

Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 04:30 PM JST

PDB ID	:	8WT1
Title	:	Crystal structure of S9 carboxypeptidase from Geobacillus sterothermophilus
Authors	:	Chandravanshi, K.; Kumar, A.; Sen, C.; Singh, R.; Bhange, G.B.; Makde,
		R.D.
Deposited on	:	2023-10-17
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	А	691	% 8 2%	12%	6%
1	В	691	85%	9%	6%
1	С	691	% 84%	10%	6%
1	D	691	83%	11%	6%
1	Е	691	84%	10%	6%
1	F	691	% 	10%	6%



Mol	Chain	Length	Quality of chain		
1	G	691	81%	12%	6%
1	Н	691	3% 85%	9%	6%

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
2	SO4	С	707	-	-	Х	-
5	ALA	А	716	-	-	Х	-
5	ALA	В	719	-	-	Х	-
5	ALA	С	713	-	Х	-	-
5	ALA	D	714	-	Х	Х	-
5	ALA	Е	715	-	Х	Х	-
5	ALA	F	713	-	Х	Х	-
5	ALA	G	709	-	Х	-	-
6	FLC	А	717	-	Х	-	-
6	FLC	Н	713	-	Х	-	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 42813 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	650	Total	С	Ν	0	S	0	0	0
1	А	050	5067	3239	873	944	11	0	0	0
1	В	650	Total	С	Ν	0	S	0	0	0
1	D	050	5063	3239	870	943	11	0	0	0
1	С	651	Total	С	Ν	0	S	0	0	0
1	U	001	5053	3232	867	943	11	0	0	0
1	1 D	640	Total	С	Ν	0	S	0	0	0
1	D	049	5032	3221	863	937	11		0	0
1	F	650	Total	С	Ν	0	S	0	0	0
1	Ľ	000	5027	3215	861	940	11		0	0
1	F	640	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	Ľ	049	5014	3211	862	930	11	0	0	0
1	С	647	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	G	047	4904	3159	829	905	11	0	0	0
1	1 II	651	Total	С	Ν	0	S	0	0	0
	п	001	4985	3203	852	919	11	0	0	

• Molecule 1 is a protein called S9 family peptidase.

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
А	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
А	-18	SER	-	expression tag	UNP A0A3L7D5Q2
А	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
А	-16	SER	-	expression tag	UNP A0A3L7D5Q2
A	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
А	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
А	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
А	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
А	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
A	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
А	-8	SER	-	expression tag	UNP A0A3L7D5Q2



Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	_	expression tag	UNP A0A3L7D5Q2
A	-6	HIS	_	expression tag	UNP A0A3L7D5Q2
A	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-4	HIS	_	expression tag	UNP A0A3L7D5Q2
A	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
A	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
А	0	SER	-	expression tag	UNP A0A3L7D5Q2
А	1	SER	-	expression tag	UNP A0A3L7D5Q2
А	2	GLY	_	expression tag	UNP A0A3L7D5Q2
А	3	SER	-	expression tag	UNP A0A3L7D5Q2
А	4	GLY	_	expression tag	UNP A0A3L7D5Q2
А	5	GLY	-	expression tag	UNP A0A3L7D5Q2
А	6	GLY	-	expression tag	UNP A0A3L7D5Q2
А	7	GLY	_	expression tag	UNP A0A3L7D5Q2
А	8	GLY	-	expression tag	UNP A0A3L7D5Q2
А	9	GLU	_	expression tag	UNP A0A3L7D5Q2
А	10	ASN	-	expression tag	UNP A0A3L7D5Q2
А	11	LEU	-	expression tag	UNP A0A3L7D5Q2
А	12	TYR	_	expression tag	UNP A0A3L7D5Q2
А	13	PHE	-	expression tag	UNP A0A3L7D5Q2
А	14	GLN	_	expression tag	UNP A0A3L7D5Q2
А	15	GLY	-	expression tag	UNP A0A3L7D5Q2
А	16	THR	_	expression tag	UNP A0A3L7D5Q2
А	332	SER	LEU	conflict	UNP A0A3L7D5Q2
В	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
В	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
В	-18	SER	-	expression tag	UNP A0A3L7D5Q2
В	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
В	-16	SER	-	expression tag	UNP A0A3L7D5Q2
В	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
В	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
В	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
В	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
В	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
В	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
В	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
В	-8	SER	-	expression tag	UNP A0A3L7D5Q2
В	-7	SER	-	expression tag	UNP A0A3L7D5Q2
В	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
В	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
В	-4	HIS	-	expression tag	UNP A0A3L7D5Q2

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
В	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
В	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
В	0	SER	-	expression tag	UNP A0A3L7D5Q2
В	1	SER	-	expression tag	UNP A0A3L7D5Q2
В	2	GLY	-	expression tag	UNP A0A3L7D5Q2
В	3	SER	_	expression tag	UNP A0A3L7D5Q2
В	4	GLY	-	expression tag	UNP A0A3L7D5Q2
В	5	GLY	-	expression tag	UNP A0A3L7D5Q2
В	6	GLY	-	expression tag	UNP A0A3L7D5Q2
В	7	GLY	-	expression tag	UNP A0A3L7D5Q2
В	8	GLY	-	expression tag	UNP A0A3L7D5Q2
В	9	GLU	-	expression tag	UNP A0A3L7D5Q2
В	10	ASN	-	expression tag	UNP A0A3L7D5Q2
В	11	LEU	-	expression tag	UNP A0A3L7D5Q2
В	12	TYR	-	expression tag	UNP A0A3L7D5Q2
В	13	PHE	-	expression tag	UNP A0A3L7D5Q2
В	14	GLN	-	expression tag	UNP A0A3L7D5Q2
В	15	GLY	-	expression tag	UNP A0A3L7D5Q2
В	16	THR	-	expression tag	UNP A0A3L7D5Q2
В	332	SER	LEU	conflict	UNP A0A3L7D5Q2
С	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
С	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
С	-18	SER	-	expression tag	UNP A0A3L7D5Q2
С	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
С	-16	SER	-	expression tag	UNP A0A3L7D5Q2
C	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
C	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
C	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
C	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
C	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
C	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
C	-8	SER	-	expression tag	UNP A0A3L7D5Q2
C	-7	SER	-	expression tag	UNP A0A3L7D5Q2
C	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
С	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
С	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
С	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
С	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
C	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
C	0	SER	-	expression tag	UNP A0A3L7D5Q2



Chain	Residue	Modelled	Actual	Comment	Reference
С	1	SER	-	expression tag	UNP A0A3L7D5Q2
С	2	GLY	-	expression tag	UNP A0A3L7D5Q2
С	3	SER	-	expression tag	UNP A0A3L7D5Q2
С	4	GLY	_	expression tag	UNP A0A3L7D5Q2
С	5	GLY	-	expression tag	UNP A0A3L7D5Q2
С	6	GLY	-	expression tag	UNP A0A3L7D5Q2
С	7	GLY	-	expression tag	UNP A0A3L7D5Q2
С	8	GLY	-	expression tag	UNP A0A3L7D5Q2
С	9	GLU	-	expression tag	UNP A0A3L7D5Q2
С	10	ASN	-	expression tag	UNP A0A3L7D5Q2
С	11	LEU	-	expression tag	UNP A0A3L7D5Q2
С	12	TYR	-	expression tag	UNP A0A3L7D5Q2
С	13	PHE	-	expression tag	UNP A0A3L7D5Q2
С	14	GLN	-	expression tag	UNP A0A3L7D5Q2
С	15	GLY	-	expression tag	UNP A0A3L7D5Q2
С	16	THR	-	expression tag	UNP A0A3L7D5Q2
С	332	SER	LEU	conflict	UNP A0A3L7D5Q2
D	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
D	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
D	-18	SER	-	expression tag	UNP A0A3L7D5Q2
D	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
D	-16	SER	-	expression tag	UNP A0A3L7D5Q2
D	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
D	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
D	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
D	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
D	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
D	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
D	-8	SER	-	expression tag	UNP A0A3L7D5Q2
D	-7	SER	-	expression tag	UNP A0A3L7D5Q2
D	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
D	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
D	0	SER	-	expression tag	UNP A0A3L7D5Q2
D	1	SER	-	expression tag	UNP A0A3L7D5Q2
D	2	GLY	-	expression tag	UNP A0A3L7D5Q2
D	3	SER	-	expression tag	UNP A0A3L7D5Q2
D	4	GLY	-	expression tag	UNP A0A3L7D5Q2



Chain	Residue	Modelled	Actual	Comment	Reference
D	5	GLY	-	expression tag	UNP A0A3L7D5Q2
D	6	GLY	_	expression tag	UNP A0A3L7D5Q2
D	7	GLY	_	expression tag	UNP A0A3L7D5Q2
D	8	GLY	_	expression tag	UNP A0A3L7D5Q2
D	9	GLU	-	expression tag	UNP A0A3L7D5Q2
D	10	ASN	-	expression tag	UNP A0A3L7D5Q2
D	11	LEU	-	expression tag	UNP A0A3L7D5Q2
D	12	TYR	-	expression tag	UNP A0A3L7D5Q2
D	13	PHE	-	expression tag	UNP A0A3L7D5Q2
D	14	GLN	-	expression tag	UNP A0A3L7D5Q2
D	15	GLY	-	expression tag	UNP A0A3L7D5Q2
D	16	THR	_	expression tag	UNP A0A3L7D5Q2
D	332	SER	LEU	conflict	UNP A0A3L7D5Q2
Е	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
Е	-19	ALA	_	expression tag	UNP A0A3L7D5Q2
Е	-18	SER	_	expression tag	UNP A0A3L7D5Q2
Е	-17	TRP	_	expression tag	UNP A0A3L7D5Q2
Е	-16	SER	-	expression tag	UNP A0A3L7D5Q2
Е	-15	HIS	_	expression tag	UNP A0A3L7D5Q2
Е	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
Е	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
Е	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
Е	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
Е	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
Е	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
Е	-8	SER	-	expression tag	UNP A0A3L7D5Q2
Е	-7	SER	-	expression tag	UNP A0A3L7D5Q2
Е	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
Е	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
Е	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
E	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
E	0	SER	-	expression tag	UNP A0A3L7D5Q2
E	1	SER	-	expression tag	UNP A0A3L7D5Q2
E	2	GLY	-	expression tag	UNP A0A3L7D5Q2
E	3	SER	-	expression tag	UNP A0A3L7D5Q2
E	4	GLY	-	expression tag	UNP A0A3L7D5 $\overline{Q2}$
E	5	GLY	-	expression tag	UNP A0A3L $\overline{7D5Q2}$
E	6	GLY	-	expression tag	UNP A0A3L7D5Q2
E	7	GLY	-	expression tag	UNP A0A3L7D5Q2
E	8	GLY	-	expression tag	UNP A0A3L7D5Q2



Chain	Residue	Modelled	Actual	Comment	Reference
Е	9	GLU	-	expression tag	UNP A0A3L7D5Q2
Е	10	ASN	-	expression tag	UNP A0A3L7D5Q2
Е	11	LEU	-	expression tag	UNP A0A3L7D5Q2
Е	12	TYR	-	expression tag	UNP A0A3L7D5Q2
Е	13	PHE	-	expression tag	UNP A0A3L7D5Q2
Е	14	GLN	-	expression tag	UNP A0A3L7D5Q2
Е	15	GLY	-	expression tag	UNP A0A3L7D5Q2
Е	16	THR	_	expression tag	UNP A0A3L7D5Q2
Е	332	SER	LEU	conflict	UNP A0A3L7D5Q2
F	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
F	-19	ALA	_	expression tag	UNP A0A3L7D5Q2
F	-18	SER	-	expression tag	UNP A0A3L7D5Q2
F	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
F	-16	SER	-	expression tag	UNP A0A3L7D5Q2
F	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
F	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
F	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
F	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
F	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
F	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
F	-8	SER	-	expression tag	UNP A0A3L7D5Q2
F	-7	SER	-	expression tag	UNP A0A3L7D5Q2
F	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
F	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
F	0	SER	_	expression tag	UNP A0A3L7D5Q2
F	1	SER	-	expression tag	UNP A0A3L7D5Q2
F	2	GLY	-	expression tag	UNP A0A3L7D5Q2
F	3	SER	-	expression tag	UNP A0A3L7D5Q2
F	4	GLY	-	expression tag	UNP A0A3L7D5Q2
F	5	GLY	-	expression tag	UNP A0A3L7D5Q2
F	6	GLY	-	expression tag	UNP A0A3L7D5 $\overline{Q2}$
F	7	GLY	-	expression tag	UNP A0A3L7D5Q2
F	8	GLY	-	expression tag	UNP A0A3L7D5Q2
F	9	GLU	-	expression tag	UNP A0A3L7D5Q2
F	10	ASN	-	expression tag	UNP A0A3L7D5Q2
F	11	LEU	-	expression tag	UNP A0A3L7D5Q2
F	12	TYR	-	expression tag	UNP A0A3L7D5Q2



