



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2016 – 11:05 AM EST

PDB ID : 1TG6  
Title : Crystallography and mutagenesis point to an essential role for the N-terminus of human mitochondrial ClpP  
Authors : Kang, S.G.; Maurizi, M.R.; Thompson, M.; Mueser, T.; Ahvazi, B.  
Deposited on : 2004-05-28  
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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028320

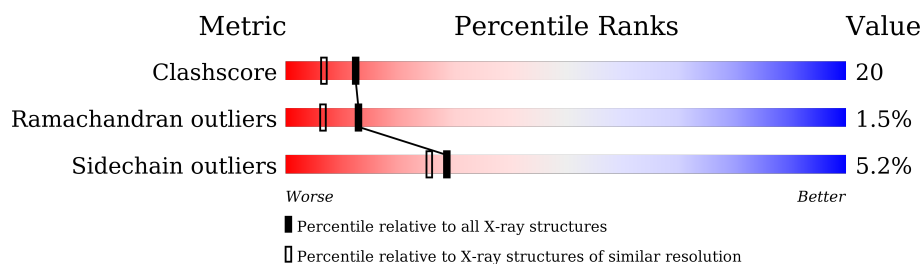
# 1 Overall quality at a glance

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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	277	
1	B	277	
1	C	277	
1	D	277	
1	E	277	
1	F	277	
1	G	277	

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
4	FME	D	1101	-	-	X	-
4	FME	D	1102	-	-	X	-
4	FME	D	1103	-	-	X	-
4	FME	D	1104	-	-	X	-
4	FME	D	1106	-	-	X	-

## 2 Entry composition [i](#)

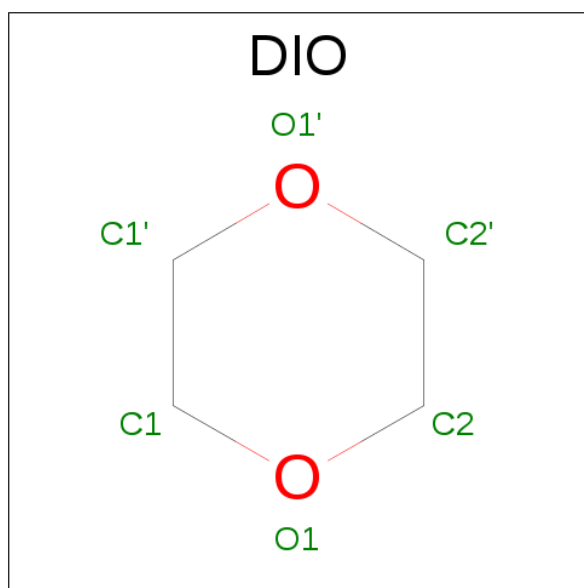
There are 6 unique types of molecules in this entry. The entry contains 11064 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative ATP-dependent Clp protease proteolytic subunit.

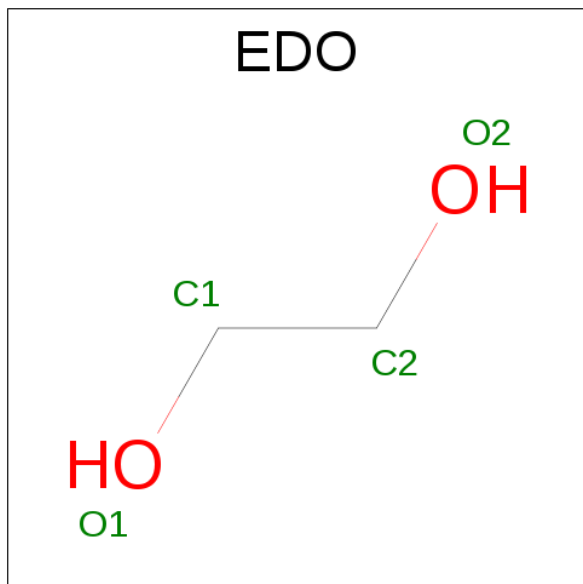
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1420	906	243	258	13			
1	B	183	Total	C	N	O	S	0	0	0
			1413	901	242	257	13			
1	C	183	Total	C	N	O	S	0	0	0
			1413	901	242	257	13			
1	D	184	Total	C	N	O	S	0	0	0
			1420	906	243	258	13			
1	E	196	Total	C	N	O	S	0	0	0
			1514	962	258	281	13			
1	F	187	Total	C	N	O	S	0	0	0
			1441	917	247	264	13			
1	G	194	Total	C	N	O	S	0	0	0
			1496	951	254	278	13			

- Molecule 2 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 4 2	0	0
2	B	1	Total C O 6 4 2	0	0
2	D	1	Total C O 6 4 2	0	0
2	E	1	Total C O 6 4 2	0	0
2	F	1	Total C O 6 4 2	0	0
2	G	1	Total C O 6 4 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



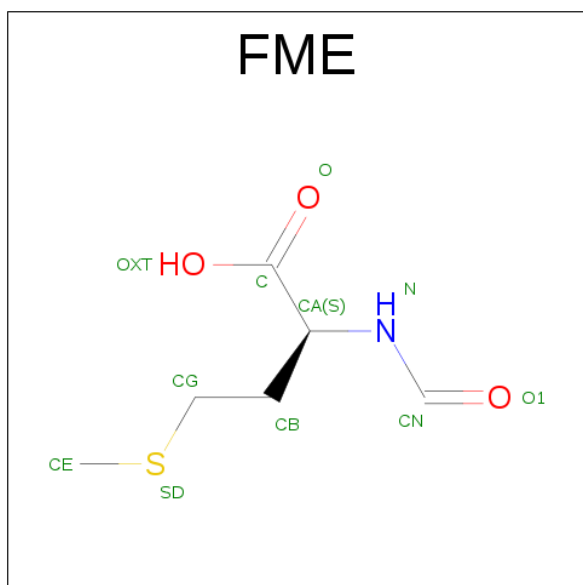
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	7	Total	C	N	O	S	0	0
			70	42	7	14	7		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O	0	0
			77	77		
6	B	90	Total	O	0	0
			90	90		
6	C	109	Total	O	0	0
			109	109		
6	D	128	Total	O	0	0
			128	128		
6	E	132	Total	O	0	0
			132	132		
6	F	126	Total	O	0	0
			126	126		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	111	Total	O	0	0
			111	111		

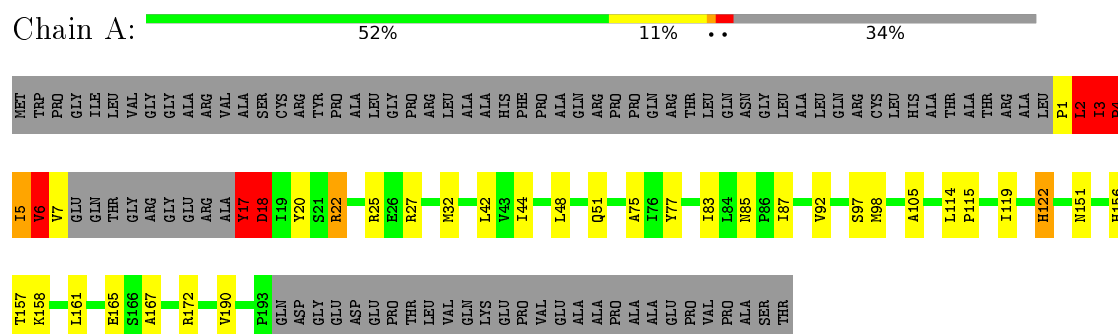


### 3 Residue-property plots

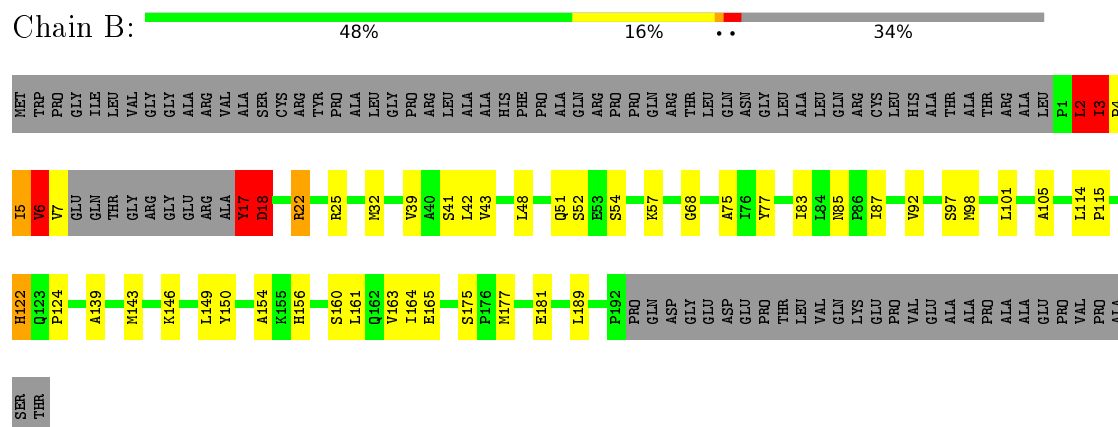
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

