



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:44 PM UTC

PDB ID : 1GLV / pdb_00001glv
Title : THREE-DIMENSIONAL STRUCTURE OF THE GLUTATHIONE SYNTHETASE FROM ESCHERICHIA COLI B AT 2.0 ANGSTROMS RESOLUTION
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Deposited on : 1993-03-12
Resolution : 2.70 Å(reported)

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

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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

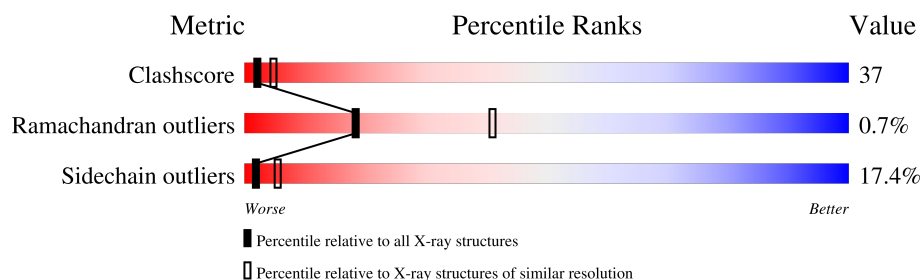
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	303	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2407 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 GLUTATHIONE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	1	0
			2389	1523	402	450	14			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P04425
A	?	-	PRO	deletion	UNP P04425
A	?	-	GLN	deletion	UNP P04425
A	?	-	GLY	deletion	UNP P04425
A	?	-	GLY	deletion	UNP P04425
A	?	-	GLU	deletion	UNP P04425
A	?	-	THR	deletion	UNP P04425
A	?	-	ARG	deletion	UNP P04425
A	?	-	GLY	deletion	UNP P04425
A	?	-	ASN	deletion	UNP P04425
A	?	-	LEU	deletion	UNP P04425
A	?	-	ALA	deletion	UNP P04425
A	?	-	ALA	deletion	UNP P04425
A	228	GLY	ARG	conflict	UNP P04425

- Molecule 2 is water.

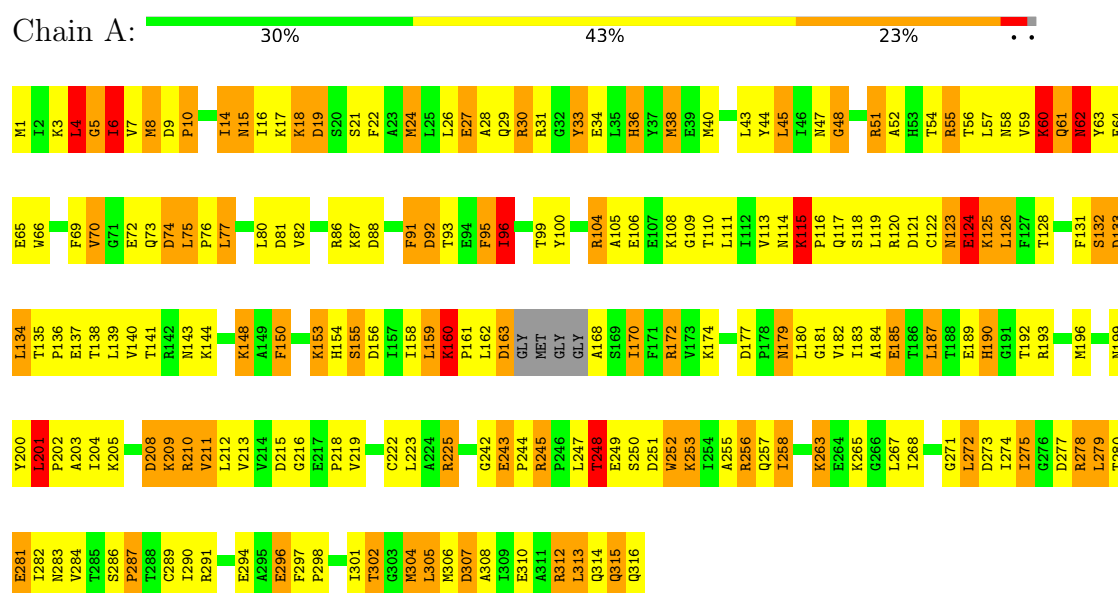
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		

