



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:50 PM UTC

PDB ID : 1AOV / pdb_00001aov
Title : APO DUCK OVOTRANSFERRIN
Authors : Rawas, A.; Muirhead, H.
Deposited on : 1996-12-11
Resolution : 4.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

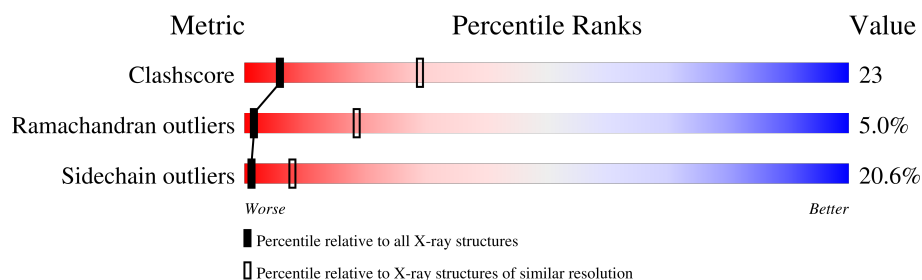
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	686	35% 42% 18% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5299 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 APO-OVOTRANSFERRIN.

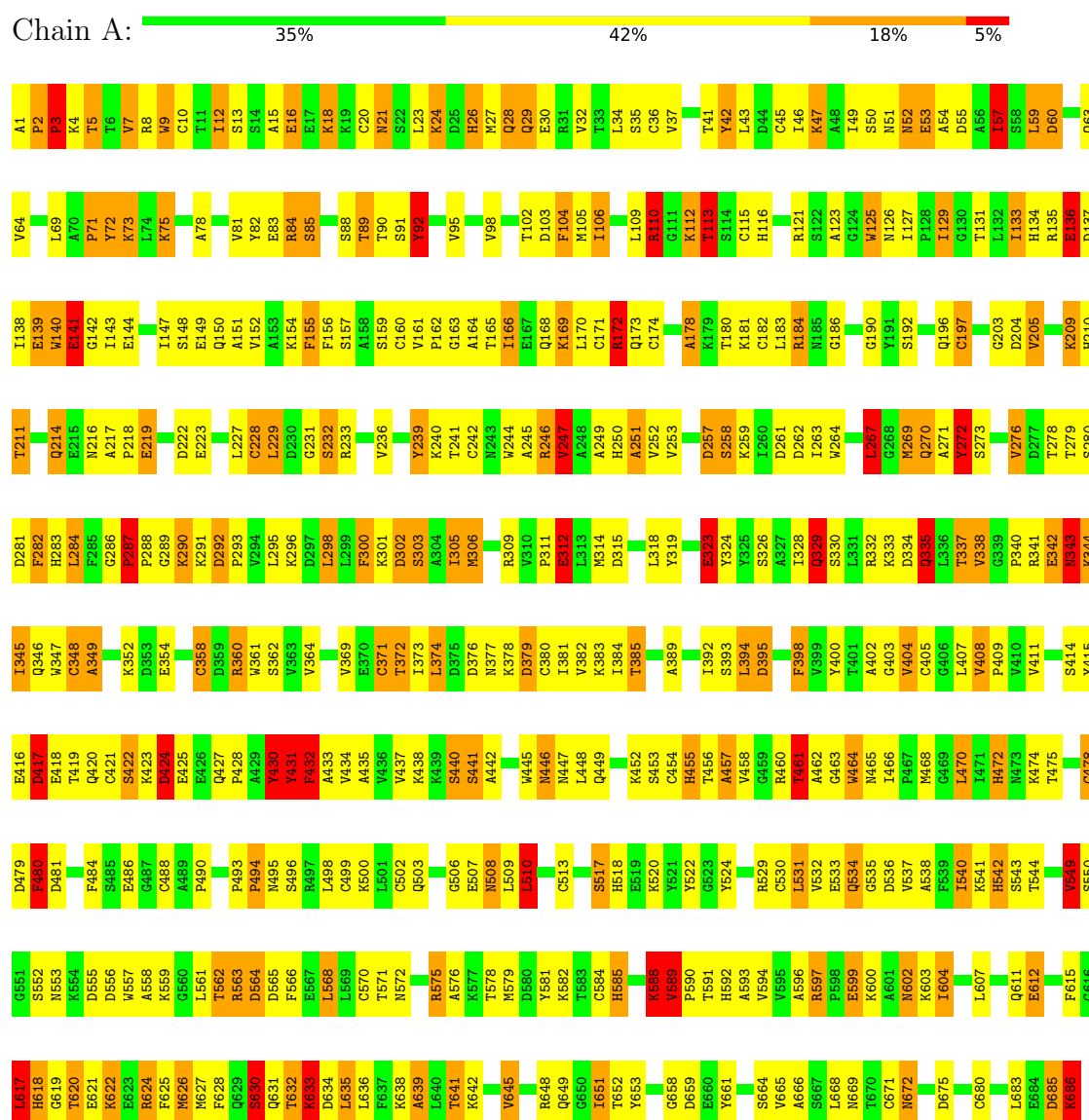
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	686	5299	3325	903	1032	39	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: APO-OVOTRANSFERRIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 98.74Å 126.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 4.00	Depositor
% Data completeness (in resolution range)	92.8 (10.00-4.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.210 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5299	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	21/5397 (0.4%)	2.28	267/7277 (3.7%)

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	4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	HIS	CD2-NE2	-7.59	1.29	1.37
1	A	472	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	247	VAL	CA-CB	6.80	1.62	1.53
1	A	455	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	542	HIS	CD2-NE2	-6.68	1.30	1.37
1	A	250	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	116	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	518	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	250	HIS	CG-ND1	-6.23	1.31	1.38
1	A	26	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	585	HIS	CG-ND1	-5.88	1.31	1.38
1	A	618	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	592	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	283	HIS	CD2-NE2	-5.62	1.31	1.37
1	A	210	HIS	CD2-NE2	-5.56	1.31	1.37
1	A	134	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	129	ILE	CA-CB	5.36	1.60	1.54
1	A	374	LEU	CA-CB	-5.25	1.46	1.53
1	A	455	HIS	CG-ND1	-5.25	1.32	1.38
1	A	244	TRP	NE1-CE2	-5.24	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	TRP	CG-CD2	-5.20	1.34	1.43

