Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:23 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

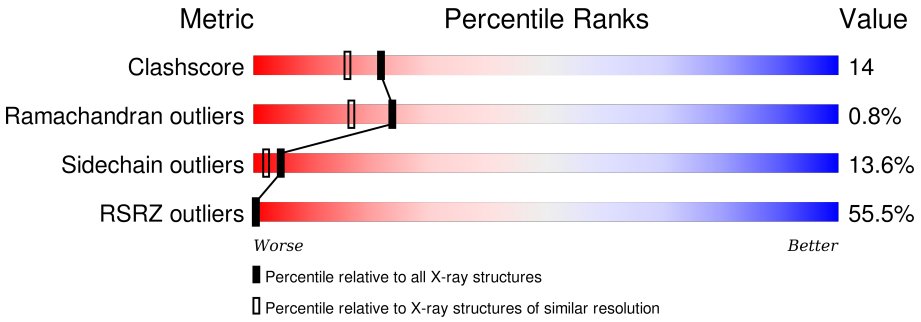
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (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 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.

Mol	Chain	Length	Quality of chain
1	A	484	55%, 47%, 34%, 14%

2 Entry composition

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
1	A	476	Total	C	N	O	S	0	0	0
			3669	2321	580	751	17			

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

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

- Molecule 3 is water.

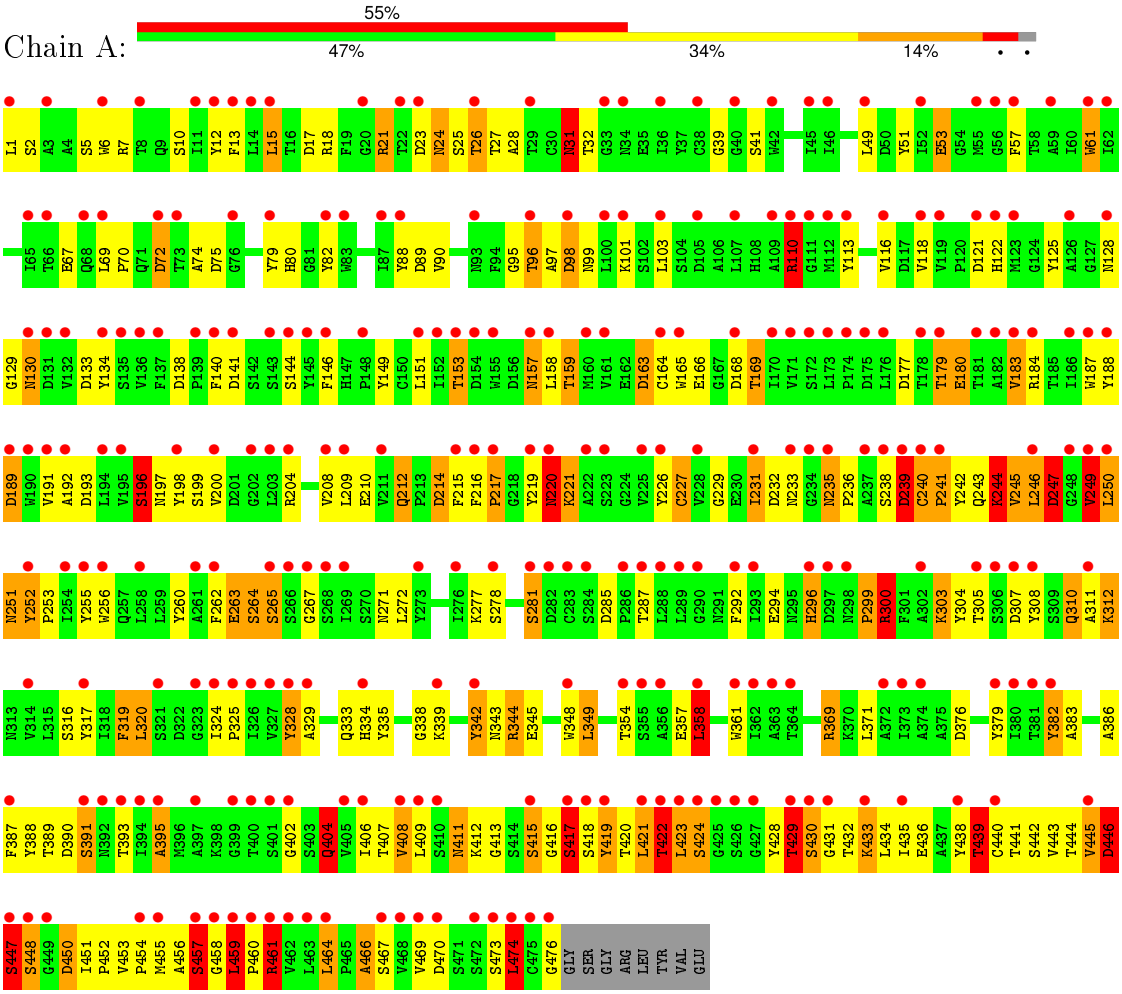
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	350	Total	O	0	0
			350	350		

