



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:37 AM UTC

PDB ID : 7FFC / pdb_00007ffc
Title : Diarylpentanoid-producing polyketide synthase (A210E mutant)
Authors : Morita, H.; Wong, C.P.; Liu, Q.; Kodama, T.; Lee, Y.; Nakashima, Y.
Deposited on : 2021-07-23
Resolution : 2.61 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

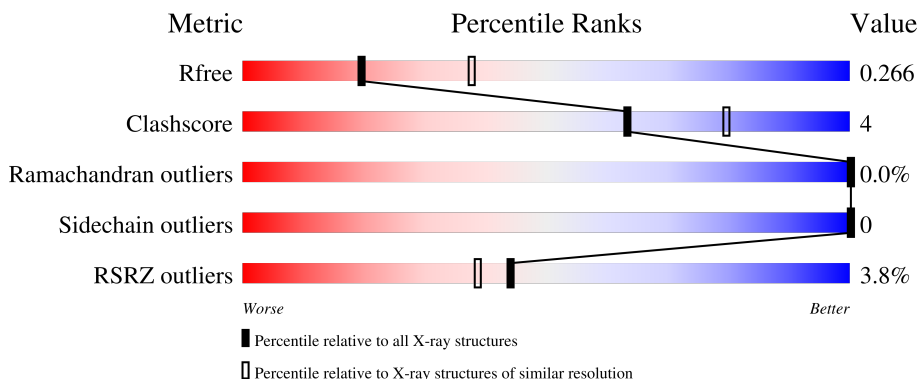
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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.



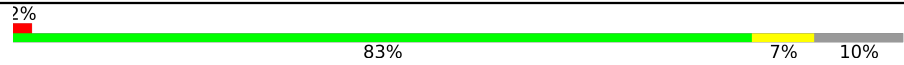
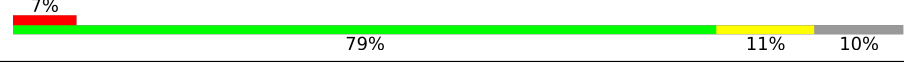

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	431	 3% 81% 10% 10%
1	B	431	 3% 78% 12% 10%
1	C	431	 7% 77% 13% 10%
1	D	431	 2% 80% 10% 10%
1	E	431	 % 83% 7% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	431	 2% 83% 7% 10%
1	G	431	 7% 79% 11% 10%
1	H	431	 % 82% 8% 10%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 24329 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	2978	1898	510	557	13	0	0	0
1	B	389	2976	1897	510	556	13	0	0	0
1	C	389	2975	1897	506	559	13	0	0	0
1	D	389	2979	1900	507	559	13	0	0	0
1	E	389	2985	1904	509	559	13	0	0	0
1	F	389	2991	1907	512	559	13	0	0	0
1	G	389	2976	1898	509	556	13	0	0	0
1	H	389	2975	1898	505	559	13	0	0	0