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	PHE	CA-CB-CG	-25.84	87.96	113.80
1	A	281	ASP	N-CA-C	16.21	133.97	113.55
1	A	83	GLU	N-CA-C	14.34	128.05	110.41
1	A	337	THR	N-CA-C	13.64	131.11	111.87
1	A	287	PRO	N-CA-C	13.10	126.69	110.70
1	A	480	PHE	CA-CB-CG	-13.05	100.75	113.80
1	A	315	ASP	CA-CB-CG	11.70	124.30	112.60
1	A	52	ASN	CA-CB-CG	11.49	124.09	112.60
1	A	581	TYR	N-CA-C	11.28	128.28	112.04
1	A	247	VAL	N-CA-C	-11.11	90.44	106.55
1	A	423	LYS	N-CA-C	-10.62	96.75	112.04
1	A	395	ASP	CA-CB-CG	10.48	123.08	112.60
1	A	270	GLN	OE1-CD-NE2	-10.23	112.37	122.60
1	A	553	ASN	OD1-CG-ND2	-10.08	112.52	122.60
1	A	685	ASP	N-CA-C	-10.07	89.36	110.80
1	A	475	THR	N-CA-C	9.73	124.50	112.23
1	A	335	GLN	CA-CB-CG	9.57	133.24	114.10
1	A	140	TRP	N-CA-CB	-9.53	94.66	110.39
1	A	335	GLN	OE1-CD-NE2	-9.46	113.14	122.60
1	A	91	SER	CA-C-N	9.43	138.68	121.70
1	A	91	SER	C-N-CA	9.43	138.68	121.70
1	A	141	GLU	N-CA-C	9.41	127.37	107.70
1	A	675	ASP	CA-CB-CG	9.41	122.01	112.60
1	A	565	ASP	CA-CB-CG	9.27	121.87	112.60
1	A	398	PHE	CA-CB-CG	-9.13	104.67	113.80
1	A	588	LYS	CA-CB-CG	-9.12	95.87	114.10
1	A	51	ASN	N-CA-C	-8.90	94.73	109.24
1	A	345	ILE	N-CA-C	-8.81	95.78	108.11
1	A	518	HIS	N-CA-C	-8.75	101.92	112.59
1	A	82	TYR	N-CA-C	8.69	126.98	114.39
1	A	52	ASN	N-CA-CB	-8.68	98.08	110.58
1	A	424	ASP	CA-CB-CG	8.66	121.26	112.60
1	A	430	TYR	CA-CB-CG	8.64	129.45	113.90
1	A	106	ILE	N-CA-C	8.58	123.01	111.17
1	A	564	ASP	CA-CB-CG	8.55	121.15	112.60
1	A	431	TYR	CA-C-O	-8.53	108.31	120.51
1	A	210	HIS	N-CA-C	8.49	121.29	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLN	OE1-CD-NE2	-8.46	114.14	122.60
1	A	139	GLU	N-CA-C	8.45	122.83	109.39
1	A	222	ASP	CA-CB-CG	8.40	121.00	112.60
1	A	335	GLN	CG-CD-NE2	8.31	128.86	116.40
1	A	563	ARG	N-CA-C	8.30	123.12	112.34
1	A	602	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	A	283	HIS	CB-CG-CD2	-8.14	120.62	131.20
1	A	302	ASP	CA-CB-CG	8.12	120.72	112.60
1	A	92	TYR	N-CA-C	-8.10	88.32	111.00
1	A	49	ILE	N-CA-C	-8.05	104.91	112.96
1	A	572	ASN	CA-CB-CG	8.05	120.66	112.60
1	A	126	ASN	OD1-CG-ND2	-8.02	114.58	122.60
1	A	589	VAL	N-CA-CB	-7.94	100.10	111.21
1	A	465	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	A	196	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	A	447	ASN	CA-CB-CG	7.79	120.39	112.60
1	A	144	GLU	N-CA-C	-7.68	102.72	112.93
1	A	26	HIS	CB-CG-CD2	-7.64	121.27	131.20
1	A	151	ALA	N-CA-C	-7.63	103.95	113.18
1	A	273	SER	N-CA-C	-7.60	102.34	111.69
1	A	16	GLU	CA-CB-CG	-7.59	98.92	114.10
1	A	503	GLN	OE1-CD-NE2	-7.55	115.05	122.60
1	A	404	VAL	N-CA-C	-7.54	103.44	110.53
1	A	633	LYS	CA-CB-CG	7.53	129.16	114.10
1	A	2	PRO	N-CA-C	7.52	119.87	110.70
1	A	686	LYS	CA-CB-CG	7.51	129.12	114.10
1	A	169	LYS	CB-CG-CD	-7.50	94.05	111.30
1	A	278	THR	N-CA-C	-7.49	97.03	109.24
1	A	377	ASN	N-CA-C	-7.46	103.08	111.14
1	A	343	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	A	417	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	323	GLU	N-CA-CB	-7.30	98.16	110.49
1	A	588	LYS	N-CA-C	7.28	131.37	111.00
1	A	73	LYS	CA-CB-CG	7.24	128.57	114.10
1	A	102	THR	N-CA-C	-7.22	99.60	110.28
1	A	394	LEU	N-CA-C	7.17	121.35	109.95
1	A	21	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	A	286	GLY	CA-C-N	7.15	127.74	120.38
1	A	286	GLY	C-N-CA	7.15	127.74	120.38
1	A	28	GLN	CG-CD-NE2	7.11	127.06	116.40
1	A	283	HIS	CB-CG-ND1	7.09	133.33	122.70
1	A	532	VAL	N-CA-C	7.08	117.21	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	ASN	OD1-CG-ND2	-7.05	115.55	122.60
1	A	649	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	214	GLN	OE1-CD-NE2	-7.02	115.58	122.60
1	A	270	GLN	CA-CB-CG	7.02	128.15	114.10
1	A	168	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	A	270	GLN	CG-CD-NE2	6.98	126.87	116.40
1	A	431	TYR	CA-C-N	-6.93	109.22	121.70
1	A	431	TYR	C-N-CA	-6.93	109.22	121.70
1	A	271	ALA	CA-C-N	-6.82	110.00	121.18
1	A	271	ALA	C-N-CA	-6.82	110.00	121.18
1	A	672	ASN	CA-CB-CG	6.80	119.40	112.60
1	A	148	SER	N-CA-C	6.80	125.29	110.80
1	A	635	LEU	N-CA-C	-6.78	96.06	107.80
1	A	462	ALA	N-CA-C	6.76	119.27	111.02
1	A	334	ASP	O-C-N	6.76	131.47	122.82
1	A	91	SER	N-CA-C	6.73	118.43	108.60
1	A	602	ASN	CB-CG-ND2	6.73	126.49	116.40
1	A	162	PRO	N-CA-C	6.73	121.63	111.14
1	A	140	TRP	CA-C-O	-6.71	113.59	120.84
1	A	414	SER	CA-C-O	6.67	127.90	120.70
1	A	134	HIS	CB-CG-CD2	-6.65	122.55	131.20
1	A	82	TYR	O-C-N	-6.60	115.39	122.19
1	A	620	THR	CA-CB-OG1	-6.57	99.74	109.60
1	A	510	LEU	N-CA-C	6.56	124.78	110.80
1	A	659	ASP	N-CA-C	6.47	119.15	111.33
1	A	134	HIS	N-CA-C	6.43	119.11	111.71
1	A	134	HIS	CA-CB-CG	-6.40	107.40	113.80
1	A	312	GLU	N-CA-C	6.39	124.42	110.80
1	A	379	ASP	CA-C-O	-6.37	114.31	121.00
1	A	73	LYS	N-CA-C	-6.34	94.94	107.69
1	A	622	LYS	N-CA-C	6.34	120.62	113.01
1	A	431	TYR	CA-CB-CG	6.34	125.31	113.90
1	A	37	VAL	N-CA-C	-6.33	99.01	108.12
1	A	258	SER	N-CA-C	6.33	116.80	107.88
1	A	267	LEU	N-CA-C	-6.33	103.52	111.11
1	A	110	ARG	O-C-N	6.32	131.31	122.77
1	A	518	HIS	CA-CB-CG	6.29	120.09	113.80
1	A	361	TRP	CG-CD2-CE3	6.28	140.18	133.90
1	A	140	TRP	CB-CA-C	6.28	121.86	111.31
1	A	3	PRO	CA-N-CD	-6.24	103.27	112.00
1	A	592	HIS	N-CA-C	-6.23	101.26	110.48
1	A	140	TRP	CB-CG-CD1	-6.22	117.57	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	SER	N-CA-C	6.19	119.79	109.95
1	A	562	THR	CA-CB-OG1	-6.17	100.34	109.60
1	A	7	VAL	N-CA-C	-6.15	99.26	108.12
1	A	373	ILE	O-C-N	6.14	129.76	123.00
1	A	136	GLU	CA-CB-CG	6.14	126.39	114.10
1	A	84	ARG	CA-CB-CG	6.13	126.35	114.10
1	A	446	ASN	CA-CB-CG	6.11	118.71	112.60
1	A	148	SER	N-CA-CB	-6.09	100.20	110.49
1	A	53	GLU	N-CA-CB	6.09	119.36	110.47
1	A	346	GLN	N-CA-C	-6.09	98.61	108.41
1	A	292	ASP	CA-C-N	6.08	126.25	119.32
1	A	292	ASP	C-N-CA	6.08	126.25	119.32
1	A	113	THR	N-CA-C	-6.07	99.81	109.76
1	A	408	VAL	CA-C-N	6.07	126.09	119.90
