



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:12 PM UTC

PDB ID : 4L7Q / pdb_00004l7q
Title : Crystal structure of gamma glutamyl hydrolase (wild-type) from zebrafish
Authors : Chuankhayan, P.; Kao, T.-T.; Chen, C.-J.; Fu, T.-F.
Deposited on : 2013-06-14
Resolution : 2.10 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

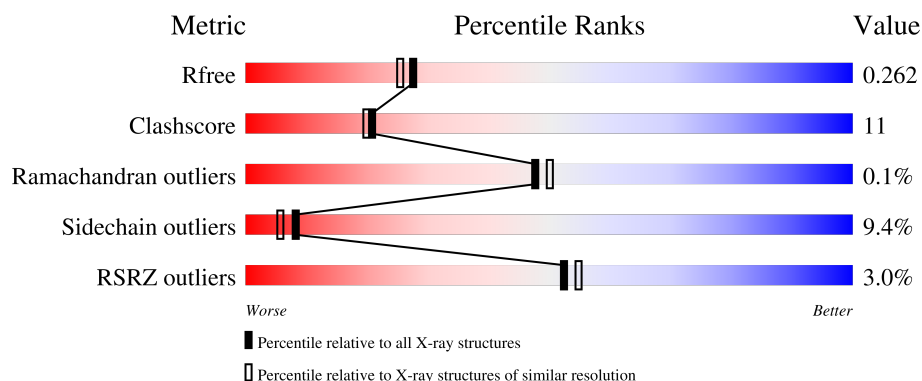
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	312	3% 67% 21% 8%
1	B	312	2% 68% 19% 8%
1	C	312	3% 71% 16% 8%
1	D	312	3% 68% 20% 8%
1	E	312	4% 65% 23% 8%

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Mol	Chain	Length	Quality of chain
1	F	312	2% 67% 21% • • 8%

2 Entry composition [i](#)

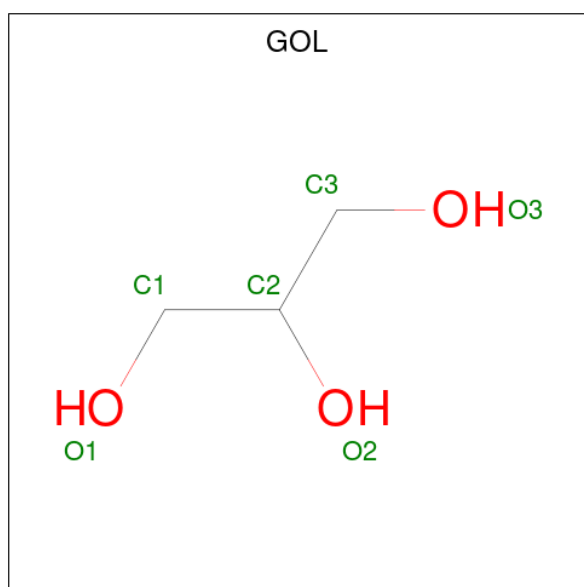
There are 3 unique types of molecules in this entry. The entry contains 14641 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gamma-glutamyl hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	287	Total	C	N	O	S	0	0	0
			2309	1492	370	442	5			
1	D	287	Total	C	N	O	S	0	0	0
			2309	1492	370	442	5			
1	A	287	Total	C	N	O	S	0	0	0
			2309	1492	370	442	5			
1	B	287	Total	C	N	O	S	0	0	0
			2309	1492	370	442	5			
1	E	287	Total	C	N	O	S	0	0	0
			2309	1492	370	442	5			
1	F	287	Total	C	N	O	S	0	0	0
			2309	1492	370	442	5			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

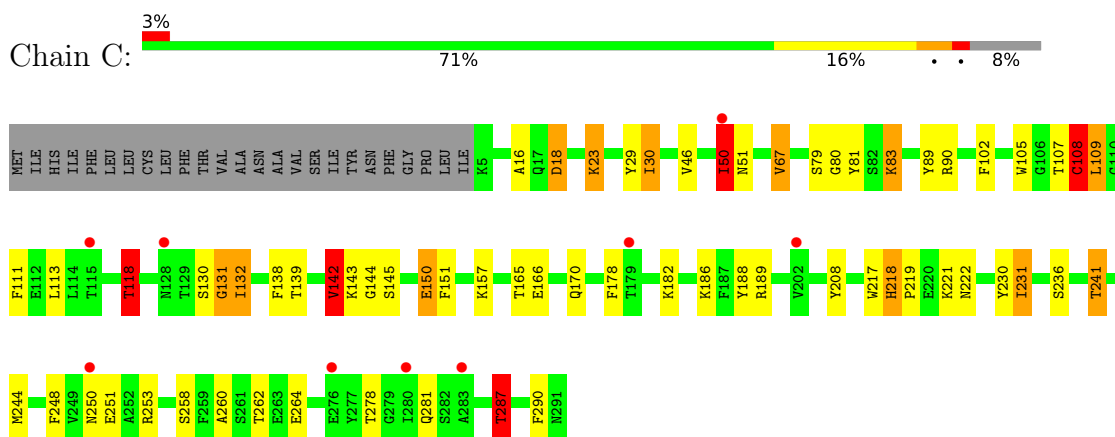
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	174	Total O 174 174	0	0
3	D	129	Total O 129 129	0	0
3	A	125	Total O 125 125	0	0
3	B	125	Total O 125 125	0	0
3	E	93	Total O 93 93	0	0
3	F	105	Total O 105 105	0	0

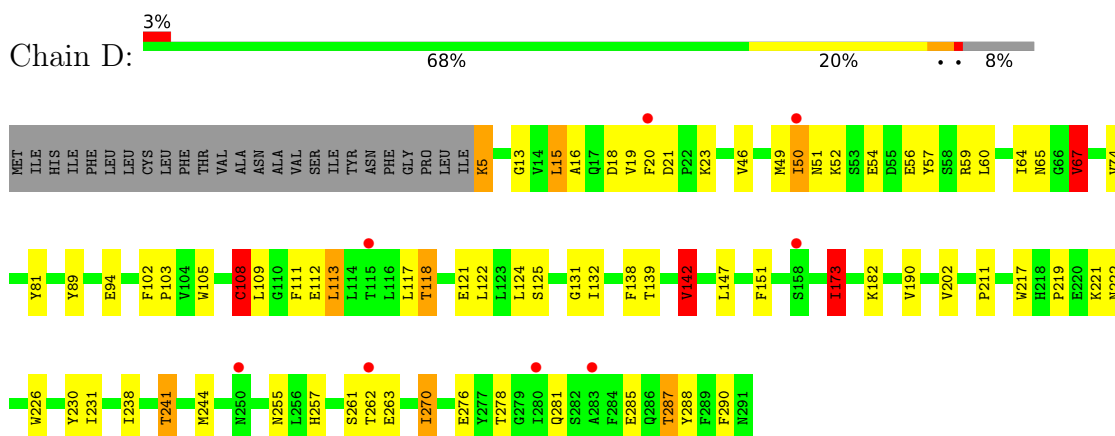
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