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.

- 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) 0.360 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 95.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 31209 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:H	1:A:296:HIS:HD2	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:HD22	1:A:157:ASN:C	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:HA	1:A:310:GLN:HE21	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:402:GLY:N	1:A:404:GLN:NE2	2.57	0.52
1:A:236:PRO:O	1:A:240:CYS:HB2	2.10	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:C	1:A:382:TYR:CD1	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:348:TRP:CD1	1:A:349:LEU:HG	2.49	0.47
1:A:265:SER:HA	1:A:411:ASN:O	2.15	0.47
1:A:446:ASP:HB2	1:A:450:ASP:N	2.29	0.46
1:A:220:ASN:ND2	1:A:246:LEU:O	2.46	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:HD22	1:A:411:ASN:C	2.19	0.45
1:A:299:PRO:HB3	1:A:303:LYS:HG2	1.99	0.44
1:A:252:TYR:N	1:A:253:PRO:CD	2.81	0.44
1:A:458:GLY:HA2	3:A:791:HOH:O	2.18	0.44
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.68	0.44
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.66	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:157:ASN:C	1:A:157:ASN:ND2	2.70	0.41
1:A:49:LEU:HA	1:A:49:LEU:HD23	1.84	0.41
1:A:395:ALA:HA	1:A:407:THR:O	2.21	0.41
1:A:97:ALA:O	1:A:101:LYS:HG3	2.20	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:444:THR:CB	3:A:791:HOH:O[3_554]	1.08	1.12
1:A:439:THR:OG1	1:A:441:THR:N[3_554]	1.08	1.12
1:A:418:SER:OG	1:A:434:LEU:CD2[3_554]	1.09	1.11
1:A:421:LEU:CG	3:A:793:HOH:O[3_554]	1.09	1.11
1:A:416:GLY:CA	1:A:431:GLY:O[3_554]	1.09	1.11
1:A:419:TYR:CD1	1:A:445:VAL:CA[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:433:LYS:CB	1:A:457:SER:CA[3_554]	1.24	0.96
1:A:416:GLY:C	1:A:431:GLY:C[3_554]	1.24	0.96
1:A:416:GLY:N	1:A:431:GLY:O[3_554]	1.25	0.95
1:A:452:PRO:O	1:A:453:VAL:C[3_554]	1.25	0.95
1:A:419:TYR:CD2	1:A:450:ASP: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:444:THR:OG1	1:A:458:GLY:CA[3_554]	1.30	0.90
1:A:417:SER:OG	1:A:429:THR:O[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: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:433:LYS:CA	1:A:457:SER:N[3_554]	1.33	0.87
1:A:439:THR:CA	1:A:440:CYS: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:417:SER:CA	1:A:432:THR:CA[3_554]	1.34	0.86
1:A:444:THR:CA	3:A:791:HOH:O[3_554]	1.35	0.85
1:A:433:LYS:CB	1:A:457:SER:CB[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:422:THR:OG1	3:A:794:HOH:O[3_554]	1.38	0.82
1:A:419:TYR:CE1	1:A:445:VAL:CA[3_554]	1.38	0.82
1:A:434:LEU:C	1:A:456:ALA:CB[3_554]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TYR:CG	1:A:450:ASP:O[3_554]	1.40	0.80
1:A:439:THR:CA	1:A:439:THR:C[3_554]	1.41	0.79
