



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:26 AM UTC

PDB ID : 1GTM / pdb_00001gtm
Title : STRUCTURE OF GLUTAMATE DEHYDROGENASE
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Deposited on : 1996-08-22
Resolution : 2.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

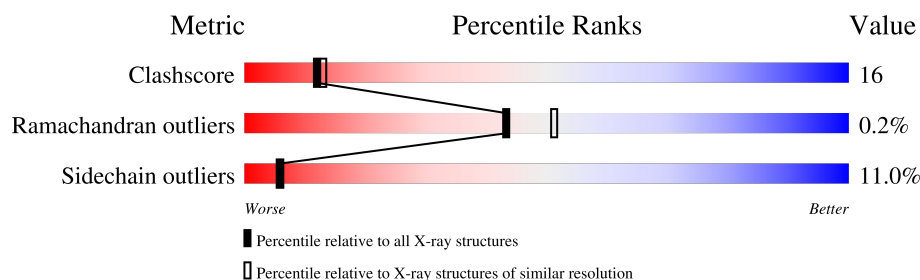
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	419	
1	B	419	
1	C	419	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	421	-	-	X	-
2	SO4	C	420	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10224 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 GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			
1	B	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			
1	C	417	Total	C	N	O	S	0	0	0
			3292	2107	554	618	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	GLN	conflict	UNP P80319
B	3	ALA	GLN	conflict	UNP P80319
C	3	ALA	GLN	conflict	UNP P80319

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

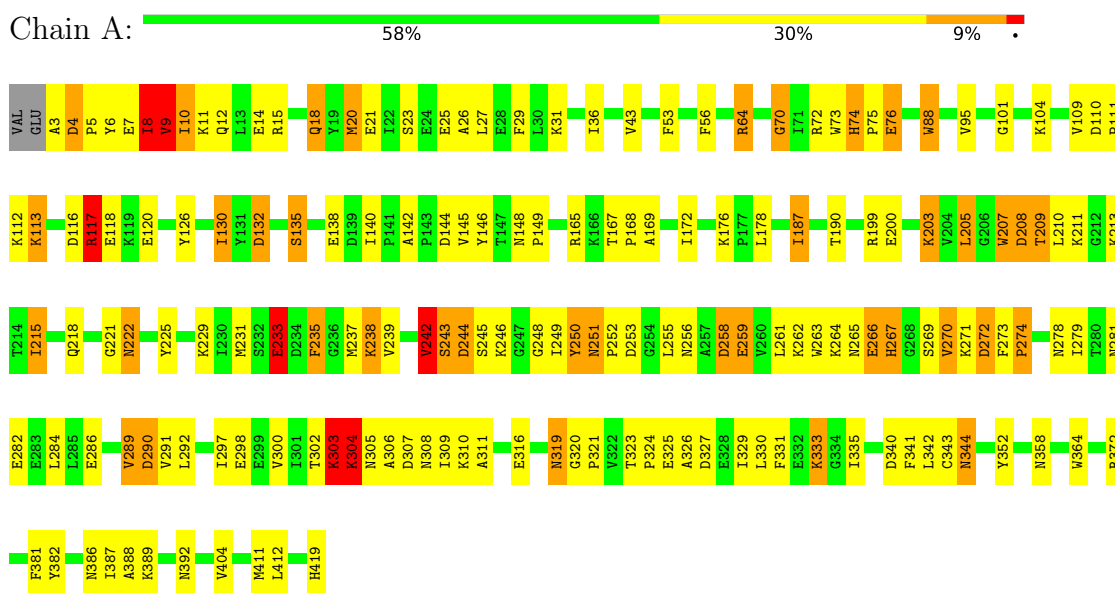
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	112	Total O 112 112	0	0
3	C	99	Total O 99 99	0	0

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: GLUTAMATE DEHYDROGENASE

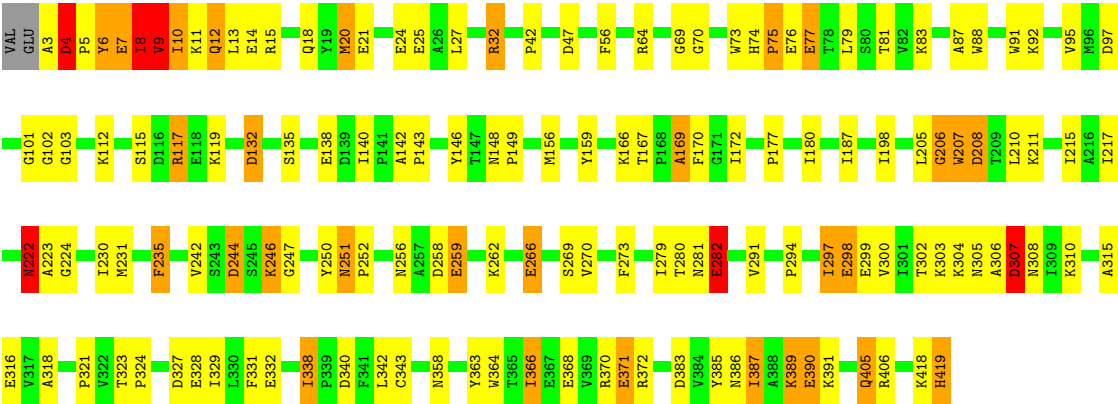


Chain C:

64%

27%

7%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.20Å 167.20Å 172.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	93.2 (10.00-2.20)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10224	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: SO4

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	1.08	0/3365	1.94	85/4560 (1.9%)
1	B	1.07	0/3365	1.92	75/4560 (1.6%)
1	C	1.07	1/3365 (0.0%)	1.93	82/4560 (1.8%)
All	All	1.07	1/10095 (0.0%)	1.93	242/13680 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	282	GLU	CD-OE2	5.16	1.35	1.25

