



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:20 AM UTC

PDB ID : 1TAH / pdb_00001tah
Title : THE CRYSTAL STRUCTURE OF TRIACYLGLYCEROL LIPASE FROM
PSEUDOMONAS GLUMAE REVEALS A PARTIALLY REDUNDANT
CATALYTIC ASPARTATE
Authors : Noble, M.E.M.; Cleasby, A.; Johnson, L.N.; Egmond, M.; Frenken, L.G.J.
Deposited on : 1993-12-21
Resolution : 3.00 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

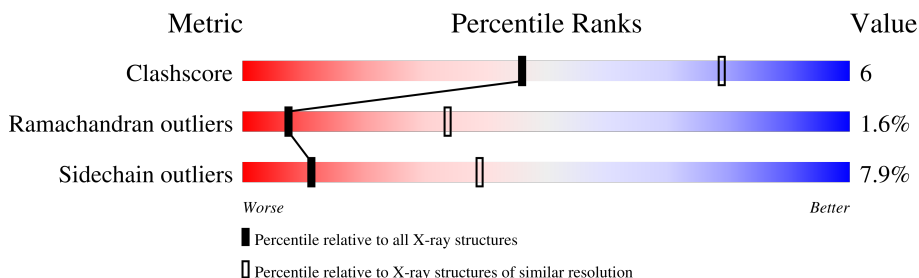
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	318	 79% 18% . .
1	B	318	 77% 18% . .
1	C	318	 81% 14% . .
1	D	318	 75% 20% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9320 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	318	Total	C	N	O	S	0	0	0
			2329	1450	410	466	3			
1	A	318	Total	C	N	O	S	0	0	0
			2329	1450	410	466	3			
1	C	318	Total	C	N	O	S	0	0	0
			2329	1450	410	466	3			
1	D	318	Total	C	N	O	S	0	0	0
			2329	1450	410	466	3			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

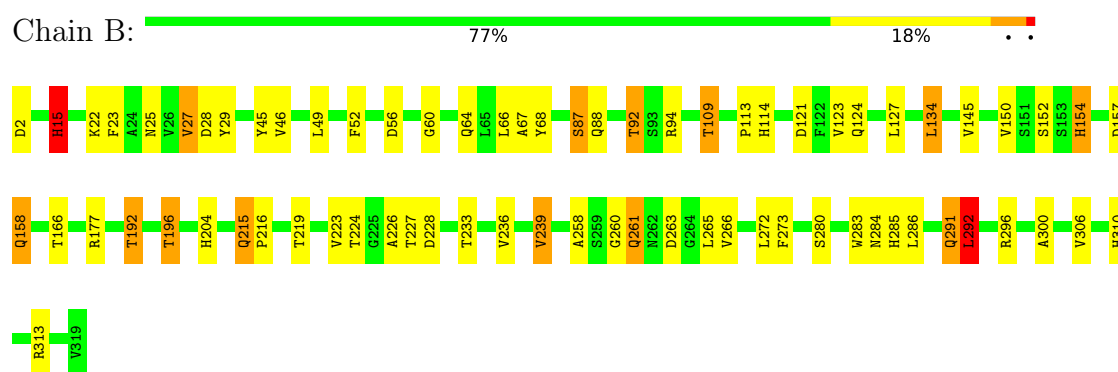
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

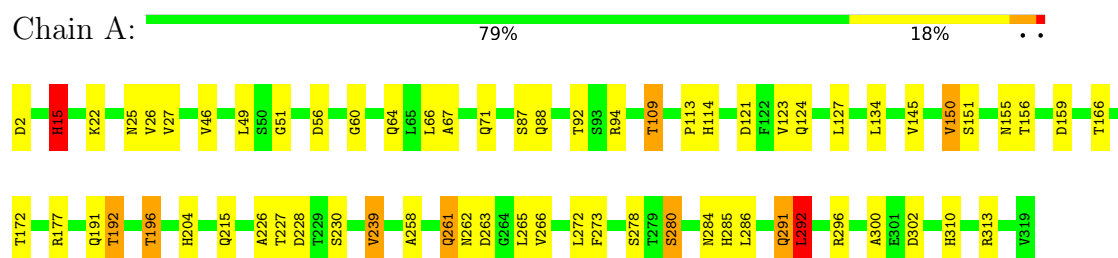
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