Chain	Residue	Modelled	Actual	Comment	Reference
F	13	PHE	_	expression tag	UNP A0A3L7D5Q2
F	14	GLN	_	expression tag	UNP A0A3L7D5Q2
F	15	GLY	-	expression tag	UNP A0A3L7D5Q2
F	16	THR	-	expression tag	UNP A0A3L7D5Q2
F	332	SER	LEU	conflict	UNP A0A3L7D5Q2
G	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
G	-19	ALA	-	expression tag	UNP A0A3L7D5Q2
G	-18	SER	-	expression tag	UNP A0A3L7D5Q2
G	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
G	-16	SER	-	expression tag	UNP A0A3L7D5Q2
G	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
G	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
G	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
G	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
G	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
G	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
G	-8	SER	-	expression tag	UNP A0A3L7D5Q2
G	-7	SER	-	expression tag	UNP A0A3L7D5Q2
G	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
G	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
G	0	SER	-	expression tag	UNP A0A3L7D5Q2
G	1	SER	-	expression tag	UNP A0A3L7D5Q2
G	2	GLY	-	expression tag	UNP A0A3L7D5Q2
G	3	SER	-	expression tag	UNP A0A3L7D5Q2
G	4	GLY	-	expression tag	UNP A0A3L7D5Q2
G	5	GLY	-	expression tag	UNP A0A3L7D5Q2
G	6	GLY	-	expression tag	UNP A0A3L7D5Q2
G	7	GLY	-	expression tag	UNP A0A3L7D5Q2
G	8	GLY	-	expression tag	UNP A0A3L7D5Q2
G	9	GLU	-	expression tag	UNP A0A3L7D5Q2
G	10	ASN	-	expression tag	UNP A0A3L7D5Q2
G	11	LEU	-	expression tag	UNP A0A3L7D5Q2
G	12	TYR	-	expression tag	UNP A0A3L7D5Q2
G	13	PHE	_	expression tag	UNP A0A3L7D5Q2
G	14	GLN	-	expression tag	UNP A0A3L7D5Q2
G	15	GLY	-	expression tag	UNP A0A3L7D5Q2
G	16	THR	-	expression tag	UNP A0A3L7D5Q2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	332	SER	LEU	conflict	UNP A0A3L7D5Q2
Н	-20	MET	-	initiating methionine	UNP A0A3L7D5Q2
Н	-19	ALA	_	expression tag	UNP A0A3L7D5Q2
Н	-18	SER	-	expression tag	UNP A0A3L7D5Q2
Н	-17	TRP	-	expression tag	UNP A0A3L7D5Q2
Н	-16	SER	-	expression tag	UNP A0A3L7D5Q2
Н	-15	HIS	-	expression tag	UNP A0A3L7D5Q2
Н	-14	PRO	-	expression tag	UNP A0A3L7D5Q2
Н	-13	GLN	-	expression tag	UNP A0A3L7D5Q2
Н	-12	PHE	-	expression tag	UNP A0A3L7D5Q2
Н	-11	GLU	-	expression tag	UNP A0A3L7D5Q2
Н	-10	LYS	-	expression tag	UNP A0A3L7D5Q2
Н	-9	GLY	-	expression tag	UNP A0A3L7D5Q2
Н	-8	SER	-	expression tag	UNP A0A3L7D5Q2
Н	-7	SER	-	expression tag	UNP A0A3L7D5Q2
Н	-6	HIS	-	expression tag	UNP A0A3L7D5Q2
Н	-5	HIS	-	expression tag	UNP A0A3L7D5Q2
Н	-4	HIS	-	expression tag	UNP A0A3L7D5Q2
Н	-3	HIS	-	expression tag	UNP A0A3L7D5Q2
Н	-2	HIS	-	expression tag	UNP A0A3L7D5Q2
Н	-1	HIS	-	expression tag	UNP A0A3L7D5Q2
Н	0	SER	-	expression tag	UNP A0A3L7D5Q2
Н	1	SER	-	expression tag	UNP A0A3L7D5Q2
Н	2	GLY	-	expression tag	UNP A0A3L7D5Q2
Н	3	SER	-	expression tag	UNP A0A3L7D5Q2
Н	4	GLY	-	expression tag	UNP A0A3L7D5Q2
Н	5	GLY	-	expression tag	UNP A0A3L7D5Q2
H	6	GLY	-	expression tag	UNP A0A3L7D5Q2
H	7	GLY	-	expression tag	UNP A0A3L7D5Q2
H	8	GLY	-	expression tag	UNP A0A3L7D5Q2
H	9	GLU	-	expression tag	UNP A0A3L7D5Q2
Н	10	ASN	-	expression tag	UNP A0A3L7D5Q2
Н	11	LEU	-	expression tag	UNP A0A3L7D5Q2
Н	12	TYR	-	expression tag	UNP A0A3L7D5 $\overline{Q2}$
Н	13	PHE	-	expression tag	UNP A0A3L7D5 $\overline{Q2}$
Н	14	GLN	-	expression tag	UNP A0A3L7D5Q2
Н	15	GLY	-	expression tag	UNP A0A3L7D5Q2
H	16	THR	-	expression tag	UNP A0A3L7D5Q2
Н	332	SER	LEU	conflict	UNP A0A3L7D5Q2

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total O S	0	0
			5 4 1	-	-
2	В	1	Total O S $5 4 1$	0	0
2	B	1	Total O S	0	0
2	D	I	5 4 1	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	Total O S	0	0
		-			Ű
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	Total O S $5 4 1$	0	0
			$\begin{array}{ccc} 5 & 4 & 1 \\ \hline Total & O & S \end{array}$		
2	С	1	$\begin{bmatrix} 10tar & 0 & 3 \\ 5 & 4 & 1 \end{bmatrix}$	0	0
2	С	1	Total O S	0	0
2	U	I	5 4 1	0	0
2	С	1	Total O S	0	0
		-	5 4 1		0
2	С	1	Total O S	0	0
			$\begin{array}{ccc} 0 & 4 & 1 \\ \hline Total & O & S \end{array}$		
2	\mathbf{C}	1	$\begin{bmatrix} 10ta1 & 0 & 3 \\ 5 & 4 & 1 \end{bmatrix}$	0	0
0	C	1	Total O S	0	0
2	C	1	5 4 1	0	0
2	р	1	Total O S	0	0
		T	5 4 1	0	0
2	D	1	Total O S	0	0
			5 4 1	-	_
2	D	1	$\begin{array}{c ccc} Total & O & S \\ 5 & 4 & 1 \end{array}$	0	0
			Total O S		
2	D	1	$5 \ 4 \ 1$	0	0
2	D	1	Total O S	0	0
		1	5 4 1	0	U
2	D	1	Total O S	0	0
			$\begin{bmatrix} 0 & 4 & 1 \\ T_{a} + a \end{bmatrix}$		
2	D	1	$\begin{bmatrix} 10tal & O & S \\ 5 & 4 & 1 \end{bmatrix}$	0	0
			Total O S		
2	D	1	5 4 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S	0	0
		1	5 4 1	0	0
2	E	1	Total O S	0	0
		1	5 4 1		0
2	Е	1	Total O S	0	0
		_	5 4 1	-	
2	Е	1	Total O S	0	0
			5 4 1		
2	Ε	1	Iotal O S	0	0
			$\begin{array}{ccc} 0 & 4 & 1 \\ \hline \\ Total & O & S \end{array}$		
2	Ε	1	$\begin{array}{ccc} 10tal & O & S \\ 5 & 4 & 1 \end{array}$	0	0
			Total O S		
2	Ε	1	5 4 1	0	0
			Total O S		
2	E	1	5 4 1	0	0
	Б		Total O S	0	0
2	E	1	5 4 1	0	0
0	F	1	Total O S	0	0
	Г	L	$5 \ 4 \ 1$	0	0
2	F	1	Total O S	0	0
	Ľ	1	5 4 1	0	0
2	F	1	Total O S	0	0
	1	1	5 4 1	0	0
2	F	1	Total O S	0	0
	_	_	5 4 1	-	
2	F	1	Total O S	0	0
			5 4 1		
2	F	1	Total O S	0	0
			$\begin{array}{ccc} 0 & 4 & 1 \\ \hline \\ \hline \\ \hline \\ \\ \hline \\ \\ \hline \\ \\ \\ \\ \\ \\ \\$		
2	F	1	$\begin{array}{ccc} 10tal & O & S \\ 5 & 4 & 1 \end{array}$	0	0
			Total O S		
2	G	1	5 4 1	0	0
			Total O S		
2	G	1	5 4 1	0	0
	C		Total O S		0
2	G		5 4 1	0	0
0	C	1	Total O S	0	0
	G		5 4 1	0	U
2	С	1	Total O S	Ο	Ο
	G		5 4 1		U



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	4	Total Na 4 4	0	0
3	В	4	Total Na 4 4	0	0
3	С	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	Е	2	Total Na 2 2	0	0
3	G	1	Total Na 1 1	0	0
3	Н	1	Total Na 1 1	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

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• Molecule 5 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	А	ton	ns		ZeroOcc	AltConf
5	А	1	Total 6	С 3	N 1	O 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 6 & 3 & 1 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{c} \hline 0 & 3 & 1 \\ \hline 1 & 1 \\ \hline 1 & 2 \\ \hline 1 & 1 \\ \hline 1 & 2 \\ \hline 1 &$	0	0
5	D	1	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0	0
5	Е	1	Total C N O 6 3 1 2	0	0
5	F	1	O J I Z Total C N O 6 3 1 2	0	0
5	G	1	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0	0
5	Н	1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0

• Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total C O 13 6 7	0	0
6	Н	1	Total C O 13 6 7	0	0

• Molecule 7 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	337	Total O 342 342	0	5
7	В	342	Total O 347 347	0	5
7	С	302	Total O 307 307	0	5
7	D	225	Total O 228 228	0	3
7	Ε	301	Total O 305 305	0	4
7	F	250	Total O 255 255	0	5
7	G	121	Total O 123 123	0	2
7	Н	203	$\begin{array}{ccc} {\rm Total} & {\rm O} \\ 204 & 204 \end{array}$	0	1



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: S9 family peptidase

1644 R356 E144 W663 R358 E146 M663 R358 E146 L668 P435 CU L435 CU CU L435 AG CU L448 L155 L166 L448 L177 L161 L448 L1233 L177 L448 L1233 L177 L456 L1233 L1233 L603 L504 L1233 L504 L1233 L1233 L504 L1233 L1233 L504 L1233 L1233 L504 L1233 L273 L505 L516 L233 L504 L1233 L233 L505 <thL50</th> <thL335</th> <thL516</th>

• Molecule 1: S9 family peptidase



- Molecule 1: S9 family peptidase











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	194.12Å 75.44Å 219.74Å	Depositor
a, b, c, α , β , γ	90.00° 93.27° 90.00°	Depositor
Bosolution (Å)	48.94 - 2.00	Depositor
Resolution (A)	48.94 - 2.00	EDS
% Data completeness	91.7 (48.94-2.00)	Depositor
(in resolution range)	91.9 (48.94 - 2.00)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.52 (at 2.00 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.212 , 0.256	Depositor
n, n_{free}	0.213 , 0.256	DCC
R_{free} test set	19886 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	29.4	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.36 , 46.5	EDS
L-test for $twinning^2$	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	42813	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 68.23 % 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 4.5178e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: NA, GOL, SO4, FLC

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).

