



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:16 AM UTC

PDB ID : 1BRO / pdb_00001bro
Title : BROMOPEROXIDASE A2
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Deposited on : 1996-06-01
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

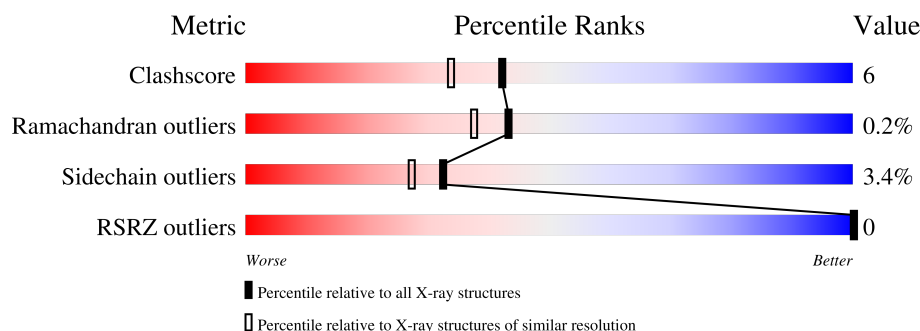
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	277	47% 40% 13%
1	B	277	46% 46% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4529 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 BROMOPEROXIDASE A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2147	1372	356	418	1			
1	B	277	Total	C	N	O	S	0	0	0
			2147	1372	356	418	1			

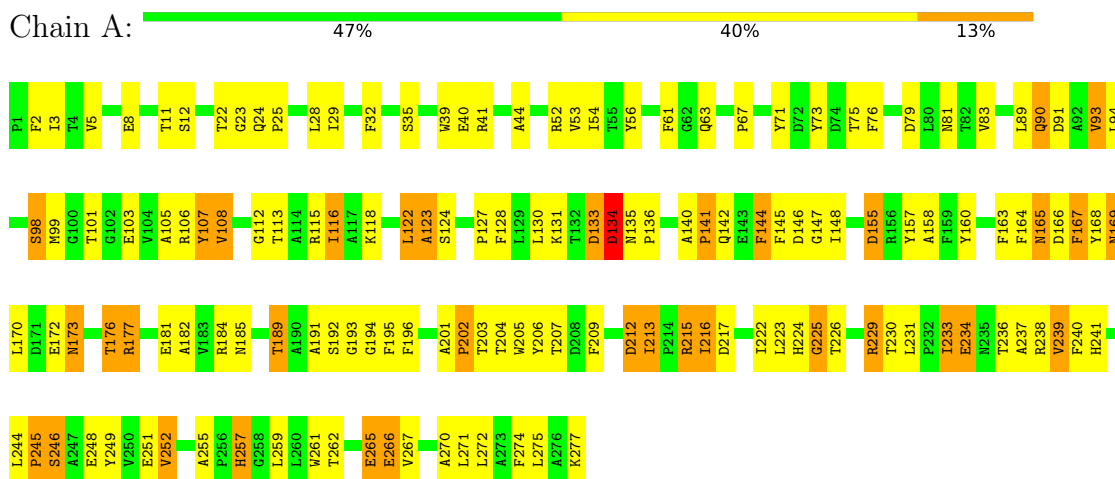
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	141	Total	O	0	0
			141	141		

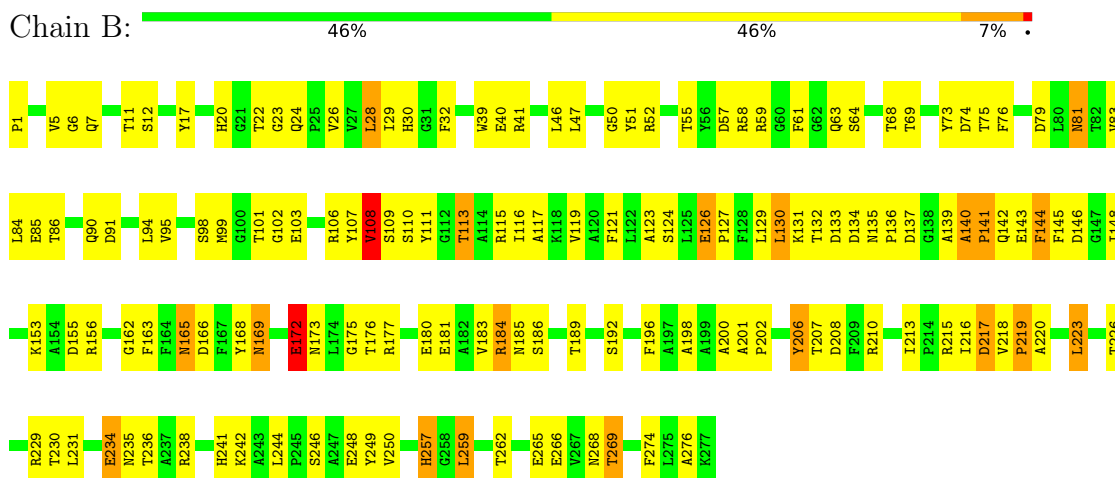
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: BROMOPEROXIDASE A2



• Molecule 1: BROMOPEROXIDASE A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	126.50Å 126.50Å 126.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 10.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (10.00-2.05) 97.2 (10.00-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.05Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.165 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4529	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	1.51	12/2205 (0.5%)	2.76	206/3010 (6.8%)
1	B	1.63	20/2205 (0.9%)	2.87	240/3010 (8.0%)
All	All	1.57	32/4410 (0.7%)	2.82	446/6020 (7.4%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	ILE	CA-CB	9.91	1.59	1.54
1	B	217	ASP	CA-CB	8.09	1.67	1.53
1	A	116	ILE	CA-CB	7.64	1.63	1.54
1	B	184	ARG	NE-CZ	7.16	1.41	1.33
1	B	184	ARG	CZ-NH2	6.71	1.42	1.33
1	B	184	ARG	CZ-NH1	6.46	1.41	1.32
1	A	41	ARG	NE-CZ	6.29	1.40	1.33
1	A	272	LEU	C-O	6.28	1.31	1.24
1	B	23	GLY	N-CA	5.86	1.52	1.45
1	A	213	ILE	C-O	5.84	1.29	1.24
1	B	103	GLU	C-O	5.80	1.30	1.24
1	B	24	GLN	N-CA	5.72	1.53	1.45
1	B	116	ILE	CA-CB	5.63	1.60	1.54
1	A	213	ILE	CA-CB	5.55	1.56	1.54
1	B	189	THR	CA-CB	5.54	1.61	1.53
1	A	215	ARG	CZ-NH2	5.49	1.40	1.33
1	B	226	THR	C-O	5.45	1.31	1.24
1	B	23	GLY	C-O	5.39	1.28	1.23
1	B	11	THR	CA-CB	5.36	1.62	1.53
1	B	215	ARG	NE-CZ	5.31	1.38	1.33
1	B	230	THR	CA-CB	5.30	1.62	1.53
1	A	11	THR	CA-CB	5.29	1.62	1.53
1	A	22	THR	CB-OG1	5.27	1.52	1.43
1	A	236	THR	CA-CB	5.18	1.61	1.53
1	B	262	THR	CA-CB	5.10	1.61	1.53
1	B	215	ARG	CZ-NH2	5.10	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	TYR	N-CA	5.08	1.52	1.45
1	B	29	ILE	CA-CB	5.07	1.59	1.53
1	A	262	THR	N-CA	5.02	1.52	1.46
1	B	94	LEU	CA-C	5.02	1.59	1.52
1	B	41	ARG	NE-CZ	5.01	1.38	1.33
1	A	112	GLY	N-CA	5.00	1.50	1.45

All (446) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASN	OD1-CG-ND2	22.21	144.81	122.60
1	B	217	ASP	CA-CB-CG	-18.46	94.14	112.60
1	B	165	ASN	OD1-CG-ND2	16.96	139.56	122.60
1	B	165	ASN	CA-CB-CG	-15.29	97.31	112.60
1	B	76	PHE	CA-CB-CG	13.66	127.46	113.80
1	B	218	VAL	N-CA-CB	-13.65	102.41	111.83
1	A	265	GLU	N-CA-C	13.37	125.37	111.07
1	B	217	ASP	N-CA-C	12.56	128.99	113.17
1	B	166	ASP	CA-CB-CG	-12.37	100.23	112.60
