Full wwPDB X-ray Structure Validation Report (i)

Sep 27, 2023 – 08:34 AM EDT

PDB ID	:	8U5F
Title	:	Crystal Structure of Trypsinized Clostridium perfringens Enterotoxin
Authors	:	Kapoor, S.; Ogbu, C.P.; Vecchio, A.J.
Deposited on	:	2023-09-12
Resolution	:	2.32 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:

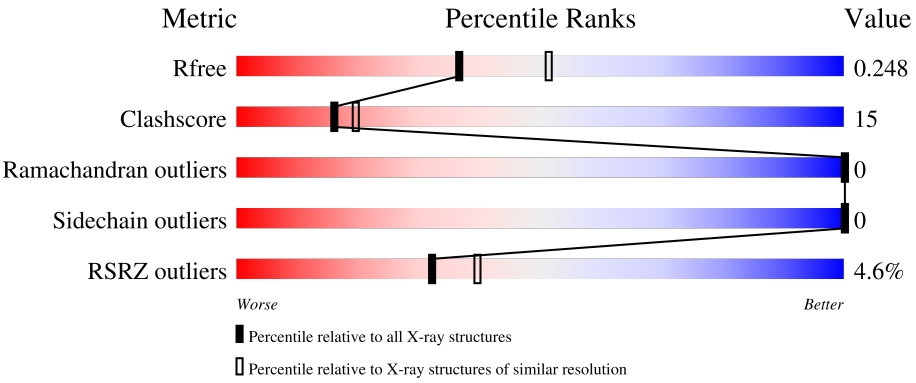
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	A	348	2% 63% 19% 18%
1	B	348	64% 18% 18%
1	C	348	3% 64% 18% 18%
1	D	348	2% 62% 20% 18%
1	E	348	5% 62% 21% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	348	8% 55% 27% 18%
1	G	348	% 61% 20% 18%
1	H	348	10% 44% 38% 18%

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	PO4	A	404	-	-	-	X
2	PO4	B	403	-	-	-	X
2	PO4	B	404	-	-	-	X
2	PO4	E	402	-	-	-	X
3	GOL	A	420	-	-	-	X
3	GOL	B	412	-	-	X	X
3	GOL	B	415	-	-	-	X
3	GOL	B	419	-	-	X	-
3	GOL	D	410	-	-	-	X
3	GOL	E	407	-	-	-	X
4	MES	B	422	-	-	-	X
4	MES	E	410	-	-	-	X
4	MES	E	411	-	-	-	X
4	MES	G	414	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19218 atoms, of which 369 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 Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2220	1407	363	448	2			
1	B	286	Total	C	N	O	S	0	0	0
			2223	1408	364	449	2			
1	C	286	Total	C	N	O	S	0	0	0
			2230	1415	364	449	2			
1	D	286	Total	C	N	O	S	0	0	0
			2230	1415	364	449	2			
1	E	287	Total	C	N	O	S	0	1	0
			2242	1423	366	451	2			
1	F	286	Total	C	N	O	S	0	0	0
			2219	1405	364	448	2			
1	G	285	Total	C	N	O	S	0	0	0
			2223	1410	363	448	2			
1	H	285	Total	C	N	O	S	0	0	0
			2223	1410	363	448	2			

There are 232 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP P01558
A	321	LEU	-	expression tag	UNP P01558
A	322	VAL	-	expression tag	UNP P01558
A	323	PRO	-	expression tag	UNP P01558
A	324	ARG	-	expression tag	UNP P01558
A	325	GLY	-	expression tag	UNP P01558
A	326	SER	-	expression tag	UNP P01558
A	327	GLY	-	expression tag	UNP P01558
A	328	GLY	-	expression tag	UNP P01558
A	329	GLY	-	expression tag	UNP P01558
A	330	GLY	-	expression tag	UNP P01558
A	331	SER	-	expression tag	UNP P01558
A	332	GLY	-	expression tag	UNP P01558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	333	GLY	-	expression tag	UNP P01558
A	334	GLY	-	expression tag	UNP P01558
A	335	GLY	-	expression tag	UNP P01558
A	336	SER	-	expression tag	UNP P01558
A	337	GLY	-	expression tag	UNP P01558
A	338	GLY	-	expression tag	UNP P01558
A	339	HIS	-	expression tag	UNP P01558
A	340	HIS	-	expression tag	UNP P01558
A	341	HIS	-	expression tag	UNP P01558
A	342	HIS	-	expression tag	UNP P01558
A	343	HIS	-	expression tag	UNP P01558
A	344	HIS	-	expression tag	UNP P01558
A	345	HIS	-	expression tag	UNP P01558
A	346	HIS	-	expression tag	UNP P01558
A	347	HIS	-	expression tag	UNP P01558
A	348	HIS	-	expression tag	UNP P01558
B	320	GLY	-	expression tag	UNP P01558
B	321	LEU	-	expression tag	UNP P01558
B	322	VAL	-	expression tag	UNP P01558
B	323	PRO	-	expression tag	UNP P01558
B	324	ARG	-	expression tag	UNP P01558
B	325	GLY	-	expression tag	UNP P01558
B	326	SER	-	expression tag	UNP P01558
B	327	GLY	-	expression tag	UNP P01558
B	328	GLY	-	expression tag	UNP P01558
B	329	GLY	-	expression tag	UNP P01558
B	330	GLY	-	expression tag	UNP P01558
B	331	SER	-	expression tag	UNP P01558
B	332	GLY	-	expression tag	UNP P01558
B	333	GLY	-	expression tag	UNP P01558
B	334	GLY	-	expression tag	UNP P01558
B	335	GLY	-	expression tag	UNP P01558
B	336	SER	-	expression tag	UNP P01558
B	337	GLY	-	expression tag	UNP P01558
B	338	GLY	-	expression tag	UNP P01558
B	339	HIS	-	expression tag	UNP P01558
B	340	HIS	-	expression tag	UNP P01558
B	341	HIS	-	expression tag	UNP P01558
B	342	HIS	-	expression tag	UNP P01558
B	343	HIS	-	expression tag	UNP P01558
B	344	HIS	-	expression tag	UNP P01558
B	345	HIS	-	expression tag	UNP P01558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	346	HIS	-	expression tag	UNP P01558
B	347	HIS	-	expression tag	UNP P01558
B	348	HIS	-	expression tag	UNP P01558
C	320	GLY	-	expression tag	UNP P01558
C	321	LEU	-	expression tag	UNP P01558
C	322	VAL	-	expression tag	UNP P01558
C	323	PRO	-	expression tag	UNP P01558
C	324	ARG	-	expression tag	UNP P01558
C	325	GLY	-	expression tag	UNP P01558
C	326	SER	-	expression tag	UNP P01558
C	327	GLY	-	expression tag	UNP P01558
C	328	GLY	-	expression tag	UNP P01558
C	329	GLY	-	expression tag	UNP P01558
C	330	GLY	-	expression tag	UNP P01558
C	331	SER	-	expression tag	UNP P01558
C	332	GLY	-	expression tag	UNP P01558
C	333	GLY	-	expression tag	UNP P01558
C	334	GLY	-	expression tag	UNP P01558
C	335	GLY	-	expression tag	UNP P01558
C	336	SER	-	expression tag	UNP P01558
C	337	GLY	-	expression tag	UNP P01558
C	338	GLY	-	expression tag	UNP P01558
C	339	HIS	-	expression tag	UNP P01558
C	340	HIS	-	expression tag	UNP P01558
C	341	HIS	-	expression tag	UNP P01558
C	342	HIS	-	expression tag	UNP P01558
C	343	HIS	-	expression tag	UNP P01558
C	344	HIS	-	expression tag	UNP P01558
C	345	HIS	-	expression tag	UNP P01558
C	346	HIS	-	expression tag	UNP P01558
C	347	HIS	-	expression tag	UNP P01558
C	348	HIS	-	expression tag	UNP P01558
D	320	GLY	-	expression tag	UNP P01558
D	321	LEU	-	expression tag	UNP P01558
D	322	VAL	-	expression tag	UNP P01558
D	323	PRO	-	expression tag	UNP P01558
D	324	ARG	-	expression tag	UNP P01558
D	325	GLY	-	expression tag	UNP P01558
D	326	SER	-	expression tag	UNP P01558
D	327	GLY	-	expression tag	UNP P01558
D	328	GLY	-	expression tag	UNP P01558
D	329	GLY	-	expression tag	UNP P01558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	330	GLY	-	expression tag	UNP P01558
D	331	SER	-	expression tag	UNP P01558
D	332	GLY	-	expression tag	UNP P01558
D	333	GLY	-	expression tag	UNP P01558
D	334	GLY	-	expression tag	UNP P01558
D	335	GLY	-	expression tag	UNP P01558
D	336	SER	-	expression tag	UNP P01558
D	337	GLY	-	expression tag	UNP P01558
D	338	GLY	-	expression tag	UNP P01558
D	339	HIS	-	expression tag	UNP P01558
D	340	HIS	-	expression tag	UNP P01558
D	341	HIS	-	expression tag	UNP P01558
D	342	HIS	-	expression tag	UNP P01558
D	343	HIS	-	expression tag	UNP P01558
D	344	HIS	-	expression tag	UNP P01558
D	345	HIS	-	expression tag	UNP P01558
D	346	HIS	-	expression tag	UNP P01558
D	347	HIS	-	expression tag	UNP P01558
D	348	HIS	-	expression tag	UNP P01558
E	320	GLY	-	expression tag	UNP P01558
E	321	LEU	-	expression tag	UNP P01558
E	322	VAL	-	expression tag	UNP P01558
E	323	PRO	-	expression tag	UNP P01558
E	324	ARG	-	expression tag	UNP P01558
E	325	GLY	-	expression tag	UNP P01558
E	326	SER	-	expression tag	UNP P01558
E	327	GLY	-	expression tag	UNP P01558
E	328	GLY	-	expression tag	UNP P01558
E	329	GLY	-	expression tag	UNP P01558
E	330	GLY	-	expression tag	UNP P01558
E	331	SER	-	expression tag	UNP P01558
E	332	GLY	-	expression tag	UNP P01558
E	333	GLY	-	expression tag	UNP P01558
E	334	GLY	-	expression tag	UNP P01558
E	335	GLY	-	expression tag	UNP P01558
E	336	SER	-	expression tag	UNP P01558
E	337	GLY	-	expression tag	UNP P01558
E	338	GLY	-	expression tag	UNP P01558
E	339	HIS	-	expression tag	UNP P01558
E	340	HIS	-	expression tag	UNP P01558
E	341	HIS	-	expression tag	UNP P01558
E	342	HIS	-	expression tag	UNP P01558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	343	HIS	-	expression tag	UNP P01558
E	344	HIS	-	expression tag	UNP P01558
E	345	HIS	-	expression tag	UNP P01558
E	346	HIS	-	expression tag	UNP P01558
E	347	HIS	-	expression tag	UNP P01558
E	348	HIS	-	expression tag	UNP P01558
F	320	GLY	-	expression tag	UNP P01558
F	321	LEU	-	expression tag	UNP P01558
F	322	VAL	-	expression tag	UNP P01558
F	323	PRO	-	expression tag	UNP P01558
F	324	ARG	-	expression tag	UNP P01558
F	325	GLY	-	expression tag	UNP P01558
F	326	SER	-	expression tag	UNP P01558
F	327	GLY	-	expression tag	UNP P01558
F	328	GLY	-	expression tag	UNP P01558
F	329	GLY	-	expression tag	UNP P01558
F	330	GLY	-	expression tag	UNP P01558
F	331	SER	-	expression tag	UNP P01558
F	332	GLY	-	expression tag	UNP P01558
F	333	GLY	-	expression tag	UNP P01558
F	334	GLY	-	expression tag	UNP P01558
F	335	GLY	-	expression tag	UNP P01558
F	336	SER	-	expression tag	UNP P01558
F	337	GLY	-	expression tag	UNP P01558
F	338	GLY	-	expression tag	UNP P01558
F	339	HIS	-	expression tag	UNP P01558
F	340	HIS	-	expression tag	UNP P01558
F	341	HIS	-	expression tag	UNP P01558
F	342	HIS	-	expression tag	UNP P01558
F	343	HIS	-	expression tag	UNP P01558
F	344	HIS	-	expression tag	UNP P01558
F	345	HIS	-	expression tag	UNP P01558
F	346	HIS	-	expression tag	UNP P01558
F	347	HIS	-	expression tag	UNP P01558
F	348	HIS	-	expression tag	UNP P01558
G	320	GLY	-	expression tag	UNP P01558
G	321	LEU	-	expression tag	UNP P01558
G	322	VAL	-	expression tag	UNP P01558
G	323	PRO	-	expression tag	UNP P01558
G	324	ARG	-	expression tag	UNP P01558
G	325	GLY	-	expression tag	UNP P01558
G	326	SER	-	expression tag	UNP P01558