1	A	408	VAL	C-N-CA	6.07	126.09	119.90
1	A	282	PHE	N-CA-C	-6.06	100.86	109.96
1	A	612	GLU	CA-C-O	-6.04	114.47	120.82
1	A	178	ALA	N-CA-C	-6.04	97.94	110.80
1	A	441	SER	CA-CB-OG	6.03	123.16	111.10
1	A	478	CYS	N-CA-C	-6.01	104.55	112.72
1	A	251	ALA	N-CA-C	5.96	118.45	108.73
1	A	472	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	57	ILE	CB-CA-C	-5.93	99.81	110.48
1	A	549	VAL	N-CA-CB	-5.91	101.48	111.23
1	A	140	TRP	CE2-CD2-CG	-5.88	100.14	107.20
1	A	344	LYS	N-CA-C	-5.85	98.33	110.80
1	A	337	THR	N-CA-CB	-5.84	102.27	111.39
1	A	553	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	358	CYS	CA-CB-SG	-5.84	100.97	114.40
1	A	503	GLN	CG-CD-NE2	5.84	125.16	116.40
1	A	9	TRP	N-CA-C	-5.83	101.85	110.48
1	A	236	VAL	N-CA-CB	-5.83	101.61	111.23
1	A	456	THR	N-CA-C	5.83	118.38	111.33
1	A	126	ASN	CB-CG-ND2	5.82	125.13	116.40
1	A	480	PHE	N-CA-C	5.81	123.18	110.80
1	A	334	ASP	N-CA-C	5.81	117.79	110.24
1	A	272	TYR	CB-CG-CD2	-5.77	112.14	120.80
1	A	344	LYS	N-CA-CB	5.77	120.25	110.49
1	A	638	LYS	CA-C-O	-5.77	114.41	120.58
1	A	495	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	218	PRO	CA-C-N	5.75	130.31	120.71
1	A	218	PRO	C-N-CA	5.75	130.31	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	ILE	N-CA-C	-5.75	104.90	110.42
1	A	244	TRP	CG-CD2-CE3	5.74	139.64	133.90
1	A	223	GLU	CB-CG-CD	5.73	122.35	112.60
1	A	155	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	329	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	186	GLY	CA-C-N	5.68	125.39	119.82
1	A	186	GLY	C-N-CA	5.68	125.39	119.82
1	A	542	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	A	352	LYS	CA-CB-CG	5.66	125.41	114.10
1	A	634	ASP	N-CA-C	-5.65	96.48	107.62
1	A	372	THR	CA-CB-OG1	-5.65	101.12	109.60
1	A	442	ALA	N-CA-C	-5.65	106.93	113.88
1	A	484	PHE	CA-CB-CG	5.64	119.44	113.80
1	A	474	LYS	CB-CG-CD	-5.63	98.34	111.30
1	A	507	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	197	CYS	CA-C-O	5.62	126.91	120.90
1	A	361	TRP	O-C-N	5.62	127.93	122.09
1	A	347	TRP	N-CA-C	-5.61	100.53	109.96
1	A	553	ASN	N-CA-C	-5.60	100.05	109.07
1	A	267	LEU	CA-C-O	-5.60	114.91	120.90
1	A	550	SER	CA-C-O	5.59	127.84	121.58
1	A	680	CYS	CA-CB-SG	-5.59	101.54	114.40
1	A	630	SER	N-CA-CB	-5.57	102.18	111.20
1	A	553	ASN	CB-CG-ND2	5.57	124.75	116.40
1	A	53	GLU	CB-CA-C	-5.56	99.51	109.24
1	A	576	ALA	N-CA-C	5.55	115.88	108.38
1	A	290	LYS	CA-CB-CG	-5.55	103.00	114.10
1	A	622	LYS	CA-CB-CG	5.54	125.18	114.10
1	A	140	TRP	O-C-N	-5.49	116.12	122.87
1	A	161	VAL	N-CA-C	-5.47	97.06	108.88
1	A	653	TYR	CA-CB-CG	5.47	123.75	113.90
1	A	110	ARG	CA-CB-CG	-5.47	103.16	114.10
1	A	85	SER	N-CA-C	-5.46	100.39	109.46
1	A	631	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	A	257	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	306	MET	CA-CB-CG	5.44	124.99	114.10
1	A	442	ALA	CA-C-O	5.44	125.39	119.24
1	A	53	GLU	N-CA-C	-5.44	106.78	113.41
1	A	575	ARG	CB-CG-CD	-5.41	98.85	111.30
1	A	147	ILE	N-CA-C	-5.41	102.60	109.58
1	A	52	ASN	CB-CA-C	5.41	120.49	111.83
1	A	556	ASP	CA-C-O	-5.40	114.82	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	A	348	CYS	CA-CB-SG	-5.38	102.01	114.40
1	A	104	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	342	GLU	CA-C-N	5.37	131.79	121.54
1	A	342	GLU	C-N-CA	5.37	131.79	121.54
1	A	361	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	A	641	THR	N-CA-C	-5.34	100.99	109.96
1	A	172	ARG	N-CA-C	5.34	117.52	111.11
1	A	593	ALA	CA-C-O	-5.32	115.21	121.44
1	A	669	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	288	PRO	O-C-N	5.31	129.81	122.64
1	A	624	ARG	N-CA-C	-5.31	103.44	111.56
1	A	168	GLN	CG-CD-NE2	5.30	124.35	116.40
1	A	209	LYS	O-C-N	-5.29	117.05	123.03
1	A	140	TRP	CG-CD2-CE3	5.28	139.18	133.90
1	A	449	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	A	290	LYS	CA-C-O	5.24	128.01	120.51
1	A	342	GLU	O-C-N	5.24	129.56	122.59
1	A	369	VAL	CB-CA-C	5.24	118.43	110.62
1	A	632	THR	N-CA-C	-5.24	99.64	110.80
1	A	125	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	A	559	LYS	N-CA-C	5.22	119.98	111.37
1	A	342	GLU	N-CA-C	5.21	121.91	110.80
1	A	334	ASP	CA-C-O	5.21	127.07	121.44
1	A	9	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	A	645	VAL	N-CA-C	5.20	115.80	109.30
1	A	103	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	557	TRP	CG-CD2-CE3	5.20	139.09	133.90
1	A	593	ALA	O-C-N	-5.18	116.42	123.15
1	A	281	ASP	N-CA-CB	-5.17	102.90	110.40
1	A	672	ASN	N-CA-CB	-5.17	104.63	111.40
1	A	581	TYR	CA-CB-CG	-5.16	104.61	113.90
1	A	349	ALA	O-C-N	5.16	128.85	123.03
1	A	455	HIS	CA-C-O	-5.16	115.08	121.11
1	A	60	ASP	CA-C-O	-5.15	115.18	121.36
1	A	283	HIS	CA-C-N	-5.14	112.49	122.06
1	A	283	HIS	C-N-CA	-5.14	112.49	122.06
1	A	273	SER	CA-C-O	5.14	125.95	120.24
1	A	445	TRP	CB-CG-CD1	-5.14	119.19	126.90
1	A	123	ALA	N-CA-C	5.13	117.53	111.33
1	A	557	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	A	337	THR	O-C-N	-5.12	115.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ILE	N-CA-C	-5.12	105.61	110.42
1	A	251	ALA	O-C-N	-5.12	117.39	123.22
1	A	617	LEU	N-CA-C	5.11	121.69	110.80
1	A	541	LYS	CA-CB-CG	5.11	124.32	114.10
1	A	562	THR	CA-CB-CG2	5.11	119.18	110.50
1	A	597	ARG	CA-C-N	5.08	124.69	119.05
1	A	597	ARG	C-N-CA	5.08	124.69	119.05
1	A	1	ALA	CA-C-N	5.07	125.60	120.38
1	A	1	ALA	C-N-CA	5.07	125.60	120.38
1	A	532	VAL	O-C-N	-5.07	116.94	121.91
1	A	508	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	164	ALA	CA-C-O	5.05	125.93	120.43
1	A	435	ALA	N-CA-C	-5.04	99.06	107.99
1	A	652	THR	N-CA-CB	5.04	117.66	110.06
1	A	116	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	343	ASN	O-C-N	5.03	129.28	122.59
1	A	184	ARG	CA-C-O	5.03	125.54	119.61
1	A	599	GLU	CB-CA-C	-5.03	102.31	110.85
1	A	300	PHE	O-C-N	-5.02	116.62	123.15
1	A	55	ASP	N-CA-C	5.01	120.25	114.04