1	A	79	ASP	CA-CB-CG	12.14	124.74	112.60
1	B	145	PHE	CA-CB-CG	-11.76	102.04	113.80
1	B	140	ALA	O-C-N	11.66	130.16	121.65
1	A	2	PHE	CA-CB-CG	-11.65	102.15	113.80
1	A	41	ARG	CD-NE-CZ	-11.50	108.31	124.40
1	B	169	ASN	OD1-CG-ND2	-11.35	111.25	122.60
1	B	184	ARG	NE-CZ-NH2	11.32	129.39	119.20
1	A	184	ARG	CD-NE-CZ	11.16	140.02	124.40
1	A	216	ILE	CA-C-N	11.06	145.19	121.64
1	A	216	ILE	C-N-CA	11.06	145.19	121.64
1	A	165	ASN	CA-CB-CG	-10.94	101.66	112.60
1	B	91	ASP	CA-CB-CG	-10.83	101.77	112.60
1	B	216	ILE	CA-C-N	10.47	139.81	122.54
1	B	216	ILE	C-N-CA	10.47	139.81	122.54
1	A	266	GLU	N-CA-C	-10.27	100.17	111.36
1	B	23	GLY	N-CA-C	-10.05	100.07	111.63
1	B	268	ASN	O-C-N	9.88	132.59	122.12
1	B	168	TYR	CA-C-O	-9.75	107.94	119.35
1	A	41	ARG	NH1-CZ-NH2	-9.60	106.82	119.30
1	A	173	ASN	N-CA-C	9.59	125.12	113.23
1	A	184	ARG	NE-CZ-NH1	9.52	131.02	121.50
1	B	79	ASP	O-C-N	9.49	131.85	122.07
1	A	41	ARG	NE-CZ-NH2	9.46	127.71	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	ASP	N-CA-CB	-9.44	96.52	110.49
1	B	39	TRP	CA-C-O	-9.44	107.86	119.28
1	A	172	GLU	CB-CG-CD	9.33	128.46	112.60
1	A	165	ASN	N-CA-CB	-9.32	96.50	110.01
1	B	79	ASP	CA-C-O	-9.30	111.05	120.82
1	B	74	ASP	CA-C-O	-9.26	110.61	120.42
1	B	135	ASN	CA-CB-CG	-9.15	103.44	112.60
1	A	177	ARG	NE-CZ-NH1	9.08	130.58	121.50
1	A	146	ASP	CA-C-N	9.05	129.99	119.94
1	A	146	ASP	C-N-CA	9.05	129.99	119.94
1	B	146	ASP	CA-CB-CG	9.02	121.61	112.60
1	B	183	VAL	O-C-N	-9.01	113.14	121.87
1	B	84	LEU	O-C-N	8.97	131.63	122.12
1	B	6	GLY	O-C-N	8.96	132.39	123.88
1	B	135	ASN	CA-C-O	8.94	131.12	121.28
1	A	142	GLN	CG-CD-NE2	-8.90	103.04	116.40
1	B	109	SER	CA-C-O	8.89	129.84	120.42
1	A	217	ASP	N-CA-C	8.85	124.76	112.45
1	B	63	GLN	CA-C-O	-8.69	108.76	119.28
1	A	217	ASP	N-CA-CB	-8.67	97.34	110.26
1	A	195	PHE	O-C-N	-8.66	112.94	122.12
1	B	215	ARG	NE-CZ-NH1	8.64	130.15	121.50
1	B	23	GLY	O-C-N	8.64	131.27	123.06
1	A	122	LEU	CA-C-O	-8.61	111.00	120.38
1	A	234	GLU	CG-CD-OE2	8.47	137.89	118.40
1	A	252	VAL	CA-C-O	8.39	130.48	120.66
1	A	246	SER	N-CA-CB	-8.31	97.43	110.22
1	B	175	GLY	O-C-N	-8.30	111.55	122.42
1	B	75	THR	CA-CB-OG1	-8.29	97.16	109.60
1	B	184	ARG	CG-CD-NE	8.29	130.25	112.00
1	B	173	ASN	N-CA-C	8.29	123.70	113.50
1	A	225	GLY	O-C-N	8.28	129.47	123.35
1	B	213	ILE	N-CA-CB	8.27	116.06	110.52
1	A	270	ALA	CA-C-O	8.23	129.46	120.82
1	B	165	ASN	CB-CG-ND2	-8.22	104.06	116.40
1	A	127	PRO	N-CD-CG	-8.20	93.96	103.80
1	A	106	ARG	CD-NE-CZ	8.16	135.82	124.40
1	B	217	ASP	CB-CA-C	-8.14	96.50	110.09
1	A	91	ASP	N-CA-CB	-8.13	99.73	111.84
1	A	184	ARG	NE-CZ-NH2	-8.12	111.89	119.20
1	A	116	ILE	N-CA-C	8.02	119.69	107.99
1	B	196	PHE	CA-CB-CG	-7.98	105.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TYR	CA-C-O	-7.97	109.83	119.32
1	B	153	LYS	O-C-N	7.94	131.51	122.22
1	B	101	THR	CA-C-N	7.92	128.57	119.94
1	B	101	THR	C-N-CA	7.92	128.57	119.94
1	B	115	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	A	67	PRO	CA-C-O	7.91	133.47	122.31
1	A	52	ARG	NE-CZ-NH2	7.91	126.32	119.20
1	B	133	ASP	CB-CA-C	-7.91	98.46	110.88
1	A	244	LEU	CA-C-N	7.91	127.98	119.28
