



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 08:08 am BST

PDB ID : 2GDG
Title : Crystal structure of covalently modified macrophage inhibitory factor
Authors : Golubkov, P.A.; Hackert, M.L.
Deposited on : 2006-03-16
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
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

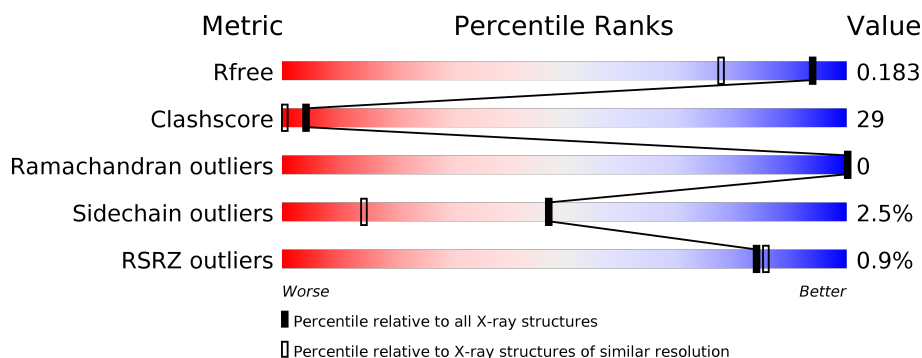
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 ≥ 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	114	<div> <div>50%</div> <div>39%</div> <div>8%</div> <div>•</div> </div>
1	B	114	<div> <div>51%</div> <div>38%</div> <div>8%</div> <div>•</div> </div>
1	C	114	<div> <div>3%</div> <div>46%</div> <div>39%</div> <div>10%</div> <div>5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3072 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 Macrophage migration inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			869	548	151	164	6			
1	B	114	Total	C	N	O	S	0	0	0
			869	548	151	164	6			
1	C	114	Total	C	N	O	S	0	0	0
			869	548	151	164	6			

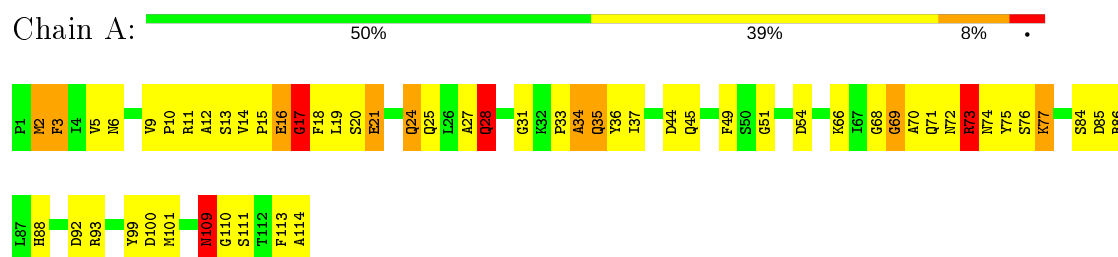
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	170	Total	O	0	0
			170	170		
2	B	159	Total	O	0	0
			159	159		
2	C	136	Total	O	0	0
			136	136		

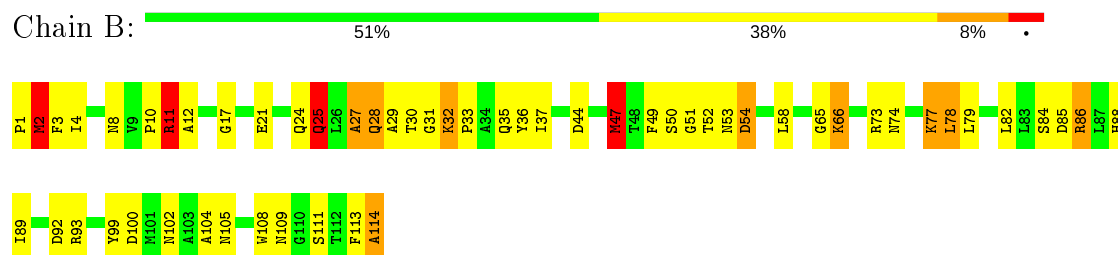
3 Residue-property plots [i](#)

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.

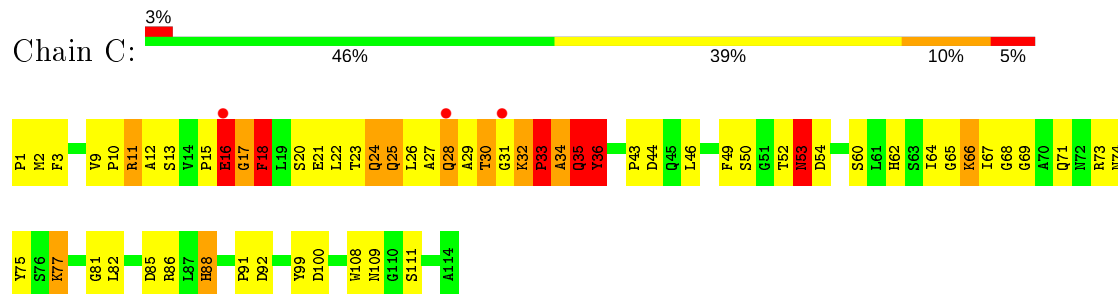
- Molecule 1: Macrophage migration inhibitory factor



- Molecule 1: Macrophage migration inhibitory factor



- Molecule 1: Macrophage migration inhibitory factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	94.70 Å 94.70 Å 87.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.45 23.80 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-1.45) 97.4 (23.80-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.45 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.147 , 0.183 0.147 , 0.183	Depositor DCC
R_{free} test set	3872 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3072	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	3.44	75/889 (8.4%)	2.78	74/1209 (6.1%)
1	B	4.41	84/889 (9.4%)	3.57	82/1209 (6.8%)
1	C	6.83	111/889 (12.5%)	4.85	130/1209 (10.8%)
All	All	5.09	270/2667 (10.1%)	3.83	286/3627 (7.9%)

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
1	B	0	6
1	C	0	10
All	All	0	19