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP A0A385MEG6
A	-32	GLY	-	expression tag	UNP A0A385MEG6
A	-31	SER	-	expression tag	UNP A0A385MEG6
A	-30	SER	-	expression tag	UNP A0A385MEG6
A	-29	HIS	-	expression tag	UNP A0A385MEG6
A	-28	HIS	-	expression tag	UNP A0A385MEG6
A	-27	HIS	-	expression tag	UNP A0A385MEG6
A	-26	HIS	-	expression tag	UNP A0A385MEG6
A	-25	HIS	-	expression tag	UNP A0A385MEG6
A	-24	HIS	-	expression tag	UNP A0A385MEG6
A	-23	SER	-	expression tag	UNP A0A385MEG6
A	-22	SER	-	expression tag	UNP A0A385MEG6
A	-21	GLY	-	expression tag	UNP A0A385MEG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	LEU	-	expression tag	UNP A0A385MEG6
A	-19	VAL	-	expression tag	UNP A0A385MEG6
A	-18	PRO	-	expression tag	UNP A0A385MEG6
A	-17	ARG	-	expression tag	UNP A0A385MEG6
A	-16	GLY	-	expression tag	UNP A0A385MEG6
A	-15	SER	-	expression tag	UNP A0A385MEG6
A	-14	HIS	-	expression tag	UNP A0A385MEG6
A	-13	MET	-	expression tag	UNP A0A385MEG6
A	-12	ALA	-	expression tag	UNP A0A385MEG6
A	-11	SER	-	expression tag	UNP A0A385MEG6
A	-10	MET	-	expression tag	UNP A0A385MEG6
A	-9	THR	-	expression tag	UNP A0A385MEG6
A	-8	GLY	-	expression tag	UNP A0A385MEG6
A	-7	GLY	-	expression tag	UNP A0A385MEG6
A	-6	GLN	-	expression tag	UNP A0A385MEG6
A	-5	GLN	-	expression tag	UNP A0A385MEG6
A	-4	MET	-	expression tag	UNP A0A385MEG6
A	-3	GLY	-	expression tag	UNP A0A385MEG6
A	-2	ARG	-	expression tag	UNP A0A385MEG6
A	-1	GLY	-	expression tag	UNP A0A385MEG6
A	0	SER	-	expression tag	UNP A0A385MEG6
A	210	GLU	ALA	engineered mutation	UNP A0A385MEG6
B	-33	MET	-	initiating methionine	UNP A0A385MEG6
B	-32	GLY	-	expression tag	UNP A0A385MEG6
B	-31	SER	-	expression tag	UNP A0A385MEG6
B	-30	SER	-	expression tag	UNP A0A385MEG6
B	-29	HIS	-	expression tag	UNP A0A385MEG6
B	-28	HIS	-	expression tag	UNP A0A385MEG6
B	-27	HIS	-	expression tag	UNP A0A385MEG6
B	-26	HIS	-	expression tag	UNP A0A385MEG6
B	-25	HIS	-	expression tag	UNP A0A385MEG6
B	-24	HIS	-	expression tag	UNP A0A385MEG6
B	-23	SER	-	expression tag	UNP A0A385MEG6
B	-22	SER	-	expression tag	UNP A0A385MEG6
B	-21	GLY	-	expression tag	UNP A0A385MEG6
B	-20	LEU	-	expression tag	UNP A0A385MEG6
B	-19	VAL	-	expression tag	UNP A0A385MEG6
B	-18	PRO	-	expression tag	UNP A0A385MEG6
B	-17	ARG	-	expression tag	UNP A0A385MEG6
B	-16	GLY	-	expression tag	UNP A0A385MEG6
B	-15	SER	-	expression tag	UNP A0A385MEG6
B	-14	HIS	-	expression tag	UNP A0A385MEG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	expression tag	UNP A0A385MEG6
B	-12	ALA	-	expression tag	UNP A0A385MEG6
B	-11	SER	-	expression tag	UNP A0A385MEG6
B	-10	MET	-	expression tag	UNP A0A385MEG6
B	-9	THR	-	expression tag	UNP A0A385MEG6
B	-8	GLY	-	expression tag	UNP A0A385MEG6
B	-7	GLY	-	expression tag	UNP A0A385MEG6
B	-6	GLN	-	expression tag	UNP A0A385MEG6
B	-5	GLN	-	expression tag	UNP A0A385MEG6
B	-4	MET	-	expression tag	UNP A0A385MEG6
B	-3	GLY	-	expression tag	UNP A0A385MEG6
B	-2	ARG	-	expression tag	UNP A0A385MEG6
B	-1	GLY	-	expression tag	UNP A0A385MEG6
B	0	SER	-	expression tag	UNP A0A385MEG6
B	210	GLU	ALA	engineered mutation	UNP A0A385MEG6
C	-33	MET	-	initiating methionine	UNP A0A385MEG6
C	-32	GLY	-	expression tag	UNP A0A385MEG6
C	-31	SER	-	expression tag	UNP A0A385MEG6
C	-30	SER	-	expression tag	UNP A0A385MEG6
C	-29	HIS	-	expression tag	UNP A0A385MEG6
C	-28	HIS	-	expression tag	UNP A0A385MEG6
C	-27	HIS	-	expression tag	UNP A0A385MEG6
C	-26	HIS	-	expression tag	UNP A0A385MEG6
C	-25	HIS	-	expression tag	UNP A0A385MEG6
C	-24	HIS	-	expression tag	UNP A0A385MEG6
C	-23	SER	-	expression tag	UNP A0A385MEG6
C	-22	SER	-	expression tag	UNP A0A385MEG6
C	-21	GLY	-	expression tag	UNP A0A385MEG6
C	-20	LEU	-	expression tag	UNP A0A385MEG6
C	-19	VAL	-	expression tag	UNP A0A385MEG6
C	-18	PRO	-	expression tag	UNP A0A385MEG6
C	-17	ARG	-	expression tag	UNP A0A385MEG6
C	-16	GLY	-	expression tag	UNP A0A385MEG6
C	-15	SER	-	expression tag	UNP A0A385MEG6
C	-14	HIS	-	expression tag	UNP A0A385MEG6
C	-13	MET	-	expression tag	UNP A0A385MEG6
C	-12	ALA	-	expression tag	UNP A0A385MEG6
C	-11	SER	-	expression tag	UNP A0A385MEG6
C	-10	MET	-	expression tag	UNP A0A385MEG6
C	-9	THR	-	expression tag	UNP A0A385MEG6
C	-8	GLY	-	expression tag	UNP A0A385MEG6
C	-7	GLY	-	expression tag	UNP A0A385MEG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLN	-	expression tag	UNP A0A385MEG6
C	-5	GLN	-	expression tag	UNP A0A385MEG6
C	-4	MET	-	expression tag	UNP A0A385MEG6
C	-3	GLY	-	expression tag	UNP A0A385MEG6
C	-2	ARG	-	expression tag	UNP A0A385MEG6
C	-1	GLY	-	expression tag	UNP A0A385MEG6
C	0	SER	-	expression tag	UNP A0A385MEG6
C	210	GLU	ALA	engineered mutation	UNP A0A385MEG6
D	-33	MET	-	initiating methionine	UNP A0A385MEG6
D	-32	GLY	-	expression tag	UNP A0A385MEG6
D	-31	SER	-	expression tag	UNP A0A385MEG6
D	-30	SER	-	expression tag	UNP A0A385MEG6
D	-29	HIS	-	expression tag	UNP A0A385MEG6
D	-28	HIS	-	expression tag	UNP A0A385MEG6
D	-27	HIS	-	expression tag	UNP A0A385MEG6
D	-26	HIS	-	expression tag	UNP A0A385MEG6
D	-25	HIS	-	expression tag	UNP A0A385MEG6
D	-24	HIS	-	expression tag	UNP A0A385MEG6
D	-23	SER	-	expression tag	UNP A0A385MEG6
D	-22	SER	-	expression tag	UNP A0A385MEG6
D	-21	GLY	-	expression tag	UNP A0A385MEG6
D	-20	LEU	-	expression tag	UNP A0A385MEG6
D	-19	VAL	-	expression tag	UNP A0A385MEG6
D	-18	PRO	-	expression tag	UNP A0A385MEG6
D	-17	ARG	-	expression tag	UNP A0A385MEG6
D	-16	GLY	-	expression tag	UNP A0A385MEG6
D	-15	SER	-	expression tag	UNP A0A385MEG6
D	-14	HIS	-	expression tag	UNP A0A385MEG6
D	-13	MET	-	expression tag	UNP A0A385MEG6
D	-12	ALA	-	expression tag	UNP A0A385MEG6
D	-11	SER	-	expression tag	UNP A0A385MEG6
D	-10	MET	-	expression tag	UNP A0A385MEG6
D	-9	THR	-	expression tag	UNP A0A385MEG6
D	-8	GLY	-	expression tag	UNP A0A385MEG6
D	-7	GLY	-	expression tag	UNP A0A385MEG6
D	-6	GLN	-	expression tag	UNP A0A385MEG6
D	-5	GLN	-	expression tag	UNP A0A385MEG6
D	-4	MET	-	expression tag	UNP A0A385MEG6
D	-3	GLY	-	expression tag	UNP A0A385MEG6
D	-2	ARG	-	expression tag	UNP A0A385MEG6
D	-1	GLY	-	expression tag	UNP A0A385MEG6
D	0	SER	-	expression tag	UNP A0A385MEG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	210	GLU	ALA	engineered mutation	UNP A0A385MEG6
E	-33	MET	-	initiating methionine	UNP A0A385MEG6
E	-32	GLY	-	expression tag	UNP A0A385MEG6
E	-31	SER	-	expression tag	UNP A0A385MEG6
E	-30	SER	-	expression tag	UNP A0A385MEG6
E	-29	HIS	-	expression tag	UNP A0A385MEG6
E	-28	HIS	-	expression tag	UNP A0A385MEG6
E	-27	HIS	-	expression tag	UNP A0A385MEG6
E	-26	HIS	-	expression tag	UNP A0A385MEG6
E	-25	HIS	-	expression tag	UNP A0A385MEG6
E	-24	HIS	-	expression tag	UNP A0A385MEG6
E	-23	SER	-	expression tag	UNP A0A385MEG6
E	-22	SER	-	expression tag	UNP A0A385MEG6
E	-21	GLY	-	expression tag	UNP A0A385MEG6
E	-20	LEU	-	expression tag	UNP A0A385MEG6
E	-19	VAL	-	expression tag	UNP A0A385MEG6
E	-18	PRO	-	expression tag	UNP A0A385MEG6
E	-17	ARG	-	expression tag	UNP A0A385MEG6
E	-16	GLY	-	expression tag	UNP A0A385MEG6
E	-15	SER	-	expression tag	UNP A0A385MEG6
E	-14	HIS	-	expression tag	UNP A0A385MEG6
E	-13	MET	-	expression tag	UNP A0A385MEG6
E	-12	ALA	-	expression tag	UNP A0A385MEG6
E	-11	SER	-	expression tag	UNP A0A385MEG6
E	-10	MET	-	expression tag	UNP A0A385MEG6
E	-9	THR	-	expression tag	UNP A0A385MEG6
E	-8	GLY	-	expression tag	UNP A0A385MEG6
E	-7	GLY	-	expression tag	UNP A0A385MEG6
E	-6	GLN	-	expression tag	UNP A0A385MEG6
E	-5	GLN	-	expression tag	UNP A0A385MEG6
E	-4	MET	-	expression tag	UNP A0A385MEG6
E	-3	GLY	-	expression tag	UNP A0A385MEG6
E	-2	ARG	-	expression tag	UNP A0A385MEG6
E	-1	GLY	-	expression tag	UNP A0A385MEG6
E	0	SER	-	expression tag	UNP A0A385MEG6
E	210	GLU	ALA	engineered mutation	UNP A0A385MEG6
F	-33	MET	-	initiating methionine	UNP A0A385MEG6
F	-32	GLY	-	expression tag	UNP A0A385MEG6
F	-31	SER	-	expression tag	UNP A0A385MEG6
F	-30	SER	-	expression tag	UNP A0A385MEG6
F	-29	HIS	-	expression tag	UNP A0A385MEG6
F	-28	HIS	-	expression tag	UNP A0A385MEG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-27	HIS	-	expression tag	UNP A0A385MEG6
F	-26	HIS	-	expression tag	UNP A0A385MEG6
F	-25	HIS	-	expression tag	UNP A0A385MEG6
F	-24	HIS	-	expression tag	UNP A0A385MEG6
F	-23	SER	-	expression tag	UNP A0A385MEG6
F	-22	SER	-	expression tag	UNP A0A385MEG6
F	-21	GLY	-	expression tag	UNP A0A385MEG6
F	-20	LEU	-	expression tag	UNP A0A385MEG6
F	-19	VAL	-	expression tag	UNP A0A385MEG6
F	-18	PRO	-	expression tag	UNP A0A385MEG6
F	-17	ARG	-	expression tag	UNP A0A385MEG6
F	-16	GLY	-	expression tag	UNP A0A385MEG6
F	-15	SER	-	expression tag	UNP A0A385MEG6
F	-14	HIS	-	expression tag	UNP A0A385MEG6
F	-13	MET	-	expression tag	UNP A0A385MEG6
F	-12	ALA	-	expression tag	UNP A0A385MEG6
F	-11	SER	-	expression tag	UNP A0A385MEG6
F	-10	MET	-	expression tag	UNP A0A385MEG6
F	-9	THR	-	expression tag	UNP A0A385MEG6
F	-8	GLY	-	expression tag	UNP A0A385MEG6
F	-7	GLY	-	expression tag	UNP A0A385MEG6
F	-6	GLN	-	expression tag	UNP A0A385MEG6
F	-5	GLN	-	expression tag	UNP A0A385MEG6
F	-4	MET	-	expression tag	UNP A0A385MEG6
F	-3	GLY	-	expression tag	UNP A0A385MEG6
F	-2	ARG	-	expression tag	UNP A0A385MEG6
F	-1	GLY	-	expression tag	UNP A0A385MEG6
F	0	SER	-	expression tag	UNP A0A385MEG6
F	210	GLU	ALA	engineered mutation	UNP A0A385MEG6
G	-33	MET	-	initiating methionine	UNP A0A385MEG6
G	-32	GLY	-	expression tag	UNP A0A385MEG6
G	-31	SER	-	expression tag	UNP A0A385MEG6
G	-30	SER	-	expression tag	UNP A0A385MEG6
G	-29	HIS	-	expression tag	UNP A0A385MEG6
G	-28	HIS	-	expression tag	UNP A0A385MEG6
G	-27	HIS	-	expression tag	UNP A0A385MEG6
G	-26	HIS	-	expression tag	UNP A0A385MEG6
G	-25	HIS	-	expression tag	UNP A0A385MEG6
G	-24	HIS	-	expression tag	UNP A0A385MEG6
G	-23	SER	-	expression tag	UNP A0A385MEG6
G	-22	SER	-	expression tag	UNP A0A385MEG6
G	-21	GLY	-	expression tag	UNP A0A385MEG6

