



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:50 pm BST

PDB ID : 4L7Q  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

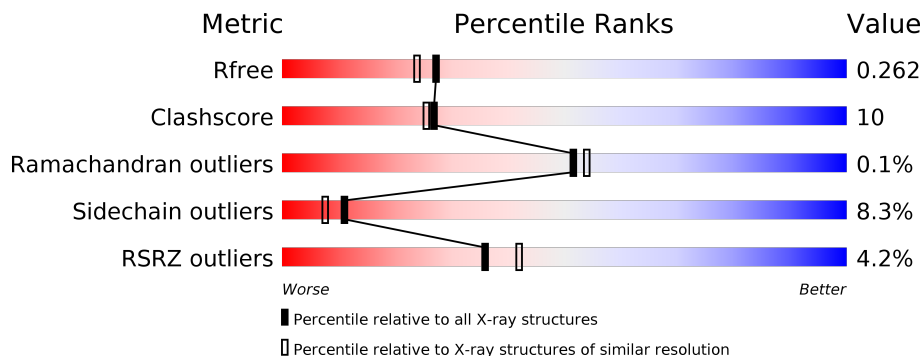
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	5% (Poor fit), 69% (0 outliers), 19% (1 outlier), 8% (2+ outliers)
1	B	312	3% (Poor fit), 73% (0 outliers), 14% (1 outlier), 8% (2+ outliers)
1	C	312	2% (Poor fit), 73% (0 outliers), 13% (1 outlier), 5% (2 outliers), 8% (3+ outliers)
1	D	312	3% (Poor fit), 72% (0 outliers), 16% (1 outlier), 8% (2+ outliers)
1	E	312	5% (Poor fit), 69% (0 outliers), 21% (1 outlier), 8% (2+ outliers)
1	F	312	5% (Poor fit), 68% (0 outliers), 21% (1 outlier), 8% (2+ outliers)

## 2 Entry composition [i](#)

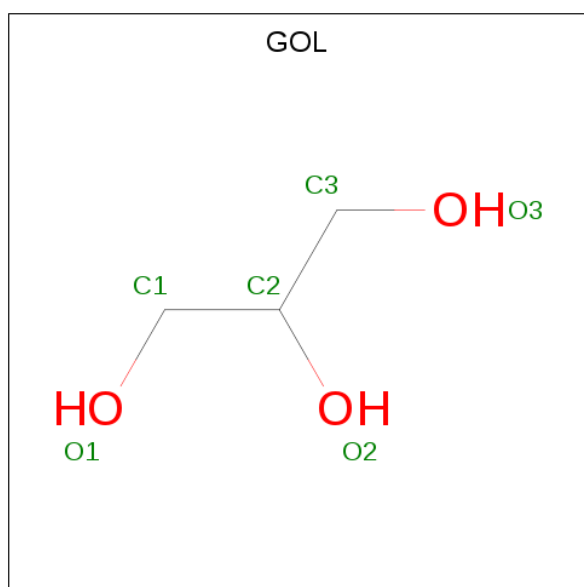
There are 3 unique types of molecules in this entry. The entry contains 14641 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	C	287	Total 2309	C 1492	N 370	O 442	S 5	0	0	0
1	D	287	Total 2309	C 1492	N 370	O 442	S 5	0	0	0
1	A	287	Total 2309	C 1492	N 370	O 442	S 5	0	0	0
1	B	287	Total 2309	C 1492	N 370	O 442	S 5	0	0	0
1	E	287	Total 2309	C 1492	N 370	O 442	S 5	0	0	0
1	F	287	Total 2309	C 1492	N 370	O 442	S 5	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