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: GLUTATHIONE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.70Å 87.70Å 169.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2407	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	1.42	8/2435 (0.3%)	2.58	170/3294 (5.2%)

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	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	THR	N-CA	6.88	1.54	1.46
1	A	51	ARG	CD-NE	5.83	1.54	1.46
1	A	272	LEU	N-CA	5.77	1.53	1.46
1	A	6	ILE	N-CA	-5.34	1.40	1.46
1	A	113	VAL	C-N	-5.32	1.25	1.33
1	A	115	LYS	N-CA	5.22	1.52	1.45
1	A	170	ILE	CA-CB	5.17	1.60	1.54
1	A	141	THR	CA-CB	5.04	1.62	1.53

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	VAL	CA-C-N	32.31	179.86	121.70
1	A	113	VAL	C-N-CA	32.31	179.86	121.70
1	A	124	GLU	CA-CB-CG	12.08	138.26	114.10
1	A	190	HIS	CA-CB-CG	-11.53	102.27	113.80
1	A	219	VAL	N-CA-C	-11.06	98.11	108.95
1	A	51	ARG	CD-NE-CZ	-10.66	109.48	124.40
1	A	51	ARG	NE-CZ-NH1	-10.49	111.00	121.50
1	A	143	ASN	CA-CB-CG	-10.08	102.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	VAL	CB-CA-C	9.59	124.25	111.88
1	A	60	LYS	O-C-N	9.49	134.30	123.48
1	A	56	THR	CB-CA-C	9.23	124.94	109.80
1	A	281	GLU	CA-CB-CG	8.93	131.96	114.10
1	A	124	GLU	CB-CG-CD	8.77	127.51	112.60
1	A	181	GLY	CA-C-N	8.52	132.54	120.53
1	A	181	GLY	C-N-CA	8.52	132.54	120.53
1	A	95	PHE	CA-CB-CG	8.33	122.13	113.80
1	A	160	LYS	O-C-N	8.29	127.70	121.65
1	A	19	ASP	CA-CB-CG	-8.26	104.34	112.60
1	A	70	VAL	N-CA-CB	-8.12	101.61	112.16
1	A	177	ASP	CA-CB-CG	-8.10	104.50	112.60
1	A	51	ARG	NE-CZ-NH2	7.92	126.33	119.20
1	A	282	ILE	N-CA-CB	-7.88	102.61	112.15
1	A	86	ARG	CA-C-N	7.70	131.73	120.95
1	A	86	ARG	C-N-CA	7.70	131.73	120.95
1	A	140	VAL	CA-C-O	-7.57	110.85	120.69
1	A	219	VAL	CB-CA-C	7.54	119.03	110.89
1	A	75	LEU	O-C-N	7.51	129.96	121.32
1	A	115	LYS	CB-CA-C	7.38	121.18	109.52
1	A	36	HIS	CA-CB-CG	-7.33	106.47	113.80
1	A	47	ASN	CA-C-O	-7.33	113.46	122.03
1	A	210	ARG	NE-CZ-NH2	7.19	125.67	119.20
1	A	5	GLY	CA-C-N	7.18	133.16	122.75
1	A	5	GLY	C-N-CA	7.18	133.16	122.75
1	A	120	ARG	CA-C-N	7.14	130.43	120.29
1	A	120	ARG	C-N-CA	7.14	130.43	120.29
1	A	91	PHE	CA-CB-CG	7.10	120.90	113.80
1	A	60	LYS	CA-C-O	-7.09	112.07	120.43
1	A	125	LYS	CB-CA-C	-7.08	97.60	110.56
1	A	48	GLY	CA-C-N	-7.04	113.00	122.72
1	A	48	GLY	C-N-CA	-7.04	113.00	122.72
1	A	15	ASN	CA-CB-CG	6.94	119.54	112.60
1	A	304	MET	O-C-N	6.88	129.46	122.03
1	A	256	ARG	CA-C-N	6.80	132.22	120.58
1	A	256	ARG	C-N-CA	6.80	132.22	120.58
1	A	139	LEU	CA-C-O	-6.80	113.02	120.36
1	A	5	GLY	N-CA-C	-6.74	100.99	112.51
1	A	279	LEU	CA-C-O	-6.71	113.02	120.60
1	A	267	LEU	CA-C-O	-6.69	114.68	122.37