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	TYR	Sidechain
1	A	42	TYR	Sidechain
1	A	431	TYR	Sidechain
1	A	432	PHE	Sidechain

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	5299	0	5218	232	0
All	All	5299	0	5218	232	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 23.

All (232) 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:454:CYS:HG	1:A:530:CYS:HG	1.01	0.91
1:A:394:LEU:HD13	1:A:398:PHE:HB3	1.51	0.89
1:A:358:CYS:SG	1:A:371:CYS:HB3	2.14	0.87
1:A:228:CYS:HG	1:A:242:CYS:HG	1.10	0.86
1:A:430:TYR:HB3	1:A:590:PRO:HA	1.58	0.85
1:A:246:ARG:NH2	1:A:686:LYS:HB2	1.92	0.84
1:A:478:CYS:HG	1:A:671:CYS:HG	0.89	0.82
1:A:7:VAL:HG11	1:A:263:ILE:HG23	1.64	0.80
1:A:314:MET:HE1	1:A:683:LEU:HD11	1.63	0.79
1:A:454:CYS:SG	1:A:535:GLY:HA3	2.23	0.78
1:A:20:CYS:HG	1:A:36:CYS:HG	1.01	0.76
1:A:437:VAL:HA	1:A:531:LEU:HD21	1.67	0.76
1:A:115:CYS:SG	1:A:203:GLY:HA3	2.26	0.75
1:A:81:VAL:HB	1:A:306:MET:HB3	1.68	0.75
1:A:140:TRP:H	1:A:337:THR:HG21	1.51	0.74
1:A:457:ALA:HB3	1:A:460:ARG:HD3	1.68	0.74
1:A:141:GLU:HA	1:A:335:GLN:HB3	1.69	0.74
1:A:163:GLY:HA3	1:A:184:ARG:HG2	1.71	0.73
1:A:98:VAL:HG11	1:A:227:LEU:HD13	1.71	0.72
1:A:9:TRP:HB2	1:A:34:LEU:HD11	1.70	0.72
1:A:26:HIS:CE1	1:A:282:PHE:HB2	2.26	0.70
1:A:10:CYS:HB3	1:A:57:ILE:HG23	1.75	0.69
1:A:135:ARG:HA	1:A:340:PRO:HB3	1.74	0.68
1:A:209:LYS:HE2	1:A:211:THR:OG1	1.95	0.67
1:A:127:ILE:HD12	1:A:245:ALA:HB3	1.75	0.67
1:A:228:CYS:CB	1:A:242:CYS:SG	2.83	0.67
1:A:228:CYS:HB3	1:A:242:CYS:SG	2.35	0.67
1:A:434:VAL:HG21	1:A:568:LEU:HG	1.77	0.67
1:A:140:TRP:CE2	1:A:335:GLN:HG2	2.30	0.66
1:A:228:CYS:CB	1:A:242:CYS:HG	2.08	0.66
1:A:15:ALA:O	1:A:18:LYS:HB3	1.96	0.65
1:A:343:ASN:ND2	1:A:343:ASN:H	1.95	0.65
1:A:23:LEU:HD12	1:A:27:MET:HE1	1.79	0.65
1:A:59:LEU:HG	1:A:63:GLN:HB3	1.79	0.65
1:A:140:TRP:CE3	1:A:335:GLN:HA	2.32	0.64
1:A:452:LYS:HA	1:A:486:GLU:O	1.98	0.64
1:A:267:LEU:HA	1:A:270:GLN:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLN:HE21	1:A:329:GLN:HA	1.61	0.64
1:A:105:MET:SD	1:A:233:ARG:HG3	2.38	0.63
1:A:382:VAL:HA	1:A:385:THR:OG1	1.99	0.63
1:A:115:CYS:CB	1:A:197:CYS:HG	2.12	0.62
1:A:150:GLN:HE21	1:A:166:ILE:HG13	1.64	0.62
1:A:432:PHE:HB3	1:A:433:ALA:N	2.13	0.62
1:A:113:THR:OG1	1:A:203:GLY:HA2	1.99	0.62
1:A:245:ALA:HB2	1:A:323:GLU:HB3	1.82	0.62
1:A:454:CYS:CB	1:A:530:CYS:HG	2.13	0.62
1:A:192:SER:HB3	1:A:216:ASN:HD21	1.65	0.61
1:A:106:ILE:HG22	1:A:231:GLY:HA2	1.82	0.61
1:A:421:CYS:H	1:A:424:ASP:HB3	1.65	0.61
1:A:420:GLN:HA	1:A:424:ASP:O	2.00	0.61
1:A:566:PHE:O	1:A:578:THR:HG23	2.00	0.61
1:A:59:LEU:HD23	1:A:64:VAL:HA	1.83	0.61
1:A:409:PRO:HG2	1:A:651:ILE:HG23	1.83	0.59
1:A:47:LYS:HA	1:A:50:SER:OG	2.02	0.59
1:A:630:SER:HB3	1:A:635:LEU:HD12	1.85	0.59
1:A:437:VAL:HG12	1:A:536:ASP:O	2.04	0.58
1:A:106:ILE:HD13	1:A:229:LEU:HA	1.86	0.58
1:A:20:CYS:HG	1:A:36:CYS:CB	2.16	0.57
1:A:129:ILE:HD12	1:A:152:VAL:HG11	1.86	0.57
1:A:142:GLY:H	1:A:335:GLN:HB2	1.68	0.57
1:A:364:VAL:HG23	1:A:624:ARG:NH1	2.18	0.57
1:A:633:LYS:O	1:A:639:ALA:HB2	2.04	0.57
1:A:109:LEU:HD23	1:A:112:LYS:HG2	1.87	0.57
1:A:430:TYR:CE2	1:A:588:LYS:HG2	2.40	0.57
1:A:10:CYS:SG	1:A:45:CYS:HB3	2.44	0.56
1:A:400:TYR:O	1:A:404:VAL:HG23	2.05	0.56
1:A:626:MET:SD	1:A:628:PHE:HB2	2.45	0.56
1:A:140:TRP:HZ3	1:A:330:SER:O	1.88	0.56
1:A:374:LEU:HD11	1:A:383:LYS:HG3	1.87	0.56
1:A:499:CYS:CB	1:A:513:CYS:HG	2.18	0.56
1:A:81:VAL:HA	1:A:89:THR:O	2.05	0.56
1:A:21:ASN:HA	1:A:24:LYS:HG2	1.87	0.55
1:A:21:ASN:O	1:A:24:LYS:HG3	2.06	0.55