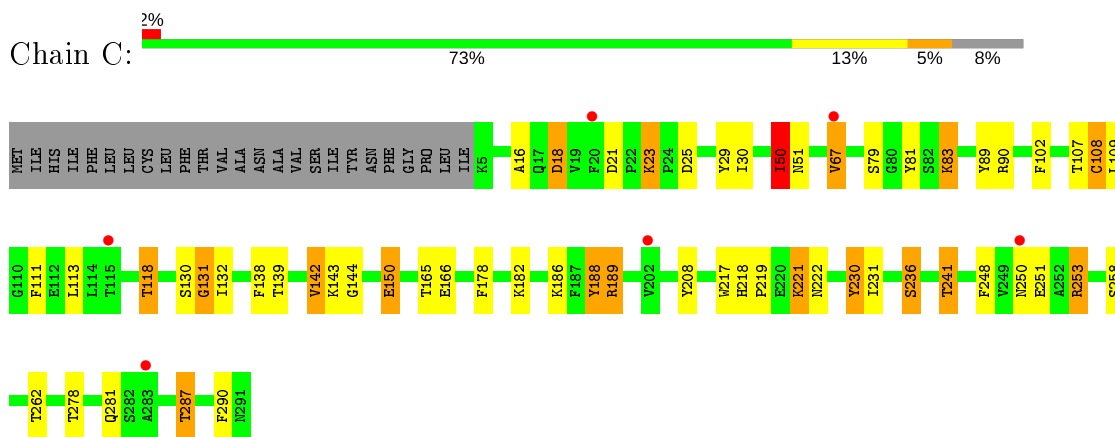
- Molecule 3 is water.

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

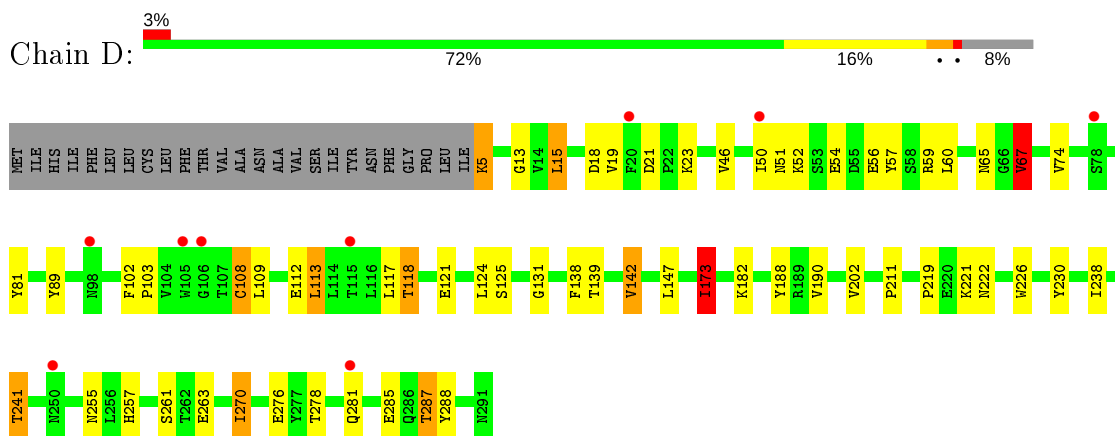
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