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	HIS	CA-CB-CG	-12.76	101.04	113.80
1	A	251	ASN	CA-C-N	10.83	130.43	119.82
1	A	251	ASN	C-N-CA	10.83	130.43	119.82
1	B	386	ASN	CA-CB-CG	-10.11	102.49	112.60
1	B	208	ASP	CA-CB-CG	9.39	121.99	112.60
1	B	101	GLY	CA-C-N	-9.22	113.86	122.80
1	B	101	GLY	C-N-CA	-9.22	113.86	122.80
1	B	207	TRP	CA-C-N	9.20	133.15	120.63
1	B	207	TRP	C-N-CA	9.20	133.15	120.63
1	B	18	GLN	CB-CA-C	-9.16	93.08	110.67
1	C	251	ASN	CA-C-N	9.11	128.75	119.82
1	C	251	ASN	C-N-CA	9.11	128.75	119.82
1	C	9	VAL	N-CA-CB	-8.65	100.42	110.55
1	A	14	GLU	N-CA-C	8.61	120.67	111.28
1	A	340	ASP	CA-CB-CG	8.50	121.10	112.60
1	C	208	ASP	CA-CB-CG	8.39	120.99	112.60
1	C	97	ASP	CA-CB-CG	8.35	120.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	PHE	CA-CB-CG	-8.33	105.47	113.80
1	C	282	GLU	CB-CG-CD	8.33	126.76	112.60
1	A	9	VAL	N-CA-CB	-8.18	100.10	110.57
1	B	298	GLU	CB-CG-CD	-8.17	98.71	112.60
1	B	207	TRP	O-C-N	7.87	132.15	122.86
1	C	307	ASP	CA-CB-CG	-7.87	104.73	112.60
1	C	21	GLU	N-CA-CB	7.86	123.23	110.43
1	B	7	GLU	CA-C-N	-7.84	107.86	121.97
1	B	7	GLU	C-N-CA	-7.84	107.86	121.97
1	B	207	TRP	N-CA-CB	7.66	121.20	110.17
1	C	207	TRP	CA-C-N	7.63	130.82	120.44
1	C	207	TRP	C-N-CA	7.63	130.82	120.44
1	B	7	GLU	CB-CA-C	-7.62	98.13	110.79
1	B	332	GLU	CB-CA-C	-7.59	98.20	110.79
1	B	332	GLU	CB-CG-CD	-7.58	99.72	112.60
1	A	274	PRO	CB-CA-C	-7.49	102.40	111.46
1	A	64	ARG	NE-CZ-NH2	-7.44	112.50	119.20
1	A	253	ASP	CA-CB-CG	-7.43	105.17	112.60
1	A	290	ASP	CA-CB-CG	-7.37	105.23	112.60
1	B	266	GLU	CB-CG-CD	-7.36	100.08	112.60
1	A	233	GLU	CA-C-N	-7.31	109.00	122.09
1	A	233	GLU	C-N-CA	-7.31	109.00	122.09
1	B	307	ASP	CA-CB-CG	-7.28	105.32	112.60
1	B	64	ARG	NE-CZ-NH2	-7.25	112.68	119.20
1	B	74	HIS	CA-CB-CG	-7.25	106.56	113.80
1	C	282	GLU	CB-CA-C	7.17	122.86	110.68
1	C	170	PHE	CA-CB-CG	-7.15	106.65	113.80
1	B	372	ARG	CA-CB-CG	-7.14	99.82	114.10
1	A	344	ASN	CA-CB-CG	-7.13	105.47	112.60
1	A	165	ARG	NE-CZ-NH1	-7.07	114.43	121.50
1	A	331	PHE	CA-C-N	7.07	130.46	120.28
1	A	331	PHE	C-N-CA	7.07	130.46	120.28
1	A	8	ILE	N-CA-C	7.06	118.66	110.62
1	C	371	GLU	N-CA-CB	7.03	121.18	110.28
1	B	9	VAL	CA-C-N	-7.01	111.56	120.60
1	B	9	VAL	C-N-CA	-7.01	111.56	120.60
1	C	207	TRP	N-CA-CB	6.99	120.81	109.69
1	B	32	ARG	NE-CZ-NH1	6.97	128.47	121.50
1	B	177	PRO	N-CA-CB	6.95	109.39	103.35
1	A	319	ASN	CA-CB-CG	6.94	119.54	112.60
1	C	247	GLY	N-CA-C	6.91	119.17	111.85
1	C	187	ILE	N-CA-C	6.86	117.62	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	LEU	N-CA-C	-6.85	103.57	112.68
1	B	32	ARG	CD-NE-CZ	6.83	133.97	124.40
1	B	169	ALA	N-CA-C	6.81	119.54	111.71
1	A	272	ASP	CA-C-O	6.79	124.75	119.18
1	A	270	VAL	N-CA-C	-6.78	103.85	113.07
1	C	91	TRP	CA-C-O	6.64	127.46	120.42
1	C	338	ILE	CA-C-N	6.64	126.67	119.90
1	C	338	ILE	C-N-CA	6.64	126.67	119.90
1	A	110	ASP	CA-C-O	6.62	125.07	119.71
1	C	206	GLY	CA-C-N	-6.58	111.62	120.90
1	C	206	GLY	C-N-CA	-6.58	111.62	120.90
1	C	332	GLU	CA-CB-CG	-6.57	100.96	114.10
1	B	251	ASN	CA-C-N	6.56	126.19	119.56
1	B	251	ASN	C-N-CA	6.56	126.19	119.56
1	B	373	LEU	CA-C-O	6.56	127.50	120.55
1	A	207	TRP	N-CA-CB	6.55	120.11	109.69
1	A	250	TYR	N-CA-C	6.46	120.05	109.72
1	A	298	GLU	CB-CG-CD	-6.44	101.65	112.60
1	C	358	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	270	VAL	N-CA-C	-6.43	103.04	112.04
1	A	267	HIS	N-CA-C	6.41	121.17	113.23
1	B	278	ASN	CA-CB-CG	6.41	119.00	112.60
1	A	104	LYS	CA-C-N	-6.39	114.70	121.48
1	A	104	LYS	C-N-CA	-6.39	114.70	121.48
1	B	135	SER	CA-C-N	6.39	126.08	119.56
1	B	135	SER	C-N-CA	6.39	126.08	119.56
1	C	101	GLY	CA-C-N	-6.38	116.61	122.80
1	C	101	GLY	C-N-CA	-6.38	116.61	122.80
1	C	222	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	C	8	ILE	CA-C-O	6.32	127.84	121.27
1	A	14	GLU	CA-CB-CG	-6.27	101.56	114.10
1	B	234	ASP	N-CA-CB	6.27	119.73	110.33
1	B	234	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	102	GLY	CA-C-O	6.18	126.70	120.64
1	B	267	HIS	CA-CB-CG	-6.18	107.62	113.80
1	B	198	ILE	N-CA-C	-6.17	104.73	110.53
1	A	209	THR	N-CA-CB	6.13	122.28	111.49
1	C	6	TYR	N-CA-C	-6.12	104.52	111.07
1	A	342	LEU	N-CA-C	-6.09	104.58	112.68
1	A	382	TYR	CA-CB-CG	-6.09	102.93	113.90
1	C	391	LYS	CA-C-O	6.08	126.56	119.32
1	B	210	LEU	CA-C-O	6.06	125.81	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	LYS	N-CA-CB	6.04	118.76	110.01
1	A	36	ILE	CA-C-N	-6.03	115.25	123.14
1	A	36	ILE	C-N-CA	-6.03	115.25	123.14
1	C	266	GLU	CB-CG-CD	-6.02	102.36	112.60
1	A	190	THR	N-CA-C	6.01	117.50	111.07
1	B	287	LEU	CA-C-O	6.00	128.47	121.87
1	B	5	PRO	N-CA-C	-5.97	104.94	113.47
1	B	187	ILE	N-CA-C	5.96	116.70	110.62
1	C	370	ARG	CA-C-N	-5.96	111.25	120.31
1	C	370	ARG	C-N-CA	-5.96	111.25	120.31
1	B	309	ILE	CB-CA-C	5.95	120.20	111.33
1	B	327	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	307	ASP	CA-CB-CG	-5.90	106.70	112.60
1	C	4	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	140	ILE	N-CA-C	5.89	113.98	108.15
1	C	273	PHE	CA-CB-CG	-5.87	107.93	113.80
1	C	42	PRO	CB-CA-C	-5.86	104.26	111.11
1	C	24	GLU	O-C-N	5.86	128.33	122.12
1	C	235	PHE	CA-CB-CG	-5.85	107.95	113.80
1	C	132	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	21	GLU	CA-CB-CG	-5.80	102.51	114.10
1	A	258	ASP	N-CA-C	5.78	117.25	111.07
1	B	76	GLU	CB-CA-C	-5.78	102.16	111.28