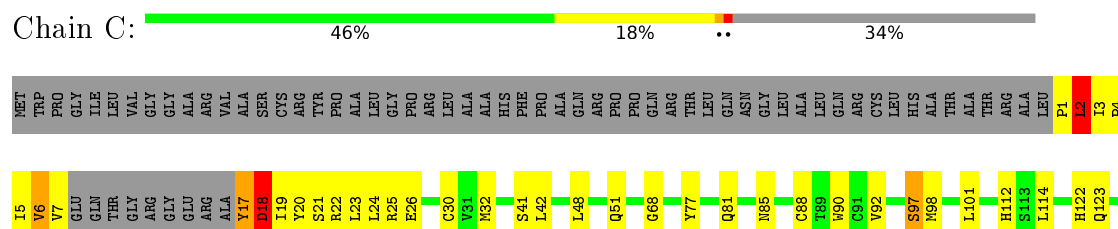
- Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit

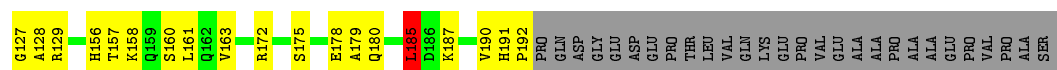


- Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit

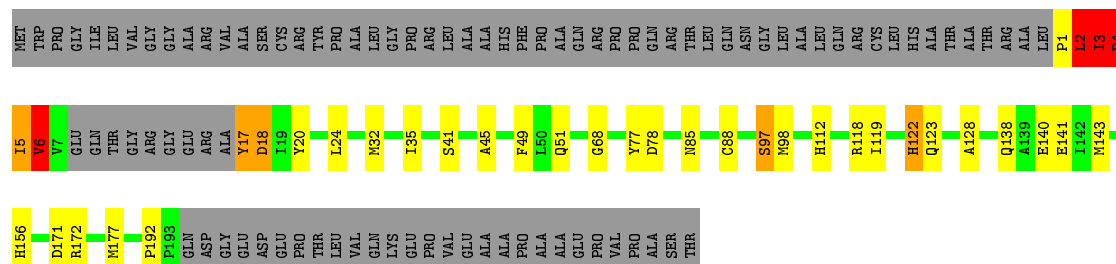


- Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit

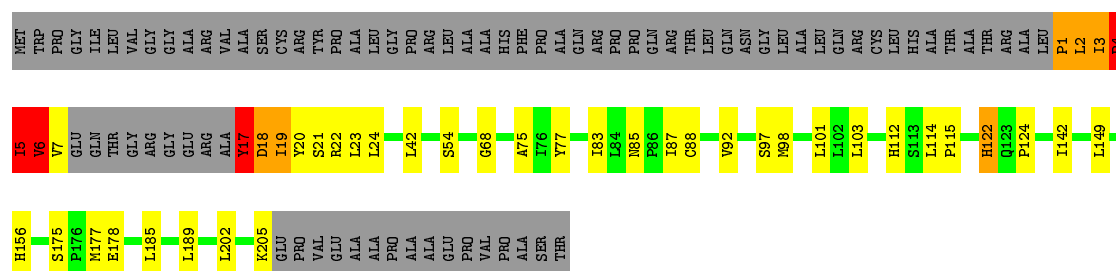




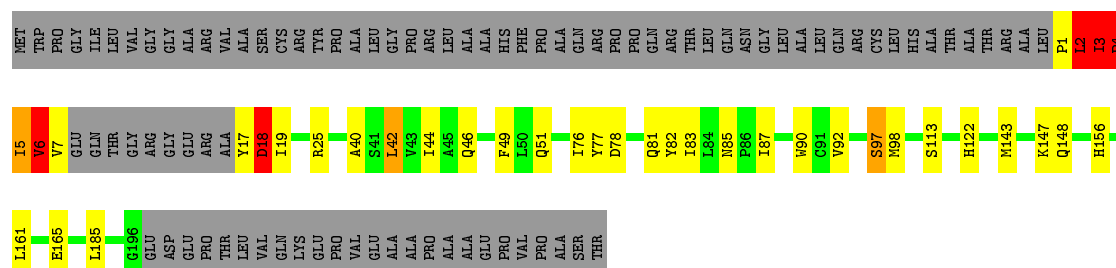
- Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit



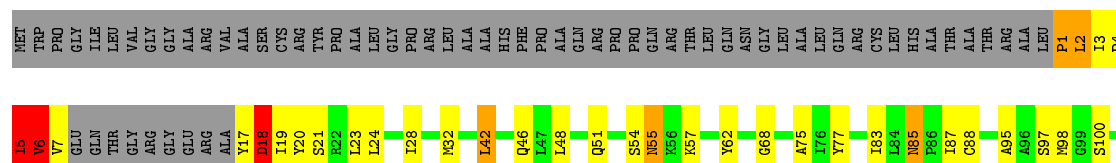
- Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit



- Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit



- Molecule 1: Putative ATP-dependent Clp protease proteolytic subunit



H112	S113	L114	I119	M120	H121	H122	L149	Y150	N151	H156	L161	D171	R172	S175	E178	K187	H188	L189	P192	L202	V203	GLN	LYS	GLU	PRO	VAL	GLU	ALA	ALA	PRO	ALA	ALA	GLU	PRO	VAL	PRO	ALA	SER	TER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.57Å 119.00Å 118.65Å 90.00° 130.16° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.224 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.53	2/1447 (0.1%)	1.19	10/1959 (0.5%)
1	B	0.53	3/1439 (0.2%)	0.89	10/1947 (0.5%)
1	C	0.39	0/1439	0.78	5/1947 (0.3%)
1	D	0.52	2/1447 (0.1%)	1.15	14/1959 (0.7%)
1	E	0.62	6/1542 (0.4%)	0.95	12/2088 (0.6%)
1	F	1.14	4/1468 (0.3%)	1.24	17/1987 (0.9%)
1	G	0.53	1/1524 (0.1%)	0.74	4/2065 (0.2%)
All	All	0.65	18/10306 (0.2%)	1.01	72/13952 (0.5%)

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	E	0	2
1	F	0	3
1	G	0	3
All	All	0	10

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	6	VAL	C-N	-31.14	0.62	1.34
1	F	7	VAL	N-CA	-23.52	0.99	1.46
1	G	6	VAL	C-N	-13.38	1.03	1.34
1	B	17	TYR	C-N	11.32	1.60	1.34
1	E	17	TYR	C-N	9.72	1.56	1.34
1	A	6	VAL	C-N	9.57	1.56	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	6	VAL	C-N	-8.06	1.15	1.34
1	F	3	ILE	C-N	6.97	1.47	1.34
1	E	5	ILE	N-CA	-6.58	1.33	1.46
1	E	4	PRO	N-CA	6.11	1.57	1.47
1	A	4	PRO	N-CA	5.93	1.57	1.47
1	D	4	PRO	N-CA	5.47	1.56	1.47
1	E	1	PRO	C-N	-5.33	1.21	1.34
1	E	3	ILE	C-N	5.26	1.44	1.34
1	D	2	LEU	C-N	-5.21	1.22	1.34
1	F	4	PRO	CA-C	-5.17	1.42	1.52
1	B	6	VAL	C-N	-5.16	1.22	1.34
1	B	5	ILE	C-N	-5.05	1.22	1.34