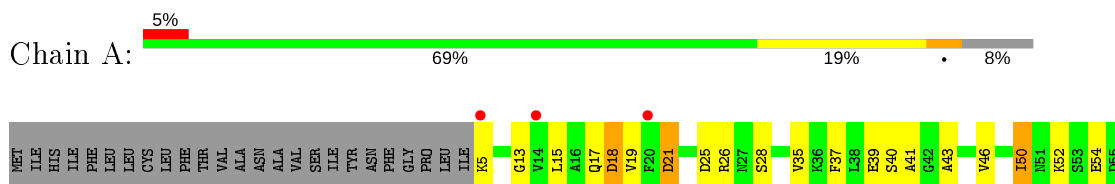
- Molecule 1: Gamma-glutamyl hydrolase

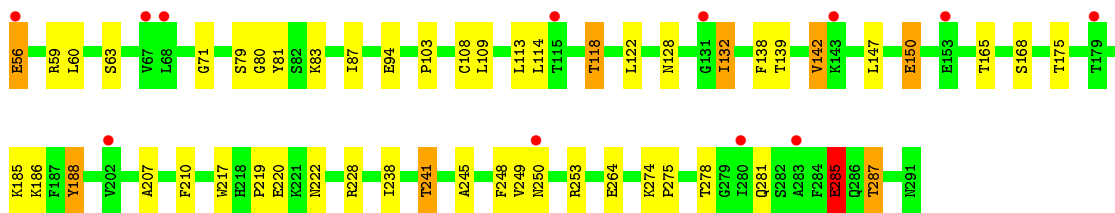


- Molecule 1: Gamma-glutamyl hydrolase

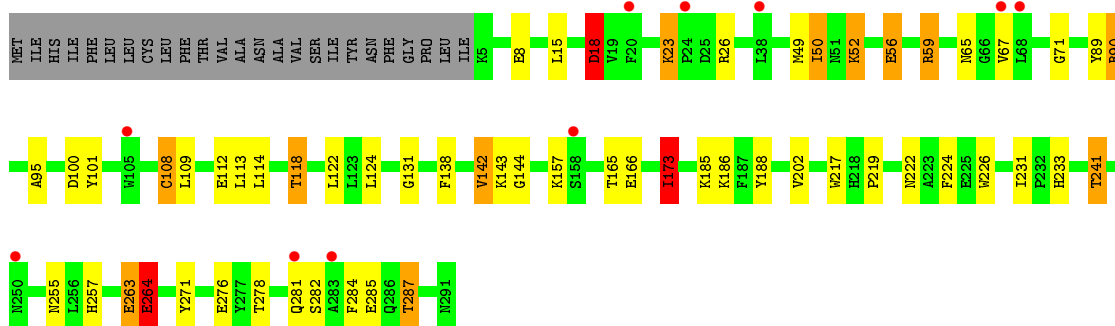


- Molecule 1: Gamma-glutamyl hydrolase

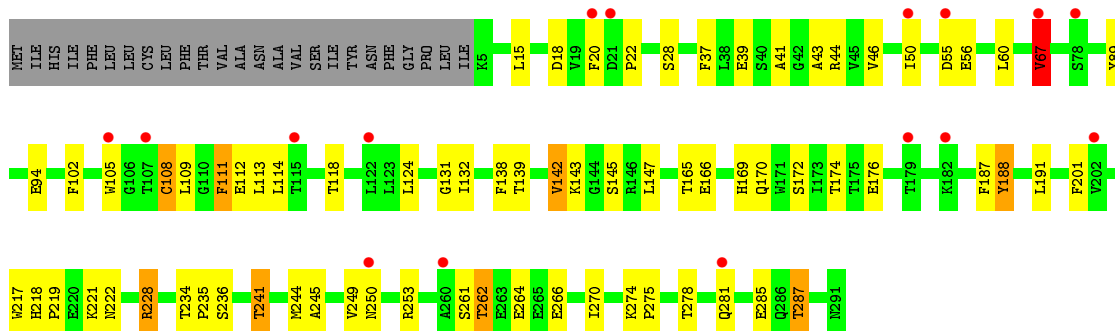




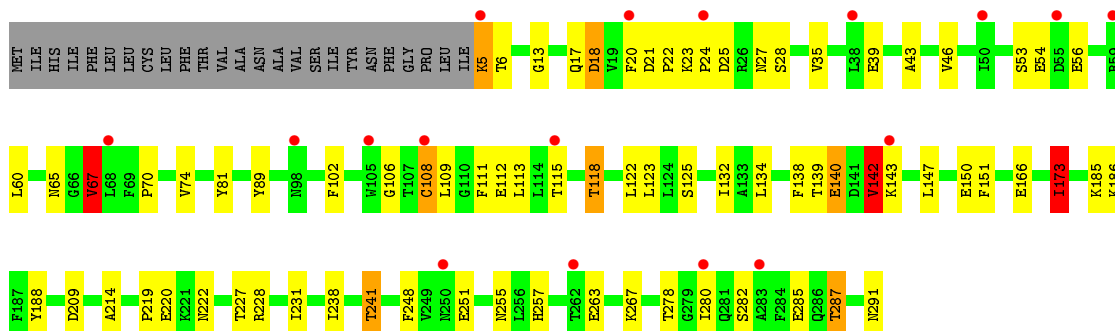
- Molecule 1: Gamma-glutamyl hydrolase



- 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, $\alpha$ , $\beta$ , $\gamma$	271.61Å 62.05Å 123.94Å 90.00° 95.41° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 28.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-2.10) 97.1 (28.20-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.198 , 0.263 0.201 , 0.262	Depositor DCC
$R_{free}$ test set	5869 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14641	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	1.14	6/2374 (0.3%)	0.92	1/3221 (0.0%)
1	B	1.18	8/2374 (0.3%)	1.02	8/3221 (0.2%)
1	C	1.27	9/2374 (0.4%)	1.05	14/3221 (0.4%)
1	D	1.06	2/2374 (0.1%)	0.95	2/3221 (0.1%)
1	E	0.98	1/2374 (0.0%)	0.92	3/3221 (0.1%)
1	F	1.04	5/2374 (0.2%)	0.92	4/3221 (0.1%)
All	All	1.12	31/14244 (0.2%)	0.97	32/19326 (0.2%)

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	ARG	C-N	10.43	1.54	1.34
1	C	150	GLU	CD-OE1	9.04	1.35	1.25
1	B	263	GLU	CG-CD	-9.00	1.38	1.51
1	B	56	GLU	CB-CG	8.52	1.68	1.52
1	A	285	GLU	CD-OE1	-7.95	1.17	1.25
1	A	150	GLU	CD-OE1	7.81	1.34	1.25
1	B	59	ARG	CZ-NH2	7.76	1.43	1.33
1	C	188	TYR	CD2-CE2	-7.25	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	GLU	CB-CG	-7.19	1.38	1.52
1	B	263	GLU	CB-CG	7.19	1.65	1.52
1	C	67	VAL	CB-CG2	-6.54	1.39	1.52
1	B	142	VAL	CB-CG1	-6.41	1.39	1.52
1	A	188	TYR	CD2-CE2	-6.27	1.29	1.39
1	C	150	GLU	CG-CD	6.26	1.61	1.51
1	B	56	GLU	CG-CD	6.12	1.61	1.51
1	A	35	VAL	CB-CG1	5.82	1.65	1.52
1	F	151	PHE	CD1-CE1	5.78	1.50	1.39
1	E	188	TYR	CD2-CE2	-5.76	1.30	1.39
