:HB2	1:A:450:ASP:N	2.29	0.46
1:A:263:GLU:CD	3:A:609:HOH:O	2.53	0.46
1:A:159:THR:O	1:A:163:ASP:HB2	2.17	0.45
1:A:95:GLY:C	3:A:581:HOH:O	2.51	0.45
1:A:446:ASP:CG	1:A:450:ASP:HB2	2.37	0.45
1:A:338:GLY:O	1:A:343:ASN:HB3	2.15	0.45
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.66	0.45
1:A:371:LEU:CD2	1:A:474:LEU:HD23	2.45	0.45
1:A:411:ASN:C	1:A:411:ASN:HD22	2.19	0.45
1:A:252:TYR:N	1:A:253:PRO:CD	2.81	0.44
1:A:299:PRO:HB3	1:A:303:LYS:HG2	1.99	0.44
1:A:458:GLY:HA2	3:A:791:HOH:O	2.18	0.44
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.66	0.44
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.68	0.44
1:A:31:ASN:ND2	3:A:491:HOH:O	2.49	0.43
1:A:260:TYR:CE2	3:A:719:HOH:O	2.53	0.43
1:A:416:GLY:O	1:A:417:SER:CB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLY:N	1:A:404:GLN:HE22	1.98	0.42
1:A:430:SER:HG	1:A:447:SER:HA	1.83	0.42
1:A:130:ASN:HD22	1:A:130:ASN:HA	1.49	0.42
1:A:231:ILE:CD1	1:A:249:VAL:CG2	2.98	0.41
1:A:208:VAL:HG21	1:A:229:GLY:HA3	2.03	0.41
1:A:328:TYR:O	1:A:329:ALA:C	2.59	0.41
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.84	0.41
1:A:157:ASN:C	1:A:157:ASN:ND2	2.70	0.41
1:A:97:ALA:O	1:A:101:LYS:HG3	2.20	0.41
1:A:395:ALA:HA	1:A:407:THR:O	2.21	0.41
1:A:422:THR:CG2	1:A:450:ASP:CB	2.87	0.40
1:A:235:ASN:HD22	1:A:236:PRO:HD2	1.87	0.40
1:A:324:ILE:HA	1:A:325:PRO:HD2	1.84	0.40
1:A:69:LEU:HA	1:A:70:PRO:HD3	1.96	0.40

All (249) 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:A:442:SER:N	1:A:461:ARG:NH1[3_554]	0.51	1.69
1:A:420:THR:C	1:A:451:ILE:O[3_554]	0.58	1.62
1:A:436:GLU:OE1	1:A:441:THR:OG1[3_554]	0.64	1.56
1:A:419:TYR:CD2	1:A:450:ASP:O[3_554]	0.66	1.54
1:A:416:GLY:O	1:A:431:GLY:C[3_554]	0.67	1.53
1:A:420:THR:N	1:A:451:ILE:CB[3_554]	0.68	1.52
1:A:439:THR:C	1:A:439:THR:C[3_554]	0.69	1.51
1:A:446:ASP:OD2	3:A:779:HOH:O[3_554]	0.72	1.48
1:A:412:LYS:NZ	3:A:808:HOH:O[3_554]	0.74	1.46
1:A:416:GLY:O	1:A:432:THR:N[3_554]	0.76	1.44
1:A:413:GLY:O	1:A:433:LYS:CE[3_554]	0.77	1.43
1:A:452:PRO:C	1:A:453:VAL:O[3_554]	0.77	1.43
1:A:417:SER:N	1:A:432:THR:CA[3_554]	0.80	1.40
1:A:417:SER:N	1:A:432:THR:C[3_554]	0.80	1.40