All (270) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	GLU	CD-OE1	135.93	2.75	1.25
1	B	11	ARG	CZ-NH2	71.56	2.26	1.33
1	C	16	GLU	CG-CD	67.64	2.53	1.51
1	C	11	ARG	CZ-NH2	35.29	1.78	1.33
1	C	36	TYR	CE2-CZ	34.77	1.83	1.38
1	C	16	GLU	CA-CB	30.03	2.20	1.53
1	C	16	GLU	CD-OE2	28.01	1.56	1.25
1	C	36	TYR	CD1-CE1	26.73	1.79	1.39
1	B	11	ARG	CZ-NH1	26.61	1.67	1.33
1	B	66	LYS	CG-CD	-26.36	0.62	1.52
1	A	28	GLN	CD-OE1	24.91	1.78	1.24
1	C	36	TYR	CE1-CZ	24.56	1.70	1.38
1	C	16	GLU	CA-C	24.15	2.15	1.52
1	C	53	ASN	CG-ND2	22.26	1.88	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	GLN	CD-NE2	21.39	1.86	1.32
1	B	11	ARG	CD-NE	21.30	1.82	1.46
1	A	16	GLU	CD-OE1	21.12	1.48	1.25
1	A	16	GLU	CG-CD	21.09	1.83	1.51
1	A	28	GLN	CD-NE2	20.59	1.84	1.32
1	A	17	GLY	N-CA	19.46	1.75	1.46
1	C	36	TYR	CZ-OH	19.38	1.70	1.37
1	B	77	LYS	CE-NZ	19.23	1.97	1.49
1	B	11	ARG	NE-CZ	18.94	1.57	1.33
1	B	66	LYS	CD-CE	18.65	1.97	1.51
1	A	21	GLU	CG-CD	18.52	1.79	1.51
1	A	73	ARG	NE-CZ	18.21	1.56	1.33
1	A	73	ARG	CZ-NH1	18.12	1.56	1.33
1	C	53	ASN	CB-CG	-17.79	1.10	1.51
1	C	32	LYS	CE-NZ	17.63	1.93	1.49
1	B	25	GLN	CD-OE1	16.65	1.60	1.24
1	B	2	MET	CB-CG	-16.63	0.98	1.51
1	B	32	LYS	CD-CE	16.18	1.91	1.51
1	C	36	TYR	CG-CD1	16.14	1.60	1.39
1	A	86	ARG	CZ-NH1	15.32	1.52	1.33
1	C	31	GLY	C-O	15.23	1.48	1.23
1	C	36	TYR	CB-CG	15.21	1.74	1.51
1	B	25	GLN	CB-CG	14.88	1.92	1.52
1	B	114	ALA	C-OXT	14.82	1.51	1.23
1	C	30	THR	C-N	-14.34	1.07	1.33
1	C	36	TYR	CD2-CE2	14.33	1.60	1.39
1	C	11	ARG	CD-NE	14.26	1.70	1.46
1	C	17	GLY	CA-C	14.23	1.74	1.51
1	A	24	GLN	CG-CD	13.48	1.82	1.51
1	C	86	ARG	CZ-NH2	13.29	1.50	1.33
1	C	88	HIS	CD2-NE2	13.04	1.69	1.42
1	B	28	GLN	CD-NE2	12.89	1.65	1.32
1	C	16	GLU	C-O	12.59	1.47	1.23
1	B	36	TYR	CE1-CZ	-12.57	1.22	1.38
1	B	52	THR	C-O	12.15	1.46	1.23
1	B	36	TYR	CE2-CZ	12.08	1.54	1.38
1	C	13	SER	CB-OG	11.89	1.57	1.42
1	A	16	GLU	CA-CB	11.81	1.79	1.53
1	A	35	GLN	CG-CD	11.78	1.78	1.51
1	C	34	ALA	C-O	11.67	1.45	1.23
1	C	17	GLY	N-CA	11.67	1.63	1.46
1	A	35	GLN	CD-OE1	11.63	1.49	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	GLN	CD-NE2	11.53	1.61	1.32
1	C	35	GLN	CA-CB	11.44	1.79	1.53
1	B	28	GLN	CD-OE1	11.40	1.49	1.24
1	B	36	TYR	CD2-CE2	11.38	1.56	1.39
1	B	25	GLN	CG-CD	-11.35	1.25	1.51
1	C	32	LYS	CA-CB	11.18	1.78	1.53
1	C	2	MET	CB-CG	-10.99	1.16	1.51
1	C	36	TYR	CG-CD2	10.92	1.53	1.39
1	C	11	ARG	CZ-NH1	10.75	1.47	1.33
1	A	13	SER	CB-OG	10.64	1.56	1.42
1	C	28	GLN	CD-NE2	10.52	1.59	1.32
1	A	113	PHE	CG-CD1	10.38	1.54	1.38
1	A	2	MET	CG-SD	10.34	2.08	1.81
1	B	36	TYR	CZ-OH	10.32	1.55	1.37
1	C	35	GLN	CD-OE1	10.32	1.46	1.24
1	C	27	ALA	CA-CB	10.30	1.74	1.52
1	C	77	LYS	CD-CE	10.30	1.76	1.51
1	C	33	PRO	N-CD	10.29	1.62	1.47
1	B	31	GLY	C-N	10.27	1.57	1.34
1	A	11	ARG	CZ-NH1	10.18	1.46	1.33
1	A	73	ARG	CZ-NH2	10.18	1.46	1.33
1	B	29	ALA	C-O	10.13	1.42	1.23
1	B	49	PHE	CD1-CE1	10.08	1.59	1.39
1	C	15	PRO	N-CA	10.02	1.64	1.47
1	C	71	GLN	CD-NE2	9.91	1.57	1.32
1	C	44	ASP	CB-CG	9.88	1.72	1.51
1	A	86	ARG	NE-CZ	-9.75	1.20	1.33
1	B	99	TYR	CE2-CZ	-9.74	1.25	1.38
1	A	24	GLN	CD-OE1	9.73	1.45	1.24
1	C	32	LYS	CG-CD	-9.71	1.19	1.52
1	B	30	THR	C-O	9.55	1.41	1.23
1	C	24	GLN	CD-NE2	9.50	1.56	1.32
1	A	73	ARG	CG-CD	9.36	1.75	1.51
1	B	51	GLY	C-O	9.27	1.38	1.23
1	A	77	LYS	CE-NZ	9.19	1.72	1.49
1	B	28	GLN	CG-CD	9.19	1.72	1.51
1	C	24	GLN	CG-CD	9.14	1.72	1.51
1	C	24	GLN	CA-CB	9.09	1.74	1.53
1	B	50	SER	CA-CB	8.99	1.66	1.52
1	B	88	HIS	CA-CB	8.96	1.73	1.53
1	C	99	TYR	CE2-CZ	-8.95	1.26	1.38
1	A	20	SER	CA-CB	8.91	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	SER	CA-CB	8.85	1.66	1.52
1	B	47	MET	SD-CE	-8.84	1.28	1.77
1	A	2	MET	CB-CG	-8.80	1.23	1.51
1	A	73	ARG	CD-NE	-8.55	1.31	1.46
1	C	81	GLY	C-O	8.55	1.37	1.23
1	B	114	ALA	CA-CB	-8.47	1.34	1.52
1	C	12	ALA	C-O	8.46	1.39	1.23
1	B	11	ARG	CB-CG	-8.44	1.29	1.52
1	C	25	GLN	CB-CG	8.38	1.75	1.52
1	B	24	GLN	C-O	8.38	1.39	1.23
1	A	15	PRO	N-CD	8.32	1.59	1.47
1	A	31	GLY	N-CA	8.31	1.58	1.46
1	A	113	PHE	C-O	8.28	1.39	1.23
1	C	16	GLU	CB-CG	-8.27	1.36	1.52
1	A	113	PHE	CE2-CZ	8.21	1.52	1.37
1	C	85	ASP	CG-OD2	8.13	1.44	1.25
1	B	27	ALA	C-O	7.98	1.38	1.23
1	B	54	ASP	CA-C	7.97	1.73	1.52
1	B	114	ALA	C-O	7.93	1.38	1.23
1	C	75	TYR	CZ-OH	7.92	1.51	1.37
1	B	53	ASN	CB-CG	-7.90	1.32	1.51
1	C	28	GLN	CD-OE1	7.88	1.41	1.24
1	A	111	SER	CA-CB	7.83	1.64	1.52
1	A	18	PHE	CB-CG	7.82	1.64	1.51
1	B	78	LEU	CG-CD1	7.82	1.80	1.51
1	A	35	GLN	CA-CB	7.80	1.71	1.53
1	C	1	PRO	N-CD	-7.70	1.37	1.47
1	C	65	GLY	C-O	7.66	1.35	1.23
1	C	34	ALA	CA-C	-7.63	1.33	1.52
1	C	85	ASP	C-O	7.59	1.37	1.23
1	B	66	LYS	CB-CG	7.58	1.73	1.52
1	B	113	PHE	C-O	7.55	1.37	1.23
1	C	73	ARG	NE-CZ	7.51	1.42	1.33
1	C	69	GLY	C-O	-7.51	1.11	1.23
1	A	27	ALA	N-CA	7.49	1.61	1.46