Continued on next page...

Continued from previous page...

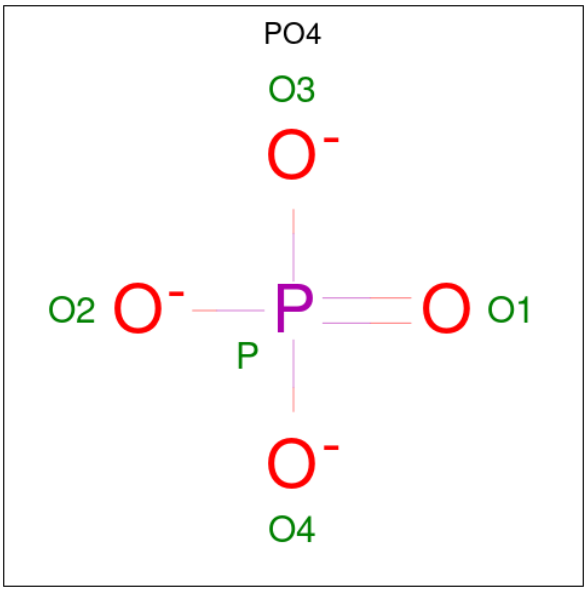
Chain	Residue	Modelled	Actual	Comment	Reference
G	327	GLY	-	expression tag	UNP P01558
G	328	GLY	-	expression tag	UNP P01558
G	329	GLY	-	expression tag	UNP P01558
G	330	GLY	-	expression tag	UNP P01558
G	331	SER	-	expression tag	UNP P01558
G	332	GLY	-	expression tag	UNP P01558
G	333	GLY	-	expression tag	UNP P01558
G	334	GLY	-	expression tag	UNP P01558
G	335	GLY	-	expression tag	UNP P01558
G	336	SER	-	expression tag	UNP P01558
G	337	GLY	-	expression tag	UNP P01558
G	338	GLY	-	expression tag	UNP P01558
G	339	HIS	-	expression tag	UNP P01558
G	340	HIS	-	expression tag	UNP P01558
G	341	HIS	-	expression tag	UNP P01558
G	342	HIS	-	expression tag	UNP P01558
G	343	HIS	-	expression tag	UNP P01558
G	344	HIS	-	expression tag	UNP P01558
G	345	HIS	-	expression tag	UNP P01558
G	346	HIS	-	expression tag	UNP P01558
G	347	HIS	-	expression tag	UNP P01558
G	348	HIS	-	expression tag	UNP P01558
H	320	GLY	-	expression tag	UNP P01558
H	321	LEU	-	expression tag	UNP P01558
H	322	VAL	-	expression tag	UNP P01558
H	323	PRO	-	expression tag	UNP P01558
H	324	ARG	-	expression tag	UNP P01558
H	325	GLY	-	expression tag	UNP P01558
H	326	SER	-	expression tag	UNP P01558
H	327	GLY	-	expression tag	UNP P01558
H	328	GLY	-	expression tag	UNP P01558
H	329	GLY	-	expression tag	UNP P01558
H	330	GLY	-	expression tag	UNP P01558
H	331	SER	-	expression tag	UNP P01558
H	332	GLY	-	expression tag	UNP P01558
H	333	GLY	-	expression tag	UNP P01558
H	334	GLY	-	expression tag	UNP P01558
H	335	GLY	-	expression tag	UNP P01558
H	336	SER	-	expression tag	UNP P01558
H	337	GLY	-	expression tag	UNP P01558
H	338	GLY	-	expression tag	UNP P01558
H	339	HIS	-	expression tag	UNP P01558

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	340	HIS	-	expression tag	UNP P01558
H	341	HIS	-	expression tag	UNP P01558
H	342	HIS	-	expression tag	UNP P01558
H	343	HIS	-	expression tag	UNP P01558
H	344	HIS	-	expression tag	UNP P01558
H	345	HIS	-	expression tag	UNP P01558
H	346	HIS	-	expression tag	UNP P01558
H	347	HIS	-	expression tag	UNP P01558
H	348	HIS	-	expression tag	UNP P01558

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



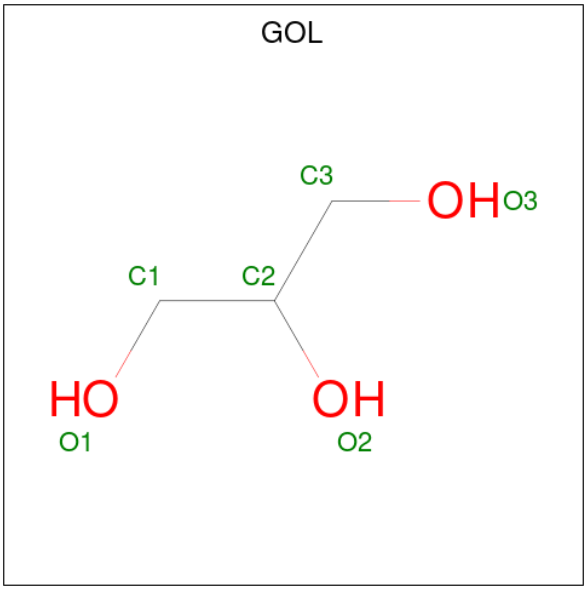
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C H O 14 3 8 3	0	0
3	E	1	Total C H O 14 3 8 3	0	0
3	E	1	Total C H O 14 3 8 3	0	0
3	E	1	Total C H O 14 3 8 3	0	0
3	E	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

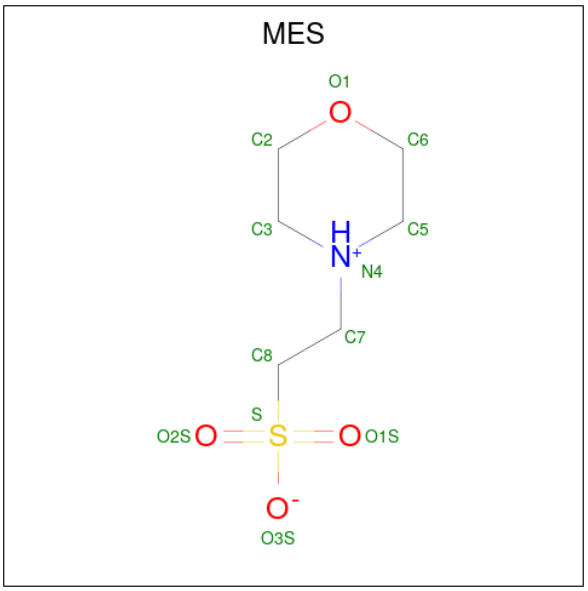
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C H O 14 3 8 3	0	0
3	F	1	Total C H O 14 3 8 3	0	0
3	F	1	Total C H O 14 3 8 3	0	0
3	F	1	Total C H O 14 3 8 3	0	0
3	F	1	Total C H O 14 3 8 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C H O 14 3 8 3	0	0
3	G	1	Total C H O 14 3 8 3	0	0
3	G	1	Total C H O 14 3 8 3	0	0
3	G	1	Total C H O 14 3 8 3	0	0
3	G	1	Total C H O 14 3 8 3	0	0
3	G	1	Total C H O 14 3 8 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H N O S 25 6 13 1 4 1	0	0
4	E	1	Total C H N O S 25 6 13 1 4 1	0	0
4	E	1	Total C H N O S 25 6 13 1 4 1	0	0
4	G	1	Total C H N O S 25 6 13 1 4 1	0	0
4	H	1	Total C H N O S 25 6 13 1 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0

Continued on next page...