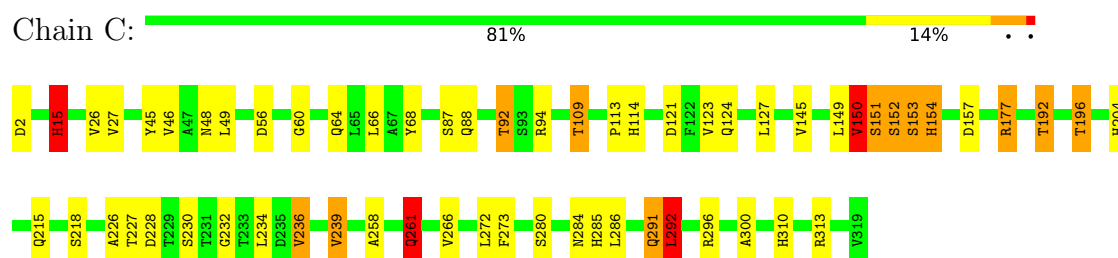
• Molecule 1: LIPASE



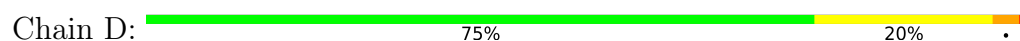
• Molecule 1: LIPASE

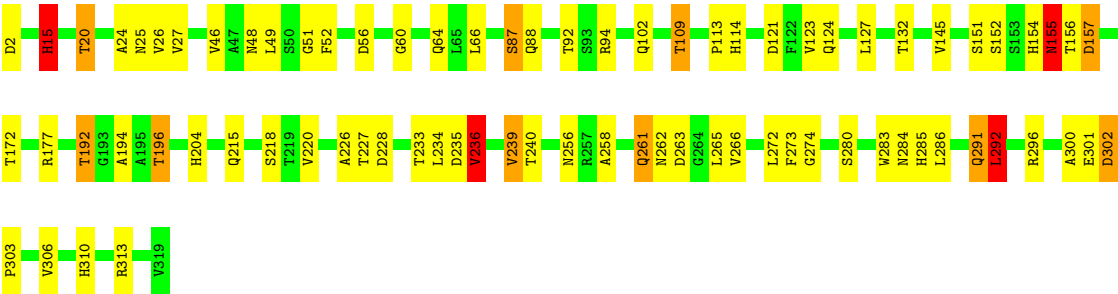


• Molecule 1: LIPASE



• Molecule 1: LIPASE





4 Data and refinement statistics

Xtrriage (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	158.16Å 158.64Å 63.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.159 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9320	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	1/2371 (0.0%)	1.59	26/3242 (0.8%)
1	B	0.73	2/2371 (0.1%)	1.63	35/3242 (1.1%)
1	C	0.73	3/2371 (0.1%)	1.65	37/3242 (1.1%)
1	D	0.73	1/2371 (0.0%)	1.62	32/3242 (1.0%)
All	All	0.73	7/9484 (0.1%)	1.62	130/12968 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	VAL	CA-C	6.32	1.60	1.52
1	A	46	VAL	CA-CB	5.84	1.61	1.54
1	B	92	THR	CA-CB	5.32	1.62	1.53
1	C	92	THR	CA-CB	5.26	1.62	1.53
1	C	46	VAL	CA-CB	5.18	1.60	1.54
1	D	46	VAL	CA-CB	5.15	1.60	1.54
1	B	46	VAL	CA-CB	5.02	1.60	1.54