1	C	33	PRO	C-N	-7.46	1.16	1.34
1	A	16	GLU	CD-OE2	-7.45	1.17	1.25
1	C	33	PRO	CG-CD	7.44	1.75	1.50
1	B	77	LYS	CB-CG	7.37	1.72	1.52
1	B	73	ARG	CZ-NH1	7.34	1.42	1.33
1	C	66	LYS	CE-NZ	7.34	1.67	1.49
1	B	1	PRO	CA-CB	-7.29	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	GLY	C-N	7.26	1.46	1.33
1	C	31	GLY	N-CA	-7.24	1.35	1.46
1	B	77	LYS	CD-CE	-7.23	1.33	1.51
1	B	44	ASP	CB-CG	7.21	1.67	1.51
1	C	33	PRO	CA-CB	7.11	1.67	1.53
1	A	11	ARG	CD-NE	7.11	1.58	1.46
1	C	88	HIS	CG-ND1	-7.10	1.23	1.38
1	B	84	SER	C-O	7.08	1.36	1.23
1	C	73	ARG	CZ-NH1	6.94	1.42	1.33
1	A	15	PRO	N-CA	6.93	1.59	1.47
1	A	15	PRO	CA-C	-6.92	1.39	1.52
1	B	12	ALA	CA-CB	6.87	1.66	1.52
1	A	9	VAL	CB-CG2	6.84	1.67	1.52
1	B	114	ALA	N-CA	6.83	1.60	1.46
1	C	66	LYS	CD-CE	6.82	1.68	1.51
1	C	21	GLU	CG-CD	6.80	1.62	1.51
1	A	49	PHE	CD1-CE1	6.72	1.52	1.39
1	A	18	PHE	CD1-CE1	6.68	1.52	1.39
1	A	99	TYR	CD1-CE1	6.68	1.49	1.39
1	C	18	PHE	CD1-CE1	6.67	1.52	1.39
1	C	20	SER	CB-OG	6.65	1.50	1.42
1	C	50	SER	C-O	6.61	1.35	1.23
1	C	65	GLY	N-CA	6.59	1.55	1.46
1	A	99	TYR	CE2-CZ	-6.59	1.29	1.38
1	B	99	TYR	CD1-CE1	6.57	1.49	1.39
1	B	102	ASN	CG-ND2	6.54	1.49	1.32
1	B	50	SER	C-O	6.52	1.35	1.23
1	A	2	MET	CA-CB	-6.50	1.39	1.53
1	A	20	SER	CA-C	-6.46	1.36	1.52
1	A	12	ALA	C-O	6.44	1.35	1.23
1	A	99	TYR	CZ-OH	6.42	1.48	1.37
1	C	2	MET	CG-SD	6.41	1.97	1.81
1	A	12	ALA	CA-C	-6.40	1.36	1.52
1	C	52	THR	C-O	6.39	1.35	1.23
1	B	32	LYS	CA-CB	6.34	1.68	1.53
1	C	109	ASN	CG-ND2	-6.33	1.17	1.32
1	B	82	LEU	C-O	6.33	1.35	1.23
1	C	35	GLN	CD-NE2	6.33	1.48	1.32
1	A	36	TYR	CG-CD2	-6.30	1.30	1.39
1	B	51	GLY	C-N	-6.29	1.19	1.34
1	B	33	PRO	C-O	6.23	1.35	1.23
1	A	69	GLY	N-CA	-6.21	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	PRO	N-CA	6.20	1.57	1.47
1	B	47	MET	CB-CG	-6.20	1.31	1.51
1	B	31	GLY	CA-C	-6.17	1.42	1.51
1	C	88	HIS	CE1-NE2	-6.17	1.18	1.32
1	B	2	MET	SD-CE	6.07	2.11	1.77
1	B	99	TYR	CZ-OH	6.07	1.48	1.37
1	A	34	ALA	CA-CB	6.05	1.65	1.52
1	A	28	GLN	CG-CD	-6.04	1.37	1.51
1	A	113	PHE	CD2-CE2	-5.99	1.27	1.39
1	C	17	GLY	C-N	-5.95	1.20	1.34
1	C	18	PHE	CG-CD1	-5.94	1.29	1.38
1	A	9	VAL	C-N	5.94	1.45	1.34
1	B	79	LEU	C-O	5.92	1.34	1.23
1	C	30	THR	CA-CB	-5.92	1.38	1.53
1	B	85	ASP	CB-CG	5.91	1.64	1.51
1	C	111	SER	CB-OG	5.91	1.50	1.42
1	B	35	GLN	CD-OE1	5.90	1.36	1.24
1	C	82	LEU	C-N	5.86	1.47	1.34
1	A	36	TYR	CD1-CE1	5.84	1.48	1.39
1	A	68	GLY	CA-C	-5.83	1.42	1.51
1	C	108	TRP	CE3-CZ3	5.83	1.48	1.38
1	A	93	ARG	CZ-NH1	5.82	1.40	1.33
1	B	50	SER	CA-C	-5.82	1.37	1.52
1	C	109	ASN	CG-OD1	5.82	1.36	1.24
1	C	26	LEU	N-CA	5.80	1.57	1.46
1	A	71	GLN	CD-OE1	5.78	1.36	1.24
1	A	12	ALA	N-CA	5.78	1.57	1.46
1	C	30	THR	N-CA	5.78	1.57	1.46
1	C	88	HIS	CG-CD2	-5.77	1.25	1.35
1	A	17	GLY	CA-C	-5.75	1.42	1.51
1	B	111	SER	CB-OG	5.72	1.49	1.42
1	C	18	PHE	CG-CD2	5.72	1.47	1.38
1	A	14	VAL	CB-CG2	5.70	1.64	1.52
1	B	27	ALA	C-N	-5.69	1.21	1.34
1	C	77	LYS	CE-NZ	5.69	1.63	1.49
1	C	71	GLN	CB-CG	5.66	1.67	1.52
1	A	36	TYR	CE2-CZ	-5.64	1.31	1.38
1	C	15	PRO	N-CD	-5.63	1.40	1.47
1	C	66	LYS	CA-CB	-5.63	1.41	1.53
1	B	8	ASN	C-O	5.62	1.34	1.23
1	C	29	ALA	CA-CB	5.61	1.64	1.52
1	A	114	ALA	N-CA	5.58	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	ALA	N-CA	5.58	1.57	1.46
1	B	93	ARG	CZ-NH1	5.57	1.40	1.33
1	C	81	GLY	CA-C	-5.56	1.43	1.51
1	B	78	LEU	C-O	5.56	1.33	1.23
1	C	88	HIS	CB-CG	5.55	1.60	1.50
1	C	1	PRO	CA-CB	-5.54	1.42	1.53
1	C	3	PHE	CB-CG	5.51	1.60	1.51
1	C	54	ASP	CG-OD1	-5.48	1.12	1.25
1	C	12	ALA	CA-C	-5.46	1.38	1.52
1	C	27	ALA	C-O	5.45	1.33	1.23
1	A	76	SER	CA-CB	5.43	1.61	1.52
1	A	69	GLY	C-O	5.42	1.32	1.23
1	C	86	ARG	CG-CD	5.42	1.65	1.51
1	A	109	ASN	CG-ND2	-5.41	1.19	1.32
1	B	31	GLY	C-O	5.41	1.32	1.23
1	B	50	SER	N-CA	5.39	1.57	1.46
1	C	18	PHE	CB-CG	5.33	1.60	1.51
1	B	77	LYS	C-O	5.33	1.33	1.23
1	A	84	SER	CB-OG	5.33	1.49	1.42
1	B	35	GLN	CA-CB	5.30	1.65	1.53
1	B	88	HIS	C-N	5.29	1.46	1.34
1	C	67	ILE	C-O	5.25	1.33	1.23
1	C	44	ASP	CG-OD2	-5.25	1.13	1.25
1	B	65	GLY	C-O	5.24	1.32	1.23
1	A	74	ASN	CG-ND2	5.23	1.46	1.32
1	A	85	ASP	CB-CG	5.22	1.62	1.51
1	B	2	MET	CG-SD	5.22	1.94	1.81
1	C	74	ASN	CB-CG	5.21	1.63	1.51
1	A	28	GLN	CA-C	-5.19	1.39	1.52
1	C	77	LYS	N-CA	5.19	1.56	1.46
1	B	11	ARG	CG-CD	5.16	1.64	1.51
1	B	54	ASP	CA-CB	5.16	1.65	1.53
1	C	10	PRO	CA-CB	5.16	1.63	1.53
1	C	28	GLN	CB-CG	5.15	1.66	1.52
1	A	111	SER	CB-OG	-5.11	1.35	1.42
1	C	92	ASP	CG-OD2	5.11	1.37	1.25
1	A	110	GLY	C-O	5.09	1.31	1.23
1	B	54	ASP	C-N	-5.07	1.24	1.34
1	B	12	ALA	N-CA	5.06	1.56	1.46
1	A	2	MET	SD-CE	-5.05	1.49	1.77
1	B	10	PRO	N-CD	5.04	1.54	1.47
1	C	54	ASP	CB-CG	5.04	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	LYS	CD-CE	5.04	1.63	1.51
1	A	18	PHE	CG-CD1	-5.03	1.31	1.38
1	B	93	ARG	N-CA	5.01	1.56	1.46
1	B	93	ARG	CZ-NH2	5.00	1.39	1.33