Continued from previous page...

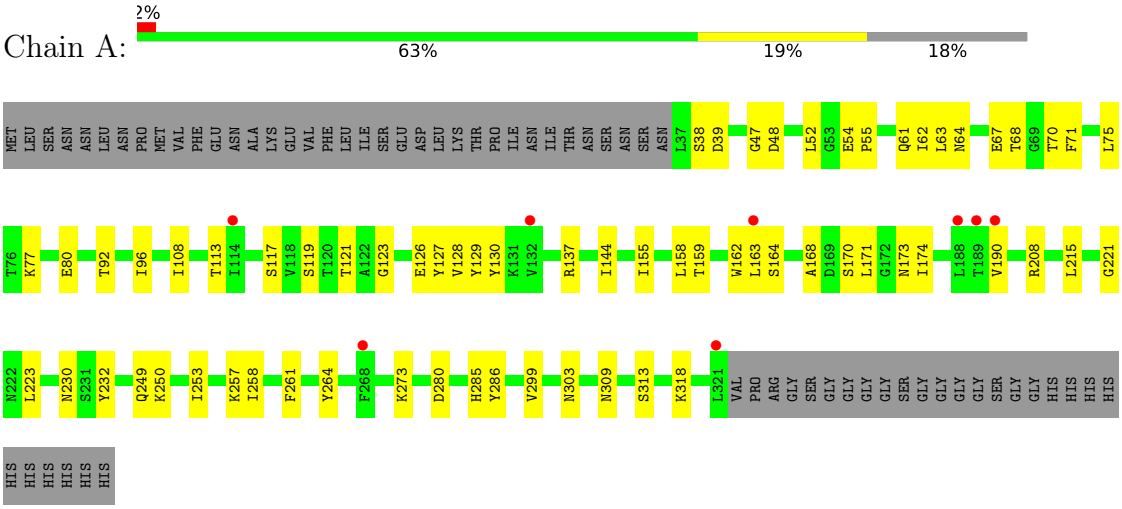
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	58	Total O 58 58	0	0
5	C	53	Total O 53 53	0	0
5	D	62	Total O 62 62	0	0
5	E	38	Total O 38 38	0	0
5	F	28	Total O 28 28	0	0
5	G	54	Total O 54 54	0	0
5	H	21	Total O 21 21	0	0

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.

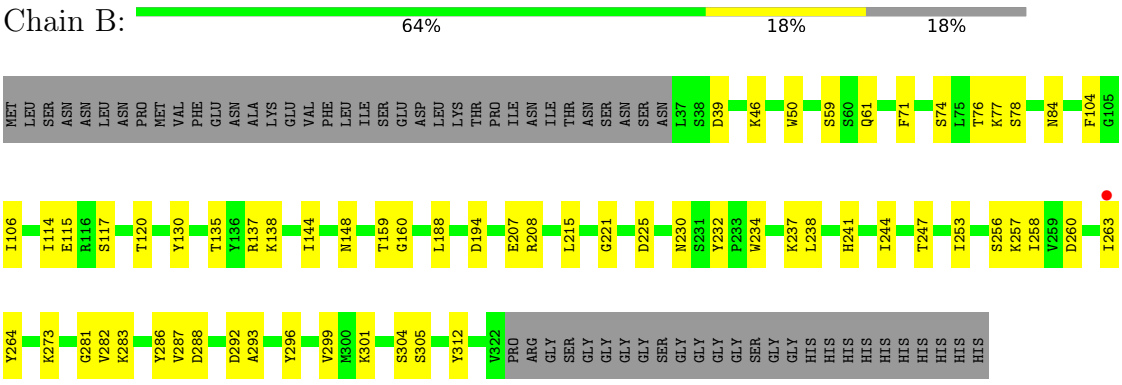
• Molecule 1: Heat-labile enterotoxin B chain

Chain A:



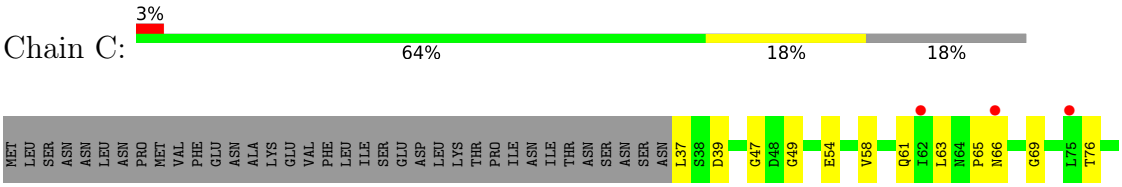
• Molecule 1: Heat-labile enterotoxin B chain

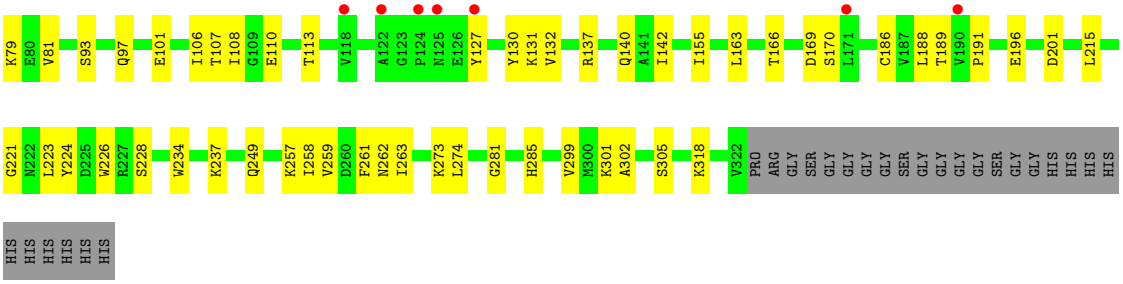
Chain B:

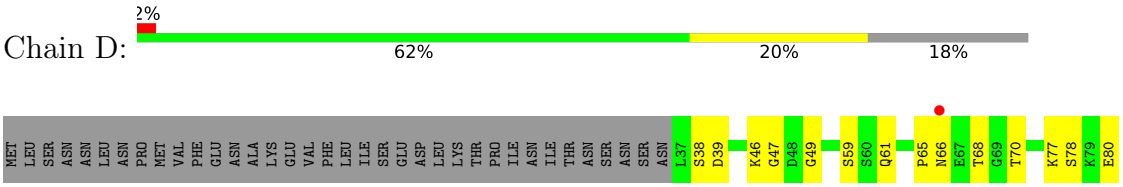


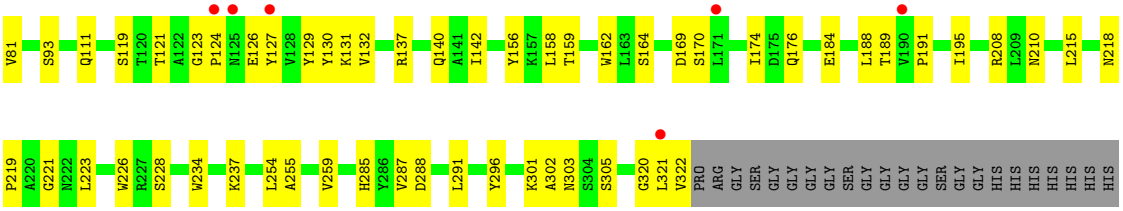
• Molecule 1: Heat-labile enterotoxin B chain

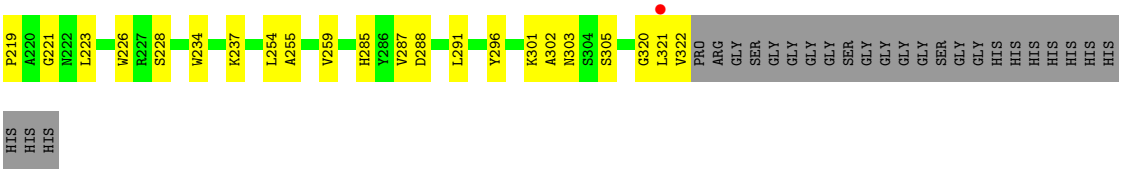
Chain C:









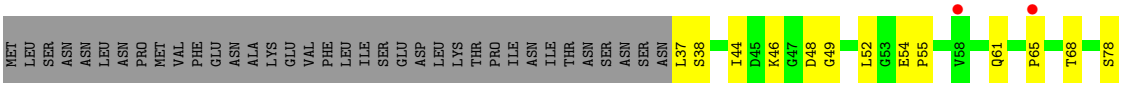


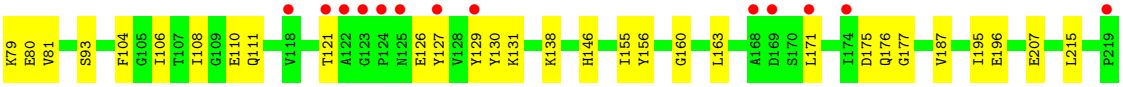
• Molecule 1: Heat-labile enterotoxin B chain

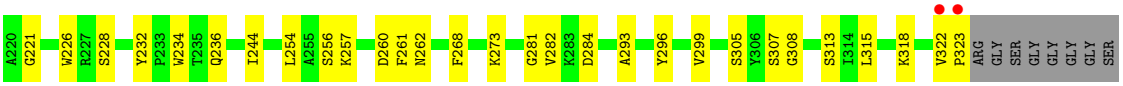
Chain D:

• Molecule 1: Heat-labile enterotoxin B chain

Chain E:

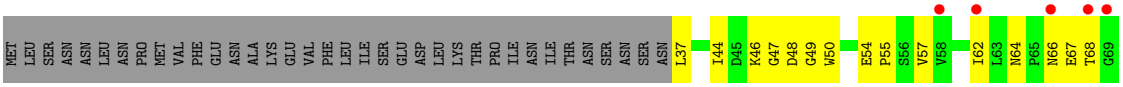


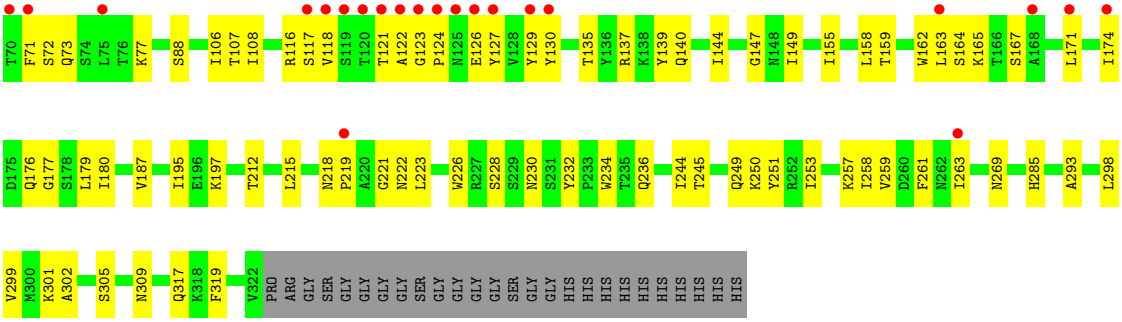




• Molecule 1: Heat-labile enterotoxin B chain

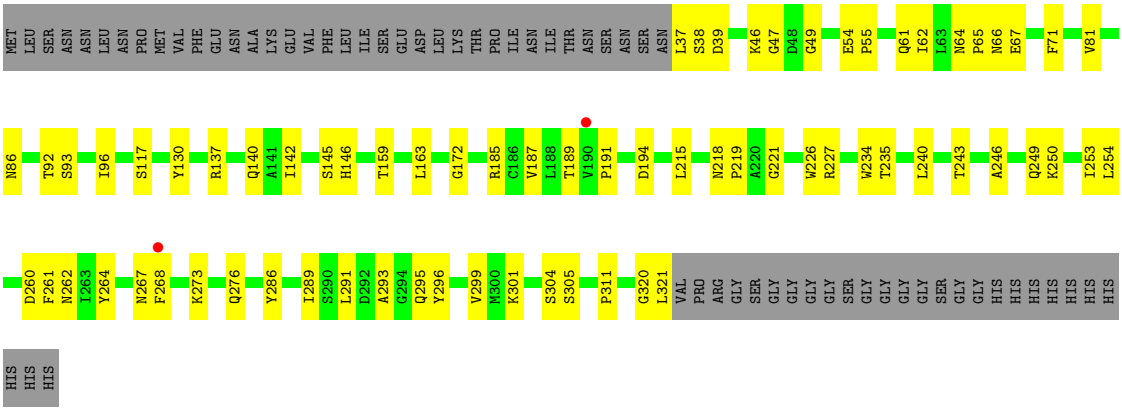
Chain F:





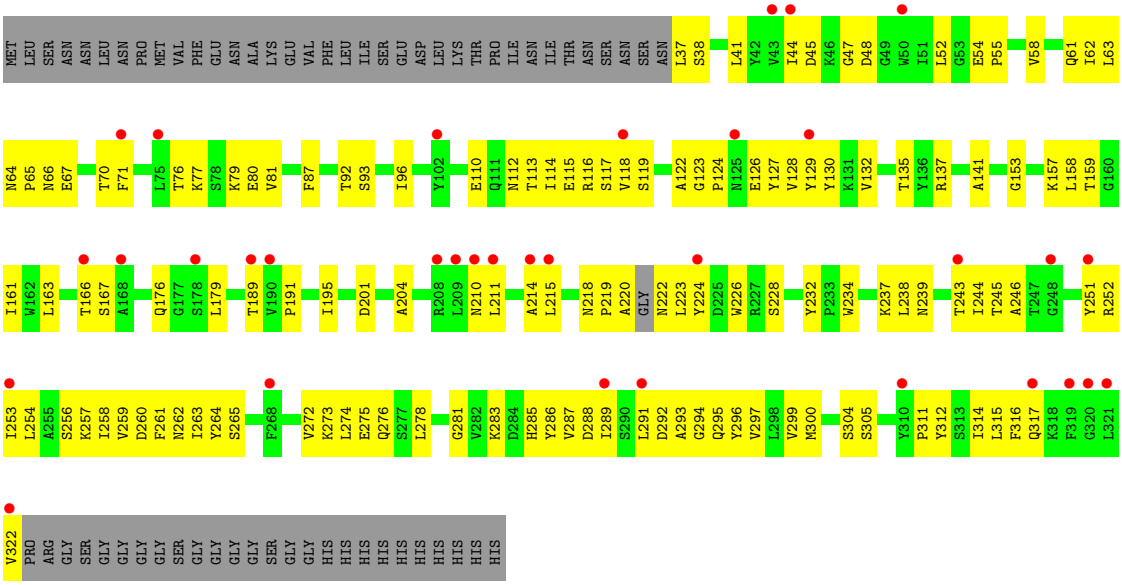
• Molecule 1: Heat-labile enterotoxin B chain

Chain G:



• Molecule 1: Heat-labile enterotoxin B chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	200.33Å 200.33Å 254.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.78 – 2.32 66.78 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.6 (66.78-2.32) 86.1 (66.78-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.37 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.224 , 0.248 0.226 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19218	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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 20.75 % 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 8.1179e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, MES

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	0.28	0/2264	0.48	0/3077
1	B	0.29	0/2267	0.48	0/3080
1	C	0.26	0/2274	0.46	0/3091
1	D	0.29	0/2274	0.49	0/3091
1	E	0.27	0/2290	0.48	0/3114
1	F	0.27	0/2262	0.47	0/3073
1	G	0.26	0/2267	0.47	0/3081
1	H	0.26	0/2266	0.48	0/3079
All	All	0.27	0/18164	0.48	0/24686

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

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	2220	0	2161	61	0
1	B	2223	0	2161	52	0
1	C	2230	0	2179	45	0
1	D	2230	0	2179	62	0
1	E	2242	0	2192	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2219	0	2163	78	0
1	G	2223	0	2170	50	0
1	H	2223	0	2166	129	0
2	A	20	0	0	1	0
2	B	20	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	1	0
2	G	10	0	0	0	0
2	H	5	0	0	0	0
3	A	96	56	128	9	0
3	B	102	48	136	18	0
3	C	72	40	95	6	0
3	D	78	40	104	18	0
3	E	42	32	56	5	0
3	F	66	40	88	5	0
3	G	66	48	88	11	0
3	H	12	0	16	3	0
4	B	12	13	13	0	0
4	E	24	26	25	3	0
4	G	12	13	13	2	0
4	H	12	13	13	0	0
5	A	51	0	0	2	0
5	B	58	0	0	0	0
5	C	53	0	0	1	0
5	D	62	0	0	1	0
5	E	38	0	0	1	0
5	F	28	0	0	0	0
5	G	54	0	0	1	0
5	H	21	0	0	3	0
All	All	18849	369	18146	532	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 15.