1	A	242	GLY	CA-C-O	-6.66	115.32	121.18
1	A	24	MET	CA-CB-CG	-6.65	100.80	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	CB-CA-C	6.62	121.38	110.78
1	A	81	ASP	O-C-N	6.56	130.75	122.23
1	A	273	ASP	CA-CB-CG	-6.54	106.06	112.60
1	A	143	ASN	N-CA-C	6.52	119.33	108.96
1	A	179	ASN	N-CA-C	6.52	122.04	113.30
1	A	190	HIS	CA-C-N	6.52	129.96	120.11
1	A	190	HIS	C-N-CA	6.52	129.96	120.11
1	A	113	VAL	CA-C-O	6.50	128.65	121.04
1	A	56	THR	CA-CB-OG1	-6.47	99.89	109.60
1	A	69	PHE	CB-CA-C	6.46	120.41	109.75
1	A	3	LYS	O-C-N	6.45	131.64	123.12
1	A	273	ASP	O-C-N	6.40	130.75	122.87
1	A	104	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	213	VAL	CB-CA-C	6.35	119.60	110.33
1	A	60	LYS	CA-CB-CG	6.35	126.79	114.10
1	A	123	ASN	CA-C-N	6.34	128.78	120.28
1	A	123	ASN	C-N-CA	6.34	128.78	120.28
1	A	172	ARG	O-C-N	6.33	130.44	123.22
1	A	105	ALA	O-C-N	6.32	129.35	122.15
1	A	80	LEU	CB-CA-C	6.28	120.15	109.53
1	A	4	LEU	CA-C-N	-6.28	115.00	122.16
1	A	4	LEU	C-N-CA	-6.28	115.00	122.16
1	A	150	PHE	CA-C-N	6.28	128.60	120.44
1	A	150	PHE	C-N-CA	6.28	128.60	120.44
1	A	27	GLU	CG-CD-OE1	6.26	132.80	118.40
1	A	189	GLU	CB-CG-CD	6.24	123.21	112.60
1	A	58	ASN	CA-C-O	-6.21	113.66	120.30
1	A	274	ILE	CA-C-O	-6.21	113.89	120.53
1	A	104	ARG	NE-CZ-NH1	-6.18	115.31	121.50
1	A	209	LYS	CA-C-O	6.18	127.52	120.54
1	A	109	GLY	O-C-N	-6.18	116.23	122.65
1	A	249	GLU	CA-CB-CG	6.17	126.43	114.10
1	A	109	GLY	N-CA-C	6.13	122.21	114.25
1	A	184	ALA	O-C-N	6.13	128.46	122.09
1	A	243	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	57	LEU	N-CA-C	6.11	118.90	109.07
1	A	200	TYR	CA-C-O	6.05	127.88	120.92
1	A	115	LYS	CA-C-N	6.04	125.25	118.97
1	A	115	LYS	C-N-CA	6.04	125.25	118.97
1	A	296	GLU	N-CA-C	6.04	120.48	113.18
1	A	282	ILE	CA-C-O	-6.03	112.86	120.69
1	A	29	GLN	OE1-CD-NE2	-6.02	116.58	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ASN	CA-C-O	-6.01	112.16	119.32
1	A	93	THR	CA-C-N	6.01	128.33	120.28
1	A	93	THR	C-N-CA	6.01	128.33	120.28
1	A	91	PHE	CA-C-N	6.00	134.38	123.27
1	A	91	PHE	C-N-CA	6.00	134.38	123.27
1	A	117	GLN	O-C-N	5.99	128.24	122.07
1	A	3	LYS	N-CA-CB	5.97	120.09	110.65
1	A	55	ARG	CA-CB-CG	5.94	125.97	114.10
1	A	104	ARG	N-CA-CB	5.93	119.47	110.28
1	A	122	CYS	N-CA-C	5.93	118.97	108.24
1	A	62	ASN	CA-C-N	5.92	128.81	120.28
1	A	62	ASN	C-N-CA	5.92	128.81	120.28
1	A	122	CYS	CA-C-O	-5.92	115.44	122.13
1	A	72	GLU	CA-CB-CG	5.92	125.94	114.10
1	A	81	ASP	CA-C-O	-5.90	113.69	120.24
1	A	278	ARG	NE-CZ-NH1	5.89	127.39	121.50
1	A	9	ASP	N-CA-C	-5.89	102.17	110.29
1	A	302	THR	CA-CB-CG2	5.86	120.45	110.50
1	A	92	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	113	VAL	O-C-N	-5.84	115.78	122.62
