



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 12:18 AM EST

PDB ID : 1YVB  
Title : the Plasmodium falciparum Cysteine Protease Falcipain-2  
Authors : Wang, S.X.  
Deposited on : 2005-02-15  
Resolution : 2.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

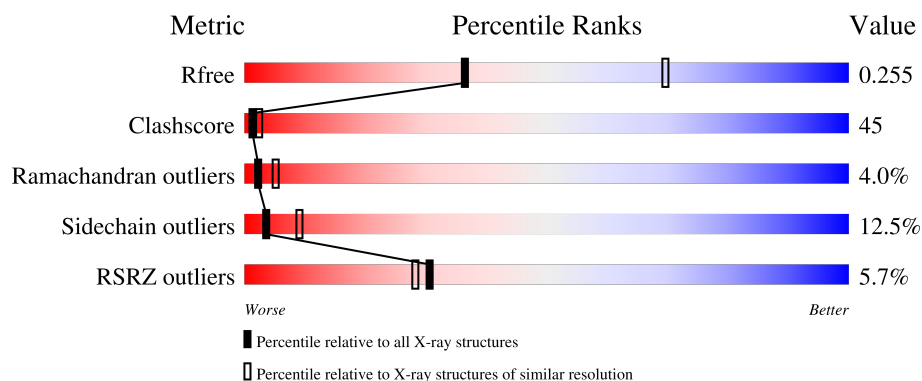
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	241	<div> <div>3%</div> <div>52%</div> <div>34%</div> <div>9%</div> <div>5%</div> </div>
2	I	111	<div> <div>12%</div> <div>32%</div> <div>30%</div> <div>23%</div> <div>14%</div> </div>

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
3	GOL	A	1001	-	X	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2809 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 falcipain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1908	1210	315	369	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0K	ARG	LYS	engineered mutation	UNP Q9N6S8
A	0M	GLU	ASN	engineered mutation	UNP Q9N6S8
A	82	PRO	THR	engineered mutation	UNP Q9N6S8
A	84	GLY	ASP	engineered mutation	UNP Q9N6S8

- Molecule 2 is a protein called Cystatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	111	Total	C	N	O	S	8	0	0
			881	553	153	169	6			

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		

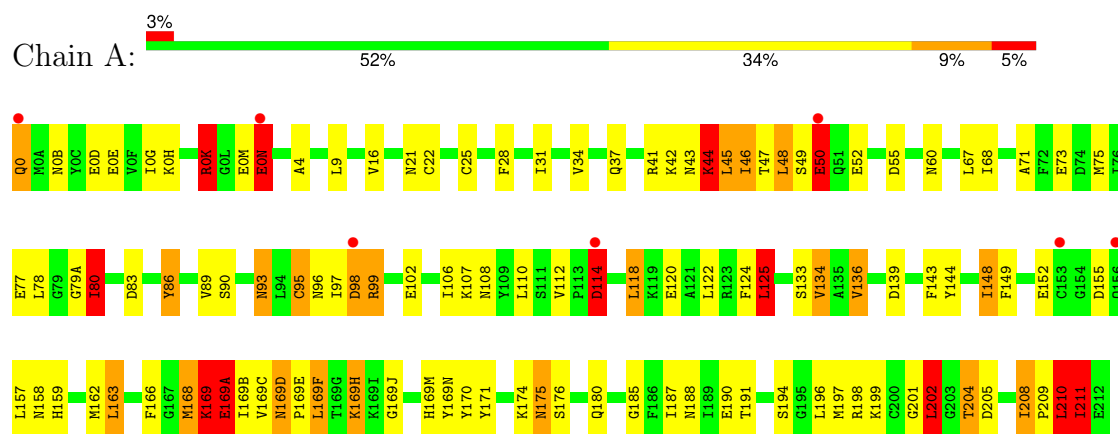
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		

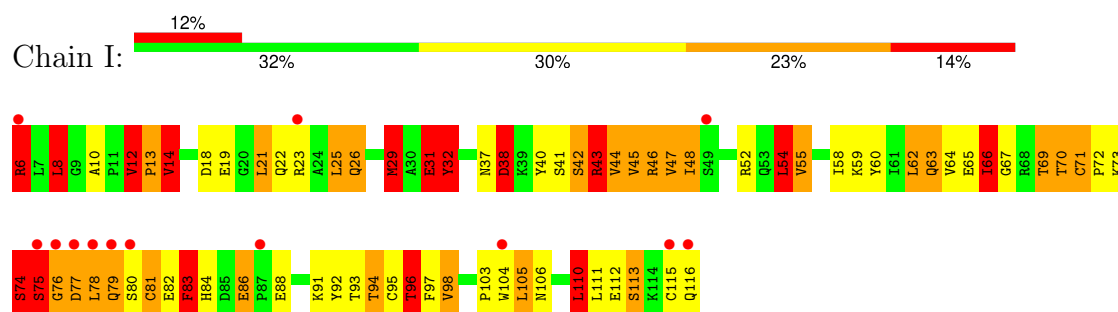
### 3 Residue-property plots [i](#)

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: falcipain 2



#### • Molecule 2: Cystatin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.04Å 96.04Å 124.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.00-2.70) 95.6 (40.00-2.71)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.264 0.226 , 0.255	Depositor DCC
$R_{free}$ test set	769 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 67.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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	0.71	2/1951 (0.1%)	1.67	65/2630 (2.5%)
2	I	1.21	8/896 (0.9%)	3.26	82/1209 (6.8%)
All	All	0.90	10/2847 (0.4%)	2.29	147/3839 (3.8%)