Mal	Chain	Bond	Bond lengths		Bond angles		
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.43	0/5201	0.64	0/7069		
1	В	0.42	0/5197	0.64	0/7062		
1	С	0.43	0/5187	0.64	2/7052~(0.0%)		
1	D	0.42	0/5165	0.62	0/7022		
1	Е	0.42	0/5161	0.63	0/7020		
1	F	0.42	0/5146	0.64	0/6990		
1	G	0.38	0/5037	0.59	0/6862		
1	Н	0.38	0/5118	0.60	0/6963		
All	All	0.41	0/41212	0.62	2/56040~(0.0%)		

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	С	124	ASP	CB-CG-OD1	5.55	123.29	118.30
1	С	25	ARG	CA-CB-CG	-5.41	101.51	113.40

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	А	5067	0	4822	52	0



8	V	V	η	Γ	1	
---	---	---	---	---	---	--

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5063	0	4830	46	0
1	C	5053	0	4803	42	0
1	D	5032	0	4774	48	0
1	Е	5027	0	4752	41	0
1	F	5014	0	4732	50	0
1	G	4904	0	4560	51	0
1	Н	4985	0	4700	40	0
2	А	40	0	0	1	0
2	В	60	0	0	2	0
2	С	35	0	0	3	0
2	D	40	0	0	1	0
2	Е	45	0	0	0	0
2	F	35	0	0	1	0
2	G	25	0	0	1	0
2	Н	45	0	0	2	0
3	А	4	0	0	0	0
3	В	4	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Е	2	0	0	0	0
3	G	1	0	0	0	0
3	Н	1	0	0	0	0
4	А	18	0	23	0	0
4	В	12	0	15	0	0
4	С	24	0	31	3	0
4	D	24	0	32	1	0
4	E	18	0	24	2	0
4	F	30	0	40	8	0
4	G	12	0	16	1	0
4	Н	6	0	8	1	0
5	A	6	0	4	4	0
5	B	6	0	4	8	0
5	C	6	0	4	2	0
5	D	6	0	4	7	0
5	E	6	0	4	4	0
5	F	6	0	4	8	0
5	G	6	0	4	0	0
5	H	6	0	4	0	0
6	A	13	0	5	3	0
6	H	13	0	5	2	0
7	A	342	0	0	1	0
7	В	347	0	0	7	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
7	С	307	0	0	3	0	
7	D	228	0	0	5	0	
7	Ε	305	0	0	4	0	
7	F	255	0	0	7	0	
7	G	123	0	0	4	0	
7	Н	204	0	0	1	0	
All	All	42813	0	38204	370	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 5.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:552:ARG:HH11	5:B:719:ALA:HB2	1.30	0.96
1:D:552:ARG:HH11	5:D:714:ALA:HB2	1.33	0.94
1:F:552:ARG:HH11	5:F:713:ALA:HB2	1.39	0.84
1:H:139:THR:HG23	1:H:141:GLU:H	1.45	0.82
1:C:82:GLU:OE1	1:C:102:ASN:ND2	2.12	0.82
1:G:139:THR:HG23	1:G:141:GLU:H	1.44	0.81
1:H:261:THR:HG23	1:H:262:LYS:HG3	1.63	0.80
1:F:551:GLN:HB3	5:F:713:ALA:HB1	1.65	0.78
1:B:552:ARG:NH1	5:B:719:ALA:HB2	2.00	0.77
1:D:50:ARG:HH11	1:D:69:ARG:HA	1.49	0.76
1:D:656:ARG:HE	5:D:714:ALA:HB3	1.51	0.76
1:F:233:LEU:HB2	1:F:242:THR:HG23	1.68	0.74
1:B:22:ARG:NH1	1:B:40:GLU:OE2	2.19	0.74
1:A:50:ARG:HG3	1:A:69:ARG:HH21	1.52	0.73
1:F:316:PRO:HG3	1:F:361:LEU:HB3	1.70	0.73
1:C:398:ARG:HH22	4:C:711:GOL:H31	1.54	0.73
1:D:551:GLN:HB3	5:D:714:ALA:HB1	1.71	0.72
1:B:402:ALA:O	1:B:406:GLU:HG3	1.90	0.71
1:F:656:ARG:HE	5:F:713:ALA:HB3	1.57	0.70
1:B:551:GLN:HB3	5:B:719:ALA:HB1	1.71	0.69
1:D:284:GLU:HG2	1:D:287:ARG:HB2	1.75	0.69
1:D:82:GLU:HG2	1:D:83:ILE:HG13	1.74	0.68
1:B:138:GLU:O	1:B:197:ARG:NH2	2.23	0.68
1:F:14:GLN:HB3	4:F:710:GOL:H32	1.74	0.68
1:D:316:PRO:HG3	1:D:361:LEU:HB3	1.74	0.68
1:F:599:ARG:HH12	4:F:712:GOL:H32	1.59	0.68
1:G:178:ARG:HD2	1:G:197:ARG:CB	2.24	0.67



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:E:715:ALA:HB2	7:E:844:HOH:O	1.93	0.67	
1:F:552:ARG:NH1	5:F:713:ALA:HB2	2.09	0.67	
1:H:124:ASP:OD1	1:H:126:THR:HG22	1.96	0.66	
1:H:653:ARG:NH1	6:H:713:FLC:OG2	2.23	0.66	
1:D:552:ARG:NH1	5:D:714:ALA:HB2	2.07	0.66	
1:B:656:ARG:HE	5:B:719:ALA:HB3	1.62	0.65	
1:E:656:ARG:HD2	5:E:715:ALA:HA	1.78	0.65	
1:A:248:CYS:SG	1:A:290:LYS:NZ	2.69	0.64	
1:H:614:PRO:HB2	1:H:616:GLU:HG3	1.80	0.64	
1:A:656:ARG:HD2	5:A:716:ALA:HA	1.80	0.64	
1:D:656:ARG:NE	5:D:714:ALA:HB3	2.12	0.64	
1:D:177:LYS:HG3	2:D:706:SO4:O1	1.98	0.63	
1:F:656:ARG:NE	5:F:713:ALA:HB3	2.12	0.63	
1:C:448:HIS:HB3	1:C:455:TYR:CZ	2.32	0.63	
1:A:99:LEU:HD12	1:A:100:PRO:HD2	1.81	0.63	
1:A:131:LEU:HD11	1:A:179:ALA:HB1	1.80	0.63	
1:A:82:GLU:HG2	1:A:83:ILE:HG13	1.80	0.63	
2:B:709:SO4:O3	7:B:801:HOH:O	2.15	0.63	
1:G:178:ARG:HD2	1:G:197:ARG:HB3	1.81	0.62	
1:B:34:THR:O	1:B:58:ALA:HB2	2.00	0.62	
1:F:366:SER:N	7:F:806:HOH:O	2.31	0.62	
1:F:22:ARG:NE	1:F:40:GLU:OE2	2.33	0.62	
1:G:308:ASP:OD2	7:G:801:HOH:O	2.16	0.62	
1:F:448:HIS:HB3	1:F:455:TYR:CZ	2.33	0.62	
1:B:22:ARG:HD3	1:B:40:GLU:OE2	1.99	0.62	
1:F:398:ARG:HH22	4:F:711:GOL:H12	1.65	0.62	
5:A:716:ALA:HB2	7:A:828:HOH:O	2.00	0.61	
1:B:342:VAL:HG22	1:B:348:ILE:HG12	1.82	0.60	
1:E:233:LEU:HB2	1:E:242:THR:HG23	1.84	0.60	
1:A:206:ILE:HD12	1:A:212:THR:O	2.02	0.59	
1:B:442:PRO:HB3	1:B:522:ARG:HB2	1.85	0.59	
1:D:619:GLU:OE2	1:D:636:ARG:NH1	2.28	0.59	
1:B:96:LEU:HD21	1:B:128:LEU:HD22	1.85	0.59	
1:G:614:PRO:HB2	1:G:616:GLU:HG3	1.85	0.58	
1:A:455:TYR:CE2	1:A:475:PHE:HB2	2.39	0.57	
1:C:305:MET:HG3	1:C:306:VAL:N	2.19	0.57	
1:H:16:THR:HG23	4:H:711:GOL:H32	1.86	0.57	
1:B:609:ARG:HD3	1:B:639:ASP:HA	1.86	0.57	
1:E:552:ARG:HH11	5:E:715:ALA:N	2.02	0.57	
1:E:386:VAL:HG22	1:E:393:LYS:HG2	1.86	0.57	
1:B:656:ARG:NE	5:B:719:ALA:HB3	2.20	0.57	



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:173:PHE:HZ	1:F:636:ARG:CZ	2.18	0.57	
1:B:343:SER:HB2	7:B:952:HOH:O	2.04	0.57	
1:G:358:LEU:HD11	1:G:372:ALA:HB1	1.86	0.57	
1:H:653:ARG:HH12	6:H:713:FLC:CGC	2.15	0.56	
1:C:41:LYS:HD3	4:C:709:GOL:H32	1.86	0.56	
1:A:436:ASP:N	1:A:439:GLU:OE2	2.35	0.56	
1:A:653:ARG:HH12	6:A:717:FLC:CAC	2.18	0.56	
1:H:126:THR:HG23	1:H:127:PHE:HD1	1.70	0.56	
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.71	0.56	
1:H:390:ASP:OD1	1:H:391:GLY:N	2.39	0.56	
1:A:50:ARG:HG3	1:A:69:ARG:NH2	2.20	0.56	
4:F:712:GOL:HO3	4:F:712:GOL:HO1	1.52	0.56	
1:D:50:ARG:HH11	1:D:69:ARG:CA	2.17	0.55	
1:F:110:THR:HG22	1:F:184:ILE:HD13	1.88	0.55	
1:F:653:ARG:HH12	4:F:708:GOL:H11	1.72	0.55	
1:A:448:HIS:HB3	1:A:455:TYR:CZ	2.42	0.54	
1:A:305:MET:HG3	1:A:306:VAL:N	2.21	0.54	
1:B:177:LYS:HE2	2:B:703:SO4:O4	2.08	0.54	
1:E:14:GLN:HB3	4:E:712:GOL:H12	1.88	0.54	
1:C:448:HIS:HB3	1:C:455:TYR:CE2	2.43	0.54	
1:D:596:LYS:NZ	7:D:806:HOH:O	2.40	0.53	
1:E:572:LYS:HD3	1:E:577:CYS:HA	1.90	0.53	
1:G:181:LEU:HD12	1:G:195:THR:HG21	1.91	0.53	
1:F:395:ARG:HE	4:F:711:GOL:H32	1.73	0.53	
1:E:242:THR:HG22	7:E:1065:HOH:O	2.09	0.53	
1:A:664:PHE:O	1:A:668:LEU:HB2	2.09	0.52	
1:D:385:ALA:HB3	1:D:394:THR:HG23	1.91	0.52	
1:E:24:VAL:HG12	1:E:40:GLU:HG3	1.90	0.52	
1:A:436:ASP:O	1:A:439:GLU:HG3	2.09	0.52	
1:H:547:ALA:HB2	1:H:667:TYR:HB2	1.91	0.52	
1:B:239:LYS:O	1:B:239:LYS:HG2	2.10	0.52	
1:G:131:LEU:HD21	1:G:179:ALA:HB1	1.91	0.52	
1:E:50:ARG:HD2	1:E:69:ARG:HA	1.90	0.52	
1:F:447:ILE:HD13	1:F:534:MET:HG3	1.92	0.52	
1:G:56:TRP:NE1	1:G:396:LEU:HD22	2.25	0.52	
1:D:452:HIS:NE2	1:D:574:GLU:OE2	2.32	0.51	
1:C:25:ARG:HD3	2:C:701:SO4:O2	2.10	0.51	
1:D:450:GLY:O	4:D:712:GOL:H31	2.09	0.51	
1:E:547:ALA:HB2	1:E:667:TYR:HB2	1.91	0.51	
1:A:122:SER:HB2	1:A:127:PHE:CZ	2.46	0.51	
1:C:395:ARG:HE	4:C:711:GOL:H2	1.75	0.51	