All (532) 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:320:GLY:C	1:D:321:LEU:HD12	1.35	1.46
1:D:320:GLY:O	1:D:321:LEU:HD12	1.00	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:GLY:C	1:D:321:LEU:CD1	2.14	1.14
1:D:320:GLY:O	1:D:321:LEU:CD1	1.95	1.13
1:H:38:SER:HB2	1:H:273:LYS:HE3	1.40	1.00
1:B:59:SER:HA	3:B:413:GOL:H31	1.45	0.98
1:F:130:TYR:HB2	1:F:163:LEU:HD21	1.49	0.93
1:C:81:VAL:HG21	1:C:93:SER:HB2	1.49	0.92
1:F:37:LEU:N	3:F:403:GOL:HO1	1.67	0.91
1:A:63:LEU:HB2	1:A:128:VAL:HG13	1.53	0.90
1:D:81:VAL:HG21	1:D:93:SER:HB2	1.56	0.88
1:H:263:ILE:HG23	1:H:274:LEU:HB2	1.58	0.84
1:D:77:LYS:HB2	1:D:158:LEU:HD22	1.58	0.84
1:C:215:LEU:O	1:C:221:GLY:HA2	1.84	0.78
1:A:137:ARG:HB2	1:A:159:THR:HG21	1.64	0.77
1:B:253:ILE:HD12	1:B:263:ILE:HD13	1.67	0.77
1:G:61:GLN:HB3	1:G:130:TYR:CE2	2.22	0.74
1:B:253:ILE:HD12	1:B:263:ILE:CD1	2.18	0.74
1:F:163:LEU:HD11	1:F:165:LYS:HD2	1.70	0.74
1:E:108:ILE:HD13	1:E:155:ILE:HD13	1.69	0.74
1:G:254:LEU:HD12	1:G:286:TYR:HB3	1.70	0.73
1:B:215:LEU:O	1:B:221:GLY:HA2	1.89	0.73
1:D:215:LEU:O	1:D:221:GLY:HA2	1.88	0.73
1:D:237:LYS:HE2	3:D:411:GOL:H11	1.71	0.72
1:A:190:VAL:HG12	5:A:503:HOH:O	1.88	0.72
1:H:76:THR:HG23	1:H:113:THR:HG22	1.69	0.72
1:C:223:LEU:HD11	1:H:322:VAL:HG13	1.70	0.71
1:A:121:THR:HG21	1:F:116:ARG:NE	2.06	0.71
1:D:129:TYR:CE2	1:D:176:GLN:HG2	2.27	0.70
1:D:174:ILE:HD12	1:D:174:ILE:O	1.91	0.70
1:E:61:GLN:HB3	1:E:130:TYR:CE2	2.26	0.70
1:A:47:GLY:O	1:A:137:ARG:HD2	1.92	0.69
1:H:252:ARG:HA	1:H:287:VAL:O	1.92	0.69
1:C:39:ASP:HB3	3:C:410:GOL:H11	1.74	0.69
1:E:322:VAL:HG13	1:E:323:PRO:HD3	1.75	0.69
1:A:77:LYS:HB2	1:A:158:LEU:HD22	1.75	0.69
1:H:38:SER:CB	1:H:273:LYS:HE3	2.19	0.69
1:H:66:ASN:OD1	1:H:124:PRO:HA	1.93	0.69
1:D:189:THR:O	1:D:191:PRO:HD3	1.93	0.68
1:D:59:SER:HA	3:D:410:GOL:H2	1.76	0.68
1:E:129:TYR:CE2	1:E:176:GLN:HG3	2.28	0.68
1:A:63:LEU:HB2	1:A:128:VAL:CG1	2.23	0.68
1:B:188:LEU:HD23	3:B:412:GOL:H31	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:LEU:HB2	1:H:128:VAL:HG13	1.76	0.67
1:E:38:SER:HB2	1:E:273:LYS:NZ	2.09	0.67
1:D:78:SER:HA	1:D:111:GLN:HG2	1.76	0.66
1:H:264:TYR:HB2	1:H:297:VAL:HG13	1.77	0.66
3:B:412:GOL:O2	3:B:420:GOL:H32	1.95	0.66
1:H:252:ARG:HB2	1:H:288:ASP:OD1	1.95	0.66
1:D:140:GLN:NE2	1:D:142:ILE:HD11	2.11	0.66
1:G:215:LEU:O	1:G:221:GLY:HA2	1.96	0.66
1:H:226:TRP:HB3	1:H:316:PHE:HE2	1.61	0.65
1:H:264:TYR:HB2	1:H:297:VAL:CG1	2.26	0.65
1:C:262:ASN:HD22	1:C:273:LYS:HE2	1.61	0.64
1:H:63:LEU:HB2	1:H:128:VAL:CG1	2.27	0.64
1:F:49:GLY:O	1:F:187:VAL:HG22	1.98	0.63
1:F:68:THR:HG22	1:F:121:THR:HA	1.81	0.63
1:H:118:VAL:HG11	1:H:163:LEU:HB2	1.78	0.63
1:H:295:GLN:HA	1:H:295:GLN:NE2	2.12	0.63
1:F:164:SER:OG	1:F:179:LEU:HD22	1.99	0.63
1:A:171:LEU:O	3:A:410:GOL:H31	1.98	0.63
1:B:84:ASN:HB2	3:B:419:GOL:C3	2.29	0.63
1:E:81:VAL:HG21	1:E:93:SER:HB3	1.81	0.63
1:E:322:VAL:CG1	1:E:323:PRO:HD3	2.29	0.63
1:G:37:LEU:N	3:G:407:GOL:HO3	1.97	0.63
1:G:246:ALA:O	1:G:293:ALA:HB2	1.98	0.63
1:H:215:LEU:O	1:H:218:ASN:HB3	1.99	0.63
1:H:244:ILE:HG23	1:H:294:GLY:H	1.64	0.62
1:E:108:ILE:CD1	1:E:155:ILE:HD13	2.29	0.62
1:G:38:SER:HB2	1:G:273:LYS:NZ	2.14	0.62
1:C:140:GLN:NE2	1:C:142:ILE:HD11	2.15	0.62
1:E:65:PRO:HB3	1:E:126:GLU:H	1.65	0.62
1:E:68:THR:HB	1:E:121:THR:HG23	1.80	0.62
1:H:118:VAL:HG23	1:H:161:ILE:HD11	1.82	0.62
1:G:49:GLY:O	1:G:187:VAL:HG22	2.00	0.62
3:C:404:GOL:H32	1:G:172:GLY:HA2	1.81	0.62
1:E:130:TYR:HB2	1:E:163:LEU:HD21	1.81	0.61
1:B:137:ARG:HB2	1:B:159:THR:HG21	1.83	0.61
1:H:292:ASP:OD1	1:H:293:ALA:N	2.33	0.61
1:C:81:VAL:HG21	1:C:93:SER:CB	2.27	0.61
1:F:37:LEU:HB2	1:F:147:GLY:O	2.01	0.61
1:G:304:SER:HA	3:G:408:GOL:H11	1.81	0.61
1:H:246:ALA:O	1:H:293:ALA:HB2	2.00	0.61
1:A:39:ASP:O	1:A:273:LYS:NZ	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:PRO:O	1:C:66:ASN:HB2	1.99	0.61
1:D:301:LYS:NZ	3:D:403:GOL:H32	2.15	0.61
1:F:67:GLU:HG2	1:F:68:THR:H	1.65	0.61
1:F:163:LEU:CD1	1:F:165:LYS:HD2	2.31	0.60
3:G:408:GOL:H12	1:H:87:PHE:HB3	1.82	0.60
1:H:76:THR:CG2	1:H:113:THR:HG22	2.31	0.60
1:B:39:ASP:O	1:B:273:LYS:NZ	2.32	0.60
1:A:285:HIS:HB2	3:A:419:GOL:H12	1.83	0.60
1:E:38:SER:HB2	1:E:273:LYS:HZ3	1.66	0.60
1:F:215:LEU:O	1:F:221:GLY:HA2	2.01	0.60
1:H:275:GLU:HG2	1:H:287:VAL:CG1	2.31	0.60
1:H:189:THR:O	1:H:191:PRO:HD3	2.02	0.60
1:H:226:TRP:CB	1:H:316:PHE:HE2	2.14	0.60
1:F:62:ILE:HD13	1:F:171:LEU:HD11	1.83	0.60
3:A:410:GOL:H12	1:E:293:ALA:O	2.01	0.60
1:D:169:ASP:OD1	1:D:170:SER:N	2.33	0.60
1:F:218:ASN:OD1	1:F:219:PRO:HD2	2.02	0.60
1:C:76:THR:OG1	1:C:113:THR:HB	2.01	0.60
1:E:61:GLN:HB3	1:E:130:TYR:CZ	2.36	0.59
1:D:38:SER:H	3:D:414:GOL:HO3	1.49	0.59
1:H:244:ILE:HG23	1:H:294:GLY:N	2.18	0.59
1:F:106:ILE:HG22	1:F:107:THR:H	1.67	0.59
1:B:234:TRP:CD2	1:B:305:SER:HA	2.38	0.59
1:D:208:ARG:NH2	5:D:502:HOH:O	2.35	0.59
1:H:79:LYS:HE2	1:H:110:GLU:OE1	2.03	0.59
1:H:166:THR:HG22	5:H:508:HOH:O	2.03	0.58
1:H:289:ILE:HG23	1:H:291:LEU:HG	1.84	0.58
1:A:208:ARG:NH2	1:C:166:THR:OG1	2.36	0.58
1:G:227:ARG:HH11	1:G:311:PRO:HG2	1.68	0.58
1:A:62:ILE:HG12	1:A:171:LEU:HD22	1.85	0.58
1:B:305:SER:H	3:B:410:GOL:C3	2.16	0.58
1:D:285:HIS:HA	3:D:413:GOL:C1	2.33	0.58
1:G:163:LEU:H	3:G:406:GOL:H32	1.67	0.58
1:H:265:SER:HB3	1:H:274:LEU:HD21	1.84	0.58
1:H:223:LEU:HA	1:H:316:PHE:O	2.03	0.57
3:D:404:GOL:O3	3:D:407:GOL:H12	2.05	0.57
1:C:234:TRP:CD2	1:C:305:SER:HA	2.40	0.57
1:G:320:GLY:O	1:G:321:LEU:HB2	2.05	0.57
1:B:104:PHE:O	1:B:106:ILE:HG23	2.05	0.57
1:C:257:LYS:HD2	1:C:281:GLY:O	2.04	0.57
1:F:253:ILE:HD12	1:F:263:ILE:CD1	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG12	1:A:171:LEU:CD2	2.35	0.57
1:B:84:ASN:HB2	3:B:419:GOL:O3	2.05	0.57