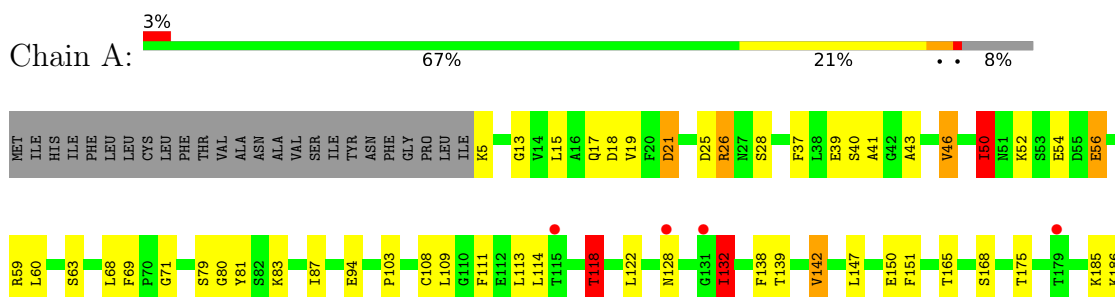
- Molecule 1: Gamma-glutamyl hydrolase



- Molecule 1: Gamma-glutamyl hydrolase

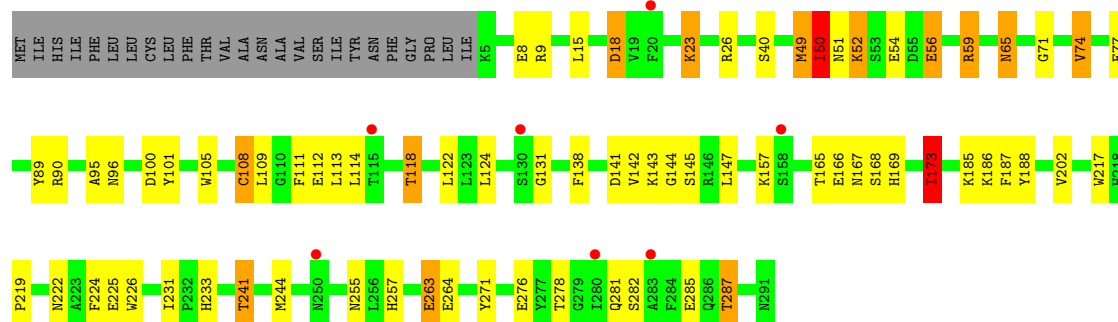


- Molecule 1: Gamma-glutamyl hydrolase

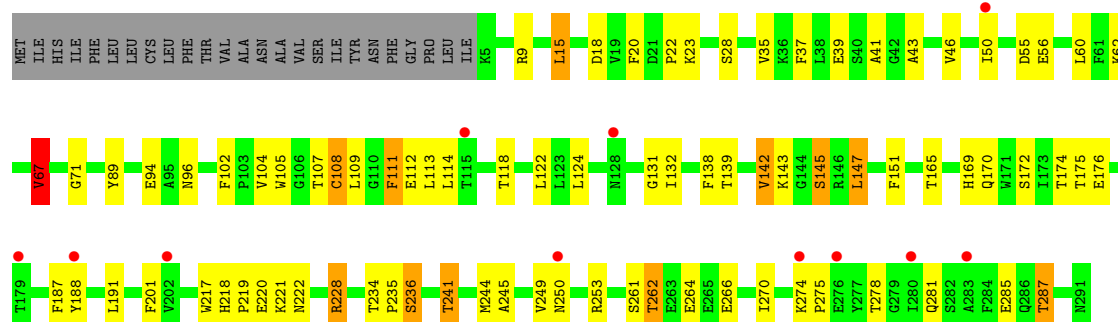




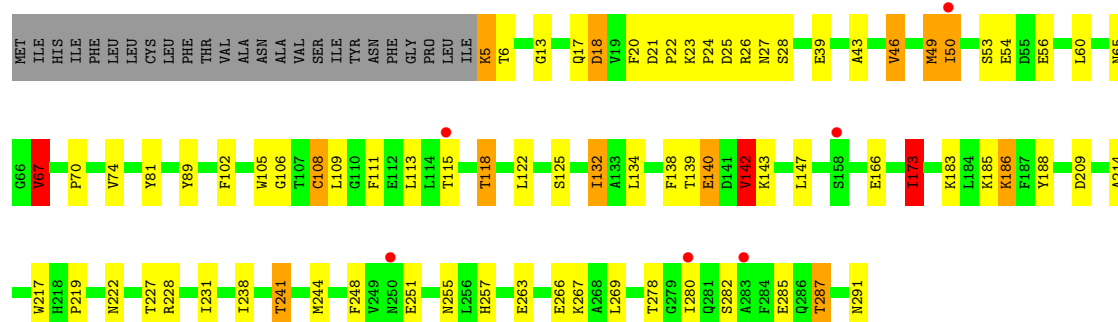
• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.61Å 62.05Å 123.94Å 90.00° 95.41° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-2.10) 97.1 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.263 0.201 , 0.262	Depositor DCC
R_{free} test set	6047 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14641	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.34	7/2374 (0.3%)	1.22	13/3221 (0.4%)
1	B	1.31	8/2374 (0.3%)	1.31	16/3221 (0.5%)
1	C	1.43	11/2374 (0.5%)	1.35	20/3221 (0.6%)
1	D	1.26	5/2374 (0.2%)	1.25	16/3221 (0.5%)
1	E	1.14	1/2374 (0.0%)	1.23	12/3221 (0.4%)
1	F	1.19	1/2374 (0.0%)	1.23	9/3221 (0.3%)
All	All	1.28	33/14244 (0.2%)	1.27	86/19326 (0.4%)