1	C	281	ASN	CA-C-N	5.77	128.29	120.38
1	C	281	ASN	C-N-CA	5.77	128.29	120.38
1	A	251	ASN	O-C-N	5.76	127.94	121.32
1	A	130	ILE	N-CA-C	5.72	118.40	112.90
1	A	76	GLU	CB-CA-C	-5.72	101.81	111.02
1	B	390	GLU	CA-C-N	-5.71	113.12	122.54
1	B	390	GLU	C-N-CA	-5.71	113.12	122.54
1	C	383	ASP	N-CA-CB	5.71	118.28	110.01
1	A	297	ILE	CB-CA-C	-5.68	103.40	111.19
1	A	300	VAL	CB-CA-C	5.68	120.61	111.29
1	A	412	LEU	CB-CA-C	-5.68	101.92	110.90
1	C	270	VAL	N-CA-C	-5.66	104.11	112.04
1	A	70	GLY	N-CA-C	5.66	119.83	112.25
1	C	281	ASN	CA-C-O	5.65	126.75	120.82
1	A	74	HIS	CA-CB-CG	-5.64	108.16	113.80
1	C	244	ASP	CB-CA-C	5.63	121.62	110.42
1	A	291	VAL	N-CA-C	5.62	116.09	107.77
1	A	392	ASN	CA-C-N	-5.62	114.83	122.92
1	A	392	ASN	C-N-CA	-5.62	114.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	PHE	CA-CB-CG	-5.61	108.19	113.80
1	B	354	GLU	CA-C-N	5.59	128.08	120.54
1	B	354	GLU	C-N-CA	5.59	128.08	120.54
1	C	308	ASN	CA-CB-CG	-5.56	107.04	112.60
1	C	258	ASP	CA-C-N	-5.52	112.88	120.28
1	C	258	ASP	C-N-CA	-5.52	112.88	120.28
1	A	187	ILE	N-CA-C	5.51	116.25	110.62
1	B	165	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	B	53	PHE	CA-CB-CG	-5.49	108.31	113.80
1	B	352	TYR	CA-C-O	5.48	126.36	120.55
1	C	92	LYS	N-CA-CB	-5.47	102.06	110.16
1	C	386	ASN	N-CA-C	5.47	117.24	111.28
1	B	149	PRO	N-CA-CB	5.47	109.30	103.39
1	A	101	GLY	CA-C-N	-5.46	117.50	122.80
1	A	101	GLY	C-N-CA	-5.46	117.50	122.80
1	A	116	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	208	ASP	N-CA-C	-5.44	105.43	111.36
1	A	308	ASN	CA-C-N	-5.44	112.92	121.62
1	A	308	ASN	C-N-CA	-5.44	112.92	121.62
1	C	87	ALA	CA-C-O	5.44	126.32	120.55
1	A	113	LYS	CA-C-N	-5.44	114.11	122.87
1	A	113	LYS	C-N-CA	-5.44	114.11	122.87
1	C	64	ARG	NE-CZ-NH2	-5.44	114.31	119.20
1	C	307	ASP	N-CA-C	5.43	117.96	111.71
1	C	327	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	75	PRO	CA-C-N	-5.43	113.99	122.73
1	C	75	PRO	C-N-CA	-5.43	113.99	122.73
1	A	386	ASN	CA-CB-CG	-5.42	107.18	112.60
1	B	9	VAL	CA-C-O	5.42	126.51	120.71
1	B	297	ILE	CB-CA-C	-5.42	103.75	111.34
1	C	8	ILE	CB-CA-C	-5.42	104.94	111.88
1	C	169	ALA	N-CA-C	5.41	117.94	111.71
1	A	388	ALA	CA-C-N	5.41	127.80	120.44
1	A	388	ALA	C-N-CA	5.41	127.80	120.44
1	A	331	PHE	CA-CB-CG	-5.39	108.41	113.80
1	C	406	ARG	NE-CZ-NH1	5.38	126.89	121.50
1	A	244	ASP	N-CA-CB	5.38	120.29	111.31
1	A	26	ALA	CA-C-O	5.37	126.46	120.82
1	A	238	LYS	CA-C-N	-5.37	115.77	122.48
1	A	238	LYS	C-N-CA	-5.37	115.77	122.48
1	A	238	LYS	CB-CA-C	-5.36	101.40	110.19
1	C	370	ARG	CD-NE-CZ	-5.34	116.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	389	LYS	CB-CA-C	-5.34	102.74	110.96
1	A	135	SER	N-CA-CB	5.33	119.86	110.37
1	B	237	MET	CA-C-N	-5.33	115.68	122.77
1	B	237	MET	C-N-CA	-5.33	115.68	122.77
1	A	327	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	352	TYR	N-CA-CB	-5.30	102.32	110.12
1	B	189	ALA	N-CA-C	5.30	117.47	111.11
1	B	210	LEU	N-CA-C	-5.30	106.98	113.50
1	A	117	ARG	CB-CG-CD	5.30	123.48	111.30
1	B	74	HIS	ND1-CG-CD2	5.28	111.38	106.10
1	A	208	ASP	CB-CA-C	5.27	119.82	110.85
1	B	64	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	B	262	LYS	CA-CB-CG	-5.24	103.61	114.10
1	B	392	ASN	N-CA-C	-5.24	104.19	111.52
1	A	130	ILE	O-C-N	5.23	126.92	122.16
1	B	386	ASN	N-CA-C	5.22	116.97	111.28
1	A	18	GLN	CA-C-N	-5.22	114.46	122.60
1	A	18	GLN	C-N-CA	-5.22	114.46	122.60
1	B	414	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	C	42	PRO	N-CA-CB	5.21	107.69	103.36
1	C	177	PRO	N-CA-CB	5.21	108.18	103.33
1	A	74	HIS	CA-C-N	5.21	124.87	119.56
1	A	74	HIS	C-N-CA	5.21	124.87	119.56
1	B	298	GLU	O-C-N	5.19	128.76	122.94
1	C	230	ILE	N-CA-C	5.19	115.41	110.53
1	A	208	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	273	PHE	CA-C-O	5.16	124.60	119.75
1	A	242	VAL	N-CA-CB	5.16	122.57	112.00
1	A	20	MET	CG-SD-CE	-5.14	89.59	100.90
1	B	408	TYR	CA-C-N	-5.14	112.88	120.28
1	B	408	TYR	C-N-CA	-5.14	112.88	120.28
1	C	81	THR	N-CA-CB	-5.13	102.63	110.07
1	C	331	PHE	CA-CB-CG	-5.12	108.68	113.80
1	C	9	VAL	CA-C-N	-5.12	113.31	120.53
1	C	9	VAL	C-N-CA	-5.12	113.31	120.53
1	C	329	ILE	CB-CA-C	-5.11	105.43	111.97
1	B	323	THR	CA-C-O	5.10	126.59	120.88
1	A	72	ARG	CA-CB-CG	-5.09	103.91	114.10
1	B	405	GLN	N-CA-CB	-5.09	102.63	110.16
1	C	318	ALA	N-CA-C	-5.09	103.96	110.53
1	B	384	VAL	CA-C-N	5.09	127.10	120.28
1	B	384	VAL	C-N-CA	5.09	127.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ILE	CB-CA-C	-5.08	105.00	110.85
1	B	394	HIS	CA-CB-CG	-5.07	108.73	113.80
1	C	222	ASN	CA-CB-CG	-5.06	107.54	112.60
1	C	332	GLU	CB-CA-C	5.06	118.82	110.88
1	B	25	GLU	N-CA-CB	-5.05	102.42	109.94
1	C	332	GLU	N-CA-CB	5.05	117.33	110.01
1	C	302	THR	CB-CA-C	-5.04	101.81	114.11
1	C	419	HIS	ND1-CG-CD2	5.03	111.13	106.10
1	A	132	ASP	N-CA-C	5.03	118.51	112.38
1	C	21	GLU	CB-CA-C	5.02	118.04	109.75
1	C	224	GLY	CA-C-N	-5.02	113.92	120.44
1	C	224	GLY	C-N-CA	-5.02	113.92	120.44
1	A	303	LYS	N-CA-CB	-5.01	101.62	109.78
1	C	167	THR	N-CA-CB	-5.00	104.19	111.25
1	A	118	GLU	CG-CD-OE2	5.00	129.90	118.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3292	0	3290	115	0
1	B	3292	0	3290	95	0
1	C	3292	0	3290	102	0
2	A	10	0	0	3	0
2	B	10	0	0	0	0
2	C	10	0	0	3	0
3	A	107	0	0	0	0
3	B	112	0	0	0	0
3	C	99	0	0	0	0
All	All	10224	0	9870	310	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 16.