1:A:62:ILE:HD11	1:A:174:ILE:HD12	1.87	0.57
1:E:234:TRP:CD2	1:E:305:SER:HA	2.39	0.57
1:H:253:ILE:O	1:H:286:TYR:HA	2.05	0.57
1:A:123:GLY:HA3	1:A:126:GLU:HG2	1.87	0.56
1:C:189:THR:O	1:C:191:PRO:HD3	2.05	0.56
1:D:287:VAL:HA	3:D:404:GOL:H12	1.87	0.56
1:B:288:ASP:N	2:B:404:PO4:O3	2.28	0.56
1:H:128:VAL:HG23	1:H:166:THR:O	2.05	0.56
1:C:223:LEU:CD1	1:H:322:VAL:HG13	2.36	0.56
1:H:176:GLN:HB2	3:H:403:GOL:H32	1.86	0.56
1:B:78:SER:H	3:B:417:GOL:C1	2.19	0.56
1:E:65:PRO:HD3	1:E:127:TYR:CD2	2.41	0.56
1:A:68:THR:HG22	1:A:121:THR:OG1	2.06	0.55
1:A:52:LEU:CD1	1:A:80:GLU:HG3	2.36	0.55
1:B:263:ILE:HD12	1:B:287:VAL:HG21	1.89	0.55
1:D:237:LYS:HE2	3:D:411:GOL:C1	2.37	0.55
1:H:244:ILE:HG21	1:H:296:TYR:CE2	2.41	0.55
1:A:47:GLY:C	1:A:137:ARG:HD2	2.27	0.55
1:A:64:ASN:HA	1:A:127:TYR:CD2	2.40	0.55
1:B:257:LYS:HD2	1:B:281:GLY:O	2.07	0.55
1:E:262:ASN:HD22	1:E:273:LYS:HE2	1.71	0.55
1:G:92:THR:O	1:G:96:ILE:HG13	2.07	0.55
1:H:260:ASP:HB3	1:H:278:LEU:HD23	1.89	0.55
1:C:113:THR:HG22	5:C:526:HOH:O	2.06	0.55
1:A:71:PHE:O	1:A:117:SER:HA	2.06	0.55
1:H:275:GLU:HG2	1:H:287:VAL:HG11	1.89	0.55
1:A:168:ALA:HB1	1:A:173:ASN:HB2	1.88	0.55
1:D:68:THR:OG1	1:D:121:THR:HG22	2.07	0.55
1:B:263:ILE:CD1	1:B:287:VAL:HG21	2.37	0.55
1:D:66:ASN:OD1	1:D:124:PRO:HA	2.07	0.55
1:E:254:LEU:HD23	1:E:315:LEU:HD23	1.89	0.55
1:E:215:LEU:O	1:E:221:GLY:HA2	2.06	0.54
1:A:121:THR:HG21	1:F:116:ARG:CD	2.38	0.54
1:C:169:ASP:OD1	1:C:170:SER:N	2.41	0.54
1:C:305:SER:HB3	1:E:305:SER:HB3	1.89	0.54
1:D:285:HIS:HA	3:D:413:GOL:H11	1.89	0.54
1:H:127:TYR:O	1:H:167:SER:HA	2.08	0.54
1:C:237:LYS:HG2	1:C:301:LYS:HD3	1.89	0.54
1:H:219:PRO:O	1:H:220:ALA:CB	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HG13	1:A:190:VAL:O	2.08	0.54
1:F:162:TRP:CH2	1:F:164:SER:HB2	2.43	0.54
1:F:269:ASN:OD1	3:F:404:GOL:H32	2.08	0.54
1:G:137:ARG:HB2	1:G:159:THR:HG21	1.90	0.53
1:H:228:SER:HB3	1:H:311:PRO:HB2	1.90	0.53
1:H:52:LEU:CD1	1:H:80:GLU:HG3	2.38	0.53
1:H:76:THR:OG1	1:H:113:THR:HG22	2.07	0.53
1:H:71:PHE:O	1:H:117:SER:HA	2.06	0.53
1:H:61:GLN:HB3	1:H:130:TYR:CE2	2.44	0.53
1:A:62:ILE:HD12	1:A:129:TYR:HB2	1.89	0.53
1:E:160:GLY:HA3	3:E:407:GOL:H32	1.89	0.53
1:F:47:GLY:C	1:F:137:ARG:HD2	2.29	0.53
1:D:195:ILE:N	1:D:195:ILE:HD12	2.24	0.53
1:E:257:LYS:HD2	1:E:281:GLY:O	2.09	0.53
1:F:77:LYS:HB2	1:F:158:LEU:HD22	1.89	0.53
1:H:219:PRO:O	1:H:220:ALA:HB3	2.09	0.53
1:A:250:LYS:HE3	5:A:527:HOH:O	2.08	0.53
1:E:256:SER:HA	1:E:284:ASP:OD1	2.09	0.53
1:H:264:TYR:CD1	1:H:273:LYS:HA	2.44	0.52
1:B:77:LYS:HA	3:B:417:GOL:H11	1.92	0.52
1:F:68:THR:HG22	1:F:121:THR:CB	2.39	0.52
1:B:61:GLN:HB2	1:B:130:TYR:CZ	2.44	0.52
1:F:67:GLU:HG2	1:F:68:THR:N	2.24	0.52
1:H:96:ILE:HG23	1:H:141:ALA:HB3	1.91	0.52
1:F:64:ASN:HB2	1:F:67:GLU:OE1	2.09	0.52
1:H:214:ALA:HB1	1:H:224:TYR:CD2	2.45	0.52
1:H:243:THR:HG22	1:H:295:GLN:HE22	1.73	0.52
1:C:65:PRO:HD3	1:C:127:TYR:CE2	2.44	0.52
1:F:123:GLY:H	1:F:126:GLU:HB3	1.73	0.52
1:F:195:ILE:N	1:F:195:ILE:HD12	2.25	0.52
1:F:257:LYS:HG3	1:F:258:ILE:HG23	1.92	0.52
1:D:65:PRO:HD3	1:D:127:TYR:CE2	2.44	0.52
1:F:66:ASN:N	1:F:122:ALA:HB3	2.25	0.52
1:H:251:TYR:CD1	1:H:291:LEU:HB2	2.44	0.52
1:A:137:ARG:HB2	1:A:159:THR:CG2	2.37	0.51
1:C:97:GLN:O	1:C:101:GLU:HG3	2.09	0.51
1:H:226:TRP:CZ2	1:H:228:SER:HA	2.45	0.51
1:G:37:LEU:N	3:G:407:GOL:HO2	2.08	0.51
1:H:166:THR:OG1	1:H:179:LEU:HD11	2.10	0.51
1:D:49:GLY:HA3	1:D:188:LEU:HG	1.91	0.51
1:A:48:ASP:OD1	1:A:137:ARG:HD3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:TRP:CD2	1:G:305:SER:HA	2.45	0.51
1:F:234:TRP:CD2	1:F:305:SER:HA	2.46	0.51
1:G:267:ASN:HA	3:G:405:GOL:H11	1.91	0.51
1:B:188:LEU:CD2	3:B:412:GOL:H31	2.41	0.51
1:B:301:LYS:HB3	3:B:416:GOL:H12	1.91	0.51
1:D:46:LYS:HE3	1:D:140:GLN:OE1	2.10	0.51
1:E:232:TYR:HD1	1:E:236:GLN:HG2	1.76	0.51
1:H:245:THR:HG21	5:H:509:HOH:O	2.10	0.51
1:H:232:TYR:CE2	1:H:238:LEU:HD13	2.46	0.50
1:A:313:SER:HB2	3:A:414:GOL:H11	1.93	0.50
1:F:258:ILE:O	1:F:258:ILE:HD12	2.10	0.50
1:H:210:ASN:HA	1:H:243:THR:OG1	2.11	0.50
1:C:223:LEU:HD23	1:C:224:TYR:N	2.26	0.50
1:D:301:LYS:HZ1	3:D:403:GOL:H32	1.75	0.50
1:F:66:ASN:HD21	1:F:124:PRO:HA	1.76	0.50
1:G:189:THR:O	1:G:191:PRO:HD3	2.12	0.50
1:H:137:ARG:HB2	1:H:159:THR:HG21	1.93	0.50
1:F:309:ASN:H	3:F:409:GOL:H11	1.77	0.50
1:G:260:ASP:HB2	3:G:410:GOL:H2	1.94	0.50
1:G:289:ILE:HD13	1:G:291:LEU:HD21	1.94	0.50
1:H:92:THR:O	1:H:96:ILE:HG13	2.11	0.50
1:C:106:ILE:HG22	1:C:107:THR:N	2.27	0.50
1:F:137:ARG:HB2	1:F:159:THR:HG21	1.94	0.50
1:A:309:ASN:H	3:A:417:GOL:H11	1.77	0.50
1:D:291:LEU:HA	3:D:412:GOL:H31	1.94	0.50
1:E:52:LEU:CD1	1:E:80:GLU:HG3	2.42	0.50
1:F:123:GLY:HA3	1:F:126:GLU:HB3	1.93	0.50
1:D:38:SER:N	3:D:414:GOL:O3	2.33	0.49
1:H:61:GLN:HB3	1:H:130:TYR:CZ	2.47	0.49
1:B:244:ILE:O	1:B:293:ALA:HA	2.12	0.49
1:D:210:ASN:HD22	3:D:406:GOL:H31	1.75	0.49
1:H:115:GLU:O	1:H:116:ARG:NE	2.45	0.49
1:E:244:ILE:HD12	1:E:296:TYR:CE2	2.48	0.49
1:D:288:ASP:HB2	3:D:404:GOL:H32	1.95	0.49
1:H:204:ALA:HB3	1:H:239:ASN:ND2	2.27	0.49
1:C:261:PHE:HA	1:C:299:VAL:O	2.13	0.49
1:D:59:SER:HB3	1:D:132:VAL:HB	1.94	0.49
1:G:268:PHE:H	3:G:405:GOL:H11	1.78	0.49
1:H:58:VAL:HG22	1:H:132:VAL:O	2.12	0.49
1:H:166:THR:CG2	1:H:179:LEU:HD11	2.43	0.49
1:F:197:LYS:HE2	2:F:401:PO4:O1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:O	1:A:221:GLY:HA2	2.12	0.49
1:F:117:SER:O	1:F:118:VAL:HG13	2.12	0.49
1:A:123:GLY:CA	1:A:126:GLU:HG2	2.43	0.49
1:H:265:SER:CB	1:H:274:LEU:HD21	2.42	0.49
1:H:228:SER:HB3	1:H:311:PRO:CB	2.43	0.48
1:G:38:SER:HB2	1:G:273:LYS:HZ2	1.77	0.48
1:H:122:ALA:HB2	1:H:128:VAL:HG12	1.95	0.48
1:H:222:ASN:O	1:H:317:GLN:HA	2.12	0.48
1:H:65:PRO:HD3	1:H:127:TYR:CD2	2.48	0.48