1	A	244	LEU	C-N-CA	7.91	127.98	119.28
1	A	192	SER	CA-C-N	7.90	129.46	120.53
1	A	192	SER	C-N-CA	7.90	129.46	120.53
1	A	168	TYR	CA-C-O	-7.90	110.11	119.35
1	A	75	THR	CA-CB-OG1	-7.90	97.76	109.60
1	A	196	PHE	O-C-N	7.88	130.60	122.09
1	B	107	TYR	CA-C-N	7.86	131.22	120.46
1	B	107	TYR	C-N-CA	7.86	131.22	120.46
1	B	116	ILE	CA-C-O	-7.84	112.17	120.48
1	B	81	ASN	CB-CG-ND2	7.82	128.13	116.40
1	A	172	GLU	CA-CB-CG	7.79	129.69	114.10
1	B	177	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	A	105	ALA	O-C-N	7.78	130.08	122.07
1	A	257	HIS	CA-C-O	7.72	128.93	120.82
1	A	145	PHE	CA-CB-CG	-7.72	106.08	113.80
1	B	183	VAL	CA-C-N	7.72	130.96	120.54
1	B	183	VAL	C-N-CA	7.72	130.96	120.54
1	B	74	ASP	CA-CB-CG	-7.66	104.94	112.60
1	B	129	LEU	N-CA-C	7.65	120.69	111.82
1	B	119	VAL	O-C-N	-7.65	114.81	123.00
1	A	177	ARG	NE-CZ-NH2	-7.64	112.33	119.20
1	B	131	LYS	CA-CB-CG	-7.63	98.83	114.10
1	B	52	ARG	NE-CZ-NH2	7.56	126.00	119.20
1	A	54	ILE	O-C-N	-7.55	115.25	123.18
1	A	229	ARG	NE-CZ-NH2	-7.55	112.41	119.20
1	A	248	GLU	N-CA-C	-7.51	98.34	110.20
1	B	265	GLU	CG-CD-OE1	7.45	135.54	118.40
1	A	166	ASP	O-C-N	7.42	132.27	122.33
1	A	90	GLN	O-C-N	7.41	132.86	123.23
1	A	75	THR	O-C-N	7.39	129.68	122.07
1	B	234	GLU	N-CA-CB	7.39	121.73	110.28
1	A	133	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	234	GLU	CG-CD-OE1	-7.34	101.53	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ALA	CA-C-O	-7.33	111.55	118.73
1	B	210	ARG	NE-CZ-NH1	7.30	128.80	121.50
1	A	157	TYR	CA-C-N	7.30	130.66	120.29
1	A	157	TYR	C-N-CA	7.30	130.66	120.29
1	B	144	PHE	CA-CB-CG	-7.29	106.51	113.80
1	B	208	ASP	CA-C-O	-7.28	112.27	120.43
1	B	186	SER	O-C-N	7.26	129.82	122.12
1	B	90	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	103	GLU	N-CA-CB	7.24	120.51	110.01
1	B	103	GLU	CB-CG-CD	7.24	124.91	112.60
1	A	238	ARG	O-C-N	7.23	129.78	122.12
1	A	170	LEU	CA-C-O	-7.21	112.91	120.55
1	A	160	TYR	O-C-N	7.19	129.74	122.12
1	B	81	ASN	CA-C-O	7.15	128.55	120.90
1	B	106	ARG	NE-CZ-NH1	7.15	128.65	121.50
1	B	201	ALA	O-C-N	7.14	126.84	120.48
1	B	185	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	196	PHE	CA-C-O	-7.12	113.37	120.70
1	A	245	PRO	CA-C-O	7.12	130.37	119.55
1	B	153	LYS	CA-C-O	-7.10	112.08	120.10
1	A	238	ARG	CA-C-O	-7.05	113.08	120.55
1	B	24	GLN	O-C-N	7.04	128.55	121.30
1	B	115	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	A	238	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	A	8	GLU	CA-C-O	-6.99	112.78	120.33
1	A	238	ARG	NE-CZ-NH1	-6.98	114.52	121.50
1	A	265	GLU	CB-CA-C	-6.97	99.93	110.88
1	B	266	GLU	OE1-CD-OE2	-6.93	106.28	122.90
1	A	277	LYS	CB-CG-CD	-6.92	95.38	111.30
1	B	181	GLU	CG-CD-OE1	6.91	134.28	118.40
1	B	238	ARG	CA-C-O	-6.90	113.24	120.55
1	B	189	THR	O-C-N	6.89	129.42	122.12
1	A	73	TYR	CA-C-N	-6.88	110.53	120.29
1	A	73	TYR	C-N-CA	-6.88	110.53	120.29
1	B	186	SER	CA-C-O	-6.86	113.28	120.55
1	B	207	THR	N-CA-C	-6.85	100.14	110.28
1	A	212	ASP	CA-CB-CG	-6.85	105.75	112.60
1	B	133	ASP	OD1-CG-OD2	6.85	139.33	122.90
1	A	52	ARG	NH1-CZ-NH2	-6.84	110.41	119.30
1	B	257	HIS	CE1-NE2-CD2	6.82	115.82	109.00