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLN	O-C-N	10.44	136.76	123.19
1	C	291	GLN	O-C-N	10.43	136.75	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	GLN	O-C-N	10.16	136.40	123.19
1	D	155	ASN	CA-CB-CG	10.10	122.70	112.60
1	D	291	GLN	O-C-N	9.88	136.04	123.19
1	C	157	ASP	CA-CB-CG	9.88	122.48	112.60
1	C	153	SER	N-CA-C	-9.82	93.63	108.46
1	C	150	VAL	N-CA-CB	-9.32	95.86	111.23
1	C	284	ASN	CA-CB-CG	9.19	121.79	112.60
1	D	284	ASN	CA-CB-CG	9.14	121.74	112.60
1	B	284	ASN	CA-CB-CG	9.09	121.69	112.60
1	A	284	ASN	CA-CB-CG	8.97	121.57	112.60
1	C	291	GLN	CA-C-N	8.74	138.23	121.54
1	C	291	GLN	C-N-CA	8.74	138.23	121.54
1	A	291	GLN	CA-C-N	8.66	138.07	121.54
1	A	291	GLN	C-N-CA	8.66	138.07	121.54
1	B	291	GLN	CA-C-N	8.63	138.02	121.54
1	B	291	GLN	C-N-CA	8.63	138.02	121.54
1	A	15	HIS	CA-CB-CG	8.56	122.36	113.80
1	D	291	GLN	CA-C-N	8.48	137.74	121.54
1	D	291	GLN	C-N-CA	8.48	137.74	121.54
1	A	2	ASP	CA-CB-CG	8.41	121.01	112.60
1	D	2	ASP	CA-CB-CG	8.40	121.00	112.60
1	C	2	ASP	CA-CB-CG	8.30	120.90	112.60
1	B	15	HIS	CA-CB-CG	8.20	122.00	113.80
1	C	15	HIS	CA-CB-CG	8.19	121.99	113.80
1	B	2	ASP	CA-CB-CG	8.16	120.76	112.60
1	C	150	VAL	N-CA-C	7.82	125.59	109.34
1	D	15	HIS	CA-CB-CG	7.80	121.60	113.80
1	A	291	GLN	N-CA-C	7.78	122.17	109.72
1	D	233	THR	N-CA-C	7.75	119.50	111.14
1	D	291	GLN	N-CA-C	7.66	121.97	109.72
1	B	291	GLN	N-CA-C	7.57	121.83	109.72
1	D	157	ASP	CA-CB-CG	7.44	120.04	112.60
1	C	291	GLN	N-CA-C	7.24	121.31	109.72
1	C	150	VAL	CA-CB-CG2	-7.23	98.12	110.40
1	C	150	VAL	O-C-N	-7.20	113.56	122.57
1	B	261	GLN	N-CA-C	-6.97	95.96	110.80
1	C	261	GLN	N-CA-C	-6.90	96.09	110.80
1	C	236	VAL	CA-CB-CG1	-6.89	98.68	110.40
1	B	152	SER	N-CA-C	-6.86	100.12	110.28
1	B	28	ASP	N-CA-C	6.85	120.60	112.93
1	D	220	VAL	N-CA-C	-6.82	97.68	107.77
1	A	261	GLN	N-CA-C	-6.79	96.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	LEU	N-CA-C	-6.70	98.28	109.07
1	C	152	SER	O-C-N	6.64	131.57	122.41
1	D	261	GLN	N-CA-C	-6.59	96.77	110.80
1	D	132	THR	N-CA-CB	-6.56	100.90	110.47
1	A	88	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	C	88	GLN	OE1-CD-NE2	-6.50	116.10	122.60
1	A	292	LEU	N-CA-C	-6.48	97.00	110.80
1	C	292	LEU	N-CA-C	-6.43	97.10	110.80
1	B	88	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	D	88	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	A	239	VAL	CB-CA-C	-6.29	103.69	111.92
1	B	292	LEU	N-CA-C	-6.25	97.48	110.80
1	B	261	GLN	N-CA-CB	6.24	121.03	110.49
1	D	261	GLN	N-CA-CB	6.21	120.99	110.49
1	B	285	HIS	N-CA-C	6.19	118.83	111.71
1	C	152	SER	N-CA-C	6.19	119.62	108.17
1	A	159	ASP	O-C-N	6.17	128.43	122.07
1	B	29	TYR	N-CA-C	-6.09	104.56	111.14
1	B	27	VAL	CB-CA-C	-6.09	102.39	112.26
1	C	239	VAL	CB-CA-C	-6.09	103.94	111.92
1	A	261	GLN	N-CA-CB	6.07	120.74	110.49
1	D	239	VAL	CB-CA-C	-6.07	103.97	111.92
1	C	261	GLN	N-CA-CB	6.06	120.73	110.49
1	D	235	ASP	N-CA-C	6.06	118.06	108.67
1	D	292	LEU	N-CA-C	-6.05	97.91	110.80
1	B	216	PRO	CA-C-O	-6.05	114.39	121.95
1	D	263	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	239	VAL	CB-CA-C	-5.97	104.10	111.92
1	D	285	HIS	N-CA-C	5.94	118.54	111.71
1	C	232	GLY	N-CA-C	-5.86	103.64	112.89
1	B	88	GLN	CG-CD-NE2	5.84	125.16	116.40
1	C	149	LEU	CA-C-N	5.73	132.28	121.97
1	C	149	LEU	C-N-CA	5.73	132.28	121.97
1	C	88	GLN	CG-CD-NE2	5.71	124.97	116.40
1	B	157	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	258	ALA	N-CA-C	5.69	119.53	112.24
1	C	285	HIS	N-CA-C	5.64	118.20	111.71
1	B	158	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	C	150	VAL	CA-CB-CG1	5.62	119.96	110.40
1	D	88	GLN	CG-CD-NE2	5.62	124.83	116.40
1	A	263	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	302	ASP	CA-C-N	5.51	125.61	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ASP	C-N-CA	5.51	125.61	119.32
