



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:49 PM UTC

PDB ID : 6Y73 / pdb_00006y73
Title : The crystal structure of human MACROD2 in space group P43
Authors : Wazir, S.; Maksimainen, M.M.; Lehtio, L.
Deposited on : 2020-02-28
Resolution : 1.70 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

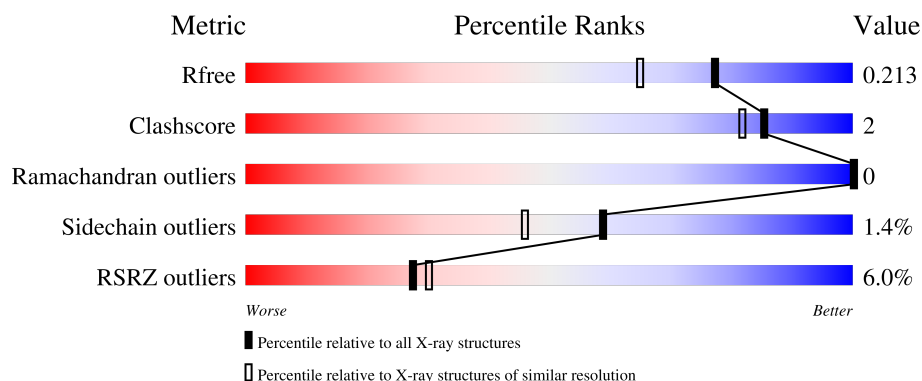
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 ≥ 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	366	
1	B	366	
1	C	366	
1	D	366	
1	E	366	

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Mol	Chain	Length	Quality of chain
1	F	366	
1	G	366	
1	H	366	

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	TLA	C	401	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15593 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 ADP-ribose glycohydrolase MACROD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	4	0
			1729	1103	302	311	13			
1	B	215	Total	C	N	O	S	0	7	0
			1745	1115	304	314	12			
1	C	215	Total	C	N	O	S	0	4	0
			1722	1098	301	310	13			
1	D	218	Total	C	N	O	S	0	3	0
			1741	1110	303	313	15			
1	E	218	Total	C	N	O	S	0	7	0
			1760	1121	308	318	13			
1	F	215	Total	C	N	O	S	0	7	0
			1746	1117	302	313	14			
1	G	215	Total	C	N	O	S	0	4	0
			1720	1097	300	310	13			
1	H	217	Total	C	N	O	S	0	5	0
			1739	1111	300	316	12			

