



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 PM UTC

PDB ID : 1N8S / pdb_00001n8s
Title : Structure of the pancreatic lipase-colipase complex
Authors : van Tilbeurgh, H.; Sarda, L.; Verger, R.; Cambillau, C.
Deposited on : 2002-11-21
Resolution : 3.04 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

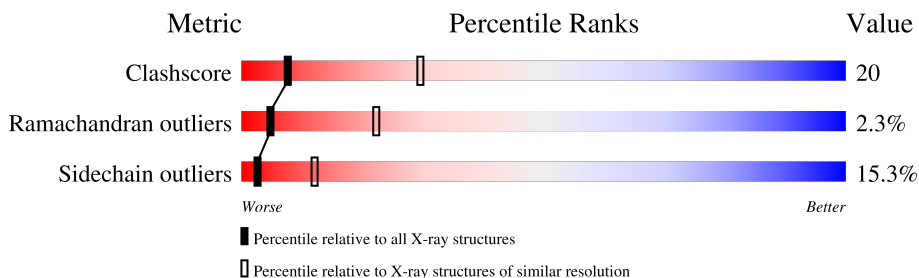
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)

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	449	
2	C	95	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4131 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 Triacylglycerol lipase, pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3491	2212	600	661	18			

- Molecule 2 is a protein called colipase II.

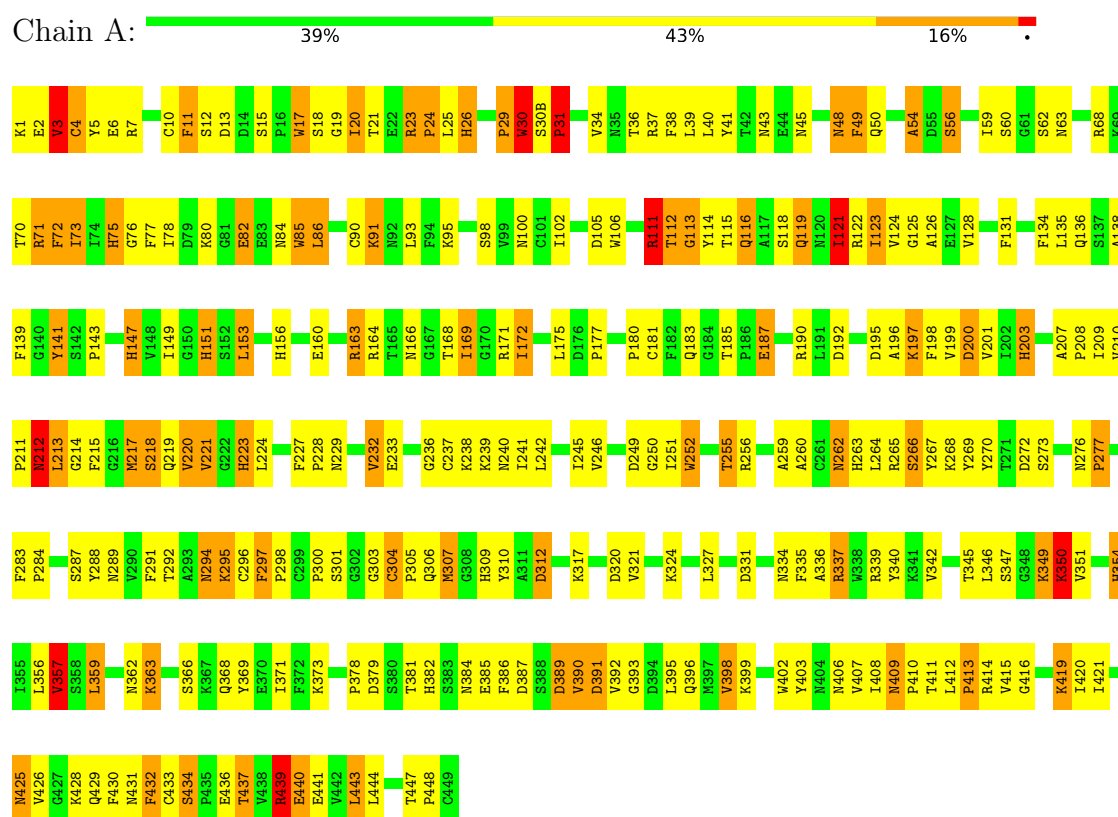
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	85	Total	C	N	O	S	0	0	0
			640	392	111	127	10			