1:A:141:GLU:CA	1:A:335:GLN:HB3	2.35	0.55
1:A:590:PRO:HD2	1:A:661:TYR:HD2	1.71	0.55
1:A:43:LEU:O	1:A:46:ILE:HB	2.07	0.55
1:A:402:ALA:HB1	1:A:407:LEU:HD12	1.87	0.55
1:A:600:LYS:O	1:A:604:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:HE3	1:A:314:MET:O	2.06	0.55
1:A:618:HIS:HA	1:A:622:LYS:NZ	2.22	0.55
1:A:171:CYS:C	1:A:174:CYS:HG	2.15	0.54
1:A:457:ALA:HA	1:A:490:PRO:HD2	1.90	0.54
1:A:324:TYR:CE1	1:A:328:ILE:HD11	2.43	0.54
1:A:524:TYR:HA	1:A:540:ILE:HD11	1.90	0.54
1:A:328:ILE:O	1:A:332:ARG:HB3	2.08	0.54
1:A:392:ILE:HG12	1:A:393:SER:N	2.22	0.53
1:A:251:ALA:HB2	1:A:319:TYR:HE2	1.73	0.53
1:A:324:TYR:CZ	1:A:328:ILE:HD11	2.44	0.53
1:A:60:ASP:O	1:A:64:VAL:HG12	2.08	0.53
1:A:292:ASP:O	1:A:295:LEU:HB2	2.10	0.52
1:A:472:HIS:CE1	1:A:671:CYS:SG	3.03	0.52
1:A:57:ILE:HD12	1:A:59:LEU:HD13	1.90	0.52
1:A:180:THR:HA	1:A:183:LEU:HG	1.90	0.52
1:A:171:CYS:O	1:A:174:CYS:SG	2.68	0.52
1:A:267:LEU:O	1:A:270:GLN:HG3	2.10	0.52
1:A:428:PRO:HD3	1:A:645:VAL:HG11	1.91	0.51
1:A:493:PRO:HG2	1:A:496:SER:HB2	1.92	0.51
1:A:590:PRO:HD2	1:A:661:TYR:CD2	2.45	0.51
1:A:420:GLN:HB3	1:A:425:GLU:HA	1.93	0.51
1:A:142:GLY:H	1:A:335:GLN:CB	2.23	0.51
1:A:468:MET:HE3	1:A:480:PHE:HD1	1.76	0.51
1:A:570:CYS:CB	1:A:584:CYS:HG	2.21	0.51
1:A:59:LEU:HG	1:A:63:GLN:CB	2.41	0.51
1:A:42:TYR:HA	1:A:45:CYS:SG	2.51	0.51
1:A:438:LYS:HG3	1:A:531:LEU:HD22	1.93	0.51
1:A:282:PHE:CE2	1:A:284:LEU:HD22	2.47	0.50
1:A:282:PHE:HE2	1:A:284:LEU:HD22	1.77	0.50
1:A:488:CYS:CB	1:A:502:CYS:HG	2.24	0.50
1:A:160:CYS:HB2	1:A:173:GLN:HB2	1.93	0.50
1:A:264:TRP:CZ2	1:A:309:ARG:HB2	2.47	0.50
1:A:494:PRO:HA	1:A:499:CYS:SG	2.51	0.50
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.76	0.49
1:A:343:ASN:H	1:A:343:ASN:HD22	1.58	0.49
1:A:422:SER:O	1:A:425:GLU:HG2	2.12	0.49
1:A:5:THR:O	1:A:32:VAL:HA	2.13	0.49
1:A:464:TRP:CH2	1:A:468:MET:HE2	2.47	0.49
1:A:10:CYS:SG	1:A:45:CYS:SG	3.10	0.49
1:A:392:ILE:HG23	1:A:394:LEU:HG	1.95	0.49
1:A:568:LEU:CD1	1:A:578:THR:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:LEU:O	1:A:611:GLN:HG2	2.12	0.49
1:A:10:CYS:HG	1:A:45:CYS:HB3	1.77	0.49
1:A:291:LYS:HD3	1:A:296:LYS:HE3	1.94	0.49
1:A:432:PHE:CZ	1:A:582:LYS:HA	2.47	0.48
1:A:121:ARG:CZ	1:A:190:GLY:HA2	2.44	0.48
1:A:524:TYR:HD1	1:A:540:ILE:HG13	1.78	0.48
1:A:457:ALA:HB2	1:A:522:TYR:HE1	1.78	0.48
1:A:174:CYS:HB2	1:A:181:LYS:HD2	1.94	0.48
1:A:121:ARG:NH2	1:A:190:GLY:HA2	2.28	0.48
1:A:104:PHE:CZ	1:A:204:ASP:HB3	2.48	0.48
1:A:142:GLY:N	1:A:335:GLN:HB2	2.29	0.48
1:A:520:LYS:HE2	1:A:529:ARG:NH2	2.29	0.48
1:A:12:ILE:HG22	1:A:45:CYS:SG	2.54	0.48
1:A:16:GLU:OE2	1:A:298:LEU:HA	2.13	0.48
1:A:159:SER:HB2	1:A:170:LEU:HA	1.94	0.48
1:A:98:VAL:HG12	1:A:205:VAL:HG12	1.96	0.47
1:A:165:THR:H	1:A:166:ILE:HD13	1.79	0.47
1:A:292:ASP:H	1:A:295:LEU:HD12	1.79	0.47
1:A:488:CYS:CB	1:A:502:CYS:SG	3.02	0.47
1:A:104:PHE:H	1:A:233:ARG:NH2	2.11	0.47
1:A:380:CYS:O	1:A:384:ILE:HG13	2.14	0.47
1:A:403:GLY:HA2	1:A:407:LEU:O	2.14	0.47
1:A:284:LEU:HD12	1:A:300:PHE:HD2	1.79	0.47
1:A:360:ARG:HH11	1:A:625:PHE:HB2	1.79	0.47
1:A:531:LEU:HG	1:A:538:ALA:HB2	1.96	0.47
1:A:341:ARG:O	1:A:343:ASN:N	2.47	0.47
1:A:348:CYS:HB2	1:A:389:ALA:HB1	1.96	0.47
1:A:125:TRP:O	1:A:129:ILE:HB	2.15	0.47
1:A:393:SER:HA	1:A:594:VAL:HG12	1.97	0.47
1:A:138:ILE:HG12	1:A:155:PHE:CG	2.49	0.47
1:A:92:TYR:O	1:A:247:VAL:N	2.49	0.46
1:A:455:HIS:HD2	1:A:463:GLY:O	1.99	0.46
1:A:481:ASP:HA	1:A:498:LEU:HD11	1.98	0.46
1:A:169:LYS:HG2	1:A:172:ARG:NH1	2.31	0.46