There are 1032 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-122	MET	-	initiating methionine	UNP A1Z1Q3
A	-121	HIS	-	expression tag	UNP A1Z1Q3
A	-120	HIS	-	expression tag	UNP A1Z1Q3
A	-119	HIS	-	expression tag	UNP A1Z1Q3
A	-118	HIS	-	expression tag	UNP A1Z1Q3
A	-117	HIS	-	expression tag	UNP A1Z1Q3
A	-116	HIS	-	expression tag	UNP A1Z1Q3
A	-115	SER	-	expression tag	UNP A1Z1Q3
A	-114	SER	-	expression tag	UNP A1Z1Q3
A	-113	GLY	-	expression tag	UNP A1Z1Q3
A	-112	MET	-	expression tag	UNP A1Z1Q3
A	-111	SER	-	expression tag	UNP A1Z1Q3
A	-110	ASP	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-109	LYS	-	expression tag	UNP A1Z1Q3
A	-108	ILE	-	expression tag	UNP A1Z1Q3
A	-107	ILE	-	expression tag	UNP A1Z1Q3
A	-106	HIS	-	expression tag	UNP A1Z1Q3
A	-105	LEU	-	expression tag	UNP A1Z1Q3
A	-104	THR	-	expression tag	UNP A1Z1Q3
A	-103	ASP	-	expression tag	UNP A1Z1Q3
A	-102	ASP	-	expression tag	UNP A1Z1Q3
A	-101	SER	-	expression tag	UNP A1Z1Q3
A	-100	PHE	-	expression tag	UNP A1Z1Q3
A	-99	ASP	-	expression tag	UNP A1Z1Q3
A	-98	THR	-	expression tag	UNP A1Z1Q3
A	-97	ASP	-	expression tag	UNP A1Z1Q3
A	-96	VAL	-	expression tag	UNP A1Z1Q3
A	-95	LEU	-	expression tag	UNP A1Z1Q3
A	-94	LYS	-	expression tag	UNP A1Z1Q3
A	-93	ALA	-	expression tag	UNP A1Z1Q3
A	-92	ASP	-	expression tag	UNP A1Z1Q3
A	-91	GLY	-	expression tag	UNP A1Z1Q3
A	-90	ALA	-	expression tag	UNP A1Z1Q3
A	-89	ILE	-	expression tag	UNP A1Z1Q3
A	-88	LEU	-	expression tag	UNP A1Z1Q3
A	-87	VAL	-	expression tag	UNP A1Z1Q3
A	-86	ASP	-	expression tag	UNP A1Z1Q3
A	-85	PHE	-	expression tag	UNP A1Z1Q3
A	-84	TRP	-	expression tag	UNP A1Z1Q3
A	-83	ALA	-	expression tag	UNP A1Z1Q3
A	-82	GLU	-	expression tag	UNP A1Z1Q3
A	-81	TRP	-	expression tag	UNP A1Z1Q3
A	-80	CYS	-	expression tag	UNP A1Z1Q3
A	-79	GLY	-	expression tag	UNP A1Z1Q3
A	-78	PRO	-	expression tag	UNP A1Z1Q3
A	-77	CYS	-	expression tag	UNP A1Z1Q3
A	-76	LYS	-	expression tag	UNP A1Z1Q3
A	-75	MET	-	expression tag	UNP A1Z1Q3
A	-74	ILE	-	expression tag	UNP A1Z1Q3
A	-73	ALA	-	expression tag	UNP A1Z1Q3
A	-72	PRO	-	expression tag	UNP A1Z1Q3
A	-71	ILE	-	expression tag	UNP A1Z1Q3
A	-70	LEU	-	expression tag	UNP A1Z1Q3
A	-69	ASP	-	expression tag	UNP A1Z1Q3
A	-68	GLU	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-67	ILE	-	expression tag	UNP A1Z1Q3
A	-66	ALA	-	expression tag	UNP A1Z1Q3
A	-65	ASP	-	expression tag	UNP A1Z1Q3
A	-64	GLU	-	expression tag	UNP A1Z1Q3
A	-63	TYR	-	expression tag	UNP A1Z1Q3
A	-62	GLN	-	expression tag	UNP A1Z1Q3
A	-61	GLY	-	expression tag	UNP A1Z1Q3
A	-60	LYS	-	expression tag	UNP A1Z1Q3
A	-59	LEU	-	expression tag	UNP A1Z1Q3
A	-58	THR	-	expression tag	UNP A1Z1Q3
A	-57	VAL	-	expression tag	UNP A1Z1Q3
A	-56	ALA	-	expression tag	UNP A1Z1Q3
A	-55	LYS	-	expression tag	UNP A1Z1Q3
A	-54	LEU	-	expression tag	UNP A1Z1Q3
A	-53	ASN	-	expression tag	UNP A1Z1Q3
A	-52	ILE	-	expression tag	UNP A1Z1Q3
A	-51	ASP	-	expression tag	UNP A1Z1Q3
A	-50	GLN	-	expression tag	UNP A1Z1Q3
A	-49	ASN	-	expression tag	UNP A1Z1Q3
A	-48	PRO	-	expression tag	UNP A1Z1Q3
A	-47	GLY	-	expression tag	UNP A1Z1Q3
A	-46	THR	-	expression tag	UNP A1Z1Q3
A	-45	ALA	-	expression tag	UNP A1Z1Q3
A	-44	PRO	-	expression tag	UNP A1Z1Q3
A	-43	LYS	-	expression tag	UNP A1Z1Q3
A	-42	TYR	-	expression tag	UNP A1Z1Q3
A	-41	GLY	-	expression tag	UNP A1Z1Q3
A	-40	ILE	-	expression tag	UNP A1Z1Q3
A	-39	ARG	-	expression tag	UNP A1Z1Q3
A	-38	GLY	-	expression tag	UNP A1Z1Q3
A	-37	ILE	-	expression tag	UNP A1Z1Q3
A	-36	PRO	-	expression tag	UNP A1Z1Q3
A	-35	THR	-	expression tag	UNP A1Z1Q3
A	-34	LEU	-	expression tag	UNP A1Z1Q3
A	-33	LEU	-	expression tag	UNP A1Z1Q3
A	-32	LEU	-	expression tag	UNP A1Z1Q3
A	-31	PHE	-	expression tag	UNP A1Z1Q3
A	-30	LYS	-	expression tag	UNP A1Z1Q3
A	-29	ASN	-	expression tag	UNP A1Z1Q3
A	-28	GLY	-	expression tag	UNP A1Z1Q3
A	-27	GLU	-	expression tag	UNP A1Z1Q3
A	-26	VAL	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	ALA	-	expression tag	UNP A1Z1Q3
A	-24	ALA	-	expression tag	UNP A1Z1Q3
A	-23	THR	-	expression tag	UNP A1Z1Q3
A	-22	LYS	-	expression tag	UNP A1Z1Q3
A	-21	VAL	-	expression tag	UNP A1Z1Q3
A	-20	GLY	-	expression tag	UNP A1Z1Q3
A	-19	ALA	-	expression tag	UNP A1Z1Q3
A	-18	LEU	-	expression tag	UNP A1Z1Q3
A	-17	SER	-	expression tag	UNP A1Z1Q3
A	-16	LYS	-	expression tag	UNP A1Z1Q3
A	-15	GLY	-	expression tag	UNP A1Z1Q3
A	-14	GLN	-	expression tag	UNP A1Z1Q3
A	-13	LEU	-	expression tag	UNP A1Z1Q3
A	-12	LYS	-	expression tag	UNP A1Z1Q3
A	-11	GLU	-	expression tag	UNP A1Z1Q3
A	-10	PHE	-	expression tag	UNP A1Z1Q3
A	-9	LEU	-	expression tag	UNP A1Z1Q3
A	-8	ASP	-	expression tag	UNP A1Z1Q3
A	-7	ALA	-	expression tag	UNP A1Z1Q3
A	-6	ASN	-	expression tag	UNP A1Z1Q3
A	-5	LEU	-	expression tag	UNP A1Z1Q3
A	-4	ALA	-	expression tag	UNP A1Z1Q3
A	-3	GLY	-	expression tag	UNP A1Z1Q3
A	-2	THR	-	expression tag	UNP A1Z1Q3
A	-1	GLU	-	expression tag	UNP A1Z1Q3
A	0	ASN	-	expression tag	UNP A1Z1Q3
A	1	LEU	-	expression tag	UNP A1Z1Q3
A	2	TYR	-	expression tag	UNP A1Z1Q3
A	3	PHE	-	expression tag	UNP A1Z1Q3
A	4	GLN	-	expression tag	UNP A1Z1Q3
A	5	SER	-	expression tag	UNP A1Z1Q3
A	6	MET	-	expression tag	UNP A1Z1Q3
B	-122	MET	-	initiating methionine	UNP A1Z1Q3
B	-121	HIS	-	expression tag	UNP A1Z1Q3
B	-120	HIS	-	expression tag	UNP A1Z1Q3
B	-119	HIS	-	expression tag	UNP A1Z1Q3
B	-118	HIS	-	expression tag	UNP A1Z1Q3
B	-117	HIS	-	expression tag	UNP A1Z1Q3
B	-116	HIS	-	expression tag	UNP A1Z1Q3
B	-115	SER	-	expression tag	UNP A1Z1Q3
B	-114	SER	-	expression tag	UNP A1Z1Q3
B	-113	GLY	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-112	MET	-	expression tag	UNP A1Z1Q3
B	-111	SER	-	expression tag	UNP A1Z1Q3
B	-110	ASP	-	expression tag	UNP A1Z1Q3
B	-109	LYS	-	expression tag	UNP A1Z1Q3
B	-108	ILE	-	expression tag	UNP A1Z1Q3
B	-107	ILE	-	expression tag	UNP A1Z1Q3
B	-106	HIS	-	expression tag	UNP A1Z1Q3
B	-105	LEU	-	expression tag	UNP A1Z1Q3
B	-104	THR	-	expression tag	UNP A1Z1Q3
B	-103	ASP	-	expression tag	UNP A1Z1Q3
B	-102	ASP	-	expression tag	UNP A1Z1Q3
B	-101	SER	-	expression tag	UNP A1Z1Q3
B	-100	PHE	-	expression tag	UNP A1Z1Q3
B	-99	ASP	-	expression tag	UNP A1Z1Q3
B	-98	THR	-	expression tag	UNP A1Z1Q3
B	-97	ASP	-	expression tag	UNP A1Z1Q3
B	-96	VAL	-	expression tag	UNP A1Z1Q3
B	-95	LEU	-	expression tag	UNP A1Z1Q3
B	-94	LYS	-	expression tag	UNP A1Z1Q3
B	-93	ALA	-	expression tag	UNP A1Z1Q3
B	-92	ASP	-	expression tag	UNP A1Z1Q3
B	-91	GLY	-	expression tag	UNP A1Z1Q3
B	-90	ALA	-	expression tag	UNP A1Z1Q3
B	-89	ILE	-	expression tag	UNP A1Z1Q3
B	-88	LEU	-	expression tag	UNP A1Z1Q3
B	-87	VAL	-	expression tag	UNP A1Z1Q3
B	-86	ASP	-	expression tag	UNP A1Z1Q3
B	-85	PHE	-	expression tag	UNP A1Z1Q3
B	-84	TRP	-	expression tag	UNP A1Z1Q3
B	-83	ALA	-	expression tag	UNP A1Z1Q3
B	-82	GLU	-	expression tag	UNP A1Z1Q3
B	-81	TRP	-	expression tag	UNP A1Z1Q3
B	-80	CYS	-	expression tag	UNP A1Z1Q3
B	-79	GLY	-	expression tag	UNP A1Z1Q3
B	-78	PRO	-	expression tag	UNP A1Z1Q3
B	-77	CYS	-	expression tag	UNP A1Z1Q3
B	-76	LYS	-	expression tag	UNP A1Z1Q3
B	-75	MET	-	expression tag	UNP A1Z1Q3
B	-74	ILE	-	expression tag	UNP A1Z1Q3
B	-73	ALA	-	expression tag	UNP A1Z1Q3
B	-72	PRO	-	expression tag	UNP A1Z1Q3
B	-71	ILE	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-70	LEU	-	expression tag	UNP A1Z1Q3
B	-69	ASP	-	expression tag	UNP A1Z1Q3
B	-68	GLU	-	expression tag	UNP A1Z1Q3
B	-67	ILE	-	expression tag	UNP A1Z1Q3
B	-66	ALA	-	expression tag	UNP A1Z1Q3
B	-65	ASP	-	expression tag	UNP A1Z1Q3
B	-64	GLU	-	expression tag	UNP A1Z1Q3
B	-63	TYR	-	expression tag	UNP A1Z1Q3
B	-62	GLN	-	expression tag	UNP A1Z1Q3
B	-61	GLY	-	expression tag	UNP A1Z1Q3
B	-60	LYS	-	expression tag	UNP A1Z1Q3
B	-59	LEU	-	expression tag	UNP A1Z1Q3
B	-58	THR	-	expression tag	UNP A1Z1Q3
B	-57	VAL	-	expression tag	UNP A1Z1Q3
B	-56	ALA	-	expression tag	UNP A1Z1Q3
B	-55	LYS	-	expression tag	UNP A1Z1Q3
B	-54	LEU	-	expression tag	UNP A1Z1Q3
B	-53	ASN	-	expression tag	UNP A1Z1Q3
B	-52	ILE	-	expression tag	UNP A1Z1Q3
B	-51	ASP	-	expression tag	UNP A1Z1Q3
B	-50	GLN	-	expression tag	UNP A1Z1Q3
B	-49	ASN	-	expression tag	UNP A1Z1Q3
B	-48	PRO	-	expression tag	UNP A1Z1Q3
B	-47	GLY	-	expression tag	UNP A1Z1Q3
B	-46	THR	-	expression tag	UNP A1Z1Q3
B	-45	ALA	-	expression tag	UNP A1Z1Q3
B	-44	PRO	-	expression tag	UNP A1Z1Q3
B	-43	LYS	-	expression tag	UNP A1Z1Q3
B	-42	TYR	-	expression tag	UNP A1Z1Q3
B	-41	GLY	-	expression tag	UNP A1Z1Q3
B	-40	ILE	-	expression tag	UNP A1Z1Q3
B	-39	ARG	-	expression tag	UNP A1Z1Q3
B	-38	GLY	-	expression tag	UNP A1Z1Q3
B	-37	ILE	-	expression tag	UNP A1Z1Q3
B	-36	PRO	-	expression tag	UNP A1Z1Q3
B	-35	THR	-	expression tag	UNP A1Z1Q3
B	-34	LEU	-	expression tag	UNP A1Z1Q3
B	-33	LEU	-	expression tag	UNP A1Z1Q3
B	-32	LEU	-	expression tag	UNP A1Z1Q3
B	-31	PHE	-	expression tag	UNP A1Z1Q3
B	-30	LYS	-	expression tag	UNP A1Z1Q3
B	-29	ASN	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-28	GLY	-	expression tag	UNP A1Z1Q3
B	-27	GLU	-	expression tag	UNP A1Z1Q3
B	-26	VAL	-	expression tag	UNP A1Z1Q3
B	-25	ALA	-	expression tag	UNP A1Z1Q3
B	-24	ALA	-	expression tag	UNP A1Z1Q3
B	-23	THR	-	expression tag	UNP A1Z1Q3
B	-22	LYS	-	expression tag	UNP A1Z1Q3
B	-21	VAL	-	expression tag	UNP A1Z1Q3
B	-20	GLY	-	expression tag	UNP A1Z1Q3
B	-19	ALA	-	expression tag	UNP A1Z1Q3
B	-18	LEU	-	expression tag	UNP A1Z1Q3
B	-17	SER	-	expression tag	UNP A1Z1Q3
B	-16	LYS	-	expression tag	UNP A1Z1Q3
B	-15	GLY	-	expression tag	UNP A1Z1Q3
B	-14	GLN	-	expression tag	UNP A1Z1Q3
B	-13	LEU	-	expression tag	UNP A1Z1Q3
B	-12	LYS	-	expression tag	UNP A1Z1Q3
B	-11	GLU	-	expression tag	UNP A1Z1Q3
B	-10	PHE	-	expression tag	UNP A1Z1Q3
B	-9	LEU	-	expression tag	UNP A1Z1Q3
B	-8	ASP	-	expression tag	UNP A1Z1Q3
B	-7	ALA	-	expression tag	UNP A1Z1Q3
B	-6	ASN	-	expression tag	UNP A1Z1Q3
B	-5	LEU	-	expression tag	UNP A1Z1Q3
B	-4	ALA	-	expression tag	UNP A1Z1Q3
B	-3	GLY	-	expression tag	UNP A1Z1Q3
B	-2	THR	-	expression tag	UNP A1Z1Q3
B	-1	GLU	-	expression tag	UNP A1Z1Q3
B	0	ASN	-	expression tag	UNP A1Z1Q3
B	1	LEU	-	expression tag	UNP A1Z1Q3
B	2	TYR	-	expression tag	UNP A1Z1Q3
B	3	PHE	-	expression tag	UNP A1Z1Q3
B	4	GLN	-	expression tag	UNP A1Z1Q3
B	5	SER	-	expression tag	UNP A1Z1Q3
B	6	MET	-	expression tag	UNP A1Z1Q3
C	-122	MET	-	initiating methionine	UNP A1Z1Q3
C	-121	HIS	-	expression tag	UNP A1Z1Q3
C	-120	HIS	-	expression tag	UNP A1Z1Q3
C	-119	HIS	-	expression tag	UNP A1Z1Q3
C	-118	HIS	-	expression tag	UNP A1Z1Q3
C	-117	HIS	-	expression tag	UNP A1Z1Q3
C	-116	HIS	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-115	SER	-	expression tag	UNP A1Z1Q3
C	-114	SER	-	expression tag	UNP A1Z1Q3
C	-113	GLY	-	expression tag	UNP A1Z1Q3
C	-112	MET	-	expression tag	UNP A1Z1Q3
C	-111	SER	-	expression tag	UNP A1Z1Q3
C	-110	ASP	-	expression tag	UNP A1Z1Q3
C	-109	LYS	-	expression tag	UNP A1Z1Q3
C	-108	ILE	-	expression tag	UNP A1Z1Q3
C	-107	ILE	-	expression tag	UNP A1Z1Q3
C	-106	HIS	-	expression tag	UNP A1Z1Q3
C	-105	LEU	-	expression tag	UNP A1Z1Q3
C	-104	THR	-	expression tag	UNP A1Z1Q3
C	-103	ASP	-	expression tag	UNP A1Z1Q3
C	-102	ASP	-	expression tag	UNP A1Z1Q3
C	-101	SER	-	expression tag	UNP A1Z1Q3
C	-100	PHE	-	expression tag	UNP A1Z1Q3
C	-99	ASP	-	expression tag	UNP A1Z1Q3
C	-98	THR	-	expression tag	UNP A1Z1Q3
C	-97	ASP	-	expression tag	UNP A1Z1Q3
C	-96	VAL	-	expression tag	UNP A1Z1Q3
C	-95	LEU	-	expression tag	UNP A1Z1Q3
C	-94	LYS	-	expression tag	UNP A1Z1Q3
C	-93	ALA	-	expression tag	UNP A1Z1Q3
C	-92	ASP	-	expression tag	UNP A1Z1Q3
C	-91	GLY	-	expression tag	UNP A1Z1Q3
C	-90	ALA	-	expression tag	UNP A1Z1Q3
C	-89	ILE	-	expression tag	UNP A1Z1Q3
C	-88	LEU	-	expression tag	UNP A1Z1Q3
C	-87	VAL	-	expression tag	UNP A1Z1Q3
C	-86	ASP	-	expression tag	UNP A1Z1Q3
C	-85	PHE	-	expression tag	UNP A1Z1Q3
C	-84	TRP	-	expression tag	UNP A1Z1Q3
C	-83	ALA	-	expression tag	UNP A1Z1Q3
C	-82	GLU	-	expression tag	UNP A1Z1Q3
C	-81	TRP	-	expression tag	UNP A1Z1Q3
C	-80	CYS	-	expression tag	UNP A1Z1Q3
C	-79	GLY	-	expression tag	UNP A1Z1Q3
C	-78	PRO	-	expression tag	UNP A1Z1Q3
C	-77	CYS	-	expression tag	UNP A1Z1Q3
C	-76	LYS	-	expression tag	UNP A1Z1Q3
C	-75	MET	-	expression tag	UNP A1Z1Q3
C	-74	ILE	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-73	ALA	-	expression tag	UNP A1Z1Q3
C	-72	PRO	-	expression tag	UNP A1Z1Q3
C	-71	ILE	-	expression tag	UNP A1Z1Q3
C	-70	LEU	-	expression tag	UNP A1Z1Q3
C	-69	ASP	-	expression tag	UNP A1Z1Q3
C	-68	GLU	-	expression tag	UNP A1Z1Q3
C	-67	ILE	-	expression tag	UNP A1Z1Q3
C	-66	ALA	-	expression tag	UNP A1Z1Q3
C	-65	ASP	-	expression tag	UNP A1Z1Q3
C	-64	GLU	-	expression tag	UNP A1Z1Q3
C	-63	TYR	-	expression tag	UNP A1Z1Q3
C	-62	GLN	-	expression tag	UNP A1Z1Q3
C	-61	GLY	-	expression tag	UNP A1Z1Q3
C	-60	LYS	-	expression tag	UNP A1Z1Q3
C	-59	LEU	-	expression tag	UNP A1Z1Q3
C	-58	THR	-	expression tag	UNP A1Z1Q3
C	-57	VAL	-	expression tag	UNP A1Z1Q3
C	-56	ALA	-	expression tag	UNP A1Z1Q3
C	-55	LYS	-	expression tag	UNP A1Z1Q3
C	-54	LEU	-	expression tag	UNP A1Z1Q3
C	-53	ASN	-	expression tag	UNP A1Z1Q3
C	-52	ILE	-	expression tag	UNP A1Z1Q3
C	-51	ASP	-	expression tag	UNP A1Z1Q3
C	-50	GLN	-	expression tag	UNP A1Z1Q3
C	-49	ASN	-	expression tag	UNP A1Z1Q3
C	-48	PRO	-	expression tag	UNP A1Z1Q3
C	-47	GLY	-	expression tag	UNP A1Z1Q3
C	-46	THR	-	expression tag	UNP A1Z1Q3
C	-45	ALA	-	expression tag	UNP A1Z1Q3
C	-44	PRO	-	expression tag	UNP A1Z1Q3
C	-43	LYS	-	expression tag	UNP A1Z1Q3
C	-42	TYR	-	expression tag	UNP A1Z1Q3
C	-41	GLY	-	expression tag	UNP A1Z1Q3
C	-40	ILE	-	expression tag	UNP A1Z1Q3
C	-39	ARG	-	expression tag	UNP A1Z1Q3
C	-38	GLY	-	expression tag	UNP A1Z1Q3
C	-37	ILE	-	expression tag	UNP A1Z1Q3
C	-36	PRO	-	expression tag	UNP A1Z1Q3
C	-35	THR	-	expression tag	UNP A1Z1Q3
C	-34	LEU	-	expression tag	UNP A1Z1Q3
C	-33	LEU	-	expression tag	UNP A1Z1Q3
C	-32	LEU	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	PHE	-	expression tag	UNP A1Z1Q3
C	-30	LYS	-	expression tag	UNP A1Z1Q3
C	-29	ASN	-	expression tag	UNP A1Z1Q3
C	-28	GLY	-	expression tag	UNP A1Z1Q3
C	-27	GLU	-	expression tag	UNP A1Z1Q3
C	-26	VAL	-	expression tag	UNP A1Z1Q3
C	-25	ALA	-	expression tag	UNP A1Z1Q3
C	-24	ALA	-	expression tag	UNP A1Z1Q3
C	-23	THR	-	expression tag	UNP A1Z1Q3
C	-22	LYS	-	expression tag	UNP A1Z1Q3
C	-21	VAL	-	expression tag	UNP A1Z1Q3
C	-20	GLY	-	expression tag	UNP A1Z1Q3
C	-19	ALA	-	expression tag	UNP A1Z1Q3
C	-18	LEU	-	expression tag	UNP A1Z1Q3
C	-17	SER	-	expression tag	UNP A1Z1Q3
C	-16	LYS	-	expression tag	UNP A1Z1Q3
C	-15	GLY	-	expression tag	UNP A1Z1Q3
C	-14	GLN	-	expression tag	UNP A1Z1Q3
C	-13	LEU	-	expression tag	UNP A1Z1Q3
C	-12	LYS	-	expression tag	UNP A1Z1Q3
C	-11	GLU	-	expression tag	UNP A1Z1Q3
C	-10	PHE	-	expression tag	UNP A1Z1Q3
C	-9	LEU	-	expression tag	UNP A1Z1Q3
C	-8	ASP	-	expression tag	UNP A1Z1Q3
C	-7	ALA	-	expression tag	UNP A1Z1Q3
C	-6	ASN	-	expression tag	UNP A1Z1Q3
C	-5	LEU	-	expression tag	UNP A1Z1Q3
C	-4	ALA	-	expression tag	UNP A1Z1Q3
C	-3	GLY	-	expression tag	UNP A1Z1Q3
C	-2	THR	-	expression tag	UNP A1Z1Q3
C	-1	GLU	-	expression tag	UNP A1Z1Q3
C	0	ASN	-	expression tag	UNP A1Z1Q3
C	1	LEU	-	expression tag	UNP A1Z1Q3
C	2	TYR	-	expression tag	UNP A1Z1Q3
C	3	PHE	-	expression tag	UNP A1Z1Q3
C	4	GLN	-	expression tag	UNP A1Z1Q3
C	5	SER	-	expression tag	UNP A1Z1Q3
C	6	MET	-	expression tag	UNP A1Z1Q3
D	-122	MET	-	initiating methionine	UNP A1Z1Q3
D	-121	HIS	-	expression tag	UNP A1Z1Q3
D	-120	HIS	-	expression tag	UNP A1Z1Q3
D	-119	HIS	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-118	HIS	-	expression tag	UNP A1Z1Q3
D	-117	HIS	-	expression tag	UNP A1Z1Q3
D	-116	HIS	-	expression tag	UNP A1Z1Q3
D	-115	SER	-	expression tag	UNP A1Z1Q3
D	-114	SER	-	expression tag	UNP A1Z1Q3
D	-113	GLY	-	expression tag	UNP A1Z1Q3
D	-112	MET	-	expression tag	UNP A1Z1Q3
D	-111	SER	-	expression tag	UNP A1Z1Q3
D	-110	ASP	-	expression tag	UNP A1Z1Q3
D	-109	LYS	-	expression tag	UNP A1Z1Q3
D	-108	ILE	-	expression tag	UNP A1Z1Q3
D	-107	ILE	-	expression tag	UNP A1Z1Q3
D	-106	HIS	-	expression tag	UNP A1Z1Q3
D	-105	LEU	-	expression tag	UNP A1Z1Q3
D	-104	THR	-	expression tag	UNP A1Z1Q3
D	-103	ASP	-	expression tag	UNP A1Z1Q3
D	-102	ASP	-	expression tag	UNP A1Z1Q3
D	-101	SER	-	expression tag	UNP A1Z1Q3
D	-100	PHE	-	expression tag	UNP A1Z1Q3
D	-99	ASP	-	expression tag	UNP A1Z1Q3
D	-98	THR	-	expression tag	UNP A1Z1Q3
D	-97	ASP	-	expression tag	UNP A1Z1Q3
D	-96	VAL	-	expression tag	UNP A1Z1Q3
D	-95	LEU	-	expression tag	UNP A1Z1Q3
D	-94	LYS	-	expression tag	UNP A1Z1Q3
D	-93	ALA	-	expression tag	UNP A1Z1Q3
D	-92	ASP	-	expression tag	UNP A1Z1Q3
D	-91	GLY	-	expression tag	UNP A1Z1Q3
D	-90	ALA	-	expression tag	UNP A1Z1Q3
D	-89	ILE	-	expression tag	UNP A1Z1Q3
D	-88	LEU	-	expression tag	UNP A1Z1Q3
D	-87	VAL	-	expression tag	UNP A1Z1Q3
D	-86	ASP	-	expression tag	UNP A1Z1Q3
D	-85	PHE	-	expression tag	UNP A1Z1Q3
D	-84	TRP	-	expression tag	UNP A1Z1Q3
D	-83	ALA	-	expression tag	UNP A1Z1Q3
D	-82	GLU	-	expression tag	UNP A1Z1Q3
D	-81	TRP	-	expression tag	UNP A1Z1Q3
D	-80	CYS	-	expression tag	UNP A1Z1Q3
D	-79	GLY	-	expression tag	UNP A1Z1Q3
D	-78	PRO	-	expression tag	UNP A1Z1Q3
D	-77	CYS	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-76	LYS	-	expression tag	UNP A1Z1Q3
D	-75	MET	-	expression tag	UNP A1Z1Q3
D	-74	ILE	-	expression tag	UNP A1Z1Q3
D	-73	ALA	-	expression tag	UNP A1Z1Q3
D	-72	PRO	-	expression tag	UNP A1Z1Q3
D	-71	ILE	-	expression tag	UNP A1Z1Q3
D	-70	LEU	-	expression tag	UNP A1Z1Q3
D	-69	ASP	-	expression tag	UNP A1Z1Q3
D	-68	GLU	-	expression tag	UNP A1Z1Q3
D	-67	ILE	-	expression tag	UNP A1Z1Q3
D	-66	ALA	-	expression tag	UNP A1Z1Q3
D	-65	ASP	-	expression tag	UNP A1Z1Q3
D	-64	GLU	-	expression tag	UNP A1Z1Q3
D	-63	TYR	-	expression tag	UNP A1Z1Q3
D	-62	GLN	-	expression tag	UNP A1Z1Q3
D	-61	GLY	-	expression tag	UNP A1Z1Q3
D	-60	LYS	-	expression tag	UNP A1Z1Q3
D	-59	LEU	-	expression tag	UNP A1Z1Q3
D	-58	THR	-	expression tag	UNP A1Z1Q3
D	-57	VAL	-	expression tag	UNP A1Z1Q3
D	-56	ALA	-	expression tag	UNP A1Z1Q3
D	-55	LYS	-	expression tag	UNP A1Z1Q3
D	-54	LEU	-	expression tag	UNP A1Z1Q3
D	-53	ASN	-	expression tag	UNP A1Z1Q3
D	-52	ILE	-	expression tag	UNP A1Z1Q3
D	-51	ASP	-	expression tag	UNP A1Z1Q3
D	-50	GLN	-	expression tag	UNP A1Z1Q3
D	-49	ASN	-	expression tag	UNP A1Z1Q3
D	-48	PRO	-	expression tag	UNP A1Z1Q3
D	-47	GLY	-	expression tag	UNP A1Z1Q3
D	-46	THR	-	expression tag	UNP A1Z1Q3
D	-45	ALA	-	expression tag	UNP A1Z1Q3
D	-44	PRO	-	expression tag	UNP A1Z1Q3
D	-43	LYS	-	expression tag	UNP A1Z1Q3
D	-42	TYR	-	expression tag	UNP A1Z1Q3
D	-41	GLY	-	expression tag	UNP A1Z1Q3
D	-40	ILE	-	expression tag	UNP A1Z1Q3
D	-39	ARG	-	expression tag	UNP A1Z1Q3
D	-38	GLY	-	expression tag	UNP A1Z1Q3
D	-37	ILE	-	expression tag	UNP A1Z1Q3
D	-36	PRO	-	expression tag	UNP A1Z1Q3
D	-35	THR	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-34	LEU	-	expression tag	UNP A1Z1Q3
D	-33	LEU	-	expression tag	UNP A1Z1Q3
D	-32	LEU	-	expression tag	UNP A1Z1Q3
D	-31	PHE	-	expression tag	UNP A1Z1Q3
D	-30	LYS	-	expression tag	UNP A1Z1Q3
D	-29	ASN	-	expression tag	UNP A1Z1Q3
D	-28	GLY	-	expression tag	UNP A1Z1Q3
D	-27	GLU	-	expression tag	UNP A1Z1Q3
D	-26	VAL	-	expression tag	UNP A1Z1Q3
D	-25	ALA	-	expression tag	UNP A1Z1Q3
D	-24	ALA	-	expression tag	UNP A1Z1Q3
D	-23	THR	-	expression tag	UNP A1Z1Q3
D	-22	LYS	-	expression tag	UNP A1Z1Q3
D	-21	VAL	-	expression tag	UNP A1Z1Q3