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	3
2	I	0	8
All	All	0	11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	31	GLU	C-N	-23.80	0.79	1.34
1	A	43	ASN	C-N	-18.62	0.91	1.34
1	A	0	GLN	C-N	-15.94	0.97	1.34
2	I	76	GLY	N-CA	-6.75	1.35	1.46
2	I	75	SER	C-N	-6.74	1.21	1.33
2	I	43	ARG	N-CA	-6.36	1.33	1.46
2	I	81	CYS	C-O	-6.35	1.11	1.23
2	I	74	SER	C-N	6.16	1.48	1.34
2	I	81	CYS	CA-C	6.13	1.68	1.52
2	I	76	GLY	C-N	6.03	1.48	1.34

All (147) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	23	ARG	NE-CZ-NH1	-36.33	102.14	120.30
2	I	23	ARG	NE-CZ-NH2	32.35	136.48	120.30
2	I	6	ARG	NE-CZ-NH2	-32.09	104.26	120.30
2	I	46	ARG	NE-CZ-NH1	-31.97	104.31	120.30
2	I	6	ARG	NE-CZ-NH1	29.62	135.11	120.30
2	I	46	ARG	NE-CZ-NH2	28.98	134.79	120.30
2	I	8	LEU	O-C-N	-22.79	84.47	123.20
1	A	0(K)	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	A	114	ASP	CB-CG-OD2	-20.07	100.24	118.30
1	A	114	ASP	CB-CG-OD1	19.90	136.21	118.30
1	A	155	ASP	CB-CG-OD1	-17.46	102.59	118.30
2	I	6	ARG	CD-NE-CZ	-16.16	100.97	123.60
1	A	98	ASP	CB-CG-OD1	-15.66	104.21	118.30
1	A	155	ASP	CB-CG-OD2	15.15	131.94	118.30
1	A	99	ARG	NE-CZ-NH1	-14.83	112.89	120.30
2	I	31	GLU	O-C-N	-14.80	99.02	122.70
1	A	98	ASP	CB-CG-OD2	13.91	130.82	118.30
1	A	43	ASN	C-N-CA	13.27	154.88	121.70
1	A	0(K)	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	A	43	ASN	O-C-N	-12.95	101.99	122.70
2	I	111	LEU	CB-CG-CD2	12.15	131.66	111.00
2	I	83	PHE	CB-CG-CD1	-11.91	112.47	120.80
2	I	29	MET	CG-SD-CE	-11.83	81.27	100.20
1	A	204	THR	CA-CB-CG2	-11.79	95.89	112.40
1	A	78	LEU	CB-CG-CD2	11.04	129.76	111.00
2	I	93	THR	CA-CB-CG2	10.88	127.64	112.40
2	I	98	VAL	CA-CB-CG1	-10.64	94.94	110.90
2	I	64	VAL	CA-CB-CG2	-10.62	94.97	110.90
2	I	64	VAL	CA-CB-CG1	10.29	126.33	110.90
2	I	38	ASP	CB-CG-OD2	-10.16	109.16	118.30
2	I	12	VAL	CA-CB-CG2	-10.02	95.88	110.90
1	A	99	ARG	NE-CZ-NH2	9.92	125.26	120.30
2	I	25	LEU	CB-CG-CD2	9.71	127.50	111.00
1	A	80	ILE	CA-CB-CG1	-9.51	92.93	111.00
1	A	210	LEU	CB-CG-CD2	-9.51	94.84	111.00
2	I	8	LEU	CB-CG-CD1	9.45	127.06	111.00
2	I	12	VAL	CA-CB-CG1	9.39	124.98	110.90
2	I	47	VAL	CA-CB-CG2	-9.30	96.95	110.90
2	I	63	GLN	CG-CD-OE1	9.08	139.76	121.60
1	A	78	LEU	CB-CG-CD1	-8.85	95.95	111.00
2	I	62	LEU	CB-CG-CD1	-8.71	96.20	111.00
1	A	43	ASN	CA-C-N	8.51	135.93	117.20
1	A	89	VAL	CA-CB-CG1	8.50	123.65	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASP	CA-CB-CG	-8.35	95.04	113.40
2	I	6	ARG	CG-CD-NE	-8.30	94.38	111.80
2	I	63	GLN	CG-CD-NE2	-8.29	96.81	116.70
2	I	86	GLU	CG-CD-OE2	-8.29	101.72	118.30
2	I	38	ASP	CB-CG-OD1	8.18	125.66	118.30
2	I	66	ILE	CA-CB-CG1	8.17	126.53	111.00
2	I	86	GLU	CG-CD-OE1	8.17	134.63	118.30
1	A	202	LEU	CB-CG-CD2	8.15	124.85	111.00
1	A	169(A)	GLU	CG-CD-OE1	8.11	134.53	118.30
2	I	96	THR	CA-CB-OG1	-8.11	91.97	109.00
1	A	210	LEU	CB-CG-CD1	8.08	124.74	111.00
1	A	93	ASN	CB-CG-OD1	8.04	137.68	121.60
2	I	31	GLU	C-N-CA	8.04	141.80	121.70
2	I	22	GLN	CA-CB-CG	-7.99	95.83	113.40
1	A	0(N)	GLU	CB-CG-CD	-7.98	92.65	114.20
1	A	169	LYS	CD-CE-NZ	-7.95	93.42	111.70
2	I	111	LEU	CB-CG-CD1	-7.94	97.50	111.00
1	A	169(A)	GLU	CG-CD-OE2	-7.92	102.46	118.30
2	I	54	LEU	CB-CG-CD2	-7.88	97.59	111.00
2	I	6	ARG	CA-CB-CG	-7.88	96.07	113.40
1	A	98	ASP	CA-CB-CG	-7.85	96.12	113.40
1	A	44	LYS	O-C-N	-7.81	110.21	122.70
1	A	125	LEU	CA-CB-CG	-7.80	97.35	115.30
1	A	118	LEU	CA-CB-CG	-7.80	97.36	115.30
2	I	29	MET	CA-CB-CG	-7.79	100.05	113.30
2	I	21	LEU	CB-CG-CD1	-7.78	97.78	111.00
2	I	74	SER	O-C-N	-7.77	110.26	122.70
2	I	8	LEU	CB-CG-CD2	-7.77	97.80	111.00
2	I	31	GLU	CA-C-N	7.77	134.29	117.20
1	A	93	ASN	CB-CG-ND2	-7.62	98.41	116.70