1	A	33	TYR	N-CA-C	-5.84	102.67	110.55
1	A	216	GLY	CA-C-N	5.84	129.45	121.74
1	A	216	GLY	C-N-CA	5.84	129.45	121.74
1	A	57	LEU	N-CA-CB	-5.83	101.42	110.57
1	A	17	LYS	O-C-N	5.81	129.78	122.23
1	A	45	LEU	O-C-N	5.77	130.66	123.28
1	A	277	ASP	CA-CB-CG	-5.76	106.84	112.60
1	A	81	ASP	N-CA-CB	5.75	118.76	110.20
1	A	9	ASP	N-CA-CB	5.73	116.96	110.03
1	A	133	ASP	CA-CB-CG	-5.73	106.87	112.60
1	A	252	TRP	O-C-N	5.68	128.00	122.09
1	A	7	VAL	CA-C-O	-5.68	114.45	120.53
1	A	92	ASP	CB-CA-C	-5.67	100.65	111.48
1	A	307	ASP	CA-C-N	5.66	127.86	120.28
1	A	307	ASP	C-N-CA	5.66	127.86	120.28
1	A	296	GLU	CB-CG-CD	5.64	122.19	112.60
1	A	287	PRO	CA-C-N	5.64	129.60	122.16
1	A	287	PRO	C-N-CA	5.64	129.60	122.16
1	A	281	GLU	CG-CD-OE2	5.63	131.36	118.40
1	A	114	ASN	CB-CA-C	5.63	120.80	110.10
1	A	131	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	120	ARG	NE-CZ-NH1	5.60	127.10	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	SER	CA-CB-OG	-5.59	99.93	111.10
1	A	54	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	272	LEU	CA-C-O	-5.56	114.70	120.70
1	A	187	LEU	CA-C-O	-5.54	114.68	120.55
1	A	121	ASP	CA-C-O	5.51	126.26	120.42
1	A	125	LYS	N-CA-CB	5.48	118.68	110.19
1	A	192	THR	CA-C-O	5.45	125.04	119.05
1	A	271	GLY	CA-C-N	-5.45	114.77	122.94
1	A	271	GLY	C-N-CA	-5.45	114.77	122.94
1	A	160	LYS	N-CA-C	5.43	114.55	108.25
1	A	96	ILE	O-C-N	5.39	127.10	121.87
1	A	282	ILE	CA-CB-CG2	5.38	119.64	110.50
1	A	278	ARG	NE-CZ-NH2	-5.37	114.36	119.20
1	A	281	GLU	N-CA-CB	5.36	119.71	111.56
1	A	312	ARG	N-CA-C	-5.36	105.51	111.36
1	A	248	THR	CA-CB-OG1	-5.35	101.57	109.60
1	A	201	LEU	CA-C-O	5.34	124.64	119.99
1	A	61	GLN	CB-CG-CD	5.32	121.64	112.60
1	A	115	LYS	CA-CB-CG	5.32	124.73	114.10
1	A	193	ARG	CA-C-O	-5.29	114.57	120.66
1	A	30	ARG	CD-NE-CZ	-5.23	117.08	124.40
1	A	150	PHE	CB-CA-C	5.22	119.45	110.79
1	A	153	LYS	CA-C-O	-5.20	112.98	119.38
1	A	304	MET	N-CA-C	-5.20	105.26	111.03
1	A	27	GLU	CA-C-O	-5.12	115.44	120.82
1	A	138	THR	N-CA-C	5.12	117.25	108.90
1	A	8	MET	N-CA-C	5.12	115.81	108.74
1	A	96	ILE	N-CA-CB	5.11	117.48	110.54
1	A	74	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	243	GLU	CB-CA-C	-5.08	104.98	110.98
1	A	274	ILE	CA-C-N	5.07	131.10	121.97
1	A	274	ILE	C-N-CA	5.07	131.10	121.97
1	A	40	MET	O-C-N	5.07	127.94	122.11
1	A	200	TYR	CB-CA-C	5.05	117.86	109.53
1	A	100	TYR	CA-CB-CG	5.01	122.92	113.90
1	A	117	GLN	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	ARG	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	2389	0	2406	179	0
2	A	18	0	0	1	0
All	All	2407	0	2406	179	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 37.