D	-20	GLY	-	expression tag	UNP A1Z1Q3
D	-19	ALA	-	expression tag	UNP A1Z1Q3
D	-18	LEU	-	expression tag	UNP A1Z1Q3
D	-17	SER	-	expression tag	UNP A1Z1Q3
D	-16	LYS	-	expression tag	UNP A1Z1Q3
D	-15	GLY	-	expression tag	UNP A1Z1Q3
D	-14	GLN	-	expression tag	UNP A1Z1Q3
D	-13	LEU	-	expression tag	UNP A1Z1Q3
D	-12	LYS	-	expression tag	UNP A1Z1Q3
D	-11	GLU	-	expression tag	UNP A1Z1Q3
D	-10	PHE	-	expression tag	UNP A1Z1Q3
D	-9	LEU	-	expression tag	UNP A1Z1Q3
D	-8	ASP	-	expression tag	UNP A1Z1Q3
D	-7	ALA	-	expression tag	UNP A1Z1Q3
D	-6	ASN	-	expression tag	UNP A1Z1Q3
D	-5	LEU	-	expression tag	UNP A1Z1Q3
D	-4	ALA	-	expression tag	UNP A1Z1Q3
D	-3	GLY	-	expression tag	UNP A1Z1Q3
D	-2	THR	-	expression tag	UNP A1Z1Q3
D	-1	GLU	-	expression tag	UNP A1Z1Q3
D	0	ASN	-	expression tag	UNP A1Z1Q3
D	1	LEU	-	expression tag	UNP A1Z1Q3
D	2	TYR	-	expression tag	UNP A1Z1Q3
D	3	PHE	-	expression tag	UNP A1Z1Q3
D	4	GLN	-	expression tag	UNP A1Z1Q3
D	5	SER	-	expression tag	UNP A1Z1Q3
D	6	MET	-	expression tag	UNP A1Z1Q3
E	-122	MET	-	initiating methionine	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-121	HIS	-	expression tag	UNP A1Z1Q3
E	-120	HIS	-	expression tag	UNP A1Z1Q3
E	-119	HIS	-	expression tag	UNP A1Z1Q3
E	-118	HIS	-	expression tag	UNP A1Z1Q3
E	-117	HIS	-	expression tag	UNP A1Z1Q3
E	-116	HIS	-	expression tag	UNP A1Z1Q3
E	-115	SER	-	expression tag	UNP A1Z1Q3
E	-114	SER	-	expression tag	UNP A1Z1Q3
E	-113	GLY	-	expression tag	UNP A1Z1Q3
E	-112	MET	-	expression tag	UNP A1Z1Q3
E	-111	SER	-	expression tag	UNP A1Z1Q3
E	-110	ASP	-	expression tag	UNP A1Z1Q3
E	-109	LYS	-	expression tag	UNP A1Z1Q3
E	-108	ILE	-	expression tag	UNP A1Z1Q3
E	-107	ILE	-	expression tag	UNP A1Z1Q3
E	-106	HIS	-	expression tag	UNP A1Z1Q3
E	-105	LEU	-	expression tag	UNP A1Z1Q3
E	-104	THR	-	expression tag	UNP A1Z1Q3
E	-103	ASP	-	expression tag	UNP A1Z1Q3
E	-102	ASP	-	expression tag	UNP A1Z1Q3
E	-101	SER	-	expression tag	UNP A1Z1Q3
E	-100	PHE	-	expression tag	UNP A1Z1Q3
E	-99	ASP	-	expression tag	UNP A1Z1Q3
E	-98	THR	-	expression tag	UNP A1Z1Q3
E	-97	ASP	-	expression tag	UNP A1Z1Q3
E	-96	VAL	-	expression tag	UNP A1Z1Q3
E	-95	LEU	-	expression tag	UNP A1Z1Q3
E	-94	LYS	-	expression tag	UNP A1Z1Q3
E	-93	ALA	-	expression tag	UNP A1Z1Q3
E	-92	ASP	-	expression tag	UNP A1Z1Q3
E	-91	GLY	-	expression tag	UNP A1Z1Q3
E	-90	ALA	-	expression tag	UNP A1Z1Q3
E	-89	ILE	-	expression tag	UNP A1Z1Q3
E	-88	LEU	-	expression tag	UNP A1Z1Q3
E	-87	VAL	-	expression tag	UNP A1Z1Q3
E	-86	ASP	-	expression tag	UNP A1Z1Q3
E	-85	PHE	-	expression tag	UNP A1Z1Q3
E	-84	TRP	-	expression tag	UNP A1Z1Q3
E	-83	ALA	-	expression tag	UNP A1Z1Q3
E	-82	GLU	-	expression tag	UNP A1Z1Q3
E	-81	TRP	-	expression tag	UNP A1Z1Q3
E	-80	CYS	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-79	GLY	-	expression tag	UNP A1Z1Q3
E	-78	PRO	-	expression tag	UNP A1Z1Q3
E	-77	CYS	-	expression tag	UNP A1Z1Q3
E	-76	LYS	-	expression tag	UNP A1Z1Q3
E	-75	MET	-	expression tag	UNP A1Z1Q3
E	-74	ILE	-	expression tag	UNP A1Z1Q3
E	-73	ALA	-	expression tag	UNP A1Z1Q3
E	-72	PRO	-	expression tag	UNP A1Z1Q3
E	-71	ILE	-	expression tag	UNP A1Z1Q3
E	-70	LEU	-	expression tag	UNP A1Z1Q3
E	-69	ASP	-	expression tag	UNP A1Z1Q3
E	-68	GLU	-	expression tag	UNP A1Z1Q3
E	-67	ILE	-	expression tag	UNP A1Z1Q3
E	-66	ALA	-	expression tag	UNP A1Z1Q3
E	-65	ASP	-	expression tag	UNP A1Z1Q3
E	-64	GLU	-	expression tag	UNP A1Z1Q3
E	-63	TYR	-	expression tag	UNP A1Z1Q3
E	-62	GLN	-	expression tag	UNP A1Z1Q3
E	-61	GLY	-	expression tag	UNP A1Z1Q3
E	-60	LYS	-	expression tag	UNP A1Z1Q3
E	-59	LEU	-	expression tag	UNP A1Z1Q3
E	-58	THR	-	expression tag	UNP A1Z1Q3
E	-57	VAL	-	expression tag	UNP A1Z1Q3
E	-56	ALA	-	expression tag	UNP A1Z1Q3
E	-55	LYS	-	expression tag	UNP A1Z1Q3
E	-54	LEU	-	expression tag	UNP A1Z1Q3
E	-53	ASN	-	expression tag	UNP A1Z1Q3
E	-52	ILE	-	expression tag	UNP A1Z1Q3
E	-51	ASP	-	expression tag	UNP A1Z1Q3
E	-50	GLN	-	expression tag	UNP A1Z1Q3
E	-49	ASN	-	expression tag	UNP A1Z1Q3
E	-48	PRO	-	expression tag	UNP A1Z1Q3
E	-47	GLY	-	expression tag	UNP A1Z1Q3
E	-46	THR	-	expression tag	UNP A1Z1Q3
E	-45	ALA	-	expression tag	UNP A1Z1Q3
E	-44	PRO	-	expression tag	UNP A1Z1Q3
E	-43	LYS	-	expression tag	UNP A1Z1Q3
E	-42	TYR	-	expression tag	UNP A1Z1Q3
E	-41	GLY	-	expression tag	UNP A1Z1Q3
E	-40	ILE	-	expression tag	UNP A1Z1Q3
E	-39	ARG	-	expression tag	UNP A1Z1Q3
E	-38	GLY	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-37	ILE	-	expression tag	UNP A1Z1Q3
E	-36	PRO	-	expression tag	UNP A1Z1Q3
E	-35	THR	-	expression tag	UNP A1Z1Q3
E	-34	LEU	-	expression tag	UNP A1Z1Q3
E	-33	LEU	-	expression tag	UNP A1Z1Q3
E	-32	LEU	-	expression tag	UNP A1Z1Q3
E	-31	PHE	-	expression tag	UNP A1Z1Q3
E	-30	LYS	-	expression tag	UNP A1Z1Q3
E	-29	ASN	-	expression tag	UNP A1Z1Q3
E	-28	GLY	-	expression tag	UNP A1Z1Q3
E	-27	GLU	-	expression tag	UNP A1Z1Q3
E	-26	VAL	-	expression tag	UNP A1Z1Q3
E	-25	ALA	-	expression tag	UNP A1Z1Q3
E	-24	ALA	-	expression tag	UNP A1Z1Q3
E	-23	THR	-	expression tag	UNP A1Z1Q3
E	-22	LYS	-	expression tag	UNP A1Z1Q3
E	-21	VAL	-	expression tag	UNP A1Z1Q3
E	-20	GLY	-	expression tag	UNP A1Z1Q3
E	-19	ALA	-	expression tag	UNP A1Z1Q3
E	-18	LEU	-	expression tag	UNP A1Z1Q3
E	-17	SER	-	expression tag	UNP A1Z1Q3
E	-16	LYS	-	expression tag	UNP A1Z1Q3
E	-15	GLY	-	expression tag	UNP A1Z1Q3
E	-14	GLN	-	expression tag	UNP A1Z1Q3
E	-13	LEU	-	expression tag	UNP A1Z1Q3
E	-12	LYS	-	expression tag	UNP A1Z1Q3
E	-11	GLU	-	expression tag	UNP A1Z1Q3
E	-10	PHE	-	expression tag	UNP A1Z1Q3
E	-9	LEU	-	expression tag	UNP A1Z1Q3
E	-8	ASP	-	expression tag	UNP A1Z1Q3
E	-7	ALA	-	expression tag	UNP A1Z1Q3
E	-6	ASN	-	expression tag	UNP A1Z1Q3
E	-5	LEU	-	expression tag	UNP A1Z1Q3
E	-4	ALA	-	expression tag	UNP A1Z1Q3
E	-3	GLY	-	expression tag	UNP A1Z1Q3
E	-2	THR	-	expression tag	UNP A1Z1Q3
E	-1	GLU	-	expression tag	UNP A1Z1Q3
E	0	ASN	-	expression tag	UNP A1Z1Q3
E	1	LEU	-	expression tag	UNP A1Z1Q3
E	2	TYR	-	expression tag	UNP A1Z1Q3
E	3	PHE	-	expression tag	UNP A1Z1Q3
E	4	GLN	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	5	SER	-	expression tag	UNP A1Z1Q3
E	6	MET	-	expression tag	UNP A1Z1Q3
F	-122	MET	-	initiating methionine	UNP A1Z1Q3
F	-121	HIS	-	expression tag	UNP A1Z1Q3
F	-120	HIS	-	expression tag	UNP A1Z1Q3
F	-119	HIS	-	expression tag	UNP A1Z1Q3
F	-118	HIS	-	expression tag	UNP A1Z1Q3
F	-117	HIS	-	expression tag	UNP A1Z1Q3
F	-116	HIS	-	expression tag	UNP A1Z1Q3
F	-115	SER	-	expression tag	UNP A1Z1Q3
F	-114	SER	-	expression tag	UNP A1Z1Q3
F	-113	GLY	-	expression tag	UNP A1Z1Q3
F	-112	MET	-	expression tag	UNP A1Z1Q3
F	-111	SER	-	expression tag	UNP A1Z1Q3
F	-110	ASP	-	expression tag	UNP A1Z1Q3
F	-109	LYS	-	expression tag	UNP A1Z1Q3
F	-108	ILE	-	expression tag	UNP A1Z1Q3
F	-107	ILE	-	expression tag	UNP A1Z1Q3
F	-106	HIS	-	expression tag	UNP A1Z1Q3
F	-105	LEU	-	expression tag	UNP A1Z1Q3
F	-104	THR	-	expression tag	UNP A1Z1Q3
F	-103	ASP	-	expression tag	UNP A1Z1Q3
F	-102	ASP	-	expression tag	UNP A1Z1Q3
F	-101	SER	-	expression tag	UNP A1Z1Q3
F	-100	PHE	-	expression tag	UNP A1Z1Q3
F	-99	ASP	-	expression tag	UNP A1Z1Q3
F	-98	THR	-	expression tag	UNP A1Z1Q3
F	-97	ASP	-	expression tag	UNP A1Z1Q3
F	-96	VAL	-	expression tag	UNP A1Z1Q3
F	-95	LEU	-	expression tag	UNP A1Z1Q3
F	-94	LYS	-	expression tag	UNP A1Z1Q3
F	-93	ALA	-	expression tag	UNP A1Z1Q3
F	-92	ASP	-	expression tag	UNP A1Z1Q3
F	-91	GLY	-	expression tag	UNP A1Z1Q3
F	-90	ALA	-	expression tag	UNP A1Z1Q3
F	-89	ILE	-	expression tag	UNP A1Z1Q3
F	-88	LEU	-	expression tag	UNP A1Z1Q3
F	-87	VAL	-	expression tag	UNP A1Z1Q3
F	-86	ASP	-	expression tag	UNP A1Z1Q3
F	-85	PHE	-	expression tag	UNP A1Z1Q3
F	-84	TRP	-	expression tag	UNP A1Z1Q3
F	-83	ALA	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-82	GLU	-	expression tag	UNP A1Z1Q3
F	-81	TRP	-	expression tag	UNP A1Z1Q3
F	-80	CYS	-	expression tag	UNP A1Z1Q3
F	-79	GLY	-	expression tag	UNP A1Z1Q3
F	-78	PRO	-	expression tag	UNP A1Z1Q3
F	-77	CYS	-	expression tag	UNP A1Z1Q3
F	-76	LYS	-	expression tag	UNP A1Z1Q3
F	-75	MET	-	expression tag	UNP A1Z1Q3
F	-74	ILE	-	expression tag	UNP A1Z1Q3
F	-73	ALA	-	expression tag	UNP A1Z1Q3
F	-72	PRO	-	expression tag	UNP A1Z1Q3
F	-71	ILE	-	expression tag	UNP A1Z1Q3
F	-70	LEU	-	expression tag	UNP A1Z1Q3
F	-69	ASP	-	expression tag	UNP A1Z1Q3
F	-68	GLU	-	expression tag	UNP A1Z1Q3
F	-67	ILE	-	expression tag	UNP A1Z1Q3
F	-66	ALA	-	expression tag	UNP A1Z1Q3
F	-65	ASP	-	expression tag	UNP A1Z1Q3
F	-64	GLU	-	expression tag	UNP A1Z1Q3
F	-63	TYR	-	expression tag	UNP A1Z1Q3
F	-62	GLN	-	expression tag	UNP A1Z1Q3
F	-61	GLY	-	expression tag	UNP A1Z1Q3
F	-60	LYS	-	expression tag	UNP A1Z1Q3
F	-59	LEU	-	expression tag	UNP A1Z1Q3
F	-58	THR	-	expression tag	UNP A1Z1Q3
F	-57	VAL	-	expression tag	UNP A1Z1Q3
F	-56	ALA	-	expression tag	UNP A1Z1Q3
F	-55	LYS	-	expression tag	UNP A1Z1Q3
F	-54	LEU	-	expression tag	UNP A1Z1Q3
F	-53	ASN	-	expression tag	UNP A1Z1Q3
F	-52	ILE	-	expression tag	UNP A1Z1Q3
F	-51	ASP	-	expression tag	UNP A1Z1Q3
F	-50	GLN	-	expression tag	UNP A1Z1Q3
F	-49	ASN	-	expression tag	UNP A1Z1Q3
F	-48	PRO	-	expression tag	UNP A1Z1Q3
F	-47	GLY	-	expression tag	UNP A1Z1Q3
F	-46	THR	-	expression tag	UNP A1Z1Q3
F	-45	ALA	-	expression tag	UNP A1Z1Q3
F	-44	PRO	-	expression tag	UNP A1Z1Q3
F	-43	LYS	-	expression tag	UNP A1Z1Q3
F	-42	TYR	-	expression tag	UNP A1Z1Q3
F	-41	GLY	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-40	ILE	-	expression tag	UNP A1Z1Q3
F	-39	ARG	-	expression tag	UNP A1Z1Q3
F	-38	GLY	-	expression tag	UNP A1Z1Q3
F	-37	ILE	-	expression tag	UNP A1Z1Q3
F	-36	PRO	-	expression tag	UNP A1Z1Q3
F	-35	THR	-	expression tag	UNP A1Z1Q3
F	-34	LEU	-	expression tag	UNP A1Z1Q3
F	-33	LEU	-	expression tag	UNP A1Z1Q3
F	-32	LEU	-	expression tag	UNP A1Z1Q3
F	-31	PHE	-	expression tag	UNP A1Z1Q3
F	-30	LYS	-	expression tag	UNP A1Z1Q3
F	-29	ASN	-	expression tag	UNP A1Z1Q3
F	-28	GLY	-	expression tag	UNP A1Z1Q3
F	-27	GLU	-	expression tag	UNP A1Z1Q3
F	-26	VAL	-	expression tag	UNP A1Z1Q3
F	-25	ALA	-	expression tag	UNP A1Z1Q3
F	-24	ALA	-	expression tag	UNP A1Z1Q3
F	-23	THR	-	expression tag	UNP A1Z1Q3
F	-22	LYS	-	expression tag	UNP A1Z1Q3
F	-21	VAL	-	expression tag	UNP A1Z1Q3
F	-20	GLY	-	expression tag	UNP A1Z1Q3
F	-19	ALA	-	expression tag	UNP A1Z1Q3
F	-18	LEU	-	expression tag	UNP A1Z1Q3
F	-17	SER	-	expression tag	UNP A1Z1Q3
F	-16	LYS	-	expression tag	UNP A1Z1Q3
F	-15	GLY	-	expression tag	UNP A1Z1Q3
F	-14	GLN	-	expression tag	UNP A1Z1Q3
F	-13	LEU	-	expression tag	UNP A1Z1Q3
F	-12	LYS	-	expression tag	UNP A1Z1Q3
F	-11	GLU	-	expression tag	UNP A1Z1Q3
F	-10	PHE	-	expression tag	UNP A1Z1Q3
F	-9	LEU	-	expression tag	UNP A1Z1Q3
F	-8	ASP	-	expression tag	UNP A1Z1Q3
F	-7	ALA	-	expression tag	UNP A1Z1Q3
F	-6	ASN	-	expression tag	UNP A1Z1Q3
F	-5	LEU	-	expression tag	UNP A1Z1Q3
F	-4	ALA	-	expression tag	UNP A1Z1Q3
F	-3	GLY	-	expression tag	UNP A1Z1Q3
F	-2	THR	-	expression tag	UNP A1Z1Q3
F	-1	GLU	-	expression tag	UNP A1Z1Q3
F	0	ASN	-	expression tag	UNP A1Z1Q3
F	1	LEU	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2	TYR	-	expression tag	UNP A1Z1Q3
F	3	PHE	-	expression tag	UNP A1Z1Q3
F	4	GLN	-	expression tag	UNP A1Z1Q3
F	5	SER	-	expression tag	UNP A1Z1Q3
F	6	MET	-	expression tag	UNP A1Z1Q3
G	-122	MET	-	initiating methionine	UNP A1Z1Q3
G	-121	HIS	-	expression tag	UNP A1Z1Q3
G	-120	HIS	-	expression tag	UNP A1Z1Q3
G	-119	HIS	-	expression tag	UNP A1Z1Q3
G	-118	HIS	-	expression tag	UNP A1Z1Q3
G	-117	HIS	-	expression tag	UNP A1Z1Q3
G	-116	HIS	-	expression tag	UNP A1Z1Q3
G	-115	SER	-	expression tag	UNP A1Z1Q3
G	-114	SER	-	expression tag	UNP A1Z1Q3
G	-113	GLY	-	expression tag	UNP A1Z1Q3
G	-112	MET	-	expression tag	UNP A1Z1Q3
G	-111	SER	-	expression tag	UNP A1Z1Q3
G	-110	ASP	-	expression tag	UNP A1Z1Q3
G	-109	LYS	-	expression tag	UNP A1Z1Q3
G	-108	ILE	-	expression tag	UNP A1Z1Q3
G	-107	ILE	-	expression tag	UNP A1Z1Q3
G	-106	HIS	-	expression tag	UNP A1Z1Q3
G	-105	LEU	-	expression tag	UNP A1Z1Q3
G	-104	THR	-	expression tag	UNP A1Z1Q3
G	-103	ASP	-	expression tag	UNP A1Z1Q3
G	-102	ASP	-	expression tag	UNP A1Z1Q3
G	-101	SER	-	expression tag	UNP A1Z1Q3
G	-100	PHE	-	expression tag	UNP A1Z1Q3
G	-99	ASP	-	expression tag	UNP A1Z1Q3
G	-98	THR	-	expression tag	UNP A1Z1Q3
G	-97	ASP	-	expression tag	UNP A1Z1Q3
G	-96	VAL	-	expression tag	UNP A1Z1Q3
G	-95	LEU	-	expression tag	UNP A1Z1Q3
G	-94	LYS	-	expression tag	UNP A1Z1Q3
G	-93	ALA	-	expression tag	UNP A1Z1Q3
G	-92	ASP	-	expression tag	UNP A1Z1Q3
G	-91	GLY	-	expression tag	UNP A1Z1Q3
G	-90	ALA	-	expression tag	UNP A1Z1Q3
G	-89	ILE	-	expression tag	UNP A1Z1Q3
G	-88	LEU	-	expression tag	UNP A1Z1Q3
G	-87	VAL	-	expression tag	UNP A1Z1Q3
G	-86	ASP	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-85	PHE	-	expression tag	UNP A1Z1Q3
G	-84	TRP	-	expression tag	UNP A1Z1Q3
G	-83	ALA	-	expression tag	UNP A1Z1Q3
G	-82	GLU	-	expression tag	UNP A1Z1Q3
G	-81	TRP	-	expression tag	UNP A1Z1Q3
G	-80	CYS	-	expression tag	UNP A1Z1Q3
G	-79	GLY	-	expression tag	UNP A1Z1Q3
G	-78	PRO	-	expression tag	UNP A1Z1Q3
G	-77	CYS	-	expression tag	UNP A1Z1Q3
G	-76	LYS	-	expression tag	UNP A1Z1Q3
G	-75	MET	-	expression tag	UNP A1Z1Q3
G	-74	ILE	-	expression tag	UNP A1Z1Q3
G	-73	ALA	-	expression tag	UNP A1Z1Q3
G	-72	PRO	-	expression tag	UNP A1Z1Q3
G	-71	ILE	-	expression tag	UNP A1Z1Q3
G	-70	LEU	-	expression tag	UNP A1Z1Q3
G	-69	ASP	-	expression tag	UNP A1Z1Q3
G	-68	GLU	-	expression tag	UNP A1Z1Q3
G	-67	ILE	-	expression tag	UNP A1Z1Q3
G	-66	ALA	-	expression tag	UNP A1Z1Q3
G	-65	ASP	-	expression tag	UNP A1Z1Q3
G	-64	GLU	-	expression tag	UNP A1Z1Q3
G	-63	TYR	-	expression tag	UNP A1Z1Q3
G	-62	GLN	-	expression tag	UNP A1Z1Q3
G	-61	GLY	-	expression tag	UNP A1Z1Q3
G	-60	LYS	-	expression tag	UNP A1Z1Q3
G	-59	LEU	-	expression tag	UNP A1Z1Q3
G	-58	THR	-	expression tag	UNP A1Z1Q3
G	-57	VAL	-	expression tag	UNP A1Z1Q3
G	-56	ALA	-	expression tag	UNP A1Z1Q3
G	-55	LYS	-	expression tag	UNP A1Z1Q3
G	-54	LEU	-	expression tag	UNP A1Z1Q3
G	-53	ASN	-	expression tag	UNP A1Z1Q3
G	-52	ILE	-	expression tag	UNP A1Z1Q3
G	-51	ASP	-	expression tag	UNP A1Z1Q3
G	-50	GLN	-	expression tag	UNP A1Z1Q3
G	-49	ASN	-	expression tag	UNP A1Z1Q3
G	-48	PRO	-	expression tag	UNP A1Z1Q3
G	-47	GLY	-	expression tag	UNP A1Z1Q3
G	-46	THR	-	expression tag	UNP A1Z1Q3
G	-45	ALA	-	expression tag	UNP A1Z1Q3
G	-44	PRO	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-43	LYS	-	expression tag	UNP A1Z1Q3
G	-42	TYR	-	expression tag	UNP A1Z1Q3
G	-41	GLY	-	expression tag	UNP A1Z1Q3
G	-40	ILE	-	expression tag	UNP A1Z1Q3
G	-39	ARG	-	expression tag	UNP A1Z1Q3
G	-38	GLY	-	expression tag	UNP A1Z1Q3
G	-37	ILE	-	expression tag	UNP A1Z1Q3
G	-36	PRO	-	expression tag	UNP A1Z1Q3
G	-35	THR	-	expression tag	UNP A1Z1Q3
G	-34	LEU	-	expression tag	UNP A1Z1Q3
G	-33	LEU	-	expression tag	UNP A1Z1Q3
G	-32	LEU	-	expression tag	UNP A1Z1Q3
G	-31	PHE	-	expression tag	UNP A1Z1Q3
G	-30	LYS	-	expression tag	UNP A1Z1Q3
G	-29	ASN	-	expression tag	UNP A1Z1Q3
G	-28	GLY	-	expression tag	UNP A1Z1Q3
G	-27	GLU	-	expression tag	UNP A1Z1Q3
G	-26	VAL	-	expression tag	UNP A1Z1Q3
G	-25	ALA	-	expression tag	UNP A1Z1Q3
G	-24	ALA	-	expression tag	UNP A1Z1Q3
G	-23	THR	-	expression tag	UNP A1Z1Q3
G	-22	LYS	-	expression tag	UNP A1Z1Q3
G	-21	VAL	-	expression tag	UNP A1Z1Q3
G	-20	GLY	-	expression tag	UNP A1Z1Q3
G	-19	ALA	-	expression tag	UNP A1Z1Q3
G	-18	LEU	-	expression tag	UNP A1Z1Q3
G	-17	SER	-	expression tag	UNP A1Z1Q3
G	-16	LYS	-	expression tag	UNP A1Z1Q3
G	-15	GLY	-	expression tag	UNP A1Z1Q3
G	-14	GLN	-	expression tag	UNP A1Z1Q3
G	-13	LEU	-	expression tag	UNP A1Z1Q3
G	-12	LYS	-	expression tag	UNP A1Z1Q3
G	-11	GLU	-	expression tag	UNP A1Z1Q3
G	-10	PHE	-	expression tag	UNP A1Z1Q3
G	-9	LEU	-	expression tag	UNP A1Z1Q3
G	-8	ASP	-	expression tag	UNP A1Z1Q3
G	-7	ALA	-	expression tag	UNP A1Z1Q3
G	-6	ASN	-	expression tag	UNP A1Z1Q3
G	-5	LEU	-	expression tag	UNP A1Z1Q3
G	-4	ALA	-	expression tag	UNP A1Z1Q3
G	-3	GLY	-	expression tag	UNP A1Z1Q3
G	-2	THR	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLU	-	expression tag	UNP A1Z1Q3
G	0	ASN	-	expression tag	UNP A1Z1Q3
G	1	LEU	-	expression tag	UNP A1Z1Q3
G	2	TYR	-	expression tag	UNP A1Z1Q3
G	3	PHE	-	expression tag	UNP A1Z1Q3
G	4	GLN	-	expression tag	UNP A1Z1Q3
G	5	SER	-	expression tag	UNP A1Z1Q3
G	6	MET	-	expression tag	UNP A1Z1Q3
H	-122	MET	-	initiating methionine	UNP A1Z1Q3
H	-121	HIS	-	expression tag	UNP A1Z1Q3
H	-120	HIS	-	expression tag	UNP A1Z1Q3
H	-119	HIS	-	expression tag	UNP A1Z1Q3
H	-118	HIS	-	expression tag	UNP A1Z1Q3
H	-117	HIS	-	expression tag	UNP A1Z1Q3
H	-116	HIS	-	expression tag	UNP A1Z1Q3
H	-115	SER	-	expression tag	UNP A1Z1Q3
H	-114	SER	-	expression tag	UNP A1Z1Q3
H	-113	GLY	-	expression tag	UNP A1Z1Q3
H	-112	MET	-	expression tag	UNP A1Z1Q3
H	-111	SER	-	expression tag	UNP A1Z1Q3
H	-110	ASP	-	expression tag	UNP A1Z1Q3
H	-109	LYS	-	expression tag	UNP A1Z1Q3
H	-108	ILE	-	expression tag	UNP A1Z1Q3
H	-107	ILE	-	expression tag	UNP A1Z1Q3
H	-106	HIS	-	expression tag	UNP A1Z1Q3
H	-105	LEU	-	expression tag	UNP A1Z1Q3
H	-104	THR	-	expression tag	UNP A1Z1Q3
H	-103	ASP	-	expression tag	UNP A1Z1Q3
H	-102	ASP	-	expression tag	UNP A1Z1Q3
H	-101	SER	-	expression tag	UNP A1Z1Q3
H	-100	PHE	-	expression tag	UNP A1Z1Q3
H	-99	ASP	-	expression tag	UNP A1Z1Q3
H	-98	THR	-	expression tag	UNP A1Z1Q3
H	-97	ASP	-	expression tag	UNP A1Z1Q3
H	-96	VAL	-	expression tag	UNP A1Z1Q3
H	-95	LEU	-	expression tag	UNP A1Z1Q3
H	-94	LYS	-	expression tag	UNP A1Z1Q3
H	-93	ALA	-	expression tag	UNP A1Z1Q3
H	-92	ASP	-	expression tag	UNP A1Z1Q3
H	-91	GLY	-	expression tag	UNP A1Z1Q3
H	-90	ALA	-	expression tag	UNP A1Z1Q3
H	-89	ILE	-	expression tag	UNP A1Z1Q3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-88	LEU	-	expression tag	UNP A1Z1Q3
H	-87	VAL	-	expression tag	UNP A1Z1Q3
H	-86	ASP	-	expression tag	UNP A1Z1Q3
H	-85	PHE	-	expression tag	UNP A1Z1Q3
H	-84	TRP	-	expression tag	UNP A1Z1Q3
H	-83	ALA	-	expression tag	UNP A1Z1Q3
H	-82	GLU	-	expression tag	UNP A1Z1Q3
H	-81	TRP	-	expression tag	UNP A1Z1Q3
H	-80	CYS	-	expression tag	UNP A1Z1Q3
H	-79	GLY	-	expression tag	UNP A1Z1Q3
H	-78	PRO	-	expression tag	UNP A1Z1Q3
H	-77	CYS	-	expression tag	UNP A1Z1Q3
H	-76	LYS	-	expression tag	UNP A1Z1Q3
H	-75	MET	-	expression tag	UNP A1Z1Q3
H	-74	ILE	-	expression tag	UNP A1Z1Q3
H	-73	ALA	-	expression tag	UNP A1Z1Q3
H	-72	PRO	-	expression tag	UNP A1Z1Q3
H	-71	ILE	-	expression tag	UNP A1Z1Q3
H	-70	LEU	-	expression tag	UNP A1Z1Q3
H	-69	ASP	-	expression tag	UNP A1Z1Q3
H	-68	GLU	-	expression tag	UNP A1Z1Q3
H	-67	ILE	-	expression tag	UNP A1Z1Q3
H	-66	ALA	-	expression tag	UNP A1Z1Q3
H	-65	ASP	-	expression tag	UNP A1Z1Q3
H	-64	GLU	-	expression tag	UNP A1Z1Q3
H	-63	TYR	-	expression tag	UNP A1Z1Q3
H	-62	GLN	-	expression tag	UNP A1Z1Q3
H	-61	GLY	-	expression tag	UNP A1Z1Q3
H	-60	LYS	-	expression tag	UNP A1Z1Q3
H	-59	LEU	-	expression tag	UNP A1Z1Q3
H	-58	THR	-	expression tag	UNP A1Z1Q3
H	-57	VAL	-	expression tag	UNP A1Z1Q3
H	-56	ALA	-	expression tag	UNP A1Z1Q3
H	-55	LYS	-	expression tag	UNP A1Z1Q3
H	-54	LEU	-	expression tag	UNP A1Z1Q3
H	-53	ASN	-	expression tag	UNP A1Z1Q3
H	-52	ILE	-	expression tag	UNP A1Z1Q3
H	-51	ASP	-	expression tag	UNP A1Z1Q3
H	-50	GLN	-	expression tag	UNP A1Z1Q3
H	-49	ASN	-	expression tag	UNP A1Z1Q3
H	-48	PRO	-	expression tag	UNP A1Z1Q3
H	-47	GLY	-	expression tag	UNP A1Z1Q3