1	C	67	VAL	CB-CG1	5.59	1.64	1.52
1	F	150	GLU	CG-CD	5.59	1.60	1.51
1	A	150	GLU	CG-CD	5.58	1.60	1.51
1	F	35	VAL	CB-CG1	5.54	1.64	1.52
1	D	188	TYR	CZ-OH	-5.53	1.28	1.37
1	C	150	GLU	CD-OE2	5.53	1.31	1.25
1	F	220	GLU	CD-OE2	5.44	1.31	1.25
1	C	131	GLY	C-N	-5.35	1.21	1.34
1	C	230	TYR	CE1-CZ	5.34	1.45	1.38
1	C	236	SER	CB-OG	-5.21	1.35	1.42
1	D	188	TYR	CD1-CE1	-5.14	1.31	1.39
1	F	112	GLU	CB-CG	5.07	1.61	1.52
1	B	284	PHE	CB-CG	-5.02	1.42	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	ARG	O-C-N	-10.25	101.62	121.10
1	B	59	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	C	131	GLY	N-CA-C	7.57	132.03	113.10
1	B	50	ILE	C-N-CA	-7.53	102.87	121.70
1	B	173	ILE	CB-CA-C	-7.06	97.49	111.60
1	B	90	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	E	67	VAL	CB-CA-C	-6.85	98.39	111.40
1	C	50	ILE	C-N-CA	-6.75	104.82	121.70
1	C	236	SER	CB-CA-C	6.62	122.69	110.10
1	F	173	ILE	CB-CA-C	-6.56	98.47	111.60
1	B	67	VAL	CG1-CB-CG2	-6.43	100.62	110.90
1	D	67	VAL	CB-CA-C	-6.37	99.29	111.40
1	D	173	ILE	CB-CA-C	-6.27	99.06	111.60
1	C	189	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	E	44	ARG	NE-CZ-NH2	-6.18	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	F	142	VAL	CB-CA-C	-5.88	100.22	111.40
1	B	122	LEU	CA-CB-CG	5.77	128.57	115.30
1	F	67	VAL	CB-CA-C	-5.66	100.65	111.40
1	C	131	GLY	O-C-N	-5.56	113.80	122.70
1	A	18	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	189	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	107	THR	C-N-CA	5.49	135.42	121.70
1	C	130	SER	N-CA-C	-5.46	96.27	111.00
1	B	50	ILE	O-C-N	-5.44	114.00	122.70
1	C	21	ASP	CB-CG-OD1	5.36	123.12	118.30
1	F	123	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	C	221	LYS	CD-CE-NZ	-5.10	99.98	111.70
1	C	25	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	107	THR	O-C-N	-5.03	114.66	122.70
1	C	253	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	B	18	ASP	CB-CG-OD1	5.00	122.80	118.30