All (179) 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:38:MET:HE1	1:A:77:LEU:HD11	1.30	1.13
1:A:38:MET:CE	1:A:77:LEU:HD11	1.80	1.11
1:A:252:TRP:O	1:A:256:ARG:HB2	1.53	1.09
1:A:48:GLY:O	1:A:104:ARG:NH1	1.87	1.08
1:A:208:ASP:O	1:A:225:ARG:HG2	1.51	1.08
1:A:168:ALA:HB1	1:A:170:ILE:HD12	1.28	1.07
1:A:316:GLN:O	1:A:316:GLN:HG2	1.50	1.05
1:A:16:ILE:HD11	1:A:63:TYR:CE1	2.01	0.96
1:A:16:ILE:HD11	1:A:63:TYR:CD1	1.99	0.96
1:A:4:LEU:C	1:A:4:LEU:HD12	1.93	0.94
1:A:137:GLU:HB2	1:A:199:ASN:OD1	1.67	0.92
1:A:61:GLN:HE22	1:A:291:ARG:HH22	1.11	0.91
1:A:168:ALA:HB1	1:A:170:ILE:CD1	2.00	0.91
1:A:91:PHE:CE1	1:A:95:PHE:CD1	2.60	0.90
1:A:159:LEU:HD23	1:A:183:ILE:HG21	1.55	0.87
1:A:51:ARG:NH1	1:A:74:ASP:OD1	2.08	0.87
1:A:159:LEU:HD23	1:A:183:ILE:CG2	2.06	0.85
1:A:95:PHE:O	1:A:99:THR:HG23	1.77	0.85
1:A:75:LEU:HB2	1:A:76:PRO:HD2	1.59	0.84
1:A:91:PHE:HE1	1:A:95:PHE:CD1	1.97	0.82
1:A:225:ARG:HH11	1:A:225:ARG:HB3	1.45	0.82
1:A:44:TYR:OH	1:A:51:ARG:NH1	2.13	0.81
1:A:210:ARG:CG	1:A:225:ARG:HD3	2.11	0.80
1:A:91:PHE:CE2	1:A:96:ILE:HD11	2.17	0.79
1:A:244:PRO:HB2	1:A:297:PHE:HE2	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:MET:HE3	1:A:52:ALA:CB	2.14	0.78
1:A:38:MET:HE3	1:A:52:ALA:HB3	1.66	0.78
1:A:156:ASP:OD2	1:A:172:ARG:NH2	2.17	0.77
1:A:315:GLN:HG3	1:A:316:GLN:H	1.48	0.76
1:A:4:LEU:C	1:A:4:LEU:CD1	2.61	0.73
1:A:144:LYS:HZ1	1:A:185:GLU:CD	1.96	0.73
1:A:215:ASP:O	1:A:263:LYS:HG3	1.88	0.73
1:A:248:THR:CG2	1:A:250:SER:H	2.01	0.73
1:A:297:PHE:HB3	1:A:298:PRO:HD2	1.70	0.73
1:A:6:ILE:HG12	1:A:8:MET:HE3	1.71	0.72
1:A:204:ILE:HD12	1:A:275:ILE:CD1	2.19	0.72
1:A:268:ILE:HD11	1:A:312:ARG:HD2	1.72	0.71
1:A:202:PRO:O	1:A:205:LYS:HG2	1.90	0.71
1:A:61:GLN:HE22	1:A:291:ARG:NH2	1.87	0.71
1:A:38:MET:HE1	1:A:77:LEU:CD1	2.15	0.70
1:A:62:ASN:HD22	1:A:62:ASN:C	1.99	0.70
1:A:91:PHE:CE1	1:A:95:PHE:HD1	2.09	0.70
1:A:225:ARG:HB3	1:A:225:ARG:NH1	2.06	0.70
1:A:210:ARG:HG2	1:A:225:ARG:HD3	1.73	0.70
1:A:4:LEU:HD13	1:A:5:GLY:O	1.91	0.69
1:A:204:ILE:HD12	1:A:275:ILE:HD11	1.75	0.68
1:A:202:PRO:O	1:A:205:LYS:CG	2.41	0.68
1:A:210:ARG:NE	1:A:225:ARG:HE	1.92	0.68
1:A:38:MET:HE3	1:A:77:LEU:HD11	1.73	0.67
1:A:248:THR:HG23	1:A:250:SER:H	1.60	0.67
1:A:118:SER:OG	1:A:265:LYS:O	2.06	0.67
1:A:134:LEU:HD21	1:A:257:GLN:OE1	1.94	0.66
1:A:315:GLN:CG	1:A:316:GLN:H	2.09	0.66
1:A:45:LEU:HD11	1:A:104:ARG:HG3	1.78	0.65
1:A:135:THR:HB	1:A:136:PRO:HD2	1.79	0.65
1:A:315:GLN:O	1:A:316:GLN:HB3	1.95	0.65
1:A:210:ARG:HE	1:A:225:ARG:HE	1.44	0.65
1:A:4:LEU:HA	1:A:82:VAL:O	1.98	0.64
1:A:27:GLU:OE2	1:A:31:ARG:NE	2.24	0.64
1:A:275:ILE:HG13	1:A:280:THR:HG21	1.80	0.63