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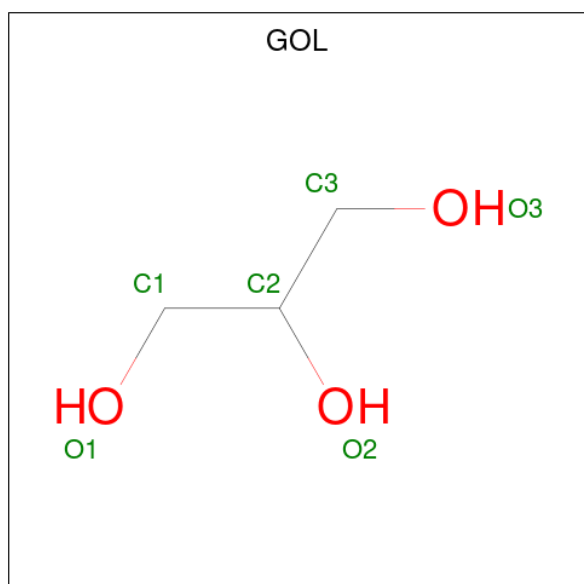
Chain	Residue	Modelled	Actual	Comment	Reference
H	-46	THR	-	expression tag	UNP A1Z1Q3
H	-45	ALA	-	expression tag	UNP A1Z1Q3
H	-44	PRO	-	expression tag	UNP A1Z1Q3
H	-43	LYS	-	expression tag	UNP A1Z1Q3
H	-42	TYR	-	expression tag	UNP A1Z1Q3
H	-41	GLY	-	expression tag	UNP A1Z1Q3
H	-40	ILE	-	expression tag	UNP A1Z1Q3
H	-39	ARG	-	expression tag	UNP A1Z1Q3
H	-38	GLY	-	expression tag	UNP A1Z1Q3
H	-37	ILE	-	expression tag	UNP A1Z1Q3
H	-36	PRO	-	expression tag	UNP A1Z1Q3
H	-35	THR	-	expression tag	UNP A1Z1Q3
H	-34	LEU	-	expression tag	UNP A1Z1Q3
H	-33	LEU	-	expression tag	UNP A1Z1Q3
H	-32	LEU	-	expression tag	UNP A1Z1Q3
H	-31	PHE	-	expression tag	UNP A1Z1Q3
H	-30	LYS	-	expression tag	UNP A1Z1Q3
H	-29	ASN	-	expression tag	UNP A1Z1Q3
H	-28	GLY	-	expression tag	UNP A1Z1Q3
H	-27	GLU	-	expression tag	UNP A1Z1Q3
H	-26	VAL	-	expression tag	UNP A1Z1Q3
H	-25	ALA	-	expression tag	UNP A1Z1Q3
H	-24	ALA	-	expression tag	UNP A1Z1Q3
H	-23	THR	-	expression tag	UNP A1Z1Q3
H	-22	LYS	-	expression tag	UNP A1Z1Q3
H	-21	VAL	-	expression tag	UNP A1Z1Q3
H	-20	GLY	-	expression tag	UNP A1Z1Q3
H	-19	ALA	-	expression tag	UNP A1Z1Q3
H	-18	LEU	-	expression tag	UNP A1Z1Q3
H	-17	SER	-	expression tag	UNP A1Z1Q3
H	-16	LYS	-	expression tag	UNP A1Z1Q3
H	-15	GLY	-	expression tag	UNP A1Z1Q3
H	-14	GLN	-	expression tag	UNP A1Z1Q3
H	-13	LEU	-	expression tag	UNP A1Z1Q3
H	-12	LYS	-	expression tag	UNP A1Z1Q3
H	-11	GLU	-	expression tag	UNP A1Z1Q3
H	-10	PHE	-	expression tag	UNP A1Z1Q3
H	-9	LEU	-	expression tag	UNP A1Z1Q3
H	-8	ASP	-	expression tag	UNP A1Z1Q3
H	-7	ALA	-	expression tag	UNP A1Z1Q3
H	-6	ASN	-	expression tag	UNP A1Z1Q3
H	-5	LEU	-	expression tag	UNP A1Z1Q3