Continued on next page...

Continued from previous page...

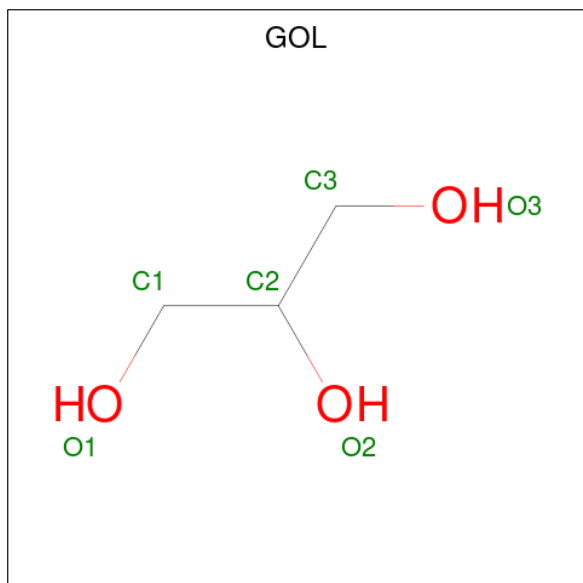
Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	LEU	-	expression tag	UNP A0A385MEG6
G	-19	VAL	-	expression tag	UNP A0A385MEG6
G	-18	PRO	-	expression tag	UNP A0A385MEG6
G	-17	ARG	-	expression tag	UNP A0A385MEG6
G	-16	GLY	-	expression tag	UNP A0A385MEG6
G	-15	SER	-	expression tag	UNP A0A385MEG6
G	-14	HIS	-	expression tag	UNP A0A385MEG6
G	-13	MET	-	expression tag	UNP A0A385MEG6
G	-12	ALA	-	expression tag	UNP A0A385MEG6
G	-11	SER	-	expression tag	UNP A0A385MEG6
G	-10	MET	-	expression tag	UNP A0A385MEG6
G	-9	THR	-	expression tag	UNP A0A385MEG6
G	-8	GLY	-	expression tag	UNP A0A385MEG6
G	-7	GLY	-	expression tag	UNP A0A385MEG6
G	-6	GLN	-	expression tag	UNP A0A385MEG6
G	-5	GLN	-	expression tag	UNP A0A385MEG6
G	-4	MET	-	expression tag	UNP A0A385MEG6
G	-3	GLY	-	expression tag	UNP A0A385MEG6
G	-2	ARG	-	expression tag	UNP A0A385MEG6
G	-1	GLY	-	expression tag	UNP A0A385MEG6
G	0	SER	-	expression tag	UNP A0A385MEG6
G	210	GLU	ALA	engineered mutation	UNP A0A385MEG6
H	-33	MET	-	initiating methionine	UNP A0A385MEG6
H	-32	GLY	-	expression tag	UNP A0A385MEG6
H	-31	SER	-	expression tag	UNP A0A385MEG6
H	-30	SER	-	expression tag	UNP A0A385MEG6
H	-29	HIS	-	expression tag	UNP A0A385MEG6
H	-28	HIS	-	expression tag	UNP A0A385MEG6
H	-27	HIS	-	expression tag	UNP A0A385MEG6
H	-26	HIS	-	expression tag	UNP A0A385MEG6
H	-25	HIS	-	expression tag	UNP A0A385MEG6
H	-24	HIS	-	expression tag	UNP A0A385MEG6
H	-23	SER	-	expression tag	UNP A0A385MEG6
H	-22	SER	-	expression tag	UNP A0A385MEG6
H	-21	GLY	-	expression tag	UNP A0A385MEG6
H	-20	LEU	-	expression tag	UNP A0A385MEG6
H	-19	VAL	-	expression tag	UNP A0A385MEG6
H	-18	PRO	-	expression tag	UNP A0A385MEG6
H	-17	ARG	-	expression tag	UNP A0A385MEG6
H	-16	GLY	-	expression tag	UNP A0A385MEG6
H	-15	SER	-	expression tag	UNP A0A385MEG6
H	-14	HIS	-	expression tag	UNP A0A385MEG6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-13	MET	-	expression tag	UNP A0A385MEG6
H	-12	ALA	-	expression tag	UNP A0A385MEG6
H	-11	SER	-	expression tag	UNP A0A385MEG6
H	-10	MET	-	expression tag	UNP A0A385MEG6
H	-9	THR	-	expression tag	UNP A0A385MEG6
H	-8	GLY	-	expression tag	UNP A0A385MEG6
H	-7	GLY	-	expression tag	UNP A0A385MEG6
H	-6	GLN	-	expression tag	UNP A0A385MEG6
H	-5	GLN	-	expression tag	UNP A0A385MEG6
H	-4	MET	-	expression tag	UNP A0A385MEG6
H	-3	GLY	-	expression tag	UNP A0A385MEG6
H	-2	ARG	-	expression tag	UNP A0A385MEG6
H	-1	GLY	-	expression tag	UNP A0A385MEG6
H	0	SER	-	expression tag	UNP A0A385MEG6
H	210	GLU	ALA	engineered mutation	UNP A0A385MEG6

- 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	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