	lo uo puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:56:TRP:NE1	1:A:396:LEU:HD22	2.26	0.51	
1:D:127:PHE:CD2	1:D:183:ARG:HG3	2.46	0.51	
1:F:233:LEU:HB2	1:F:242:THR:CG2	2.38	0.51	
1:A:552:ARG:HH11	5:A:716:ALA:N	2.09	0.51	
1:H:65:TRP:HE3	1:H:99:LEU:HD21	1.76	0.51	
1:D:593:LYS:HD3	1:D:594:TYR:CZ	2.45	0.51	
1:F:614:PRO:HB2	1:F:616:GLU:HG3	1.93	0.50	
1:F:82:GLU:HG2	1:F:83:ILE:HG13	1.93	0.50	
1:F:127:PHE:CD2	1:F:183:ARG:HG3	2.46	0.50	
1:F:572:LYS:NZ	7:F:807:HOH:O	2.44	0.50	
1:A:455:TYR:CD2	1:A:475:PHE:HB2	2.46	0.50	
1:D:55:ILE:HG13	1:D:65:TRP:CE2	2.46	0.50	
1:E:15:GLY:H	4:E:712:GOL:H2	1.76	0.50	
1:G:75:PRO:HA	1:G:85:ALA:O	2.11	0.50	
1:E:455:TYR:CE2	1:E:475:PHE:HB2	2.47	0.50	
1:C:539:VAL:HG23	1:C:598:MET:HG2	1.93	0.49	
1:F:579:VAL:HG23	7:F:948:HOH:O	2.12	0.49	
1:F:656:ARG:HE	5:F:713:ALA:CB	2.23	0.49	
1:F:117:ARG:NH1	1:F:201:ILE:O	2.44	0.49	
1:G:604:ILE:HD12	1:G:622:PHE:HB2	1.95	0.49	
1:A:463:LEU:HD22	1:A:473:VAL:HG11	1.94	0.49	
1:A:113:LYS:HA	1:A:144:GLU:HA	1.94	0.49	
1:B:634:LEU:HB3	1:C:161:VAL:HB	1.95	0.49	
1:G:127:PHE:CD1	1:G:183:ARG:HG3	2.48	0.49	
1:D:402:ALA:O	1:D:406:GLU:HG3	2.13	0.49	
1:D:579:VAL:HG22	1:D:586:LEU:HD12	1.95	0.48	
1:E:440:LYS:HB3	1:E:519:ASP:HB2	1.93	0.48	
1:G:432:PRO:HG2	1:G:435:LEU:HD22	1.95	0.48	
1:H:658:ARG:HG2	1:H:658:ARG:HH11	1.78	0.48	
1:C:245:THR:HG21	1:C:251:PHE:CE2	2.47	0.48	
1:D:455:TYR:CE2	1:D:475:PHE:HB2	2.49	0.48	
1:B:41:LYS:NZ	1:B:312:ASP:OD2	2.47	0.48	
1:C:209:ASN:ND2	1:C:211:ARG:HD3	2.27	0.48	
1:E:131:LEU:HD11	1:E:179:ALA:HB1	1.94	0.48	
1:G:99:LEU:HD12	1:G:100:PRO:HD2	1.94	0.48	
1:F:599:ARG:NH1	4:F:712:GOL:H32	2.27	0.48	
1:E:368:GLN:NE2	7:E:815:HOH:O	2.47	0.48	
1:C:44:ASP:HB3	1:C:50:ARG:HD2	1.95	0.47	
1:E:78:SER:HB3	1:E:121:TRP:CZ2	2.49	0.47	
1:B:364:HIS:CE1	1:B:367:GLU:HG3	2.49	0.47	
5:D:714:ALA:N	7:D:811:HOH:O	2.47	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:448:HIS:HB3	1:D:455:TYR:CZ	2.49	0.47	
1:G:181:LEU:HB2	1:G:195:THR:HG23	1.96	0.47	
1:H:177:LYS:HE2	2:H:707:SO4:O3	2.13	0.47	
1:D:96:LEU:HD21	1:D:128:LEU:HD22	1.96	0.47	
1:F:616:GLU:O	1:F:620:GLN:HG3	2.14	0.47	
1:A:309:THR:HA	6:A:717:FLC:HA2	1.96	0.47	
1:C:318:PRO:HB2	1:C:327:LEU:HD22	1.95	0.47	
1:C:614:PRO:HB2	1:C:616:GLU:HG3	1.97	0.47	
1:D:126:THR:O	1:D:186:VAL:HG22	2.14	0.47	
1:E:603:LEU:HD22	1:E:663:TRP:HB2	1.97	0.47	
1:G:455:TYR:CD2	1:G:475:PHE:HB2	2.50	0.47	
1:B:552:ARG:HH11	5:B:719:ALA:CB	2.14	0.47	
1:D:123:PRO:HD2	7:D:999:HOH:O	2.14	0.47	
2:F:706:SO4:O4	4:F:708:GOL:O3	2.24	0.47	
1:C:127:PHE:CD2	1:C:183:ARG:HG3	2.49	0.47	
1:G:18:LEU:HA	1:G:21:LEU:HG	1.96	0.47	
1:A:351:VAL:HG12	1:A:352:ILE:HG13	1.97	0.46	
1:G:358:LEU:CD1	1:G:372:ALA:HB1	2.44	0.46	
1:H:61:SER:HB2	1:H:63:ARG:HE	1.81	0.46	
1:B:666:ARG:HD2	1:B:666:ARG:O	2.14	0.46	
1:C:570:PHE:CZ	1:C:574:GLU:HG3	2.50	0.46	
1:H:68:GLY:HA3	1:H:70:TRP:CH2	2.50	0.46	
1:A:198:GLU:HG3	1:A:201:ILE:HD11	1.98	0.46	
1:D:542:THR:OG1	1:D:544:ARG:HG3	2.15	0.46	
1:F:18:LEU:HB3	1:F:461:HIS:CE1	2.51	0.46	
1:G:88:SER:OG	1:G:90:ARG:HG2	2.15	0.46	
1:D:119:TYR:HA	1:D:129:ILE:O	2.16	0.46	
1:F:552:ARG:HD3	5:F:713:ALA:HA	1.97	0.46	
1:A:135:GLY:N	1:A:177:LYS:HG2	2.30	0.46	
1:B:430:MET:HB2	1:B:473:VAL:HB	1.97	0.46	
1:C:336:ARG:HD3	1:C:355:ASN:OD1	2.15	0.46	
1:D:385:ALA:HB3	1:D:394:THR:CG2	2.46	0.46	
1:E:448:HIS:HB3	1:E:455:TYR:CZ	2.50	0.46	
1:G:455:TYR:CE2	1:G:475:PHE:HB2	2.51	0.46	
1:A:614:PRO:HB2	1:A:616:GLU:HG3	1.97	0.46	
1:C:554:ILE:HD13	1:C:557:TRP:CH2	2.51	0.46	
1:B:455:TYR:CE2	1:B:475:PHE:HB2	2.51	0.45	
1:D:656:ARG:HE	5:D:714:ALA:CB	2.24	0.45	
1:G:283:PHE:CD2	1:G:290:LYS:HB3	2.51	0.45	
1:G:547:ALA:HB2	1:G:667:TYR:HB2	1.98	0.45	
1:H:609:ARG:HD2	7:H:987:HOH:O	2.16	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:131:LEU:HD11	1:C:179:ALA:HB1	1.97	0.45	
1:E:96:LEU:HD21	1:E:128:LEU:HD22	1.96	0.45	
1:F:619:GLU:OE2	1:F:636:ARG:NH1	2.39	0.45	
1:H:75:PRO:HA	1:H:85:ALA:O	2.16	0.45	
1:C:273:LEU:HD13	1:C:573:TRP:CD1	2.52	0.45	
1:D:664:PHE:O	1:D:668:LEU:HB2	2.17	0.45	
1:G:449:GLY:HA2	1:G:530:TYR:HB3	1.98	0.45	
1:A:25:ARG:HD3	2:A:701:SO4:O2	2.17	0.45	
1:A:213:LEU:HB2	1:A:236:LEU:HD11	1.98	0.45	
1:F:547:ALA:HB2	1:F:667:TYR:HB2	1.97	0.45	
1:G:179:ALA:HB3	1:G:201:ILE:HG13	1.99	0.45	
1:A:126:THR:O	1:A:186:VAL:HG22	2.17	0.45	
1:C:293:LEU:HD11	1:C:344:LEU:HD23	1.98	0.45	
1:D:558:LEU:HD23	1:D:579:VAL:HG13	1.98	0.45	
1:G:236:LEU:HD23	1:G:236:LEU:HA	1.80	0.45	
1:H:358:LEU:HD11	1:H:372:ALA:HB1	1.99	0.45	
1:A:418:ARG:HG2	1:A:422:GLY:O	2.16	0.45	
1:B:603:LEU:HB2	1:B:663:TRP:CD2	2.51	0.45	
1:D:178:ARG:HD2	1:D:197:ARG:HB3	1.98	0.45	
1:G:178:ARG:HD2	1:G:197:ARG:HB2	1.98	0.45	
1:B:552:ARG:HD3	5:B:719:ALA:HA	1.99	0.45	
1:B:558:LEU:HD12	1:B:558:LEU:H	1.81	0.45	
1:C:350:PRO:HG3	1:F:353:GLU:OE1	2.16	0.45	
1:D:572:LYS:HD2	1:D:577:CYS:HA	1.99	0.45	
1:H:455:TYR:CE2	1:H:475:PHE:HB2	2.51	0.45	
1:B:354:GLY:HA3	1:B:356:PHE:CE2	2.52	0.45	
1:C:479:ARG:HA	1:C:488:PHE:CE2	2.52	0.45	
1:A:570:PHE:CE2	1:A:574:GLU:HG3	2.51	0.44	
1:G:603:LEU:HB2	1:G:663:TRP:CD2	2.52	0.44	
1:C:616:GLU:O	1:C:620:GLN:HG3	2.16	0.44	
1:A:644:LEU:HD12	1:A:648:GLY:HA3	1.98	0.44	
1:B:626:LYS:NZ	7:B:808:HOH:O	2.36	0.44	
1:G:73:MET:HE2	1:G:73:MET:HB3	1.91	0.44	
1:C:113:LYS:HA	1:C:144:GLU:HA	1.99	0.44	
1:D:219:ARG:NH2	1:D:241:GLU:OE1	2.50	0.44	
1:F:522:ARG:HD2	1:F:668:LEU:O	2.16	0.44	
1:C:177:LYS:HE2	2:C:707:SO4:O1	2.18	0.44	
1:F:97:TRP:CH2	1:F:108:GLN:HB2	2.52	0.44	
1:H:626:LYS:HA	1:H:626:LYS:HD2	1.83	0.44	
1:D:96:LEU:HB3	1:D:110:THR:HG23	1.98	0.44	
1:A:619:GLU:OE2	1:A:636:ARG:NH1	2.40	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:364:HIS:ND1	1:E:365:PRO:HD2	2.33	0.44	
1:G:431:LYS:O	1:G:433:PRO:HD3	2.18	0.44	
1:D:537:TRP:CE2	1:D:541:HIS:CE1	3.06	0.44	
1:E:34:THR:O	1:E:58:ALA:HB2	2.18	0.44	
1:E:55:ILE:HG13	1:E:65:TRP:CE2	2.53	0.44	
1:B:318:PRO:HB3	1:B:329:VAL:HG12	2.00	0.43	
1:F:318:PRO:HB2	1:F:327:LEU:HD22	1.99	0.43	
1:C:111:PHE:O	1:C:143:ARG:HA	2.18	0.43	
1:F:22:ARG:HD3	7:F:1026:HOH:O	2.19	0.43	
1:G:96:LEU:HD23	1:G:109:LEU:HD23	2.00	0.43	
1:F:97:TRP:CZ2	1:F:108:GLN:HB2	2.53	0.43	
1:G:461:HIS:HD2	7:G:801:HOH:O	2.01	0.43	
1:H:78:SER:HB3	1:H:121:TRP:CZ2	2.54	0.43	
1:E:78:SER:HB3	1:E:121:TRP:CH2	2.54	0.43	
1:F:448:HIS:HB3	1:F:455:TYR:CE2	2.52	0.43	
1:B:455:TYR:CD2	1:B:475:PHE:HB2	2.54	0.43	
1:B:448:HIS:HB3	1:B:455:TYR:CZ	2.53	0.43	
1:H:156:LEU:HA	1:H:156:LEU:HD23	1.73	0.43	
1:B:213:LEU:HB2	1:B:236:LEU:HD11	2.00	0.43	
1:B:616:GLU:O	1:B:620:GLN:HG3	2.17	0.43	
1:C:442:PRO:HB2	1:C:668:LEU:HD13	2.00	0.43	
1:A:620:GLN:HA	1:H:562:GLY:HA3	2.01	0.43	
1:D:370:ALA:HB2	1:D:388:LEU:HD21	2.01	0.43	
1:C:442:PRO:HB3	1:C:522:ARG:HB3	2.01	0.43	
1:E:99:LEU:HD12	1:E:100:PRO:HD2	2.01	0.43	
1:E:448:HIS:HB3	1:E:455:TYR:CE2	2.54	0.43	
1:B:656:ARG:HE	5:B:719:ALA:CB	2.31	0.42	
1:H:181:LEU:HG	1:H:201:ILE:HD13	2.00	0.42	
1:H:398:ARG:NH2	2:H:708:SO4:O3	2.51	0.42	
1:A:56:TRP:HE1	1:A:396:LEU:HD22	1.84	0.42	
1:A:320:TRP:CE2	1:A:327:LEU:HD21	2.54	0.42	
1:F:509:ASP:OD2	1:F:544:ARG:NH2	2.53	0.42	
1:G:509:ASP:OD1	1:G:544:ARG:NH1	2.51	0.42	
1:B:131:LEU:HD11	1:B:179:ALA:HB1	2.01	0.42	
1:F:178:ARG:HD2	7:F:1022:HOH:O	2.18	0.42	
1:F:603:LEU:HB2	1:F:663:TRP:CD2	2.54	0.42	
1:H:390:ASP:OD1	1:H:392:THR:HG23	2.20	0.42	
1:H:390:ASP:CG	1:H:392:THR:HG23	2.39	0.42	
1:H:658:ARG:HG2	1:H:658:ARG:NH1	2.34	0.42	
1:A:122:SER:HB3	1:A:127:PHE:O	2.19	0.42	
1:A:549:VAL:HG11	1:A:660:ILE:HG12	2.02	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:388:LEU:O	7:B:802:HOH:O	2.22	0.42	
1:C:603:LEU:HB2	1:C:663:TRP:CD2	2.55	0.42	
1:H:218:ASN:OD1	1:H:220:ASN:ND2	2.52	0.42	
1:A:552:ARG:HD3	5:A:716:ALA:HB3	2.01	0.42	
1:C:157:LYS:N	7:C:803:HOH:O	2.35	0.42	
1:C:273:LEU:HD13	1:C:573:TRP:CG	2.55	0.42	
1:D:50:ARG:HD3	1:D:69:ARG:HA	2.02	0.42	
1:D:515:PHE:HB3	1:D:517:PHE:CE2	2.54	0.42	
1:E:596:LYS:HB2	7:E:905:HOH:O	2.19	0.42	
1:F:528:GLY:HA2	1:F:551:GLN:O	2.19	0.42	
1:G:233:LEU:HG	1:G:244:LEU:HD23	2.01	0.42	
1:A:427:GLY:HA2	1:A:476:THR:HA	2.01	0.42	
1:C:155:ASP:HB3	7:C:1044:HOH:O	2.19	0.42	
1:A:68:GLY:HA3	1:A:70:TRP:CH2	2.55	0.42	
1:D:656:ARG:HD3	7:D:891:HOH:O	2.18	0.42	
1:E:552:ARG:HD3	5:E:715:ALA:CB	2.49	0.42	
1:F:516:ASP:OD1	7:F:801:HOH:O	2.21	0.42	
1:G:528:GLY:HA2	1:G:551:GLN:O	2.19	0.42	
1:G:616:GLU:O	1:G:620:GLN:HG3	2.20	0.42	
1:H:245:THR:HG21	1:H:251:PHE:CE2	2.54	0.42	
1:A:626:LYS:HA	1:A:626:LYS:HD2	1.87	0.42	
1:B:609:ARG:NE	7:B:823:HOH:O	2.51	0.42	
1:D:603:LEU:HD21	1:D:605:LEU:HD21	2.02	0.42	
1:H:29:TYR:CZ	1:H:371:ILE:HG13	2.55	0.42	
1:A:638:PRO:HD3	1:H:158:PRO:HA	2.02	0.42	
1:D:190:LYS:HB3	1:D:190:LYS:HE2	1.75	0.42	
1:G:25:ARG:HD3	2:G:704:SO4:O2	2.19	0.42	
1:B:546:LYS:NZ	7:B:818:HOH:O	2.47	0.41	
1:C:25:ARG:HG3	1:C:39:VAL:HB	2.01	0.41	
1:F:514:LYS:HG2	1:F:515:PHE:CZ	2.55	0.41	
1:G:386:VAL:HA	1:G:392:THR:O	2.19	0.41	
1:G:596:LYS:HB2	7:G:828:HOH:O	2.19	0.41	
1:G:644:LEU:HD12	1:G:648:GLY:HA3	2.02	0.41	
1:H:145:GLU:HA	1:H:146:PRO:HD3	1.91	0.41	
1:A:570:PHE:CZ	1:A:574:GLU:HG3	2.55	0.41	
1:C:644:LEU:HD23	5:C:713:ALA:HB3	2.02	0.41	
1:D:554:ILE:HD13	1:D:557:TRP:CH2	2.55	0.41	
1:G:331:ALA:O	1:G:337:VAL:HA	2.21	0.41	
1:E:577:CYS:SG	1:E:582:ASP:HB3	2.61	0.41	
1:G:183:ARG:HB2	1:G:194:LEU:HD21	2.02	0.41	
1:B:333:GLU:HG2	7:B:1087:HOH:O	2.19	0.41	