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
1	B	0	1
1	C	0	1
1	E	0	1
All	All	0	4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	ARG	C-N	18.83	1.54	1.34
1	C	131	GLY	C-N	-9.68	1.21	1.33
1	A	132	ILE	C-N	9.12	1.45	1.33
1	A	190	VAL	C-O	7.76	1.32	1.23
1	C	108	CYS	N-CA	7.48	1.55	1.46
1	B	59	ARG	CZ-NH2	7.45	1.43	1.33
1	A	231	ILE	N-CA	7.01	1.51	1.46
1	C	118	THR	CA-CB	6.88	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	ASN	C-N	6.58	1.43	1.33
1	B	225	GLU	N-CA	6.14	1.53	1.46
1	D	173	ILE	CA-CB	6.03	1.61	1.54
1	C	46	VAL	C-O	-5.99	1.17	1.24
1	C	260	ALA	CA-CB	5.82	1.62	1.53
1	B	51	ASN	N-CA	5.72	1.54	1.46
1	C	287	THR	CA-CB	5.71	1.63	1.53
1	A	274	LYS	CA-C	-5.68	1.48	1.52
1	F	26	ARG	C-O	-5.64	1.17	1.23
1	D	108	CYS	C-O	-5.61	1.17	1.24
1	B	168	SER	C-O	-5.54	1.17	1.24
1	A	46	VAL	CA-CB	5.50	1.58	1.54
1	C	109	LEU	C-O	-5.47	1.17	1.24
1	B	263	GLU	CG-CD	-5.44	1.38	1.52
1	C	236	SER	CA-C	5.43	1.60	1.52
1	E	236	SER	CA-C	5.42	1.60	1.52
1	C	150	GLU	CD-OE1	5.39	1.35	1.25
1	B	56	GLU	CB-CG	5.30	1.68	1.52
1	D	262	THR	CA-CB	5.23	1.62	1.53
1	D	132	ILE	N-CA	5.22	1.52	1.46
1	D	231	ILE	CA-CB	5.17	1.60	1.54
1	A	118	THR	CA-CB	5.14	1.61	1.53
1	B	40	SER	N-CA	-5.11	1.40	1.46
1	C	264	GLU	N-CA	5.10	1.52	1.46
1	C	30	ILE	CA-C	-5.01	1.46	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	ARG	O-C-N	-17.13	101.62	121.32
1	B	50	ILE	CA-C-N	-14.73	102.87	123.20
1	B	50	ILE	C-N-CA	-14.73	102.87	123.20
1	C	130	SER	N-CA-C	-9.60	96.27	110.48
1	B	50	ILE	N-CA-C	9.51	119.47	110.53
1	C	151	PHE	CA-C-N	-9.41	110.09	119.78
1	C	151	PHE	C-N-CA	-9.41	110.09	119.78
1	C	50	ILE	N-CA-C	9.10	123.63	111.44
1	F	173	ILE	CB-CA-C	-9.09	98.47	110.84
1	B	173	ILE	CB-CA-C	-8.95	97.49	110.83
1	C	50	ILE	CA-C-N	-8.75	104.82	121.54
1	C	50	ILE	C-N-CA	-8.75	104.82	121.54
1	D	173	ILE	CB-CA-C	-8.70	99.06	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	GLY	N-CA-C	7.96	132.03	113.18
1	B	9	ARG	CA-C-N	-7.78	111.89	120.14
1	B	9	ARG	C-N-CA	-7.78	111.89	120.14
1	F	142	VAL	CB-CA-C	-7.70	100.22	112.16
1	B	50	ILE	O-C-N	-7.60	114.00	121.90
1	E	35	VAL	N-CA-C	-7.46	103.58	110.82
1	D	67	VAL	CB-CA-C	-7.41	99.29	110.55
1	C	107	THR	O-C-N	-7.30	114.66	123.27
1	F	50	ILE	N-CA-C	7.28	118.08	110.72
1	C	107	THR	CA-C-N	7.27	135.42	121.54
1	C	107	THR	C-N-CA	7.27	135.42	121.54
1	B	145	SER	N-CA-C	7.07	120.46	110.50
1	A	50	ILE	N-CA-C	7.06	117.88	111.81
1	A	228	ARG	CA-C-N	-6.89	112.60	120.04
1	A	228	ARG	C-N-CA	-6.89	112.60	120.04
1	E	67	VAL	CB-CA-C	-6.88	98.39	110.71
1	C	131	GLY	O-C-N	-6.84	113.80	122.70
1	D	50	ILE	CA-C-N	-6.83	112.56	122.06
1	D	50	ILE	C-N-CA	-6.83	112.56	122.06
1	B	65	ASN	N-CA-C	6.80	121.73	113.17
1	A	151	PHE	CA-C-N	-6.72	112.86	119.78
1	A	151	PHE	C-N-CA	-6.72	112.86	119.78
1	D	151	PHE	CA-C-N	-6.54	113.05	119.78
1	D	151	PHE	C-N-CA	-6.54	113.05	119.78
1	B	141	ASP	N-CA-C	6.51	120.32	112.38
1	E	220	GLU	N-CA-C	6.50	120.31	112.38
1	C	231	ILE	CB-CA-C	-6.42	103.84	110.71
1	D	142	VAL	CB-CA-C	-6.42	102.22	112.16
1	E	145	SER	N-CA-C	6.40	119.06	110.35
1	F	142	VAL	N-CA-CB	6.38	121.56	110.65
1	F	67	VAL	CB-CA-C	-6.28	100.65	110.69
1	A	50	ILE	CA-C-N	-6.15	109.80	121.54
1	A	50	ILE	C-N-CA	-6.15	109.80	121.54
1	D	132	ILE	CA-C-N	6.09	130.78	122.19
1	D	132	ILE	C-N-CA	6.09	130.78	122.19
1	D	173	ILE	N-CA-CB	6.08	118.32	111.21
1	D	111	PHE	N-CA-C	-6.00	104.65	111.07
1	C	142	VAL	CB-CA-C	-5.98	102.89	112.16
1	B	74	VAL	CB-CA-C	5.96	119.72	111.19
1	A	287	THR	CB-CA-C	5.94	121.11	109.35
1	C	236	SER	CB-CA-C	5.92	122.69	110.31
1	A	274	LYS	CA-C-N	5.89	126.08	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	LYS	C-N-CA	5.89	126.08	120.31
1	C	30	ILE	CB-CA-C	-5.84	101.80	110.33
1	C	132	ILE	N-CA-C	5.82	116.03	108.35
1	B	169	HIS	N-CA-C	5.81	118.86	109.40
1	E	15	LEU	N-CA-C	5.81	118.13	109.59
1	E	9	ARG	CA-C-N	-5.76	114.03	119.85
1	E	9	ARG	C-N-CA	-5.76	114.03	119.85
1	F	183	LYS	N-CA-C	5.55	117.33	111.28
1	A	69	PHE	CB-CA-C	-5.47	105.51	110.44
1	B	187	PHE	N-CA-C	5.45	117.02	111.14
1	C	218	HIS	CB-CA-C	-5.43	105.00	110.65
1	A	196	ASP	N-CA-C	-5.42	105.98	112.59
1	F	49	MET	CA-C-N	5.40	128.09	120.42
1	F	49	MET	C-N-CA	5.40	128.09	120.42
1	F	269	LEU	N-CA-C	5.36	117.20	110.24
1	D	20	PHE	CA-C-N	-5.33	116.71	123.15
1	D	20	PHE	C-N-CA	-5.33	116.71	123.15
1	C	142	VAL	N-CA-CB	5.31	119.73	110.65
1	C	170	GLN	N-CA-C	-5.30	106.86	113.38
1	D	142	VAL	N-CA-CB	5.29	119.70	110.65
1	D	64	ILE	N-CA-C	5.29	116.76	109.46
1	E	151	PHE	N-CA-C	-5.28	103.39	109.93
1	C	145	SER	N-CA-C	5.27	117.94	110.50
1	B	56	GLU	N-CA-CB	5.17	117.82	110.16
1	D	16	ALA	N-CA-C	-5.16	103.87	110.53
1	E	104	VAL	CB-CA-C	-5.16	102.79	110.33
1	B	263	GLU	N-CA-CB	-5.15	102.54	110.01
1	E	71	GLY	N-CA-C	-5.13	104.35	112.66
1	A	132	ILE	O-C-N	-5.12	116.17	122.57
1	B	96	ASN	N-CA-C	5.10	117.23	111.11
1	E	96	ASN	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ILE	Mainchain
1	B	144	GLY	Peptide
1	C	144	GLY	Peptide
1	E	228	ARG	Mainchain

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	2309	0	2229	50	0
1	B	2309	0	2229	57	0
1	C	2309	0	2229	43	0
1	D	2309	0	2229	47	0
1	E	2309	0	2229	50	0
1	F	2309	0	2229	63	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
3	A	125	0	0	3	0
3	B	125	0	0	5	0
3	C	174	0	0	5	0
3	D	129	0	0	1	0
3	E	93	0	0	1	0
3	F	105	0	0	4	0
All	All	14641	0	13422	302	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 11.