1:H:275:GLU:HG2	1:H:287:VAL:HG13	1.96	0.48
1:F:171:LEU:O	1:F:174:ILE:HG13	2.14	0.48
1:F:301:LYS:HD3	1:F:302:ALA:O	2.14	0.48
1:D:137:ARG:HB2	1:D:159:THR:HG21	1.95	0.48
1:F:129:TYR:CE1	1:F:176:GLN:HG2	2.48	0.48
1:H:211:LEU:O	1:H:214:ALA:N	2.45	0.48
1:E:129:TYR:OH	1:E:131:LYS:HD3	2.13	0.48
1:E:175:ASP:O	1:E:177:GLY:N	2.45	0.48
1:F:177:GLY:HA2	1:F:180:ILE:HG13	1.95	0.48
1:G:86:ASN:O	1:H:281:GLY:HA3	2.13	0.48
1:G:65:PRO:O	1:G:66:ASN:HB2	2.14	0.48
1:H:65:PRO:HD3	1:H:127:TYR:CE2	2.49	0.48
1:H:64:ASN:HB2	1:H:67:GLU:CD	2.34	0.48
1:A:62:ILE:CD1	1:A:129:TYR:HB2	2.44	0.48
1:A:108:ILE:HD12	1:A:155:ILE:HD13	1.96	0.48
1:H:265:SER:OG	1:H:272:VAL:HB	2.14	0.48
1:A:52:LEU:HD11	1:A:80:GLU:HG3	1.96	0.47
1:D:47:GLY:C	1:D:137:ARG:HD2	2.35	0.47
1:E:104:PHE:O	1:E:106:ILE:HG23	2.14	0.47
1:F:48:ASP:OD1	1:F:137:ARG:HD3	2.13	0.47
1:F:144:ILE:CD1	1:F:149:ILE:HG12	2.43	0.47
1:F:253:ILE:HD12	1:F:263:ILE:HD13	1.96	0.47
1:D:65:PRO:O	1:D:66:ASN:HB2	2.14	0.47
1:E:196:GLU:OE2	3:E:409:GOL:H12	2.14	0.47
1:A:48:ASP:OD1	1:A:159:THR:HG21	2.15	0.47
1:A:170:SER:HG	1:A:173:ASN:CG	2.12	0.47
1:C:37:LEU:HD22	3:C:413:GOL:C3	2.44	0.47
1:E:79:LYS:HE2	1:E:110:GLU:OE1	2.14	0.47
1:H:300:MET:HG3	1:H:312:TYR:CD2	2.49	0.47
1:F:218:ASN:HD22	1:F:221:GLY:N	2.12	0.47
1:A:253:ILE:O	1:A:286:TYR:HA	2.15	0.47
1:B:253:ILE:O	1:B:286:TYR:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:TYR:CD2	1:B:273:LYS:HA	2.50	0.47
1:C:257:LYS:HG3	1:C:258:ILE:HG23	1.97	0.47
1:F:68:THR:HG22	1:F:121:THR:CA	2.43	0.47
1:E:48:ASP:HB3	5:E:503:HOH:O	2.15	0.47
1:F:54:GLU:N	1:F:55:PRO:CD	2.77	0.47
1:F:230:ASN:HB2	1:F:232:TYR:CZ	2.50	0.47
1:G:71:PHE:O	1:G:117:SER:HA	2.14	0.47
1:F:123:GLY:CA	1:F:126:GLU:HB3	2.45	0.47
1:F:249:GLN:HB2	1:F:251:TYR:CZ	2.49	0.47
1:H:265:SER:HB3	1:H:274:LEU:HD11	1.97	0.47
1:B:253:ILE:HD12	1:B:263:ILE:HD11	1.95	0.46
1:F:259:VAL:O	1:F:285:HIS:NE2	2.45	0.46
1:H:263:ILE:HG23	1:H:263:ILE:O	2.15	0.46
1:B:76:THR:O	3:B:415:GOL:H2	2.15	0.46
1:F:50:TRP:O	1:F:135:THR:HA	2.15	0.46
1:H:254:LEU:HB3	1:H:315:LEU:HB3	1.98	0.46
1:C:49:GLY:HA3	1:C:188:LEU:HG	1.98	0.46
1:E:221:GLY:O	1:E:318:LYS:HE3	2.16	0.46
1:F:106:ILE:HG22	1:F:107:THR:N	2.30	0.46
1:B:208:ARG:HG2	1:B:241:HIS:HB2	1.97	0.46
1:E:37:LEU:N	3:E:406:GOL:H31	2.30	0.46
1:F:174:ILE:CD1	1:F:176:GLN:HG3	2.46	0.46
1:H:81:VAL:HG11	1:H:93:SER:HA	1.96	0.46
1:G:253:ILE:O	1:G:286:TYR:HA	2.14	0.46
1:F:261:PHE:HA	1:F:299:VAL:O	2.15	0.46
1:D:123:GLY:H	1:D:126:GLU:HG2	1.80	0.46
1:D:234:TRP:CD2	1:D:305:SER:HA	2.51	0.46
1:F:226:TRP:CH2	1:F:228:SER:HB3	2.51	0.46
1:D:218:ASN:OD1	1:D:219:PRO:HD2	2.16	0.46
1:D:234:TRP:HE1	3:D:408:GOL:H12	1.81	0.46
1:F:46:LYS:HE3	1:F:140:GLN:OE1	2.16	0.46
1:C:196:GLU:OE2	3:C:413:GOL:H11	2.16	0.46
1:E:49:GLY:O	1:E:187:VAL:HG22	2.16	0.46
1:H:237:LYS:HD3	1:H:299:VAL:CG1	2.46	0.46
1:D:61:GLN:HB3	1:D:130:TYR:CE2	2.50	0.45
1:F:88:SER:OG	3:F:408:GOL:H31	2.15	0.45
1:H:62:ILE:HD12	1:H:129:TYR:HB2	1.98	0.45
1:A:62:ILE:HD13	1:E:268:PHE:CD1	2.51	0.45
1:D:303:ASN:HA	3:D:403:GOL:H31	1.99	0.45
1:H:62:ILE:CD1	1:H:129:TYR:HB2	2.46	0.45
1:H:118:VAL:HG12	1:H:119:SER:N	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:SER:HA	3:B:410:GOL:H32	1.99	0.45
1:C:54:GLU:OE1	1:C:131:LYS:NZ	2.49	0.45
1:D:39:ASP:HB3	3:D:411:GOL:H2	1.97	0.45
1:E:127:TYR:CD2	1:E:171:LEU:HD13	2.52	0.45
1:G:38:SER:HB2	1:G:273:LYS:HZ3	1.82	0.45
1:A:70:THR:HG22	1:A:119:SER:CB	2.47	0.45
1:F:127:TYR:O	1:F:167:SER:HA	2.17	0.45
1:H:41:LEU:HD22	1:H:201:ASP:HA	1.98	0.45
1:B:120:THR:HG21	1:B:130:TYR:CD2	2.52	0.45
1:G:218:ASN:OD1	1:G:219:PRO:HD2	2.17	0.45
1:D:321:LEU:CD1	1:D:321:LEU:N	2.73	0.45
1:E:234:TRP:CG	1:E:305:SER:HA	2.52	0.45
1:E:244:ILE:O	1:E:293:ALA:HA	2.16	0.45
1:E:254:LEU:HD11	1:E:284:ASP:HB3	1.99	0.45
1:F:309:ASN:H	3:F:409:GOL:C1	2.30	0.45
1:B:74:SER:OG	1:B:115:GLU:OE2	2.33	0.45
1:B:77:LYS:HA	3:B:417:GOL:C1	2.47	0.45
1:F:72:SER:O	1:F:73:GLN:HB3	2.16	0.45
1:G:249:GLN:HA	1:G:249:GLN:OE1	2.17	0.45
1:A:230:ASN:HB2	1:A:232:TYR:CZ	2.52	0.44
1:D:70:THR:OG1	1:D:119:SER:HB3	2.17	0.44
1:G:54:GLU:N	1:G:55:PRO:CD	2.80	0.44
1:F:174:ILE:C	1:F:174:ILE:HD12	2.38	0.44
1:G:39:ASP:OD2	1:G:146:HIS:N	2.48	0.44
1:G:261:PHE:HA	1:G:299:VAL:O	2.17	0.44
1:H:234:TRP:CD2	1:H:305:SER:HA	2.52	0.44
1:C:201:ASP:OD2	1:C:237:LYS:HE2	2.16	0.44
1:E:307:SER:HA	4:E:411:MES:H51	1.98	0.44
1:F:223:LEU:C	1:F:223:LEU:HD23	2.37	0.44
1:G:62:ILE:HG23	1:G:62:ILE:O	2.18	0.44
1:H:37:LEU:N	1:H:37:LEU:HD12	2.32	0.44
1:H:232:TYR:HE2	1:H:238:LEU:HD22	1.83	0.44
1:A:144:ILE:CD1	3:A:405:GOL:H31	2.47	0.44
1:D:320:GLY:CA	1:D:321:LEU:CD1	2.94	0.44
1:E:232:TYR:CD1	1:E:236:GLN:HG2	2.52	0.44
1:H:137:ARG:N	1:H:157:LYS:O	2.34	0.44
1:B:46:LYS:HD3	1:B:194:ASP:CG	2.37	0.44
1:H:244:ILE:HG21	1:H:296:TYR:HE2	1.83	0.44
1:H:314:ILE:HG22	1:H:315:LEU:N	2.33	0.44
1:C:237:LYS:HD3	3:C:410:GOL:O1	2.17	0.44
1:B:260:ASP:HB2	3:B:416:GOL:H2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:VAL:O	1:D:285:HIS:NE2	2.50	0.44
1:E:78:SER:HA	1:E:111:GLN:HA	2.00	0.44
1:A:223:LEU:C	1:A:223:LEU:HD23	2.39	0.44
1:B:256:SER:OG	1:B:257:LYS:N	2.51	0.44
1:G:145:SER:HB3	3:G:403:GOL:H11	2.00	0.44
1:G:185:ARG:HH12	3:G:412:GOL:H31	1.83	0.44
1:A:39:ASP:HB3	3:A:420:GOL:H32	1.99	0.43
1:B:84:ASN:HB2	3:B:419:GOL:H31	1.99	0.43
1:F:108:ILE:HD12	1:F:155:ILE:HD13	1.99	0.43
1:F:222:ASN:O	1:F:317:GLN:HA	2.18	0.43
1:F:261:PHE:CD1	1:F:298:LEU:HD11	2.53	0.43
1:G:243:THR:HG23	1:G:295:GLN:NE2	2.33	0.43
1:B:234:TRP:CG	1:B:305:SER:HA	2.52	0.43
1:G:81:VAL:HG11	1:G:93:SER:CB	2.47	0.43
1:G:140:GLN:NE2	1:G:142:ILE:HD11	2.32	0.43
1:G:291:LEU:HD22	1:G:296:TYR:CE1	2.53	0.43