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:364:HIS:ND1	1:B:365:PRO:HD2	2.36	0.41
1:H:358:LEU:CD1	1:H:372:ALA:HB1	2.49	0.41
1:B:551:GLN:O	1:B:552:ARG:C	2.58	0.41
5:C:713:ALA:HB1	7:C:930:HOH:O	2.21	0.41
1:E:98:LEU:HD11	1:E:109:LEU:HD22	2.03	0.41
1:E:554:ILE:HD13	1:E:557:TRP:CH2	2.56	0.41
1:C:177:LYS:HB2	2:C:707:SO4:O1	2.20	0.41
1:E:58:ALA:C	1:E:60:GLY:H	2.22	0.41
1:E:454:MET:HG2	1:E:455:TYR:O	2.21	0.41
1:F:28:HIS:HB3	7:F:923:HOH:O	2.20	0.41
1:H:198:GLU:OE2	1:H:219:ARG:NH2	2.53	0.41
1:A:646:ARG:O	6:A:717:FLC:HA1	2.21	0.41
1:D:620:GLN:HA	1:G:562:GLY:HA3	2.01	0.41
1:E:455:TYR:CD2	1:E:475:PHE:HB2	2.55	0.41
1:E:585:ARG:O	1:E:589:HIS:HD2	2.03	0.41
1:G:279:ARG:NH1	1:G:297:TRP:O	2.53	0.41
1:A:603:LEU:HB2	1:A:663:TRP:CD2	2.56	0.41
1:D:577:CYS:SG	1:D:582:ASP:HB3	2.61	0.41
1:F:656:ARG:CD	5:F:713:ALA:HB3	2.50	0.41
1:H:354:GLY:HA3	1:H:356:PHE:CE2	2.56	0.41
1:C:528:GLY:HA2	1:C:551:GLN:O	2.20	0.41
1:D:532:GLY:HA3	1:D:553:SER:HB3	2.03	0.41
1:E:320:TRP:CE2	1:E:327:LEU:HD21	2.56	0.41
1:H:328:TYR:HB3	1:H:339:LEU:HD11	2.03	0.41
1:H:411:ASP:OD1	1:H:412:ALA:N	2.50	0.41
1:B:533:PHE:HB2	1:B:554:ILE:HB	2.01	0.41
1:C:352:ILE:CG1	1:C:386:VAL:HG11	2.51	0.41
1:G:59:ASP:OD1	1:G:59:ASP:C	2.59	0.41
1:A:119:TYR:HA	1:A:129:ILE:O	2.22	0.40
1:B:657:LEU:HD23	1:B:657:LEU:HA	1.91	0.40
1:E:64:GLN:NE2	1:E:66:THR:O	2.48	0.40
1:G:103:GLY:HA2	7:G:820:HOH:O	2.21	0.40
1:G:359:TYR:CZ	1:G:373:ALA:HB1	2.56	0.40
1:G:499:MET:HE1	1:G:502:GLU:HB2	2.03	0.40
1:A:308:ASP:HA	1:A:646:ARG:HG2	2.04	0.40
1:C:596:LYS:HB2	1:C:596:LYS:HE2	1.88	0.40
1:G:273:LEU:HD13	1:G:573:TRP:CD1	2.56	0.40
1:H:139:THR:HG23	1:H:141:GLU:N	2.25	0.40
1:A:11:LEU:O	1:A:408:VAL:HG23	2.21	0.40
1:A:93:ARG:HH11	1:A:93:ARG:CG	2.35	0.40
1:C:233:LEU:O	1:C:241:GLU:HA	2.20	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:493:ARG:HD2	1:F:573:TRP:O	2.21	0.40
1:G:25:ARG:NH2	4:G:707:GOL:H32	2.35	0.40
1:G:134:LEU:HD11	1:G:140:ILE:HG22	2.02	0.40
1:A:385:ALA:O	1:A:393:LYS:HA	2.21	0.40
1:B:119:TYR:HA	1:B:129:ILE:O	2.21	0.40
1:B:554:ILE:HD13	1:B:557:TRP:CH2	2.56	0.40
1:C:504:ILE:O	1:C:508:VAL:HG23	2.21	0.40
1:E:528:GLY:HA2	1:E:551:GLN:O	2.21	0.40
1:H:278:HIS:CG	1:H:300:HIS:HE1	2.39	0.40
1:D:112:PHE:HB3	7:D:867:HOH:O	2.22	0.40
1:E:442:PRO:HB3	1:E:522:ARG:HB3	2.03	0.40
1:E:614:PRO:HB2	1:E:616:GLU:HG3	2.02	0.40
1:E:634:LEU:HB3	1:F:161:VAL:HB	2.03	0.40
1:F:514:LYS:HG2	1:F:515:PHE:CE1	2.57	0.40
1:G:283:PHE:CE2	1:G:290:LYS:HD3	2.56	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	Perce	ntiles
1	А	646/691~(94%)	623~(96%)	23~(4%)	0	100	100
1	В	646/691~(94%)	631~(98%)	15 (2%)	0	100	100
1	С	647/691~(94%)	631~(98%)	16 (2%)	0	100	100
1	D	643/691~(93%)	623~(97%)	20 (3%)	0	100	100
1	Е	646/691~(94%)	631~(98%)	15 (2%)	0	100	100
1	F	643/691~(93%)	627~(98%)	16 (2%)	0	100	100
1	G	641/691~(93%)	621 (97%)	20 (3%)	0	100	100
1	Н	645/691~(93%)	620 (96%)	25 (4%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percent	tiles
All	All	5157/5528~(93%)	5007~(97%)	150 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	509/568~(90%)	500~(98%)	9(2%)	59	63
1	В	509/568~(90%)	504 (99%)	5 (1%)	76	81
1	С	507/568~(89%)	499~(98%)	8 (2%)	62	67
1	D	504/568~(89%)	494 (98%)	10 (2%)	55	58
1	Ε	505/568~(89%)	494 (98%)	11 (2%)	52	55
1	F	496/568~(87%)	487 (98%)	9(2%)	59	63
1	G	469/568~(83%)	458 (98%)	11 (2%)	50	53
1	Н	486/568~(86%)	475 (98%)	11 (2%)	50	53
All	All	3985/4544 (88%)	3911 (98%)	74 (2%)	57	61

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	23	SER
1	А	73	MET
1	А	118	ASP
1	А	122	SER
1	А	327	LEU
1	А	460	PHE
1	А	529	SER
1	А	533	PHE
1	А	561	SER
1	В	117	ARG
1	В	343	SER
1	В	387	SER


Mol	Chain	Res	Type
1	В	434	GLU
1	В	460	PHE
1	С	13	PHE
1	С	178	ARG
1	С	279	ARG
1	С	327	LEU
1	С	432	PRO
1	С	460	PHE
1	С	468	SER
1	С	599	ARG
1	D	13	PHE
1	D	73	MET
1	D	93	ARG
1	D	122	SER
1	D	137	ASP
1	D	186	VAL
1	D	387	SER
1	D	460	PHE
1	D	468	SER
1	D	606	HIS
1	Е	13	PHE
1	Е	25	ARG
1	E	62	VAL
1	E	93	ARG
1	E	186	VAL
1	E	236	LEU
1	E	242	THR
1	E	460	PHE
1	E	513	SER
1	E	572	LYS
1	E	626	LYS
1	F	11	LEU
1	F	13	PHE
1	F	48	GLN
1	F	118	ASP
1	F'	322	SER
1	F	343	SER
1	F	434	GLU
1	F	460	PHE
1	F	468	SER
1	G	13	PHE
1	G	23	SER



Mol	Chain	Res	Type
1	G	35	ARG
1	G	59	ASP
1	G	73	MET
1	G	118	ASP
1	G	289	THR
1	G	327	LEU
1	G	363	ILE
1	G	398	ARG
1	G	460	PHE
1	Н	23	SER
1	Н	25	ARG
1	Н	50	ARG
1	Н	107	ARG
1	Н	122	SER
1	Н	171	SER
1	Н	278	HIS
1	Н	398	ARG
1	Н	460	PHE
1	Н	529	SER
1	Н	579	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	368	GLN
1	В	28	HIS
1	Е	14	GLN
1	Е	48	GLN
1	G	28	HIS
1	Н	278	HIS
1	Н	300	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 113 ligands modelled in this entry, 14 are monoatomic - leaving 99 for Mogul analysis.

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).