All (302) 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:56:GLU:HG3	1:B:59:ARG:NH2	1.41	1.32
1:F:65:ASN:HD22	1:F:255:ASN:ND2	1.50	1.07
1:F:132:ILE:HD13	1:F:134:LEU:HD21	1.42	1.02
1:B:49:MET:HE3	1:B:49:MET:HA	1.36	1.01
1:B:56:GLU:CG	1:B:59:ARG:NH2	2.24	1.00
1:B:56:GLU:HG3	1:B:59:ARG:HH22	1.14	0.97
1:B:65:ASN:HD22	1:B:255:ASN:HD22	1.11	0.96
1:F:115:THR:HG21	1:F:173:ILE:CD1	1.97	0.94
1:F:219:PRO:O	1:F:241:THR:HB	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:PHE:HB3	1:E:142:VAL:HG21	1.51	0.92
1:D:65:ASN:HD22	1:D:255:ASN:HD22	1.18	0.90
1:F:65:ASN:ND2	1:F:255:ASN:HD22	1.70	0.90
1:F:65:ASN:HD22	1:F:255:ASN:HD22	0.90	0.89
1:A:52:LYS:HB3	1:A:56:GLU:HG2	1.57	0.86
1:A:222:ASN:HB2	1:A:241:THR:CG2	2.06	0.85
1:F:25:ASP:H	1:F:291:ASN:ND2	1.75	0.85
1:B:56:GLU:HG3	1:B:59:ARG:HH21	1.39	0.84
1:C:16:ALA:HA	1:C:30:ILE:HD11	1.60	0.82
1:F:115:THR:HG21	1:F:173:ILE:HD12	1.61	0.82
1:A:219:PRO:O	1:A:241:THR:HB	1.81	0.81
1:B:118:THR:HG21	1:B:188:TYR:OH	1.81	0.81
1:F:115:THR:HG21	1:F:173:ILE:HD11	1.62	0.81
1:E:222:ASN:HB2	1:E:241:THR:CG2	2.12	0.80
1:B:56:GLU:CG	1:B:59:ARG:HH22	1.90	0.80
1:C:16:ALA:HA	1:C:30:ILE:CD1	2.12	0.78
1:F:222:ASN:HB2	1:F:241:THR:CG2	2.11	0.78
1:B:222:ASN:HB2	1:B:241:THR:CG2	2.13	0.78
1:D:222:ASN:HB2	1:D:241:THR:CG2	2.14	0.76
1:D:50:ILE:HD11	1:D:81:TYR:CA	2.15	0.76
1:B:49:MET:HE3	1:B:49:MET:CA	2.09	0.76
1:E:118:THR:HG21	1:E:188:TYR:OH	1.85	0.76
1:D:219:PRO:O	1:D:241:THR:HB	1.87	0.74
1:D:50:ILE:HD11	1:D:81:TYR:HA	1.70	0.73
1:C:231:ILE:HD11	3:C:521:HOH:O	1.88	0.71
1:B:219:PRO:O	1:B:241:THR:HB	1.90	0.71
1:A:287:THR:HG21	3:A:407:HOH:O	1.91	0.70
1:F:25:ASP:N	1:F:291:ASN:HD22	1.88	0.70
1:A:139:THR:O	1:A:142:VAL:HG22	1.92	0.70
1:F:255:ASN:HD21	1:F:257:HIS:HB2	1.58	0.69
1:D:278:THR:HG21	1:D:287:THR:HG23	1.73	0.69
1:C:222:ASN:HB2	1:C:241:THR:CG2	2.22	0.69
1:A:118:THR:HG21	1:A:188:TYR:OH	1.93	0.68
1:C:16:ALA:CA	1:C:30:ILE:HD11	2.24	0.68
1:C:219:PRO:O	1:C:241:THR:HB	1.94	0.67
1:F:108:CYS:SG	1:F:109:LEU:N	2.67	0.67
1:B:108:CYS:SG	1:B:109:LEU:N	2.68	0.66
1:A:50:ILE:HD11	1:A:81:TYR:HA	1.77	0.66
1:D:50:ILE:HD11	1:D:81:TYR:N	2.10	0.66
1:F:132:ILE:CD1	1:F:134:LEU:HD21	2.23	0.66
1:F:118:THR:HG21	1:F:188:TYR:OH	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:LYS:HE3	1:F:5:LYS:HA	1.78	0.66
1:B:138:PHE:CD2	1:B:142:VAL:HG11	2.30	0.66
1:F:25:ASP:H	1:F:291:ASN:HD22	1.39	0.65
1:E:28:SER:HB3	1:E:50:ILE:CD1	2.27	0.65
1:C:138:PHE:CD2	1:C:142:VAL:HG11	2.31	0.65
1:E:169:HIS:CE1	1:E:172:SER:OG	2.49	0.65
1:F:222:ASN:HB2	1:F:241:THR:HG21	1.78	0.65
1:B:114:LEU:O	1:B:118:THR:HG23	1.96	0.65
1:C:278:THR:HG21	1:C:287:THR:HG23	1.78	0.65
1:B:90:ARG:NH2	3:B:444:HOH:O	2.22	0.65
1:E:139:THR:O	1:E:142:VAL:HG23	1.97	0.64
1:B:52:LYS:NZ	3:B:485:HOH:O	2.30	0.64
1:B:264:GLU:HG3	3:B:475:HOH:O	1.95	0.64
1:F:139:THR:O	1:F:142:VAL:HG22	1.97	0.64
1:F:140:GLU:HG3	1:F:143:LYS:NZ	2.12	0.64
1:E:278:THR:HG21	1:E:287:THR:HG23	1.80	0.64
1:B:65:ASN:HD22	1:B:255:ASN:ND2	1.90	0.64
1:E:50:ILE:HG12	3:E:482:HOH:O	1.95	0.64
1:F:25:ASP:N	1:F:291:ASN:ND2	2.44	0.63
1:B:26:ARG:NH2	1:B:276:GLU:OE2	2.31	0.63
1:B:217:TRP:H	1:B:217:TRP:CD1	2.17	0.62
1:A:285:GLU:HG3	1:B:271:TYR:CE1	2.35	0.62
1:F:231:ILE:HD11	3:F:413:HOH:O	1.98	0.62
1:A:114:LEU:O	1:A:118:THR:HG23	1.99	0.61
1:E:222:ASN:HB2	1:E:241:THR:HG22	1.81	0.61
1:E:105:TRP:HH2	1:E:244:MET:HE3	1.65	0.61
1:D:89:TYR:OH	1:D:118:THR:HG22	2.01	0.60
1:C:139:THR:O	1:C:142:VAL:HG22	2.02	0.60
1:C:258:SER:HB2	3:C:485:HOH:O	2.00	0.60
1:A:222:ASN:HB2	1:A:241:THR:HG21	1.81	0.60
1:F:89:TYR:OH	1:F:118:THR:HB	2.01	0.60
1:E:89:TYR:OH	1:E:118:THR:HG22	2.02	0.60
1:E:114:LEU:O	1:E:118:THR:HG23	2.02	0.60
1:A:25:ASP:O	1:A:26:ARG:HG3	2.02	0.59
1:D:19:VAL:HG12	1:D:21:ASP:H	1.67	0.59
1:B:278:THR:OG1	1:B:287:THR:HG23	2.03	0.59
1:F:105:TRP:CH2	1:F:244:MET:HE3	2.38	0.59
1:E:253:ARG:NH2	1:F:238:ILE:HD13	2.18	0.59
1:C:287:THR:HG21	3:C:431:HOH:O	2.01	0.58
1:E:250:ASN:ND2	1:E:253:ARG:HH11	2.00	0.58
1:D:113:LEU:HD22	1:D:117:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:THR:HG21	1:F:287:THR:HG23	1.85	0.58
1:F:105:TRP:HH2	1:F:244:MET:HE3	1.68	0.58
1:A:39:GLU:HA	1:A:43:ALA:O	2.02	0.58
1:C:29:TYR:O	1:C:30:ILE:HD13	2.04	0.58
1:B:118:THR:CG2	1:B:188:TYR:OH	2.51	0.58
1:C:18:ASP:OD2	1:C:18:ASP:N	2.36	0.58
1:F:67:VAL:HG22	1:F:102:PHE:HE2	1.67	0.58
1:C:50:ILE:HD11	1:C:81:TYR:HA	1.86	0.57
1:B:49:MET:HA	1:B:49:MET:CE	2.23	0.57
1:E:28:SER:HB3	1:E:50:ILE:HG12	1.87	0.57
1:E:169:HIS:HE1	1:E:172:SER:OG	1.86	0.57