All (310) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ILE:CD1	1:B:8:ILE:C	2.03	1.31
1:B:8:ILE:CD1	1:B:9:VAL:N	1.99	1.25
1:B:8:ILE:C	1:B:8:ILE:HD13	1.55	1.24
1:B:8:ILE:HD12	1:B:9:VAL:N	1.52	1.23
1:A:25:GLU:OE1	1:A:419:HIS:HD2	1.28	1.16
1:A:3:ALA:O	1:A:5:PRO:HD2	1.52	1.07
1:B:3:ALA:O	1:B:7:GLU:N	1.93	1.00
1:C:4:ASP:O	1:C:7:GLU:HB3	1.62	0.99
1:A:256:ASN:ND2	1:A:259:GLU:H	1.61	0.98
1:C:10:ILE:HD13	1:C:10:ILE:H	1.30	0.94
1:A:323:THR:HB	1:A:324:PRO:HD2	1.51	0.93
1:A:25:GLU:OE1	1:A:419:HIS:CD2	2.21	0.93
1:C:3:ALA:O	1:C:4:ASP:C	2.11	0.92
1:B:8:ILE:HD12	1:B:9:VAL:H	1.34	0.92
1:B:12:GLN:HE21	1:B:12:GLN:HA	1.32	0.92
1:A:148:ASN:HB2	1:A:149:PRO:HD2	1.53	0.90
1:A:286:GLU:O	1:A:310:LYS:NZ	2.05	0.90
1:A:256:ASN:HD22	1:A:259:GLU:HB2	1.37	0.90
1:C:10:ILE:HD13	1:C:10:ILE:N	1.86	0.90
1:C:250:TYR:CZ	1:C:252:PRO:HG3	2.08	0.89
1:C:385:TYR:OH	1:C:389:LYS:HE3	1.73	0.89
1:B:117:ARG:HA	1:B:117:ARG:NE	1.89	0.88
1:B:258:ASP:O	1:B:262:LYS:HG3	1.73	0.87
1:C:8:ILE:HG22	1:C:9:VAL:N	1.88	0.87
1:C:4:ASP:HB3	1:C:5:PRO:HD3	1.57	0.86
1:B:323:THR:HB	1:B:324:PRO:HD2	1.59	0.84
1:C:5:PRO:O	1:C:8:ILE:HB	1.78	0.83
1:B:3:ALA:O	1:B:6:TYR:N	2.13	0.82
1:A:272:ASP:O	1:A:273:PHE:C	2.21	0.82
1:C:10:ILE:N	1:C:10:ILE:CD1	2.41	0.82
1:B:4:ASP:O	1:B:8:ILE:HG23	1.79	0.82
1:B:8:ILE:C	1:B:8:ILE:HD12	1.89	0.82
1:A:3:ALA:O	1:A:5:PRO:CD	2.27	0.81
1:A:326:ALA:O	1:A:330:LEU:HG	1.81	0.81
1:C:3:ALA:C	1:C:5:PRO:HD2	2.06	0.80
1:A:243:SER:OG	1:A:281:ASN:ND2	2.13	0.80
1:C:9:VAL:HG12	1:C:10:ILE:CD1	2.16	0.76
1:B:12:GLN:HA	1:B:12:GLN:NE2	2.00	0.76
1:C:117:ARG:HA	1:C:117:ARG:NE	2.00	0.76
1:C:148:ASN:HB2	1:C:149:PRO:HD2	1.66	0.76
1:B:245:SER:OG	1:B:246:LYS:HE3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:O	1:C:83:LYS:HG3	1.86	0.75
1:A:256:ASN:ND2	1:A:259:GLU:HB2	2.01	0.75
1:B:12:GLN:HE21	1:B:12:GLN:CA	1.98	0.75
1:A:256:ASN:HD22	1:A:259:GLU:H	1.31	0.75
1:B:8:ILE:HD13	1:B:9:VAL:N	1.77	0.74
1:C:25:GLU:OE2	1:C:419:HIS:ND1	2.19	0.73
1:B:148:ASN:HB2	1:B:149:PRO:HD2	1.71	0.73
1:C:3:ALA:O	1:C:5:PRO:N	2.21	0.73
1:A:4:ASP:HB3	1:A:5:PRO:HD3	1.70	0.73
1:A:329:ILE:O	1:A:333:LYS:HG3	1.89	0.73
1:A:229:LYS:O	1:A:233:GLU:HG3	1.89	0.73
1:C:117:ARG:HA	1:C:117:ARG:HE	1.53	0.72
1:C:368:GLU:O	1:C:372:ARG:HG3	1.89	0.72
1:A:221:GLY:HA3	2:A:421:SO4:O2	1.90	0.71
1:A:316:GLU:O	1:A:343:CYS:HB3	1.90	0.71
1:A:9:VAL:HG12	1:A:10:ILE:N	2.04	0.71
1:B:148:ASN:HB2	1:B:149:PRO:CD	2.20	0.71
1:C:305:ASN:O	1:C:306:ALA:C	2.34	0.70
1:A:6:TYR:O	1:A:10:ILE:HD12	1.92	0.69
1:C:148:ASN:HB2	1:C:149:PRO:CD	2.21	0.69
1:B:250:TYR:CE2	1:B:252:PRO:HG3	2.27	0.69
1:C:3:ALA:O	1:C:6:TYR:N	2.26	0.69
1:C:9:VAL:HG12	1:C:10:ILE:HD13	1.75	0.68
1:A:244:ASP:OD2	1:A:270:VAL:HG22	1.93	0.68
1:A:323:THR:HB	1:A:324:PRO:CD	2.22	0.67
1:A:148:ASN:HB2	1:A:149:PRO:CD	2.22	0.67
1:A:271:LYS:HG3	1:A:278:ASN:HD21	1.59	0.67
1:B:74:HIS:HE1	1:B:76:GLU:HB2	1.60	0.67
1:B:74:HIS:CE1	1:B:76:GLU:HB2	2.30	0.67
1:C:3:ALA:O	1:C:5:PRO:HD2	1.95	0.67
1:C:280:THR:HB	1:C:282:GLU:HG2	1.77	0.67
1:C:3:ALA:O	1:C:5:PRO:CD	2.42	0.66
1:B:74:HIS:CD2	1:B:75:PRO:HD2	2.31	0.66
1:C:3:ALA:HB3	1:C:6:TYR:HB3	1.76	0.65
1:B:117:ARG:HA	1:B:117:ARG:HE	1.61	0.65
1:C:244:ASP:OD2	1:C:269:SER:HA	1.96	0.65
1:A:213:LYS:HB3	1:A:290:ASP:OD2	1.97	0.65
1:C:3:ALA:CB	1:C:6:TYR:HB3	2.27	0.65
1:A:263:TRP:CZ3	1:A:274:PRO:HD3	2.31	0.65