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 [\(i\)](#)

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	46	0
1	B	2309	0	2229	53	0
1	C	2309	0	2227	40	0
1	D	2309	0	2229	44	0
1	E	2309	0	2229	46	0
1	F	2309	0	2229	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	13420	278	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 10.

All (278) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:MET:HA	1:B:49:MET:HE3	1.62	0.80
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: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:B:49:MET:HA	1:B:49:MET:CE	2.23	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
1:F:5:LYS:HA	1:F:5:LYS:HE3	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:264:GLU:HG3	3:B:475:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:NZ	3:B:485:HOH:O	2.30	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: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:D:221:LYS:HZ1	2:D:301:GOL:H31	1.65	0.61
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: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: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
1:F:278:THR:HG21	1:F:287:THR:HG23	1.85	0.58
1:A:39:GLU:HA	1:A:43:ALA:O	2.02	0.58
1:B:118:THR:CG2	1:B:188:TYR:OH	2.51	0.58
1:C:29:TYR:O	1:C:30:ILE:HD13	2.04	0.58
1:C:18:ASP:N	1:C:18:ASP:OD2	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:E:28:SER:HB3	1:E:50:ILE:HG12	1.87	0.57
1:F:140:GLU:HG3	1:F:143:LYS:HZ2	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:278:THR:OG1	1:A:287:THR:CG2	2.54	0.55
1:D:222:ASN:HB2	1:D:241:THR:HG22	1.87	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:53:SER:OG	1:F:56:GLU:HG3	2.07	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: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:B:49:MET:CA	1:B:49:MET:CE	2.84	0.53
1:D:13:GLY:HA2	1:D:46:VAL:O	2.09	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
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:173:ILE:CD1	1:D:202:VAL:HB	2.40	0.52
1:E:105:TRP:HH2	1:E:244:MET:HE3	1.75	0.52
1:D:221:LYS:NZ	2:D:301:GOL:H31	2.24	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:108:CYS:SG	1:C:109:LEU:N	2.84	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:O	1:A:132:ILE:HG23	2.10	0.49
1:A:79:SER:O	1:A:83:LYS:HG2	2.12	0.49
1:D:222:ASN:HB2	1:D:241:THR:HG21	1.94	0.49
1:A:250:ASN:ND2	1:A:253:ARG:HH11	2.10	0.49
1:A:94:GLU:HG2	3:A:501:HOH:O	2.12	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:B:282:SER:HB2	3:B:518:HOH:O	2.12	0.49
1:C:253:ARG:NH2	1:D:238:ILE:HD13	2.27	0.49
1:B:18:ASP:N	1:B:18:ASP:OD2	2.46	0.48
1:D:50:ILE:HG23	1:D:51:ASN:ND2	2.28	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:E:41:ALA:HB3	1:E:249:VAL:HG21	1.95	0.48
1:B:226:TRP:HB2	1:B:285:GLU:OE1	2.14	0.48
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:D:226:TRP:HB2	1:D:285:GLU:OE1	2.14	0.47
1:F:18:ASP:N	1:F:18:ASP:OD2	2.44	0.47
1:A:37:PHE:CE2	1:A:245:ALA:HB2	2.50	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:B:71:GLY:HA2	1:B:109:LEU:H	1.80	0.47
1:D:270:ILE:CD1	1:D:288:TYR:CZ	2.97	0.47
1:C:90:ARG:HD2	3:C:402:HOH:O	2.15	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:B:138:PHE:HD2	1:B:142:VAL:HG11	1.77	0.47
1:C:89:TYR:OH	1:C:118:THR:HG22	2.14	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:A:108:CYS:SG	1:A:109:LEU:N	2.88	0.46