1:A:269:MET:HA	1:A:272:TYR:HE1	1.81	0.46
1:A:276:VAL:HG11	1:A:305:ILE:HG22	1.97	0.46
1:A:506:GLY:HA2	1:A:520:LYS:HE3	1.97	0.46
1:A:78:ALA:HB3	1:A:252:VAL:HB	1.98	0.46
1:A:454:CYS:HB3	1:A:530:CYS:SG	2.56	0.46
1:A:466:ILE:O	1:A:470:LEU:HD22	2.16	0.46
1:A:3:PRO:HG3	1:A:262:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HB3	1:A:64:VAL:HB	1.98	0.46
1:A:142:GLY:N	1:A:335:GLN:CB	2.79	0.46
1:A:84:ARG:HG2	1:A:85:SER:H	1.81	0.45
1:A:246:ARG:CZ	1:A:686:LYS:HB2	2.45	0.45
1:A:461:THR:CG2	1:A:589:VAL:HG21	2.46	0.45
1:A:329:GLN:HA	1:A:329:GLN:NE2	2.29	0.45
1:A:272:TYR:CD1	1:A:272:TYR:N	2.84	0.45
1:A:341:ARG:O	1:A:603:LYS:HE2	2.17	0.45
1:A:8:ARG:HB2	1:A:54:ALA:HA	1.99	0.45
1:A:416:GLU:C	1:A:418:GLU:H	2.25	0.45
1:A:589:VAL:HG22	1:A:661:TYR:CE2	2.52	0.45
1:A:295:LEU:O	1:A:298:LEU:HD22	2.17	0.45
1:A:599:GLU:CD	1:A:599:GLU:H	2.25	0.44
1:A:8:ARG:HA	1:A:35:SER:HB3	1.99	0.44
1:A:301:LYS:HB3	1:A:303:SER:OG	2.18	0.44
1:A:157:SER:O	1:A:169:LYS:HD3	2.17	0.44
1:A:381:ILE:HG23	1:A:407:LEU:HD11	1.98	0.44
1:A:533:GLU:HB3	1:A:534:GLN:OE1	2.17	0.44
1:A:155:PHE:HD2	1:A:156:PHE:CD2	2.35	0.44
1:A:415:TYR:HD1	1:A:641:THR:HA	1.82	0.44
1:A:420:GLN:HA	1:A:425:GLU:HA	1.99	0.44
1:A:597:ARG:HE	1:A:597:ARG:HB3	1.69	0.44
1:A:344:LYS:O	1:A:345:ILE:N	2.50	0.44
1:A:615:PHE:CE1	1:A:621:GLU:HB2	2.53	0.44
1:A:131:THR:HG22	1:A:135:ARG:HD2	1.99	0.44
1:A:71:PRO:HD2	1:A:72:TYR:CE1	2.53	0.43
1:A:136:GLU:O	1:A:139:GLU:HG3	2.18	0.43
1:A:420:GLN:HG2	1:A:427:GLN:O	2.18	0.43
1:A:481:ASP:HA	1:A:498:LEU:CD1	2.49	0.43
1:A:81:VAL:HG13	1:A:89:THR:H	1.84	0.43
1:A:267:LEU:CA	1:A:270:GLN:HG3	2.45	0.43
1:A:479:ASP:O	1:A:481:ASP:N	2.52	0.43
1:A:358:CYS:HG	1:A:371:CYS:HB3	1.81	0.43
1:A:619:GLY:H	1:A:622:LYS:HD3	1.83	0.43
1:A:135:ARG:O	1:A:340:PRO:HD3	2.18	0.43
1:A:349:ALA:HB1	1:A:354:GLU:HB3	2.00	0.43
1:A:407:LEU:HA	1:A:596:ALA:O	2.19	0.42
1:A:457:ALA:HB3	1:A:460:ARG:CD	2.44	0.42
1:A:71:PRO:HD2	1:A:72:TYR:CZ	2.53	0.42
1:A:408:VAL:HA	1:A:409:PRO:HD2	1.87	0.42
1:A:416:GLU:HB2	1:A:419:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:HB3	1:A:642:LYS:HD2	2.01	0.42
1:A:540:ILE:HG12	1:A:544:THR:OG1	2.20	0.42
1:A:42:TYR:O	1:A:46:ILE:HG13	2.20	0.42
1:A:7:VAL:O	1:A:35:SER:N	2.52	0.42
1:A:110:ARG:HG2	1:A:155:PHE:CE1	2.54	0.42
1:A:420:GLN:CA	1:A:425:GLU:HA	2.50	0.42
1:A:314:MET:SD	1:A:318:LEU:HB2	2.59	0.42
1:A:329:GLN:O	1:A:333:LYS:HB2	2.19	0.42
1:A:438:LYS:HG2	1:A:566:PHE:HE1	1.85	0.42
1:A:287:PRO:HB3	1:A:302:ASP:HB3	2.02	0.42
1:A:432:PHE:CE2	1:A:585:HIS:ND1	2.88	0.41
1:A:10:CYS:HG	1:A:45:CYS:CB	2.32	0.41
1:A:217:ALA:O	1:A:219:GLU:N	2.54	0.41
1:A:376:ASP:HB2	1:A:379:ASP:H	1.85	0.41
1:A:105:MET:HE3	1:A:232:SER:HA	2.02	0.41
1:A:589:VAL:HA	1:A:590:PRO:HD2	1.98	0.41
1:A:81:VAL:HG11	1:A:88:SER:HB2	2.02	0.41
1:A:133:ILE:HG21	1:A:330:SER:HB3	2.02	0.41
1:A:668:LEU:O	1:A:671:CYS:HB2	2.20	0.41
1:A:239:TYR:CZ	1:A:240:LYS:HE3	2.56	0.41
1:A:305:ILE:HD13	1:A:305:ILE:HG21	1.89	0.41
1:A:582:LYS:O	1:A:585:HIS:CE1	2.74	0.41
1:A:582:LYS:O	1:A:585:HIS:HE1	2.04	0.41
1:A:440:SER:O	1:A:575:ARG:NH2	2.55	0.40
1:A:458:VAL:HG13	1:A:464:TRP:CE2	2.56	0.40
1:A:665:VAL:HG13	1:A:666:ALA:N	2.35	0.40
1:A:282:PHE:HE2	1:A:284:LEU:CD2	2.35	0.40
1:A:630:SER:HB2	1:A:632:THR:O	2.22	0.40
1:A:27:MET:N	1:A:27:MET:SD	2.94	0.40
1:A:420:GLN:CB	1:A:425:GLU:HA	2.52	0.40
1:A:558:ALA:HA	1:A:561:LEU:HD12	2.04	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	674/686 (98%)	555 (82%)	85 (13%)	34 (5%)	1	18