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	6	VAL	O-C-N	-28.91	76.45	122.70
1	A	17	TYR	CB-CG-CD2	-24.05	106.57	121.00
1	A	17	TYR	CB-CG-CD1	23.23	134.94	121.00
1	D	17	TYR	CB-CG-CD1	-17.59	110.45	121.00
1	D	17	TYR	CB-CG-CD2	16.41	130.84	121.00
1	F	6	VAL	CA-C-N	15.61	151.55	117.20
1	E	6	VAL	O-C-N	-15.50	97.90	122.70
1	D	6	VAL	O-C-N	14.60	146.06	122.70
1	A	6	VAL	CA-C-N	-13.64	87.18	117.20
1	D	6	VAL	CA-C-N	-13.60	87.29	117.20
1	B	6	VAL	CA-C-N	-13.43	87.65	117.20
1	A	6	VAL	C-N-CA	-13.22	88.64	121.70
1	A	6	VAL	O-C-N	12.87	143.29	122.70
1	F	7	VAL	N-CA-C	12.32	144.26	111.00
1	B	6	VAL	C-N-CA	-11.79	92.23	121.70
1	E	4	PRO	CA-N-CD	-11.52	95.37	111.50
1	D	3	ILE	N-CA-C	11.50	142.05	111.00
1	F	3	ILE	N-CA-C	11.22	141.28	111.00
1	D	3	ILE	CA-C-N	10.92	147.68	117.10
1	D	6	VAL	C-N-CA	-10.84	94.61	121.70
1	F	1	PRO	C-N-CA	10.80	148.70	121.70
1	E	17	TYR	C-N-CA	10.73	148.53	121.70
1	E	5	ILE	CA-C-N	-10.09	95.00	117.20
1	B	17	TYR	CA-C-N	-10.07	95.05	117.20
1	D	17	TYR	CB-CA-C	-9.79	90.82	110.40
1	F	4	PRO	CA-N-CD	-9.05	98.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	VAL	CA-C-N	8.54	135.99	117.20
1	C	17	TYR	C-N-CA	8.33	142.53	121.70
1	B	3	ILE	N-CA-C	8.12	132.93	111.00
1	F	2	LEU	C-N-CA	8.10	141.95	121.70
1	B	6	VAL	O-C-N	8.06	135.60	122.70
1	F	1	PRO	CA-C-N	-7.96	99.70	117.20
1	F	2	LEU	CB-CA-C	7.89	125.19	110.20
1	D	3	ILE	O-C-N	-7.86	106.16	121.10
1	E	17	TYR	O-C-N	-7.76	110.28	122.70
1	F	6	VAL	C-N-CA	7.71	140.96	121.70
1	A	17	TYR	CA-CB-CG	7.62	127.88	113.40
1	F	1	PRO	CB-CA-C	7.53	130.84	112.00
1	F	2	LEU	CA-C-N	-7.32	101.10	117.20
1	G	5	ILE	N-CA-C	-7.28	91.36	111.00
1	G	18	ASP	N-CA-CB	-7.23	97.59	110.60
1	C	17	TYR	CA-C-N	-6.97	101.87	117.20
1	E	5	ILE	O-C-N	6.91	133.75	122.70
1	G	1	PRO	O-C-N	6.68	133.39	122.70
1	B	17	TYR	O-C-N	6.66	133.36	122.70
1	D	3	ILE	CA-C-O	-6.66	106.11	120.10
1	A	3	ILE	N-CA-C	6.46	128.44	111.00
1	D	17	TYR	CA-C-N	-6.21	103.53	117.20
1	A	3	ILE	CB-CA-C	-6.16	99.29	111.60
1	F	1	PRO	O-C-N	6.07	132.40	122.70
1	D	4	PRO	CA-N-CD	-5.97	103.14	111.50
1	E	4	PRO	N-CA-C	5.94	127.53	112.10
1	E	4	PRO	C-N-CA	-5.83	107.12	121.70
1	B	18	ASP	N-CA-CB	-5.82	100.12	110.60
1	B	2	LEU	C-N-CA	5.78	136.16	121.70
1	F	4	PRO	C-N-CA	-5.78	107.24	121.70
1	D	17	TYR	C-N-CA	5.77	136.13	121.70
1	E	4	PRO	N-CD-CG	5.71	111.77	103.20
1	E	3	ILE	N-CA-C	5.71	126.42	111.00
1	C	185	LEU	CA-CB-CG	5.55	128.06	115.30
1	F	3	ILE	N-CA-CB	-5.53	98.09	110.80
1	D	3	ILE	N-CA-CB	-5.49	98.18	110.80
1	B	17	TYR	CA-C-O	5.47	131.58	120.10
1	B	3	ILE	N-CA-CB	-5.35	98.50	110.80
1	E	5	ILE	CA-C-O	5.30	131.23	120.10
1	F	4	PRO	N-CA-CB	5.29	109.66	103.30
1	G	5	ILE	C-N-CA	-5.23	108.63	121.70
1	C	2	LEU	N-CA-C	5.20	125.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	TYR	O-C-N	5.18	130.99	122.70
1	F	18	ASP	N-CA-CB	-5.16	101.31	110.60
1	A	18	ASP	CB-CA-C	5.16	120.71	110.40
1	A	3	ILE	CA-C-N	5.11	131.41	117.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	VAL	Mainchain
1	B	6	VAL	Mainchain
1	E	17	TYR	Peptide
1	E	6	VAL	Mainchain
1	F	2	LEU	Peptide
1	F	6	VAL	Mainchain,Peptide
1	G	5	ILE	Mainchain
1	G	6	VAL	Mainchain,Peptide

## 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	1420	0	1465	50	0
1	B	1413	0	1458	60	0
1	C	1413	0	1458	64	0
1	D	1420	0	1463	67	0
1	E	1514	0	1550	53	0
1	F	1441	0	1479	68	0
1	G	1496	0	1529	105	0
2	A	6	0	8	1	0
2	B	6	0	8	2	0
2	D	6	0	8	1	0
2	E	6	0	8	2	0
2	F	6	0	8	1	0
2	G	6	0	8	0	0
3	A	4	0	5	1	0
3	B	8	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	10	1	0
3	D	4	0	5	0	0
3	F	4	0	5	0	0
3	G	4	0	5	0	0
4	D	70	0	70	55	0
5	B	12	0	8	3	0
5	C	6	0	4	0	0
5	D	6	0	4	2	0
5	E	6	0	4	0	0
5	F	6	0	4	1	0
6	A	77	0	0	3	0
6	B	90	0	0	4	0
6	C	109	0	0	2	0
6	D	128	0	0	6	0
6	E	132	0	0	1	0
6	F	126	0	0	3	0
6	G	111	0	0	5	0
All	All	11064	0	10584	407	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 20.