1:F:27:ASN:ND2	1:F:291:ASN:O	2.32	0.57
1:D:255:ASN:HD21	1:D:257:HIS:CG	2.23	0.56
1:B:222:ASN:HB2	1:B:241:THR:HG21	1.87	0.56
1:F:24:PRO:O	1:F:25:ASP:HB2	2.05	0.56
1:F:65:ASN:ND2	1:F:255:ASN:ND2	2.35	0.56
1:F:278:THR:OG1	1:F:287:THR:HG22	2.04	0.56
1:D:270:ILE:HD11	1:D:288:TYR:CZ	2.41	0.56
1:D:278:THR:CG2	1:D:287:THR:HG23	2.35	0.56
1:B:118:THR:HG21	1:B:188:TYR:CZ	2.41	0.55
1:E:219:PRO:O	1:E:241:THR:HB	2.05	0.55
1:D:222:ASN:HB2	1:D:241:THR:HG22	1.87	0.55
1:A:278:THR:OG1	1:A:287:THR:CG2	2.54	0.55
1:E:108:CYS:SG	1:E:109:LEU:N	2.79	0.55
1:F:20:PHE:O	1:F:22:PRO:HD3	2.06	0.55
1:E:222:ASN:HB2	1:E:241:THR:HG21	1.88	0.55
1:F:140:GLU:HG3	1:F:143:LYS:HZ1	1.69	0.55
1:F:53:SER:OG	1:F:56:GLU:HG3	2.07	0.54
1:F:49:MET:HE3	1:F:49:MET:HA	1.87	0.54
1:F:132:ILE:HD13	1:F:134:LEU:CD2	2.28	0.54
1:D:270:ILE:HD11	1:D:288:TYR:CE2	2.42	0.54
1:E:118:THR:HG21	1:E:188:TYR:CZ	2.43	0.53
1:F:217:TRP:CD1	1:F:217:TRP:H	2.26	0.53
1:A:138:PHE:CD2	1:A:142:VAL:HG11	2.43	0.53
1:F:255:ASN:HD21	1:F:257:HIS:CB	2.21	0.53
1:C:217:TRP:H	1:C:217:TRP:CD1	2.26	0.53
1:D:13:GLY:HA2	1:D:46:VAL:O	2.09	0.53
1:B:49:MET:CA	1:B:49:MET:CE	2.84	0.53
1:E:261:SER:O	1:E:264:GLU:HB2	2.08	0.53
1:C:30:ILE:HG12	1:C:290:PHE:HE1	1.74	0.53
1:E:278:THR:CG2	1:E:287:THR:HG23	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:TRP:CH2	1:E:244:MET:HE3	2.45	0.52
1:A:222:ASN:HB2	1:A:241:THR:HG22	1.90	0.52
1:C:67:VAL:HG23	1:C:102:PHE:CE2	2.45	0.52
1:D:221:LYS:NZ	2:D:301:GOL:H31	2.24	0.52
1:D:173:ILE:CD1	1:D:202:VAL:HB	2.40	0.52
1:A:25:ASP:C	1:A:26:ARG:HG3	2.35	0.51
1:F:222:ASN:HB2	1:F:241:THR:HG22	1.92	0.51
1:F:17:GLN:O	1:F:28:SER:HA	2.10	0.51
1:C:278:THR:OG1	1:C:287:THR:CG2	2.59	0.51
1:E:28:SER:HB3	1:E:50:ILE:HD13	1.92	0.51
1:F:5:LYS:HG3	1:F:5:LYS:O	2.11	0.51
1:F:70:PRO:HD2	1:F:81:TYR:HE1	1.76	0.51
1:A:217:TRP:CD1	1:A:217:TRP:H	2.29	0.50
1:B:89:TYR:OH	1:B:118:THR:HB	2.10	0.50
1:C:278:THR:CG2	1:C:287:THR:HG23	2.40	0.50
1:C:50:ILE:HG23	1:C:51:ASN:ND2	2.27	0.50
1:D:217:TRP:H	1:D:217:TRP:CD1	2.29	0.50
1:C:108:CYS:SG	1:C:109:LEU:N	2.84	0.50
1:E:28:SER:HB3	1:E:50:ILE:CG1	2.42	0.50
1:E:37:PHE:CE2	1:E:245:ALA:HB2	2.46	0.50
1:A:165:THR:HB	1:A:217:TRP:CE3	2.47	0.50
1:B:222:ASN:HB2	1:B:241:THR:HG22	1.92	0.50
1:A:79:SER:O	1:A:83:LYS:HG2	2.12	0.49
1:A:132:ILE:HG23	1:A:132:ILE:O	2.10	0.49
1:D:222:ASN:HB2	1:D:241:THR:HG21	1.94	0.49
1:A:94:GLU:HG2	3:A:501:HOH:O	2.12	0.49
1:A:250:ASN:ND2	1:A:253:ARG:HH11	2.10	0.49
1:F:278:THR:OG1	1:F:287:THR:CG2	2.61	0.49
1:F:209:ASP:HB3	3:F:433:HOH:O	2.12	0.49
1:C:105:TRP:CH2	1:C:244:MET:HE3	2.48	0.49
1:C:253:ARG:NH2	1:D:238:ILE:HD13	2.27	0.49
1:B:282:SER:HB2	3:B:518:HOH:O	2.12	0.49
1:D:50:ILE:HG23	1:D:51:ASN:ND2	2.28	0.48
1:B:18:ASP:OD2	1:B:18:ASP:N	2.46	0.48
1:E:111:PHE:C	1:E:111:PHE:CD2	2.91	0.48
1:E:262:THR:O	1:E:266:GLU:HG3	2.12	0.48
1:C:131:GLY:HA2	1:C:230:TYR:CD1	2.49	0.48
1:C:218:HIS:CG	1:C:221:LYS:HE2	2.48	0.48
1:D:139:THR:O	1:D:142:VAL:HG22	2.14	0.48
1:C:178:PHE:C	1:C:178:PHE:CD2	2.92	0.48
1:E:41:ALA:HB3	1:E:249:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:TRP:HB2	1:B:285:GLU:OE1	2.14	0.48
1:F:49:MET:HE3	1:F:50:ILE:H	1.79	0.47
1:D:226:TRP:HB2	1:D:285:GLU:OE1	2.14	0.47
1:A:83:LYS:O	1:A:87:ILE:HG12	2.13	0.47
1:B:165:THR:HB	1:B:217:TRP:CD2	2.49	0.47
1:E:234:THR:O	1:E:235:PRO:C	2.57	0.47
1:F:18:ASP:OD2	1:F:18:ASP:N	2.44	0.47
1:A:37:PHE:CE2	1:A:245:ALA:HB2	2.50	0.47
1:B:71:GLY:HA2	1:B:109:LEU:H	1.80	0.47
1:B:231:ILE:HG22	1:B:233:HIS:CE1	2.48	0.47
1:B:255:ASN:HD21	1:B:257:HIS:CG	2.33	0.47
1:C:90:ARG:HD2	3:C:402:HOH:O	2.15	0.47
1:D:270:ILE:CD1	1:D:288:TYR:CZ	2.97	0.47
1:B:18:ASP:CG	1:B:50:ILE:HD11	2.39	0.47
1:C:166:GLU:HG3	1:C:231:ILE:HD12	1.96	0.47
1:D:52:LYS:HB3	1:D:56:GLU:OE1	2.15	0.47
1:F:138:PHE:CD2	1:F:142:VAL:HG11	2.50	0.47
1:C:89:TYR:OH	1:C:118:THR:HG22	2.14	0.47
1:B:138:PHE:HD2	1:B:142:VAL:HG11	1.77	0.47
1:E:278:THR:OG1	1:E:287:THR:CG2	2.62	0.47
1:A:41:ALA:HB3	1:A:249:VAL:HG21	1.97	0.47
1:A:50:ILE:HD12	1:A:50:ILE:HA	1.61	0.47
1:C:186:LYS:HD2	1:C:186:LYS:HA	1.67	0.46
1:C:250:ASN:ND2	1:C:253:ARG:HH11	2.13	0.46
1:A:108:CYS:SG	1:A:109:LEU:N	2.88	0.46
1:D:89:TYR:CG	1:D:117:LEU:HD13	2.50	0.46
1:E:147:LEU:HD11	1:E:244:MET:HE1	1.98	0.46
1:E:20:PHE:O	1:E:22:PRO:HD3	2.15	0.46
1:F:113:LEU:HD23	1:F:113:LEU:O	2.16	0.46
1:C:189:ARG:HB2	1:C:208:TYR:CE2	2.50	0.46
1:B:105:TRP:CH2	1:B:244:MET:HE3	2.51	0.46
1:F:5:LYS:HE3	1:F:5:LYS:CA	2.44	0.46
1:D:15:LEU:HD13	1:D:81:TYR:CD1	2.50	0.45
1:B:165:THR:HB	1:B:217:TRP:CE3	2.52	0.45