1	B	86	THR	O-C-N	6.80	129.07	122.07
1	B	248	GLU	N-CA-C	-6.79	98.97	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	PHE	CA-CB-CG	-6.77	107.03	113.80
1	B	109	SER	N-CA-CB	-6.77	100.14	110.16
1	B	235	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	B	246	SER	CA-C-O	-6.76	110.27	119.05
1	B	109	SER	O-C-N	-6.76	114.45	122.15
1	A	213	ILE	N-CA-C	6.75	121.11	112.67
1	A	22	THR	CA-C-O	-6.73	113.26	121.06
1	A	274	PHE	CA-C-O	-6.72	113.76	120.82
1	A	233	ILE	O-C-N	-6.68	115.16	121.90
1	B	133	ASP	CA-CB-CG	-6.67	105.92	112.60
1	B	116	ILE	N-CA-C	6.67	117.50	108.17
1	A	213	ILE	CA-C-N	6.66	126.35	119.56
1	A	213	ILE	C-N-CA	6.66	126.35	119.56
1	B	106	ARG	NH1-CZ-NH2	-6.65	110.65	119.30
1	A	267	VAL	O-C-N	-6.63	115.01	121.90
1	B	7	GLN	CB-CG-CD	6.60	123.83	112.60
1	B	185	ASN	O-C-N	-6.60	115.27	122.07
1	B	59	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	B	91	ASP	CB-CA-C	-6.58	102.19	111.80
1	B	259	LEU	CA-C-O	-6.56	111.31	119.38
1	A	23	GLY	N-CA-C	-6.54	101.68	110.97
1	B	111	TYR	O-C-N	6.54	130.15	122.24
1	A	35	SER	CA-C-O	-6.54	114.31	121.31
1	B	7	GLN	CG-CD-NE2	6.53	126.20	116.40
1	B	86	THR	CA-C-O	-6.52	113.98	120.82
1	B	215	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	B	162	GLY	O-C-N	6.50	128.49	122.19
1	B	61	PHE	O-C-N	6.49	131.22	123.24
1	B	219	PRO	N-CA-CB	-6.49	97.54	103.25
1	A	5	VAL	N-CA-CB	-6.48	104.61	112.33
1	B	180	GLU	N-CA-CB	-6.48	100.59	110.12
1	B	234	GLU	CB-CA-C	-6.47	98.24	110.67
1	A	165	ASN	CB-CG-ND2	-6.47	106.70	116.40
1	B	133	ASP	O-C-N	6.47	128.73	122.07
1	A	141	PRO	CB-CA-C	6.44	119.49	110.60
1	A	234	GLU	CB-CG-CD	6.44	123.54	112.60
1	B	137	ASP	O-C-N	6.42	131.81	122.43
1	A	29	ILE	CB-CG1-CD1	6.41	127.26	113.80
1	A	195	PHE	CA-C-O	6.39	127.33	120.55
1	A	239	VAL	CB-CA-C	6.39	122.58	112.16
1	B	124	SER	N-CA-C	6.39	119.51	110.50
1	A	177	ARG	CA-CB-CG	-6.38	101.34	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LEU	O-C-N	6.38	128.66	122.03
1	B	85	GLU	CA-C-N	6.37	128.72	120.44
1	B	85	GLU	C-N-CA	6.37	128.72	120.44
1	B	220	ALA	O-C-N	-6.36	115.41	123.24
1	B	269	THR	OG1-CB-CG2	-6.36	96.58	109.30
1	A	249	TYR	N-CA-CB	-6.36	100.13	110.81
1	A	166	ASP	CA-CB-CG	-6.35	106.25	112.60
1	A	76	PHE	CA-CB-CG	6.34	120.14	113.80
1	A	147	GLY	CA-C-O	6.34	127.84	121.00
1	B	121	PHE	CA-C-O	-6.32	113.76	120.40
1	B	83	VAL	CA-C-O	-6.30	114.49	121.17
1	A	54	ILE	CA-C-O	6.29	127.15	120.48
1	A	22	THR	O-C-N	6.28	130.55	123.27
1	A	185	ASN	CA-CB-CG	-6.28	106.32	112.60
1	B	198	ALA	N-CA-C	-6.27	104.36	111.07
1	A	128	PHE	CA-CB-CG	6.27	120.07	113.80
1	A	101	THR	CA-CB-OG1	-6.26	100.21	109.60
1	A	224	HIS	CA-C-N	6.24	127.61	121.62
1	A	224	HIS	C-N-CA	6.24	127.61	121.62
1	A	181	GLU	CA-C-N	6.23	128.54	120.44
1	A	181	GLU	C-N-CA	6.23	128.54	120.44
1	A	165	ASN	CB-CG-OD1	-6.23	108.34	120.80
1	B	208	ASP	O-C-N	6.23	130.29	123.13
1	B	249	TYR	CA-C-O	-6.23	113.63	120.36
1	A	131	LYS	CB-CG-CD	-6.23	96.97	111.30
1	B	26	VAL	CA-C-O	-6.20	113.94	120.39
1	A	83	VAL	O-C-N	6.17	127.96	121.91
1	A	191	ALA	CA-C-O	6.17	127.07	120.10
1	A	81	ASN	CA-CB-CG	-6.14	106.46	112.60
1	B	229	ARG	CD-NE-CZ	6.13	132.99	124.40
1	A	272	LEU	CA-C-O	-6.13	114.05	120.55