3 Residue-property plots

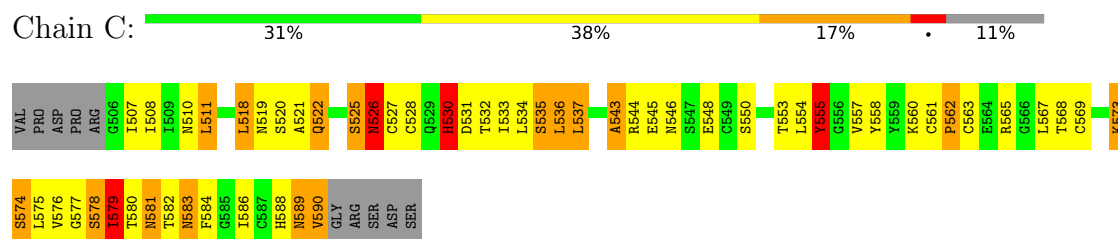
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 2: colipase II



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	80.30 Å 80.30 Å 251.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.04	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.04)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4131	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	1.36	22/3583 (0.6%)	2.17	147/4864 (3.0%)
2	C	1.31	4/647 (0.6%)	2.36	41/872 (4.7%)
All	All	1.35	26/4230 (0.6%)	2.20	188/5736 (3.3%)

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	2
2	C	0	1
All	All	0	3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	TRP	C-O	-10.20	1.11	1.24
1	A	75	HIS	CD2-NE2	-7.77	1.29	1.37
1	A	309	HIS	CD2-NE2	-7.75	1.29	1.37
1	A	141	TYR	CA-CB	-7.61	1.43	1.52
1	A	382	HIS	CD2-NE2	-7.51	1.29	1.37
1	A	147	HIS	CD2-NE2	-7.40	1.29	1.37
1	A	337	ARG	CA-CB	-7.01	1.42	1.53
2	C	530	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	203	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	223	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	263	HIS	CD2-NE2	-6.46	1.30	1.37
2	C	588	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	151	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	354	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	149	ILE	CA-CB	5.97	1.61	1.54
1	A	357	VAL	CA-CB	-5.86	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	508	ILE	CA-CB	-5.84	1.47	1.54
1	A	295	LYS	CA-CB	-5.52	1.46	1.54
1	A	151	HIS	CG-ND1	-5.45	1.32	1.38
1	A	223	HIS	CG-ND1	-5.24	1.32	1.38
1	A	309	HIS	CG-ND1	-5.22	1.32	1.38
1	A	305	PRO	CA-CB	-5.17	1.48	1.54
2	C	532	THR	CA-CB	5.17	1.62	1.53
1	A	30	TRP	C-N	-5.14	1.22	1.34
1	A	413	PRO	CA-CB	-5.05	1.46	1.53
1	A	26	HIS	CD2-NE2	-5.03	1.32	1.37