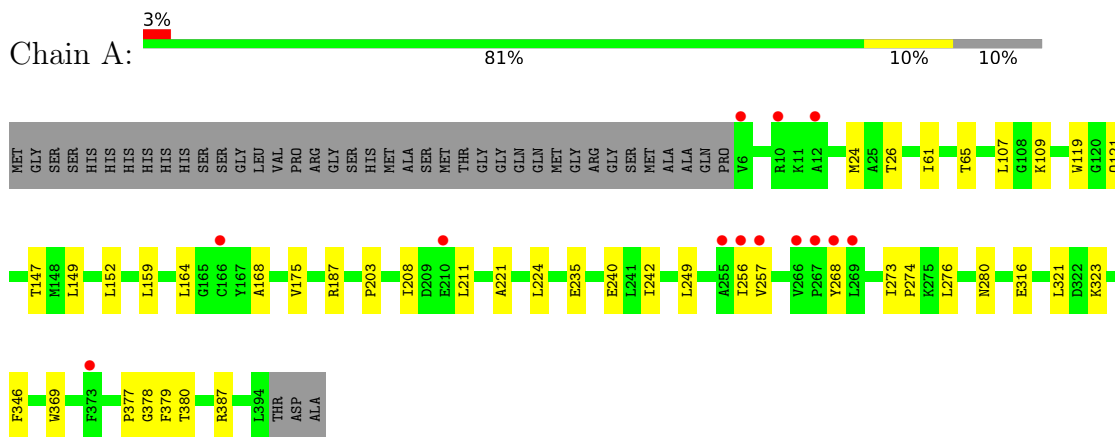
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total 56	O 56	0	0
3	B	55	Total 55	O 55	0	0
3	C	23	Total 23	O 23	0	0
3	D	68	Total 68	O 68	0	0
3	E	62	Total 62	O 62	0	0
3	F	58	Total 58	O 58	0	0
3	G	20	Total 20	O 20	0	0
3	H	62	Total 62	O 62	0	0

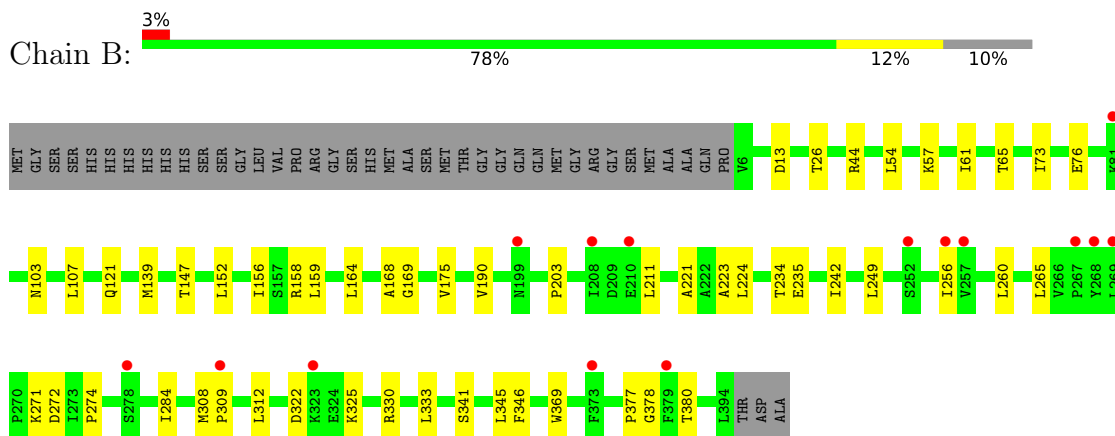
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

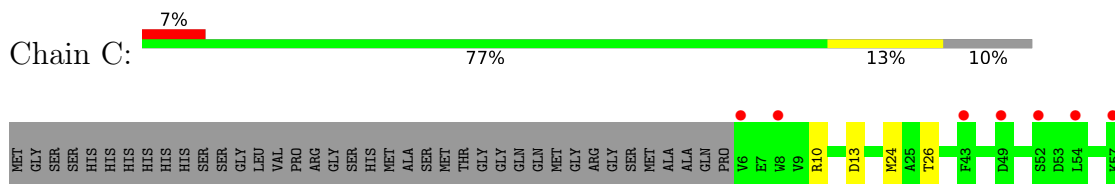
- Molecule 1: Type III polyketide synthase

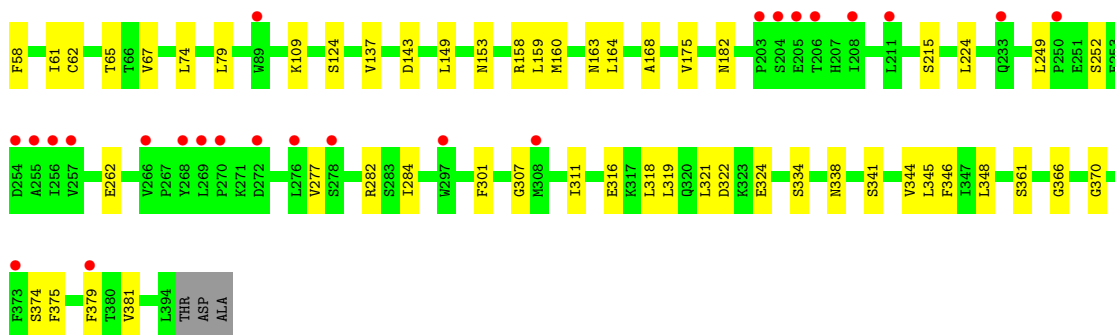


- Molecule 1: Type III polyketide synthase

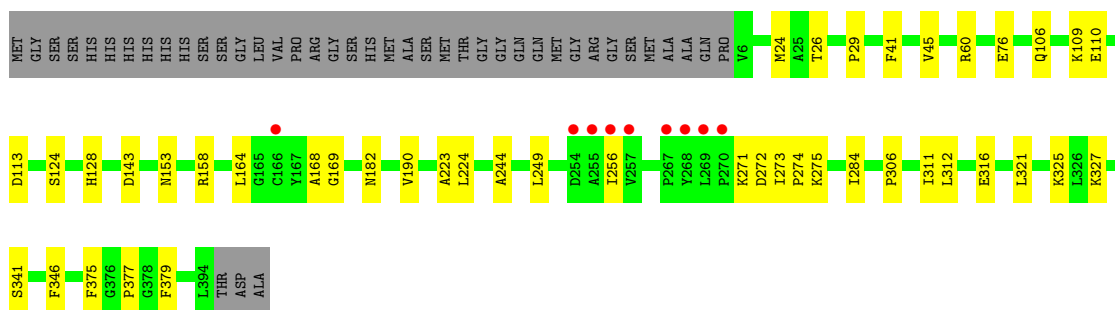
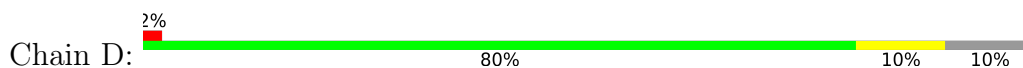


- Molecule 1: Type III polyketide synthase

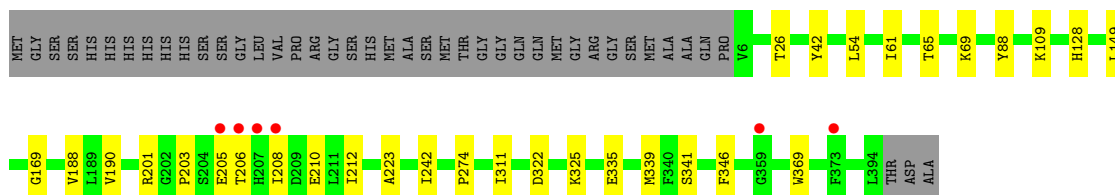
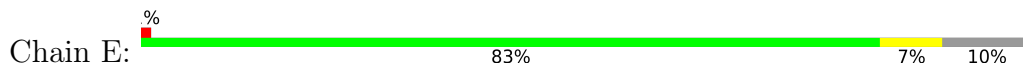




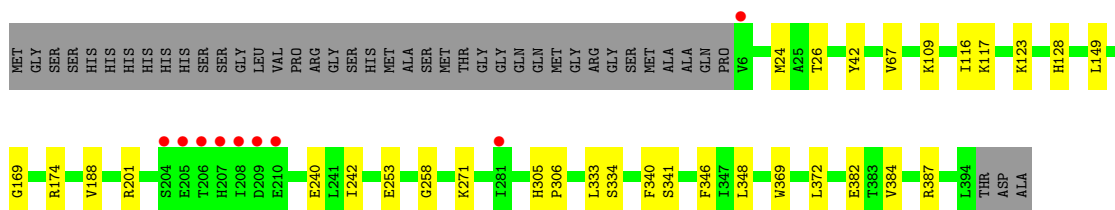
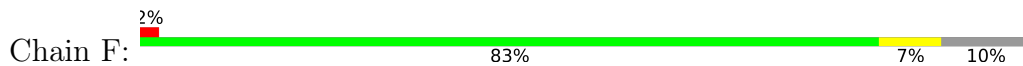
- Molecule 1: Type III polyketide synthase