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	136	GLU
1	A	249	ALA
1	A	289	GLY
1	A	290	LYS
1	A	312	GLU
1	A	342	GLU
1	A	343	ASN
1	A	440	SER
1	A	480	PHE
1	A	510	LEU
1	A	685	ASP
1	A	259	LYS
1	A	323	GLU
1	A	430	TYR
1	A	509	LEU
1	A	579	MET
1	A	639	ALA
1	A	422	SER
1	A	461	THR
1	A	517	SER
1	A	29	GLN
1	A	178	ALA
1	A	457	ALA
1	A	591	THR
1	A	617	LEU
1	A	636	LEU
1	A	311	PRO
1	A	417	ASP
1	A	137	ASP
1	A	335	GLN
1	A	549	VAL
1	A	658	GLY
1	A	338	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	578/578 (100%)	459 (79%)	119 (21%)	1 8

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	3	PRO
1	A	4	LYS
1	A	5	THR
1	A	12	ILE
1	A	13	SER
1	A	18	LYS
1	A	24	LYS
1	A	28	GLN
1	A	29	GLN
1	A	30	GLU
1	A	41	THR
1	A	47	LYS
1	A	52	ASN
1	A	53	GLU
1	A	57	ILE
1	A	59	LEU
1	A	69	LEU
1	A	71	PRO
1	A	72	TYR
1	A	73	LYS
1	A	75	LYS
1	A	89	THR
1	A	90	THR
1	A	92	TYR
1	A	95	VAL
1	A	110	ARG
1	A	112	LYS
1	A	113	THR
1	A	136	GLU