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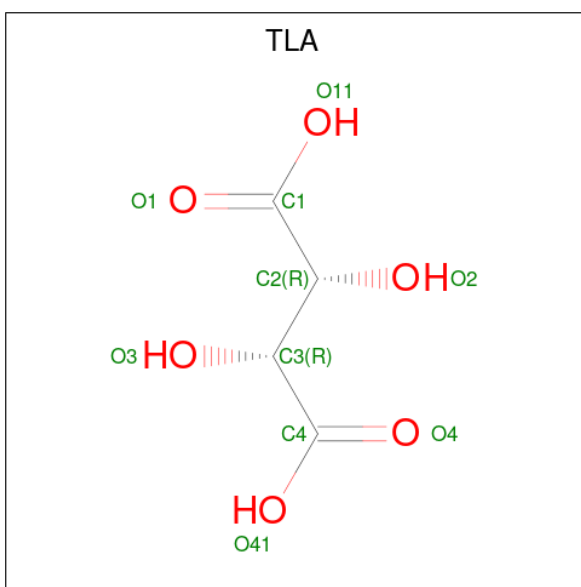
Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	ALA	-	expression tag	UNP A1Z1Q3
H	-3	GLY	-	expression tag	UNP A1Z1Q3
H	-2	THR	-	expression tag	UNP A1Z1Q3
H	-1	GLU	-	expression tag	UNP A1Z1Q3
H	0	ASN	-	expression tag	UNP A1Z1Q3
H	1	LEU	-	expression tag	UNP A1Z1Q3
H	2	TYR	-	expression tag	UNP A1Z1Q3
H	3	PHE	-	expression tag	UNP A1Z1Q3
H	4	GLN	-	expression tag	UNP A1Z1Q3
H	5	SER	-	expression tag	UNP A1Z1Q3
H	6	MET	-	expression tag	UNP A1Z1Q3