1:A:443:VAL:CG1	1:A:454:PRO:O[3_554]	1.42	0.78
1:A:433:LYS:CD	1:A:457:SER:C[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:453:VAL:N	1:A:453:VAL:O[3_554]	1.48	0.72
1:A:436:GLU:OE1	1:A:441:THR:CB[3_554]	1.48	0.72
1:A:443:VAL:O	1:A:456:ALA:CA[3_554]	1.49	0.71
1:A:417:SER:CB	1:A:429:THR:O[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:419:TYR:C	1:A:451:ILE:CA[3_554]	1.51	0.69
1:A:416:GLY:C	1:A:432:THR: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:443:VAL:O	1:A:456:ALA:C[3_554]	1.52	0.68
1:A:420:THR:CA	1:A:451:ILE:C[3_554]	1.52	0.68
1:A:453:VAL:CA	1:A:453:VAL:C[3_554]	1.53	0.67
1:A:418:SER:CB	1:A:434:LEU:CD1[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:421:LEU:N	1:A:452:PRO:CA[3_554]	1.56	0.64
1:A:416:GLY:C	1:A:431:GLY:O[3_554]	1.56	0.64
1:A:439:THR:O	1:A:440:CYS:N[3_554]	1.56	0.64
1:A:433:LYS:CG	1:A:457:SER:CA[3_554]	1.56	0.64
1:A:419:TYR:CE2	1:A:450:ASP:O[3_554]	1.56	0.64
1:A:443:VAL:C	1:A:456:ALA:N[3_554]	1.56	0.64
1:A:453:VAL:N	1:A:453:VAL:N[3_554]	1.57	0.63
1:A:444:THR:CA	3:A:792:HOH:O[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:443:VAL:O	1:A:456:ALA:O[3_554]	1.59	0.61
1:A:441:THR:C	1:A:461:ARG:NH1[3_554]	1.59	0.61
1:A:441:THR:O	1:A:461:ARG:NH2[3_554]	1.60	0.60
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: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: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:418:SER:CB	1:A:434:LEU:CD2[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:443:VAL:CG2	1:A:455:MET:C[3_554]	1.66	0.54
1:A:442:SER:N	1:A:461:ARG:CZ[3_554]	1.66	0.54
1:A:422:THR:N	1:A:422:THR:OG1[3_554]	1.68	0.52
1:A:420:THR:CA	1:A:451:ILE:CB[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:443:VAL:C	3:A:790:HOH: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:416:GLY:C	1:A:432:THR:C[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:433:LYS:CD	1:A:458:GLY:N[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: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:417:SER:CB	1:A:432:THR:CB[3_554]	1.76	0.44
1:A:442:SER:C	1:A:461:ARG:CZ[3_554]	1.77	0.43
1:A:433:LYS:CD	1:A:457:SER:CA[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:452:PRO:CG	1:A:455:MET:CG[3_554]	1.85	0.35
1:A:438:TYR:O	1:A:440:CYS:O[3_554]	1.85	0.35
1:A:420:THR:CA	1:A:451:ILE:CA[3_554]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:SER:CA	1:A:461:ARG:CZ[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:441:THR:CG2	1:A:461:ARG:NE[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:419:TYR:CZ	1:A:446:ASP:N[3_554]	1.88	0.32
1:A:415:SER:O	3:A:660:HOH:O[3_554]	1.89	0.31
1:A:412:LYS:CE	3:A:808:HOH:O[3_554]	1.89	0.31
1:A:439:THR:CA	1:A:439:THR:O[3_554]	1.89	0.31
3:A:657:HOH:O	3:A:796:HOH:O[3_554]	1.90	0.30
1:A:413:GLY:C	1:A:433:LYS:CE[3_554]	1.90	0.30