1:A:282:GLU:O	1:A:286:GLU:HG3	1.96	0.64
1:A:258:ASP:O	1:A:261:LEU:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:TYR:CZ	1:C:389:LYS:HE3	2.33	0.64
1:A:88:TRP:CZ3	1:A:341:PHE:HB3	2.34	0.63
1:A:243:SER:HA	1:A:248:GLY:HA2	1.82	0.62
1:C:206:GLY:O	1:C:207:TRP:C	2.40	0.62
1:C:223:ALA:N	2:C:420:SO4:O3	2.28	0.62
1:A:244:ASP:CG	1:A:270:VAL:HG22	2.25	0.62
1:B:8:ILE:HD13	1:B:8:ILE:O	1.97	0.61
1:C:6:TYR:O	1:C:9:VAL:HB	2.00	0.61
1:B:266:GLU:HB2	1:B:267:HIS:ND1	2.14	0.61
1:C:4:ASP:HB3	1:C:5:PRO:CD	2.27	0.61
1:A:289:VAL:O	1:A:311:ALA:HA	2.00	0.61
1:A:305:ASN:O	1:A:309:ILE:HD12	2.01	0.60
1:C:297:ILE:HD12	1:C:298:GLU:O	2.01	0.60
1:B:4:ASP:HB3	1:B:5:PRO:HD3	1.83	0.60
1:A:117:ARG:HA	1:A:117:ARG:NE	2.17	0.60
1:C:316:GLU:HB2	1:C:338:ILE:O	2.01	0.60
1:C:115:SER:O	1:C:119:LYS:HG3	2.02	0.59
1:B:302:THR:O	1:B:306:ALA:HB2	2.01	0.59
1:A:251:ASN:C	1:A:251:ASN:OD1	2.44	0.59
1:B:4:ASP:N	1:B:5:PRO:HD2	2.18	0.59
1:A:4:ASP:O	1:A:8:ILE:CD1	2.51	0.59
1:B:3:ALA:O	1:B:6:TYR:CA	2.51	0.59
1:B:207:TRP:CD1	1:B:207:TRP:N	2.69	0.58
1:C:8:ILE:O	1:C:11:LYS:HB2	2.04	0.58
1:C:207:TRP:CD1	1:C:207:TRP:N	2.71	0.58
1:A:74:HIS:HE1	1:A:76:GLU:CG	2.16	0.58
1:B:8:ILE:HD11	1:B:9:VAL:HG23	1.84	0.58
1:B:16:ALA:O	1:B:20:MET:HG2	2.03	0.58
1:A:9:VAL:CG1	1:A:10:ILE:N	2.66	0.58
1:C:74:HIS:CG	1:C:75:PRO:HD2	2.38	0.58
1:C:74:HIS:CE1	1:C:76:GLU:H	2.21	0.58
1:A:176:LYS:HZ1	1:A:358:ASN:HD21	1.53	0.57
1:A:311:ALA:O	1:A:335:ILE:HG12	2.05	0.57
1:B:6:TYR:O	1:B:9:VAL:HB	2.05	0.57
1:B:9:VAL:HG12	1:B:10:ILE:HD12	1.87	0.57
1:A:256:ASN:HD21	1:A:259:GLU:H	1.49	0.57
1:C:9:VAL:O	1:C:10:ILE:C	2.47	0.56
1:A:74:HIS:CG	1:A:75:PRO:HD2	2.40	0.56
1:B:297:ILE:HD13	1:B:297:ILE:H	1.69	0.56
1:B:10:ILE:CD1	1:B:10:ILE:N	2.69	0.56
1:A:200:GLU:OE2	1:A:203:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ASP:O	1:C:7:GLU:CB	2.46	0.55
1:A:256:ASN:HD22	1:A:259:GLU:N	2.04	0.55
1:C:250:TYR:CE2	1:C:252:PRO:HG3	2.42	0.55
1:B:5:PRO:O	1:B:8:ILE:CD1	2.55	0.55
1:C:169:ALA:O	1:C:172:ILE:HG22	2.07	0.55
1:B:323:THR:HB	1:B:324:PRO:CD	2.35	0.54
1:C:73:TRP:O	1:C:146:TYR:HD2	1.90	0.54
1:B:25:GLU:OE2	1:B:418:LYS:N	2.37	0.54
1:C:256:ASN:HB3	1:C:259:GLU:CD	2.33	0.54
1:B:9:VAL:O	1:B:10:ILE:C	2.45	0.53
1:B:280:THR:OG1	1:B:283:GLU:HG3	2.08	0.53
1:C:6:TYR:O	1:C:10:ILE:HD13	2.09	0.53
1:A:207:TRP:N	1:A:207:TRP:CD1	2.77	0.52
1:A:271:LYS:HG3	1:A:278:ASN:ND2	2.23	0.52
1:A:256:ASN:HD22	1:A:259:GLU:CB	2.17	0.52
1:A:305:ASN:O	1:A:309:ILE:CD1	2.57	0.52
1:A:344:ASN:OD1	1:A:344:ASN:C	2.51	0.52
1:A:209:THR:OG1	1:A:210:LEU:N	2.40	0.52
1:A:23:SER:OG	1:A:419:HIS:OXT	2.18	0.52
1:B:323:THR:CB	1:B:324:PRO:CD	2.88	0.52
1:C:323:THR:HB	1:C:324:PRO:HD2	1.90	0.52
1:A:4:ASP:O	1:A:8:ILE:HD13	2.10	0.52
1:A:4:ASP:O	1:A:8:ILE:HD12	2.10	0.51
1:A:323:THR:CB	1:A:324:PRO:CD	2.80	0.51
1:B:3:ALA:O	1:B:6:TYR:C	2.53	0.51
1:B:7:GLU:O	1:B:8:ILE:C	2.49	0.51
1:B:10:ILE:HD13	1:B:10:ILE:H	1.76	0.51
1:C:20:MET:HE3	1:C:405:GLN:HG3	1.93	0.51
1:C:256:ASN:CG	1:C:259:GLU:HG3	2.35	0.51
1:B:109:VAL:O	1:B:111:PRO:HD3	2.11	0.51
1:C:215:ILE:HA	1:C:291:VAL:O	2.10	0.51
1:A:109:VAL:O	1:A:111:PRO:HD3	2.10	0.50
1:A:302:THR:OG1	1:A:304:LYS:HG3	2.11	0.50
1:C:246:LYS:HG3	1:C:269:SER:HB2	1.93	0.50
1:A:221:GLY:CA	2:A:421:SO4:O2	2.59	0.50
1:A:251:ASN:HB3	1:A:255:LEU:HD21	1.92	0.50
1:A:221:GLY:O	1:A:225:TYR:HB3	2.11	0.50
1:B:12:GLN:NE2	1:B:12:GLN:CA	2.67	0.50