1	B	32	PHE	CA-CB-CG	6.13	119.93	113.80
1	B	135	ASN	O-C-N	-6.13	116.27	121.23
1	B	7	GLN	CA-C-O	6.12	128.16	121.06
1	B	176	THR	O-C-N	6.11	129.09	121.95
1	B	226	THR	CA-C-O	-6.09	111.89	119.38
1	B	81	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	B	73	TYR	O-C-N	6.06	129.31	122.22
1	B	7	GLN	CG-CD-OE1	-6.05	108.69	120.80
1	B	186	SER	N-CA-C	-6.05	104.68	111.28
1	A	134	ASP	CB-CA-C	6.03	122.60	109.99
1	B	156	ARG	CD-NE-CZ	6.03	132.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	TYR	O-C-N	-6.02	115.87	122.07
1	B	57	ASP	CA-C-O	-6.00	113.94	120.36
1	B	183	VAL	CA-C-O	6.00	127.19	120.95
1	A	229	ARG	NE-CZ-NH1	6.00	127.50	121.50
1	A	32	PHE	CA-CB-CG	5.98	119.78	113.80
1	B	142	GLN	CB-CG-CD	-5.96	102.47	112.60
1	A	106	ARG	NH1-CZ-NH2	-5.96	111.56	119.30
1	B	85	GLU	CG-CD-OE2	5.92	132.01	118.40
1	B	99	MET	CG-SD-CE	-5.90	87.92	100.90
1	A	40	GLU	CA-C-O	-5.89	114.27	120.63
1	B	79	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	166	ASP	CB-CG-OD1	5.86	131.87	118.40
1	B	12	SER	CA-CB-OG	-5.86	99.39	111.10
1	B	59	ARG	NH1-CZ-NH2	-5.85	111.69	119.30
1	B	64	SER	CA-C-N	5.85	129.59	120.75
1	B	64	SER	C-N-CA	5.85	129.59	120.75
1	A	241	HIS	N-CA-CB	5.85	119.23	110.22
1	A	22	THR	CA-CB-CG2	5.85	120.44	110.50
1	A	251	GLU	N-CA-CB	5.84	119.96	110.43
1	B	51	TYR	CA-CB-CG	-5.84	103.39	113.90
1	B	206	TYR	CA-C-N	5.83	129.14	120.87
1	B	206	TYR	C-N-CA	5.83	129.14	120.87
1	B	41	ARG	NE-CZ-NH1	5.82	127.31	121.50
1	B	169	ASN	CB-CG-ND2	5.81	125.11	116.40
1	A	44	ALA	CA-C-O	-5.80	114.40	120.55
1	B	5	VAL	N-CA-C	-5.80	107.11	113.43
1	A	71	TYR	CA-CB-CG	-5.79	103.47	113.90
1	B	46	LEU	CA-C-O	-5.79	114.28	120.42
1	B	52	ARG	CB-CG-CD	-5.79	97.98	111.30
1	B	134	ASP	CB-CG-OD2	-5.78	105.10	118.40
1	A	212	ASP	O-C-N	5.78	129.74	122.23
1	B	68	THR	CB-CA-C	5.77	120.43	111.13
1	A	73	TYR	CA-CB-CG	-5.77	103.51	113.90
1	A	90	GLN	CA-C-O	-5.76	114.47	120.70
1	B	22	THR	CA-C-N	-5.74	113.39	122.92
1	B	22	THR	C-N-CA	-5.74	113.39	122.92
1	A	12	SER	CA-CB-OG	-5.74	99.63	111.10
1	A	63	GLN	CA-CB-CG	-5.73	102.64	114.10
1	A	93	VAL	O-C-N	-5.73	117.16	123.18
1	A	155	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	274	PHE	CA-CB-CG	-5.71	108.09	113.80
1	B	148	ILE	CA-CB-CG1	-5.71	100.69	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	THR	CA-CB-OG1	-5.71	101.04	109.60
1	B	136	PRO	CA-C-O	5.70	126.73	118.86
1	B	111	TYR	CA-C-N	-5.70	114.78	121.85
1	B	111	TYR	C-N-CA	-5.70	114.78	121.85
1	A	265	GLU	CG-CD-OE2	-5.69	105.31	118.40
1	B	238	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	B	175	GLY	CA-C-O	5.68	125.29	119.10
1	B	126	GLU	CB-CG-CD	5.68	122.25	112.60
1	B	29	ILE	O-C-N	5.68	130.57	122.62
1	B	244	LEU	N-CA-CB	-5.68	102.02	110.99
1	B	177	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	B	119	VAL	CA-C-N	5.66	131.84	122.33
1	B	119	VAL	C-N-CA	5.66	131.84	122.33
1	B	106	ARG	CD-NE-CZ	5.65	132.31	124.40
1	A	240	PHE	CA-C-N	5.64	128.41	120.28
1	A	240	PHE	C-N-CA	5.64	128.41	120.28
1	A	115	ARG	CA-C-N	5.63	130.11	122.90
1	A	115	ARG	C-N-CA	5.63	130.11	122.90
1	A	261	TRP	N-CA-CB	5.62	118.91	110.14