Mal	Twpe Chain Pe		Dec	Ros Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	SO4	G	703	-	4,4,4	0.15	0	$6,\!6,\!6$	0.19	0	
2	SO4	В	706	-	4,4,4	0.16	0	$6,\!6,\!6$	0.21	0	
4	GOL	С	709	-	$5,\!5,\!5$	0.91	0	$5,\!5,\!5$	0.81	0	
4	GOL	F	712	-	$5,\!5,\!5$	1.09	0	$5,\!5,\!5$	0.83	0	
4	GOL	В	718	-	$5,\!5,\!5$	1.02	0	$5,\!5,\!5$	1.08	0	
2	SO4	Н	709	-	4,4,4	0.22	0	$6,\!6,\!6$	0.14	0	
5	ALA	G	709	-	$5,\!5,\!5$	1.10	1 (20%)	$6,\!6,\!6$	1.65	2 (33%)	
2	SO4	G	704	-	4,4,4	0.13	0	6,6,6	0.21	0	
2	SO4	А	702	3	4,4,4	0.14	0	$6,\!6,\!6$	0.49	0	
4	GOL	G	707	-	$5,\!5,\!5$	0.59	0	$5,\!5,\!5$	1.42	1 (20%)	
5	ALA	Е	715	-	$5,\!5,\!5$	1.73	1 (20%)	$6,\!6,\!6$	1.07	1 (16%)	
2	SO4	С	707	-	4,4,4	0.14	0	$6,\!6,\!6$	0.28	0	
6	FLC	А	717	-	12,12,12	2.06	5 (41%)	17,17,17	2.52	7 (41%)	
2	SO4	Н	707	-	4,4,4	0.19	0	$6,\!6,\!6$	0.14	0	
4	GOL	D	710	-	$5,\!5,\!5$	0.97	0	$5,\!5,\!5$	1.15	1 (20%)	
2	SO4	G	701	-	4,4,4	0.15	0	$6,\!6,\!6$	0.50	0	
2	SO4	А	708	-	4,4,4	0.11	0	$6,\!6,\!6$	0.27	0	
2	SO4	С	701	-	4,4,4	0.13	0	$6,\!6,\!6$	0.19	0	
2	SO4	G	702	-	4,4,4	0.18	0	$6,\!6,\!6$	0.17	0	
2	SO4	А	706	-	4,4,4	0.15	0	$6,\!6,\!6$	0.36	0	
4	GOL	Ε	713	-	$5,\!5,\!5$	0.63	0	$5,\!5,\!5$	1.10	0	
2	SO4	С	706	-	$4,\!4,\!4$	0.16	0	$6,\!6,\!6$	0.23	0	
2	SO4	В	710	-	4,4,4	0.18	0	$6,\!6,\!6$	0.21	0	
2	SO4	С	705	-	4,4,4	0.15	0	6,6,6	0.09	0	
4	GOL	С	710		5,5,5	1.28	1 (20%)	$5,\!5,\!5$	1.10	0	
2	SO4	D	707	-	4,4,4	0.28	0	$6,\!6,\!6$	0.28	0	



	T	Chain	Dag	T : 1-	Bo	ond leng	ths	Bond angles			
IVIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	SO4	Н	708	-	4,4,4	0.11	0	$6,\!6,\!6$	0.18	0	
2	SO4	D	701	-	$4,\!4,\!4$	0.22	0	$6,\!6,\!6$	0.21	0	
2	SO4	В	711	-	4,4,4	0.17	0	$6,\!6,\!6$	0.14	0	
2	SO4	Н	704	-	4,4,4	0.14	0	$6,\!6,\!6$	0.15	0	
4	GOL	E	712	-	$5,\!5,\!5$	0.82	0	$5,\!5,\!5$	1.21	0	
2	SO4	E	709	-	4,4,4	0.28	0	$6,\!6,\!6$	0.30	0	
5	ALA	А	716	3	$5,\!5,\!5$	1.94	2 (40%)	$6,\!6,\!6$	1.60	1 (16%)	
2	SO4	Е	707	-	$4,\!4,\!4$	0.13	0	$6,\!6,\!6$	0.28	0	
2	SO4	Е	702	-	$4,\!4,\!4$	0.15	0	$6,\!6,\!6$	0.32	0	
2	SO4	А	704	-	4,4,4	0.20	0	$6,\!6,\!6$	0.27	0	
2	SO4	F	704	-	$4,\!4,\!4$	0.16	0	$6,\!6,\!6$	0.27	0	
5	ALA	В	719	-	$5,\!5,\!5$	1.53	2 (40%)	$6,\!6,\!6$	1.64	2 (33%)	
2	SO4	Н	703	-	4,4,4	0.15	0	$6,\!6,\!6$	0.21	0	
2	SO4	D	705	-	$4,\!4,\!4$	0.27	0	$6,\!6,\!6$	0.24	0	
2	SO4	Ε	703	-	4,4,4	0.17	0	$6,\!6,\!6$	0.27	0	
2	SO4	Н	702	-	4,4,4	0.18	0	$6,\!6,\!6$	0.31	0	
2	SO4	В	704	-	4,4,4	0.23	0	$6,\!6,\!6$	0.14	0	
2	SO4	В	702	-	4,4,4	0.14	0	$6,\!6,\!6$	0.28	0	
2	SO4	F	702	-	$4,\!4,\!4$	0.11	0	$6,\!6,\!6$	0.46	0	
2	SO4	Ε	708	-	$4,\!4,\!4$	0.13	0	$6,\!6,\!6$	0.57	0	
4	GOL	F	711	-	$5,\!5,\!5$	0.81	0	$5,\!5,\!5$	1.08	0	
2	SO4	В	712	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.12	0	
2	SO4	В	709	3	4,4,4	0.13	0	$6,\!6,\!6$	0.29	0	
2	SO4	В	708	-	4,4,4	0.16	0	$6,\!6,\!6$	0.07	0	
4	GOL	G	708	-	$5,\!5,\!5$	0.82	0	$5,\!5,\!5$	1.13	0	
5	ALA	С	713	-	$5,\!5,\!5$	1.39	1 (20%)	$6,\!6,\!6$	1.55	2 (33%)	
2	SO4	В	703	-	4,4,4	0.18	0	$6,\!6,\!6$	0.31	0	
2	SO4	D	702	-	4,4,4	0.13	0	$6,\!6,\!6$	0.30	0	
4	GOL	Е	714	-	$5,\!5,\!5$	0.75	0	$5,\!5,\!5$	0.98	0	
4	GOL	F	709	-	$5,\!5,\!5$	0.96	0	$5,\!5,\!5$	0.97	0	
2	SO4	Е	704	-	$4,\!4,\!4$	0.23	0	$6,\!6,\!6$	0.35	0	
2	SO4	G	705	-	4,4,4	0.17	0	$6,\!6,\!6$	0.21	0	
5	ALA	F	713	-	$5,\!5,\!5$	1.68	2 (40%)	$6,\!6,\!6$	1.48	2 (33%)	
2	SO4	D	708	-	4,4,4	0.13	0	$6,\!6,\!6$	0.20	0	
6	FLC	Н	713	-	12,12,12	1.95	6 (50%)	17,17,17	2.36	6 (35%)	
4	GOL	D	713	-	$5,\!5,\!5$	0.96	0	$5,\!5,\!5$	0.93	0	
2	SO4	F	705	_	4,4,4	0.19	0	$6,\!6,\!6$	0.22	0	
4	GOL	В	717	_	5, 5, 5	1.21	1 (20%)	$5,\!5,\!5$	1.13	1 (20%)	
2	SO4	Н	701	-	4,4,4	0.14	0	6,6,6	0.31	0	
2	SO4	С	704	-	4,4,4	0.12	0	$6,\!6,\!6$	0.18	0	
2	SO4	F	707	-	4,4,4	0.20	0	$6,\!6,\!6$	0.13	0	
2	SO4	D	704	-	4,4,4	0.19	0	6,6,6	0.19	0	



Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	Bond angles			
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	SO4	Е	706	-	4,4,4	0.16	0	$6,\!6,\!6$	0.10	0	
2	SO4	Н	705	-	4,4,4	0.31	0	$6,\!6,\!6$	0.17	0	
2	SO4	Е	701	-	$4,\!4,\!4$	0.18	0	$6,\!6,\!6$	0.35	0	
2	SO4	С	703	-	$4,\!4,\!4$	0.24	0	$6,\!6,\!6$	0.18	0	
2	SO4	В	701	-	$4,\!4,\!4$	0.15	0	$6,\!6,\!6$	0.12	0	
2	SO4	F	701	-	$4,\!4,\!4$	0.20	0	$6,\!6,\!6$	0.31	0	
2	SO4	D	703	-	4,4,4	0.24	0	$6,\!6,\!6$	0.27	0	
4	GOL	D	712	-	$5,\!5,\!5$	0.87	0	$5,\!5,\!5$	0.97	0	
2	SO4	F	706	-	$4,\!4,\!4$	0.29	0	$6,\!6,\!6$	0.13	0	
4	GOL	А	714	-	$5,\!5,\!5$	0.88	0	$5,\!5,\!5$	1.15	1 (20%)	
2	SO4	А	703	-	4,4,4	0.11	0	$6,\!6,\!6$	0.27	0	
4	GOL	С	712	-	$5,\!5,\!5$	0.85	0	$5,\!5,\!5$	1.03	0	
2	SO4	А	707	-	$4,\!4,\!4$	0.13	0	$6,\!6,\!6$	0.31	0	
2	SO4	Н	706	-	$4,\!4,\!4$	0.12	0	$6,\!6,\!6$	0.19	0	
2	SO4	С	702	-	4,4,4	0.15	0	$6,\!6,\!6$	0.34	0	
4	GOL	F	708	-	$5,\!5,\!5$	0.98	0	$5,\!5,\!5$	0.94	0	
4	GOL	Н	711	-	$5,\!5,\!5$	0.77	0	$5,\!5,\!5$	1.10	0	
2	SO4	А	701	-	$4,\!4,\!4$	0.34	0	$6,\!6,\!6$	0.27	0	
4	GOL	А	713	-	$5,\!5,\!5$	1.36	1 (20%)	$5,\!5,\!5$	0.73	0	
5	ALA	D	714	-	$5,\!5,\!5$	2.05	2 (40%)	$6,\!6,\!6$	1.34	2 (33%)	
2	SO4	F	703	3	4,4,4	0.17	0	$6,\!6,\!6$	0.16	0	
5	ALA	Н	712	-	$5,\!5,\!5$	1.32	1 (20%)	$6,\!6,\!6$	1.10	1 (16%)	
2	SO4	Е	705	-	4,4,4	0.15	0	6,6,6	0.42	0	
2	SO4	А	705	-	4,4,4	0.18	0	$6,\!6,\!6$	0.31	0	
2	SO4	D	706	-	4,4,4	0.24	0	$6,\!6,\!6$	0.32	0	
4	GOL	D	711	-	$5,\!5,\!5$	1.05	0	$5,\!5,\!5$	1.19	0	
2	SO4	В	707	-	4,4,4	0.18	0	6,6,6	0.23	0	
4	GOL	F	710	-	$5,\!5,\!5$	1.00	0	$5,\!5,\!5$	0.99	0	
4	GOL	А	715	-	$5,\!5,\!5$	1.20	1 (20%)	$5,\!5,\!5$	1.02	0	
4	GOL	С	711	-	$5,\!5,\!5$	0.96	0	$5,\!5,\!5$	0.89	0	
2	SO4	В	705	-	4,4,4	0.15	0	$6,\!6,\!6$	0.25	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
4	GOL	С	710	-	-	2/4/4/4	-
4	GOL	D	712	-	-	2/4/4/4	-
4	GOL	А	714	-	-	4/4/4/4	-



8	W	Т	1

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	С	709	-	-	3/4/4/4	-
4	GOL	G	708	-	_	4/4/4/4	_
4	GOL	F	712	-	-	0/4/4/4	-
4	GOL	В	718	-	-	0/4/4/4	-
4	GOL	С	712	-	-	2/4/4/4	-
5	ALA	С	713	-	-	4/4/4/4	-
5	ALA	G	709	-	-	4/4/4/4	-
4	GOL	F	708	-	-	4/4/4/4	-
4	GOL	Н	711	-	-	4/4/4/4	-
4	GOL	Е	712	-	-	3/4/4/4	-
4	GOL	G	707	-	_	4/4/4/4	-
4	GOL	Е	714	-	-	4/4/4/4	-
5	ALA	А	716	3	-	0/4/4/4	-
5	ALA	Е	715	-	-	4/4/4/4	-
4	GOL	А	713	-	-	0/4/4/4	-
4	GOL	F	709	-	-	4/4/4/4	-
5	ALA	D	714	-	-	3/4/4/4	-
5	ALA	В	719	-	-	0/4/4/4	-
5	ALA	F	713	-	-	3/4/4/4	-
6	FLC	А	717	-	-	8/16/16/16	-
6	FLC	Н	713	-	-	9/16/16/16	-
4	GOL	D	713	-	-	2/4/4/4	-
5	ALA	Н	712	-	-	2/4/4/4	-
4	GOL	В	717	-	-	2/4/4/4	-
4	GOL	D	710	-	-	2/4/4/4	-
4	GOL	D	711	-	-	2/4/4/4	-
4	GOL	F	710	-	-	4/4/4/4	-
4	GOL	А	715	-	-	4/4/4/4	-
4	GOL	С	711	-	-	3/4/4/4	-
4	GOL	Е	713	-	-	2/4/4/4	-
4	GOL	F	711	-	-	2/4/4/4	-