1	A	112	VAL	CA-CB-CG1	7.62	122.33	110.90
2	I	22	GLN	CG-CD-NE2	-7.62	98.41	116.70
1	A	0(N)	GLU	CA-CB-CG	-7.57	96.75	113.40
2	I	62	LEU	CA-CB-CG	-7.56	97.91	115.30
2	I	25	LEU	CA-CB-CG	-7.47	98.13	115.30
1	A	169(H)	LYS	CD-CE-NZ	-7.46	94.55	111.70
1	A	118	LEU	CB-CG-CD1	-7.38	98.46	111.00
2	I	69	THR	CA-CB-OG1	-7.37	93.53	109.00
2	I	23	ARG	CA-CB-CG	-7.37	97.19	113.40
1	A	45	LEU	CB-CG-CD2	7.35	123.49	111.00
2	I	62	LEU	CB-CG-CD2	7.29	123.40	111.00
2	I	48	ILE	CA-CB-CG1	7.28	124.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	105	LEU	CB-CG-CD1	-7.25	98.68	111.00
2	I	32	TYR	CA-C-N	-7.21	101.34	117.20
2	I	22	GLN	CG-CD-OE1	7.18	135.97	121.60
1	A	169(F)	LEU	CA-CB-CG	-7.17	98.80	115.30
1	A	211	ILE	CA-CB-CG1	7.16	124.60	111.00
1	A	134	VAL	CA-CB-CG2	7.08	121.52	110.90
1	A	204	THR	CA-CB-OG1	7.05	123.81	109.00
2	I	14	VAL	CA-CB-CG1	-7.01	100.38	110.90
2	I	112	GLU	CA-CB-CG	6.99	128.79	113.40
2	I	8	LEU	CA-CB-CG	-6.99	99.23	115.30
2	I	70	THR	CA-CB-OG1	-6.92	94.46	109.00
2	I	26	GLN	CA-CB-CG	6.92	128.63	113.40
2	I	44	VAL	O-C-N	-6.87	111.71	122.70
1	A	202	LEU	CB-CG-CD1	-6.74	99.55	111.00
1	A	125	LEU	CB-CG-CD1	-6.69	99.63	111.00
2	I	83	PHE	CB-CG-CD2	6.65	125.45	120.80
1	A	48	LEU	CB-CG-CD1	-6.64	99.72	111.00
2	I	14	VAL	CA-CB-CG2	-6.63	100.95	110.90
1	A	77	GLU	CG-CD-OE1	-6.60	105.10	118.30
1	A	208	ILE	CB-CG1-CD1	-6.54	95.60	113.90
1	A	47	THR	CA-CB-CG2	6.53	121.55	112.40
2	I	23	ARG	CB-CG-CD	6.51	128.53	111.60
2	I	75	SER	CA-C-O	6.47	133.69	120.10
1	A	45	LEU	CA-CB-CG	6.39	130.00	115.30
2	I	6	ARG	CB-CG-CD	6.36	128.14	111.60
1	A	169(H)	LYS	CB-CG-CD	6.21	127.75	111.60
1	A	9	LEU	CB-CG-CD2	6.21	121.55	111.00
2	I	32	TYR	C-N-CA	-6.19	106.23	121.70
1	A	136	VAL	CA-CB-CG2	-6.17	101.65	110.90
2	I	65	GLU	CA-CB-CG	6.10	126.81	113.40
2	I	46	ARG	CG-CD-NE	6.08	124.57	111.80
2	I	23	ARG	CG-CD-NE	6.03	124.46	111.80
1	A	0(N)	GLU	CG-CD-OE1	-6.01	106.28	118.30
2	I	70	THR	CA-CB-CG2	5.98	120.77	112.40
1	A	80	ILE	CB-CG1-CD1	-5.91	97.34	113.90
2	I	46	ARG	CB-CG-CD	5.89	126.91	111.60
2	I	46	ARG	CD-NE-CZ	5.83	131.76	123.60
1	A	90	SER	CA-CB-OG	5.79	126.84	111.20
2	I	112	GLU	CG-CD-OE2	-5.76	106.79	118.30
1	A	50	GLU	CG-CD-OE1	-5.75	106.80	118.30
2	I	44	VAL	CA-C-O	5.75	132.17	120.10
2	I	42	SER	CA-C-O	5.69	132.06	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	GLU	CG-CD-OE2	5.63	129.56	118.30
2	I	63	GLN	CB-CG-CD	5.60	126.16	111.60
1	A	169(H)	LYS	CA-CB-CG	5.58	125.68	113.40
1	A	169	LYS	CG-CD-CE	5.55	128.56	111.90
2	I	81	CYS	CA-C-N	-5.53	105.04	117.20
1	A	169(F)	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	A	211	ILE	CA-CB-CG2	-5.47	99.95	110.90
2	I	65	GLU	CG-CD-OE1	-5.38	107.54	118.30
1	A	0(N)	GLU	CG-CD-OE2	5.38	129.05	118.30
1	A	80	ILE	CA-CB-CG2	5.35	121.61	110.90
2	I	86	GLU	CA-CB-CG	5.33	125.12	113.40
1	A	47	THR	CA-CB-OG1	-5.33	97.81	109.00
1	A	78	LEU	CA-CB-CG	-5.25	103.24	115.30
2	I	110	LEU	CA-CB-CG	5.24	127.34	115.30
2	I	45	VAL	CA-CB-CG2	5.22	118.72	110.90
2	I	29	MET	CB-CG-SD	5.21	128.03	112.40
2	I	66	ILE	CA-CB-CG2	-5.16	100.58	110.90
2	I	110	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	9	LEU	CA-CB-CG	5.06	126.94	115.30
2	I	110	LEU	CB-CG-CD1	-5.04	102.42	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	GLN	Mainchain
1	A	0(K)	ARG	Sidechain
1	A	44	LYS	Mainchain
2	I	10	ALA	Mainchain
2	I	31	GLU	Mainchain
2	I	32	TYR	Mainchain
2	I	6	ARG	Sidechain
2	I	74	SER	Mainchain
2	I	77	ASP	Mainchain
2	I	8	LEU	Mainchain
2	I	83	PHE	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1908	0	1825	137	0
2	I	881	0	873	110	0
3	A	6	0	4	8	0
4	A	14	0	0	1	0
All	All	2809	0	2702	244	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 45.