All (407) 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:F:17:TYR:CG	1:G:5:ILE:HD11	1.27	1.66
1:G:5:ILE:HG22	1:G:17:TYR:CE2	1.37	1.58
1:F:17:TYR:CD2	1:G:5:ILE:HD11	1.04	1.55
1:F:17:TYR:CE2	1:G:5:ILE:CD1	1.91	1.51
1:F:17:TYR:CD2	1:G:5:ILE:CD1	1.90	1.49
1:G:5:ILE:CG2	1:G:17:TYR:CE2	1.99	1.44
1:A:6:VAL:CG2	1:A:7:VAL:H	1.03	1.39
1:C:17:TYR:CD1	1:D:5:ILE:HG21	1.58	1.37
1:A:2:LEU:H	1:A:2:LEU:CD2	1.36	1.33
1:F:17:TYR:HD2	1:F:18:ASP:CB	1.42	1.32
1:A:6:VAL:HG23	1:A:7:VAL:N	1.15	1.31
1:F:17:TYR:CZ	1:G:5:ILE:CD1	2.13	1.30
1:F:17:TYR:CE1	1:G:5:ILE:HD12	1.66	1.30
1:A:2:LEU:N	1:A:2:LEU:HD23	1.37	1.28
1:F:17:TYR:CE2	1:G:5:ILE:HD11	1.63	1.22
1:E:6:VAL:O	1:E:7:VAL:CG2	1.88	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:VAL:O	1:E:7:VAL:HG23	1.41	1.20
1:F:17:TYR:CD2	1:F:18:ASP:CB	2.24	1.19
1:B:6:VAL:N	1:B:17:TYR:O	1.74	1.18
1:F:17:TYR:CG	1:G:5:ILE:CD1	2.14	1.18
1:F:17:TYR:HD2	1:F:18:ASP:HB3	0.98	1.14
1:D:2:LEU:HG	1:D:20:TYR:HE2	1.04	1.14
1:D:1:PRO:O	1:D:2:LEU:HB2	1.44	1.12
1:F:17:TYR:CD1	1:G:5:ILE:CD1	2.31	1.12
1:A:42:LEU:HD11	1:B:2:LEU:HG	1.15	1.11
1:F:17:TYR:CE2	1:G:5:ILE:HD13	1.66	1.10
1:F:17:TYR:CD2	1:F:18:ASP:HB2	1.87	1.10
1:G:6:VAL:HG12	1:G:7:VAL:N	1.56	1.09
1:C:6:VAL:HG23	1:C:7:VAL:N	1.67	1.08
1:G:5:ILE:HG21	1:G:17:TYR:CZ	1.89	1.07
1:F:17:TYR:CD1	1:G:5:ILE:HD11	1.88	1.06
1:F:17:TYR:CE1	1:G:5:ILE:CD1	2.32	1.06
1:F:17:TYR:CZ	1:G:5:ILE:HD12	1.83	1.05
4:D:1106:FME:HA	1:G:97:SER:OG	1.57	1.05
1:F:17:TYR:CD2	1:F:18:ASP:HB3	1.88	1.05
1:G:6:VAL:CG1	1:G:7:VAL:N	2.14	1.03
1:F:25:ARG:HH22	1:G:7:VAL:HG22	1.23	1.02
1:C:6:VAL:HG23	1:C:7:VAL:H	1.17	1.01
1:D:2:LEU:CG	1:D:20:TYR:HE2	1.72	1.01
1:D:2:LEU:HG	1:D:20:TYR:CE2	1.93	1.01
1:C:17:TYR:HD1	1:D:5:ILE:CG2	1.73	1.01
1:C:97:SER:OG	4:D:1102:FME:HA	1.62	0.99
1:A:6:VAL:CG2	1:A:7:VAL:N	1.77	0.99
1:D:97:SER:OG	4:D:1103:FME:HA	1.63	0.99
1:G:5:ILE:HG21	1:G:17:TYR:CE2	1.92	0.98
1:A:42:LEU:CD1	1:B:2:LEU:HG	1.94	0.98
1:G:88:CYS:HB3	6:G:914:HOH:O	1.63	0.97
1:F:40:ALA:HA	1:F:76:ILE:HD11	1.47	0.97
1:D:5:ILE:HG13	1:D:6:VAL:N	1.80	0.95
1:D:1:PRO:O	1:D:2:LEU:CB	2.08	0.93
1:F:17:TYR:CE2	1:F:18:ASP:HB2	2.03	0.93
1:G:83:ILE:HD11	1:G:87:ILE:HD11	1.48	0.93
1:F:25:ARG:NH2	1:G:7:VAL:CG2	2.32	0.92
1:C:17:TYR:HD1	1:D:5:ILE:HG21	0.78	0.91
1:G:5:ILE:HG22	1:G:17:TYR:CD2	2.04	0.91
1:F:25:ARG:NH2	1:G:7:VAL:HG22	1.88	0.88
1:G:6:VAL:HG13	1:G:7:VAL:HG23	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:TYR:CD1	1:G:5:ILE:HD12	1.99	0.88
1:D:2:LEU:C	1:D:3:ILE:HG13	1.95	0.87
4:D:1105:FME:HG2	1:F:97:SER:OG	1.75	0.87
1:G:5:ILE:HG22	1:G:17:TYR:HE2	1.08	0.87
1:G:2:LEU:HD23	1:G:2:LEU:C	1.96	0.86
1:B:2:LEU:O	1:B:4:PRO:HD3	1.76	0.84
1:E:103:LEU:HD11	1:E:185:LEU:HD21	1.60	0.84
1:G:2:LEU:HD23	1:G:3:ILE:N	1.93	0.83
1:B:17:TYR:CD2	1:B:18:ASP:N	2.47	0.83
6:A:975:HOH:O	1:B:2:LEU:HD21	1.78	0.83
1:G:2:LEU:CD2	1:G:2:LEU:C	2.47	0.83
1:A:97:SER:OG	4:D:1100:FME:HA	1.79	0.82
1:F:17:TYR:CD2	1:F:18:ASP:N	2.48	0.82
1:C:6:VAL:CG2	1:C:7:VAL:N	2.38	0.82
1:C:17:TYR:CD1	1:D:5:ILE:CG2	2.55	0.82
1:E:17:TYR:HB3	1:E:21:SER:HB2	1.60	0.81
1:A:17:TYR:HD1	1:A:18:ASP:H	1.26	0.81
1:B:17:TYR:C	1:B:17:TYR:HD2	1.84	0.81
1:D:2:LEU:CG	1:D:20:TYR:CE2	2.55	0.81
1:A:5:ILE:HD12	1:G:21:SER:OG	1.81	0.80
1:A:2:LEU:N	1:A:2:LEU:CD2	2.11	0.80
1:G:6:VAL:HG12	1:G:7:VAL:HB	1.64	0.79
1:C:42:LEU:HD21	1:D:2:LEU:C	2.03	0.78
1:G:6:VAL:CG1	1:G:7:VAL:HB	2.14	0.78
1:B:42:LEU:HD11	1:C:4:PRO:HD2	1.67	0.77
1:A:2:LEU:H	1:A:2:LEU:HD23	0.62	0.76
4:D:1106:FME:HE1	1:G:149:LEU:HD13	1.67	0.76
1:D:6:VAL:HG13	1:D:17:TYR:O	1.86	0.76
1:C:6:VAL:CG1	1:C:18:ASP:C	2.54	0.76
1:F:25:ARG:HH22	1:G:7:VAL:CG2	1.93	0.75
1:B:17:TYR:C	1:B:17:TYR:CD2	2.58	0.75
1:A:151:ASN:HD22	1:A:161:LEU:HD21	1.52	0.75
1:A:1:PRO:O	1:A:3:ILE:HG23	1.86	0.74
1:B:41:SER:HB2	1:C:32:MET:HE1	1.67	0.74
1:A:83:ILE:HD11	1:A:87:ILE:HD11	1.70	0.73
1:A:167:ALA:HA	1:A:172:ARG:HH12	1.52	0.72
1:F:161:LEU:O	1:F:165:GLU:HG3	1.89	0.72
1:D:68:GLY:H	4:D:1103:FME:C	2.02	0.72
1:G:6:VAL:HG12	1:G:7:VAL:CA	2.20	0.71
1:D:98:MET:HG2	4:D:1103:FME:HB2	1.72	0.71
1:A:6:VAL:HG23	1:A:7:VAL:H	0.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:VAL:HG12	1:G:7:VAL:CB	2.21	0.70
1:E:42:LEU:HD11	1:F:3:ILE:HG13	1.74	0.69
1:F:5:ILE:HG13	1:F:6:VAL:N	2.07	0.69
1:G:6:VAL:CG1	1:G:7:VAL:CB	2.71	0.69
1:D:3:ILE:O	1:D:4:PRO:C	2.31	0.69
1:F:42:LEU:HD12	1:F:46:GLN:NE2	2.08	0.69
1:G:6:VAL:HG13	1:G:7:VAL:CG2	2.23	0.69
1:A:151:ASN:ND2	1:A:161:LEU:HD21	2.08	0.68
1:A:98:MET:HG2	4:D:1100:FME:HB2	1.76	0.68
2:A:800:DIO:H2'2	1:G:48:LEU:HD21	1.75	0.68
4:D:1104:FME:HE3	1:E:122:HIS:O	1.94	0.68
1:B:149:LEU:HD13	4:D:1101:FME:HE1	1.76	0.68
1:A:42:LEU:HD11	1:B:2:LEU:CG	2.09	0.67
1:B:3:ILE:HG22	1:B:3:ILE:O	1.95	0.66
1:G:1:PRO:HD2	1:G:2:LEU:HD13	1.75	0.66
1:F:40:ALA:CA	1:F:76:ILE:HD11	2.23	0.66
1:C:98:MET:HG2	4:D:1102:FME:HB2	1.76	0.66
1:D:2:LEU:HD11	1:D:20:TYR:OH	1.97	0.65
1:E:6:VAL:O	1:E:7:VAL:CB	2.17	0.65
1:B:98:MET:HG2	4:D:1101:FME:HB2	1.78	0.65
4:D:1104:FME:HA	1:E:97:SER:HB3	1.79	0.65
1:B:122:HIS:O	4:D:1101:FME:HE2	1.97	0.65
1:D:41:SER:HA	2:E:803:DIO:H21	1.78	0.65
1:F:3:ILE:HD13	1:F:18:ASP:OD1	1.97	0.65
1:F:44:ILE:HG13	1:F:76:ILE:HD13	1.78	0.65
1:C:18:ASP:OD1	1:C:21:SER:OG	2.05	0.65
1:G:54:SER:OG	1:G:57:LYS:HG3	1.97	0.64
1:G:55:ASN:HA	1:G:85:ASN:HD22	1.63	0.64
1:F:3:ILE:HD11	1:F:19:ILE:HG22	1.80	0.64
1:C:6:VAL:HG13	1:C:18:ASP:C	2.19	0.63
1:D:2:LEU:CD1	1:D:20:TYR:CE2	2.82	0.63
1:G:5:ILE:HG21	1:G:17:TYR:OH	1.99	0.63
1:F:25:ARG:NH2	1:G:7:VAL:HG23	2.13	0.62
1:C:68:GLY:H	4:D:1102:FME:C	2.10	0.62
1:C:6:VAL:CG1	1:C:19:ILE:N	2.63	0.62
1:C:42:LEU:HD11	1:D:2:LEU:HA	1.82	0.62
1:D:49:PHE:CE2	1:E:6:VAL:HG12	2.35	0.62
1:G:151:ASN:HD22	1:G:161:LEU:HD21	1.65	0.61
1:C:42:LEU:HD21	1:D:2:LEU:CA	2.30	0.61
1:F:156:HIS:HD2	6:F:1008:HOH:O	1.84	0.61
1:D:2:LEU:HD11	1:D:20:TYR:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:DIO:H22	1:C:114:LEU:HD11	1.81	0.61