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ARG	CA-CB-CG	-12.61	88.88	114.10
1	A	31	PRO	O-C-N	-12.11	108.32	122.24
1	A	389	ASP	CA-CB-CG	10.89	123.49	112.60
1	A	63	ASN	CA-CB-CG	-10.60	102.00	112.60
1	A	72	PHE	CA-CB-CG	10.35	124.15	113.80
1	A	277	PRO	N-CA-C	9.67	126.44	114.35
1	A	60	SER	N-CA-C	9.51	122.84	111.33
2	C	510	ASN	N-CA-C	9.49	124.24	112.47
1	A	166	ASN	CA-CB-CG	-9.47	103.13	112.60
1	A	406	ASN	CA-CB-CG	9.34	121.94	112.60
1	A	45	ASN	CA-CB-CG	9.28	121.88	112.60
1	A	296	CYS	N-CA-C	-9.18	93.44	108.41
2	C	565	ARG	N-CA-C	8.99	123.78	110.30
2	C	582	THR	N-CA-C	8.39	124.54	113.30
2	C	573	LYS	N-CA-C	-8.06	93.26	108.17
1	A	220	VAL	N-CA-CB	-8.04	101.76	110.53
2	C	535	SER	N-CA-C	7.94	121.27	110.55
1	A	240	ASN	CA-CB-CG	7.74	120.34	112.60
1	A	334	ASN	N-CA-C	-7.67	96.74	109.24
1	A	156	HIS	CB-CG-CD2	-7.63	121.28	131.20
1	A	262	ASN	OD1-CG-ND2	-7.61	115.00	122.60
2	C	589	ASN	OD1-CG-ND2	-7.58	115.02	122.60
2	C	530	HIS	CA-CB-CG	7.44	121.24	113.80
1	A	121	ILE	CA-CB-CG1	-7.42	97.79	110.40
1	A	136	GLN	CA-C-O	-7.39	113.09	120.70
1	A	434	SER	CA-C-O	7.39	126.76	119.22
1	A	71	ARG	CA-CB-CG	7.37	128.84	114.10
1	A	263	HIS	CB-CG-CD2	-7.37	121.62	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	589	ASN	CB-CG-ND2	7.34	127.41	116.40
1	A	15	SER	N-CA-C	-7.33	100.52	109.83
1	A	82	GLU	N-CA-C	7.29	121.87	113.19
1	A	237	CYS	N-CA-C	7.28	120.53	108.96
1	A	289	ASN	CA-C-O	-7.25	113.39	121.00
2	C	582	THR	CA-CB-OG1	-7.22	98.77	109.60
1	A	265	ARG	CA-C-O	-7.18	112.88	120.63
1	A	1	LYS	CA-C-N	7.14	133.58	121.87
1	A	1	LYS	C-N-CA	7.14	133.58	121.87
1	A	309	HIS	N-CA-C	7.12	120.86	111.75
1	A	85	TRP	CB-CG-CD1	-7.09	116.26	126.90
1	A	249	ASP	CA-CB-CG	7.08	119.67	112.60
1	A	121	ILE	CA-CB-CG2	7.03	122.45	110.50
2	C	543	ALA	N-CA-C	7.02	120.41	110.23
1	A	163	ARG	NE-CZ-NH1	-7.01	114.49	121.50
1	A	187	GLU	N-CA-C	7.01	120.72	111.75
1	A	387	ASP	CA-C-O	6.98	128.66	120.70
2	C	582	THR	N-CA-CB	-6.97	100.08	110.61
2	C	530	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	A	425	ASN	CA-CB-CG	6.90	119.50	112.60
1	A	437	THR	N-CA-C	-6.90	98.92	109.41
1	A	396	GLN	N-CA-C	-6.84	102.95	112.12
1	A	306	GLN	O-C-N	-6.82	114.36	122.96
2	C	582	THR	CA-CB-CG2	6.79	122.04	110.50
1	A	3	VAL	N-CA-C	-6.76	99.40	108.06
1	A	190	ARG	N-CA-C	6.73	118.35	108.86
2	C	544	ARG	NE-CZ-NH2	6.73	125.26	119.20
1	A	357	VAL	N-CA-CB	-6.56	103.34	112.52
1	A	85	TRP	CG-CD2-CE3	6.55	140.45	133.90
1	A	166	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	A	347	SER	CA-CB-OG	6.48	124.07	111.10
2	C	544	ARG	CB-CG-CD	-6.46	96.43	111.30
1	A	29	PRO	O-C-N	-6.46	113.92	122.64
1	A	384	ASN	CA-CB-CG	-6.44	106.16	112.60
1	A	113	GLY	N-CA-C	-6.40	104.35	112.54
1	A	312	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	276	ASN	O-C-N	-6.38	116.15	121.12
1	A	116	GLN	N-CA-C	-6.37	103.95	111.03
1	A	2	GLU	N-CA-C	-6.33	99.53	108.96
1	A	391	ASP	N-CA-C	-6.31	99.60	109.25
1	A	37	ARG	O-C-N	-6.25	115.91	123.16
1	A	220	VAL	CB-CA-C	6.21	119.22	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ILE	O-C-N	6.19	129.19	122.63
1	A	48	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	38	PHE	CA-CB-CG	-6.14	107.66	113.80
1	A	223	HIS	N-CA-C	-6.14	105.61	113.23
2	C	565	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	A	26	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	382	HIS	CB-CG-CD2	-6.08	123.29	131.20
1	A	440	GLU	CA-C-N	6.08	130.76	122.19
1	A	440	GLU	C-N-CA	6.08	130.76	122.19
2	C	577	GLY	N-CA-C	-6.06	98.81	113.18
2	C	518	LEU	CA-C-O	6.04	125.62	118.79
1	A	259	ALA	N-CA-C	-6.01	97.42	107.99
2	C	532	THR	N-CA-CB	6.00	120.63	110.49
1	A	245	ILE	CA-C-N	-5.98	115.39	123.10
1	A	245	ILE	C-N-CA	-5.98	115.39	123.10
1	A	396	GLN	CA-CB-CG	-5.98	102.14	114.10
1	A	21	THR	N-CA-C	5.96	119.38	111.75
2	C	555	TYR	CA-CB-CG	-5.95	103.19	113.90
1	A	217	MET	N-CA-C	-5.95	102.52	110.55
1	A	371	ILE	CA-C-O	-5.93	114.31	119.29
1	A	381	THR	O-C-N	-5.92	116.43	123.06
1	A	3	VAL	O-C-N	-5.92	117.51	123.19
1	A	163	ARG	CG-CD-NE	-5.91	98.99	112.00
2	C	565	ARG	CB-CG-CD	-5.91	97.71	111.30
1	A	4	CYS	CA-CB-SG	-5.91	100.81	114.40
2	C	562	PRO	CB-CA-C	5.91	118.74	111.12
2	C	550	SER	N-CA-C	-5.89	99.80	109.40
1	A	432	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	390	VAL	CB-CA-C	-5.87	101.77	110.33