All (244) 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)
2:I:63:GLN:HE22	2:I:96:THR:CG2	1.04	1.60
1:A:114:ASP:CG	3:A:1001:GOL:H11	1.37	1.45
2:I:63:GLN:NE2	2:I:96:THR:CG2	1.82	1.41
1:A:114:ASP:OD1	3:A:1001:GOL:C3	1.70	1.39
2:I:13:PRO:O	2:I:14:VAL:HG12	1.18	1.31
1:A:79(A):GLY:C	1:A:80:ILE:CD1	1.99	1.28
1:A:202:LEU:HD12	1:A:202:LEU:O	1.25	1.26
2:I:63:GLN:NE2	2:I:96:THR:HG23	1.45	1.26
2:I:31:GLU:O	2:I:32:TYR:N	1.56	1.25
1:A:80:ILE:CD1	1:A:80:ILE:N	1.98	1.23
2:I:78:LEU:HD23	2:I:78:LEU:O	1.35	1.23
2:I:77:ASP:HB3	2:I:79:GLN:CG	1.59	1.21
1:A:79(A):GLY:O	1:A:80:ILE:CD1	1.91	1.18
1:A:114:ASP:OD2	3:A:1001:GOL:C1	1.91	1.18
1:A:114:ASP:OD1	3:A:1001:GOL:H11	1.22	1.18
2:I:78:LEU:O	2:I:78:LEU:CD2	1.93	1.15
1:A:201:GLY:O	1:A:204:THR:HG23	1.46	1.15
2:I:31:GLU:C	2:I:32:TYR:CA	2.14	1.15
1:A:125:LEU:CD1	1:A:125:LEU:N	2.07	1.14
1:A:114:ASP:CG	3:A:1001:GOL:C1	2.15	1.14
1:A:114:ASP:OD2	3:A:1001:GOL:H11	1.47	1.13
2:I:6:ARG:HD2	2:I:6:ARG:O	1.46	1.13
2:I:41:SER:O	2:I:69:THR:HG22	1.48	1.12
1:A:125:LEU:N	1:A:125:LEU:HD13	1.58	1.12
2:I:31:GLU:CA	2:I:32:TYR:N	2.15	1.10
2:I:31:GLU:HG2	2:I:110:LEU:HD23	1.35	1.07
1:A:114:ASP:OD2	3:A:1001:GOL:O1	1.71	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD11	1:A:163:LEU:HD22	1.26	1.07
1:A:79(A):GLY:C	1:A:80:ILE:HD13	1.66	1.07
1:A:80:ILE:N	1:A:80:ILE:HD13	1.59	1.07
2:I:77:ASP:OD2	2:I:79:GLN:HB2	1.55	1.06
1:A:79(A):GLY:O	1:A:80:ILE:HD12	1.51	1.05
2:I:63:GLN:HE22	2:I:96:THR:HG21	1.20	1.02
2:I:63:GLN:HE22	2:I:96:THR:HG23	0.96	1.00
2:I:6:ARG:NH1	2:I:6:ARG:HG2	1.38	0.99
1:A:124:PHE:C	1:A:125:LEU:CD1	2.31	0.99
2:I:13:PRO:O	2:I:14:VAL:CG1	2.12	0.98
1:A:202:LEU:HD12	1:A:202:LEU:C	1.84	0.97
1:A:114:ASP:OD1	3:A:1001:GOL:C2	2.11	0.96
1:A:209:PRO:C	1:A:210:LEU:HD22	1.85	0.96
1:A:210:LEU:N	1:A:210:LEU:CD2	2.29	0.95
2:I:63:GLN:NE2	2:I:96:THR:HG22	1.81	0.92
1:A:98:ASP:OD1	1:A:98:ASP:N	1.87	0.90
2:I:104:TRP:O	2:I:105:LEU:HD23	1.70	0.90
2:I:110:LEU:HD11	2:I:113:SER:HB3	1.52	0.90
1:A:79(A):GLY:C	1:A:80:ILE:HD12	1.74	0.89
1:A:124:PHE:C	1:A:125:LEU:HD13	1.92	0.89
2:I:21:LEU:C	2:I:21:LEU:HD23	1.93	0.89
2:I:78:LEU:HD23	2:I:78:LEU:C	1.93	0.88
1:A:202:LEU:O	1:A:202:LEU:CD1	2.18	0.88
1:A:201:GLY:O	1:A:204:THR:CG2	2.21	0.87
2:I:63:GLN:HE22	2:I:96:THR:HG22	1.31	0.87
2:I:69:THR:OG1	2:I:82:GLU:O	1.94	0.85
2:I:77:ASP:HB3	2:I:79:GLN:HG3	1.58	0.85
2:I:31:GLU:C	2:I:32:TYR:N	0.79	0.84
2:I:77:ASP:CB	2:I:79:GLN:HB2	2.08	0.82
1:A:124:PHE:C	1:A:125:LEU:HD12	1.98	0.82
2:I:21:LEU:HD23	2:I:21:LEU:O	1.80	0.82
1:A:209:PRO:C	1:A:210:LEU:CD2	2.47	0.81
2:I:31:GLU:HG2	2:I:110:LEU:CD2	2.08	0.81
1:A:210:LEU:HD22	1:A:210:LEU:N	1.91	0.81
2:I:77:ASP:HB3	2:I:79:GLN:CB	2.10	0.81
1:A:210:LEU:N	1:A:210:LEU:HD23	1.95	0.80
2:I:6:ARG:O	2:I:6:ARG:CD	2.30	0.80
2:I:12:VAL:HG22	2:I:13:PRO:HD2	1.63	0.80
2:I:77:ASP:O	2:I:78:LEU:HB3	1.80	0.80
1:A:136:VAL:CG2	1:A:158:ASN:HD21	1.94	0.80
1:A:209:PRO:O	1:A:210:LEU:HD22	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:C	1:A:202:LEU:CD1	2.51	0.79
2:I:77:ASP:CG	2:I:79:GLN:HB2	2.03	0.78
1:A:148:ILE:HD12	1:A:170:TYR:HB3	1.63	0.78
2:I:54:LEU:HD22	2:I:55:VAL:N	1.98	0.78
1:A:124:PHE:O	1:A:125:LEU:HD12	1.84	0.78
1:A:134:VAL:HG23	1:A:202:LEU:HB3	1.65	0.78
2:I:12:VAL:HG22	2:I:13:PRO:CD	2.15	0.77
1:A:175:ASN:ND2	1:A:176:SER:H	1.83	0.75
1:A:198:ARG:HH12	1:A:204:THR:HG22	1.52	0.75
2:I:67:GLY:HA3	2:I:83:PHE:CE2	2.21	0.75
1:A:168:MET:HE2	1:A:169:LYS:C	2.08	0.74
2:I:67:GLY:CA	2:I:83:PHE:HE2	2.01	0.74
2:I:47:VAL:HG23	2:I:47:VAL:O	1.86	0.74
2:I:77:ASP:CB	2:I:79:GLN:CG	2.53	0.74
2:I:113:SER:O	2:I:113:SER:OG	2.05	0.73
2:I:77:ASP:OD2	2:I:79:GLN:CB	2.36	0.72