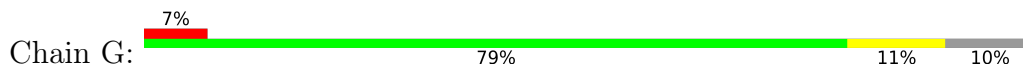
- Molecule 1: Type III polyketide synthase

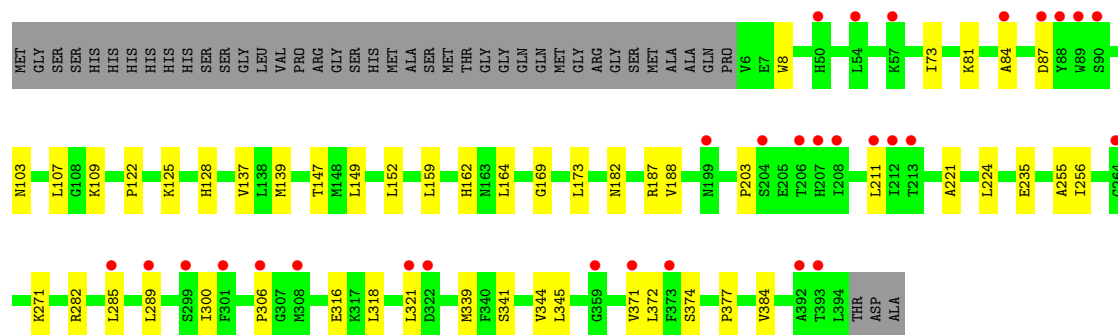


- Molecule 1: Type III polyketide synthase

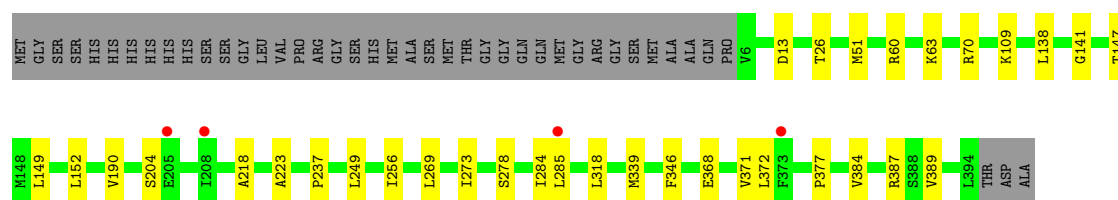
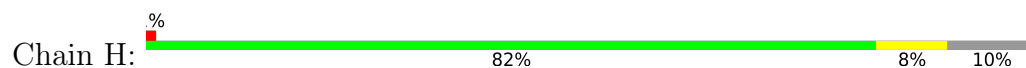


- Molecule 1: Type III polyketide synthase





- Molecule 1: Type III polyketide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.02Å 126.89Å 118.17Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	49.13 – 2.61 49.13 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.13-2.61) 99.4 (49.13-2.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.219 , 0.269 0.220 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtrriage
Anisotropy	0.880	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24329	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7538e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.10	0/3039	0.28	0/4129
1	B	0.10	0/3037	0.28	0/4126
1	C	0.11	0/3036	0.29	0/4127
1	D	0.10	0/3040	0.29	0/4131
1	E	0.10	0/3046	0.29	0/4137
1	F	0.10	0/3052	0.29	0/4144
1	G	0.12	0/3037	0.30	0/4127
1	H	0.10	0/3036	0.29	0/4126
All	All	0.10	0/24323	0.29	0/33047

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	2978	0	3002	24	0
1	B	2976	0	3003	29	0
1	C	2975	0	2993	36	0
1	D	2979	0	3004	29	0
1	E	2985	0	3022	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2991	0	3033	17	0
1	G	2976	0	3003	30	0
1	H	2975	0	3000	19	0
2	A	12	0	16	0	0
2	B	12	0	16	1	0
2	C	18	0	24	1	0
2	D	30	0	40	4	0
2	E	6	0	8	0	0
2	H	12	0	16	1	0
3	A	56	0	0	0	0
3	B	55	0	0	0	0
3	C	23	0	0	0	0
3	D	68	0	0	0	0
3	E	62	0	0	0	0
3	F	58	0	0	0	0
3	G	20	0	0	0	0
3	H	62	0	0	0	0
All	All	24329	0	24180	191	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 4.