All (27) bond length outliers are listed below:

10101	Ullaill	res	Type	Atoms	Z	Observed(A)	Ideal(A)
6	А	717	FLC	OA1-CAC	3.30	1.33	1.22



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	D	714	ALA	CA-C	-3.29	1.50	1.54
6	А	717	FLC	CA-CB	3.13	1.57	1.53
6	Н	713	FLC	OA1-CAC	3.06	1.32	1.22
6	А	717	FLC	OB1-CBC	2.98	1.31	1.22
6	Н	713	FLC	OG1-CGC	2.95	1.31	1.22
6	Н	713	FLC	OB1-CBC	2.89	1.31	1.22
5	А	716	ALA	OXT-C	-2.85	1.21	1.30
5	D	714	ALA	OXT-C	-2.75	1.21	1.30
6	Н	713	FLC	OG2-CGC	-2.66	1.21	1.30
6	А	717	FLC	OG1-CGC	2.66	1.31	1.22
5	А	716	ALA	CA-C	-2.53	1.51	1.54
6	А	717	FLC	OG2-CGC	-2.53	1.22	1.30
4	С	710	GOL	O2-C2	-2.46	1.36	1.43
6	Н	713	FLC	OA2-CAC	-2.43	1.22	1.30
5	В	719	ALA	CB-CA	-2.39	1.43	1.52
5	Е	715	ALA	OXT-C	-2.39	1.22	1.30
5	F	713	ALA	OXT-C	-2.33	1.22	1.30
5	F	713	ALA	CB-CA	-2.29	1.43	1.52
4	В	717	GOL	O2-C2	-2.25	1.36	1.43
4	А	715	GOL	O2-C2	-2.24	1.36	1.43
5	С	713	ALA	OXT-C	-2.23	1.23	1.30
4	A	713	GOL	C1-C2	2.16	1.60	1.51
5	Н	712	ALA	OXT-C	-2.15	1.23	1.30
5	В	719	ALA	OXT-C	-2.14	1.23	1.30
6	Н	713	FLC	OB2-CBC	-2.08	1.22	1.30
5	G	709	ALA	OXT-C	-2.03	1.23	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	А	717	FLC	OB1-CBC-CB	-6.06	113.67	122.25
6	Н	713	FLC	OB1-CBC-CB	-6.00	113.76	122.25
6	Н	713	FLC	OB2-CBC-CB	5.39	122.41	113.05
6	А	717	FLC	OB2-CBC-CB	5.01	121.75	113.05
5	G	709	ALA	OXT-C-O	-3.34	116.50	124.09
5	А	716	ALA	OXT-C-O	-3.31	116.58	124.09
6	А	717	FLC	OA1-CAC-CA	-3.30	113.31	122.94
6	А	717	FLC	OG1-CGC-CG	-3.07	113.96	122.94
5	С	713	ALA	OXT-C-O	-3.05	117.15	124.09
6	А	717	FLC	OA2-CAC-CA	2.87	123.56	114.35
5	В	719	ALA	OXT-C-O	-2.86	117.59	124.09
4	G	707	GOL	C3-C2-C1	-2.83	100.70	111.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	717	FLC	OG2-CGC-CG	2.82	123.42	114.35
6	Н	713	FLC	OA1-CAC-CA	-2.74	114.93	122.94
6	Н	713	FLC	OG2-CGC-CG	2.51	122.41	114.35
5	D	714	ALA	OXT-C-O	-2.40	118.64	124.09
5	Н	712	ALA	OXT-C-O	-2.40	118.64	124.09
5	F	713	ALA	OXT-C-CA	2.39	122.70	114.06
6	Н	713	FLC	OA2-CAC-CA	2.36	121.92	114.35
6	Н	713	FLC	OG1-CGC-CG	-2.35	116.06	122.94
5	F	713	ALA	OXT-C-O	-2.26	118.97	124.09
5	G	709	ALA	OXT-C-CA	2.21	122.05	114.06
5	Е	715	ALA	OXT-C-O	-2.14	119.24	124.09
4	D	710	GOL	C3-C2-C1	-2.13	103.43	111.70
5	В	719	ALA	C-CA-N	2.12	115.54	107.60
5	С	713	ALA	OXT-C-CA	2.12	121.71	114.06
5	D	714	ALA	OXT-C-CA	2.09	121.62	114.06
6	A	717	FLC	CB-CA-CAC	2.08	118.85	113.81
4	В	717	GOL	C3-C2-C1	-2.04	103.78	111.70
4	А	714	GOL	C3-C2-C1	-2.00	103.91	111.70

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	715	GOL	O1-C1-C2-C3
4	А	715	GOL	C1-C2-C3-O3
4	В	717	GOL	O1-C1-C2-C3
4	С	710	GOL	O1-C1-C2-C3
4	С	712	GOL	O1-C1-C2-C3
4	D	711	GOL	C1-C2-C3-O3
4	D	712	GOL	O1-C1-C2-O2
4	D	712	GOL	O1-C1-C2-C3
4	Е	713	GOL	C1-C2-C3-O3
4	Ε	714	GOL	C1-C2-C3-O3
4	F	708	GOL	O1-C1-C2-C3
4	F	708	GOL	C1-C2-C3-O3
4	F	708	GOL	O2-C2-C3-O3
4	F	711	GOL	O1-C1-C2-C3
4	G	707	GOL	O1-C1-C2-C3
4	G	708	GOL	O1-C1-C2-C3
4	G	708	GOL	C1-C2-C3-O3
4	G	708	GOL	O2-C2-C3-O3
5	C	713	ALA	O-C-CA-N



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Mol	Chain	Res	Type	Atoms			
5 D		714	ALA	OXT-C-CA-N			
5	D	714	ALA	OXT-C-CA-CB			
5	Е	715	ALA	O-C-CA-N			
5	Е	715	ALA	OXT-C-CA-N			
5	G	709	ALA	OXT-C-CA-N			
6	A	717	FLC	CA-CB-CBC-OB1			
6	A	717	FLC	CA-CB-CBC-OB2			
6	А	717	FLC	OHB-CB-CBC-OB1			
6	А	717	FLC	OHB-CB-CBC-OB2			
6	Н	713	FLC	CAC-CA-CB-CBC			
6	Н	713	FLC	CAC-CA-CB-CG			
6	Н	713	FLC	CA-CB-CBC-OB1			
6	Н	713	FLC	CA-CB-CBC-OB2			
6	Н	713	FLC	OHB-CB-CBC-OB1			
6	Н	713	FLC	OHB-CB-CBC-OB2			
4	А	714	GOL	O2-C2-C3-O3			
6	Н	713	FLC	CAC-CA-CB-OHB			
4	А	714	GOL	O1-C1-C2-C3			
4	А	714	GOL	C1-C2-C3-O3			
4	С	709	GOL	C1-C2-C3-O3			
4	С	711	GOL	C1-C2-C3-O3			
4	Е	712	GOL	C1-C2-C3-O3			
4	Е	714	GOL	O1-C1-C2-C3			
4	F	709	GOL	O1-C1-C2-C3			
4	F	710	GOL	O1-C1-C2-C3			
4	F	710	GOL	C1-C2-C3-O3			
4	G	707	GOL	C1-C2-C3-O3			
4	Н	711	GOL	O1-C1-C2-C3			
4	Н	711	GOL	C1-C2-C3-O3			
4	А	715	GOL	O1-C1-C2-O2			
4	А	715	GOL	O2-C2-C3-O3			
4	В	717	GOL	O1-C1-C2-O2			
4	С	710	GOL	O1-C1-C2-O2			
4	F	709	GOL	O1-C1-C2-O2			
4	G	707	GOL	O1-C1-C2-O2			
4	Н	711	GOL	O1-C1-C2-O2			
4	Н	711	GOL	O2-C2-C3-O3			
5	С	713	ALA	OXT-C-CA-N			
6	А	717	FLC	CAC-CA-CB-CG			
5	С	713	ALA	O-C-CA-CB			
5	С	713	ALA	OXT-C-CA-CB			
5	D	714	ALA	O-C-CA-CB			

Continued from previous page...



Mol	Chain Res T		Type	Atoms	
5	Е	715	ALA	O-C-CA-CB	
5	Е	715	ALA	OXT-C-CA-CB	
4	D	711	GOL	O2-C2-C3-O3	
4	F	708	GOL	O1-C1-C2-O2	
4	F	710	GOL	O1-C1-C2-O2	
4	F	710	GOL	O2-C2-C3-O3	
4	F	711	GOL	O1-C1-C2-O2	
6	Н	713	FLC	CG-CB-CBC-OB1	
6	Н	713	FLC	CG-CB-CBC-OB2	
4	А	714	GOL	O1-C1-C2-O2	
4	С	709	GOL	O1-C1-C2-O2	
4	С	711	GOL	O2-C2-C3-O3	
4	D	713	GOL	O2-C2-C3-O3	
4	Е	714	GOL	O2-C2-C3-O3	
4	F	709	GOL	O2-C2-C3-O3	
5	Н	712	ALA	OXT-C-CA-N	
6	А	717	FLC	CAC-CA-CB-CBC	
5	Н	712	ALA	O-C-CA-N	
5	F	713	ALA	OXT-C-CA-CB	
5	G	709	ALA	O-C-CA-CB	
5	G	709	ALA	OXT-C-CA-CB	
4	С	712	GOL	O1-C1-C2-O2	
4	Ε	713	GOL	O2-C2-C3-O3	
4	G	707	GOL	O2-C2-C3-O3	
4	G	708	GOL	O1-C1-C2-O2	
6	А	717	FLC	CAC-CA-CB-OHB	
4	Е	712	GOL	O1-C1-C2-C3	
4	Ε	712	GOL	O2-C2-C3-O3	
4	D	710	GOL	C1-C2-C3-O3	
4	D	713	GOL	C1-C2-C3-O3	
5	F	713	ALA	O-C-CA-CB	
4	С	709	GOL	O2-C2-C3-O3	
4	D	710	GOL	O2-C2-C3-O3	
4	Е	714	GOL	O1-C1-C2-O2	
6	A	717	FLC	CA-CB-CG-CGC	
4	F	709	GOL	C1-C2-C3-O3	
5	G	709	ALA	O-C-CA-N	
5	F	713	ALA	OXT-C-CA-N	
4	С	711	GOL	01-C1-C2-O2	

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There are no ring outliers.

28 monomers are involved in 64 short contacts:



$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	nes
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
2 H 707 SO4 1 0 2 C 701 SO4 1 0 2 H 708 SO4 1 0 2 H 708 SO4 1 0 4 E 712 GOL 2 0 5 A 716 ALA 4 0 5 B 719 ALA 8 0 4 F 711 GOL 2 0 5 B 709 SO4 1 0 5 C 713 ALA 2 0 2 B 703 SO4 1 0 5 F 713 ALA 8 0 6 H 713 FLC 2 0 4 D 712 GOL 1 0 2 F 706 SO4 1 0 4 F 708 GOL 2 0 4 <t< td=""><td></td></t<>	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
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6 H 713 FLC 2 0 4 D 712 GOL 1 0 2 F 706 SO4 1 0 4 F 708 GOL 2 0 4 H 711 GOL 1 0	
4 D 712 GOL 1 0 2 F 706 SO4 1 0 4 F 708 GOL 2 0 4 H 711 GOL 1 0	
2 F 706 SO4 1 0 4 F 708 GOL 2 0 4 H 711 GOL 1 0	
4 F 708 GOL 2 0 4 H 711 GOL 1 0	
4 H 711 GOL 1 0	
2 A 701 SO4 1 0	
5 D 714 ALA 7 0	
2 D 706 SO4 1 0	
4 F 710 GOL 1 0	
4 C 711 GOL 2 0	

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.































































































































































































































































































































