1:A:419:TYR:C	1:A:451:ILE:CB[3_554]	0.82	1.38
1:A:436:GLU:CD	1:A:441:THR:OG1[3_554]	0.87	1.33
1:A:417:SER:CA	1:A:432:THR:CB[3_554]	0.91	1.29
1:A:419:TYR:CA	1:A:451:ILE:CG1[3_554]	0.92	1.28
1:A:439:THR:CA	1:A:440:CYS:N[3_554]	0.96	1.24
1:A:439:THR:C	1:A:440:CYS:N[3_554]	0.98	1.22
1:A:422:THR:CB	3:A:794:HOH:O[3_554]	0.99	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:VAL:CG1	3:A:806:HOH:O[3_554]	0.99	1.21
1:A:422:THR:O	3:A:795:HOH:O[3_554]	1.03	1.17
1:A:454:PRO:CD	1:A:454:PRO:CD[3_554]	1.06	1.14
1:A:439:THR:OG1	1:A:441:THR:N[3_554]	1.08	1.12
1:A:444:THR:CB	3:A:791:HOH:O[3_554]	1.08	1.12
1:A:416:GLY:CA	1:A:431:GLY:O[3_554]	1.09	1.11
1:A:418:SER:OG	1:A:434:LEU:CD2[3_554]	1.09	1.11
1:A:419:TYR:CD1	1:A:445:VAL:CA[3_554]	1.09	1.11
1:A:421:LEU:CG	3:A:793:HOH:O[3_554]	1.09	1.11
1:A:420:THR:C	1:A:451:ILE:C[3_554]	1.14	1.06
1:A:452:PRO:O	1:A:453:VAL:O[3_554]	1.14	1.06
1:A:416:GLY:C	1:A:432:THR:N[3_554]	1.16	1.04
1:A:442:SER:CA	1:A:461:ARG:NH1[3_554]	1.18	1.02
1:A:439:THR:CB	1:A:441:THR:N[3_554]	1.19	1.01
1:A:416:GLY:C	1:A:431:GLY:C[3_554]	1.24	0.96
1:A:433:LYS:CB	1:A:457:SER:CA[3_554]	1.24	0.96
1:A:416:GLY:N	1:A:431:GLY:O[3_554]	1.25	0.95
1:A:419:TYR:CD2	1:A:450:ASP:C[3_554]	1.25	0.95
1:A:452:PRO:O	1:A:453:VAL:C[3_554]	1.25	0.95
1:A:421:LEU:N	1:A:451:ILE:O[3_554]	1.26	0.94
1:A:421:LEU:CD2	3:A:797:HOH:O[3_554]	1.27	0.93
1:A:443:VAL:CG2	1:A:455:MET:CA[3_554]	1.28	0.92
1:A:417:SER:OG	1:A:429:THR:O[3_554]	1.30	0.90
1:A:444:THR:OG1	1:A:458:GLY:CA[3_554]	1.30	0.90
1:A:423:LEU:O	3:A:659:HOH:O[3_554]	1.32	0.88
1:A:434:LEU:CA	1:A:456:ALA:CB[3_554]	1.32	0.88
1:A:433:LYS:CA	1:A:457:SER:N[3_554]	1.33	0.87
1:A:439:THR:N	1:A:439:THR:O[3_554]	1.33	0.87
1:A:443:VAL:O	1:A:456:ALA:N[3_554]	1.33	0.87
1:A:417:SER:CA	1:A:432:THR:CA[3_554]	1.34	0.86
1:A:419:TYR:C	1:A:451:ILE:CG1[3_554]	1.34	0.86
1:A:439:THR:CA	1:A:440:CYS:CA[3_554]	1.34	0.86
1:A:433:LYS:CB	1:A:457:SER:CB[3_554]	1.35	0.85
1:A:444:THR:CA	3:A:791:HOH:O[3_554]	1.35	0.85
1:A:420:THR:CA	1:A:451:ILE:O[3_554]	1.36	0.84
1:A:420:THR:N	1:A:451:ILE:CA[3_554]	1.37	0.83
1:A:421:LEU:N	1:A:451:ILE:C[3_554]	1.37	0.83