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



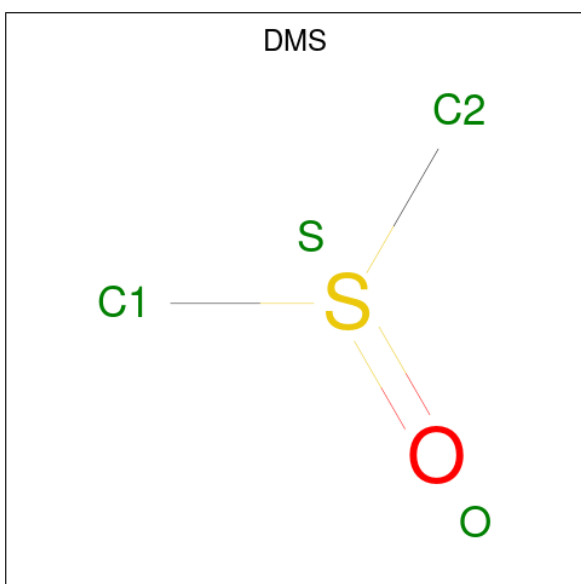
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	F	1	Total	C	O	0	0
			10	4	6		
3	G	1	Total	C	O	0	0
			10	4	6		
3	H	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

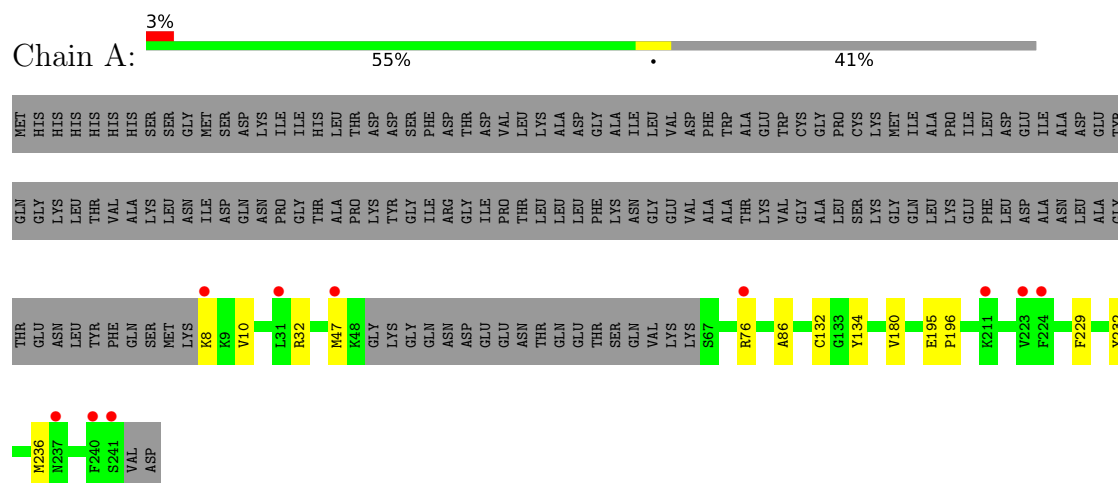
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	240	Total O 241 241	0	1
5	B	216	Total O 216 216	0	0
5	C	166	Total O 166 166	0	0
5	D	167	Total O 168 168	0	1
5	E	197	Total O 199 199	0	2
5	F	175	Total O 178 178	0	3
5	G	216	Total O 217 217	0	1
5	H	216	Total O 218 218	0	2

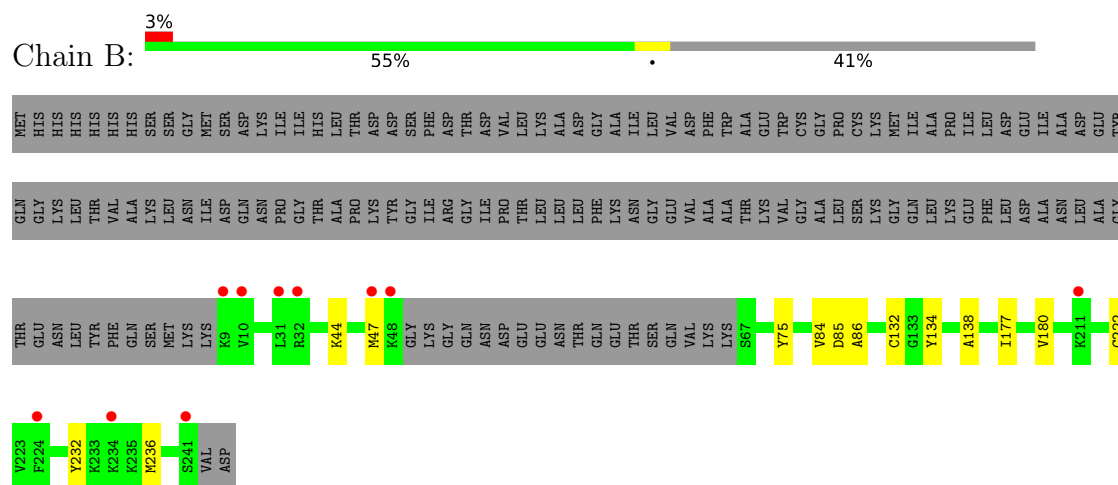
3 Residue-property plots

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.