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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	А	650/691~(94%)	-0.13	5 (0%)	86	85	23, 32, 45, 62	0
1	В	650/691~(94%)	-0.25	3~(0%)	91	90	23, 33, 46, 69	0
1	С	651/691~(94%)	-0.13	6 (0%)	84	83	24, 32, 45, 68	0
1	D	649/691~(93%)	-0.07	6 (0%)	84	83	24, 35, 49, 75	0
1	Ε	650/691~(94%)	-0.23	1 (0%)	95	94	22, 33, 48, 74	0
1	F	649/691~(93%)	-0.05	5 (0%)	86	85	22, 34, 49, 67	0
1	G	647/691~(93%)	0.22	33~(5%)	28	27	31, 42, 58, 80	0
1	Н	651/691~(94%)	0.10	18 (2%)	53	51	26, 39, 56, 71	0
All	All	5197/5528~(94%)	-0.07	77 (1%)	73	72	22, 35, 52, 80	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	58	ALA	6.2
1	Е	146	PRO	4.7
1	D	146	PRO	4.5
1	А	146	PRO	3.9
1	F	146	PRO	3.5
1	G	146	PRO	3.5
1	G	140	ILE	3.5
1	Н	437	GLU	3.5
1	G	433	PRO	3.4
1	G	518	ILE	3.3
1	С	155	ASP	3.3
1	G	283	PHE	3.3
1	G	517	PHE	3.3
1	D	12	TYR	3.3
1	G	232	VAL	3.3
1	G	240	ALA	3.3



Mol	Iol Chain Re		Type	RSRZ
1	Н	242	THR	3.2
1	Н	140	ILE	3.2
1	А	436	ASP	3.1
1	G	515	PHE	3.1
1	В	146	PRO	3.0
1	G	58	ALA	3.0
1	G	12	TYR	3.0
1	Н	154	ALA	3.0
1	F	438	GLY	2.9
1	G	242	THR	2.9
1	С	434	GLU	2.9
1	Н	155	ASP	2.9
1	А	137	ASP	2.9
1	Н	234	LEU	2.8
1	G	238	SER	2.8
1	Н	146	PRO	2.7
1	G	194	LEU	2.7
1	G	111	PHE	2.7
1	Н	193	ALA	2.6
1	G	244	LEU	2.6
1	G	134	LEU	2.5
1	G	234	LEU	2.5
1	С	12	TYR	2.5
1	С	146	PRO	2.5
1	F	346	GLY	2.5
1	А	134	LEU	2.4
1	G	233	LEU	2.4
1	G	178	ARG	2.4
1	Н	139	THR	2.4
1	G	254	LEU	2.4
1	G	195	THR	2.4
1	Н	613	CYS	2.3
1	G	112	PHE	2.3
1	G	235	ASP	2.3
1	Н	244	LEU	2.3
1	С	438	GLY	2.3
1	Н	233	LEU	2.2
1	G	661	VAL	2.2
1	А	139	THR	2.2
1	G	243	ASN	2.2
1	D	134	LEU	2.2
1	С	436	ASP	2.2



Mol	Chain	Res	Type	RSRZ
1	G	263	LEU	2.2
1	G	403	LEU	2.2
1	Н	517	PHE	2.2
1	В	12	TYR	2.1
1	G	217	ALA	2.1
1	G	435	LEU	2.1
1	G	180	VAL	2.1
1	Н	111	PHE	2.1
1	D	137	ASP	2.1
1	Н	212	THR	2.1
1	В	156	LEU	2.1
1	Н	134	LEU	2.1
1	G	28	HIS	2.0
1	Н	195	THR	2.0
1	F	436	ASP	2.0
1	G	468	SER	2.0
1	D	140	ILE	2.0
1	D	634	LEU	2.0
1	F	137	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	FLC	А	717	13/13	0.54	0.34	$38,\!47,\!54,\!56$	0
6	FLC	Н	713	13/13	0.60	0.34	47,53,59,60	0
4	GOL	G	707	6/6	0.68	0.21	42,46,48,57	0
4	GOL	D	710	6/6	0.74	0.17	40,42,48,57	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors(A^2)	Q<0.9			
2	SO4	D	707	5/5	0.74	0.23	61,66,70,84	0			
4	GOL	D	712	6/6	0.78	0.20	36,39,48,48	0			
4	GOL	Н	711	6/6	0.78	0.24	46,49,55,59	0			
5	ALA	G	709	6/6	0.80	0.22	32,35,37,38	0			
4	GOL	С	709	6/6	0.81	0.15	36,40,42,42	0			
4	GOL	D	711	6/6	0.82	0.24	41,47,49,50	0			
4	GOL	G	708	6/6	0.82	0.12	$50,\!54,\!56,\!58$	0			
4	GOL	С	712	6/6	0.82	0.20	$42,\!45,\!51,\!53$	0			
4	GOL	А	713	6/6	0.84	0.19	$35,\!38,\!40,\!44$	0			
2	SO4	D	706	5/5	0.84	0.17	$50,\!56,\!64,\!69$	0			
2	SO4	F	705	5/5	0.84	0.26	$53,\!60,\!72,\!77$	0			
4	GOL	Е	712	6/6	0.84	0.29	42,46,47,57	0			
4	GOL	Е	714	6/6	0.84	0.26	45,51,51,55	0			
4	GOL	F	709	6/6	0.84	0.21	46,51,55,55	0			
3	NA	А	712	1/1	0.85	0.13	41,41,41,41	0			
4	GOL	D	713	6/6	0.86	0.17	44,45,48,61	0			
4	GOL	С	710	6/6	0.86	0.16	38,42,45,46	0			
4	GOL	F	712	6/6	0.86	0.27	47,52,54,63	0			
4	GOL	F	711	6/6	0.87	0.12	50,52,57,58	0			
2	SO4	Н	708	5/5	0.87	0.20	72,74,82,86	0			
5	ALA	С	713	6/6	0.88	0.19	22,28,30,30	0			
2	SO4	G	702	5/5	0.88	0.21	58,63,71,74	0			
2	SO4	Е	709	5/5	0.88	0.20	41,51,55,67	0			
4	GOL	В	718	6/6	0.88	0.12	39,42,46,46	0			
3	NA	G	706	1/1	0.89	0.16	48,48,48,48	0			
4	GOL	С	711	6/6	0.89	0.13	46,48,53,58	0			
4	GOL	Е	713	6/6	0.89	0.18	40,48,56,60	0			
2	SO4	F	706	5/5	0.89	0.21	34,37,42,45	5			
4	GOL	F	708	6/6	0.89	0.17	40,43,46,48	0			
5	ALA	Н	712	6/6	0.90	0.20	27,28,33,34	0			
5	ALA	F	713	6/6	0.90	0.22	25,28,32,33	0			
3	NA	Н	710	1/1	0.90	0.29	49,49,49,49	0			
4	GOL	F	710	6/6	0.91	0.28	40,51,57,64	0			
4	GOL	А	715	6/6	0.91	0.15	38,41,42,50	0			
2	SO4	В	712	5/5	0.91	0.20	60,61,73,80	0			
4	GOL	А	714	6/6	0.91	0.21	36,41,46,48	0			
2	SO4	Н	709	5/5	0.92	0.17	58,64,78,82	0			
2	SO4	F	707	5/5	0.92	0.34	59,60,76,86	0			
2	SO4	А	705	5/5	0.92	0.18	53,54,60,63	0			
4	GOL	В	717	6/6	0.92	0.20	39,48,50,52	0			
2	SO4	A	707	$\frac{1}{5/5}$	0.92	0.21	62,70,74,86	0			
5	ALA	Е	715	6/6	0.93	0.22	21,29,36,37	0			

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Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(A^2)$	Q < 0.9			
2	SO4	С	706	5/5	0.93	0.17	$50,\!57,\!66,\!70$	0			
3	NA	A	710	1/1	0.93	0.13	42,42,42,42	0			
2	SO4	A	708	5/5	0.94	0.24	59,60,74,79	0			
2	SO4	E	708	5/5	0.94	0.16	54,57,60,62	0			
3	NA	А	711	1/1	0.94	0.10	43,43,43,43	0			
5	ALA	В	719	6/6	0.94	0.20	$26,\!27,\!30,\!32$	0			
2	SO4	В	707	5/5	0.94	0.10	$46,\!48,\!65,\!65$	0			
3	NA	В	716	1/1	0.94	0.32	40,40,40,40	0			
3	NA	D	709	1/1	0.94	0.31	$47,\!47,\!47,\!47$	0			
3	NA	Е	711	1/1	0.94	0.22	42,42,42,42	0			
2	SO4	Н	704	5/5	0.94	0.11	$56,\!57,\!58,\!60$	0			
2	SO4	Н	706	5/5	0.94	0.16	$51,\!58,\!68,\!72$	0			
2	SO4	В	711	5/5	0.94	0.18	65,70,78,78	0			
2	SO4	G	705	5/5	0.95	0.09	$59,\!61,\!65,\!65$	0			
2	SO4	В	708	5/5	0.95	0.11	61,64,75,81	0			
2	SO4	Н	705	5/5	0.95	0.12	40,41,47,48	0			
2	SO4	С	707	5/5	0.95	0.14	52,53,55,58	0			
2	SO4	Е	707	5/5	0.95	0.17	62,63,68,68	0			
5	ALA	D	714	6/6	0.95	0.25	25,30,33,34	0			
2	SO4	D	708	5/5	0.96	0.15	62,65,69,69	0			
2	SO4	Е	705	5/5	0.96	0.10	45,51,60,61	0			
2	SO4	F	702	5/5	0.96	0.14	33,34,38,40	0			
3	NA	В	713	1/1	0.96	0.12	40,40,40,40	0			
3	NA	В	715	1/1	0.96	0.17	34,34,34,34	0			
2	SO4	G	703	5/5	0.96	0.17	58,59,63,64	0			
5	ALA	А	716	6/6	0.96	0.28	24,29,34,36	0			
2	SO4	D	705	5/5	0.96	0.08	42,44,50,56	0			
2	SO4	С	705	5/5	0.97	0.17	50,55,68,71	0			
2	SO4	Н	707	5/5	0.97	0.19	53,54,56,60	0			
2	SO4	В	704	5/5	0.97	0.09	44,45,46,49	0			
2	SO4	В	706	5/5	0.97	0.12	$29,\!32,\!35,\!36$	5			
3	NA	А	709	1/1	0.97	0.09	$35,\!35,\!35,\!35$	0			
2	SO4	F	703	5/5	0.97	0.08	41,42,48,51	0			
2	SO4	D	702	5/5	0.97	0.10	44,49,53,53	0			
2	SO4	А	702	5/5	0.97	0.14	36,37,41,43	0			
2	SO4	А	706	5/5	0.97	0.11	23,35,40,43	5			
3	NA	В	714	1/1	0.97	0.10	35,35,35,35	0			
2	SO4	G	701	5/5	0.97	0.14	40,45,49,49	0			
2	SO4	А	703	5/5	0.97	0.10	46,47,50,55	0			
2	SO4	А	704	5/5	0.97	0.19	45,46,56,58	0			
3	NA	Е	710	1/1	0.97	0.11	40,40,40,40	0			
2	SO4	Е	701	5/5	0.97	0.12	26,30,33,36	5			



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
2	SO4	С	702	5/5	0.97	0.10	33,36,39,40	0
2	SO4	С	704	5/5	0.97	0.17	48,52,55,58	0
2	SO4	Н	701	5/5	0.98	0.08	36,37,42,44	0
2	SO4	Н	702	5/5	0.98	0.07	42,42,47,47	0
2	SO4	Н	703	5/5	0.98	0.13	36,39,41,45	0
2	SO4	D	703	5/5	0.98	0.12	36,41,41,42	0
2	SO4	D	704	5/5	0.98	0.23	49,50,56,56	0
2	SO4	С	703	5/5	0.98	0.15	31,33,39,45	0
2	SO4	F	701	5/5	0.98	0.08	33,36,44,48	0
2	SO4	В	709	5/5	0.98	0.06	40,46,48,49	0
2	SO4	В	710	5/5	0.98	0.11	49,54,57,60	0
2	SO4	F	704	5/5	0.98	0.09	52,52,52,58	0
2	SO4	В	701	5/5	0.98	0.09	32,34,36,38	0
2	SO4	В	703	5/5	0.98	0.10	49,51,52,53	0
2	SO4	Е	702	5/5	0.98	0.14	34,37,39,42	0
2	SO4	Е	703	5/5	0.98	0.08	40,42,45,47	0
2	SO4	Е	704	5/5	0.98	0.11	42,45,49,53	0
2	SO4	А	701	5/5	0.98	0.09	$25,\!27,\!37,\!38$	5
2	SO4	G	704	5/5	0.98	0.07	36, 38, 42, 43	0
3	NA	С	708	1/1	0.98	0.06	$39,\!39,\!39,\!39$	0
2	SO4	Е	706	5/5	0.98	0.10	31,32,36,36	5
2	SO4	В	702	5/5	0.99	0.09	35,37,39,42	0
2	SO4	С	701	5/5	0.99	0.08	29,32,37,38	0
2	SO4	D	701	5/5	0.99	0.07	24,31,40,41	0
2	SO4	В	705	5/5	0.99	0.11	$3\overline{6},\!3\overline{6},\!41,\!4\overline{3}$	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.






















































































































































































































































































































































































































6.5 Other polymers (i)

There are no such residues in this entry.