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:25:ASP:C	1:A:26:ARG:HG3	2.35	0.46
1:D:89:TYR:CG	1:D:117:LEU:HD13	2.50	0.46
1:B:49:MET:HE2	1:B:49:MET:HB3	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:PHE:O	1:E:22:PRO:HD3	2.15	0.46
1:F:113:LEU:O	1:F:113:LEU:HD23	2.16	0.46
1:C:189:ARG:HB2	1:C:208:TYR:CE2	2.50	0.46
1:F:5:LYS:HE3	1:F:5:LYS:CA	2.44	0.46
1:B:165:THR:HB	1:B:217:TRP:CE3	2.52	0.45
1:D:15:LEU:HD13	1:D:81:TYR:CD1	2.50	0.45
1:E:187:PHE:CE2	1:E:188:TYR:CE1	3.04	0.45
1:A:103:PRO:HB2	1:A:248:PHE:CE1	2.51	0.45
1:C:23:LYS:HE2	1:C:23:LYS:HB2	1.36	0.45
1:A:285:GLU:CG	1:B:271:TYR:CE1	3.00	0.45
1:A:278:THR:OG1	1:A:287:THR:HG23	2.16	0.45
1:E:270:ILE:HG13	1:E:270:ILE:O	2.16	0.45
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:E:278:THR:OG1	1:E:287:THR:HG23	2.16	0.45
1:E:94:GLU:HA	1:E:94:GLU:OE2	2.16	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:F:186:LYS:HG3	1:F:186:LYS:O	2.16	0.44
1:D:108:CYS:SG	1:D:109:LEU:N	2.90	0.44
1:D:103:PRO:HA	1:D:211:PRO:O	2.17	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:B:101:TYR:O	1:B:255:ASN:HB2	2.17	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: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:E:111:PHE:CD2	1:E:111:PHE:C	2.91	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:138:PHE:CD2	1:D:142:VAL:HG11	2.53	0.44
1:D:50:ILE:O	1:D:57:TYR:OH	2.35	0.44
1:B:173:ILE:HD12	1:B:202:VAL:HB	2.00	0.44
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:E:234:THR:O	1:E:235:PRO:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:178:PHE:C	1:C:178:PHE:CD2	2.92	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: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
1:A:59:ARG:NH1	1:A:264:GLU:OE1	2.53	0.42
1:A:13:GLY:HA2	1:A:46:VAL:O	2.19	0.42
1:A:207:ALA:HB3	1:A:210:PHE:O	2.20	0.42
1:A:37:PHE:HB2	1:A:220:GLU:HB2	2.01	0.42
1:D:5:LYS:HB2	1:D:5:LYS:HE3	1.73	0.42
1:D:67:VAL:HG22	1:D:102:PHE:HE2	1.84	0.42
1:B:18:ASP:CG	1:B:50:ILE:HD11	2.39	0.42
1:D:182:LYS:NZ	3:D:474:HOH:O	2.49	0.42
1:A:50:ILE:HG13	1:A:80:GLY:HA3	2.02	0.42
1:C:262:THR:HG23	3:C:546:HOH:O	2.20	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:285:GLU:HG3	1:B:271:TYR:CZ	2.54	0.42
1:A:71:GLY:HA3	1:A:108:CYS:HB3	2.02	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: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:HG21	1:B:50:ILE:HD13	1.52	0.41
1:B:263:GLU:HG2	1:B:263:GLU:H	1.35	0.41
1:A:274:LYS:HA	1:A:275:PRO:HD3	1.86	0.41
1:D:255:ASN:ND2	1:D:257:HIS:H	2.17	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:A:52:LYS:CB	1:A:56:GLU:HG2	2.39	0.41
1:D:52:LYS:HB2	1:D:57:TYR:CZ	2.56	0.41
1:C:132:ILE:HD12	1:A:128:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HG13	1:B:173:ILE:H	1.55	0.40
1:A:40:SER:HA	1:B:224:PHE:CE1	2.56	0.40
1:C:111:PHE:C	1:C:111:PHE:CD2	2.95	0.40
1:E:174:THR:HA	1:E:201:PHE:HA	2.03	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
1:F:106:GLY:O	1:F:214:ALA:HA	2.21	0.40
1:B:100:ASP:OD2	1:B:257:HIS:NE2	2.35	0.40
1:D:278:THR:OG1	1:D:287:THR:CG2	2.70	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%)	34	32
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%)	34	32
1	F	285/312 (91%)	274 (96%)	11 (4%)	0	100	100
All	All	1710/1872 (91%)	1627 (95%)	81 (5%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