1:A:419:TYR:O	1:A:451:ILE:CG2[3_554]	1.38	0.82
1:A:419:TYR:CE1	1:A:445:VAL:CA[3_554]	1.38	0.82
1:A:422:THR:OG1	3:A:794:HOH:O[3_554]	1.38	0.82
1:A:419:TYR:CG	1:A:450:ASP:O[3_554]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LEU:C	1:A:456:ALA:CB[3_554]	1.40	0.80
1:A:439:THR:CA	1:A:439:THR:C[3_554]	1.41	0.79
1:A:433:LYS:CD	1:A:457:SER:C[3_554]	1.42	0.78
1:A:443:VAL:CG1	1:A:454:PRO:O[3_554]	1.42	0.78
1:A:421:LEU:N	1:A:452:PRO:N[3_554]	1.45	0.75
1:A:419:TYR:CE1	1:A:445:VAL:C[3_554]	1.46	0.74
1:A:422:THR:CG2	3:A:794:HOH:O[3_554]	1.46	0.74
1:A:421:LEU:CD1	3:A:793:HOH:O[3_554]	1.47	0.73
1:A:436:GLU:OE1	1:A:441:THR:CB[3_554]	1.48	0.72
1:A:453:VAL:N	1:A:453:VAL:O[3_554]	1.48	0.72
1:A:417:SER:CB	1:A:429:THR:O[3_554]	1.49	0.71
1:A:443:VAL:O	1:A:456:ALA:CA[3_554]	1.49	0.71
1:A:417:SER:CB	1:A:432:THR:OG1[3_554]	1.50	0.70
1:A:452:PRO:CD	1:A:455:MET:CG[3_554]	1.50	0.70
1:A:416:GLY:C	1:A:432:THR:CA[3_554]	1.51	0.69
1:A:419:TYR:C	1:A:451:ILE:CA[3_554]	1.51	0.69
1:A:443:VAL:CG2	1:A:455:MET:N[3_554]	1.51	0.69
1:A:452:PRO:C	1:A:453:VAL:C[3_554]	1.51	0.69
1:A:453:VAL:N	1:A:453:VAL:C[3_554]	1.51	0.69
1:A:420:THR:CA	1:A:451:ILE:C[3_554]	1.52	0.68
1:A:443:VAL:O	1:A:456:ALA:C[3_554]	1.52	0.68
1:A:418:SER:CB	1:A:434:LEU:CD1[3_554]	1.53	0.67
1:A:453:VAL:CA	1:A:453:VAL:C[3_554]	1.53	0.67
1:A:447:SER:N	3:A:658:HOH:O[3_554]	1.54	0.66
1:A:446:ASP:CG	3:A:779:HOH:O[3_554]	1.55	0.65
1:A:416:GLY:C	1:A:431:GLY:O[3_554]	1.56	0.64
1:A:419:TYR:CE2	1:A:450:ASP:O[3_554]	1.56	0.64
1:A:421:LEU:N	1:A:452:PRO:CA[3_554]	1.56	0.64
1:A:433:LYS:CG	1:A:457:SER:CA[3_554]	1.56	0.64
1:A:439:THR:O	1:A:440:CYS:N[3_554]	1.56	0.64
1:A:443:VAL:C	1:A:456:ALA:N[3_554]	1.56	0.64
1:A:444:THR:CA	3:A:792:HOH:O[3_554]	1.57	0.63
1:A:453:VAL:N	1:A:453:VAL:N[3_554]	1.57	0.63
1:A:412:LYS:CE	1:A:445:VAL:O[3_554]	1.58	0.62
1:A:420:THR:OG1	1:A:423:LEU:CB[3_554]	1.58	0.62
1:A:441:THR:C	1:A:461:ARG:NH1[3_554]	1.59	0.61
1:A:443:VAL:O	1:A:456:ALA:O[3_554]	1.59	0.61
1:A:418:SER:CB	1:A:434:LEU:CG[3_554]	1.60	0.60
1:A:434:LEU:O	1:A:456:ALA:CB[3_554]	1.60	0.60
1:A:441:THR:O	1:A:461:ARG:NH2[3_554]	1.60	0.60