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	ARG	NE-CZ-NH1	52.12	146.36	120.30
1	C	86	ARG	NE-CZ-NH1	47.73	144.16	120.30
1	C	36	TYR	CZ-CE2-CD2	-45.53	78.82	119.80
1	B	11	ARG	NE-CZ-NH1	43.12	141.86	120.30
1	C	11	ARG	NE-CZ-NH2	-43.09	98.76	120.30
1	C	36	TYR	CD1-CE1-CZ	-37.98	85.62	119.80
1	C	36	TYR	CB-CG-CD2	-36.41	99.16	121.00
1	C	16	GLU	CG-CD-OE1	-31.96	54.37	118.30
1	B	11	ARG	NH1-CZ-NH2	-28.32	88.24	119.40
1	B	11	ARG	CD-NE-CZ	-27.35	85.31	123.60
1	B	36	TYR	CZ-CE2-CD2	-27.30	95.23	119.80
1	C	16	GLU	O-C-N	24.27	164.46	123.20
1	C	36	TYR	CE1-CZ-CE2	22.36	155.57	119.80
1	C	16	GLU	CG-CD-OE2	-21.51	75.29	118.30
1	B	54	ASP	CB-CG-OD2	-21.48	98.97	118.30
1	C	16	GLU	CA-C-N	-21.21	73.78	116.20
1	A	16	GLU	OE1-CD-OE2	20.84	148.30	123.30
1	C	31	GLY	O-C-N	-19.65	91.26	122.70
1	C	16	GLU	CA-CB-CG	-18.65	72.37	113.40
1	B	36	TYR	CE1-CZ-CE2	18.52	149.43	119.80
1	A	21	GLU	OE1-CD-OE2	18.29	145.24	123.30
1	B	2	MET	CG-SD-CE	-17.75	71.81	100.20
1	B	28	GLN	CG-CD-NE2	-16.83	76.30	116.70
1	B	77	LYS	CD-CE-NZ	16.64	149.97	111.70
1	C	16	GLU	C-N-CA	-15.98	88.74	122.30
1	C	44	ASP	CB-CG-OD2	-15.81	104.07	118.30
1	C	86	ARG	NE-CZ-NH2	-15.72	112.44	120.30
1	B	86	ARG	NE-CZ-NH1	15.66	128.13	120.30
1	B	28	GLN	CG-CD-OE1	15.63	152.86	121.60
1	B	36	TYR	CD1-CE1-CZ	-15.41	105.93	119.80
1	B	21	GLU	OE1-CD-OE2	-15.07	105.22	123.30
1	C	36	TYR	CE1-CZ-OH	-14.74	80.30	120.10
1	C	86	ARG	NH1-CZ-NH2	-14.69	103.24	119.40
1	C	92	ASP	CB-CG-OD2	-14.69	105.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	CB-CG-OD1	14.42	131.28	118.30
1	C	33	PRO	N-CD-CG	-14.30	81.74	103.20
1	A	73	ARG	CD-NE-CZ	-13.97	104.04	123.60
1	B	47	MET	CG-SD-CE	13.79	122.26	100.20
1	A	113	PHE	CB-CG-CD2	13.67	130.37	120.80
1	A	15	PRO	O-C-N	-13.59	100.96	122.70
1	C	18	PHE	CD1-CE1-CZ	-13.22	104.23	120.10
1	A	16	GLU	CG-CD-OE1	-13.22	91.86	118.30
1	A	35	GLN	CG-CD-NE2	12.74	147.27	116.70
1	C	33	PRO	N-CA-CB	-12.68	88.08	103.30
1	A	25	GLN	CG-CD-OE1	12.56	146.72	121.60
1	A	113	PHE	CG-CD2-CE2	12.02	134.02	120.80
1	C	85	ASP	CB-CG-OD1	11.98	129.09	118.30
1	B	86	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	B	25	GLN	CG-CD-OE1	11.96	145.51	121.60
1	C	99	TYR	CD1-CE1-CZ	-11.86	109.12	119.80
1	C	16	GLU	N-CA-CB	-11.63	89.67	110.60
1	C	33	PRO	O-C-N	11.62	141.29	122.70
1	A	11	ARG	NE-CZ-NH1	-11.61	114.50	120.30
1	B	2	MET	CA-CB-CG	11.57	132.97	113.30
1	C	36	TYR	CG-CD2-CE2	11.44	130.45	121.30
1	B	31	GLY	O-C-N	-11.42	104.43	122.70
1	C	44	ASP	OD1-CG-OD2	11.14	144.47	123.30
1	B	73	ARG	NE-CZ-NH1	-11.09	114.75	120.30
1	C	86	ARG	CD-NE-CZ	-11.08	108.09	123.60
1	C	92	ASP	CB-CG-OD1	10.96	128.16	118.30
1	B	49	PHE	CB-CG-CD2	-10.88	113.18	120.80
1	C	35	GLN	CA-CB-CG	-10.88	89.45	113.40
1	A	73	ARG	NH1-CZ-NH2	-10.76	107.56	119.40
1	B	93	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	B	77	LYS	CG-CD-CE	-10.43	80.62	111.90
1	A	16	GLU	C-N-CA	-10.35	100.56	122.30
1	A	18	PHE	CB-CG-CD2	-10.32	113.57	120.80
1	B	44	ASP	CB-CG-OD2	-10.27	109.06	118.30
1	A	93	ARG	NE-CZ-NH2	10.22	125.41	120.30
1	B	85	ASP	CB-CG-OD2	-10.18	109.13	118.30
1	C	30	THR	CA-C-O	-10.13	98.83	120.10
1	C	75	TYR	CZ-CE2-CD2	-10.13	110.69	119.80
1	A	75	TYR	CG-CD1-CE1	-10.09	113.23	121.30
1	A	92	ASP	CB-CG-OD1	9.99	127.29	118.30
1	A	75	TYR	CB-CG-CD1	-9.97	115.02	121.00
1	A	54	ASP	CB-CG-OD1	9.96	127.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	ASN	CB-CG-OD1	9.90	141.40	121.60
1	B	36	TYR	OH-CZ-CE2	-9.80	93.65	120.10
1	B	99	TYR	CD1-CE1-CZ	-9.79	110.99	119.80
1	B	29	ALA	CA-C-N	9.70	138.53	117.20
1	A	28	GLN	OE1-CD-NE2	-9.63	99.74	121.90
1	C	77	LYS	CD-CE-NZ	-9.57	89.69	111.70
1	B	92	ASP	CB-CG-OD2	-9.50	109.75	118.30
1	C	30	THR	CA-CB-CG2	9.42	125.59	112.40
1	C	16	GLU	CB-CG-CD	9.37	139.50	114.20
1	C	35	GLN	N-CA-CB	-9.31	93.83	110.60
1	A	36	TYR	CG-CD1-CE1	-9.23	113.92	121.30
1	C	100	ASP	CB-CG-OD1	9.18	126.56	118.30
1	B	36	TYR	CB-CG-CD2	-9.13	115.52	121.00
1	C	33	PRO	CA-C-O	-9.07	98.44	120.20
1	C	33	PRO	CA-N-CD	9.04	124.36	111.70
1	A	35	GLN	CG-CD-OE1	-9.01	103.58	121.60
1	C	16	GLU	CB-CA-C	-8.98	92.43	110.40
1	B	31	GLY	CA-C-O	8.98	136.76	120.60
1	A	36	TYR	CB-CG-CD1	-8.97	115.62	121.00
1	A	99	TYR	CD1-CE1-CZ	-8.91	111.78	119.80
1	B	100	ASP	CB-CG-OD1	8.89	126.30	118.30
1	A	16	GLU	N-CA-CB	-8.89	94.60	110.60
1	A	113	PHE	CD1-CG-CD2	-8.88	106.76	118.30