All (191) 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:D:244:ALA:O	2:D:404:GOL:H31	1.88	0.73
1:E:206:THR:HB	1:E:210:GLU:HB3	1.72	0.71
1:H:249:LEU:HD21	1:H:284:ILE:HD11	1.78	0.64
1:G:344:VAL:HB	1:G:372:LEU:HD11	1.80	0.64
1:H:368:GLU:OE2	1:H:387:ARG:NH1	2.32	0.62
1:D:110:GLU:OE1	1:F:117:LYS:NZ	2.31	0.62
1:G:316:GLU:HA	1:G:321:LEU:HB2	1.82	0.61
1:D:109:LYS:NZ	1:D:113:ASP:OD2	2.35	0.60
1:A:109:LYS:HD2	1:A:149:LEU:HB3	1.83	0.60
1:F:42:TYR:OH	1:F:201:ARG:O	2.19	0.60
1:H:13:ASP:HB2	2:H:401:GOL:O1	2.01	0.60
1:E:109:LYS:HD2	1:E:149:LEU:HB3	1.83	0.60
1:H:372:LEU:HB3	1:H:384:VAL:HB	1.83	0.60
1:B:242:ILE:HG13	1:B:369:TRP:HZ3	1.66	0.59
1:H:51:MET:HE1	1:H:204:SER:HB3	1.84	0.59
1:C:143:ASP:OD1	1:C:158:ARG:NH1	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:TYR:OH	1:E:201:ARG:O	2.19	0.58
1:E:88:TYR:HD2	1:E:205:GLU:HG3	1.69	0.58
1:E:242:ILE:HG13	1:E:369:TRP:HZ3	1.68	0.57
1:F:253:GLU:O	1:F:271:LYS:NZ	2.35	0.57
1:C:163:ASN:HB3	1:G:139:MET:HE2	1.86	0.57
1:H:109:LYS:HD2	1:H:149:LEU:HB3	1.86	0.57
1:A:257:VAL:HB	1:A:268:TYR:HB3	1.88	0.56
1:E:128:HIS:HB2	1:E:188:VAL:HG22	1.87	0.56
1:C:344:VAL:HG11	1:C:374:SER:HB3	1.88	0.56
1:A:24:MET:HG2	1:A:224:LEU:HG	1.88	0.55
1:F:240:GLU:HB2	1:F:387:ARG:HB3	1.88	0.55
1:B:159:LEU:HD23	1:B:175:VAL:HG11	1.89	0.55
1:D:24:MET:HG2	1:D:224:LEU:HG	1.89	0.54
1:C:375:PHE:HB2	1:C:379:PHE:CZ	2.42	0.54
1:B:54:LEU:HA	1:B:57:LYS:HD2	1.90	0.53
1:C:316:GLU:HG3	1:C:321:LEU:HB2	1.89	0.53
1:F:109:LYS:HD2	1:F:149:LEU:HB3	1.90	0.53
1:F:26:THR:HB	1:F:346:PHE:CZ	2.43	0.53
1:D:249:LEU:HD21	1:D:284:ILE:HD11	1.90	0.53
1:G:203:PRO:HB3	1:G:211:LEU:HD21	1.91	0.53
1:F:128:HIS:HB2	1:F:188:VAL:HG22	1.91	0.53
1:H:285:LEU:HD11	1:H:371:VAL:HG21	1.90	0.52
1:H:147:THR:HG23	1:H:152:LEU:HB2	1.90	0.52
1:B:234:THR:HG23	1:B:235:GLU:HG3	1.91	0.52
1:D:41:PHE:HE1	1:D:76:GLU:HG3	1.74	0.52
1:G:344:VAL:HG11	1:G:374:SER:HB3	1.92	0.52
1:C:109:LYS:HD2	1:C:149:LEU:HB3	1.92	0.52
1:C:282:ARG:HG2	1:C:319:LEU:HD21	1.91	0.51
1:H:269:LEU:HD23	1:H:273:ILE:HG13	1.92	0.51
1:B:44:ARG:NH2	1:B:76:GLU:OE2	2.43	0.51
1:F:169:GLY:N	1:F:341:SER:HB2	2.25	0.51
1:B:26:THR:HB	1:B:346:PHE:CZ	2.46	0.50
1:B:256:ILE:HB	1:B:377:PRO:HA	1.93	0.50
1:B:322:ASP:HB3	1:B:325:LYS:HG2	1.93	0.50
1:D:29:PRO:HB3	2:D:402:GOL:H31	1.94	0.50
1:G:109:LYS:HD2	1:G:149:LEU:HB3	1.93	0.50
1:B:147:THR:HG23	1:B:152:LEU:HB2	1.93	0.50
1:G:128:HIS:HB2	1:G:188:VAL:HG22	1.93	0.49
1:D:124:SER:O	1:D:153:ASN:ND2	2.44	0.49
1:G:107:LEU:HG	1:G:221:ALA:HB2	1.94	0.49
1:G:147:THR:HG23	1:G:152:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:CYS:O	1:C:65:THR:OG1	2.31	0.49
1:C:74:LEU:HD13	1:C:79:LEU:HD21	1.94	0.49
1:C:324:GLU:HG2	1:D:60:ARG:HH12	1.78	0.49
1:B:13:ASP:OD1	2:B:401:GOL:H32	2.13	0.49
1:H:256:ILE:HG12	1:H:269:LEU:HG	1.94	0.49
1:A:316:GLU:HG3	1:A:321:LEU:HB2	1.94	0.49
1:H:190:VAL:O	1:H:223:ALA:HA	2.13	0.48
1:C:26:THR:HB	1:C:346:PHE:CZ	2.48	0.48
1:G:73:ILE:HD13	1:G:103:ASN:HB3	1.95	0.48
1:A:256:ILE:HB	1:A:377:PRO:HA	1.96	0.48
1:F:242:ILE:HG13	1:F:369:TRP:HZ3	1.78	0.48
1:A:242:ILE:HG13	1:A:369:TRP:HZ3	1.79	0.48
1:G:169:GLY:N	1:G:341:SER:HB2	2.29	0.48
1:G:256:ILE:HB	1:G:377:PRO:HA	1.96	0.47
1:B:164:LEU:HB2	1:B:168:ALA:HB2	1.96	0.47
1:C:182:ASN:HB2	1:G:182:ASN:HB2	1.97	0.47
1:G:173:LEU:HD12	1:G:372:LEU:HD23	1.95	0.47
1:B:203:PRO:HB3	1:B:211:LEU:HD21	1.96	0.47
1:B:260:LEU:HD13	1:B:265:LEU:HD22	1.94	0.47
1:D:316:GLU:HG3	1:D:321:LEU:HB2	1.95	0.47
1:C:137:VAL:HG21	1:G:137:VAL:HG21	1.96	0.47
1:D:143:ASP:OD2	1:D:158:ARG:NH1	2.45	0.47
1:C:277:VAL:HG21	1:C:311:ILE:HD13	1.97	0.47
1:C:67:VAL:HA	1:C:334:SER:HA	1.95	0.47
1:E:322:ASP:HB2	1:E:325:LYS:HG2	1.96	0.47
1:G:122:PRO:HG2	1:G:125:LYS:HG2	1.97	0.47
1:A:276:LEU:O	1:A:280:ASN:ND2	2.40	0.46
1:A:249:LEU:HD22	1:A:379:PHE:HD1	1.79	0.46
1:B:312:LEU:HD23	1:B:330:ARG:HG2	1.96	0.46
1:E:26:THR:HB	1:E:346:PHE:CZ	2.51	0.46
1:E:54:LEU:HD21	1:E:203:PRO:HB2	1.97	0.46
1:A:26:THR:HB	1:A:346:PHE:CZ	2.51	0.46
1:C:24:MET:HE1	1:C:348:LEU:HB3	1.97	0.46
1:F:174:ARG:NH2	1:F:382:GLU:OE2	2.35	0.46
1:H:70:ARG:HD2	1:H:218:ALA:HB2	1.98	0.46
1:C:61:ILE:O	1:C:65:THR:HG23	2.16	0.45
1:G:255:ALA:HA	1:G:271:LYS:HB2	1.98	0.45
1:A:187:ARG:NH2	1:A:235:GLU:OE1	2.43	0.45
1:C:224:LEU:HD13	1:C:345:LEU:HD13	1.98	0.45
1:B:169:GLY:N	1:B:341:SER:HB2	2.32	0.45
1:C:159:LEU:HD13	1:C:175:VAL:HG11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:HD21	1:C:284:ILE:HD11	1.99	0.45
1:F:24:MET:HE1	1:F:348:LEU:HB3	1.98	0.45
1:F:305:HIS:HE1	1:F:340:PHE:O	2.00	0.44
1:A:147:THR:HG23	1:A:152:LEU:HB2	1.98	0.44
1:B:107:LEU:HG	1:B:221:ALA:HB2	1.99	0.44
1:B:139:MET:HB2	1:F:258:GLY:O	2.16	0.44
1:B:308:MET:HE2	1:B:308:MET:HB2	1.76	0.44
1:C:168:ALA:HB3	1:C:341:SER:HB3	1.99	0.44
1:C:322:ASP:HB3	1:D:60:ARG:NH1	2.31	0.44
1:E:208:ILE:O	1:E:212:ILE:HD12	2.17	0.44
1:A:159:LEU:HD23	1:A:175:VAL:HG11	2.00	0.44
1:D:182:ASN:OD1	2:D:401:GOL:O3	2.35	0.44
1:G:372:LEU:HB3	1:G:384:VAL:HB	1.99	0.44
1:D:273:ILE:HG22	1:D:311:ILE:HD11	2.00	0.44
1:H:60:ARG:HA	1:H:63:LYS:HE2	1.99	0.44
1:C:282:ARG:HD2	1:C:318:LEU:HD21	2.00	0.44
1:C:307:GLY:HA2	1:C:338:ASN:ND2	2.32	0.44
1:G:84:ALA:HA	1:G:87:ASP:HB2	1.99	0.44
1:B:121:GLN:OE1	1:B:234:THR:OG1	2.36	0.44
1:B:224:LEU:HD11	1:B:345:LEU:HD13	2.00	0.44
1:C:13:ASP:OD1	2:C:401:GOL:H12	2.18	0.44
1:E:190:VAL:O	1:E:223:ALA:HA	2.18	0.44
1:G:285:LEU:HD22	1:G:371:VAL:HG21	2.00	0.43
1:C:301:PHE:CE1	1:C:370:GLY:HA3	2.53	0.43
1:A:240:GLU:HB2	1:A:387:ARG:HB3	1.99	0.43