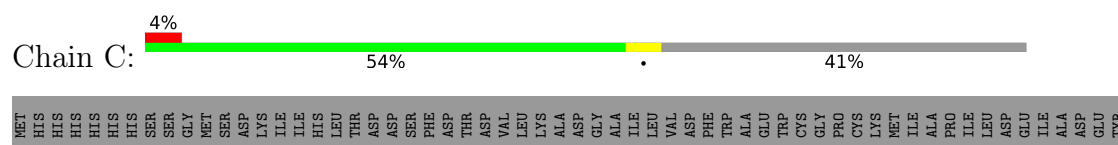
• Molecule 1: ADP-ribose glycohydrolase MACROD2

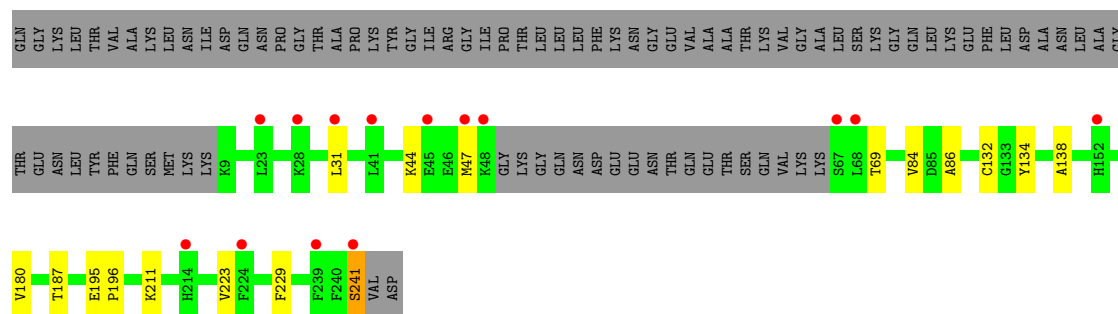


• Molecule 1: ADP-ribose glycohydrolase MACROD2

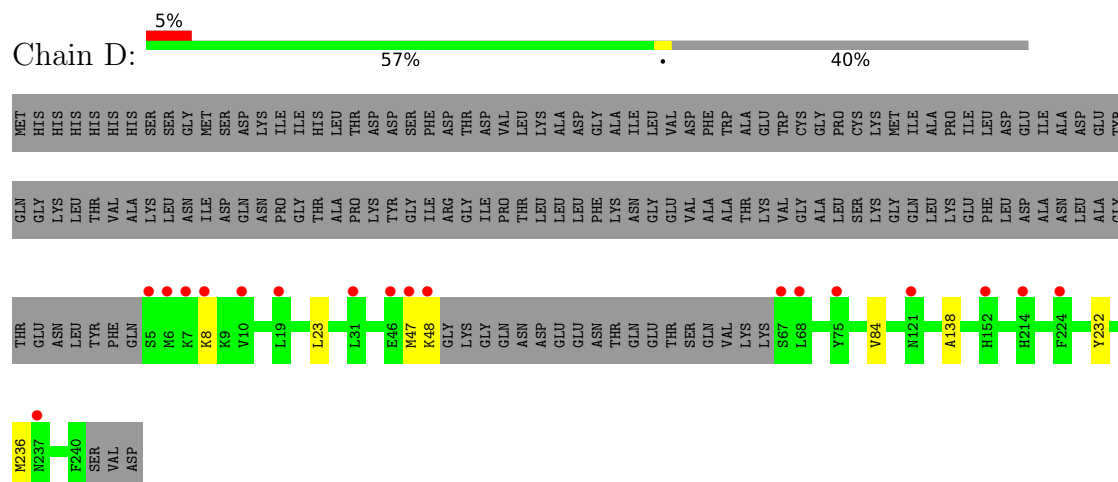


• Molecule 1: ADP-ribose glycohydrolase MACROD2

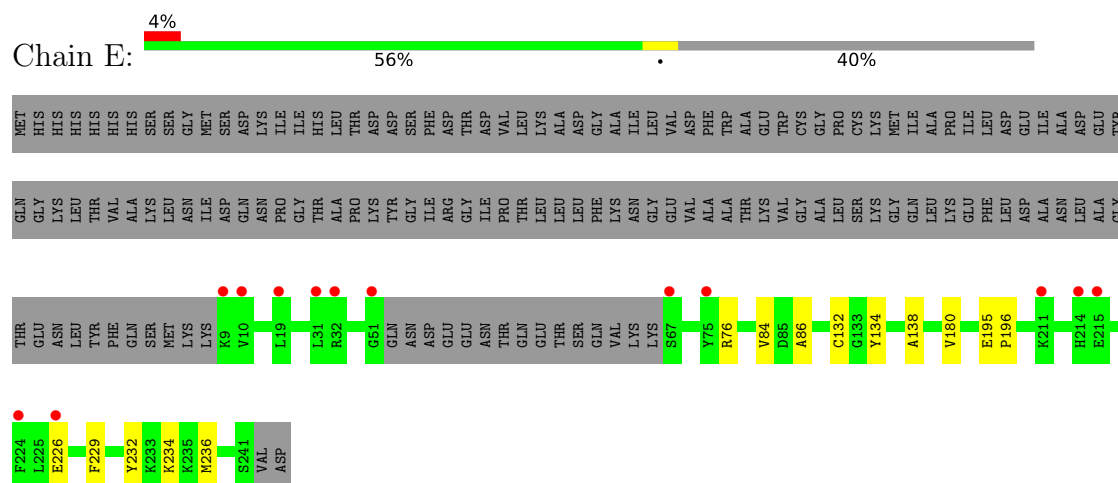




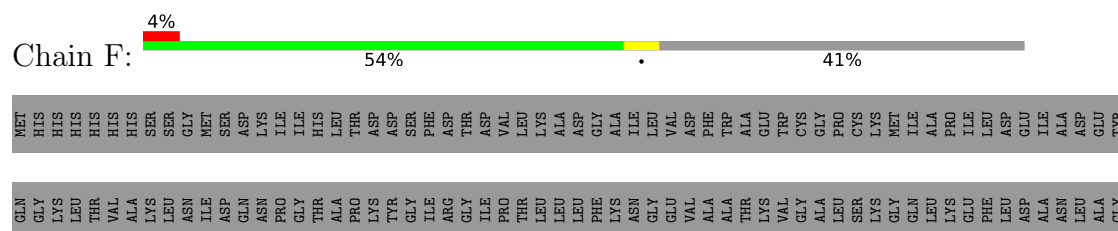
• Molecule 1: ADP-ribose glycohydrolase MACROD2



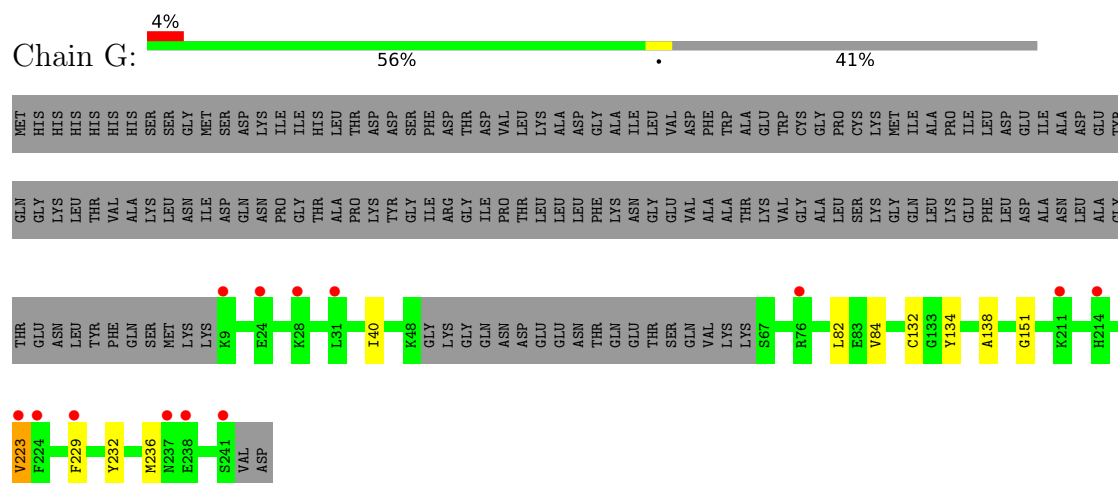
• Molecule 1: ADP-ribose glycohydrolase MACROD2



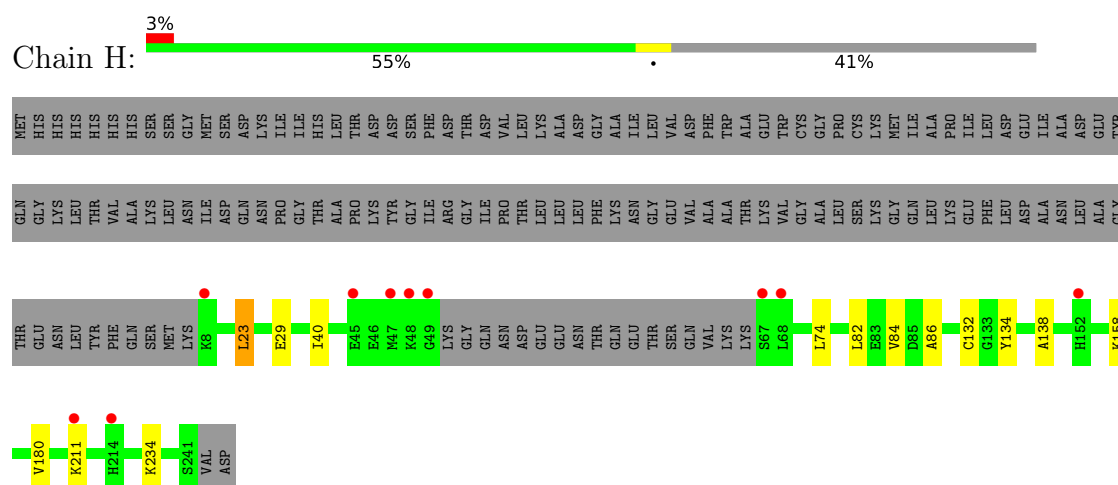
• Molecule 1: ADP-ribose glycohydrolase MACROD2



- Molecule 1: ADP-ribose glycohydrolase MACROD2



- Molecule 1: ADP-ribose glycohydrolase MACROD2



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	96.78Å 96.78Å 261.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 1.70 48.39 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.39-1.70) 100.0 (48.39-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.182 , 0.203 0.192 , 0.213	Depositor DCC
R_{free} test set	13095 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15593	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, DMS, 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	0.94	0/1774	1.20	0/2388
1	B	0.94	0/1800	1.16	0/2424
1	C	0.95	0/1767	1.22	0/2380
1	D	0.95	0/1780	1.24	0/2395
1	E	0.97	0/1811	1.21	0/2436
1	F	0.95	0/1798	1.20	0/2420
1	G	0.95	0/1765	1.24	0/2377
1	H	0.97	0/1787	1.18	0/2406
All	All	0.95	0/14282	1.21	0/19226

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1729	0	1767	7	0
1	B	1745	0	1783	10	0
1	C	1722	0	1755	8	0
1	D	1741	0	1775	4	0
1	E	1760	0	1797	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1746	0	1784	11	0
1	G	1720	0	1754	7	0
1	H	1739	0	1775	8	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	D	6	0	8	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	F	10	0	4	0	0
3	G	10	0	4	1	0
3	H	10	0	4	0	0
4	C	4	0	6	1	0
4	F	4	0	6	0	0
5	A	241	0	0	0	0
5	B	216	0	0	0	0
5	C	166	0	0	0	0
5	D	168	0	0	0	0
5	E	199	0	0	0	0
5	F	178	0	0	0	0
5	G	217	0	0	0	0
5	H	218	0	0	3	0
All	All	15593	0	14262	63	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 2.