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

### 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	250/272 (92%)	227 (91%)	23 (9%)	9	6
1	B	250/272 (92%)	233 (93%)	17 (7%)	16	13
1	C	250/272 (92%)	235 (94%)	15 (6%)	19	16
1	D	250/272 (92%)	226 (90%)	24 (10%)	8	5
1	E	250/272 (92%)	230 (92%)	20 (8%)	12	8
1	F	250/272 (92%)	225 (90%)	25 (10%)	7	5
All	All	1500/1632 (92%)	1376 (92%)	124 (8%)	11	7

All (124) 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	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	182	LYS
1	C	236	SER
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
1	D	60	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	67	VAL
1	D	74	VAL
1	D	108	CYS
1	D	113	LEU
1	D	118	THR
1	D	121	GLU
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	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
1	A	285	GLU
1	A	287	THR
1	B	15	LEU
1	B	18	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	23	LYS
1	B	52	LYS
1	B	108	CYS
1	B	113	LEU
1	B	118	THR
1	B	143	LYS
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	264	GLU
1	B	281	GLN
1	B	287	THR
1	E	15	LEU
1	E	18	ASP
1	E	55	ASP
1	E	56	GLU
1	E	67	VAL
1	E	108	CYS
1	E	111	PHE
1	E	113	LEU
1	E	142	VAL
1	E	143	LYS
1	E	147	LEU
1	E	166	GLU
1	E	170	GLN
1	E	176	GLU
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	54	GLU
1	F	60	LEU

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Mol	Chain	Res	Type
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	140	GLU
1	F	142	VAL
1	F	147	LEU
1	F	166	GLU
1	F	173	ILE
1	F	185	LYS
1	F	241	THR
1	F	263	GLU
1	F	280	ILE
1	F	282	SER
1	F	287	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	ASN
1	C	167	ASN
1	C	170	GLN
1	C	250	ASN
1	D	51	ASN
1	D	250	ASN
1	D	255	ASN
1	D	286	GLN
1	A	167	ASN
1	A	250	ASN
1	B	255	ASN
1	B	272	ASN
1	B	281	GLN
1	B	286	GLN
1	E	167	ASN
1	E	250	ASN
1	F	167	ASN
1	F	216	GLN
1	F	255	ASN
1	F	286	GLN

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Mol	Chain	Res	Type
1	F	291	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 carbohydrates 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	GOL	A	301	-	5,5,5	1.07	0	5,5,5	1.03	0
2	GOL	C	301	-	5,5,5	0.79	0	5,5,5	0.96	0
2	GOL	E	301	-	5,5,5	0.62	0	5,5,5	1.13	0
2	GOL	B	301	-	5,5,5	0.37	0	5,5,5	0.28	0
2	GOL	D	301	-	5,5,5	0.91	0	5,5,5	1.05	0
2	GOL	F	301	-	5,5,5	0.43	0	5,5,5	1.10	1 (20%)