1:A:417:SER:O	1:A:445:VAL:CG2[3_554]	1.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:MET:CE	3:A:804:HOH:O[3_554]	1.62	0.58
1:A:434:LEU:N	1:A:456:ALA:CB[3_554]	1.63	0.57
1:A:418:SER:OG	1:A:434:LEU:CG[3_554]	1.64	0.56
1:A:418:SER:CB	1:A:434:LEU:CD2[3_554]	1.64	0.56
1:A:443:VAL:CB	1:A:455:MET:CA[3_554]	1.64	0.56
1:A:443:VAL:CA	3:A:790:HOH:O[3_554]	1.64	0.56
1:A:417:SER:N	1:A:432:THR:N[3_554]	1.65	0.55
3:A:659:HOH:O	3:A:809:HOH:O[3_554]	1.65	0.55
1:A:442:SER:N	1:A:461:ARG:CZ[3_554]	1.66	0.54
1:A:443:VAL:CG2	1:A:455:MET:C[3_554]	1.66	0.54
1:A:420:THR:CA	1:A:451:ILE:CB[3_554]	1.68	0.52
1:A:422:THR:N	1:A:422:THR:OG1[3_554]	1.68	0.52
1:A:453:VAL:CA	1:A:453:VAL:CA[3_554]	1.68	0.52
1:A:419:TYR:C	1:A:451:ILE:CG2[3_554]	1.69	0.51
1:A:421:LEU:O	1:A:421:LEU:O[3_554]	1.69	0.51
1:A:433:LYS:CB	1:A:457:SER:OG[3_554]	1.69	0.51
1:A:417:SER:N	1:A:432:THR:O[3_554]	1.71	0.49
1:A:436:GLU:CG	1:A:441:THR:OG1[3_554]	1.71	0.49
1:A:443:VAL:C	3:A:790:HOH:O[3_554]	1.71	0.49
1:A:416:GLY:C	1:A:432:THR:C[3_554]	1.72	0.48
1:A:433:LYS:CD	1:A:458:GLY:N[3_554]	1.72	0.48
1:A:441:THR:C	1:A:461:ARG:CZ[3_554]	1.72	0.48
1:A:444:THR:N	3:A:791:HOH:O[3_554]	1.72	0.48
1:A:416:GLY:O	1:A:431:GLY:CA[3_554]	1.73	0.47
1:A:421:LEU:CB	1:A:452:PRO:CB[3_554]	1.73	0.47
1:A:439:THR:CA	1:A:440:CYS:C[3_554]	1.74	0.46
1:A:419:TYR:O	1:A:451:ILE:CB[3_554]	1.75	0.45
1:A:417:SER:CB	1:A:432:THR:CB[3_554]	1.76	0.44
1:A:420:THR:O	1:A:451:ILE:O[3_554]	1.76	0.44
1:A:453:VAL:N	1:A:453:VAL:CA[3_554]	1.76	0.44
1:A:433:LYS:CD	1:A:457:SER:CA[3_554]	1.77	0.43
1:A:442:SER:C	1:A:461:ARG:CZ[3_554]	1.77	0.43
1:A:444:THR:CG2	3:A:792:HOH:O[3_554]	1.78	0.42
1:A:444:THR:N	3:A:790:HOH:O[3_554]	1.80	0.40
1:A:444:THR:OG1	3:A:791:HOH:O[3_554]	1.82	0.38
1:A:416:GLY:O	1:A:431:GLY:O[3_554]	1.84	0.36
1:A:433:LYS:CA	1:A:457:SER:CA[3_554]	1.84	0.36
1:A:434:LEU:N	1:A:456:ALA:CA[3_554]	1.84	0.36
1:A:420:THR:CA	1:A:451:ILE:CA[3_554]	1.85	0.35
1:A:438:TYR:O	1:A:440:CYS:O[3_554]	1.85	0.35
1:A:442:SER:CA	1:A:461:ARG:CZ[3_554]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:PRO:CG	1:A:455:MET:CG[3_554]	1.85	0.35