1:B:215:ILE:HA	1:B:291:VAL:O	2.12	0.50
1:B:8:ILE:HD13	1:B:9:VAL:CA	2.40	0.50
1:C:3:ALA:C	1:C:5:PRO:CD	2.82	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLY:N	1:A:321:PRO:CD	2.75	0.49
1:B:8:ILE:CD1	1:B:9:VAL:CA	2.87	0.49
1:C:256:ASN:C	1:C:256:ASN:OD1	2.54	0.49
1:A:218:GLN:HG3	1:A:281:ASN:HD22	1.76	0.49
1:B:364:TRP:N	1:B:364:TRP:CD1	2.80	0.49
1:A:117:ARG:HA	1:A:117:ARG:HE	1.77	0.49
1:B:213:LYS:HB2	1:B:237:MET:HE3	1.94	0.49
1:A:176:LYS:NZ	1:A:358:ASN:HD21	2.10	0.49
1:B:256:ASN:O	1:B:260:VAL:HG23	2.12	0.49
1:B:262:LYS:O	1:B:266:GLU:HG3	2.13	0.49
1:C:251:ASN:C	1:C:251:ASN:OD1	2.55	0.49
1:C:142:ALA:HB1	1:C:143:PRO:HD2	1.95	0.49
1:A:15:ARG:O	1:A:18:GLN:N	2.36	0.49
1:C:77:GLU:OE1	1:C:77:GLU:HA	2.13	0.48
1:A:74:HIS:CD2	1:A:75:PRO:HD2	2.48	0.48
1:B:110:ASP:OD1	1:B:112:LYS:HG3	2.13	0.48
1:B:4:ASP:N	1:B:5:PRO:CD	2.77	0.47
1:B:5:PRO:O	1:B:8:ILE:HG13	2.14	0.47
1:B:3:ALA:O	1:B:4:ASP:C	2.57	0.47
1:A:306:ALA:HA	1:A:309:ILE:HD13	1.95	0.47
1:B:388:ALA:O	1:B:392:ASN:N	2.47	0.47
1:C:198:ILE:HG21	1:C:231:MET:HE2	1.96	0.47
1:C:390:GLU:O	1:C:390:GLU:HG2	2.14	0.47
1:A:222:ASN:N	2:A:421:SO4:O2	2.47	0.47
1:C:12:GLN:HG2	1:C:13:LEU:N	2.29	0.47
1:B:210:LEU:HA	1:B:213:LYS:HG3	1.97	0.47
1:B:267:HIS:ND1	1:B:267:HIS:N	2.63	0.47
1:A:167:THR:OG1	1:A:168:PRO:HD2	2.15	0.47
1:A:250:TYR:CE2	1:A:252:PRO:HG3	2.49	0.47
1:B:5:PRO:O	1:B:8:ILE:HD12	2.14	0.47
1:B:205:LEU:HD12	1:B:205:LEU:HA	1.60	0.47
1:C:70:GLY:HA2	1:C:142:ALA:O	2.14	0.47
1:C:305:ASN:C	1:C:307:ASP:N	2.68	0.47
1:A:263:TRP:CH2	1:A:274:PRO:HD3	2.50	0.47
1:A:126:TYR:O	1:A:130:ILE:HG12	2.15	0.47
1:A:251:ASN:HB3	1:A:255:LEU:CD2	2.45	0.47
1:B:72:ARG:NH2	1:B:77:GLU:OE1	2.45	0.47
1:C:222:ASN:N	2:C:420:SO4:O3	2.48	0.47
1:B:250:TYR:CZ	1:B:252:PRO:HG3	2.49	0.46
1:A:271:LYS:O	1:A:272:ASP:HB2	2.14	0.46
1:B:74:HIS:CE1	1:B:76:GLU:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:TYR:OH	1:C:252:PRO:HG3	2.13	0.46
1:B:117:ARG:NH2	1:B:120:GLU:OE1	2.48	0.46
1:B:4:ASP:O	1:B:7:GLU:HB2	2.15	0.46
1:C:69:GLY:HA3	1:C:103:GLY:O	2.16	0.46
1:C:305:ASN:O	1:C:307:ASP:N	2.49	0.46
1:A:88:TRP:HZ3	1:A:341:PHE:HB3	1.79	0.46
1:A:144:ASP:O	1:A:145:VAL:C	2.56	0.46
1:A:250:TYR:O	1:A:251:ASN:HB2	2.16	0.46
1:A:309:ILE:HD12	1:A:309:ILE:N	2.31	0.46
1:B:166:LYS:NZ	1:C:138:GLU:OE1	2.40	0.46
1:B:297:ILE:HD13	1:B:297:ILE:N	2.30	0.46
1:A:20:MET:HE1	1:A:404:VAL:HB	1.98	0.46
1:A:169:ALA:O	1:A:172:ILE:HG22	2.16	0.46
1:C:10:ILE:HG22	1:C:14:GLU:OE2	2.16	0.46
1:B:309:ILE:HD12	1:B:309:ILE:N	2.31	0.46
1:C:231:MET:O	1:C:235:PHE:HB2	2.16	0.46
1:A:29:PHE:CD1	1:A:411:MET:HE3	2.51	0.45
1:A:364:TRP:N	1:A:364:TRP:CD1	2.80	0.45
1:C:9:VAL:HG12	1:C:10:ILE:HD12	1.96	0.45
1:C:74:HIS:ND1	1:C:76:GLU:N	2.56	0.45
1:B:10:ILE:CD1	1:B:10:ILE:H	2.29	0.45
1:A:251:ASN:HA	1:A:252:PRO:HD2	1.43	0.45
1:B:201:ALA:HB1	1:B:336:LEU:HD23	1.98	0.45
1:A:262:LYS:O	1:A:265:ASN:HB2	2.16	0.45
1:C:298:GLU:O	1:C:299:GLU:HB2	2.17	0.45
1:B:251:ASN:HA	1:B:252:PRO:HD3	1.55	0.45
1:C:222:ASN:CB	2:C:420:SO4:O3	2.65	0.45
1:A:74:HIS:HE1	1:A:76:GLU:HG3	1.82	0.45
1:A:74:HIS:CE1	1:A:76:GLU:CG	2.97	0.44
1:B:325:GLU:CD	1:B:325:GLU:H	2.24	0.44
1:C:363:TYR:CD1	1:C:363:TYR:N	2.85	0.44
1:A:43:VAL:HB	1:A:53:PHE:HE1	1.81	0.44
1:B:272:ASP:O	1:B:273:PHE:C	2.58	0.44
1:B:262:LYS:HG3	1:B:262:LYS:H	1.31	0.44
1:A:73:TRP:O	1:A:146:TYR:HD2	1.99	0.44
1:A:303:LYS:HE2	1:A:303:LYS:HB3	1.58	0.44