1	B	50	GLY	N-CA-C	5.62	124.63	114.46
1	A	123	ALA	CA-C-N	5.62	129.76	120.94
1	A	123	ALA	C-N-CA	5.62	129.76	120.94
1	A	124	SER	N-CA-C	5.61	118.42	110.50
1	A	265	GLU	CA-C-O	5.61	126.71	120.82
1	A	203	THR	O-C-N	-5.61	115.37	122.27
1	B	223	LEU	CA-C-O	-5.61	114.21	120.66
1	A	230	THR	CB-CA-C	5.61	120.82	110.56
1	A	204	THR	CA-C-O	-5.60	112.36	119.31
1	B	41	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	A	217	ASP	CA-C-N	5.59	132.47	122.13
1	A	217	ASP	C-N-CA	5.59	132.47	122.13
1	A	215	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	A	205	TRP	CA-C-O	-5.58	113.79	120.10
1	A	170	LEU	O-C-N	5.58	128.03	122.12
1	B	52	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	44	ALA	CA-C-N	5.58	128.02	120.44
1	A	44	ALA	C-N-CA	5.58	128.02	120.44
1	A	112	GLY	CA-C-O	5.58	128.39	122.59
1	B	198	ALA	N-CA-CB	5.57	118.08	110.01
1	B	39	TRP	O-C-N	5.57	130.05	122.37
1	B	55	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	98	SER	CB-CA-C	5.57	121.49	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	HIS	CA-C-O	-5.57	114.52	120.42
1	B	58	ARG	CD-NE-CZ	5.55	132.16	124.40
1	B	242	LYS	CG-CD-CE	5.55	124.06	111.30
1	A	53	VAL	CA-CB-CG2	5.54	119.81	110.40
1	A	182	ALA	N-CA-CB	5.52	118.01	110.01
1	A	222	ILE	N-CA-CB	5.52	118.82	111.64
1	B	266	GLU	CB-CG-CD	5.52	121.98	112.60
1	B	236	THR	CA-C-N	5.52	129.09	120.82
1	B	236	THR	C-N-CA	5.52	129.09	120.82
1	A	252	VAL	CB-CA-C	5.50	118.84	111.19
1	A	272	LEU	CB-CA-C	5.50	119.92	110.79
1	B	108	VAL	CB-CA-C	5.50	119.56	112.14
1	B	163	PHE	CA-C-N	5.50	128.19	120.28
1	B	163	PHE	C-N-CA	5.50	128.19	120.28
1	B	242	LYS	CB-CG-CD	5.49	123.92	111.30
1	A	142	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	B	24	GLN	CA-C-O	-5.47	114.48	120.17
1	B	185	ASN	CA-C-N	5.46	127.60	120.28
1	B	185	ASN	C-N-CA	5.46	127.60	120.28
1	B	165	ASN	O-C-N	5.45	127.68	122.07
1	A	267	VAL	CA-C-N	5.45	127.52	120.44
1	A	267	VAL	C-N-CA	5.45	127.52	120.44
1	A	229	ARG	CA-CB-CG	5.44	124.98	114.10
1	B	166	ASP	CB-CG-OD2	-5.44	105.89	118.40
1	B	208	ASP	CA-C-N	-5.44	113.95	122.65
1	B	208	ASP	C-N-CA	-5.44	113.95	122.65
1	B	130	LEU	CA-C-O	5.43	126.89	120.58
1	A	270	ALA	O-C-N	-5.43	116.47	122.07
1	A	144	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	233	ILE	CA-C-N	5.41	129.76	120.72
1	A	233	ILE	C-N-CA	5.41	129.76	120.72
1	A	124	SER	CB-CA-C	-5.41	99.59	109.54
1	A	207	THR	N-CA-C	-5.40	102.29	110.28
1	A	189	THR	O-C-N	5.40	127.63	122.07
1	A	246	SER	CA-CB-OG	-5.40	100.31	111.10
1	A	5	VAL	CB-CA-C	5.39	116.44	110.62
1	B	192	SER	O-C-N	-5.39	114.56	122.43
1	A	24	GLN	O-C-N	5.38	126.09	121.30
1	B	113	THR	N-CA-CB	-5.36	102.38	111.17
1	A	146	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	210	ARG	NH1-CZ-NH2	-5.35	112.34	119.30
1	B	102	GLY	O-C-N	-5.34	117.06	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ALA	CA-C-O	-5.34	115.20	120.70
1	B	257	HIS	ND1-CE1-NE2	-5.33	103.08	108.40
1	A	176	THR	N-CA-CB	-5.31	101.52	110.49
1	B	132	THR	CA-C-N	5.30	127.33	120.44
1	B	132	THR	C-N-CA	5.30	127.33	120.44
1	B	185	ASN	CB-CG-ND2	5.30	124.35	116.40
1	B	202	PRO	O-C-N	-5.30	115.76	122.17
1	A	145	PHE	O-C-N	5.29	128.19	122.15