1:A:416:GLY:CA	1:A:431:GLY:C[3_554]	1.86	0.34
1:A:443:VAL:CG1	1:A:461:ARG:CD[3_554]	1.86	0.34
1:A:413:GLY:O	1:A:433:LYS:NZ[3_554]	1.87	0.33
1:A:417:SER:C	1:A:445:VAL:CG2[3_554]	1.88	0.32
1:A:419:TYR:CZ	1:A:446:ASP:N[3_554]	1.88	0.32
1:A:420:THR:N	1:A:451:ILE:CG1[3_554]	1.88	0.32
1:A:436:GLU:CD	1:A:441:THR:CB[3_554]	1.88	0.32
1:A:441:THR:CG2	1:A:461:ARG:NE[3_554]	1.88	0.32
1:A:412:LYS:CE	3:A:808:HOH:O[3_554]	1.89	0.31
1:A:415:SER:O	3:A:660:HOH:O[3_554]	1.89	0.31
1:A:439:THR:CA	1:A:439:THR:O[3_554]	1.89	0.31
1:A:413:GLY:C	1:A:433:LYS:CE[3_554]	1.90	0.30
1:A:434:LEU:CB	1:A:456:ALA:CB[3_554]	1.90	0.30
1:A:441:THR:O	1:A:461:ARG:CZ[3_554]	1.90	0.30
1:A:446:ASP:OD1	3:A:657:HOH:O[3_554]	1.90	0.30
3:A:657:HOH:O	3:A:796:HOH:O[3_554]	1.90	0.30
1:A:439:THR:CG2	1:A:439:THR:CG2[3_554]	1.91	0.29
1:A:417:SER:N	1:A:433:LYS:N[3_554]	1.92	0.28
1:A:417:SER:O	1:A:432:THR:O[3_554]	1.92	0.28
1:A:342:TYR:OH	3:A:510:HOH:O[8_555]	1.93	0.27
1:A:438:TYR:O	1:A:440:CYS:CB[3_554]	1.93	0.27
1:A:439:THR:C	1:A:439:THR:O[3_554]	1.93	0.27
1:A:444:THR:CB	3:A:792:HOH:O[3_554]	1.93	0.27
1:A:417:SER:CB	1:A:432:THR:N[3_554]	1.94	0.26
1:A:436:GLU:OE1	1:A:441:THR:CA[3_554]	1.94	0.26
1:A:439:THR:N	1:A:439:THR:C[3_554]	1.94	0.26
1:A:419:TYR:CD2	1:A:451:ILE:N[3_554]	1.95	0.25
1:A:422:THR:N	1:A:422:THR:CA[3_554]	1.95	0.25
1:A:417:SER:CA	1:A:432:THR:N[3_554]	1.96	0.24
1:A:419:TYR:CE1	1:A:446:ASP:N[3_554]	1.96	0.24
1:A:438:TYR:C	1:A:440:CYS:O[3_554]	1.96	0.24
1:A:443:VAL:CG2	1:A:454:PRO:C[3_554]	1.96	0.24
1:A:417:SER:CA	1:A:432:THR:OG1[3_554]	1.97	0.23
1:A:420:THR:CG2	1:A:453:VAL:CG2[3_554]	1.97	0.23
1:A:444:THR:OG1	1:A:458:GLY:N[3_554]	1.97	0.23
1:A:446:ASP:OD1	3:A:779:HOH:O[3_554]	1.97	0.23
1:A:419:TYR:CG	1:A:450:ASP:C[3_554]	1.98	0.22
1:A:421:LEU:CA	1:A:452:PRO:CA[3_554]	1.98	0.22
1:A:439:THR:OG1	1:A:441:THR:CA[3_554]	1.98	0.22
1:A:442:SER:C	1:A:461:ARG:NH1[3_554]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:SER:C	1:A:431:GLY:O[3_554]	1.99	0.21
1:A:417:SER:O	1:A:445:VAL:N[3_554]	1.99	0.21
1:A:421:LEU:CB	1:A:452:PRO:CA[3_554]	1.99	0.21
1:A:433:LYS:CG	1:A:457:SER:CB[3_554]	1.99	0.21