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	A	301	-	-	0/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-
2	GOL	E	301	-	-	2/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	D	301	-	-	2/4/4/4	-
2	GOL	F	301	-	-	3/4/4/4	-

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	2.15	118.61	109.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	287/312 (91%)	0.12	15 (5%) 27 32	17, 29, 46, 59	9 (3%)
1	B	287/312 (91%)	0.01	10 (3%) 44 50	13, 28, 43, 49	5 (1%)
1	C	287/312 (91%)	-0.16	6 (2%) 63 68	7, 22, 35, 46	9 (3%)
1	D	287/312 (91%)	0.13	9 (3%) 49 55	13, 29, 49, 59	5 (1%)
1	E	287/312 (91%)	0.26	16 (5%) 24 29	20, 36, 50, 58	9 (3%)
1	F	287/312 (91%)	0.26	17 (5%) 22 27	19, 32, 54, 61	5 (1%)
All	All	1722/1872 (91%)	0.10	73 (4%) 36 42	7, 29, 48, 61	42 (2%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	202	VAL	5.5
1	B	20	PHE	5.4
1	A	179	THR	4.5
1	E	20	PHE	4.1
1	E	50	ILE	4.1
1	A	202	VAL	4.0
1	F	250	ASN	4.0
1	B	158	SER	3.9
1	B	250	ASN	3.8
1	F	20	PHE	3.7
1	F	68	LEU	3.7
1	F	24	PRO	3.4
1	C	250	ASN	3.2
1	F	50	ILE	3.2
1	D	281	GLN	3.2
1	D	250	ASN	3.2
1	C	202	VAL	3.2
1	A	20	PHE	3.1
1	A	14	VAL	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	283	ALA	3.1
1	C	20	PHE	3.1
1	A	5	LYS	3.0
1	E	281	GLN	3.0
1	E	260	ALA	3.0
1	F	105	TRP	2.9
1	C	115	THR	2.9
1	B	281	GLN	2.9
1	D	105	TRP	2.8
1	F	280	ILE	2.8
1	A	115	THR	2.8
1	E	250	ASN	2.8
1	F	262	THR	2.7
1	F	283	ALA	2.7
1	B	105	TRP	2.7
1	B	24	PRO	2.5
1	E	115	THR	2.5
1	E	105	TRP	2.5
1	F	115	THR	2.5
1	E	182	LYS	2.5
1	B	67	VAL	2.5
1	E	55	ASP	2.4
1	D	20	PHE	2.4
1	A	68	LEU	2.4
1	F	5	LYS	2.4
1	B	68	LEU	2.4
1	E	21	ASP	2.4
1	D	115	THR	2.4
1	E	179	THR	2.4
1	D	106	GLY	2.3
1	E	122	LEU	2.3
1	A	67	VAL	2.3
1	B	283	ALA	2.3
1	A	283	ALA	2.3
1	A	250	ASN	2.3
1	F	98	ASN	2.2
1	D	78	SER	2.2
1	F	38	LEU	2.2
1	A	131	GLY	2.2
1	A	143	LYS	2.1
1	F	59	ARG	2.1
1	A	280	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	143	LYS	2.1
1	E	107	THR	2.1
1	A	153	GLU	2.1
1	B	38	LEU	2.1
1	A	56	GLU	2.1
1	E	67	VAL	2.1
1	F	55	ASP	2.0
1	C	67	VAL	2.0
1	D	98	ASN	2.0
1	E	78	SER	2.0
1	D	50	ILE	2.0
1	F	108	CYS	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 carbohydrates 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	GOL	B	301	6/6	0.70	0.21	42,45,46,46	0
2	GOL	E	301	6/6	0.80	0.22	41,46,48,48	0
2	GOL	D	301	6/6	0.82	0.14	31,33,35,36	0
2	GOL	A	301	6/6	0.85	0.17	25,30,33,35	0
2	GOL	C	301	6/6	0.87	0.16	21,28,31,32	0
2	GOL	F	301	6/6	0.89	0.14	35,44,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.