1	B	135	ASN	CA-C-N	5.29	125.37	119.87
1	B	135	ASN	C-N-CA	5.29	125.37	119.87
1	A	107	TYR	CA-C-O	5.28	126.37	120.82
1	A	106	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	259	LEU	O-C-N	5.28	129.50	122.43
1	A	25	PRO	N-CA-CB	5.27	108.00	103.36
1	A	89	LEU	O-C-N	5.25	129.18	123.04
1	B	276	ALA	N-CA-CB	5.25	119.10	110.39
1	B	172	GLU	CG-CD-OE1	-5.24	106.34	118.40
1	A	11	THR	N-CA-CB	-5.24	102.78	110.85
1	B	143	GLU	CG-CD-OE2	-5.24	106.36	118.40
1	B	175	GLY	CA-C-N	5.22	130.21	122.17
1	B	175	GLY	C-N-CA	5.22	130.21	122.17
1	A	115	ARG	CB-CG-CD	-5.21	99.31	111.30
1	A	205	TRP	CE3-CZ3-CH2	5.21	127.87	121.10
1	A	194	GLY	O-C-N	-5.21	117.48	122.84
1	A	11	THR	CA-CB-CG2	5.20	119.34	110.50
1	A	238	ARG	CA-CB-CG	-5.20	103.70	114.10
1	B	113	THR	CA-CB-OG1	-5.20	101.80	109.60
1	B	276	ALA	CA-C-O	-5.19	112.99	119.38
1	A	113	THR	CA-CB-CG2	5.19	119.33	110.50
1	B	173	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	B	28	LEU	CB-CA-C	5.19	118.59	110.19
1	A	226	THR	CA-C-O	-5.18	113.01	119.38
1	B	155	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	163	PHE	O-C-N	5.18	127.40	122.07
1	B	236	THR	CA-C-O	-5.18	116.82	119.77
1	B	109	SER	N-CA-C	5.17	117.00	111.36
1	B	248	GLU	CB-CG-CD	-5.17	103.81	112.60
1	A	3	ILE	N-CA-CB	5.16	118.84	111.82
1	B	219	PRO	CB-CA-C	5.16	118.11	111.56
1	B	20	HIS	N-CA-C	5.15	117.64	109.50
1	B	216	ILE	CA-C-O	5.14	127.09	120.76
1	B	265	GLU	OE1-CD-OE2	-5.14	110.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ASP	CB-CA-C	-5.13	100.42	110.11
1	A	252	VAL	N-CA-CB	5.13	118.13	111.67
1	A	158	ALA	N-CA-C	-5.12	105.77	111.36
1	A	204	THR	CA-C-N	5.12	127.66	120.28
1	A	204	THR	C-N-CA	5.12	127.66	120.28
1	B	40	GLU	CB-CG-CD	-5.12	103.89	112.60
1	B	86	THR	N-CA-CB	5.12	117.44	110.01
1	A	202	PRO	O-C-N	-5.12	115.98	122.17
1	A	182	ALA	N-CA-C	-5.11	105.60	111.07
1	A	251	GLU	CA-C-O	-5.10	114.87	120.43
1	B	184	ARG	NH1-CZ-NH2	-5.10	112.67	119.30
1	A	177	ARG	CD-NE-CZ	5.09	131.53	124.40
1	B	30	HIS	CA-C-O	5.09	127.79	121.99
1	B	69	THR	N-CA-C	5.09	116.92	109.24
1	B	241	HIS	O-C-N	5.08	127.50	122.12
1	B	73	TYR	CA-C-O	-5.08	114.36	120.10
1	A	73	TYR	CA-C-O	-5.08	114.36	120.10
1	A	25	PRO	O-C-N	5.07	128.78	123.10
1	A	167	PHE	N-CA-C	-5.07	105.64	111.07
1	B	110	SER	CA-C-O	-5.07	113.81	120.00
1	B	200	ALA	CA-C-O	-5.07	113.81	119.79
1	B	6	GLY	CA-C-O	-5.06	115.86	120.97
1	A	193	GLY	CA-C-N	5.05	125.47	120.31
1	A	193	GLY	C-N-CA	5.05	125.47	120.31
1	B	111	TYR	CA-CB-CG	-5.05	104.80	113.90
1	B	17	TYR	CA-C-N	5.05	130.74	122.81
1	B	17	TYR	C-N-CA	5.05	130.74	122.81
1	A	113	THR	CA-CB-OG1	-5.04	102.03	109.60
1	A	8	GLU	N-CA-CB	5.04	118.50	110.84
1	B	141	PRO	CB-CA-C	5.04	117.55	110.95
1	A	133	ASP	O-C-N	5.04	128.78	122.23
1	B	47	LEU	CA-C-O	-5.03	115.09	120.42
1	B	11	THR	O-C-N	-5.02	116.62	123.10
1	A	118	LYS	O-C-N	5.02	128.79	123.42
1	A	169	ASN	N-CA-C	-5.01	104.51	111.52
1	B	12	SER	N-CA-C	-5.00	102.66	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2147	0	2034	35	0
1	B	2147	0	2034	18	0
2	A	94	0	0	1	0
2	B	141	0	0	3	0
All	All	4529	0	4068	53	0

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 6.