1:E:187:PHE:CE2	1:E:188:TYR:CE1	3.04	0.45
1:C:23:LYS:HE2	1:C:23:LYS:HB2	1.36	0.45
1:A:103:PRO:HB2	1:A:248:PHE:CE1	2.51	0.45
1:C:111:PHE:C	1:C:111:PHE:CD2	2.95	0.45
1:A:278:THR:OG1	1:A:287:THR:HG23	2.16	0.45
1:A:285:GLU:CG	1:B:271:TYR:CE1	3.00	0.45
1:E:270:ILE:O	1:E:270:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ILE:O	1:E:132:ILE:HG23	2.16	0.45
1:F:285:GLU:HG2	3:F:428:HOH:O	2.16	0.45
1:D:49:MET:HE1	1:D:290:PHE:CG	2.52	0.45
1:E:94:GLU:OE2	1:E:94:GLU:HA	2.16	0.45
1:E:278:THR:OG1	1:E:287:THR:HG23	2.16	0.45
1:A:111:PHE:CD2	1:A:111:PHE:C	2.95	0.45
1:D:112:GLU:HB3	1:D:124:LEU:HD11	1.99	0.44
1:D:270:ILE:CD1	1:D:288:TYR:CE2	3.00	0.44
1:D:103:PRO:HA	1:D:211:PRO:O	2.17	0.44
1:D:108:CYS:SG	1:D:109:LEU:N	2.90	0.44
1:F:186:LYS:O	1:F:186:LYS:HG3	2.16	0.44
1:B:8:GLU:OE1	3:B:496:HOH:O	2.20	0.44
1:F:118:THR:HG21	1:F:188:TYR:CZ	2.52	0.44
1:C:165:THR:HB	1:C:217:TRP:CE3	2.52	0.44
1:D:89:TYR:CB	1:D:117:LEU:HD13	2.48	0.44
1:B:101:TYR:O	1:B:255:ASN:HB2	2.17	0.44
1:A:19:VAL:HG12	1:A:21:ASP:H	1.83	0.44
1:B:112:GLU:HB3	1:B:124:LEU:HD11	1.99	0.44
1:F:13:GLY:HA2	1:F:46:VAL:O	2.17	0.44
1:C:118:THR:HG21	1:C:188:TYR:OH	2.17	0.44
1:D:50:ILE:O	1:D:57:TYR:OH	2.35	0.44
1:D:138:PHE:CD2	1:D:142:VAL:HG11	2.53	0.44
1:B:173:ILE:HD12	1:B:202:VAL:HB	2.00	0.44
1:D:49:MET:HE1	1:D:290:PHE:CD2	2.53	0.43
1:B:23:LYS:HE3	1:B:23:LYS:HB2	1.90	0.43
1:E:145:SER:HB3	1:E:191:LEU:HD22	1.99	0.43
1:E:218:HIS:CG	1:E:221:LYS:HE2	2.52	0.43
1:C:248:PHE:O	1:C:251:GLU:HB2	2.19	0.43
1:C:278:THR:OG1	1:C:287:THR:HG22	2.16	0.43
1:D:131:GLY:HA2	1:D:230:TYR:CD1	2.53	0.43
1:A:50:ILE:HG13	1:A:80:GLY:C	2.43	0.43
1:C:50:ILE:HG13	1:C:80:GLY:C	2.44	0.43
1:A:168:SER:OG	2:A:301:GOL:H32	2.19	0.43
1:E:169:HIS:CD2	1:E:169:HIS:H	2.36	0.43
1:B:95:ALA:HB1	1:B:100:ASP:HB3	2.01	0.43
1:F:118:THR:CG2	1:F:188:TYR:OH	2.65	0.43
1:A:285:GLU:CG	1:B:271:TYR:CZ	3.02	0.43
1:A:68:LEU:C	1:A:68:LEU:HD23	2.44	0.43
1:C:16:ALA:HA	1:C:30:ILE:HD13	1.93	0.43
1:D:173:ILE:HD12	1:D:202:VAL:HB	2.00	0.43
1:D:139:THR:HG21	1:D:190:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:TRP:CH2	1:D:244:MET:HE3	2.55	0.42
1:A:13:GLY:HA2	1:A:46:VAL:O	2.19	0.42
1:A:59:ARG:NH1	1:A:264:GLU:OE1	2.53	0.42
1:D:5:LYS:HE3	1:D:5:LYS:HB2	1.73	0.42
1:D:67:VAL:HG22	1:D:102:PHE:HE2	1.84	0.42
1:A:37:PHE:HB2	1:A:220:GLU:HB2	2.01	0.42
1:A:207:ALA:HB3	1:A:210:PHE:O	2.20	0.42
1:D:182:LYS:NZ	3:D:474:HOH:O	2.49	0.42
1:C:262:THR:HG23	3:C:546:HOH:O	2.20	0.42
1:A:50:ILE:HG13	1:A:80:GLY:HA3	2.02	0.42
1:E:67:VAL:CG2	1:E:102:PHE:HE2	2.30	0.42
1:F:248:PHE:O	1:F:251:GLU:HB2	2.20	0.42
1:A:71:GLY:HA3	1:A:108:CYS:HB3	2.02	0.42
1:A:285:GLU:HG3	1:B:271:TYR:CZ	2.54	0.42
1:F:81:TYR:CE2	1:F:113:LEU:HD12	2.55	0.42
1:E:46:VAL:HG11	1:E:60:LEU:HD11	2.02	0.42
1:F:267:LYS:HG2	3:F:476:HOH:O	2.19	0.42
1:B:231:ILE:CG2	1:B:233:HIS:CE1	3.03	0.42
1:E:39:GLU:HA	1:E:43:ALA:O	2.20	0.41
1:F:53:SER:HG	1:F:56:GLU:HG3	1.84	0.41
1:E:165:THR:HB	1:E:217:TRP:CE3	2.55	0.41
1:F:39:GLU:HA	1:F:43:ALA:O	2.20	0.41
1:B:50:ILE:HD13	1:B:50:ILE:HG21	1.52	0.41
1:B:105:TRP:HH2	1:B:244:MET:HE3	1.85	0.41
1:B:263:GLU:H	1:B:263:GLU:HG2	1.35	0.41
1:D:255:ASN:ND2	1:D:257:HIS:H	2.17	0.41
1:A:274:LYS:HA	1:A:275:PRO:HD3	1.86	0.41
1:A:118:THR:CG2	1:A:188:TYR:OH	2.67	0.41
1:F:227:THR:O	1:F:228:ARG:HD3	2.21	0.41
1:F:278:THR:CG2	1:F:287:THR:HG23	2.48	0.41
1:C:79:SER:O	1:C:83:LYS:HD2	2.20	0.41
1:B:111:PHE:C	1:B:111:PHE:CD2	2.97	0.41
1:D:52:LYS:HB2	1:D:57:TYR:CZ	2.56	0.41
1:A:52:LYS:CB	1:A:56:GLU:HG2	2.39	0.41
1:C:132:ILE:HD12	1:A:128:ASN:HB2	2.03	0.41
1:A:40:SER:HA	1:B:224:PHE:CE1	2.56	0.40
1:B:173:ILE:H	1:B:173:ILE:HG13	1.55	0.40
1:E:174:THR:HA	1:E:201:PHE:HA	2.03	0.40
1:E:105:TRP:CD1	1:E:107:THR:HG1	2.38	0.40
1:A:56:GLU:CB	3:A:502:HOH:O	2.69	0.40
1:E:112:GLU:HB3	1:E:124:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:TRP:CD1	1:E:217:TRP:H	2.40	0.40
1:F:106:GLY:O	1:F:214:ALA:HA	2.21	0.40
1:D:278:THR:OG1	1:D:287:THR:CG2	2.70	0.40
1:B:100:ASP:OD2	1:B:257:HIS:NE2	2.35	0.40
1:E:274:LYS:HA	1:E:275:PRO:HD3	1.92	0.40
1:A:17:GLN:O	1:A:28:SER:HA	2.21	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	285/312 (91%)	271 (95%)	14 (5%)	0	100	100
1	B	285/312 (91%)	273 (96%)	11 (4%)	1 (0%)	30	28
1	C	285/312 (91%)	276 (97%)	9 (3%)	0	100	100
1	D	285/312 (91%)	269 (94%)	16 (6%)	0	100	100
1	E	285/312 (91%)	264 (93%)	20 (7%)	1 (0%)	30	28
1	F	285/312 (91%)	274 (96%)	11 (4%)	0	100	100
All	All	1710/1872 (91%)	1627 (95%)	81 (5%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	GLY
1	E	131	GLY