1:A:446:ASP:OD1	3:A:657:HOH:O[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: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:439:THR:C	1:A:439:THR:O[3_554]	1.93	0.27
1:A:438:TYR:O	1:A:440:CYS:CB[3_554]	1.93	0.27
1:A:444:THR:CB	3:A:792:HOH:O[3_554]	1.93	0.27
1:A:342:TYR:OH	3:A:510:HOH:O[8_555]	1.93	0.27
1:A:439:THR:N	1:A:439:THR:C[3_554]	1.94	0.26
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:422:THR:N	1:A:422:THR:CA[3_554]	1.95	0.25
1:A:419:TYR:CD2	1:A:451:ILE:N[3_554]	1.95	0.25
1:A:419:TYR:CE1	1:A:446:ASP:N[3_554]	1.96	0.24
1:A:417:SER:CA	1:A:432:THR: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:446:ASP:OD1	3:A:779:HOH:O[3_554]	1.97	0.23
1:A:444:THR:OG1	1:A:458:GLY:N[3_554]	1.97	0.23
1:A:420:THR:CG2	1:A:453:VAL:CG2[3_554]	1.97	0.23
1:A:421:LEU:CA	1:A:452:PRO:CA[3_554]	1.98	0.22
1:A:419:TYR:CG	1:A:450:ASP:C[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:433:LYS:CG	1:A:457:SER:CB[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:439:THR:CA	1:A:441:THR:N[3_554]	1.99	0.21
1:A:436:GLU:OE2	1:A:441:THR:OG1[3_554]	1.99	0.21
1:A:415:SER:C	1:A:431:GLY:O[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:422:THR:C	3:A:795:HOH:O[3_554]	2.01	0.19
1:A:438:TYR:C	1:A:440:CYS:C[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:420:THR:N	1:A:451:ILE:N[3_554]	2.01	0.19
3:A:655:HOH:O	3:A:662:HOH:O[3_554]	2.03	0.17
1:A:419:TYR:OH	3:A:662:HOH:O[3_554]	2.03	0.17
1:A:417:SER:N	1:A:432:THR:CB[3_554]	2.03	0.17
1:A:444:THR:C	3:A:792:HOH:O[3_554]	2.03	0.17
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:408:VAL:CG1	3:A:805:HOH:O[3_554]	2.04	0.16
1:A:419:TYR:O	1:A:451:ILE:CA[3_554]	2.04	0.16
1:A:442:SER:CB	1:A:459:LEU:CG[3_554]	2.04	0.16
1:A:418:SER:CA	1:A:434:LEU:CD1[3_554]	2.04	0.16
1:A:461:ARG:CB	3:A:807:HOH:O[3_554]	2.04	0.16
1:A:439:THR:N	1:A:441:THR:N[3_554]	2.05	0.15
1:A:433:LYS:C	1:A:457:SER: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:CD1	1:A:445:VAL:CB[3_554]	2.05	0.15
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:419:TYR:CA	1:A:451:ILE: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:442:SER:O	1:A:461:ARG:CD[3_554]	2.08	0.12
1:A:433:LYS:CG	1:A:457:SER:C[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: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: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:443:VAL:CG2	1:A:454:PRO:O[3_554]	2.13	0.07
1:A:443:VAL:N	1:A:461:ARG:NH2[3_554]	2.14	0.06
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:CA	1:A:456:ALA:N[3_554]	2.15	0.05
1:A:420:THR:O	1:A:451:ILE:N[3_554]	2.15	0.05
1:A:442:SER:OG	1:A:459:LEU:CD2[3_554]	2.15	0.05
1:A:452:PRO:O	1:A:454:PRO: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: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%)	24 17