1	A	25	LEU	CB-CA-C	-5.84	101.59	109.71
1	A	200	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	77	PHE	O-C-N	-5.83	115.08	123.07
2	C	588	HIS	CB-CG-CD2	-5.82	123.64	131.20
2	C	536	LEU	CA-C-O	5.80	126.95	120.92
2	C	522	GLN	CA-CB-CG	-5.76	102.57	114.10
2	C	590	VAL	CA-CB-CG2	-5.75	100.62	110.40
1	A	147	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	A	346	LEU	N-CA-C	5.74	119.26	110.20
2	C	530	HIS	CB-CG-ND1	5.71	131.27	122.70
2	C	579	ILE	N-CA-C	-5.71	104.56	112.50
1	A	172	ILE	N-CA-C	-5.69	100.25	108.89
1	A	218	SER	N-CA-C	-5.68	106.99	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	ASN	CA-C-N	5.67	124.87	118.97
1	A	409	ASN	C-N-CA	5.67	124.87	118.97
1	A	354	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	A	240	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	13	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	76	GLY	N-CA-C	-5.63	99.85	113.18
1	A	259	ALA	CA-C-O	5.63	126.77	120.92
1	A	56	SER	O-C-N	-5.62	116.17	122.12
1	A	84	ASN	N-CA-C	5.61	119.39	112.54
1	A	232	VAL	O-C-N	-5.59	115.58	122.57
1	A	229	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	172	ILE	O-C-N	-5.54	117.21	122.98
1	A	73	ILE	N-CA-CB	-5.53	104.93	111.90
1	A	212	ASN	N-CA-C	5.51	119.99	112.88
2	C	561	CYS	CA-CB-SG	-5.49	101.78	114.40
1	A	429	GLN	CA-CB-CG	-5.47	103.15	114.10
2	C	525	SER	N-CA-C	-5.47	96.05	107.37
1	A	68	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	199	VAL	N-CA-C	-5.46	100.25	108.12
1	A	398	VAL	O-C-N	-5.45	117.00	123.00
1	A	17	TRP	CE2-CD2-CG	-5.45	100.66	107.20
1	A	337	ARG	CG-CD-NE	-5.45	100.02	112.00
1	A	212	ASN	OD1-CG-ND2	-5.45	117.16	122.60
2	C	519	ASN	N-CA-C	-5.44	100.04	108.42
1	A	336	ALA	O-C-N	5.43	129.05	122.85
1	A	350	LYS	N-CA-C	-5.43	100.32	108.96
1	A	268	LYS	CA-CB-CG	-5.43	103.23	114.10
2	C	580	THR	N-CA-C	-5.41	106.99	113.21
1	A	439	ARG	N-CA-C	-5.40	103.25	110.55
1	A	337	ARG	NE-CZ-NH1	-5.39	116.11	121.50
2	C	565	ARG	CA-CB-CG	-5.35	103.40	114.10
1	A	304	CYS	N-CA-C	-5.34	103.40	110.40
1	A	409	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	304	CYS	CA-C-O	-5.32	115.38	120.97
1	A	213	LEU	N-CA-C	5.31	118.76	111.54
1	A	54	ALA	N-CA-C	5.31	122.10	110.80
2	C	568	THR	CA-C-N	-5.30	115.48	122.85
2	C	568	THR	C-N-CA	-5.30	115.48	122.85
1	A	354	HIS	CA-C-O	-5.30	114.60	120.38
2	C	521	ALA	O-C-N	5.29	127.73	122.12
1	A	252	TRP	CA-C-O	-5.29	115.26	120.70
1	A	116	GLN	O-C-N	5.28	127.73	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASP	CA-C-O	5.26	128.03	120.51
1	A	163	ARG	O-C-N	5.25	127.48	122.07
1	A	195	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	77	PHE	N-CA-C	5.24	118.17	110.30
1	A	111	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	441	GLU	N-CA-C	5.22	118.79	111.74
1	A	236	GLY	N-CA-C	-5.22	107.68	113.79
1	A	398	VAL	CA-C-O	-5.20	116.37	121.67
1	A	221	VAL	O-C-N	-5.18	116.10	122.57
2	C	555	TYR	N-CA-C	5.18	119.31	113.15
1	A	309	HIS	CA-CB-CG	-5.17	108.62	113.80
1	A	320	ASP	CA-C-O	5.17	126.86	121.38
1	A	49	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	60	SER	CA-C-O	-5.16	115.06	120.63
1	A	197	LYS	N-CA-C	-5.15	105.75	111.36
1	A	85	TRP	CA-CB-CG	5.14	123.38	113.60
1	A	251	ILE	N-CA-C	-5.14	105.49	110.42
1	A	112	THR	O-C-N	-5.13	116.80	122.75
2	C	543	ALA	O-C-N	-5.12	116.57	122.87
2	C	526	ASN	CA-C-N	5.11	129.17	121.40
2	C	526	ASN	C-N-CA	5.11	129.17	121.40
1	A	240	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	263	HIS	CB-CG-ND1	5.10	130.35	122.70
1	A	331	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	240	ASN	N-CA-C	-5.06	102.28	110.32
1	A	347	SER	N-CA-C	-5.06	101.51	109.50
1	A	149	ILE	N-CA-C	-5.05	100.37	107.75
1	A	86	LEU	CD1-CG-CD2	-5.05	99.68	110.80
1	A	11	PHE	CA-CB-CG	-5.04	108.76	113.80
1	A	203	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	85	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	A	147	HIS	CB-CG-ND1	5.01	130.22	122.70
1	A	147	HIS	CA-CB-CG	5.01	118.81	113.80
1	A	119	GLN	OE1-CD-NE2	-5.01	117.59	122.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	31	PRO	Mainchain
2	C	555	TYR	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	3491	0	3352	137	0
2	C	640	0	616	26	0
All	All	4131	0	3968	163	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 20.