1	C	29	ALA	CA-C-O	-8.87	101.47	120.10
1	B	85	ASP	CB-CG-OD1	-8.75	110.43	118.30
1	A	86	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	C	31	GLY	CA-C-N	8.65	136.24	117.20
1	C	44	ASP	CB-CG-OD1	-8.58	110.58	118.30
1	A	16	GLU	CA-C-N	-8.51	99.18	116.20
1	C	11	ARG	CD-NE-CZ	-8.47	111.73	123.60
1	C	73	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	C	27	ALA	N-CA-CB	-8.41	98.32	110.10
1	B	85	ASP	OD1-CG-OD2	8.36	139.19	123.30
1	C	12	ALA	CA-C-N	8.21	135.26	117.20
1	C	22	LEU	O-C-N	8.12	135.69	122.70
1	C	54	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	B	1	PRO	N-CA-CB	8.05	112.96	103.30
1	C	12	ALA	O-C-N	-7.94	109.99	122.70
1	A	12	ALA	O-C-N	-7.88	110.08	122.70
1	C	29	ALA	N-CA-CB	-7.87	99.09	110.10
1	A	2	MET	CG-SD-CE	-7.79	87.74	100.20
1	C	81	GLY	O-C-N	-7.78	110.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ALA	CA-C-N	7.78	134.31	117.20
1	A	88	HIS	CG-CD2-NE2	-7.74	94.50	109.20
1	C	73	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	A	54	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	C	36	TYR	CA-CB-CG	-7.64	98.88	113.40
1	B	114	ALA	CA-C-O	7.62	136.09	120.10
1	C	34	ALA	N-CA-CB	-7.61	99.44	110.10
1	C	3	PHE	CB-CG-CD2	-7.61	115.47	120.80
1	C	17	GLY	CA-C-O	-7.59	106.94	120.60
1	B	25	GLN	CG-CD-NE2	-7.57	98.54	116.70
1	C	109	ASN	CB-CG-OD1	-7.49	106.62	121.60
1	B	44	ASP	OD1-CG-OD2	7.35	137.26	123.30
1	C	25	GLN	O-C-N	7.35	134.45	122.70
1	A	24	GLN	CG-CD-OE1	-7.32	106.95	121.60
1	B	25	GLN	CB-CG-CD	-7.32	92.57	111.60
1	C	50	SER	CA-C-N	7.32	130.83	116.20
1	B	99	TYR	CE1-CZ-CE2	7.29	131.47	119.80
1	C	34	ALA	O-C-N	-7.28	111.05	122.70
1	B	44	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	C	20	SER	O-C-N	-7.27	111.06	122.70
1	C	18	PHE	CE1-CZ-CE2	7.15	132.87	120.00
1	A	86	ARG	NH1-CZ-NH2	-7.15	111.53	119.40
1	C	108	TRP	CD2-CE3-CZ3	-7.08	109.60	118.80
1	A	16	GLU	CA-CB-CG	-7.06	97.86	113.40
1	B	3	PHE	CB-CG-CD2	-7.06	115.86	120.80
1	C	34	ALA	CA-C-N	7.04	132.68	117.20
1	C	22	LEU	CA-C-O	-7.01	105.38	120.10
1	B	113	PHE	CB-CG-CD2	7.00	125.70	120.80
1	C	67	ILE	O-C-N	-6.95	111.38	123.20
1	C	99	TYR	CE1-CZ-CE2	6.94	130.91	119.80
1	C	85	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	114	ALA	N-CA-CB	-6.93	100.39	110.10
1	C	21	GLU	OE1-CD-OE2	6.88	131.56	123.30
1	C	53	ASN	OD1-CG-ND2	-6.85	106.14	121.90
1	A	10	PRO	N-CA-CB	-6.83	95.09	102.60
1	C	18	PHE	CG-CD1-CE1	6.81	128.29	120.80
1	A	11	ARG	CD-NE-CZ	-6.80	114.08	123.60
1	B	49	PHE	CD1-CE1-CZ	-6.80	111.94	120.10
1	A	18	PHE	CD1-CG-CD2	6.79	127.13	118.30
1	A	35	GLN	OE1-CD-NE2	-6.78	106.30	121.90
1	C	64	ILE	O-C-N	6.78	134.73	123.20
1	A	21	GLU	CG-CD-OE2	-6.77	104.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	THR	CA-C-N	6.73	129.66	116.20
1	C	18	PHE	O-C-N	6.71	133.44	122.70
1	C	82	LEU	O-C-N	-6.69	112.00	122.70
1	B	114	ALA	N-CA-C	-6.67	92.99	111.00
1	C	36	TYR	CB-CA-C	-6.66	97.08	110.40
1	A	92	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	15	PRO	CA-C-O	6.65	136.16	120.20
1	A	100	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	16	GLU	O-C-N	6.62	134.46	123.20
1	C	28	GLN	CA-C-N	6.62	131.76	117.20
1	A	70	ALA	N-CA-CB	-6.61	100.84	110.10
1	C	36	TYR	CD1-CG-CD2	6.60	125.17	117.90
1	C	16	GLU	OE1-CD-OE2	-6.57	115.42	123.30
1	C	31	GLY	C-N-CA	6.56	138.10	121.70
1	A	101	MET	O-C-N	6.55	133.19	122.70
1	A	93	ARG	NH1-CZ-NH2	-6.54	112.20	119.40
1	C	111	SER	N-CA-CB	-6.52	100.71	110.50
1	A	36	TYR	CD1-CG-CD2	6.52	125.07	117.90
1	A	35	GLN	N-CA-CB	-6.46	98.97	110.60
1	A	33	PRO	CA-N-CD	6.45	120.73	111.70
1	B	49	PHE	CD1-CG-CD2	6.44	126.67	118.30
1	C	100	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	50	SER	CA-C-N	6.41	129.03	116.20
1	C	18	PHE	CB-CG-CD1	6.41	125.29	120.80
1	B	93	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	B	74	ASN	CB-CG-OD1	-6.40	108.80	121.60
1	C	27	ALA	CA-C-O	-6.37	106.72	120.10
1	C	49	PHE	CG-CD2-CE2	-6.36	113.80	120.80
1	B	52	THR	CA-C-N	6.35	131.17	117.20
1	B	29	ALA	O-C-N	-6.32	112.59	122.70
1	C	9	VAL	CA-CB-CG2	-6.28	101.49	110.90
1	A	25	GLN	CG-CD-NE2	-6.25	101.69	116.70
1	A	70	ALA	O-C-N	6.21	132.63	122.70
1	C	28	GLN	CA-CB-CG	-6.20	99.77	113.40
1	C	30	THR	N-CA-C	-6.17	94.34	111.00
1	B	52	THR	O-C-N	-6.16	112.84	122.70
1	B	50	SER	O-C-N	-6.16	112.73	123.20
1	A	9	VAL	CA-CB-CG2	-6.14	101.69	110.90
1	A	28	GLN	N-CA-CB	-6.12	99.58	110.60
1	C	31	GLY	CA-C-O	6.10	131.59	120.60