1:A:79(A):GLY:O	1:A:80:ILE:HD11	1.88	0.72
1:A:169(C):VAL:HA	1:A:169(J):GLY:HA2	1.69	0.72
2:I:31:GLU:CG	2:I:110:LEU:HD23	2.18	0.71
2:I:14:VAL:O	2:I:14:VAL:HG13	1.89	0.71
1:A:55:ASP:OD2	1:A:93:ASN:ND2	2.24	0.71
1:A:60:ASN:HD21	1:A:67:LEU:H	1.37	0.70
2:I:6:ARG:HG3	2:I:6:ARG:NH2	1.94	0.70
2:I:67:GLY:C	2:I:83:PHE:HE2	1.94	0.70
1:A:0(K):ARG:HD3	1:A:124:PHE:CE2	2.26	0.70
1:A:60:ASN:ND2	1:A:67:LEU:H	1.88	0.69
2:I:78:LEU:O	2:I:78:LEU:HD22	1.88	0.69
2:I:54:LEU:CD2	2:I:55:VAL:N	2.55	0.69
2:I:66:ILE:HG21	2:I:95:CYS:SG	2.33	0.69
2:I:77:ASP:CB	2:I:79:GLN:CB	2.68	0.69
1:A:157:LEU:HD11	1:A:204:THR:OG1	1.93	0.69
2:I:6:ARG:HG2	2:I:6:ARG:HH11	1.54	0.68
2:I:13:PRO:C	2:I:14:VAL:HG12	2.11	0.68
1:A:44:LYS:HE3	1:A:46:ILE:HG22	1.75	0.67
1:A:169(D):ASN:ND2	1:A:169(F):LEU:H	1.92	0.67
1:A:0(K):ARG:HG2	1:A:0(K):ARG:HH11	1.59	0.67
2:I:67:GLY:CA	2:I:83:PHE:CE2	2.78	0.67
1:A:44:LYS:HE3	1:A:46:ILE:CG2	2.24	0.67
2:I:38:ASP:OD1	2:I:40:TYR:N	2.25	0.66
1:A:136:VAL:HG23	1:A:158:ASN:HD21	1.61	0.66
2:I:29:MET:O	2:I:32:TYR:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:70:THR:O	2:I:70:THR:OG1	2.15	0.65
1:A:169(D):ASN:HD22	1:A:169(E):PRO:CD	2.08	0.65
1:A:169(D):ASN:HD22	1:A:169(E):PRO:HD2	1.62	0.65
2:I:63:GLN:CD	2:I:96:THR:HG23	2.16	0.65
1:A:42:LYS:HE2	1:A:211:ILE:HD12	1.79	0.65
1:A:169:LYS:HD3	1:A:169(A):GLU:N	2.13	0.64
1:A:169(B):ILE:HD12	1:A:169(M):HIS:ND1	2.11	0.64
1:A:175:ASN:HD22	1:A:176:SER:H	1.46	0.64
2:I:31:GLU:O	2:I:32:TYR:CA	2.32	0.64
1:A:28:PHE:HA	1:A:50:GLU:OE1	1.98	0.63
2:I:94:THR:O	2:I:116:GLN:HG2	1.98	0.63
1:A:97:ILE:HG13	1:A:98:ASP:N	2.13	0.62
1:A:0(B):ASN:HB3	1:A:0(D):GLU:OE1	1.99	0.62
1:A:46:ILE:HD13	1:A:46:ILE:H	1.64	0.62
1:A:134:VAL:HG23	1:A:202:LEU:CB	2.30	0.62
2:I:32:TYR:O	2:I:32:TYR:CD2	2.54	0.61
1:A:148:ILE:HG12	1:A:148:ILE:O	2.01	0.61
2:I:8:LEU:N	2:I:8:LEU:CD1	2.63	0.61
2:I:78:LEU:CD2	2:I:78:LEU:C	2.61	0.61
2:I:67:GLY:C	2:I:83:PHE:CE2	2.75	0.60
2:I:21:LEU:C	2:I:21:LEU:CD2	2.69	0.60
1:A:0(G):ILE:O	1:A:0(K):ARG:HB3	2.02	0.59
2:I:14:VAL:CG1	2:I:14:VAL:O	2.50	0.59
1:A:136:VAL:HG21	2:I:54:LEU:HD12	1.84	0.59
2:I:19:GLU:H	2:I:19:GLU:CD	2.06	0.59
2:I:77:ASP:O	2:I:78:LEU:CB	2.45	0.59
1:A:0(K):ARG:NH1	1:A:120:GLU:OE2	2.35	0.59
1:A:185:GLY:HA2	4:A:1014:HOH:O	2.03	0.59
2:I:97:PHE:CD1	2:I:113:SER:HB2	2.37	0.59
2:I:32:TYR:CD2	2:I:32:TYR:C	2.75	0.59
2:I:25:LEU:HD23	2:I:25:LEU:O	2.02	0.58
1:A:169(D):ASN:HD22	1:A:169(E):PRO:N	2.01	0.58
2:I:41:SER:O	2:I:69:THR:CG2	2.39	0.58
2:I:54:LEU:HD22	2:I:54:LEU:C	2.24	0.58
2:I:54:LEU:CD2	2:I:55:VAL:H	2.15	0.57
1:A:37:GLN:HE22	1:A:41:ARG:HE	1.53	0.56
2:I:48:ILE:HD11	2:I:94:THR:CG2	2.35	0.56
1:A:49:SER:HB2	1:A:83:ASP:HA	1.88	0.55
2:I:97:PHE:HD1	2:I:113:SER:HB2	1.69	0.55
1:A:136:VAL:CG2	1:A:158:ASN:ND2	2.67	0.55
2:I:69:THR:OG1	2:I:70:THR:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169(D):ASN:HD22	1:A:169(D):ASN:C	2.10	0.55
1:A:194:SER:OG	1:A:196:LEU:HD13	2.07	0.55
1:A:124:PHE:O	1:A:125:LEU:CD1	2.50	0.54
1:A:175:ASN:HD22	1:A:176:SER:N	2.04	0.54
2:I:31:GLU:CG	2:I:110:LEU:CD2	2.81	0.54
1:A:98:ASP:OD1	1:A:98:ASP:C	2.33	0.53
1:A:34:VAL:HG12	1:A:209:PRO:HG3	1.90	0.53
1:A:136:VAL:HG22	1:A:158:ASN:ND2	2.23	0.53
2:I:71:CYS:SG	2:I:72:PRO:HD2	2.49	0.53
1:A:133:SER:OG	1:A:205:ASP:HB2	2.08	0.52
1:A:169:LYS:HD3	1:A:169(A):GLU:H	1.74	0.52
2:I:98:VAL:O	2:I:98:VAL:HG12	2.07	0.52
1:A:122:LEU:CD1	1:A:163:LEU:HD22	2.19	0.52
2:I:52:ARG:HD3	2:I:60:TYR:CE2	2.45	0.52
2:I:38:ASP:OD1	2:I:40:TYR:HB2	2.09	0.52
1:A:107:LYS:O	1:A:108:ASN:HB2	2.09	0.52
1:A:169(D):ASN:ND2	1:A:169(D):ASN:C	2.62	0.52
1:A:175:ASN:ND2	1:A:176:SER:N	2.57	0.52