1:B:17:TYR:HD2	1:B:18:ASP:N	1.94	0.61
1:E:75:ALA:HB1	1:F:92:VAL:HG12	1.83	0.61
1:G:5:ILE:CG2	1:G:17:TYR:CZ	2.54	0.60
1:E:83:ILE:HD11	1:E:87:ILE:HD11	1.82	0.60
1:C:97:SER:HG	4:D:1102:FME:HA	1.62	0.60
1:C:77:TYR:OH	1:C:156:HIS:HE1	1.85	0.60
6:A:975:HOH:O	1:B:2:LEU:HD11	2.02	0.59
1:B:41:SER:HB3	6:B:1061:HOH:O	2.02	0.59
1:D:2:LEU:HD11	1:D:20:TYR:CE2	2.37	0.59
1:A:77:TYR:OH	1:A:156:HIS:HE1	1.85	0.59
1:E:42:LEU:CD1	1:F:3:ILE:HG13	2.32	0.59
1:A:5:ILE:O	1:G:21:SER:HB3	2.02	0.59
1:C:175:SER:OG	1:C:178:GLU:HG3	2.01	0.59
4:D:1105:FME:HG3	1:F:98:MET:HG2	1.85	0.59
1:E:97:SER:OG	1:E:122:HIS:NE2	2.36	0.58
1:F:77:TYR:OH	1:F:156:HIS:HE1	1.84	0.58
1:D:5:ILE:CG1	1:D:6:VAL:N	2.60	0.58
4:D:1104:FME:HA	1:E:97:SER:CB	2.34	0.58
1:A:32:MET:HG2	3:A:900:EDO:O1	2.03	0.58
4:D:1106:FME:HE3	1:G:122:HIS:O	2.03	0.58
1:C:6:VAL:HG11	1:C:18:ASP:C	2.24	0.58
1:B:83:ILE:HD11	1:B:87:ILE:HD11	1.86	0.58
1:B:48:LEU:HD21	2:B:801:DIO:H2'2	1.85	0.57
1:B:97:SER:HB3	4:D:1101:FME:HA	1.87	0.57
1:B:75:ALA:HB1	1:C:92:VAL:HG12	1.85	0.57
1:A:17:TYR:CD1	1:A:18:ASP:N	2.70	0.57
1:A:6:VAL:HG22	1:A:17:TYR:O	2.04	0.57
1:D:77:TYR:OH	1:D:156:HIS:HE1	1.87	0.57
1:A:92:VAL:HG12	1:G:75:ALA:HB1	1.86	0.57
1:G:112:HIS:CD2	6:G:914:HOH:O	2.57	0.57
4:D:1104:FME:HE1	1:E:149:LEU:HD13	1.87	0.56
1:D:2:LEU:CD1	1:D:20:TYR:HE2	2.17	0.56
1:E:92:VAL:HG13	1:E:114:LEU:HD12	1.87	0.56
1:E:115:PRO:HD3	1:E:189:LEU:O	2.05	0.56
1:F:3:ILE:HG12	1:F:4:PRO:N	2.19	0.56
1:G:156:HIS:HD2	6:G:928:HOH:O	1.87	0.56
1:B:22:ARG:HG2	1:B:22:ARG:HH11	1.70	0.56
1:B:181:GLU:HG3	6:B:1056:HOH:O	2.06	0.56
1:B:105:ALA:HA	1:B:156:HIS:CD2	2.40	0.56
1:B:77:TYR:OH	1:B:156:HIS:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:VAL:HG11	1:C:19:ILE:HA	1.88	0.56
1:G:189:LEU:HG	1:G:202:LEU:CD2	2.36	0.56
1:A:51:GLN:HG3	1:A:85:ASN:OD1	2.06	0.56
1:B:51:GLN:HG3	1:B:85:ASN:OD1	2.06	0.56
1:F:49:PHE:CE2	1:G:6:VAL:HG21	2.41	0.56
1:A:167:ALA:HA	1:A:172:ARG:NH1	2.21	0.55
1:C:30:CYS:HB3	1:C:32:MET:CE	2.37	0.55
1:D:122:HIS:O	4:D:1103:FME:HE2	2.06	0.55
1:D:140:GLU:O	1:D:143:MET:CG	2.54	0.55
1:C:180:GLN:HA	1:C:185:LEU:HD22	1.87	0.55
1:C:2:LEU:C	1:C:3:ILE:HG13	2.26	0.55
1:C:32:MET:HB3	3:C:903:EDO:O2	2.06	0.55
1:E:88:CYS:SG	1:E:112:HIS:CD2	3.00	0.55
1:F:17:TYR:CZ	1:G:5:ILE:HD13	2.11	0.55
1:G:51:GLN:HG3	1:G:85:ASN:HD21	1.71	0.55
1:A:6:VAL:HG23	1:A:7:VAL:CA	2.22	0.55
6:D:1224:HOH:O	1:E:20:TYR:HE1	1.89	0.55
1:A:156:HIS:HD2	6:A:906:HOH:O	1.89	0.54
1:A:20:TYR:OH	1:G:42:LEU:HD22	2.08	0.54
1:F:17:TYR:CG	1:G:5:ILE:CG1	2.90	0.54
1:D:156:HIS:HD2	6:D:1109:HOH:O	1.90	0.54
1:G:77:TYR:OH	1:G:156:HIS:HE1	1.90	0.54
1:D:128:ALA:HA	1:D:138:GLN:OE1	2.07	0.54
1:G:112:HIS:CE1	1:G:187:LYS:HD2	2.43	0.54
1:B:115:PRO:HD3	1:B:189:LEU:O	2.08	0.54
1:D:177:MET:HG3	6:D:1122:HOH:O	2.07	0.54
1:B:160:SER:OG	1:B:163:VAL:HG23	2.08	0.54
1:E:103:LEU:HD11	1:E:185:LEU:CD2	2.35	0.54
1:F:42:LEU:HD12	1:F:46:GLN:HE21	1.72	0.54
1:G:24:LEU:O	1:G:24:LEU:HD13	2.08	0.54
1:F:42:LEU:HD11	1:G:4:PRO:HD2	1.90	0.54
4:D:1104:FME:CE	1:E:122:HIS:O	2.56	0.53
1:B:68:GLY:H	4:D:1101:FME:C	2.20	0.53
1:D:140:GLU:O	1:D:143:MET:HG3	2.08	0.53
1:E:4:PRO:C	1:E:5:ILE:HG22	2.28	0.53
4:D:1105:FME:N	1:F:97:SER:OG	2.41	0.53
1:B:32:MET:HG2	3:B:901:EDO:O2	2.09	0.53
1:B:143:MET:HE1	6:B:1022:HOH:O	2.09	0.53
1:B:22:ARG:NH1	1:B:25:ARG:HD2	2.24	0.52
1:B:154:ALA:HA	1:B:164:ILE:HD11	1.90	0.52
4:D:1104:FME:HG2	1:E:124:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:ILE:O	1:G:23:LEU:HD13	2.09	0.52
1:C:51:GLN:HG3	1:C:85:ASN:OD1	2.10	0.52
1:A:44:ILE:O	1:A:48:LEU:HD13	2.08	0.52
1:C:42:LEU:CD2	1:D:2:LEU:C	2.75	0.52
1:G:17:TYR:CD2	1:G:18:ASP:N	2.78	0.52
1:B:17:TYR:CG	1:B:18:ASP:N	2.67	0.52
1:E:189:LEU:HD22	1:E:202:LEU:CD2	2.40	0.52
1:D:68:GLY:N	4:D:1103:FME:O	2.39	0.51
1:G:83:ILE:HD12	1:G:85:ASN:OD1	2.10	0.51
4:D:1106:FME:O	1:G:68:GLY:N	2.38	0.51
1:F:143:MET:SD	1:F:147:LYS:HE3	2.50	0.51
1:F:25:ARG:HH21	1:G:7:VAL:HG23	1.75	0.51
1:D:2:LEU:CD2	1:D:20:TYR:CE2	2.93	0.51
1:E:156:HIS:HD2	6:E:1013:HOH:O	1.93	0.51
4:D:1104:FME:C	1:E:68:GLY:H	2.23	0.51
1:E:19:ILE:O	1:E:23:LEU:HD13	2.10	0.51
1:B:114:LEU:HD21	3:B:902:EDO:H21	1.93	0.51
1:C:112:HIS:CE1	1:C:187:LYS:HE3	2.46	0.51
1:D:5:ILE:HA	1:D:18:ASP:HA	1.93	0.50
1:G:42:LEU:O	1:G:46:GLN:HG3	2.12	0.50
1:F:17:TYR:CG	1:F:18:ASP:N	2.78	0.50
1:G:122:HIS:ND1	1:G:171:ASP:OD1	2.30	0.50
1:D:6:VAL:N	1:D:17:TYR:O	2.44	0.50
1:C:42:LEU:CD2	1:D:2:LEU:O	2.59	0.50
1:F:90:TRP:HB3	2:F:804:DIO:H1'2	1.92	0.50
1:G:6:VAL:HG13	1:G:7:VAL:CB	2.40	0.50
1:E:189:LEU:HD22	1:E:202:LEU:HD22	1.93	0.49
4:D:1105:FME:HB3	6:F:1122:HOH:O	2.12	0.49
1:C:123:GLN:C	4:D:1102:FME:HE2	2.33	0.49
1:B:3:ILE:O	1:B:4:PRO:C	2.49	0.49
1:C:22:ARG:HH11	1:C:25:ARG:HH11	1.59	0.49
4:D:1106:FME:C	1:G:68:GLY:O	2.60	0.49
4:D:1106:FME:HCN	6:G:1008:HOH:O	2.11	0.49
1:D:45:ALA:HB1	1:E:19:ILE:HD12	1.94	0.49
6:D:1144:HOH:O	2:E:803:DIO:H12	2.13	0.49
1:B:2:LEU:O	1:B:4:PRO:CD	2.56	0.49
1:E:189:LEU:CD2	1:E:202:LEU:HD22	2.43	0.49
1:F:17:TYR:OH	1:G:17:TYR:OH	2.31	0.49
1:F:42:LEU:HD11	1:G:4:PRO:CD	2.43	0.49
1:A:1:PRO:O	1:A:2:LEU:C	2.51	0.48
1:E:17:TYR:HB3	1:E:21:SER:CB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:CYS:SG	1:C:112:HIS:CD2	3.07	0.48
1:C:6:VAL:HG13	1:C:18:ASP:CA	2.44	0.48
1:F:113:SER:HB2	1:F:185:LEU:HD22	1.96	0.48
1:G:5:ILE:CG2	1:G:17:TYR:HE2	1.77	0.48
1:G:55:ASN:HA	1:G:85:ASN:ND2	2.28	0.48
1:C:68:GLY:N	4:D:1102:FME:O	2.39	0.47
1:F:83:ILE:HD11	1:F:87:ILE:HD11	1.96	0.47
1:F:49:PHE:CZ	1:G:6:VAL:HG21	2.48	0.47
1:B:5:ILE:HB	1:B:17:TYR:O	2.15	0.47
1:D:177:MET:HG2	6:D:1194:HOH:O	2.14	0.47
1:G:17:TYR:HD2	1:G:18:ASP:N	2.11	0.47
5:B:1001:GOL:O1	1:C:175:SER:HA	2.14	0.47
1:C:42:LEU:HD11	1:D:2:LEU:CA	2.43	0.47
1:F:78:ASP:HB3	1:G:114:LEU:HD13	1.95	0.47
1:E:17:TYR:HB2	1:F:5:ILE:HG12	1.95	0.47
1:A:75:ALA:HB1	1:B:92:VAL:HG12	1.95	0.47
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.64	0.47
1:B:41:SER:HB2	1:C:32:MET:CE	2.39	0.47