All (163) 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:342:VAL:HG21	1:A:357:VAL:HG11	1.57	0.87
2:C:533:ILE:HG23	2:C:534:LEU:HD22	1.58	0.83
1:A:356:LEU:HD23	1:A:368:GLN:HB3	1.69	0.74
1:A:227:PHE:CE2	1:A:324:LYS:HG2	2.25	0.71
1:A:209:ILE:HD12	1:A:213:LEU:HA	1.71	0.70
1:A:172:ILE:HG12	1:A:196:ALA:HB2	1.74	0.70
1:A:50:GLN:OE1	1:A:62:SER:HB2	1.94	0.68
1:A:90:CYS:HA	1:A:93:LEU:HD12	1.74	0.68
2:C:576:VAL:HA	2:C:579:ILE:HG22	1.76	0.68
1:A:210:VAL:HG13	1:A:246:VAL:HG23	1.76	0.67
1:A:73:ILE:HG22	1:A:86:LEU:HD23	1.76	0.67
1:A:227:PHE:HE2	1:A:324:LYS:HG2	1.60	0.64
1:A:18:SER:OG	1:A:26:HIS:HA	1.97	0.64
1:A:131:PHE:HE1	1:A:135:LEU:HD21	1.63	0.63
2:C:543:ALA:HB3	2:C:563:CYS:HA	1.80	0.63
1:A:297:PHE:CZ	1:A:425:ASN:HA	2.34	0.63
1:A:71:ARG:HB3	1:A:147:HIS:HB3	1.80	0.63
1:A:91:LYS:HZ2	1:A:91:LYS:HB3	1.65	0.62
1:A:29:PRO:O	1:A:30:TRP:C	2.37	0.61
1:A:363:LYS:NZ	1:A:363:LYS:HB3	2.15	0.61
1:A:29:PRO:O	1:A:30:TRP:O	2.19	0.61
2:C:575:LEU:HG	2:C:576:VAL:O	2.01	0.60
1:A:399:LYS:HD3	1:A:443:LEU:HD23	1.83	0.60
1:A:34:VAL:HG11	1:A:123:ILE:HG22	1.82	0.60
1:A:11:PHE:HE2	1:A:164:ARG:HH22	1.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:574:SER:H	2:C:583:ASN:ND2	2.00	0.59
1:A:366:SER:HB2	1:A:369:TYR:HE2	1.67	0.58
1:A:398:VAL:HG11	1:A:420:ILE:HG21	1.85	0.58
1:A:201:VAL:HG21	1:A:221:VAL:HG23	1.85	0.58
1:A:210:VAL:HG22	1:A:246:VAL:HB	1.85	0.58
1:A:7:ARG:HB2	1:A:7:ARG:HH21	1.67	0.58
2:C:574:SER:HB2	2:C:578:SER:OG	2.03	0.58
1:A:354:HIS:CE1	1:A:373:LYS:HG3	2.38	0.58
1:A:183:GLN:HG3	1:A:219:GLN:OE1	2.02	0.58
1:A:447:THR:HB	1:A:448:PRO:HD2	1.87	0.57
1:A:147:HIS:CD2	1:A:171:ARG:HG2	2.39	0.57
1:A:362:ASN:OD1	1:A:393:GLY:HA3	2.04	0.57
2:C:558:TYR:CD1	2:C:562:PRO:HD3	2.40	0.56
1:A:112:THR:HG23	1:A:113:GLY:O	2.06	0.56
1:A:414:ARG:HB3	1:A:437:THR:OG1	2.06	0.56
1:A:428:LYS:HB3	1:A:430:PHE:HE1	1.71	0.55
1:A:7:ARG:HB2	1:A:7:ARG:NH2	2.22	0.55
1:A:39:LEU:HD22	1:A:49:PHE:CE2	2.42	0.55
1:A:181:CYS:O	1:A:185:THR:HG21	2.06	0.55
1:A:356:LEU:HD11	1:A:403:TYR:HE1	1.71	0.55
1:A:17:TRP:CZ3	1:A:122:ARG:HD3	2.42	0.54
2:C:558:TYR:HB3	2:C:560:LYS:O	2.08	0.54
1:A:29:PRO:C	1:A:30:TRP:O	2.50	0.53
2:C:527:CYS:SG	2:C:562:PRO:HD2	2.49	0.53
1:A:134:PHE:CE1	1:A:138:ALA:HB2	2.43	0.52
1:A:75:HIS:CG	1:A:78:ILE:HD11	2.44	0.52
2:C:574:SER:HB2	2:C:578:SER:CB	2.40	0.52
1:A:213:LEU:HD12	1:A:213:LEU:N	2.24	0.52
1:A:413:PRO:HD2	1:A:439:ARG:NH2	2.24	0.52
1:A:233:GLU:HA	1:A:262:ASN:HD21	1.75	0.51