2:I:54:LEU:CD2	2:I:54:LEU:C	2.73	0.52
1:A:143:PHE:CE1	2:I:103:PRO:HB2	2.46	0.51
2:I:44:VAL:HG12	2:I:46:ARG:N	2.26	0.51
1:A:0(D):GLU:O	1:A:0(H):LYS:HE3	2.11	0.51
1:A:97:ILE:HG13	1:A:98:ASP:H	1.75	0.51
1:A:198:ARG:HH12	1:A:204:THR:CG2	2.22	0.51
2:I:70:THR:HG22	2:I:84:HIS:HA	1.92	0.51
1:A:99:ARG:O	1:A:99:ARG:HG2	2.11	0.51
1:A:139:ASP:OD2	1:A:152:GLU:HB2	2.10	0.51
2:I:8:LEU:N	2:I:8:LEU:HD12	2.25	0.50
2:I:69:THR:HA	2:I:83:PHE:HA	1.93	0.50
2:I:42:SER:O	2:I:43:ARG:CB	2.52	0.50
1:A:136:VAL:HG22	1:A:158:ASN:HD21	1.70	0.50
1:A:180:GLN:HA	1:A:180:GLN:NE2	2.26	0.50
1:A:122:LEU:HD21	1:A:163:LEU:O	2.12	0.50
2:I:25:LEU:HD23	2:I:25:LEU:C	2.32	0.50
1:A:55:ASP:HB3	1:A:95:CYS:HB2	1.94	0.49
1:A:134:VAL:CG2	1:A:202:LEU:HB3	2.37	0.49
2:I:62:LEU:O	2:I:96:THR:HA	2.13	0.49
2:I:58:ILE:HD12	2:I:58:ILE:N	2.27	0.49
2:I:78:LEU:HA	2:I:79:GLN:O	2.13	0.49
1:A:169(N):TYR:HB2	1:A:191:THR:O	2.13	0.48
2:I:48:ILE:HB	2:I:63:GLN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0(M):GLU:O	1:A:0(N):GLU:C	2.51	0.48
2:I:45:VAL:HG21	2:I:92:TYR:CE2	2.49	0.48
1:A:31:ILE:CD1	1:A:50:GLU:HA	2.44	0.47
2:I:73:LYS:O	2:I:74:SER:OG	2.32	0.47
1:A:68:ILE:O	1:A:71:ALA:HB3	2.14	0.47
1:A:170:TYR:HA	1:A:191:THR:HG22	1.96	0.47
1:A:168:MET:HE2	1:A:169:LYS:O	2.15	0.47
2:I:73:LYS:O	2:I:75:SER:N	2.48	0.46
1:A:148:ILE:HA	1:A:188:ASN:HB2	1.97	0.46
1:A:198:ARG:NH1	1:A:204:THR:HG22	2.25	0.46
1:A:125:LEU:HB3	1:A:208:ILE:CD1	2.46	0.46
1:A:149:PHE:CD1	1:A:149:PHE:C	2.89	0.46
2:I:45:VAL:HG21	2:I:92:TYR:HE2	1.81	0.45
2:I:103:PRO:C	2:I:105:LEU:H	2.20	0.45
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.75	0.45
1:A:125:LEU:HB3	1:A:208:ILE:HD11	1.99	0.45
1:A:144:TYR:CZ	1:A:187:ILE:HG13	2.52	0.45
1:A:199:LYS:HE2	1:A:199:LYS:HB3	1.72	0.44
1:A:80:ILE:HD12	1:A:80:ILE:HA	1.02	0.44
2:I:46:ARG:HH11	2:I:46:ARG:HD3	1.54	0.44
1:A:106:ILE:HA	1:A:211:ILE:HG22	2.00	0.44
2:I:54:LEU:HD23	2:I:55:VAL:H	1.81	0.44
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.14	0.44
1:A:168:MET:HG3	1:A:169(N):TYR:CE2	2.53	0.44
1:A:0(E):GLU:OE1	1:A:0(E):GLU:HA	2.17	0.44
1:A:0(K):ARG:HD3	1:A:124:PHE:CZ	2.52	0.44
2:I:95:CYS:HA	2:I:115:CYS:HA	1.98	0.44
1:A:50:GLU:H	1:A:50:GLU:HG2	1.37	0.43
1:A:168:MET:HE2	1:A:169:LYS:N	2.32	0.43
1:A:0(H):LYS:HE3	1:A:0(H):LYS:HB2	1.82	0.43
1:A:162:MET:SD	1:A:174:LYS:HD3	2.58	0.43
2:I:104:TRP:C	2:I:105:LEU:HD23	2.36	0.43
1:A:96:ASN:OD1	1:A:98:ASP:OD1	2.36	0.43
2:I:12:VAL:HG22	2:I:13:PRO:HD3	1.99	0.42
1:A:48:LEU:N	1:A:48:LEU:HD23	2.33	0.42
2:I:25:LEU:O	2:I:26:GLN:C	2.57	0.42
1:A:52:GLU:HA	1:A:86:TYR:CZ	2.55	0.42
1:A:52:GLU:HB2	1:A:86:TYR:CD1	2.55	0.42
1:A:190:GLU:HG2	1:A:197:MET:HE2	2.01	0.42
2:I:48:ILE:HD11	2:I:94:THR:HG21	2.01	0.42
1:A:208:ILE:HG21	1:A:208:ILE:HD13	1.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:CE2	1:A:187:ILE:HG13	2.56	0.41
1:A:163:LEU:HD21	1:A:171:TYR:CD1	2.55	0.41
1:A:21:ASN:HD21	2:I:59:LYS:HD2	1.86	0.41
1:A:25:CYS:HB3	1:A:159:HIS:CE1	2.55	0.41
2:I:18:ASP:O	2:I:21:LEU:N	2.49	0.41
1:A:71:ALA:O	1:A:75:MET:HG3	2.21	0.41
1:A:148:ILE:HD11	1:A:190:GLU:HA	2.03	0.41
1:A:169(F):LEU:HA	1:A:169(F):LEU:HD12	1.35	0.41
1:A:136:VAL:HG22	1:A:136:VAL:H	1.69	0.40
1:A:4:ALA:HA	1:A:166:PHE:CD1	2.57	0.40
1:A:97:ILE:O	1:A:99:ARG:N	2.53	0.40
2:I:54:LEU:HD23	2:I:54:LEU:HA	1.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/241 (99%)	216 (90%)	20 (8%)	3 (1%)	10	26
2	I	109/111 (98%)	85 (78%)	13 (12%)	11 (10%)	0	0
All	All	348/352 (99%)	301 (86%)	33 (10%)	14 (4%)	2	5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	75	SER
2	I	78	LEU
2	I	88	GLU
1	A	0(N)	GLU
1	A	114	ASP
2	I	55	VAL