All (63) 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:75[A]:TYR:CD2	1:F:222:CYS:SG	2.60	0.94
1:F:75[A]:TYR:CE2	1:F:222:CYS:SG	2.64	0.91
1:B:75[B]:TYR:HD2	1:B:222:CYS:HG	1.14	0.88
1:F:75[A]:TYR:HD2	1:F:222:CYS:SG	2.03	0.78
1:B:75[B]:TYR:CD2	1:B:222:CYS:SG	2.80	0.73
1:F:75[A]:TYR:HE2	1:F:222:CYS:SG	2.12	0.70
1:B:75[B]:TYR:HD2	1:B:222:CYS:SG	2.16	0.67
1:H:29[B]:GLU:HG3	5:H:1379:HOH:O	1.99	0.61
1:B:75[B]:TYR:CE2	1:B:222:CYS:SG	2.95	0.59
1:E:195:GLU:HB3	1:E:196:PRO:HD3	1.86	0.58
1:F:195:GLU:HB3	1:F:196:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:GLY:HA3	3:G:301:TLA:O2	2.06	0.56
1:G:223:VAL:HG11	1:G:229:PHE:HB2	1.89	0.55
1:G:232:TYR:O	1:G:236[A]:MET:HG2	2.06	0.55
1:A:195:GLU:HB3	1:A:196:PRO:HD3	1.90	0.54
1:D:47:MET:O	1:D:48:LYS:C	2.53	0.52
1:A:232:TYR:O	1:A:236[A]:MET:HG2	2.09	0.52
1:D:232:TYR:O	1:D:236[A]:MET:HG2	2.10	0.52
1:C:69:THR:HG21	1:C:241:SER:HB3	1.92	0.52
1:C:195:GLU:HB3	1:C:196:PRO:HD3	1.91	0.51
1:B:232:TYR:O	1:B:236[A]:MET:HG2	2.11	0.51
1:F:132:CYS:HB3	1:F:134:TYR:CZ	2.47	0.50
1:B:47:MET:HA	1:B:47:MET:HE2	1.94	0.49
1:H:158:LYS:NZ	5:H:1303:HOH:O	2.44	0.48
1:F:132:CYS:HB3	1:F:134:TYR:CE2	2.48	0.48
1:F:9[B]:LYS:HD2	1:F:9[B]:LYS:HA	1.45	0.47
1:C:223:VAL:HG21	1:C:229:PHE:HA	1.96	0.47
1:E:76:ARG:HD3	1:E:229:PHE:CD1	2.49	0.47
1:E:86:ALA:O	1:E:180:VAL:HA	2.14	0.47
1:G:132:CYS:HB3	1:G:134:TYR:CZ	2.50	0.46
1:A:76:ARG:HD2	1:A:229:PHE:CD1	2.51	0.46
1:C:132:CYS:HB3	1:C:134:TYR:CE2	2.51	0.45
1:F:84:VAL:O	1:F:138:ALA:HA	2.17	0.45
1:A:132:CYS:HB3	1:A:134:TYR:CZ	2.52	0.45
1:D:84:VAL:O	1:D:138:ALA:HA	2.17	0.45
1:H:234:LYS:HG3	5:H:1339:HOH:O	2.16	0.45
1:C:132:CYS:HB3	1:C:134:TYR:CZ	2.52	0.44
1:E:76:ARG:HD3	1:E:229:PHE:CG	2.52	0.44
1:H:132:CYS:HB3	1:H:134:TYR:CZ	2.52	0.44
1:A:86:ALA:O	1:A:180:VAL:HA	2.18	0.44
1:E:132:CYS:HB3	1:E:134:TYR:CE2	2.52	0.44
1:F:86:ALA:O	1:F:180:VAL:HA	2.18	0.44
1:A:232:TYR:O	1:A:236[B]:MET:HG2	2.17	0.44
1:H:86:ALA:O	1:H:180:VAL:HA	2.18	0.43
1:E:132:CYS:HB3	1:E:134:TYR:CZ	2.55	0.42
1:B:132:CYS:HB3	1:B:134:TYR:CZ	2.55	0.42
1:C:86:ALA:O	1:C:180:VAL:HA	2.19	0.42
1:F:9[B]:LYS:HG3	1:F:14:GLU:HB2	2.02	0.42
1:C:84:VAL:O	1:C:138:ALA:HA	2.20	0.41
1:G:40:ILE:HD11	1:G:82:LEU:HD22	2.02	0.41
1:A:132:CYS:HB3	1:A:134:TYR:CE2	2.54	0.41
1:C:187:THR:O	4:C:403:DMS:H22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:TYR:O	1:G:236[B]:MET:HG2	2.20	0.41
1:H:23:LEU:HD12	1:H:23:LEU:HA	1.83	0.41
1:H:40[A]:ILE:HD11	1:H:82:LEU:HD22	2.03	0.41
1:B:85:ASP:HB2	1:B:177:ILE:HG23	2.02	0.41
1:H:84:VAL:O	1:H:138:ALA:HA	2.21	0.41
1:D:23:LEU:HD12	1:D:23:LEU:HA	1.93	0.41
1:G:84:VAL:O	1:G:138:ALA:HA	2.21	0.41
1:B:84:VAL:O	1:B:138:ALA:HA	2.21	0.41
1:B:86:ALA:O	1:B:180:VAL:HA	2.20	0.41
1:E:232:TYR:O	1:E:236[A]:MET:HG2	2.21	0.41
1:E:84:VAL:O	1:E:138:ALA:HA	2.22	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	216/366 (59%)	212 (98%)	4 (2%)	0	100	100
1	B	218/366 (60%)	216 (99%)	2 (1%)	0	100	100
1	C	215/366 (59%)	212 (99%)	3 (1%)	0	100	100
1	D	217/366 (59%)	215 (99%)	2 (1%)	0	100	100
1	E	221/366 (60%)	218 (99%)	3 (1%)	0	100	100
1	F	217/366 (59%)	213 (98%)	4 (2%)	0	100	100
1	G	215/366 (59%)	211 (98%)	4 (2%)	0	100	100
1	H	218/366 (60%)	215 (99%)	3 (1%)	0	100	100
All	All	1737/2928 (59%)	1712 (99%)	25 (1%)	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	189/310 (61%)	185 (98%)	4 (2%)	47	30
1	B	191/310 (62%)	190 (100%)	1 (0%)	81	76
1	C	188/310 (61%)	183 (97%)	5 (3%)	39	23
1	D	190/310 (61%)	189 (100%)	1 (0%)	81	76
1	E	192/310 (62%)	190 (99%)	2 (1%)	68	58
1	F	191/310 (62%)	186 (97%)	5 (3%)	40	23
1	G	188/310 (61%)	187 (100%)	1 (0%)	81	76
1	H	190/310 (61%)	187 (98%)	3 (2%)	55	41
All	All	1519/2480 (61%)	1497 (99%)	22 (1%)	59	46

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	10	VAL
1	A	32	ARG
1	A	47	MET
1	B	44	LYS
1	C	31	LEU
1	C	44	LYS
1	C	47	MET
1	C	211	LYS
1	C	241	SER
1	D	8	LYS
1	E	226	GLU
1	E	234	LYS
1	F	21[A]	MET
1	F	21[B]	MET
1	F	31	LEU
1	F	211	LYS
1	F	214	HIS
1	G	223	VAL

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Mol	Chain	Res	Type
1	H	23	LEU
1	H	74	LEU
1	H	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	214	HIS
1	B	119	ASN
1	D	203	ASN
1	D	213	HIS
1	E	203	ASN
1	F	121	ASN
1	F	127	HIS
1	H	121	ASN
1	H	214	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	TLA	F	301	-	9,9,9	1.23	0	12,12,12	1.17	1 (8%)
3	TLA	G	301	-	9,9,9	1.07	0	12,12,12	1.23	2 (16%)
4	DMS	C	403	-	3,3,3	0.34	0	3,3,3	0.20	0
3	TLA	H	501	-	9,9,9	1.33	0	12,12,12	0.87	0
3	TLA	B	502	-	9,9,9	1.17	0	12,12,12	0.95	0
2	GOL	B	501	-	5,5,5	0.08	0	5,5,5	0.29	0
2	GOL	A	601	-	5,5,5	0.07	0	5,5,5	0.24	0
4	DMS	F	302	-	3,3,3	0.58	0	3,3,3	0.05	0
3	TLA	C	401	-	9,9,9	1.32	1 (11%)	12,12,12	3.27	6 (50%)
2	GOL	C	404	-	5,5,5	0.13	0	5,5,5	0.31	0
2	GOL	D	401	-	5,5,5	0.11	0	5,5,5	0.31	0
2	GOL	C	402	-	5,5,5	0.09	0	5,5,5	0.51	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
3	TLA	F	301	-	-	0/12/12/12	-
3	TLA	G	301	-	-	1/12/12/12	-
3	TLA	H	501	-	-	4/12/12/12	-
3	TLA	B	502	-	-	0/12/12/12	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
3	TLA	C	401	-	-	7/12/12/12	-
2	GOL	C	404	-	-	0/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	C	402	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	TLA	C2-C1	-2.39	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	TLA	C2-C3-C4	7.47	126.37	109.82
3	C	401	TLA	O3-C3-C2	-5.96	98.04	110.17
3	C	401	TLA	O41-C4-C3	3.28	122.44	113.31
3	C	401	TLA	O2-C2-C3	2.86	115.99	110.17
3	F	301	TLA	O41-C4-C3	2.61	120.58	113.31
3	G	301	TLA	O11-C1-C2	2.46	120.14	113.31
3	C	401	TLA	O41-C4-O4	-2.44	118.55	124.08
3	G	301	TLA	O41-C4-C3	2.15	119.29	113.31
3	C	401	TLA	C3-C2-C1	2.11	114.50	109.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	GOL	C1-C2-C3-O3
2	C	402	GOL	C1-C2-C3-O3
3	C	401	TLA	O1-C1-C2-O2
3	C	401	TLA	O11-C1-C2-O2
3	C	401	TLA	C1-C2-C3-C4
3	C	401	TLA	O2-C2-C3-O3
2	C	402	GOL	O2-C2-C3-O3
3	C	401	TLA	O1-C1-C2-C3
3	C	401	TLA	O11-C1-C2-C3
2	B	501	GOL	O2-C2-C3-O3
3	C	401	TLA	O2-C2-C3-C4
3	H	501	TLA	O11-C1-C2-C3
3	H	501	TLA	O1-C1-C2-C3
3	H	501	TLA	O11-C1-C2-O2
3	H	501	TLA	O1-C1-C2-O2
3	G	301	TLA	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	TLA	1	0
4	C	403	DMS	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	216/366 (59%)	0.17	10 (4%)	37	41	12, 23, 45, 63	4 (1%)
1	B	215/366 (58%)	0.04	10 (4%)	36	40	12, 21, 44, 69	7 (3%)
1	C	215/366 (58%)	0.36	14 (6%)	25	27	14, 25, 49, 76	4 (1%)
1	D	218/366 (59%)	0.36	18 (8%)	17	18	11, 25, 48, 75	3 (1%)
1	E	218/366 (59%)	0.19	13 (5%)	27	30	13, 22, 42, 59	7 (3%)
1	F	215/366 (58%)	0.24	15 (6%)	22	24	10, 22, 44, 76	7 (3%)
1	G	215/366 (58%)	0.26	13 (6%)	27	30	13, 24, 47, 61	4 (1%)
1	H	217/366 (59%)	0.07	10 (4%)	37	41	11, 20, 41, 84	5 (2%)
All	All	1729/2928 (59%)	0.21	103 (5%)	27	30	10, 23, 46, 84	41 (2%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	LEU	6.9
1	D	31	LEU	5.8
1	G	223	VAL	5.8
1	C	31	LEU	5.7
1	H	49	GLY	5.6
1	D	5	SER	4.9
1	B	31	LEU	4.4
1	F	224	PHE	4.4
1	G	31	LEU	4.4
1	D	75	TYR	4.3
1	D	6	MET	4.2
1	F	31	LEU	4.0
1	F	48	LYS	3.9
1	H	48	LYS	3.9
1	E	9	LYS	3.9
1	E	51	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	48	LYS	3.8
1	G	241	SER	3.8
1	B	48	LYS	3.7
1	F	101	VAL	3.7
1	F	9[A]	LYS	3.6
1	G	224	PHE	3.6
1	C	48	LYS	3.6
1	E	224	PHE	3.5
1	A	8	LYS	3.4
1	H	8	LYS	3.3
1	H	67	SER	3.2
1	H	47	MET	3.2
1	B	9	LYS	3.2
1	B	224	PHE	3.2
1	A	223	VAL	3.2
1	C	241	SER	3.1
1	F	47	MET	3.1
1	D	237	ASN	3.1
1	D	47	MET	3.0
1	B	241	SER	3.0
1	E	67	SER	3.0
1	A	241	SER	3.0
1	E	31	LEU	3.0
1	F	214	HIS	2.9
1	H	45	GLU	2.9
1	C	23	LEU	2.9
1	C	152	HIS	2.9
1	F	223	VAL	2.8
1	C	47	MET	2.8
1	F	222	CYS	2.8
1	D	214	HIS	2.8
1	G	76	ARG	2.8
1	E	226	GLU	2.8
1	B	47	MET	2.8
1	G	237	ASN	2.7
1	H	152	HIS	2.7
1	D	7	LYS	2.7
1	D	8	LYS	2.7
1	A	76	ARG	2.7
1	C	224	PHE	2.7
1	F	67	SER	2.7
1	F	152	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	237	ASN	2.6
1	C	214	HIS	2.6
1	A	224	PHE	2.6
1	H	68	LEU	2.6
1	B	211	LYS	2.6
1	A	240	PHE	2.5
1	G	9	LYS	2.5
1	F	241	SER	2.5
1	E	214	HIS	2.5
1	C	67	SER	2.5
1	G	229	PHE	2.5
1	G	238	GLU	2.4
1	D	10	VAL	2.4
1	C	68	LEU	2.4
1	G	28	LYS	2.4
1	A	47	MET	2.4
1	D	67	SER	2.4
1	D	152	HIS	2.4
1	E	10	VAL	2.3
1	B	32	ARG	2.3
1	D	68	LEU	2.3
1	E	19	LEU	2.3
1	D	224	PHE	2.3
1	G	24	GLU	2.3
1	G	214	HIS	2.2
1	C	41	LEU	2.2
1	B	234	LYS	2.2
1	C	239	PHE	2.2
1	H	214	HIS	2.2
1	H	211	LYS	2.2
1	F	75[A]	TYR	2.2
1	E	215	GLU	2.2
1	C	28	LYS	2.2
1	E	211	LYS	2.1
1	C	45	GLU	2.1
1	D	19	LEU	2.1
1	E	32	ARG	2.1
1	A	211	LYS	2.1
1	E	75	TYR	2.1
1	D	121	ASN	2.0
1	D	46	GLU	2.0
1	F	26[A]	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	32	ARG	2.0
1	B	10	VAL	2.0
1	G	211	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	601	6/6	0.83	0.17	44,51,55,57	0
2	GOL	C	404	6/6	0.83	0.16	38,47,51,52	0
3	TLA	C	401	10/10	0.84	0.14	32,38,46,56	0
3	TLA	G	301	10/10	0.87	0.12	37,40,41,42	0
3	TLA	B	502	10/10	0.89	0.10	31,37,41,41	0
3	TLA	H	501	10/10	0.89	0.10	39,44,50,51	0
2	GOL	B	501	6/6	0.90	0.12	28,29,35,38	0
2	GOL	D	401	6/6	0.91	0.10	30,33,36,38	0
2	GOL	C	402	6/6	0.92	0.10	27,30,33,34	0
4	DMS	F	302	4/4	0.92	0.16	25,32,32,33	0
4	DMS	C	403	4/4	0.98	0.09	23,26,26,27	0
3	TLA	F	301	10/10	0.98	0.05	20,20,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.