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	250/272 (92%)	226 (90%)	24 (10%)	8	5
1	B	250/272 (92%)	227 (91%)	23 (9%)	8	6
1	C	250/272 (92%)	234 (94%)	16 (6%)	16	14
1	D	250/272 (92%)	224 (90%)	26 (10%)	7	4
1	E	250/272 (92%)	227 (91%)	23 (9%)	8	6
1	F	250/272 (92%)	221 (88%)	29 (12%)	5	3
All	All	1500/1632 (92%)	1359 (91%)	141 (9%)	8	6

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	18	ASP
1	C	23	LYS
1	C	50	ILE
1	C	67	VAL
1	C	83	LYS
1	C	108	CYS
1	C	113	LEU
1	C	118	THR
1	C	142	VAL
1	C	143	LYS
1	C	150	GLU
1	C	157	LYS
1	C	182	LYS
1	C	241	THR
1	C	281	GLN
1	C	287	THR
1	D	5	LYS
1	D	15	LEU
1	D	18	ASP
1	D	23	LYS
1	D	54	GLU
1	D	59	ARG

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Mol	Chain	Res	Type
1	D	60	LEU
1	D	67	VAL
1	D	74	VAL
1	D	94	GLU
1	D	108	CYS
1	D	113	LEU
1	D	118	THR
1	D	121	GLU
1	D	122	LEU
1	D	125	SER
1	D	142	VAL
1	D	147	LEU
1	D	173	ILE
1	D	241	THR
1	D	261	SER
1	D	263	GLU
1	D	270	ILE
1	D	276	GLU
1	D	281	GLN
1	D	287	THR
1	A	5	LYS
1	A	15	LEU
1	A	18	ASP
1	A	21	ASP
1	A	26	ARG
1	A	50	ILE
1	A	54	GLU
1	A	56	GLU
1	A	60	LEU
1	A	63	SER
1	A	113	LEU
1	A	118	THR
1	A	122	LEU
1	A	142	VAL
1	A	147	LEU
1	A	150	GLU
1	A	175	THR
1	A	185	LYS
1	A	186	LYS
1	A	238	ILE
1	A	241	THR
1	A	281	GLN