1:A:294:ASN:OD1	1:A:385:GLU:HB2	2.10	0.51
1:A:270:TYR:O	1:A:273:SER:HB3	2.11	0.51
1:A:124:VAL:O	1:A:128:VAL:HG23	2.10	0.51
2:C:525:SER:O	2:C:527:CYS:N	2.44	0.51
1:A:208:PRO:HB2	1:A:212:ASN:OD1	2.11	0.51
1:A:116:GLN:O	1:A:119:GLN:HB2	2.12	0.50
2:C:530:HIS:HD2	2:C:535:SER:O	1.95	0.50
1:A:209:ILE:HA	1:A:214:GLY:H	1.77	0.50
1:A:217:MET:HE1	1:A:221:VAL:HG11	1.93	0.49
1:A:4:CYS:HA	1:A:10:CYS:HA	1.94	0.49
1:A:203:HIS:HE1	1:A:219:GLN:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:O	1:A:7:ARG:HB2	2.12	0.49
1:A:3:VAL:CG1	1:A:5:TYR:CE2	2.96	0.49
1:A:153:LEU:HD22	1:A:252:TRP:CH2	2.47	0.49
2:C:511:LEU:HD22	2:C:522:GLN:HB3	1.94	0.49
1:A:419:LYS:HB2	1:A:419:LYS:NZ	2.28	0.49
1:A:354:HIS:O	1:A:402:TRP:HA	2.13	0.49
1:A:43:ASN:OD1	1:A:98:SER:HA	2.12	0.49
1:A:75:HIS:HB3	1:A:86:LEU:HD21	1.95	0.48
1:A:209:ILE:HA	1:A:214:GLY:N	2.27	0.48
2:C:548:GLU:OE1	2:C:560:LYS:HE2	2.14	0.48
1:A:297:PHE:CE1	1:A:339:ARG:HG2	2.49	0.48
1:A:171:ARG:HD3	1:A:198:PHE:CD2	2.48	0.48
1:A:419:LYS:HA	1:A:432:PHE:O	2.14	0.48
1:A:171:ARG:HA	1:A:198:PHE:O	2.14	0.48
1:A:233:GLU:HA	1:A:262:ASN:ND2	2.29	0.48
1:A:390:VAL:HG12	1:A:391:ASP:O	2.13	0.48
2:C:553:THR:HG22	2:C:558:TYR:CZ	2.49	0.47
2:C:560:LYS:HG3	2:C:584:PHE:CE2	2.49	0.47
1:A:72:PHE:HA	1:A:102:ILE:O	2.14	0.47
1:A:207:ALA:HB2	1:A:232:VAL:HG13	1.95	0.47
1:A:126:ALA:HB2	1:A:164:ARG:CZ	2.45	0.47
1:A:407:VAL:HG23	1:A:409:ASN:HD21	1.79	0.47
1:A:421:ILE:HG12	1:A:431:ASN:HD22	1.80	0.47
2:C:555:TYR:O	2:C:557:VAL:HG22	2.14	0.47
1:A:419:LYS:NZ	1:A:433:CYS:SG	2.88	0.47
1:A:412:LEU:HD12	1:A:439:ARG:HE	1.80	0.47
1:A:349:LYS:HD2	1:A:349:LYS:N	2.30	0.46
1:A:298:PRO:HB2	1:A:425:ASN:O	2.16	0.46
2:C:569:CYS:SG	2:C:586:ILE:C	2.98	0.46
2:C:558:TYR:CE1	2:C:562:PRO:HD3	2.50	0.46
1:A:269:TYR:HE1	1:A:335:PHE:CD2	2.34	0.46
1:A:172:ILE:HG12	1:A:196:ALA:CB	2.44	0.45
1:A:399:LYS:HD3	1:A:443:LEU:CD2	2.45	0.45
1:A:111:ARG:HH21	1:A:111:ARG:HB2	1.81	0.45
1:A:125:GLY:HA3	1:A:160:GLU:HB3	1.98	0.45
1:A:415:VAL:HG12	1:A:416:GLY:N	2.31	0.45
1:A:112:THR:CG2	1:A:116:GLN:HB3	2.47	0.45
1:A:428:LYS:HB3	1:A:430:PHE:CE1	2.52	0.45
2:C:548:GLU:CD	2:C:560:LYS:HE2	2.42	0.45
1:A:5:TYR:CD1	1:A:31:PRO:HD2	2.52	0.45
1:A:5:TYR:CE1	1:A:30(B):SER:CB	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TYR:CE1	1:A:180:PRO:HB2	2.53	0.44
1:A:250:GLY:HA2	1:A:255:THR:OG1	2.17	0.44
1:A:407:VAL:HG23	1:A:409:ASN:ND2	2.32	0.44
2:C:563:CYS:SG	2:C:569:CYS:HB2	2.57	0.44
1:A:59:ILE:HG21	1:A:139:PHE:CE1	2.52	0.44