1	B	25	ASN	CA-CB-CG	-5.51	107.09	112.60
1	D	102	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	D	228	ASP	N-CA-C	-5.49	100.35	109.46
1	B	263	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	88	GLN	CG-CD-NE2	5.42	124.52	116.40
1	C	152	SER	CA-C-O	5.41	127.99	121.66
1	D	302	ASP	CA-C-N	5.35	125.42	119.32
1	D	302	ASP	C-N-CA	5.35	125.42	119.32
1	B	56	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	152	SER	CA-C-N	5.33	133.33	121.81
1	C	152	SER	C-N-CA	5.33	133.33	121.81
1	C	228	ASP	N-CA-C	-5.32	100.63	109.46
1	D	256	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	228	ASP	N-CA-C	-5.29	100.68	109.46
1	D	258	ALA	N-CA-C	5.29	119.01	112.24
1	C	56	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	230	SER	N-CA-C	-5.22	106.06	112.90
1	C	56	ASP	N-CA-C	5.21	119.27	113.02
1	A	56	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	154	HIS	CA-CB-CG	5.20	119.00	113.80
1	C	230	SER	N-CA-C	-5.18	106.11	112.90
1	B	87	SER	CB-CA-C	-5.18	110.62	116.63
1	D	236	VAL	CA-C-O	-5.17	115.04	120.57
1	A	285	HIS	N-CA-C	5.15	118.66	112.38
1	D	261	GLN	CB-CA-C	-5.15	100.18	110.42
1	C	236	VAL	CA-CB-CG2	5.14	119.13	110.40
1	A	150	VAL	N-CA-CB	-5.13	103.11	111.98
1	B	158	GLN	CG-CD-NE2	5.13	124.09	116.40
1	A	56	ASP	N-CA-C	5.12	119.17	113.02
1	D	56	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	87	SER	CB-CA-C	-5.10	110.71	116.63
1	B	258	ALA	N-CA-C	5.08	118.74	112.24
1	A	155	ASN	N-CA-C	5.08	120.38	113.37
1	A	262	ASN	CA-CB-CG	5.08	117.67	112.60
1	B	52	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	215	GLN	O-C-N	-5.07	116.88	121.39
1	B	27	VAL	CA-CB-CG1	-5.07	101.79	110.40
1	B	260	GLY	N-CA-C	5.04	123.00	115.64
1	B	228	ASP	N-CA-C	-5.04	101.10	109.46
1	B	261	GLN	CB-CA-C	-5.03	100.40	110.42
1	B	134	LEU	N-CA-C	5.03	121.51	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	258	ALA	N-CA-C	5.02	118.66	112.24
1	D	52	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	154	HIS	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	2329	0	2282	25	0
1	B	2329	0	2282	27	0
1	C	2329	0	2282	30	0
1	D	2329	0	2282	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	9320	0	9128	107	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 (107) 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:278:SER:OG	1:C:154:HIS:HD2	1.81	0.64
1:C:94:ARG:HH11	1:C:114:HIS:HD2	1.47	0.62
1:D:94:ARG:HH11	1:D:114:HIS:HD2	1.47	0.62
1:C:15:HIS:HE1	1:C:49:LEU:H	1.47	0.62
1:B:94:ARG:HH11	1:B:114:HIS:HD2	1.47	0.61
1:D:15:HIS:HE1	1:D:49:LEU:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:HIS:CD2	1:B:313:ARG:HD2	2.36	0.61
1:B:15:HIS:HE1	1:B:49:LEU:H	1.47	0.60
1:A:94:ARG:HH11	1:A:114:HIS:HD2	1.49	0.60
1:D:310:HIS:CD2	1:D:313:ARG:HD2	2.38	0.58
1:D:310:HIS:HD2	1:D:313:ARG:HH11	1.51	0.58
1:A:15:HIS:HE1	1:A:49:LEU:H	1.50	0.58
1:C:310:HIS:CD2	1:C:313:ARG:HD2	2.38	0.58
1:B:310:HIS:HD2	1:B:313:ARG:HH11	1.51	0.57
1:A:310:HIS:HD2	1:A:313:ARG:HH11	1.51	0.57
1:A:310:HIS:CD2	1:A:313:ARG:HD2	2.39	0.57
1:C:310:HIS:HD2	1:C:313:ARG:HH11	1.51	0.57
1:C:109:THR:HG21	1:C:114:HIS:HE1	1.68	0.57
1:D:109:THR:HG21	1:D:114:HIS:HE1	1.70	0.57
1:B:109:THR:HG21	1:B:114:HIS:HE1	1.70	0.57
1:A:109:THR:HG21	1:A:114:HIS:HE1	1.71	0.56
1:D:192:THR:HG23	1:D:272:LEU:HB3	1.88	0.56
1:C:150:VAL:HG12	1:C:151:SER:H	1.70	0.55
1:A:192:THR:HG23	1:A:272:LEU:HB3	1.88	0.55
1:A:286:LEU:HB3	1:A:291:GLN:HB3	1.89	0.55
1:C:15:HIS:CE1	1:C:49:LEU:H	2.25	0.55
1:C:150:VAL:CG1	1:C:151:SER:H	2.20	0.54
1:C:192:THR:HG23	1:C:272:LEU:HB3	1.89	0.53
1:B:15:HIS:CE1	1:B:49:LEU:H	2.26	0.53
1:B:296:ARG:HB3	1:B:300:ALA:HB3	1.91	0.53
1:B:64:GLN:O	1:B:67:ALA:HB3	2.09	0.53
1:C:286:LEU:HB3	1:C:291:GLN:HB3	1.90	0.53
1:D:15:HIS:CE1	1:D:49:LEU:H	2.27	0.52