1:A:38:MET:CE	1:A:52:ALA:CB	2.76	0.63
1:A:75:LEU:C	1:A:75:LEU:HD12	2.25	0.62
1:A:306:MET:O	1:A:310:GLU:HG3	2.00	0.62
1:A:210:ARG:HG3	1:A:225:ARG:HD3	1.80	0.62
1:A:125:LYS:HB3	1:A:196:MET:HE1	1.83	0.61
1:A:148:LYS:HG2	1:A:180:LEU:CD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:OD1	1:A:287:PRO:HD3	2.00	0.60
1:A:153:LYS:HG2	1:A:154:HIS:CD2	2.37	0.60
1:A:14:ILE:C	1:A:14:ILE:HD12	2.26	0.60
1:A:21:SER:O	1:A:24:MET:HB2	2.02	0.59
1:A:4:LEU:HD12	1:A:4:LEU:O	2.01	0.59
1:A:91:PHE:CD2	1:A:96:ILE:HD11	2.37	0.59
1:A:218:PRO:HG2	1:A:252:TRP:CZ3	2.38	0.59
1:A:248:THR:HG22	1:A:251:ASP:H	1.67	0.59
1:A:75:LEU:HD12	1:A:75:LEU:O	2.03	0.58
1:A:283:ASN:OD1	1:A:283:ASN:C	2.45	0.58
1:A:315:GLN:HG3	1:A:316:GLN:N	2.18	0.58
1:A:87:LYS:NZ	1:A:88:ASP:O	2.36	0.58
1:A:275:ILE:HG22	1:A:275:ILE:O	2.03	0.58
1:A:75:LEU:HB2	1:A:76:PRO:CD	2.33	0.58
1:A:91:PHE:CE2	1:A:96:ILE:CD1	2.86	0.57
1:A:6:ILE:HG12	1:A:8:MET:CE	2.34	0.57
1:A:144:LYS:NZ	1:A:185:GLU:CD	2.62	0.57
1:A:48:GLY:C	1:A:104:ARG:HH12	2.13	0.57
1:A:243:GLU:CD	1:A:245:ARG:HH11	2.13	0.57
1:A:91:PHE:CD1	1:A:95:PHE:CD1	2.92	0.57
1:A:247:LEU:HB3	1:A:251:ASP:HB2	1.86	0.56
1:A:248:THR:HB	1:A:251:ASP:OD2	2.05	0.56
1:A:62:ASN:ND2	1:A:64:GLU:H	2.03	0.56
1:A:159:LEU:HD23	1:A:183:ILE:HG22	1.86	0.56
1:A:310:GLU:O	1:A:314:GLN:NE2	2.37	0.56
1:A:294:GLU:OE2	1:A:301:ILE:N	2.36	0.55
1:A:248:THR:HG22	1:A:250:SER:H	1.72	0.55
1:A:16:ILE:CD1	1:A:63:TYR:CE1	2.85	0.55
1:A:51:ARG:HH12	1:A:74:ASP:CG	2.12	0.54
1:A:154:HIS:O	1:A:156:ASP:N	2.34	0.54
1:A:179:ASN:O	1:A:180:LEU:C	2.51	0.54
1:A:248:THR:HG22	1:A:250:SER:N	2.23	0.53
1:A:305:LEU:O	1:A:308:ALA:HB3	2.08	0.53
1:A:91:PHE:HE1	1:A:95:PHE:HD1	1.48	0.53
1:A:4:LEU:CD1	1:A:5:GLY:O	2.57	0.53
1:A:27:GLU:O	1:A:31:ARG:HG3	2.08	0.53
1:A:15:ASN:ND2	1:A:18:LYS:HG2	2.24	0.53
1:A:62:ASN:HD22	1:A:64:GLU:H	1.57	0.52
1:A:258:ILE:HD11	1:A:279:LEU:HD22	1.91	0.52
1:A:48:GLY:C	1:A:104:ARG:NH1	2.68	0.51
1:A:28:ALA:HB1	1:A:33:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASN:C	1:A:62:ASN:ND2	2.69	0.51
1:A:44:TYR:OH	1:A:74:ASP:OD2	2.26	0.50
1:A:62:ASN:ND2	1:A:65:GLU:H	2.09	0.50
1:A:302:THR:O	1:A:306:MET:HG2	2.12	0.50
1:A:268:ILE:CD1	1:A:312:ARG:HD2	2.40	0.50
1:A:208:ASP:O	1:A:225:ARG:CG	2.42	0.49
1:A:111:LEU:HD22	1:A:313:LEU:CD1	2.43	0.49
1:A:51:ARG:NH2	1:A:75:LEU:HA	2.27	0.49
1:A:204:ILE:HB	1:A:275:ILE:HD12	1.94	0.49
1:A:248:THR:HG22	1:A:251:ASP:N	2.27	0.49
1:A:74:ASP:OD1	1:A:74:ASP:C	2.56	0.49
1:A:92:ASP:O	1:A:96:ILE:HD12	2.13	0.48
1:A:128:THR:HB	1:A:135:THR:HG21	1.95	0.48
1:A:26:LEU:HD11	1:A:61:GLN:NE2	2.28	0.48