1:A:223:HIS:HA	1:A:321:VAL:HA	1.99	0.44
1:A:20:ILE:CG1	1:A:23:ARG:HG3	2.48	0.44
1:A:175:LEU:HB3	1:A:266:SER:HB2	1.98	0.44
1:A:283:PHE:HD2	1:A:291:PHE:HE1	1.65	0.44
1:A:339:ARG:HA	1:A:386:PHE:O	2.18	0.44
1:A:91:LYS:HB3	1:A:91:LYS:NZ	2.31	0.44
1:A:121:ILE:HD12	1:A:121:ILE:HA	1.66	0.44
1:A:409:ASN:HA	1:A:410:PRO:HD3	1.75	0.44
1:A:151:HIS:HD2	1:A:175:LEU:O	2.01	0.43
1:A:131:PHE:CE1	1:A:135:LEU:HD21	2.49	0.43
1:A:307:MET:HB3	1:A:327:LEU:HD21	2.00	0.43
1:A:395:LEU:HB2	1:A:430:PHE:CD2	2.53	0.43
1:A:277:PRO:HB3	1:A:310:TYR:CE2	2.53	0.43
1:A:151:HIS:HA	1:A:175:LEU:O	2.19	0.43
1:A:340:TYR:O	1:A:385:GLU:HA	2.19	0.43
1:A:350:LYS:HA	1:A:378:PRO:HD3	1.99	0.43
1:A:171:ARG:HD2	1:A:200:ASP:OD2	2.19	0.43
1:A:439:ARG:HD2	1:A:440:GLU:H	1.83	0.43
1:A:71:ARG:HA	1:A:147:HIS:O	2.19	0.43
1:A:177:PRO:HB2	1:A:217:MET:SD	2.59	0.43
1:A:264:LEU:HD22	1:A:267:TYR:OH	2.19	0.43
1:A:283:PHE:CD1	1:A:304:CYS:SG	3.12	0.43
1:A:359:LEU:HD11	1:A:386:PHE:HZ	1.83	0.43
2:C:553:THR:OG1	2:C:554:LEU:N	2.52	0.43
1:A:241:ILE:HD12	1:A:241:ILE:H	1.84	0.42
1:A:399:LYS:HB3	1:A:443:LEU:HD23	2.01	0.42
1:A:269:TYR:CE1	1:A:335:PHE:CD2	3.08	0.42
1:A:70:THR:HA	1:A:100:ASN:HB2	2.01	0.42
2:C:520:SER:HB3	2:C:526:ASN:C	2.44	0.42
1:A:288:TYR:O	1:A:292:THR:HG23	2.18	0.42
2:C:537:LEU:HD12	2:C:557:VAL:HG11	2.00	0.42
1:A:40:LEU:HB3	1:A:50:GLN:O	2.20	0.42
1:A:224:LEU:HD21	1:A:317:LYS:HA	2.02	0.42
1:A:228:PRO:HG3	1:A:307:MET:HE1	2.01	0.42
1:A:19:GLY:O	1:A:24:PRO:HA	2.19	0.42
1:A:106:TRP:CH2	1:A:121:ILE:CD1	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ALA:O	1:A:264:LEU:HG	2.20	0.42
2:C:528:CYS:O	2:C:557:VAL:HA	2.20	0.42
1:A:41:TYR:CZ	1:A:49:PHE:HB3	2.55	0.41
1:A:40:LEU:HD23	1:A:50:GLN:HG2	2.01	0.41
2:C:545:GLU:O	2:C:546:ASN:HB2	2.20	0.41
1:A:36:THR:HA	1:A:105:ASP:O	2.20	0.41
1:A:363:LYS:HG2	1:A:392:VAL:C	2.45	0.41
1:A:168:THR:HA	1:A:197:LYS:HE2	2.02	0.41
1:A:30(B):SER:HB2	1:A:31:PRO:HD2	2.03	0.41
1:A:398:VAL:HG12	1:A:399:LYS:N	2.35	0.41
1:A:91:LYS:HE2	1:A:95:LYS:NZ	2.36	0.41
1:A:171:ARG:HD2	1:A:171:ARG:HH21	1.75	0.40
1:A:359:LEU:H	1:A:359:LEU:HD12	1.86	0.40
1:A:5:TYR:CZ	1:A:30(B):SER:HA	2.56	0.40
1:A:82:GLU:HG3	1:A:264:LEU:HD13	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	447/449 (100%)	397 (89%)	41 (9%)	9 (2%)	6	25
2	C	83/95 (87%)	66 (80%)	14 (17%)	3 (4%)	2	13
All	All	530/544 (97%)	463 (87%)	55 (10%)	12 (2%)	5	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	30	TRP
1	A	54	ALA