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

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%)	5 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

Some 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

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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	476/484 (98%)	2.30	264 (55%)	0	0	8, 16, 31, 50	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	ILE	8.0
1	A	363	ALA	7.3
1	A	148	PRO	6.8
1	A	430	SER	6.2
1	A	132	VAL	5.8
1	A	473	SER	5.7
1	A	302	ALA	5.7
1	A	306	SER	5.6
1	A	356	ALA	5.6
1	A	288	LEU	5.3
1	A	98	ASP	5.3
1	A	165	TRP	5.2
1	A	130	ASN	5.1
1	A	62	ILE	5.0
1	A	311	ALA	5.0
1	A	458	GLY	5.0
1	A	476	GLY	5.0
1	A	88	TYR	5.0
1	A	423	LEU	4.9
1	A	374	ALA	4.9
1	A	449	GLY	4.8
1	A	463	LEU	4.6
1	A	361	TRP	4.6
1	A	421	LEU	4.5
1	A	464	LEU	4.5
1	A	395	ALA	4.5
1	A	425	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	256	TRP	4.4
1	A	255	TYR	4.4
1	A	362	ILE	4.4
1	A	40	GLY	4.4
1	A	46	ILE	4.4
1	A	293	ILE	4.4
1	A	118	VAL	4.4
1	A	176	LEU	4.3
1	A	445	VAL	4.3
1	A	170	ILE	4.2
1	A	203	LEU	4.2
1	A	381	THR	4.2
1	A	146	PHE	4.2
1	A	406	ILE	4.2
1	A	100	LEU	4.1
1	A	152	ILE	4.1
1	A	158	LEU	4.1
1	A	134	TYR	4.1
1	A	467	SER	4.0
1	A	153	THR	4.0
1	A	82	TYR	3.9
1	A	422	THR	3.9
1	A	216	PHE	3.8
1	A	231	ILE	3.8
1	A	202	GLY	3.8
1	A	447	SER	3.7
1	A	460	PRO	3.7
1	A	317	TYR	3.7
1	A	394	ILE	3.7
1	A	136	VAL	3.7
1	A	49	LEU	3.6
1	A	325	PRO	3.6
1	A	435	ILE	3.6
1	A	474	LEU	3.6
1	A	96	THR	3.6
1	A	128	ASN	3.6
1	A	391	SER	3.6
1	A	429	THR	3.5
1	A	373	ILE	3.5
1	A	418	SER	3.5
1	A	211	VAL	3.5
1	A	462	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	3.5
1	A	22	THR	3.5
1	A	195	VAL	3.5
1	A	326	ILE	3.5
1	A	281	SER	3.4
1	A	109	ALA	3.4
1	A	237	ALA	3.4
1	A	103	LEU	3.4
1	A	155	TRP	3.4
1	A	143	SER	3.4
1	A	401	SER	3.4
1	A	57	PHE	3.4
1	A	289	LEU	3.4
1	A	179	THR	3.4
1	A	427	GLY	3.4
1	A	358	LEU	3.4
1	A	292	PHE	3.4
1	A	459	LEU	3.4
1	A	157	ASN	3.4
1	A	267	GLY	3.4
1	A	126	ALA	3.3
1	A	131	ASP	3.3
1	A	468	VAL	3.3
1	A	15	LEU	3.3
1	A	215	PHE	3.3
1	A	173	LEU	3.3
1	A	66	THR	3.3
1	A	137	PHE	3.3
1	A	187	TRP	3.3
1	A	409	LEU	3.3
1	A	305	THR	3.2
1	A	431	GLY	3.2
1	A	339	LYS	3.2
1	A	282	ASP	3.2
1	A	238	SER	3.1
1	A	355	SER	3.1
1	A	419	TYR	3.1
1	A	119	VAL	3.1
1	A	225	VAL	3.1
1	A	194	LEU	3.1
1	A	258	LEU	3.1
1	A	189	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	457	SER	3.1
1	A	23	ASP	3.0
1	A	226	TYR	3.0
1	A	387	PHE	3.0
1	A	6	TRP	3.0
1	A	111	GLY	3.0
1	A	110	ARG	3.0
1	A	141	ASP	3.0
1	A	208	VAL	3.0
1	A	417	SER	2.9
1	A	45	ILE	2.9
1	A	140	PHE	2.9