1:B:115:SER:O	1:B:119:LYS:N	2.46	0.44
1:A:290:ASP:N	1:A:290:ASP:OD1	2.48	0.44
1:A:319:ASN:C	1:A:321:PRO:HD3	2.43	0.44
1:B:47:ASP:C	1:B:47:ASP:OD1	2.61	0.44
1:B:70:GLY:HA2	1:B:142:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:O	1:C:18:GLN:HG2	2.18	0.43
1:C:32:ARG:NH1	1:C:32:ARG:HG3	2.33	0.43
1:A:266:GLU:HB3	1:A:267:HIS:CE1	2.53	0.43
1:B:280:THR:HG23	1:B:283:GLU:OE1	2.18	0.43
1:C:298:GLU:HA	1:C:321:PRO:HA	1.99	0.43
1:A:8:ILE:O	1:A:11:LYS:HB2	2.18	0.43
1:C:366:ILE:O	1:C:366:ILE:HG13	2.17	0.43
1:A:387:ILE:HD12	1:A:387:ILE:HG23	1.65	0.43
1:B:8:ILE:HD12	1:B:8:ILE:N	2.31	0.43
1:A:244:ASP:OD2	1:A:264:LYS:HE2	2.18	0.43
1:A:302:THR:O	1:A:306:ALA:N	2.48	0.43
1:A:3:ALA:O	1:A:5:PRO:N	2.51	0.43
1:B:401:VAL:O	1:B:405:GLN:HB2	2.19	0.43
1:A:205:LEU:HA	1:A:205:LEU:HD12	1.63	0.43
1:B:27:LEU:HA	1:B:27:LEU:HD23	1.76	0.43
1:B:266:GLU:HB2	1:B:267:HIS:CE1	2.54	0.43
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.48	0.43
1:A:199:ARG:HA	1:A:210:LEU:HD11	1.99	0.43
1:C:47:ASP:C	1:C:47:ASP:OD1	2.62	0.43
1:C:280:THR:CB	1:C:282:GLU:HG2	2.48	0.42
1:C:387:ILE:HD12	1:C:387:ILE:HG21	1.62	0.42
1:B:3:ALA:C	1:B:5:PRO:HD2	2.44	0.42
1:A:231:MET:O	1:A:235:PHE:HB2	2.20	0.42
1:A:284:LEU:C	1:A:284:LEU:HD23	2.45	0.42
1:C:244:ASP:OD1	1:C:244:ASP:C	2.62	0.42
1:C:297:ILE:HD12	1:C:300:VAL:HG13	2.02	0.42
1:A:242:VAL:O	1:A:248:GLY:HA2	2.20	0.42
1:B:142:ALA:HB1	1:B:143:PRO:HD2	2.01	0.42
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.77	0.42
1:C:3:ALA:HB1	1:C:6:TYR:CB	2.50	0.42
1:A:248:GLY:C	1:A:249:ILE:HG23	2.45	0.42
1:B:328:GLU:O	1:B:332:GLU:HG2	2.20	0.41
1:C:6:TYR:O	1:C:7:GLU:C	2.62	0.41
1:C:25:GLU:OE1	1:C:418:LYS:N	2.51	0.41
1:A:70:GLY:HA2	1:A:142:ALA:O	2.19	0.41
1:C:159:TYR:CG	1:C:172:ILE:HG12	2.56	0.41
1:C:294:PRO:HD2	1:C:315:ALA:O	2.20	0.41
1:A:305:ASN:O	1:A:306:ALA:C	2.64	0.41
1:B:34:GLN:OE1	1:B:61:ASN:HA	2.21	0.41
1:C:217:ILE:O	1:C:242:VAL:HA	2.21	0.41
1:C:364:TRP:N	1:C:364:TRP:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:MET:CE	1:C:180:ILE:HD12	2.50	0.41
1:A:138:GLU:OE1	1:C:166:LYS:NZ	2.50	0.41
1:A:215:ILE:HG22	1:A:237:MET:HE2	2.03	0.41
1:A:239:VAL:O	1:A:255:LEU:HG	2.21	0.41
1:B:20:MET:HE3	1:B:405:GLN:HG3	2.03	0.41
1:B:246:LYS:HG3	1:B:269:SER:HB2	2.03	0.41
1:B:256:ASN:OD1	1:B:256:ASN:C	2.63	0.41
1:C:279:ILE:HG21	1:C:279:ILE:HD13	1.77	0.41
1:A:29:PHE:HB3	1:A:411:MET:HE1	2.03	0.41
1:C:11:LYS:O	1:C:12:GLN:C	2.63	0.41
1:A:4:ASP:HB3	1:A:5:PRO:CD	2.44	0.40
1:A:148:ASN:CB	1:A:149:PRO:CD	2.88	0.40
1:C:256:ASN:OD1	1:C:259:GLU:HG3	2.21	0.40
1:C:387:ILE:HD13	1:C:387:ILE:HG23	1.75	0.40
1:A:27:LEU:O	1:A:31:LYS:HG3	2.22	0.40
1:A:269:SER:HB3	1:A:271:LYS:HB3	2.03	0.40
1:A:117:ARG:HH21	1:A:120:GLU:HB2	1.86	0.40
1:B:15:ARG:O	1:B:16:ALA:C	2.64	0.40
1:C:32:ARG:HG3	1:C:32:ARG:HH11	1.86	0.40
1:C:338:ILE:HG22	1:C:343:CYS:HB2	2.03	0.40
1:A:244:ASP:C	1:A:244:ASP:OD1	2.64	0.40
1:B:173:ILE:HD13	1:B:173:ILE:HG21	1.80	0.40
1:C:316:GLU:O	1:C:340:ASP:HA	2.22	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	415/419 (99%)	393 (95%)	20 (5%)	2 (0%)	24 27
1	B	415/419 (99%)	401 (97%)	14 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	415/419 (99%)	396 (95%)	18 (4%)	1 (0%)	43	51
All	All	1245/1257 (99%)	1190 (96%)	52 (4%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	C	4	ASP
1	A	304	LYS