1:A:115:LYS:HA	1:A:116:PRO:HD3	1.71	0.48
1:A:19:ASP:OD2	1:A:21:SER:HB2	2.14	0.48
1:A:304:MET:O	1:A:307:ASP:HB2	2.13	0.48
1:A:123:ASN:HB3	1:A:126:LEU:HB2	1.94	0.48
1:A:161:PRO:HG3	1:A:187:LEU:CD2	2.44	0.48
1:A:75:LEU:CB	1:A:76:PRO:HD2	2.39	0.47
1:A:95:PHE:HE1	1:A:119:LEU:HD13	1.79	0.47
1:A:244:PRO:HB2	1:A:297:PHE:CE2	2.38	0.47
1:A:137:GLU:HA	1:A:137:GLU:OE1	2.14	0.47
1:A:209:LYS:NZ	1:A:251:ASP:OD1	2.31	0.47
1:A:222:CYS:O	1:A:244:PRO:HA	2.14	0.47
1:A:210:ARG:HG3	1:A:225:ARG:CD	2.44	0.47
1:A:134:LEU:CD1	1:A:258:ILE:HD11	2.45	0.46
1:A:211:VAL:O	1:A:272:LEU:N	2.45	0.46
1:A:258:ILE:CD1	1:A:279:LEU:HD22	2.45	0.46
1:A:18:LYS:HE3	1:A:18:LYS:HB3	1.66	0.46
1:A:38:MET:HE2	1:A:43:LEU:HD23	1.98	0.46
1:A:4:LEU:HB2	1:A:82:VAL:HG13	1.97	0.46
1:A:124:GLU:OE1	1:A:284:VAL:HG22	2.17	0.45
1:A:14:ILE:C	1:A:14:ILE:CD1	2.89	0.45
1:A:59:VAL:HA	1:A:66:TRP:O	2.15	0.45
1:A:60:LYS:HE2	1:A:65:GLU:O	2.16	0.45
1:A:244:PRO:HG2	1:A:296:GLU:HG3	1.98	0.45
1:A:158:ILE:HG23	1:A:170:ILE:HG23	1.98	0.45
1:A:91:PHE:HE1	1:A:95:PHE:CE1	2.33	0.45
1:A:22:PHE:CZ	1:A:66:TRP:HB2	2.53	0.44
1:A:75:LEU:C	1:A:75:LEU:CD1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:O	1:A:256:ARG:CB	2.44	0.44
1:A:218:PRO:HB3	1:A:255:ALA:HB1	1.99	0.44
1:A:34:GLU:OE2	1:A:36:HIS:NE2	2.36	0.44
1:A:150:PHE:O	1:A:154:HIS:HD2	2.01	0.43
1:A:144:LYS:O	1:A:148:LYS:HB2	2.18	0.43
1:A:290:ILE:O	1:A:294:GLU:HG3	2.18	0.43
1:A:223:LEU:HD22	1:A:289:CYS:SG	2.59	0.43
1:A:51:ARG:CZ	1:A:74:ASP:OD1	2.67	0.43
1:A:312:ARG:HH11	1:A:312:ARG:HD3	1.57	0.43
1:A:62:ASN:HD22	1:A:64:GLU:N	2.16	0.43
1:A:253:LYS:HB2	1:A:253:LYS:HE3	1.49	0.43
1:A:204:ILE:HB	1:A:275:ILE:CD1	2.49	0.43
1:A:52:ALA:O	1:A:74:ASP:HA	2.20	0.42
1:A:160:LYS:HA	1:A:161:PRO:HD3	1.78	0.42
1:A:203:ALA:C	1:A:205:LYS:N	2.75	0.42
1:A:185:GLU:HG3	1:A:190:HIS:ND1	2.35	0.42
1:A:297:PHE:HB3	1:A:298:PRO:CD	2.45	0.42
1:A:63:TYR:O	1:A:66:TRP:HZ3	2.03	0.41
1:A:134:LEU:HD12	1:A:258:ILE:HD11	2.01	0.41
1:A:38:MET:HE2	1:A:43:LEU:CD2	2.50	0.41
1:A:6:ILE:CG1	1:A:8:MET:HE3	2.46	0.41
1:A:316:GLN:O	1:A:316:GLN:CG	2.36	0.41
1:A:163:ASP:OD1	1:A:163:ASP:N	2.52	0.41
1:A:124:GLU:HB2	2:A:416:HOH:O	2.21	0.41
1:A:196:MET:HB2	1:A:196:MET:HE3	1.79	0.41
1:A:315:GLN:CG	1:A:316:GLN:N	2.76	0.41
1:A:201:LEU:C	1:A:203:ALA:N	2.79	0.40
1:A:48:GLY:CA	1:A:104:ARG:HH12	2.35	0.40
1:A:135:THR:HB	1:A:136:PRO:CD	2.49	0.40
1:A:106:GLU:HA	1:A:110:THR:O	2.21	0.40
1:A:154:HIS:C	1:A:155:SER:OG	2.65	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	295/303 (97%)	267 (90%)	26 (9%)	2 (1%)	18	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PRO
1	A	315	GLN