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Mol	Chain	Res	Type
1	A	141	GLU
1	A	143	ILE
1	A	149	GLU
1	A	154	LYS
1	A	166	ILE
1	A	172	ARG
1	A	182	CYS
1	A	205	VAL
1	A	211	THR
1	A	214	GLN
1	A	219	GLU
1	A	228	CYS
1	A	229	LEU
1	A	232	SER
1	A	239	TYR
1	A	241	THR
1	A	246	ARG
1	A	247	VAL
1	A	253	VAL
1	A	257	ASP
1	A	258	SER
1	A	261	ASP
1	A	267	LEU
1	A	269	MET
1	A	276	VAL
1	A	279	THR
1	A	280	SER
1	A	284	LEU
1	A	287	PRO
1	A	293	PRO
1	A	298	LEU
1	A	303	SER
1	A	305	ILE
1	A	312	GLU
1	A	326	SER
1	A	329	GLN
1	A	338	VAL
1	A	343	ASN
1	A	360	ARG
1	A	362	SER
1	A	371	CYS
1	A	372	THR

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Mol	Chain	Res	Type
1	A	378	LYS
1	A	385	THR
1	A	395	ASP
1	A	405	CYS
1	A	411	VAL
1	A	424	ASP
1	A	430	TYR
1	A	431	TYR
1	A	441	SER
1	A	446	ASN
1	A	448	LEU
1	A	461	THR
1	A	470	LEU
1	A	494	PRO
1	A	500	LYS
1	A	508	ASN
1	A	510	LEU
1	A	517	SER
1	A	531	LEU
1	A	534	GLN
1	A	537	VAL
1	A	540	ILE
1	A	542	HIS
1	A	543	SER
1	A	549	VAL
1	A	552	SER
1	A	555	ASP
1	A	562	THR
1	A	563	ARG
1	A	564	ASP
1	A	568	LEU
1	A	571	THR
1	A	588	LYS
1	A	589	VAL
1	A	602	ASN
1	A	612	GLU
1	A	617	LEU
1	A	620	THR
1	A	626	MET
1	A	627	MET
1	A	630	SER
1	A	633	LYS

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Mol	Chain	Res	Type
1	A	648	ARG
1	A	651	ILE
1	A	664	SER
1	A	672	ASN
1	A	686	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	196	GLN
1	A	214	GLN
1	A	216	ASN
1	A	243	ASN
1	A	329	GLN
1	A	343	ASN
1	A	455	HIS
1	A	508	ASN
1	A	611	GLN
1	A	669	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	245:ALA	C	246:ARG	N	4.94
1	A	587:ALA	C	588:LYS	N	3.36
1	A	432:PHE	C	433:ALA	N	3.21
1	A	92:TYR	C	93:TYR	N	3.19
1	A	344:LYS	C	345:ILE	N	2.88

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.