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Mol	Chain	Res	Type
1	A	285	GLU
1	A	287	THR
1	B	15	LEU
1	B	18	ASP
1	B	23	LYS
1	B	49	MET
1	B	50	ILE
1	B	52	LYS
1	B	54	GLU
1	B	74	VAL
1	B	77	GLU
1	B	108	CYS
1	B	113	LEU
1	B	118	THR
1	B	122	LEU
1	B	143	LYS
1	B	147	LEU
1	B	157	LYS
1	B	166	GLU
1	B	173	ILE
1	B	185	LYS
1	B	186	LYS
1	B	241	THR
1	B	281	GLN
1	B	287	THR
1	E	15	LEU
1	E	18	ASP
1	E	23	LYS
1	E	55	ASP
1	E	56	GLU
1	E	62	LYS
1	E	67	VAL
1	E	108	CYS
1	E	111	PHE
1	E	113	LEU
1	E	122	LEU
1	E	142	VAL
1	E	143	LYS
1	E	147	LEU
1	E	170	GLN
1	E	175	THR
1	E	176	GLU

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Mol	Chain	Res	Type
1	E	236	SER
1	E	241	THR
1	E	262	THR
1	E	281	GLN
1	E	285	GLU
1	E	287	THR
1	F	5	LYS
1	F	6	THR
1	F	18	ASP
1	F	21	ASP
1	F	23	LYS
1	F	46	VAL
1	F	54	GLU
1	F	60	LEU
1	F	67	VAL
1	F	74	VAL
1	F	108	CYS
1	F	111	PHE
1	F	118	THR
1	F	122	LEU
1	F	125	SER
1	F	132	ILE
1	F	140	GLU
1	F	142	VAL
1	F	147	LEU
1	F	166	GLU
1	F	173	ILE
1	F	185	LYS
1	F	186	LYS
1	F	241	THR
1	F	263	GLU
1	F	266	GLU
1	F	280	ILE
1	F	282	SER
1	F	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	ASN
1	C	126	HIS
1	C	170	GLN

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Mol	Chain	Res	Type
1	C	199	ASN
1	C	250	ASN
1	D	51	ASN
1	D	128	ASN
1	D	250	ASN
1	D	255	ASN
1	D	272	ASN
1	D	286	GLN
1	A	126	HIS
1	A	199	ASN
1	A	216	GLN
1	A	250	ASN
1	A	291	ASN
1	B	216	GLN
1	B	255	ASN
1	B	281	GLN
1	B	286	GLN
1	E	250	ASN
1	F	216	GLN
1	F	255	ASN
1	F	272	ASN
1	F	286	GLN
1	F	291	ASN

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 ⓘ

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	GOL	B	301	-	5,5,5	0.38	0	5,5,5	0.31	0
2	GOL	C	301	-	5,5,5	0.82	0	5,5,5	1.03	0
2	GOL	D	301	-	5,5,5	0.95	0	5,5,5	1.11	0
2	GOL	F	301	-	5,5,5	0.45	0	5,5,5	1.18	1 (20%)
2	GOL	E	301	-	5,5,5	0.65	0	5,5,5	1.21	0
2	GOL	A	301	-	5,5,5	1.11	0	5,5,5	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	F	301	-	-	3/4/4/4	-
2	GOL	E	301	-	-	3/4/4/4	-
2	GOL	A	301	-	-	1/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	GOL	O2-C2-C3	2.28	118.61	109.18

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	GOL	C1-C2-C3-O3
2	D	301	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	E	301	GOL	C1-C2-C3-O3
2	F	301	GOL	C1-C2-C3-O3
2	D	301	GOL	O2-C2-C3-O3
2	E	301	GOL	O2-C2-C3-O3
2	F	301	GOL	O2-C2-C3-O3
2	B	301	GOL	O1-C1-C2-O2
2	C	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-C3
2	F	301	GOL	O1-C1-C2-O2
2	E	301	GOL	O1-C1-C2-C3
2	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	GOL	1	0
2	A	301	GOL	1	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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	287/312 (91%)	-0.03	10 (3%) 47 49	9, 28, 46, 59	9 (3%)
1	B	287/312 (91%)	-0.14	7 (2%) 59 62	7, 28, 43, 49	5 (1%)
1	C	287/312 (91%)	-0.42	9 (3%) 51 54	3, 22, 35, 46	9 (3%)
1	D	287/312 (91%)	-0.10	8 (2%) 55 57	6, 29, 49, 59	5 (1%)
1	E	287/312 (91%)	0.28	11 (3%) 44 46	10, 36, 50, 58	9 (3%)
1	F	287/312 (91%)	0.06	6 (2%) 63 66	10, 32, 54, 61	5 (1%)
All	All	1722/1872 (91%)	-0.06	51 (2%) 52 55	3, 29, 48, 61	42 (2%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	THR	8.2
1	A	179	THR	8.1
1	C	179	THR	6.6
1	B	158	SER	6.1
1	F	283	ALA	6.1
1	C	283	ALA	5.5
1	B	250	ASN	5.4
1	F	250	ASN	5.3
1	A	283	ALA	5.3
1	E	50	ILE	5.2
1	E	250	ASN	5.1
1	E	202	VAL	4.8
1	F	158	SER	4.7
1	D	250	ASN	4.6
1	A	280	ILE	4.5
1	A	131	GLY	4.5
1	F	280	ILE	4.5
1	B	283	ALA	4.3
1	D	158	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	250	ASN	4.2
1	A	250	ASN	4.1
1	D	280	ILE	4.0
1	E	280	ILE	3.9
1	E	115	THR	3.7
1	B	280	ILE	3.6
1	E	283	ALA	3.4
1	D	283	ALA	3.3
1	E	128	ASN	3.2
1	C	115	THR	3.1
1	A	276	GLU	2.9
1	C	280	ILE	2.9
1	A	202	VAL	2.8
1	A	115	THR	2.7
1	D	115	THR	2.6
1	C	202	VAL	2.5
1	F	115	THR	2.5
1	F	50	ILE	2.5
1	E	274	LYS	2.5
1	E	276	GLU	2.4
1	D	262	THR	2.4
1	D	20	PHE	2.4
1	B	20	PHE	2.4
1	B	115	THR	2.4
1	D	50	ILE	2.3
1	C	276	GLU	2.2
1	E	188	TYR	2.2
1	A	128	ASN	2.2
1	C	128	ASN	2.2
1	C	50	ILE	2.1
1	B	130	SER	2.0
1	A	274	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	301	6/6	0.61	0.24	42,45,46,46	0
2	GOL	E	301	6/6	0.66	0.21	41,46,48,48	0
2	GOL	A	301	6/6	0.73	0.15	25,30,33,35	0
2	GOL	C	301	6/6	0.81	0.12	21,28,31,32	0
2	GOL	F	301	6/6	0.82	0.13	35,44,47,47	0
2	GOL	D	301	6/6	0.83	0.11	31,33,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.