1:B:286:LEU:HB3	1:B:291:GLN:HB3	1.90	0.52
1:C:177:ARG:NH1	1:D:301:GLU:OE2	2.42	0.52
1:B:192:THR:HG23	1:B:272:LEU:HB3	1.90	0.52
1:A:296:ARG:HB3	1:A:300:ALA:HB3	1.92	0.51
1:D:286:LEU:HB3	1:D:291:GLN:HB3	1.92	0.50
1:D:296:ARG:HB3	1:D:300:ALA:HB3	1.91	0.50
1:D:310:HIS:O	1:D:313:ARG:HB3	2.12	0.50
1:C:296:ARG:HB3	1:C:300:ALA:HB3	1.92	0.50
1:B:219:THR:HA	1:B:223:VAL:O	2.12	0.50
1:D:113:PRO:HB3	1:D:266:VAL:HG22	1.95	0.49
1:B:310:HIS:O	1:B:313:ARG:HB3	2.12	0.49
1:A:15:HIS:CE1	1:A:49:LEU:H	2.29	0.49
1:B:224:THR:HG21	1:A:191:GLN:HG2	1.95	0.49
1:C:310:HIS:CD2	1:C:313:ARG:HH11	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:THR:HG21	1:C:114:HIS:CE1	2.48	0.48
1:C:113:PRO:HB3	1:C:266:VAL:HG22	1.95	0.48
1:D:310:HIS:CD2	1:D:313:ARG:HH11	2.31	0.48
1:A:310:HIS:O	1:A:313:ARG:HB3	2.14	0.48
1:A:310:HIS:CD2	1:A:313:ARG:HH11	2.30	0.48
1:D:215:GLN:O	1:D:226:ALA:HA	2.14	0.48
1:C:310:HIS:O	1:C:313:ARG:HB3	2.14	0.47
1:D:109:THR:HG21	1:D:114:HIS:CE1	2.48	0.47
1:A:109:THR:HG21	1:A:114:HIS:CE1	2.49	0.47
1:D:155:ASN:O	1:D:157:ASP:N	2.47	0.47
1:A:113:PRO:HB3	1:A:266:VAL:HG22	1.96	0.47
1:B:22:LYS:HD2	1:B:23:PHE:CE2	2.50	0.47
1:B:310:HIS:CD2	1:B:313:ARG:HH11	2.30	0.47
1:C:196:THR:HA	1:C:204:HIS:O	2.15	0.47
1:B:113:PRO:HB3	1:B:266:VAL:HG22	1.96	0.46
1:D:236:VAL:HG12	1:D:240:THR:HG23	1.98	0.46
1:C:121:ASP:O	1:C:124:GLN:HG2	2.16	0.46
1:B:196:THR:HA	1:B:204:HIS:O	2.16	0.46
1:D:26:VAL:HG21	1:D:48:ASN:CG	2.41	0.46
1:D:196:THR:HA	1:D:204:HIS:O	2.15	0.46
1:D:60:GLY:O	1:D:64:GLN:HG2	2.16	0.45
1:A:196:THR:HA	1:A:204:HIS:O	2.17	0.45
1:C:60:GLY:O	1:C:64:GLN:HG2	2.15	0.45
1:D:20:THR:HA	1:D:51:GLY:HA2	1.98	0.45
1:B:60:GLY:O	1:B:64:GLN:HG2	2.16	0.45
1:B:215:GLN:O	1:B:226:ALA:HA	2.16	0.45
1:A:280:SER:HB2	1:C:154:HIS:CD2	2.51	0.45
1:B:109:THR:HG21	1:B:114:HIS:CE1	2.49	0.44
1:B:123:VAL:O	1:B:127:LEU:HG	2.17	0.44
1:C:26:VAL:HG21	1:C:48:ASN:OD1	2.16	0.44
1:A:114:HIS:CE1	1:A:273:PHE:HB2	2.53	0.44
1:A:121:ASP:O	1:A:124:GLN:HG2	2.17	0.44
1:B:22:LYS:HD2	1:B:23:PHE:CZ	2.52	0.44
1:B:121:ASP:O	1:B:124:GLN:HG2	2.18	0.44
1:A:22:LYS:HD3	1:A:51:GLY:HA3	1.99	0.44
1:A:215:GLN:O	1:A:226:ALA:HA	2.17	0.44
1:D:121:ASP:O	1:D:124:GLN:HG2	2.17	0.44
1:A:60:GLY:O	1:A:64:GLN:HG2	2.17	0.44
1:A:123:VAL:O	1:A:127:LEU:HG	2.17	0.43
1:C:123:VAL:O	1:C:127:LEU:HG	2.19	0.43
1:C:215:GLN:O	1:C:226:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASN:OD1	1:A:27:VAL:HG12	2.19	0.43
1:B:114:HIS:CE1	1:B:273:PHE:HB2	2.54	0.43
1:D:234:LEU:HA	1:D:234:LEU:HD23	1.83	0.42
1:C:114:HIS:CE1	1:C:273:PHE:HB2	2.54	0.42
1:C:150:VAL:CG1	1:C:151:SER:N	2.82	0.42
1:B:310:HIS:HD2	1:B:313:ARG:HD2	1.82	0.42
1:D:24:ALA:O	1:D:26:VAL:HG23	2.20	0.42
1:A:67:ALA:O	1:A:71:GLN:HG3	2.18	0.42
1:C:177:ARG:HG2	1:C:177:ARG:HH11	1.85	0.41
1:D:114:HIS:CE1	1:D:273:PHE:HB2	2.54	0.41
1:D:123:VAL:O	1:D:127:LEU:HG	2.19	0.41
1:C:310:HIS:HD2	1:C:313:ARG:HD2	1.86	0.41
1:C:45:TYR:HB3	1:C:68:TYR:OH	2.20	0.41
1:D:302:ASP:HA	1:D:303:PRO:HD3	1.94	0.41
1:B:283:TRP:CH2	1:B:306:VAL:HG21	2.56	0.41
1:C:215:GLN:OE1	1:C:261:GLN:HG2	2.21	0.40
1:D:194:ALA:O	1:D:274:GLY:HA2	2.22	0.40
1:B:45:TYR:HB3	1:B:68:TYR:OH	2.21	0.40
1:D:283:TRP:CH2	1:D:306:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/318 (99%)	298 (94%)	14 (4%)	4 (1%)	9	38
1	B	316/318 (99%)	295 (93%)	17 (5%)	4 (1%)	9	38
1	C	316/318 (99%)	298 (94%)	14 (4%)	4 (1%)	9	38
1	D	316/318 (99%)	291 (92%)	17 (5%)	8 (2%)	4	23
All	All	1264/1272 (99%)	1182 (94%)	62 (5%)	20 (2%)	7	34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	LEU
1	B	261	GLN
1	A	261	GLN
1	C	261	GLN
1	D	154	HIS
1	D	156	THR
1	D	218	SER
1	D	261	GLN
1	B	150	VAL
1	B	292	LEU
1	A	134	LEU
1	A	292	LEU
1	C	150	VAL
1	C	151	SER
1	C	292	LEU
1	D	292	LEU
1	A	156	THR
1	D	25	ASN
1	D	152	SER
1	D	151	SER