1:B:309:PRO:HG3	1:B:333:LEU:HD21	1.99	0.43
1:E:69:LYS:NZ	1:E:335:GLU:O	2.46	0.43
1:H:26:THR:HB	1:H:346:PHE:CZ	2.54	0.43
1:C:175:VAL:HG21	1:G:159:LEU:HD21	2.01	0.43
1:C:164:LEU:HB2	1:C:168:ALA:HB2	2.00	0.43
1:C:58:PHE:CE1	1:C:215:SER:HB3	2.53	0.43
1:G:224:LEU:HD11	1:G:345:LEU:HD13	2.01	0.43
1:C:284:ILE:HD13	1:C:381:VAL:HG11	2.00	0.43
1:D:128:HIS:NE2	2:D:403:GOL:O3	2.45	0.43
1:D:325:LYS:HD3	1:D:325:LYS:HA	1.83	0.43
1:F:306:PRO:HB2	1:F:333:LEU:HD22	2.00	0.43
1:H:256:ILE:HB	1:H:377:PRO:HA	2.01	0.43
1:B:190:VAL:O	1:B:223:ALA:HA	2.19	0.43
1:C:160:MET:HB3	1:G:164:LEU:HD21	2.01	0.42
1:D:256:ILE:HB	1:D:377:PRO:HA	2.00	0.42
1:D:106:GLN:OE1	1:D:106:GLN:N	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ILE:O	1:E:65:THR:HG23	2.19	0.42
1:A:208:ILE:HD12	1:A:208:ILE:H	1.84	0.42
1:D:190:VAL:O	1:D:223:ALA:HA	2.19	0.42
1:D:272:ASP:HB3	1:D:275:LYS:HB3	1.99	0.42
1:E:169:GLY:N	1:E:341:SER:HB2	2.34	0.42
1:A:203:PRO:HB3	1:A:211:LEU:HD21	2.02	0.42
1:C:249:LEU:O	1:C:252:SER:OG	2.30	0.42
1:G:289:LEU:HD11	1:G:300:ILE:HD13	2.01	0.42
1:B:61:ILE:O	1:B:65:THR:HG23	2.20	0.42
1:G:187:ARG:NH2	1:G:235:GLU:OE1	2.52	0.42
1:H:278:SER:HB2	1:H:318:LEU:HD13	2.01	0.42
1:D:375:PHE:HB2	1:D:379:PHE:CZ	2.55	0.42
1:B:378:GLY:HA3	1:B:380:THR:N	2.34	0.42
1:D:26:THR:HB	1:D:346:PHE:CZ	2.54	0.42
1:D:169:GLY:N	1:D:341:SER:HB2	2.35	0.42
1:A:378:GLY:HA3	1:A:380:THR:N	2.35	0.42
1:B:274:PRO:HD3	1:B:308:MET:HE3	2.01	0.41
1:A:249:LEU:HD22	1:A:379:PHE:CD1	2.55	0.41
1:C:124:SER:O	1:C:153:ASN:ND2	2.50	0.41
1:D:306:PRO:HB3	1:D:312:LEU:HD11	2.02	0.41
1:A:164:LEU:HB2	1:A:168:ALA:HB2	2.02	0.41
1:H:237:PRO:O	1:H:389:VAL:HG11	2.20	0.41
1:E:88:TYR:CD2	1:E:205:GLU:HG3	2.52	0.41
1:F:116:ILE:HD13	1:F:123:LYS:HG2	2.02	0.41
1:H:138:LEU:HB2	1:H:141:GLY:HA2	2.02	0.41
1:A:61:ILE:O	1:A:65:THR:HG23	2.20	0.41
1:D:327:LYS:HE3	1:D:327:LYS:HB3	1.96	0.41
1:G:339:MET:HE3	1:G:339:MET:HB2	1.98	0.41
1:H:339:MET:HE3	1:H:339:MET:HB2	1.98	0.41
1:A:323:LYS:HA	1:A:323:LYS:HD3	1.87	0.41
1:A:273:ILE:N	1:A:274:PRO:HD2	2.35	0.41
1:D:271:LYS:HE2	1:D:271:LYS:HB3	1.83	0.41
1:F:67:VAL:HA	1:F:334:SER:HA	2.02	0.41
1:A:119:TRP:CD2	1:A:121:GLN:HB2	2.56	0.41
1:B:156:ILE:HG23	1:B:158:ARG:HG3	2.03	0.41
1:C:262:GLU:CD	1:C:262:GLU:H	2.29	0.41
1:D:274:PRO:HA	1:D:311:ILE:HG12	2.03	0.41
1:F:372:LEU:HB3	1:F:384:VAL:HB	2.03	0.41
1:G:137:VAL:HA	1:G:162:HIS:CD2	2.56	0.41
1:B:249:LEU:HD21	1:B:284:ILE:HD11	2.02	0.41
1:B:271:LYS:HD3	1:B:272:ASP:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:MET:HE3	1:E:339:MET:HB2	1.95	0.41
1:G:81:LYS:HD2	1:G:81:LYS:HA	1.86	0.40
1:D:164:LEU:HB2	1:D:168:ALA:HB2	2.03	0.40
1:E:274:PRO:HA	1:E:311:ILE:HG12	2.03	0.40
1:G:282:ARG:HE	1:G:318:LEU:HD21	1.86	0.40
1:A:187:ARG:HH21	1:A:235:GLU:CD	2.29	0.40
1:B:73:ILE:HD13	1:B:103:ASN:HB3	2.03	0.40
1:C:10:ARG:HG3	1:G:8:TRP:CH2	2.56	0.40
1:D:45:VAL:HG11	1:D:76:GLU:HG2	2.03	0.40
1:A:107:LEU:HG	1:A:221:ALA:HB2	2.03	0.40
1:C:361:SER:HB2	1:C:366:GLY:HA2	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	387/431 (90%)	374 (97%)	13 (3%)	0	100	100
1	B	387/431 (90%)	367 (95%)	20 (5%)	0	100	100
1	C	387/431 (90%)	367 (95%)	20 (5%)	0	100	100
1	D	387/431 (90%)	372 (96%)	15 (4%)	0	100	100
1	E	387/431 (90%)	375 (97%)	12 (3%)	0	100	100
1	F	387/431 (90%)	372 (96%)	15 (4%)	0	100	100
1	G	387/431 (90%)	371 (96%)	15 (4%)	1 (0%)	36	56
1	H	387/431 (90%)	376 (97%)	11 (3%)	0	100	100
All	All	3096/3448 (90%)	2974 (96%)	121 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	306	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/353 (90%)	318 (100%)	0	100	100
1	B	318/353 (90%)	318 (100%)	0	100	100
1	C	318/353 (90%)	318 (100%)	0	100	100
1	D	319/353 (90%)	319 (100%)	0	100	100
1	E	321/353 (91%)	321 (100%)	0	100	100
1	F	322/353 (91%)	322 (100%)	0	100	100
1	G	318/353 (90%)	318 (100%)	0	100	100
1	H	319/353 (90%)	319 (100%)	0	100	100
All	All	2553/2824 (90%)	2553 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	153	ASN
1	A	163	ASN
1	A	331	HIS
1	B	103	ASN
1	D	121	GLN
1	D	331	HIS
1	E	331	HIS
1	F	207	HIS
1	F	280	ASN
1	F	331	HIS
1	G	121	GLN
1	G	153	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	280	ASN
1	H	121	GLN
1	H	128	HIS
1	H	163	ASN
1	H	298	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	C	403	-	5,5,5	0.92	0	5,5,5	1.10	0
2	GOL	A	402	-	5,5,5	0.84	0	5,5,5	1.11	0
2	GOL	A	401	-	5,5,5	0.91	0	5,5,5	1.09	0
2	GOL	D	402	-	5,5,5	0.89	0	5,5,5	1.09	0
2	GOL	B	402	-	5,5,5	0.94	0	5,5,5	1.07	0
2	GOL	H	401	-	5,5,5	0.89	0	5,5,5	1.10	0
2	GOL	C	402	-	5,5,5	0.87	0	5,5,5	1.13	0
2	GOL	D	403	-	5,5,5	0.88	0	5,5,5	1.16	1 (20%)
2	GOL	D	404	-	5,5,5	0.99	0	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	401	-	5,5,5	0.94	0	5,5,5	1.07	0
2	GOL	E	401	-	5,5,5	0.94	0	5,5,5	1.10	0
2	GOL	C	401	-	5,5,5	0.97	0	5,5,5	1.05	0
2	GOL	D	405	-	5,5,5	0.95	0	5,5,5	1.00	0
2	GOL	H	402	-	5,5,5	0.94	0	5,5,5	1.06	0
2	GOL	B	401	-	5,5,5	0.90	0	5,5,5	1.05	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	403	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	A	401	-	-	3/4/4/4	-
2	GOL	D	402	-	-	2/4/4/4	-
2	GOL	B	402	-	-	2/4/4/4	-
2	GOL	H	401	-	-	2/4/4/4	-
2	GOL	C	402	-	-	0/4/4/4	-
2	GOL	D	403	-	-	2/4/4/4	-
2	GOL	D	404	-	-	4/4/4/4	-
2	GOL	D	401	-	-	0/4/4/4	-
2	GOL	E	401	-	-	3/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
2	GOL	D	405	-	-	2/4/4/4	-
2	GOL	H	402	-	-	1/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	GOL	C3-C2-C1	-2.13	103.99	111.80