1:A:436:GLU:OE2	1:A:441:THR:OG1[3_554]	1.99	0.21
1:A:439:THR:CA	1:A:441:THR:N[3_554]	1.99	0.21
1:A:420:THR:CB	1:A:453:VAL:CG2[3_554]	2.00	0.20
1:A:419:TYR:CE1	1:A:444:THR:O[3_554]	2.01	0.19
1:A:420:THR:N	1:A:451:ILE:N[3_554]	2.01	0.19
1:A:422:THR:C	3:A:795:HOH:O[3_554]	2.01	0.19
1:A:433:LYS:CB	1:A:457:SER:N[3_554]	2.01	0.19
1:A:433:LYS:NZ	1:A:458:GLY:CA[3_554]	2.01	0.19
1:A:438:TYR:C	1:A:440:CYS:C[3_554]	2.01	0.19
1:A:417:SER:N	1:A:432:THR:CB[3_554]	2.03	0.17
1:A:419:TYR:OH	3:A:662:HOH:O[3_554]	2.03	0.17
1:A:444:THR:C	3:A:792:HOH:O[3_554]	2.03	0.17
3:A:655:HOH:O	3:A:662:HOH:O[3_554]	2.03	0.17
1:A:408:VAL:CG1	3:A:805:HOH:O[3_554]	2.04	0.16
1:A:418:SER:CA	1:A:434:LEU:CD1[3_554]	2.04	0.16
1:A:419:TYR:O	1:A:451:ILE:CA[3_554]	2.04	0.16
1:A:422:THR:N	1:A:422:THR:N[3_554]	2.04	0.16
1:A:442:SER:CA	1:A:461:ARG:NH2[3_554]	2.04	0.16
1:A:442:SER:CB	1:A:459:LEU:CG[3_554]	2.04	0.16
1:A:461:ARG:CB	3:A:807:HOH:O[3_554]	2.04	0.16
1:A:419:TYR:CD1	1:A:445:VAL:CB[3_554]	2.05	0.15
1:A:433:LYS:C	1:A:457:SER:N[3_554]	2.05	0.15
1:A:439:THR:N	1:A:441:THR:N[3_554]	2.05	0.15
1:A:446:ASP:C	3:A:658:HOH:O[3_554]	2.05	0.15
1:A:419:TYR:CA	1:A:451:ILE:CB[3_554]	2.06	0.14
1:A:420:THR:CA	1:A:451:ILE:CG2[3_554]	2.06	0.14
1:A:442:SER:CB	1:A:459:LEU:CB[3_554]	2.06	0.14
1:A:442:SER:C	1:A:461:ARG:NH2[3_554]	2.06	0.14
1:A:419:TYR:N	1:A:451:ILE:CG1[3_554]	2.07	0.13
1:A:422:THR:CA	1:A:422:THR:OG1[3_554]	2.07	0.13
1:A:433:LYS:CG	1:A:457:SER:C[3_554]	2.08	0.12
1:A:442:SER:O	1:A:461:ARG:CD[3_554]	2.08	0.12
1:A:417:SER:CA	1:A:432:THR:C[3_554]	2.09	0.11
1:A:416:GLY:O	1:A:432:THR:CA[3_554]	2.10	0.10
1:A:417:SER:C	1:A:432:THR:O[3_554]	2.10	0.10
1:A:418:SER:CA	1:A:434:LEU:CG[3_554]	2.10	0.10
1:A:72:ASP:OD2	3:A:772:HOH:O[8_555]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:C	1:A:451:ILE:CA[3_554]	2.12	0.08
1:A:420:THR:N	1:A:451:ILE:CG2[3_554]	2.12	0.08
1:A:422:THR:N	1:A:422:THR:CB[3_554]	2.12	0.08
1:A:443:VAL:CB	1:A:454:PRO:O[3_554]	2.12	0.08
1:A:443:VAL:CG2	1:A:454:PRO:O[3_554]	2.13	0.07
1:A:419:TYR:CD1	1:A:445:VAL:C[3_554]	2.14	0.06
1:A:438:TYR:O	1:A:440:CYS:C[3_554]	2.14	0.06