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Mol	Chain	Res	Type
2	I	81	CYS
2	I	14	VAL
1	A	22	CYS
2	I	79	GLN
2	I	91	LYS
2	I	106	ASN
2	I	13	PRO
2	I	76	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	206/206 (100%)	184 (89%)	22 (11%)	5	13
2	I	99/99 (100%)	83 (84%)	16 (16%)	2	5
All	All	305/305 (100%)	267 (88%)	38 (12%)	3	9

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	45	LEU
1	A	46	ILE
1	A	50	GLU
1	A	73	GLU
1	A	80	ILE
1	A	86	TYR
1	A	95	CYS
1	A	102	GLU
1	A	110	LEU
1	A	125	LEU
1	A	148	ILE
1	A	163	LEU
1	A	168	MET
1	A	169	LYS

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Mol	Chain	Res	Type
1	A	169(A)	GLU
1	A	169(D)	ASN
1	A	169(H)	LYS
1	A	175	ASN
1	A	202	LEU
1	A	210	LEU
1	A	211	ILE
2	I	6	ARG
2	I	12	VAL
2	I	29	MET
2	I	37	ASN
2	I	38	ASP
2	I	43	ARG
2	I	54	LEU
2	I	66	ILE
2	I	71	CYS
2	I	75	SER
2	I	80	SER
2	I	86	GLU
2	I	94	THR
2	I	96	THR
2	I	110	LEU
2	I	113	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	37	GLN
1	A	60	ASN
1	A	169(D)	ASN
1	A	175	ASN
1	A	180	GLN
2	I	22	GLN
2	I	53	GLN
2	I	63	GLN