5.3.2 Protein sidechains [i](#)

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	343/345 (99%)	303 (88%)	40 (12%)	5	5
1	B	343/345 (99%)	307 (90%)	36 (10%)	6	6
1	C	343/345 (99%)	306 (89%)	37 (11%)	6	6
All	All	1029/1035 (99%)	916 (89%)	113 (11%)	6	6

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	ILE
1	A	9	VAL
1	A	10	ILE
1	A	12	GLN
1	A	56	PHE
1	A	64	ARG
1	A	88	TRP
1	A	95	VAL
1	A	112	LYS
1	A	113	LYS
1	A	117	ARG

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Mol	Chain	Res	Type
1	A	132	ASP
1	A	135	SER
1	A	140	ILE
1	A	178	LEU
1	A	187	ILE
1	A	203	LYS
1	A	205	LEU
1	A	208	ASP
1	A	211	LYS
1	A	215	ILE
1	A	222	ASN
1	A	233	GLU
1	A	238	LYS
1	A	242	VAL
1	A	243	SER
1	A	245	SER
1	A	246	LYS
1	A	259	GLU
1	A	266	GLU
1	A	279	ILE
1	A	289	VAL
1	A	292	LEU
1	A	303	LYS
1	A	304	LYS
1	A	325	GLU
1	A	333	LYS
1	A	372	ARG
1	A	389	LYS
1	B	8	ILE
1	B	9	VAL
1	B	10	ILE
1	B	12	GLN
1	B	15	ARG
1	B	21	GLU
1	B	32	ARG
1	B	64	ARG
1	B	80	SER
1	B	88	TRP
1	B	95	VAL
1	B	112	LYS
1	B	113	LYS
1	B	117	ARG

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Mol	Chain	Res	Type
1	B	132	ASP
1	B	135	SER
1	B	187	ILE
1	B	205	LEU
1	B	208	ASP
1	B	222	ASN
1	B	231	MET
1	B	246	LYS
1	B	256	ASN
1	B	262	LYS
1	B	264	LYS
1	B	288	GLU
1	B	297	ILE
1	B	298	GLU
1	B	304	LYS
1	B	307	ASP
1	B	312	LYS
1	B	328	GLU
1	B	332	GLU
1	B	371	GLU
1	B	379	LYS
1	B	389	LYS
1	C	7	GLU
1	C	8	ILE
1	C	9	VAL
1	C	10	ILE
1	C	12	GLN
1	C	20	MET
1	C	27	LEU
1	C	32	ARG
1	C	56	PHE
1	C	77	GLU
1	C	88	TRP
1	C	95	VAL
1	C	112	LYS
1	C	117	ARG
1	C	132	ASP
1	C	135	SER
1	C	205	LEU
1	C	208	ASP
1	C	211	LYS
1	C	222	ASN

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Mol	Chain	Res	Type
1	C	246	LYS
1	C	259	GLU
1	C	262	LYS
1	C	266	GLU
1	C	282	GLU
1	C	297	ILE
1	C	298	GLU
1	C	303	LYS
1	C	304	LYS
1	C	307	ASP
1	C	310	LYS
1	C	328	GLU
1	C	366	ILE
1	C	371	GLU
1	C	387	ILE
1	C	390	GLU
1	C	405	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	256	ASN
1	A	265	ASN
1	A	278	ASN
1	A	281	ASN
1	A	358	ASN
1	A	386	ASN
1	A	419	HIS
1	B	12	GLN
1	B	18	GLN
1	B	222	ASN
1	B	265	ASN
1	B	308	ASN
1	B	386	ASN
1	C	18	GLN
1	C	222	ASN
1	C	265	ASN
1	C	308	ASN
1	C	386	ASN
1	C	392	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	420	-	4,4,4	0.71	0	6,6,6	0.26	0
2	SO4	C	421	-	4,4,4	0.87	0	6,6,6	0.24	0
2	SO4	A	421	-	4,4,4	1.13	0	6,6,6	0.15	0
2	SO4	C	420	-	4,4,4	0.64	0	6,6,6	0.33	0
2	SO4	B	420	-	4,4,4	0.62	0	6,6,6	0.55	0
2	SO4	B	421	-	4,4,4	0.55	0	6,6,6	0.44	0

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.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	421	SO4	3	0
2	C	420	SO4	3	0

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.