5:F:1005:GOL:O1	1:G:175:SER:HA	2.15	0.47
1:D:2:LEU:HD21	1:D:20:TYR:CE2	2.50	0.47
1:E:5:ILE:HG13	1:E:6:VAL:N	2.29	0.47
1:B:22:ARG:HG2	1:B:22:ARG:NH1	2.29	0.47
1:C:156:HIS:HD2	6:C:1012:HOH:O	1.98	0.47
1:C:30:CYS:HB3	1:C:32:MET:HE3	1.98	0.47
1:C:19:ILE:O	1:C:23:LEU:HD13	2.15	0.46
1:E:18:ASP:HB3	1:E:21:SER:HB2	1.97	0.46
1:D:17:TYR:HB3	1:D:18:ASP:HB3	1.96	0.46
1:B:97:SER:HB3	4:D:1101:FME:O	2.15	0.46
1:B:161:LEU:HG	1:B:165:GLU:OE2	2.15	0.46
1:C:30:CYS:HB3	1:C:32:MET:HE2	1.98	0.46
1:D:3:ILE:O	1:D:4:PRO:O	2.33	0.46
1:B:39:VAL:O	1:B:43:VAL:HG23	2.16	0.46
1:B:97:SER:HB3	4:D:1101:FME:C	2.46	0.46
1:E:54:SER:O	1:E:85:ASN:ND2	2.41	0.46
1:G:55:ASN:N	1:G:55:ASN:HD22	2.13	0.46
1:B:189:LEU:N	1:B:189:LEU:HD12	2.31	0.45
1:D:140:GLU:HA	1:D:143:MET:HG2	1.96	0.45
1:F:78:ASP:HB3	1:G:114:LEU:CD1	2.46	0.45
1:A:1:PRO:O	1:A:3:ILE:HD13	2.15	0.45
1:C:157:THR:O	1:C:158:LYS:HB2	2.17	0.45
1:C:42:LEU:HD21	1:D:2:LEU:HA	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:HG23	1:C:20:TYR:CD1	2.51	0.45
1:D:118:ARG:C	1:D:119:ILE:HD12	2.36	0.45
1:D:88:CYS:SG	1:D:112:HIS:NE2	2.90	0.45
1:F:82:TYR:CZ	1:G:192:PRO:HD3	2.52	0.45
1:A:115:PRO:HG3	1:A:190:VAL:HG22	1.98	0.45
1:B:122:HIS:O	4:D:1101:FME:CE	2.63	0.45
1:D:78:ASP:HB3	1:E:114:LEU:HD13	1.98	0.45
1:D:97:SER:HB3	4:D:1103:FME:O	2.17	0.45
1:C:101:LEU:HD23	1:C:101:LEU:C	2.37	0.45
1:B:139:ALA:O	1:B:143:MET:HG2	2.17	0.45
1:C:41:SER:OG	1:D:32:MET:HG3	2.16	0.44
1:G:17:TYR:HB3	1:G:18:ASP:H	1.28	0.44
1:E:24:LEU:C	1:E:24:LEU:HD13	2.37	0.44
1:F:51:GLN:HG3	1:F:85:ASN:OD1	2.18	0.44
1:B:156:HIS:HD2	6:B:1028:HOH:O	1.99	0.44
1:D:123:GLN:C	4:D:1103:FME:HE2	2.38	0.44
1:D:140:GLU:O	1:D:143:MET:HG2	2.17	0.44
1:F:77:TYR:O	1:F:81:GLN:HG2	2.18	0.44
1:G:120:MET:HA	1:G:172:ARG:O	2.17	0.44
1:G:55:ASN:H	1:G:55:ASN:ND2	2.16	0.44
1:A:1:PRO:O	1:A:3:ILE:N	2.51	0.44
1:B:6:VAL:HB	1:B:7:VAL:H	0.89	0.44
4:D:1104:FME:O	1:E:68:GLY:N	2.40	0.44
1:D:97:SER:OG	4:D:1103:FME:CA	2.49	0.44
1:E:177:MET:CE	1:E:205:LYS:HB3	2.48	0.44
4:D:1106:FME:CE	1:G:149:LEU:HD13	2.45	0.44
1:G:151:ASN:ND2	1:G:161:LEU:HD21	2.31	0.44
1:G:175:SER:OG	1:G:178:GLU:HG3	2.18	0.44
1:G:28:ILE:HD13	1:G:62:TYR:OH	2.18	0.44
1:C:6:VAL:HG13	1:C:18:ASP:HA	1.99	0.43
1:G:122:HIS:HB3	1:G:171:ASP:HA	2.00	0.43
1:G:55:ASN:HD22	1:G:55:ASN:C	2.21	0.43
1:C:190:VAL:HG12	1:C:191:HIS:CD2	2.53	0.43
1:C:191:HIS:HB3	1:C:192:PRO:HD2	2.00	0.43
1:A:119:ILE:N	1:A:119:ILE:HD12	2.34	0.43
1:C:30:CYS:CB	1:C:32:MET:HE3	2.48	0.43
1:C:81:GLN:O	1:D:192:PRO:HD2	2.19	0.43
1:E:4:PRO:O	1:E:5:ILE:CB	2.63	0.43
1:C:88:CYS:SG	1:C:90:TRP:NE1	2.91	0.43
5:B:1001:GOL:H12	6:C:1027:HOH:O	2.19	0.43
1:B:97:SER:HB3	4:D:1101:FME:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:GLY:O	1:C:128:ALA:HB2	2.19	0.43
1:E:17:TYR:CB	1:E:21:SER:HB2	2.41	0.43
1:E:5:ILE:HA	1:E:6:VAL:HG22	1.99	0.43
1:F:25:ARG:HH21	1:G:7:VAL:CG2	2.25	0.43
1:A:122:HIS:O	4:D:1100:FME:HE2	2.18	0.43
4:D:1106:FME:HB2	1:G:98:MET:HG2	1.99	0.43
1:B:124:PRO:HA	4:D:1101:FME:HG3	2.01	0.42
1:D:51:GLN:HG3	1:D:85:ASN:OD1	2.18	0.42
1:A:1:PRO:O	1:A:3:ILE:CG1	2.67	0.42
1:A:22:ARG:HD3	1:A:22:ARG:O	2.19	0.42
1:C:179:ALA:HB3	1:C:185:LEU:HD11	2.01	0.42
1:G:95:ALA:O	1:G:100:SER:HB3	2.20	0.42
1:D:6:VAL:CG1	1:D:18:ASP:C	2.88	0.42
4:D:1104:FME:N	1:E:122:HIS:NE2	2.68	0.42
4:D:1104:FME:HB2	1:E:98:MET:HG2	2.00	0.42
4:D:1106:FME:CE	1:G:122:HIS:O	2.67	0.42
1:A:5:ILE:CD1	1:G:18:ASP:HB3	2.49	0.42
1:B:17:TYR:CE1	1:C:5:ILE:HG12	2.55	0.42
1:C:129:ARG:HB2	1:C:129:ARG:CZ	2.49	0.42
1:C:48:LEU:HD11	2:D:802:DIO:H22	2.01	0.42
1:E:101:LEU:HD23	1:E:101:LEU:C	2.40	0.42
1:F:44:ILE:HG13	1:F:76:ILE:CD1	2.47	0.42
1:A:157:THR:O	1:A:158:LYS:HB2	2.19	0.42
1:D:119:ILE:HD12	1:D:119:ILE:N	2.35	0.42
1:A:105:ALA:HA	1:A:156:HIS:CD2	2.55	0.42
1:E:97:SER:HB3	1:E:98:MET:H	1.48	0.42
1:C:2:LEU:HG	1:C:2:LEU:H	1.56	0.42
1:G:51:GLN:HG3	1:G:85:ASN:ND2	2.34	0.42
1:B:101:LEU:HD23	1:B:101:LEU:C	2.41	0.41
4:D:1104:FME:HA	1:E:97:SER:OG	2.19	0.41
1:A:161:LEU:O	1:A:165:GLU:HG3	2.20	0.41
1:A:115:PRO:CG	1:A:190:VAL:HG22	2.49	0.41
1:F:148:GLN:NE2	6:F:1082:HOH:O	2.53	0.41
4:D:1105:FME:HG3	1:F:98:MET:SD	2.60	0.41
1:E:77:TYR:OH	1:E:156:HIS:HE1	2.03	0.41
5:D:1003:GOL:O1	1:E:175:SER:HA	2.19	0.41
1:G:119:ILE:N	1:G:119:ILE:HD12	2.36	0.41
1:G:24:LEU:HD12	6:G:924:HOH:O	2.19	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.91	0.41
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.85	0.41
1:A:77:TYR:OH	1:A:156:HIS:CE1	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:LEU:HD13	1:G:42:LEU:HA	1.86	0.41
1:B:54:SER:OG	1:B:57:LYS:HG3	2.21	0.41
1:C:160:SER:OG	1:C:163:VAL:HG23	2.21	0.41
1:D:2:LEU:N	1:D:3:ILE:HG13	2.36	0.41
1:B:114:LEU:HD22	1:B:114:LEU:N	2.35	0.41
1:G:55:ASN:N	1:G:55:ASN:ND2	2.68	0.41
1:D:122:HIS:HB3	1:D:171:ASP:HA	2.02	0.41
1:A:3:ILE:O	1:A:4:PRO:O	2.39	0.41
4:D:1104:FME:C	1:E:68:GLY:O	2.69	0.41
1:E:2:LEU:HD23	1:E:2:LEU:N	2.35	0.41
1:G:6:VAL:CG1	1:G:7:VAL:CA	2.88	0.41
1:B:146:LYS:HE3	1:B:150:TYR:OH	2.21	0.40
1:D:122:HIS:O	4:D:1103:FME:CE	2.69	0.40
1:G:19:ILE:HG23	1:G:20:TYR:N	2.36	0.40
1:E:175:SER:OG	1:E:178:GLU:HG3	2.20	0.40
1:E:3:ILE:H	1:E:3:ILE:HG13	1.61	0.40
1:B:175:SER:HA	5:B:1000:GOL:O1	2.21	0.40
1:D:141:GLU:OE2	5:D:1003:GOL:C3	2.70	0.40
4:D:1103:FME:HCN	6:D:1208:HOH:O	2.21	0.40
1:F:17:TYR:O	1:F:18:ASP:O	2.39	0.40
1:D:35:ILE:O	1:D:68:GLY:HA3	2.21	0.40
1:D:24:LEU:HD11	1:D:49:PHE:CE2	2.57	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	180/277 (65%)	172 (96%)	4 (2%)	4 (2%)	8	3
1	B	179/277 (65%)	170 (95%)	5 (3%)	4 (2%)	8	3
1	C	179/277 (65%)	172 (96%)	5 (3%)	2 (1%)	17	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	180/277 (65%)	174 (97%)	2 (1%)	4 (2%)	8	3
1	E	192/277 (69%)	186 (97%)	5 (3%)	1 (0%)	34	30
1	F	183/277 (66%)	174 (95%)	6 (3%)	3 (2%)	12	6
1	G	190/277 (69%)	181 (95%)	8 (4%)	1 (0%)	34	30
All	All	1283/1939 (66%)	1229 (96%)	35 (3%)	19 (2%)	13	7