1:A:443:VAL:N	1:A:461:ARG:NH2[3_554]	2.14	0.06
1:A:420:THR:O	1:A:451:ILE:N[3_554]	2.15	0.05
1:A:436:GLU:CD	1:A:441:THR:CG2[3_554]	2.15	0.05
1:A:442:SER:OG	1:A:459:LEU:CD2[3_554]	2.15	0.05
1:A:443:VAL:CA	1:A:456:ALA:N[3_554]	2.15	0.05
1:A:452:PRO:O	1:A:454:PRO:N[3_554]	2.15	0.05
1:A:454:PRO:N	1:A:454:PRO:CD[3_554]	2.16	0.04
1:A:419:TYR:CB	1:A:451:ILE:CG1[3_554]	2.17	0.03
1:A:445:VAL:N	3:A:792:HOH:O[3_554]	2.17	0.03
1:A:413:GLY:O	1:A:433:LYS:CD[3_554]	2.18	0.02
1:A:417:SER:O	1:A:445:VAL:CB[3_554]	2.18	0.02
1:A:442:SER:CB	1:A:459:LEU:CD2[3_554]	2.18	0.02
1:A:417:SER:C	1:A:432:THR:CB[3_554]	2.19	0.01
1:A:423:LEU:C	3:A:659:HOH:O[3_554]	2.19	0.01
1:A:433:LYS:C	1:A:457:SER:OG[3_554]	2.19	0.01
1:A:442:SER:O	1:A:459:LEU:O[3_554]	2.19	0.01

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	474/484 (98%)	452 (95%)	18 (4%)	4 (1%)	19 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ASP
1	A	417	SER
1	A	446	ASP
1	A	457	SER

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	403/409 (98%)	348 (86%)	55 (14%)	3 2

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	15	LEU
1	A	26	THR
1	A	31	ASN
1	A	61	TRP
1	A	96	THR
1	A	98	ASP
1	A	103	LEU
1	A	153	THR
1	A	157	ASN
1	A	169	THR
1	A	179	THR
1	A	191	VAL
1	A	196	SER
1	A	212	GLN
1	A	214	ASP
1	A	220	ASN
1	A	221	LYS
1	A	235	ASN
1	A	239	ASP
1	A	244	LYS
1	A	245	VAL
1	A	249	VAL

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Mol	Chain	Res	Type
1	A	250	LEU
1	A	251	ASN
1	A	264	SER
1	A	265	SER
1	A	277	LYS
1	A	278	SER
1	A	281	SER
1	A	296	HIS
1	A	300	ARG
1	A	303	LYS
1	A	310	GLN
1	A	320	LEU
1	A	358	LEU
1	A	391	SER
1	A	393	THR
1	A	404	GLN
1	A	409	LEU
1	A	411	ASN
1	A	415	SER
1	A	417	SER
1	A	421	LEU
1	A	422	THR
1	A	424	SER
1	A	429	THR
1	A	430	SER
1	A	439	THR
1	A	446	ASP
1	A	447	SER
1	A	457	SER
1	A	459	LEU
1	A	464	LEU
1	A	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	31	ASN
1	A	43	GLN
1	A	128	ASN
1	A	130	ASN
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	235	ASN
1	A	251	ASN
1	A	291	ASN
1	A	296	HIS
1	A	310	GLN
1	A	333	GLN
1	A	392	ASN
1	A	404	GLN
1	A	411	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.