### 5.3.3 RNA ⓘ

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](#)

1 ligand is 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	$\# Z  > 2$
3	GOL	A	1001	1	5,5,5	4.80	5 (100%)	5,5,5	5.83	3 (60%)

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
3	GOL	A	1001	1	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	GOL	C3-C2	-7.83	1.21	1.51
3	A	1001	GOL	O1-C1	4.27	1.60	1.42
3	A	1001	GOL	O2-C2	-3.90	1.32	1.43
3	A	1001	GOL	O3-C3	3.43	1.56	1.42
3	A	1001	GOL	C1-C2	-2.94	1.40	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	GOL	O3-C3-C2	10.71	158.59	110.38
3	A	1001	GOL	O2-C2-C3	6.64	136.67	109.18
3	A	1001	GOL	O1-C1-C2	3.30	125.24	110.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	GOL	O1-C1-C2-C3
3	A	1001	GOL	O1-C1-C2-O2
3	A	1001	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	GOL	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
2	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	0:GLN	C	0(A):MET	N	0.97
1	A	43:ASN	C	44:LYS	N	0.91
1	I	31:GLU	C	32:TYR	N	0.79

## 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	241/241 (100%)	-0.20	7 (2%)	54 52	15, 36, 79, 117	0
2	I	111/111 (100%)	0.95	13 (11%)	10 10	24, 72, 129, 195	4 (3%)
All	All	352/352 (100%)	0.16	20 (5%)	30 28	15, 43, 104, 195	4 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	78	LEU	4.6
1	A	98	ASP	3.8
1	A	0	GLN	3.4
2	I	80	SER	3.1
2	I	23	ARG	3.0
2	I	6	ARG	3.0
2	I	115	CYS	2.9
2	I	49	SER	2.7
1	A	50	GLU	2.7
2	I	87	PRO	2.6
1	A	0(N)	GLU	2.5
2	I	116	GLN	2.2
2	I	77	ASP	2.2
2	I	104	TRP	2.2
1	A	114	ASP	2.2
1	A	153	CYS	2.1
2	I	75	SER	2.1
1	A	156	GLN	2.0
2	I	76	GLY	2.0
2	I	79	GLN	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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1001	6/6	0.73	0.21	8,27,34,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.