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Mol	Chain	Res	Type
1	A	294	ASN
1	A	303	GLY
2	C	526	ASN
2	C	581	ASN
2	C	583	ASN
1	A	24	PRO
1	A	297	PHE
1	A	20	ILE
1	A	284	PRO

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	383/383 (100%)	328 (86%)	55 (14%)	3	14
2	C	74/83 (89%)	59 (80%)	15 (20%)	1	6
All	All	457/466 (98%)	387 (85%)	70 (15%)	3	12

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	23	ARG
1	A	48	ASN
1	A	56	SER
1	A	80	LYS
1	A	85	TRP
1	A	91	LYS
1	A	111	ARG
1	A	115	THR
1	A	118	SER
1	A	121	ILE
1	A	123	ILE
1	A	143	PRO
1	A	153	LEU

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Mol	Chain	Res	Type
1	A	163	ARG
1	A	169	ILE
1	A	187	GLU
1	A	192	ASP
1	A	211	PRO
1	A	212	ASN
1	A	215	PHE
1	A	218	SER
1	A	220	VAL
1	A	238	LYS
1	A	239	LYS
1	A	242	LEU
1	A	255	THR
1	A	256	ARG
1	A	266	SER
1	A	272	ASP
1	A	287	SER
1	A	295	LYS
1	A	300	PRO
1	A	301	SER
1	A	307	MET
1	A	312	ASP
1	A	337	ARG
1	A	345	THR
1	A	349	LYS
1	A	350	LYS
1	A	351	VAL
1	A	357	VAL
1	A	359	LEU
1	A	363	LYS
1	A	379	ASP
1	A	389	ASP
1	A	408	ILE
1	A	411	THR
1	A	419	LYS
1	A	426	VAL
1	A	434	SER
1	A	436	GLU
1	A	439	ARG
1	A	443	LEU
1	A	444	LEU
2	C	507	ILE

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Mol	Chain	Res	Type
2	C	511	LEU
2	C	518	LEU
2	C	530	HIS
2	C	531	ASP
2	C	536	LEU
2	C	537	LEU
2	C	567	LEU
2	C	573	LYS
2	C	574	SER
2	C	578	SER
2	C	579	ILE
2	C	581	ASN
2	C	589	ASN
2	C	590	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	136	GLN
1	A	151	HIS
1	A	262	ASN
1	A	404	ASN
1	A	409	ASN
1	A	431	ASN
2	C	530	HIS
2	C	583	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

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

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.