1	A	171	VAL	2.9
1	A	342	TYR	2.9
1	A	61	TRP	2.9
1	A	408	VAL	2.9
1	A	354	THR	2.9
1	A	400	THR	2.9
1	A	448	SER	2.9
1	A	204	ARG	2.9
1	A	440	CYS	2.9
1	A	438	TYR	2.8
1	A	26	THR	2.8
1	A	469	VAL	2.8
1	A	33	GLY	2.8
1	A	151	LEU	2.8
1	A	308	TYR	2.8
1	A	36	ILE	2.8
1	A	12	TYR	2.8
1	A	87	ILE	2.7
1	A	269	ILE	2.7
1	A	121	ASP	2.7
1	A	223	SER	2.7
1	A	145	TYR	2.7
1	A	29	THR	2.7
1	A	379	TYR	2.7
1	A	235	ASN	2.7
1	A	399	GLY	2.7
1	A	93	ASN	2.7
1	A	261	ALA	2.7
1	A	79	TYR	2.7
1	A	273	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	2.6
1	A	11	ILE	2.6
1	A	392	ASN	2.6
1	A	424	SER	2.6
1	A	20	GLY	2.6
1	A	233	ASN	2.6
1	A	217	PRO	2.6
1	A	172	SER	2.6
1	A	191	VAL	2.6
1	A	192	ALA	2.6
1	A	321	SER	2.6
1	A	397	ALA	2.6
1	A	307	ASP	2.6
1	A	139	PRO	2.6
1	A	284	SER	2.6
1	A	3	ALA	2.5
1	A	209	LEU	2.5
1	A	220	ASN	2.5
1	A	248	GLY	2.5
1	A	101	LYS	2.5
1	A	222	ALA	2.5
1	A	246	LEU	2.5
1	A	268	SER	2.5
1	A	164	CYS	2.5
1	A	168	ASP	2.5
1	A	327	VAL	2.5
1	A	426	SER	2.5
1	A	254	ILE	2.5
1	A	348	TRP	2.5
1	A	55	MET	2.4
1	A	65	ILE	2.4
1	A	123	MET	2.4
1	A	455	MET	2.4
1	A	323	GLY	2.4
1	A	276	ILE	2.4
1	A	265	SER	2.4
1	A	68	GLN	2.4
1	A	240	CYS	2.4
1	A	135	SER	2.4
1	A	262	PHE	2.4
1	A	266	SER	2.4
1	A	69	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	252	TYR	2.3
1	A	73	THR	2.3
1	A	250	LEU	2.3
1	A	405	VAL	2.3
1	A	324	ILE	2.3
1	A	175	ASP	2.3
1	A	174	PRO	2.3
1	A	154	ASP	2.3
1	A	56	GLY	2.3
1	A	144	SER	2.3
1	A	283	CYS	2.3
1	A	475	CYS	2.3
1	A	8	THR	2.3
1	A	402	GLY	2.2
1	A	364	THR	2.2
1	A	105	ASP	2.2
1	A	182	ALA	2.2
1	A	329	ALA	2.2
1	A	1	LEU	2.2
1	A	113	TYR	2.2
1	A	461	ARG	2.2
1	A	470	ASP	2.2
1	A	200	VAL	2.2
1	A	249	VAL	2.2
1	A	290	GLY	2.2
1	A	42	TRP	2.2
1	A	297	ASP	2.2
1	A	160	MET	2.2
1	A	34	ASN	2.2
1	A	234	GLY	2.2
1	A	188	TYR	2.2
1	A	410	SER	2.2
1	A	52	ILE	2.2
1	A	298	ASN	2.2
1	A	38	CYS	2.2
1	A	13	PHE	2.2
1	A	472	SER	2.2
1	A	328	TYR	2.2
1	A	286	PRO	2.2
1	A	454	PRO	2.2
1	A	112	MET	2.1
1	A	334	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	2.1
1	A	393	THR	2.1
1	A	83	TRP	2.1
1	A	59	ALA	2.1
1	A	219	TYR	2.1
1	A	372	ALA	2.1
1	A	382	TYR	2.1
1	A	161	VAL	2.1
1	A	241	PRO	2.1
1	A	72	ASP	2.1
1	A	415	SER	2.1
1	A	433	LYS	2.1
1	A	122	HIS	2.1
1	A	287	THR	2.1
1	A	314	VAL	2.1
1	A	380	ILE	2.1
1	A	296	HIS	2.1
1	A	278	SER	2.1
1	A	198	TYR	2.1
1	A	184	ARG	2.0
1	A	190	TRP	2.0
1	A	178	THR	2.0
1	A	181	THR	2.0
1	A	116	VAL	2.0
1	A	228	VAL	2.0
1	A	76	GLY	2.0
1	A	239	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	A	485	1/1	0.91	0.09	-4.44	17,17,17,17	0
2	CA	A	486	1/1	0.74	0.14	-	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.