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	PRO
1	B	2	LEU
1	B	3	ILE
1	C	18	ASP
1	D	2	LEU
1	D	3	ILE
1	F	18	ASP
1	G	6	VAL
1	A	6	VAL
1	B	52	SER
1	F	2	LEU
1	A	3	ILE
1	E	18	ASP
1	B	6	VAL
1	D	6	VAL
1	C	6	VAL
1	D	4	PRO
1	F	6	VAL

### 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	157/226 (70%)	149 (95%)	8 (5%)	29	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	156/226 (69%)	148 (95%)	8 (5%)	29	26
1	C	156/226 (69%)	146 (94%)	10 (6%)	22	18
1	D	157/226 (70%)	150 (96%)	7 (4%)	34	32
1	E	168/226 (74%)	159 (95%)	9 (5%)	27	24
1	F	159/226 (70%)	151 (95%)	8 (5%)	30	27
1	G	166/226 (74%)	158 (95%)	8 (5%)	31	29
All	All	1119/1582 (71%)	1061 (95%)	58 (5%)	29	25

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	ILE
1	A	5	ILE
1	A	17	TYR
1	A	18	ASP
1	A	22	ARG
1	A	25	ARG
1	A	122	HIS
1	B	2	LEU
1	B	3	ILE
1	B	6	VAL
1	B	17	TYR
1	B	18	ASP
1	B	22	ARG
1	B	122	HIS
1	B	177	MET
1	C	1	PRO
1	C	2	LEU
1	C	18	ASP
1	C	24	LEU
1	C	26	GLU
1	C	97	SER
1	C	122	HIS
1	C	161	LEU
1	C	172	ARG
1	C	185	LEU
1	D	3	ILE
1	D	4	PRO
1	D	5	ILE

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Mol	Chain	Res	Type
1	D	18	ASP
1	D	97	SER
1	D	122	HIS
1	D	172	ARG
1	E	1	PRO
1	E	2	LEU
1	E	4	PRO
1	E	5	ILE
1	E	6	VAL
1	E	19	ILE
1	E	22	ARG
1	E	122	HIS
1	E	142	ILE
1	F	2	LEU
1	F	3	ILE
1	F	4	PRO
1	F	5	ILE
1	F	6	VAL
1	F	42	LEU
1	F	97	SER
1	F	122	HIS
1	G	2	LEU
1	G	5	ILE
1	G	18	ASP
1	G	32	MET
1	G	42	LEU
1	G	55	ASN
1	G	85	ASN
1	G	122	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	81	GLN
1	A	148	GLN
1	A	151	ASN
1	A	156	HIS
1	B	51	GLN
1	B	148	GLN
1	B	151	ASN
1	B	156	HIS

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Mol	Chain	Res	Type
1	B	180	GLN
1	C	112	HIS
1	C	148	GLN
1	C	156	HIS
1	C	191	HIS
1	D	156	HIS
1	E	112	HIS
1	E	148	GLN
1	E	156	HIS
1	F	46	GLN
1	F	112	HIS
1	F	148	GLN
1	F	156	HIS
1	F	180	GLN
1	F	191	HIS
1	G	51	GLN
1	G	55	ASN
1	G	85	ASN
1	G	112	HIS
1	G	148	GLN
1	G	151	ASN
1	G	156	HIS
1	G	194	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