1	B	24	GLN	CA-C-N	6.07	130.54	117.20
1	A	111	SER	CB-CA-C	-6.06	98.58	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	GLY	CA-C-O	6.05	131.49	120.60
1	C	77	LYS	CG-CD-CE	-6.03	93.81	111.90
1	C	36	TYR	CG-CD1-CE1	-6.02	116.48	121.30
1	A	110	GLY	CA-C-O	-6.02	109.77	120.60
1	B	10	PRO	N-CD-CG	-5.99	94.22	103.20
1	C	25	GLN	CG-CD-OE1	5.98	133.57	121.60
1	A	88	HIS	ND1-CG-CD2	5.98	117.17	108.80
1	A	44	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	17	GLY	CA-C-O	-5.97	109.86	120.60
1	C	74	ASN	CB-CG-OD1	-5.96	109.67	121.60
1	C	18	PHE	CB-CG-CD2	-5.96	116.63	120.80
1	C	28	GLN	O-C-N	-5.95	113.18	122.70
1	C	82	LEU	CA-C-O	5.94	132.58	120.10
1	B	108	TRP	CG-CD2-CE3	-5.92	128.57	133.90
1	C	46	LEU	CB-CA-C	5.89	121.40	110.20
1	B	86	ARG	NH1-CZ-NH2	-5.88	112.94	119.40
1	B	27	ALA	CB-CA-C	-5.88	101.29	110.10
1	B	28	GLN	OE1-CD-NE2	-5.87	108.40	121.90
1	B	102	ASN	CB-CG-OD1	5.84	133.29	121.60
1	C	35	GLN	O-C-N	-5.82	113.38	122.70
1	A	27	ALA	N-CA-CB	-5.81	101.97	110.10
1	B	100	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	32	LYS	CG-CD-CE	-5.79	94.54	111.90
1	C	18	PHE	CA-C-O	-5.78	107.95	120.10
1	C	1	PRO	N-CA-CB	5.78	110.23	103.30
1	C	81	GLY	CA-C-N	5.78	129.90	117.20
1	A	113	PHE	O-C-N	-5.77	113.47	122.70
1	C	23	THR	CA-CB-CG2	-5.75	104.35	112.40
1	C	36	TYR	O-C-N	-5.74	113.52	122.70
1	B	25	GLN	OE1-CD-NE2	-5.73	108.71	121.90
1	A	113	PHE	CA-C-N	5.64	129.62	117.20
1	B	51	GLY	CA-C-O	-5.61	110.51	120.60
1	A	33	PRO	N-CD-CG	-5.60	94.80	103.20
1	C	29	ALA	CA-C-N	5.60	129.53	117.20
1	C	11	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	C	15	PRO	CA-C-O	5.55	133.53	120.20
1	A	51	GLY	CA-C-O	-5.55	110.61	120.60
1	A	25	GLN	OE1-CD-NE2	-5.54	109.16	121.90
1	C	99	TYR	CG-CD1-CE1	5.52	125.72	121.30
1	A	73	ARG	CB-CG-CD	-5.51	97.28	111.60
1	A	109	ASN	CB-CG-OD1	-5.50	110.59	121.60
1	B	32	LYS	CD-CE-NZ	-5.50	99.05	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	LEU	CA-C-N	5.50	129.29	117.20
1	C	18	PHE	N-CA-CB	-5.49	100.72	110.60
1	B	113	PHE	CG-CD2-CE2	5.49	126.83	120.80
1	A	75	TYR	CZ-CE2-CD2	-5.45	114.89	119.80
1	C	75	TYR	CG-CD2-CE2	5.44	125.65	121.30
1	C	25	GLN	C-N-CA	-5.44	108.11	121.70
1	B	11	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	67	ILE	CA-CB-CG1	-5.43	100.69	111.00
1	C	33	PRO	CB-CA-C	5.40	125.50	112.00
1	A	74	ASN	CB-CG-ND2	5.39	129.65	116.70
1	B	77	LYS	N-CA-CB	-5.38	100.92	110.60
1	C	66	LYS	CD-CE-NZ	5.37	124.06	111.70
1	A	19	LEU	O-C-N	-5.37	114.11	122.70
1	B	29	ALA	CA-C-O	-5.36	108.84	120.10
1	C	99	TYR	CZ-CE2-CD2	-5.35	114.99	119.80
1	A	20	SER	O-C-N	-5.33	114.17	122.70
1	B	113	PHE	CA-C-N	5.31	128.88	117.20
1	B	73	ARG	NH1-CZ-NH2	5.27	125.20	119.40
1	B	99	TYR	CE1-CZ-OH	-5.27	105.88	120.10
1	C	35	GLN	CA-C-N	5.22	128.69	117.20
1	A	15	PRO	CA-N-CD	-5.22	104.19	111.50
1	B	77	LYS	CA-CB-CG	-5.22	101.92	113.40
1	C	53	ASN	CB-CG-ND2	-5.20	104.22	116.70
1	C	88	HIS	CG-CD2-NE2	-5.20	99.33	109.20
1	B	52	THR	CB-CA-C	-5.18	97.61	111.60
1	B	109	ASN	OD1-CG-ND2	5.17	133.79	121.90
1	A	99	TYR	CE1-CZ-OH	-5.16	106.17	120.10
1	B	78	LEU	O-C-N	-5.16	114.45	122.70
1	A	3	PHE	CZ-CE2-CD2	-5.15	113.92	120.10
1	B	89	ILE	O-C-N	5.15	130.94	122.70
1	C	85	ASP	O-C-N	-5.13	114.49	122.70
1	C	32	LYS	CA-CB-CG	-5.13	102.12	113.40
1	C	15	PRO	C-N-CA	-5.12	108.90	121.70
1	C	1	PRO	N-CD-CG	5.10	110.86	103.20
1	B	113	PHE	O-C-N	-5.10	114.54	122.70
1	C	28	GLN	N-CA-CB	-5.09	101.43	110.60
1	C	26	LEU	CA-CB-CG	-5.08	103.62	115.30
1	C	75	TYR	CE1-CZ-CE2	5.07	127.91	119.80
1	B	109	ASN	CB-CG-ND2	-5.06	104.55	116.70
1	B	49	PHE	CE1-CZ-CE2	5.05	129.10	120.00
1	A	18	PHE	CD1-CE1-CZ	-5.04	114.05	120.10
1	C	18	PHE	CG-CD2-CE2	-5.01	115.29	120.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLY	Mainchain
1	A	28	GLN	Sidechain
1	A	73	ARG	Sidechain
1	B	11	ARG	Sidechain
1	B	25	GLN	Sidechain
1	B	28	GLN	Sidechain
1	B	54	ASP	Sidechain
1	B	86	ARG	Sidechain,Mainchain
1	C	16	GLU	Sidechain
1	C	18	PHE	Sidechain
1	C	24	GLN	Sidechain
1	C	28	GLN	Sidechain
1	C	33	PRO	Mainchain
1	C	34	ALA	Mainchain
1	C	35	GLN	Sidechain,Mainchain
1	C	36	TYR	Sidechain
1	C	53	ASN	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	869	0	853	41	0
1	B	869	0	852	53	0
1	C	869	0	851	60	0
2	A	170	0	0	2	0
2	B	159	0	0	2	0
2	C	136	0	0	3	0
All	All	3072	0	2556	152	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 29.