All (53) 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:B:231:LEU:HD12	1:B:257:HIS:HE1	1.49	0.77
1:A:252:VAL:HG12	1:A:255:ALA:HB2	1.69	0.75
1:A:176:THR:HG22	1:A:177:ARG:HG3	1.71	0.72
1:B:28:LEU:HD23	1:B:95:VAL:HB	1.74	0.69
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.76	0.67
1:B:140:ALA:HB1	1:B:141:PRO:HD2	1.78	0.64
1:A:130:LEU:O	1:A:135:ASN:ND2	2.31	0.62
1:A:134:ASP:C	1:A:136:PRO:HD3	2.27	0.59
1:A:212:ASP:O	1:A:215:ARG:HB2	2.02	0.59
1:A:93:VAL:HG11	1:A:275:LEU:HD21	1.85	0.58
1:B:126:GLU:HB3	1:B:127:PRO:HA	1.87	0.57
1:A:122:LEU:CD2	1:A:223:LEU:HB3	2.34	0.57
1:B:108:VAL:HG22	1:B:113:THR:HG22	1.86	0.57
1:B:1:PRO:N	2:B:374:HOH:O	2.31	0.57
1:A:231:LEU:HD12	1:A:257:HIS:HE1	1.69	0.56
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.88	0.55
1:B:231:LEU:HD12	1:B:257:HIS:CE1	2.37	0.54
1:A:94:LEU:HG	1:A:116:ILE:HD12	1.89	0.54
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.90	0.53
1:A:122:LEU:HD23	1:A:223:LEU:HB3	1.91	0.51
1:A:245:PRO:HG2	1:A:246:SER:H	1.75	0.51
1:A:141:PRO:O	1:A:144:PHE:HB3	2.10	0.50
1:A:164:PHE:HA	1:A:167:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:ND2	1:A:177:ARG:HD2	2.28	0.49
1:A:189:THR:HG21	2:A:284:HOH:O	2.11	0.49
1:B:169:ASN:HB3	1:B:172:GLU:HG3	1.93	0.49
1:A:169:ASN:HA	1:A:229:ARG:NH1	2.27	0.48
1:A:209:PHE:O	1:A:213:ILE:HG13	2.12	0.48
1:A:144:PHE:CZ	1:A:148:ILE:HD11	2.48	0.48
1:A:90:GLN:NE2	1:A:90:GLN:HA	2.29	0.47
1:B:223:LEU:HA	1:B:250:VAL:O	2.14	0.47
1:B:98:SER:HA	1:B:123:ALA:O	2.15	0.47
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.82	0.46
1:A:108:VAL:HG11	1:A:216:ILE:HG12	1.97	0.46
1:B:81:ASN:ND2	2:B:386:HOH:O	2.46	0.45
1:B:169:ASN:HB3	1:B:172:GLU:CG	2.45	0.45
1:A:265:GLU:HB2	1:A:266:GLU:OE1	2.17	0.45
1:A:233:ILE:HG13	1:A:237:ALA:HB3	1.99	0.44
1:A:98:SER:HA	1:A:123:ALA:O	2.18	0.44
1:A:225:GLY:HA2	1:A:255:ALA:HB3	2.00	0.43
1:B:126:GLU:CB	1:B:127:PRO:HA	2.47	0.43
1:A:93:VAL:HG11	1:A:275:LEU:CD2	2.48	0.43
1:A:134:ASP:O	1:A:136:PRO:HD3	2.19	0.43
1:A:140:ALA:HB1	1:A:141:PRO:HD2	2.01	0.42
1:A:201:ALA:N	1:A:202:PRO:CD	2.82	0.42
1:B:269:THR:HG21	2:B:373:HOH:O	2.21	0.41
1:A:107:TYR:CD1	1:A:107:TYR:C	2.98	0.41
1:B:141:PRO:O	1:B:144:PHE:HB3	2.20	0.41
1:A:223:LEU:C	1:A:223:LEU:HD23	2.46	0.41
1:B:117:ALA:O	1:B:219:PRO:HD2	2.21	0.41
1:A:225:GLY:CA	1:A:255:ALA:HB3	2.51	0.40
1:B:231:LEU:CD1	1:B:257:HIS:HE1	2.25	0.40
1:A:28:LEU:HB3	1:A:39:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/277 (99%)	262 (95%)	12 (4%)	1 (0%)	30	22
1	B	275/277 (99%)	266 (97%)	9 (3%)	0	100	100
All	All	550/554 (99%)	528 (96%)	21 (4%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/219 (100%)	211 (96%)	8 (4%)	30	25
1	B	219/219 (100%)	212 (97%)	7 (3%)	34	29
All	All	438/438 (100%)	423 (97%)	15 (3%)	32	27

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	MET
1	A	108	VAL
1	A	133	ASP
1	A	134	ASP
1	A	165	ASN
1	A	234	GLU
1	A	239	VAL
1	A	259	LEU
1	B	108	VAL
1	B	165	ASN
1	B	172	GLU
1	B	184	ARG

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Mol	Chain	Res	Type
1	B	217	ASP
1	B	234	GLU
1	B	259	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	173	ASN
1	A	188	ASN
1	B	42	GLN
1	B	81	ASN
1	B	169	ASN
1	B	188	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	277/277 (100%)	-0.54	0 100 100	19, 29, 49, 68	0
1	B	277/277 (100%)	-0.84	0 100 100	16, 21, 33, 55	0
All	All	554/554 (100%)	-0.69	0 100 100	16, 24, 46, 68	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.