27 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	DIO	A	800	-	6,6,6	1.65	1 (16%)	6,6,6	0.43	0
3	EDO	A	900	-	3,3,3	1.01	0	2,2,2	0.35	0
5	GOL	B	1000	-	5,5,5	4.01	3 (60%)	5,5,5	5.26	2 (40%)
5	GOL	B	1001	-	5,5,5	4.11	3 (60%)	5,5,5	5.26	2 (40%)
2	DIO	B	801	-	6,6,6	1.62	1 (16%)	6,6,6	0.41	0
3	EDO	B	901	-	3,3,3	0.97	0	2,2,2	0.35	0
3	EDO	B	902	-	3,3,3	1.00	0	2,2,2	0.36	0
5	GOL	C	1002	-	5,5,5	3.95	3 (60%)	5,5,5	5.26	2 (40%)
3	EDO	C	903	-	3,3,3	1.00	0	2,2,2	0.35	0
3	EDO	C	904	-	3,3,3	0.95	0	2,2,2	0.29	0
5	GOL	D	1003	-	5,5,5	4.04	3 (60%)	5,5,5	5.27	2 (40%)
4	FME	D	1100	-	8,9,10	0.95	0	5,9,11	1.59	2 (40%)
4	FME	D	1101	-	8,9,10	0.81	0	5,9,11	1.72	2 (40%)
4	FME	D	1102	-	8,9,10	1.03	0	5,9,11	1.91	2 (40%)
4	FME	D	1103	-	8,9,10	1.01	1 (12%)	5,9,11	1.80	2 (40%)
4	FME	D	1104	-	8,9,10	0.91	0	5,9,11	1.50	1 (20%)
4	FME	D	1105	-	8,9,10	0.83	0	5,9,11	1.49	1 (20%)
4	FME	D	1106	-	8,9,10	1.05	0	5,9,11	1.73	2 (40%)
2	DIO	D	802	-	6,6,6	1.62	1 (16%)	6,6,6	0.42	0
3	EDO	D	905	-	3,3,3	0.99	0	2,2,2	0.32	0
5	GOL	E	1004	-	5,5,5	4.13	3 (60%)	5,5,5	5.30	2 (40%)
2	DIO	E	803	-	6,6,6	1.70	1 (16%)	6,6,6	0.40	0
5	GOL	F	1005	-	5,5,5	3.87	3 (60%)	5,5,5	5.26	2 (40%)
2	DIO	F	804	-	6,6,6	1.62	1 (16%)	6,6,6	0.41	0
3	EDO	F	906	-	3,3,3	1.01	0	2,2,2	0.31	0
2	DIO	G	805	-	6,6,6	1.62	1 (16%)	6,6,6	0.40	0
3	EDO	G	907	-	3,3,3	0.97	0	2,2,2	0.30	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	DIO	A	800	-	-	0/0/6/6	0/1/1/1
3	EDO	A	900	-	-	0/1/1/1	0/0/0/0
5	GOL	B	1000	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1001	-	-	0/4/4/4	0/0/0/0
2	DIO	B	801	-	-	0/0/6/6	0/1/1/1
3	EDO	B	901	-	-	0/1/1/1	0/0/0/0
3	EDO	B	902	-	-	0/1/1/1	0/0/0/0
5	GOL	C	1002	-	-	0/4/4/4	0/0/0/0
3	EDO	C	903	-	-	0/1/1/1	0/0/0/0
3	EDO	C	904	-	-	0/1/1/1	0/0/0/0
5	GOL	D	1003	-	-	0/4/4/4	0/0/0/0
4	FME	D	1100	-	-	0/6/9/11	0/0/0/0
4	FME	D	1101	-	-	0/6/9/11	0/0/0/0
4	FME	D	1102	-	-	0/6/9/11	0/0/0/0
4	FME	D	1103	-	-	0/6/9/11	0/0/0/0
4	FME	D	1104	-	-	0/6/9/11	0/0/0/0
4	FME	D	1105	-	-	0/6/9/11	0/0/0/0
4	FME	D	1106	-	-	0/6/9/11	0/0/0/0
2	DIO	D	802	-	-	0/0/6/6	0/1/1/1
3	EDO	D	905	-	-	0/1/1/1	0/0/0/0
5	GOL	E	1004	-	-	0/4/4/4	0/0/0/0
2	DIO	E	803	-	-	0/0/6/6	0/1/1/1
5	GOL	F	1005	-	-	0/4/4/4	0/0/0/0
2	DIO	F	804	-	-	0/0/6/6	0/1/1/1
3	EDO	F	906	-	-	0/1/1/1	0/0/0/0
2	DIO	G	805	-	-	0/0/6/6	0/1/1/1
3	EDO	G	907	-	-	0/1/1/1	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1004	GOL	C3-C2	-8.08	1.20	1.52
5	D	1003	GOL	C3-C2	-8.04	1.20	1.52
5	B	1001	GOL	C3-C2	-8.02	1.20	1.52
5	B	1000	GOL	C3-C2	-7.81	1.21	1.52
5	C	1002	GOL	C3-C2	-7.76	1.21	1.52
5	F	1005	GOL	C3-C2	-7.55	1.22	1.52
2	E	803	DIO	O1-C2	-3.88	1.26	1.42
2	A	800	DIO	O1-C2	-3.74	1.27	1.42
2	D	802	DIO	O1-C2	-3.69	1.27	1.42
2	F	804	DIO	O1-C2	-3.68	1.27	1.42
2	B	801	DIO	O1-C2	-3.67	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	805	DIO	O1-C2	-3.66	1.27	1.42
5	E	1004	GOL	C1-C2	-3.31	1.39	1.52
5	B	1001	GOL	C1-C2	-3.30	1.39	1.52
5	B	1000	GOL	O2-C2	-3.30	1.33	1.43
5	F	1005	GOL	C1-C2	-3.19	1.39	1.52
5	C	1002	GOL	O2-C2	-3.06	1.34	1.43
5	B	1001	GOL	O2-C2	-2.97	1.34	1.43
5	D	1003	GOL	C1-C2	-2.93	1.40	1.52
5	E	1004	GOL	O2-C2	-2.93	1.34	1.43
5	B	1000	GOL	C1-C2	-2.87	1.40	1.52
5	C	1002	GOL	C1-C2	-2.86	1.40	1.52
5	F	1005	GOL	O2-C2	-2.81	1.35	1.43
5	D	1003	GOL	O2-C2	-2.76	1.35	1.43
4	D	1103	FME	CB-CA	-2.17	1.49	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1102	FME	O-C-CA	-2.98	117.55	125.69
4	D	1103	FME	O1-CN-N	-2.92	120.34	124.80
4	D	1106	FME	O1-CN-N	-2.85	120.44	124.80
4	D	1101	FME	O1-CN-N	-2.78	120.54	124.80
4	D	1100	FME	O1-CN-N	-2.57	120.87	124.80
4	D	1105	FME	O1-CN-N	-2.53	120.92	124.80
4	D	1102	FME	O1-CN-N	-2.52	120.94	124.80
4	D	1106	FME	O-C-CA	-2.38	119.18	125.69
4	D	1101	FME	O-C-CA	-2.20	119.69	125.69
4	D	1100	FME	O-C-CA	-2.10	119.94	125.69
4	D	1104	FME	O1-CN-N	-2.06	121.65	124.80
4	D	1103	FME	O-C-CA	-2.04	120.12	125.69
5	B	1001	GOL	O2-C2-C3	6.20	138.25	108.47
5	D	1003	GOL	O2-C2-C3	6.21	138.28	108.47
5	C	1002	GOL	O2-C2-C3	6.23	138.37	108.47
5	E	1004	GOL	O2-C2-C3	6.26	138.54	108.47
5	B	1000	GOL	O2-C2-C3	6.27	138.58	108.47
5	F	1005	GOL	O2-C2-C3	6.39	139.14	108.47
5	F	1005	GOL	O3-C3-C2	9.87	160.01	109.97
5	B	1000	GOL	O3-C3-C2	9.92	160.27	109.97
5	C	1002	GOL	O3-C3-C2	9.96	160.47	109.97
5	B	1001	GOL	O3-C3-C2	9.96	160.48	109.97
5	D	1003	GOL	O3-C3-C2	9.97	160.53	109.97
5	E	1004	GOL	O3-C3-C2	10.03	160.82	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	DIO	1	0
3	A	900	EDO	1	0
5	B	1000	GOL	1	0
5	B	1001	GOL	2	0
2	B	801	DIO	2	0
3	B	901	EDO	1	0
3	B	902	EDO	1	0
3	C	903	EDO	1	0
5	D	1003	GOL	2	0
4	D	1100	FME	3	0
4	D	1101	FME	10	0
4	D	1102	FME	6	0
4	D	1103	FME	10	0
4	D	1104	FME	12	0
4	D	1105	FME	5	0
4	D	1106	FME	9	0
2	D	802	DIO	1	0
2	E	803	DIO	2	0
5	F	1005	GOL	1	0
2	F	804	DIO	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 ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.