All (152) 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:C:36:TYR:CG	1:C:36:TYR:CB	1.74	1.69
1:C:36:TYR:CZ	1:C:36:TYR:CE2	1.83	1.65
1:C:36:TYR:CE1	1:C:36:TYR:CD1	1.79	1.64
1:C:32:LYS:CA	1:C:32:LYS:CB	1.78	1.62
1:A:73:ARG:CD	1:A:73:ARG:CG	1.75	1.59
1:C:77:LYS:CE	1:C:77:LYS:CD	1.77	1.58
1:C:35:GLN:CB	1:C:35:GLN:CA	1.79	1.57
1:A:16:GLU:CA	1:A:16:GLU:CB	1.79	1.56
1:C:25:GLN:CG	1:C:25:GLN:CB	1.75	1.55
1:C:33:PRO:CD	1:C:33:PRO:CG	1.75	1.55
1:B:78:LEU:CG	1:B:78:LEU:CD1	1.80	1.54
1:C:11:ARG:CD	1:C:11:ARG:NE	1.70	1.52
1:A:77:LYS:NZ	1:A:77:LYS:CE	1.72	1.52
1:B:11:ARG:CZ	1:B:11:ARG:NH1	1.67	1.51
1:A:21:GLU:CD	1:A:21:GLU:CG	1.79	1.50
1:C:17:GLY:C	1:C:17:GLY:CA	1.74	1.49
1:A:35:GLN:CD	1:A:35:GLN:CG	1.78	1.49
1:A:17:GLY:N	1:A:17:GLY:CA	1.75	1.49
1:B:32:LYS:CD	1:B:32:LYS:CE	1.91	1.48
1:A:16:GLU:CD	1:A:16:GLU:CG	1.83	1.47
1:A:24:GLN:CD	1:A:24:GLN:CG	1.82	1.44
1:C:11:ARG:NH2	1:C:11:ARG:CZ	1.78	1.44
1:B:66:LYS:CD	1:B:66:LYS:CB	1.96	1.43
1:B:25:GLN:CB	1:B:25:GLN:CG	1.92	1.43
1:C:16:GLU:CA	1:C:16:GLU:HG2	1.49	1.42
1:C:36:TYR:OH	1:C:36:TYR:CZ	1.70	1.42
1:B:66:LYS:CE	1:B:66:LYS:CD	1.97	1.41
1:B:11:ARG:NE	1:B:11:ARG:CD	1.82	1.41
1:A:2:MET:CG	1:A:2:MET:SD	2.08	1.40
1:B:2:MET:SD	1:B:2:MET:CE	2.11	1.38
1:C:36:TYR:CD2	1:C:36:TYR:CZ	2.19	1.30
1:C:32:LYS:NZ	1:C:32:LYS:CE	1.93	1.29
1:A:28:GLN:CD	1:A:28:GLN:NE2	1.84	1.29
1:B:25:GLN:NE2	1:B:25:GLN:CD	1.86	1.28
1:B:77:LYS:NZ	1:B:77:LYS:CE	1.97	1.28
1:C:53:ASN:ND2	1:C:53:ASN:CG	1.88	1.25
1:A:28:GLN:CD	1:A:28:GLN:OE1	1.78	1.21
1:C:16:GLU:CA	1:C:16:GLU:CB	2.20	1.19
1:C:16:GLU:CA	1:C:16:GLU:CG	2.20	1.18
1:B:66:LYS:CE	1:B:66:LYS:CG	2.23	1.16
1:C:16:GLU:CA	1:C:16:GLU:C	2.15	1.14
1:C:36:TYR:CZ	1:C:36:TYR:CD1	2.37	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:CD2	1:C:88:HIS:NE2	1.69	1.11
1:C:36:TYR:CG	1:C:36:TYR:CZ	2.40	1.09
1:B:11:ARG:CZ	1:B:11:ARG:CD	2.31	1.08
1:C:16:GLU:CA	1:C:17:GLY:N	2.18	1.07
1:B:2:MET:CE	1:B:2:MET:CG	2.38	1.01
1:C:35:GLN:CG	1:C:35:GLN:CA	2.39	1.00
1:A:73:ARG:CD	1:A:73:ARG:CB	2.41	0.98
1:B:11:ARG:CZ	1:B:11:ARG:NH2	2.26	0.98
1:C:36:TYR:CG	1:C:36:TYR:CA	2.48	0.96
1:B:25:GLN:CB	1:B:25:GLN:CD	2.34	0.95
1:C:36:TYR:CE1	1:C:36:TYR:OH	2.19	0.95
1:C:36:TYR:CD2	1:C:36:TYR:CB	2.49	0.95
1:C:77:LYS:CE	1:C:77:LYS:CG	2.48	0.91
1:C:16:GLU:OE1	1:C:16:GLU:HG2	1.72	0.90
1:A:16:GLU:C	1:A:17:GLY:CA	2.40	0.89
1:A:2:MET:CE	1:A:2:MET:CG	2.51	0.88
1:A:16:GLU:N	1:A:16:GLU:CB	2.36	0.87
1:C:11:ARG:CD	1:C:11:ARG:CZ	2.53	0.87
1:C:53:ASN:ND2	1:C:53:ASN:CB	2.40	0.85
1:B:66:LYS:CD	1:B:66:LYS:HG3	1.33	0.85
1:B:66:LYS:HG2	1:B:66:LYS:CD	1.33	0.85
1:B:66:LYS:HD3	1:B:66:LYS:CG	1.33	0.84
1:B:25:GLN:NE2	1:B:25:GLN:CG	2.39	0.84
1:B:78:LEU:CD2	1:B:78:LEU:CD1	2.56	0.83
1:C:77:LYS:NZ	1:C:77:LYS:CD	2.40	0.83
1:A:16:GLU:CA	1:A:16:GLU:CG	2.56	0.82
1:C:25:GLN:CB	1:C:25:GLN:CD	2.48	0.82
1:B:66:LYS:CG	1:B:66:LYS:HD2	1.33	0.82
1:C:35:GLN:N	1:C:35:GLN:CB	2.43	0.81
1:B:2:MET:HG3	1:B:2:MET:CE	2.10	0.80
1:C:16:GLU:HA	1:C:16:GLU:HG2	1.62	0.78
1:C:62:HIS:HD2	2:C:176:HOH:O	1.67	0.78
1:C:16:GLU:CD	1:C:16:GLU:CG	2.53	0.77
1:A:73:ARG:NE	1:A:73:ARG:CG	2.47	0.77
1:B:66:LYS:HD3	1:B:66:LYS:CA	2.15	0.77
1:C:32:LYS:CG	1:C:32:LYS:CA	2.62	0.76
1:C:30:THR:O	1:C:66:LYS:HE2	1.88	0.74
1:B:25:GLN:HB3	1:B:78:LEU:HD21	1.71	0.71
1:A:16:GLU:OE1	1:A:16:GLU:CG	2.39	0.70
1:B:32:LYS:CD	1:B:32:LYS:NZ	2.55	0.70
1:A:2:MET:HE1	2:C:163:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ARG:NH2	1:C:11:ARG:NE	2.39	0.69
1:B:66:LYS:N	1:B:66:LYS:HD3	2.08	0.69
1:C:16:GLU:CA	1:C:17:GLY:H	2.04	0.69
1:A:77:LYS:NZ	1:A:77:LYS:CD	2.55	0.68
1:A:2:MET:CB	1:A:2:MET:SD	2.79	0.68
1:B:66:LYS:CD	1:B:66:LYS:CA	2.68	0.68
1:B:11:ARG:CZ	1:B:11:ARG:HD3	2.23	0.68
1:A:21:GLU:CG	1:A:21:GLU:OE2	2.40	0.67
1:C:32:LYS:CB	1:C:32:LYS:N	2.56	0.67
1:C:16:GLU:OE1	1:C:16:GLU:CG	2.42	0.67
1:C:25:GLN:CG	1:C:25:GLN:CA	2.72	0.67
1:C:53:ASN:ND2	1:C:53:ASN:HB3	2.10	0.67