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/248 (100%)	229 (92%)	19 (8%)	12	40
1	B	248/248 (100%)	228 (92%)	20 (8%)	11	38
1	C	248/248 (100%)	229 (92%)	19 (8%)	12	40
1	D	248/248 (100%)	228 (92%)	20 (8%)	11	38
All	All	992/992 (100%)	914 (92%)	78 (8%)	11	39

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	HIS
1	B	27	VAL
1	B	66	LEU
1	B	87	SER
1	B	92	THR
1	B	109	THR
1	B	145	VAL
1	B	154	HIS
1	B	158	GLN
1	B	166	THR
1	B	177	ARG
1	B	192	THR
1	B	196	THR
1	B	227	THR
1	B	233	THR
1	B	236	VAL
1	B	239	VAL
1	B	265	LEU
1	B	280	SER
1	B	292	LEU
1	A	15	HIS
1	A	26	VAL
1	A	66	LEU
1	A	87	SER
1	A	92	THR
1	A	109	THR
1	A	145	VAL
1	A	150	VAL
1	A	151	SER
1	A	166	THR
1	A	172	THR
1	A	177	ARG
1	A	192	THR
1	A	196	THR
1	A	227	THR
1	A	239	VAL
1	A	265	LEU
1	A	280	SER
1	A	292	LEU
1	C	15	HIS
1	C	27	VAL
1	C	66	LEU
1	C	87	SER