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	260/260 (100%)	214 (82%)	46 (18%)	2	5

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	4	LEU
1	A	6	ILE
1	A	10	PRO
1	A	14	ILE
1	A	18	LYS
1	A	38	MET
1	A	55	ARG
1	A	60	LYS
1	A	62	ASN
1	A	70	VAL
1	A	73	GLN
1	A	77	LEU
1	A	96	ILE
1	A	108	LYS
1	A	115	LYS

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Mol	Chain	Res	Type
1	A	124	GLU
1	A	126	LEU
1	A	132	SER
1	A	133	ASP
1	A	134	LEU
1	A	148	LYS
1	A	155	SER
1	A	159	LEU
1	A	160	LYS
1	A	162	LEU
1	A	163	ASP
1	A	174	LYS
1	A	182	VAL
1	A	185	GLU
1	A	201	LEU
1	A	211	VAL
1	A	212	LEU
1	A	225	ARG
1	A	245	ARG
1	A	248	THR
1	A	253	LYS
1	A	258	ILE
1	A	263	LYS
1	A	275	ILE
1	A	278	ARG
1	A	281	GLU
1	A	286	SER
1	A	305	LEU
1	A	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	61	GLN
1	A	62	ASN
1	A	154	HIS
1	A	314	GLN

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](#)

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.