1:A:16:GLU:C	1:A:16:GLU:CB	2.62	0.67
1:B:66:LYS:CE	1:B:66:LYS:HG2	2.23	0.66
1:C:32:LYS:C	1:C:32:LYS:CB	2.64	0.65
1:B:2:MET:HE2	1:B:2:MET:HG3	1.77	0.65
1:C:17:GLY:O	1:C:17:GLY:CA	2.44	0.65
1:B:78:LEU:CB	1:B:78:LEU:CD1	2.69	0.65
1:B:25:GLN:CG	1:B:78:LEU:HD11	2.29	0.63
1:B:66:LYS:HD3	1:B:66:LYS:CB	1.95	0.62
1:B:66:LYS:CD	1:B:66:LYS:CG	0.62	0.62
1:B:25:GLN:NE2	1:B:25:GLN:HG3	2.15	0.62
1:C:35:GLN:CA	1:C:35:GLN:HG2	2.28	0.61
1:C:16:GLU:N	1:C:16:GLU:CB	2.65	0.60
1:C:16:GLU:OE1	1:C:17:GLY:N	2.35	0.59
1:A:21:GLU:CD	1:A:21:GLU:CB	2.67	0.58
1:B:66:LYS:NZ	1:B:66:LYS:HG3	2.19	0.58
1:A:34:ALA:HA	1:A:37:ILE:HD12	1.85	0.57
1:B:66:LYS:CE	1:B:66:LYS:HG3	2.27	0.57
1:A:16:GLU:H	1:A:16:GLU:CB	2.14	0.56
1:A:16:GLU:CD	1:A:16:GLU:CB	2.71	0.56
1:B:2:MET:CB	1:B:2:MET:CE	2.79	0.56
1:C:35:GLN:H	1:C:35:GLN:CB	2.20	0.54
1:B:66:LYS:CB	1:B:66:LYS:HD2	2.00	0.54
1:B:66:LYS:NZ	1:B:66:LYS:CG	2.70	0.54
1:C:16:GLU:OE1	1:C:16:GLU:CA	2.55	0.54
1:B:25:GLN:CG	1:B:25:GLN:CA	2.84	0.51
1:C:17:GLY:N	1:C:17:GLY:C	2.62	0.51
1:A:73:ARG:HD2	1:A:73:ARG:CB	2.35	0.51
1:C:35:GLN:C	1:C:35:GLN:CB	2.69	0.51
1:C:77:LYS:HZ2	1:C:77:LYS:CD	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:HG3	2:A:191:HOH:O	2.10	0.51
1:A:35:GLN:OE1	1:A:35:GLN:CG	2.57	0.51
1:C:17:GLY:CA	1:C:18:PHE:N	2.59	0.51
1:B:25:GLN:HG2	1:B:78:LEU:HD11	1.93	0.50
1:A:3:PHE:CE2	1:A:5:VAL:CG2	2.95	0.49
1:A:6:ASN:HD22	1:A:45:GLN:HG3	1.76	0.49
1:C:16:GLU:CG	1:C:16:GLU:OE2	2.61	0.48
1:A:2:MET:HE2	1:A:2:MET:CG	2.43	0.47
1:B:25:GLN:CA	1:B:25:GLN:CD	2.83	0.47
1:B:47:MET:CE	1:B:58:LEU:HG	2.46	0.46
1:B:2:MET:HE3	1:B:2:MET:HB2	1.97	0.46
1:C:66:LYS:HB3	1:C:66:LYS:HE3	1.65	0.46
1:B:66:LYS:CD	1:B:66:LYS:NZ	2.70	0.45
1:A:109:ASN:HD22	1:C:91:PRO:HB2	1.81	0.45
1:A:73:ARG:HB3	1:A:73:ARG:CD	2.41	0.45
1:C:62:HIS:CD2	2:C:176:HOH:O	2.53	0.45
1:B:4:ILE:HD11	2:B:211:HOH:O	2.17	0.45
1:B:2:MET:HB2	1:B:2:MET:CE	2.46	0.45
1:A:72:ASN:ND2	1:B:105:ASN:HD22	2.16	0.43
1:A:69:GLY:HA2	2:B:137:HOH:O	2.18	0.43
1:A:109:ASN:HA	1:A:109:ASN:HD22	1.59	0.43
1:B:2:MET:HE3	1:B:2:MET:CB	2.48	0.42
1:A:6:ASN:ND2	2:A:126:HOH:O	2.52	0.42
1:A:16:GLU:O	1:A:17:GLY:CA	2.66	0.41
1:A:21:GLU:CG	1:A:21:GLU:OE1	2.54	0.41
1:B:27:ALA:HA	1:B:37:ILE:HD11	2.03	0.41
1:B:104:ALA:HA	1:B:114:ALA:HB2	2.02	0.40
1:B:47:MET:HE2	1:B:58:LEU:HG	2.03	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	112/114 (98%)	112 (100%)	0	0	100	100
1	B	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
1	C	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
All	All	336/342 (98%)	331 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	95/95 (100%)	94 (99%)	1 (1%)	73	48
1	B	95/95 (100%)	91 (96%)	4 (4%)	30	4
1	C	95/95 (100%)	93 (98%)	2 (2%)	53	19
All	All	285/285 (100%)	278 (98%)	7 (2%)	47	14

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	B	2	MET
1	B	11	ARG
1	B	25	GLN
1	B	47	MET
1	C	36	TYR
1	C	43	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	109	ASN
1	B	28	GLN

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Mol	Chain	Res	Type
1	B	105	ASN
1	C	35	GLN
1	C	62	HIS
1	C	71	GLN
1	C	109	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](#)

There are no ligands in this entry.

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	C	3
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	17:GLY	C	18:PHE	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	51:GLY	C	52:THR	N	1.19
1	C	33:PRO	C	34:ALA	N	1.16
1	C	30:THR	C	31:GLY	N	1.07

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	114/114 (100%)	-0.08	0 100 100	11, 17, 28, 39	0
1	B	114/114 (100%)	-0.08	0 100 100	12, 17, 31, 44	0
1	C	114/114 (100%)	0.03	3 (2%) 56 58	13, 19, 38, 67	0
All	All	342/342 (100%)	-0.04	3 (0%) 84 86	11, 17, 33, 67	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	16	GLU	2.6
1	C	31	GLY	2.2
1	C	28	GLN	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.