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GOL	C1-C2-C3-O3
2	D	403	GOL	O1-C1-C2-C3
2	D	404	GOL	O1-C1-C2-C3
2	E	401	GOL	O1-C1-C2-C3
2	D	402	GOL	O1-C1-C2-O2
2	A	401	GOL	C1-C2-C3-O3
2	B	402	GOL	O1-C1-C2-C3
2	C	401	GOL	C1-C2-C3-O3
2	D	402	GOL	O1-C1-C2-C3
2	D	404	GOL	C1-C2-C3-O3
2	D	405	GOL	C1-C2-C3-O3
2	H	401	GOL	C1-C2-C3-O3
2	D	403	GOL	O1-C1-C2-O2
2	D	404	GOL	O1-C1-C2-O2
2	D	404	GOL	O2-C2-C3-O3
2	E	401	GOL	O1-C1-C2-O2
2	B	401	GOL	O2-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	B	402	GOL	O1-C1-C2-O2
2	D	405	GOL	O2-C2-C3-O3
2	E	401	GOL	O2-C2-C3-O3
2	C	401	GOL	O1-C1-C2-C3
2	H	402	GOL	O1-C1-C2-C3
2	A	401	GOL	O2-C2-C3-O3
2	H	401	GOL	O2-C2-C3-O3
2	C	401	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	402	GOL	1	0
2	H	401	GOL	1	0
2	D	403	GOL	1	0
2	D	404	GOL	1	0
2	D	401	GOL	1	0
2	C	401	GOL	1	0
2	B	401	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	389/431 (90%)	0.17	13 (3%) 49 44	21, 35, 70, 100	0
1	B	389/431 (90%)	0.25	15 (3%) 43 38	19, 37, 78, 99	0
1	C	389/431 (90%)	0.69	31 (7%) 18 14	32, 52, 94, 121	0
1	D	389/431 (90%)	0.09	9 (2%) 61 56	17, 29, 65, 93	0
1	E	389/431 (90%)	0.06	6 (1%) 72 68	22, 35, 55, 87	0
1	F	389/431 (90%)	0.12	9 (2%) 61 56	19, 35, 59, 106	0
1	G	389/431 (90%)	0.82	30 (7%) 19 15	31, 55, 91, 122	0
1	H	389/431 (90%)	0.05	4 (1%) 79 76	18, 31, 58, 83	0
All	All	3112/3448 (90%)	0.28	117 (3%) 44 39	17, 38, 79, 122	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	TRP	5.7
1	G	322	ASP	4.7
1	B	268	TYR	4.5
1	C	268	TYR	4.3
1	G	208	ILE	4.2
1	G	308	MET	4.2
1	G	204	SER	4.2
1	G	207	HIS	4.0
1	A	166	CYS	3.8
1	A	10	ARG	3.8
1	G	87	ASP	3.8
1	B	269	LEU	3.7
1	G	373	PHE	3.7
1	C	257	VAL	3.7
1	H	373	PHE	3.7
1	C	308	MET	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	208	ILE	3.6
1	F	207	HIS	3.5
1	E	205	GLU	3.5
1	F	205	GLU	3.5
1	F	208	ILE	3.4
1	C	373	PHE	3.3
1	C	54	LEU	3.1
1	C	269	LEU	3.1
1	D	269	LEU	3.1
1	B	210	GLU	3.1
1	B	257	VAL	3.1
1	C	211	LEU	3.1
1	F	209	ASP	3.1
1	C	256	ILE	3.1
1	D	268	TYR	3.0
1	C	379	PHE	3.0
1	F	204	SER	3.0
1	B	256	ILE	2.9
1	B	379	PHE	2.9
1	C	254	ASP	2.8
1	F	210	GLU	2.8
1	G	321	LEU	2.8
1	H	205	GLU	2.8
1	G	206	THR	2.7
1	A	6	VAL	2.7
1	D	255	ALA	2.7
1	E	373	PHE	2.7
1	D	256	ILE	2.7
1	C	297	TRP	2.7
1	E	206	THR	2.7
1	C	270	PRO	2.7
1	A	268	TYR	2.7
1	C	205	GLU	2.7
1	G	89	TRP	2.7
1	A	257	VAL	2.7
1	G	84	ALA	2.7
1	G	392	ALA	2.7
1	G	88	TYR	2.6
1	B	252	SER	2.6
1	D	267	PRO	2.6
1	A	256	ILE	2.6
1	E	208	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	266	VAL	2.6
1	C	255	ALA	2.6
1	H	208	ILE	2.5
1	B	309	PRO	2.5
1	F	6	VAL	2.5
1	B	208	ILE	2.5
1	B	278	SER	2.5
1	E	207	HIS	2.5
1	G	306	PRO	2.5
1	G	54	LEU	2.5
1	A	210	GLU	2.5
1	G	57	LYS	2.4
1	D	254	ASP	2.4
1	C	6	VAL	2.4
1	F	206	THR	2.4
1	C	57	LYS	2.4
1	C	266	VAL	2.4
1	A	269	LEU	2.4
1	C	272	ASP	2.4
1	A	373	PHE	2.4
1	G	199	ASN	2.4
1	B	323	LYS	2.4
1	A	267	PRO	2.4
1	D	257	VAL	2.4
1	G	301	PHE	2.4
1	G	393	THR	2.3
1	G	359	GLY	2.3
1	C	52	SER	2.3
1	G	289	LEU	2.3
1	A	255	ALA	2.3
1	A	12	ALA	2.2
1	D	166	CYS	2.2
1	F	281	ILE	2.2
1	E	359	GLY	2.2
1	C	49	ASP	2.2
1	B	373	PHE	2.2
1	B	199	ASN	2.2
1	C	203	PRO	2.2
1	D	270	PRO	2.2
1	C	204	SER	2.2
1	C	278	SER	2.2
1	G	211	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	264	GLY	2.2
1	C	8	TRP	2.2
1	B	81	LYS	2.1
1	H	285	LEU	2.1
1	G	50	HIS	2.1
1	C	206	THR	2.1
1	C	250	PRO	2.1
1	C	233	GLN	2.1
1	G	212	ILE	2.1
1	G	90	SER	2.1
1	G	213	THR	2.1
1	G	285	LEU	2.1
1	C	43	PHE	2.1
1	G	299	SER	2.0
1	G	371	VAL	2.0
1	B	267	PRO	2.0
1	C	276	LEU	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	H	402	6/6	0.54	0.21	53,54,59,60	0
2	GOL	C	402	6/6	0.65	0.19	45,49,52,54	0
2	GOL	C	401	6/6	0.72	0.17	46,51,52,54	0
2	GOL	C	403	6/6	0.79	0.15	44,51,51,54	0
2	GOL	B	402	6/6	0.79	0.16	40,46,47,49	0
2	GOL	E	401	6/6	0.80	0.17	45,48,50,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	D	405	6/6	0.84	0.16	46,52,56,56	0
2	GOL	H	401	6/6	0.86	0.12	31,38,42,47	0
2	GOL	D	404	6/6	0.87	0.14	28,37,41,47	0
2	GOL	D	401	6/6	0.88	0.13	33,46,49,51	0
2	GOL	A	402	6/6	0.88	0.15	29,31,34,34	0
2	GOL	D	403	6/6	0.89	0.10	35,40,43,44	0
2	GOL	B	401	6/6	0.90	0.10	31,37,38,40	0
2	GOL	D	402	6/6	0.90	0.12	32,34,34,35	0
2	GOL	A	401	6/6	0.91	0.09	32,34,37,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.