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Mol	Chain	Res	Type
1	C	92	THR
1	C	109	THR
1	C	145	VAL
1	C	150	VAL
1	C	152	SER
1	C	153	SER
1	C	177	ARG
1	C	192	THR
1	C	196	THR
1	C	218	SER
1	C	227	THR
1	C	236	VAL
1	C	239	VAL
1	C	280	SER
1	C	292	LEU
1	D	15	HIS
1	D	20	THR
1	D	27	VAL
1	D	66	LEU
1	D	87	SER
1	D	92	THR
1	D	109	THR
1	D	145	VAL
1	D	155	ASN
1	D	172	THR
1	D	177	ARG
1	D	192	THR
1	D	196	THR
1	D	227	THR
1	D	236	VAL
1	D	239	VAL
1	D	262	ASN
1	D	265	LEU
1	D	280	SER
1	D	292	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	HIS
1	B	71	GLN
1	B	114	HIS

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Mol	Chain	Res	Type
1	B	284	ASN
1	B	310	HIS
1	A	15	HIS
1	A	71	GLN
1	A	114	HIS
1	A	171	GLN
1	A	262	ASN
1	A	284	ASN
1	A	310	HIS
1	C	15	HIS
1	C	114	HIS
1	C	154	HIS
1	C	284	ASN
1	C	310	HIS
1	D	15	HIS
1	D	71	GLN
1	D	114	HIS
1	D	284	ASN
1	D	310	HIS

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 ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.