1:H:45:ASP:OD2	1:H:137:ARG:NH1	2.51	0.43
1:H:237:LYS:HG2	1:H:238:LEU:N	2.32	0.43
1:D:80:GLU:HB2	1:D:156:TYR:HB2	2.01	0.43
1:D:320:GLY:C	1:D:321:LEU:HD13	2.26	0.43
1:G:61:GLN:HB3	1:G:130:TYR:CZ	2.51	0.43
1:H:77:LYS:HB2	1:H:158:LEU:HD22	2.00	0.43
1:H:112:ASN:ND2	1:H:158:LEU:O	2.52	0.43
1:A:92:THR:O	1:A:96:ILE:HG13	2.18	0.43
1:D:123:GLY:HA3	1:D:126:GLU:HG2	2.00	0.43
1:E:261:PHE:HA	1:E:299:VAL:O	2.18	0.43
1:H:262:ASN:OD1	1:H:276:GLN:HB2	2.18	0.43
1:A:64:ASN:HD22	1:A:67:GLU:CD	2.22	0.43
1:B:71:PHE:O	1:B:117:SER:HA	2.17	0.43
1:D:162:TRP:CH2	1:D:164:SER:HB2	2.53	0.43
1:H:48:ASP:OD1	1:H:137:ARG:HB2	2.19	0.43
1:C:49:GLY:O	1:C:186:CYS:HA	2.18	0.43
1:F:123:GLY:N	1:F:126:GLU:HB3	2.33	0.43
1:D:254:LEU:HD23	1:D:255:ALA:N	2.33	0.43
1:B:188:LEU:HD21	3:B:412:GOL:H11	2.00	0.43
1:C:234:TRP:CG	1:C:305:SER:HA	2.53	0.43
1:E:308:GLY:H	4:E:411:MES:H21	1.84	0.43
1:G:64:ASN:HB2	1:G:67:GLU:CD	2.39	0.43
1:A:61:GLN:HB3	1:A:130:TYR:CE2	2.54	0.43
1:D:285:HIS:HA	3:D:413:GOL:H12	2.00	0.43
1:E:257:LYS:HD3	1:E:282:VAL:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:GLY:C	1:H:137:ARG:HD3	2.38	0.43
1:H:253:ILE:HD12	1:H:316:PHE:CD1	2.54	0.43
1:A:257:LYS:HG3	1:A:258:ILE:HG23	2.00	0.43
1:C:61:GLN:HB3	1:C:130:TYR:CE2	2.53	0.43
1:F:163:LEU:HD22	1:F:164:SER:N	2.34	0.43
1:F:236:GLN:OE1	1:F:236:GLN:HA	2.18	0.43
1:C:259:VAL:O	1:C:285:HIS:NE2	2.51	0.42
1:F:66:ASN:ND2	1:F:124:PRO:HA	2.34	0.42
1:H:251:TYR:HE1	1:H:291:LEU:O	2.02	0.42
1:A:38:SER:HG	1:A:273:LYS:HZ2	1.64	0.42
1:B:247:THR:HG22	1:B:293:ALA:H	1.84	0.42
3:C:402:GOL:H32	4:E:410:MES:H81	2.00	0.42
1:F:250:LYS:HG2	1:F:319:PHE:CD2	2.54	0.42
1:H:54:GLU:N	1:H:55:PRO:CD	2.81	0.42
1:H:253:ILE:O	1:H:286:TYR:CA	2.67	0.42
1:B:207:GLU:HG3	1:B:238:LEU:HD11	2.01	0.42
1:C:63:LEU:HD21	1:C:69:GLY:CA	2.49	0.42
1:G:250:LYS:HE2	5:G:517:HOH:O	2.19	0.42
1:B:144:ILE:HA	1:B:148:ASN:O	2.18	0.42
1:F:106:ILE:HD13	1:F:139:TYR:OH	2.20	0.42
1:B:225:ASP:OD2	3:E:404:GOL:H12	2.20	0.42
1:D:301:LYS:HG2	1:D:302:ALA:O	2.20	0.42
1:F:244:ILE:HG22	1:F:293:ALA:HA	2.00	0.42
1:H:244:ILE:HD13	1:H:292:ASP:O	2.19	0.42
1:A:68:THR:HG22	1:A:121:THR:CB	2.49	0.42
1:C:263:ILE:HG23	1:C:274:LEU:HB2	2.02	0.42
1:D:223:LEU:C	1:D:223:LEU:HD23	2.40	0.42
1:E:108:ILE:HG21	1:E:155:ILE:HD11	2.00	0.42
1:H:283:LYS:HB2	1:H:283:LYS:HE3	1.76	0.42
1:H:163:LEU:C	1:H:163:LEU:HD23	2.40	0.42
1:B:257:LYS:HG3	1:B:258:ILE:HG23	2.02	0.42
1:C:39:ASP:O	1:C:273:LYS:NZ	2.45	0.42
1:E:65:PRO:HG3	1:E:126:GLU:N	2.34	0.42
1:E:207:GLU:OE2	1:E:228:SER:HB2	2.20	0.42
1:H:70:THR:HG23	1:H:118:VAL:O	2.20	0.42
1:H:176:GLN:HB2	3:H:403:GOL:C3	2.49	0.42
1:H:261:PHE:HA	1:H:299:VAL:O	2.20	0.42
1:A:39:ASP:CB	3:A:420:GOL:H32	2.49	0.42
1:A:249:GLN:HG3	1:A:318:LYS:HD2	2.00	0.42
1:C:47:GLY:C	1:C:137:ARG:HD2	2.40	0.42
1:G:235:THR:O	1:G:301:LYS:HE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:ILE:HD12	1:H:44:ILE:N	2.35	0.42
1:H:123:GLY:N	1:H:126:GLU:HG2	2.35	0.42
1:H:157:LYS:NZ	5:H:501:HOH:O	2.52	0.42
1:H:258:ILE:HD11	3:H:402:GOL:H31	2.02	0.42
1:H:264:TYR:HA	1:H:272:VAL:O	2.20	0.42
1:E:46:LYS:HB2	1:E:138:LYS:HB3	2.02	0.42
1:F:212:THR:HG21	1:F:245:THR:OG1	2.20	0.42
1:H:135:THR:O	1:H:158:LEU:HD12	2.20	0.42
1:B:50:TRP:O	1:B:135:THR:HA	2.20	0.41
1:B:230:ASN:HB2	1:B:232:TYR:CZ	2.54	0.41
1:C:301:LYS:HG3	1:C:302:ALA:O	2.20	0.41
1:D:226:TRP:CZ2	1:D:228:SER:HA	2.55	0.41
1:D:291:LEU:HD22	1:D:296:TYR:CE1	2.55	0.41
1:H:96:ILE:HD13	1:H:153:GLY:HA3	2.02	0.41
1:H:251:TYR:CE1	1:H:291:LEU:HB2	2.55	0.41
1:F:54:GLU:O	1:F:57:VAL:HG23	2.20	0.41
1:G:226:TRP:CZ2	1:G:240:LEU:HD13	2.56	0.41
1:A:54:GLU:N	1:A:55:PRO:CD	2.83	0.41
1:C:249:GLN:OE1	1:C:318:LYS:HD2	2.20	0.41
1:E:37:LEU:N	3:E:406:GOL:C3	2.83	0.41
1:E:54:GLU:N	1:E:55:PRO:CD	2.83	0.41
1:A:75:LEU:O	1:A:113:THR:HA	2.20	0.41
1:G:227:ARG:HH11	1:G:311:PRO:CG	2.32	0.41
1:G:254:LEU:CD1	1:G:286:TYR:HB3	2.43	0.41
1:B:292:ASP:O	1:B:296:TYR:OH	2.28	0.41
1:C:79:LYS:HE2	1:C:110:GLU:OE1	2.20	0.41
1:E:80:GLU:HB2	1:E:156:TYR:HB2	2.02	0.41
1:F:253:ILE:HD12	1:F:263:ILE:HD11	2.01	0.41
1:A:64:ASN:HA	1:A:127:TYR:CE2	2.55	0.41
1:B:312:TYR:HA	3:B:411:GOL:H12	2.02	0.41
1:C:108:ILE:HD12	1:C:155:ILE:HD13	2.01	0.41
1:E:44:ILE:HD12	1:E:44:ILE:N	2.36	0.41
1:E:195:ILE:HD12	1:E:195:ILE:N	2.35	0.41
1:F:44:ILE:N	1:F:44:ILE:HD12	2.35	0.41
1:A:280:ASP:HA	2:A:403:PO4:O4	2.21	0.41
1:E:38:SER:HB2	1:E:273:LYS:HZ2	1.82	0.41
1:G:47:GLY:O	1:G:137:ARG:HD2	2.21	0.41
3:G:403:GOL:H12	4:G:414:MES:O3S	2.20	0.41
1:H:244:ILE:HG23	1:H:293:ALA:HA	2.02	0.41
1:A:163:LEU:HD23	1:A:163:LEU:C	2.41	0.41
1:A:261:PHE:HA	1:A:299:VAL:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:VAL:HG22	1:C:132:VAL:O	2.21	0.41
1:C:226:TRP:CH2	1:C:228:SER:HB3	2.56	0.41
1:D:174:ILE:H	1:D:174:ILE:HG13	1.70	0.41
1:F:108:ILE:CD1	1:F:155:ILE:HD13	2.51	0.41
1:G:46:LYS:HD2	1:G:194:ASP:OD1	2.21	0.41
1:G:262:ASN:OD1	1:G:276:GLN:HB2	2.21	0.41
1:G:264:TYR:CD2	1:G:273:LYS:HA	2.56	0.41
4:G:414:MES:O1	1:H:304:SER:HA	2.21	0.41
1:H:76:THR:CB	1:H:113:THR:HG22	2.51	0.41
1:H:118:VAL:HG23	1:H:161:ILE:CD1	2.50	0.41
1:H:195:ILE:N	1:H:195:ILE:HD12	2.36	0.41
1:H:243:THR:HA	1:H:295:GLN:HE22	1.85	0.41
1:H:256:SER:OG	1:H:257:LYS:N	2.54	0.41
1:D:129:TYR:OH	1:D:131:LYS:HD3	2.21	0.41
1:H:179:LEU:HD12	1:H:179:LEU:N	2.36	0.41
1:A:162:TRP:CH2	1:A:164:SER:HB2	2.57	0.40
1:A:258:ILE:HA	1:A:303:ASN:OD1	2.20	0.40
1:A:313:SER:HB3	3:A:414:GOL:O1	2.20	0.40
1:B:138:LYS:CE	3:B:419:GOL:H12	2.50	0.40
1:H:52:LEU:HD11	1:H:80:GLU:HG3	2.02	0.40
1:H:214:ALA:HB1	1:H:224:TYR:CE2	2.56	0.40
1:H:64:ASN:HB2	1:H:67:GLU:OE2	2.22	0.40
1:H:257:LYS:HG3	1:H:258:ILE:HG23	2.03	0.40
1:B:114:ILE:HD12	1:B:160:GLY:HA2	2.03	0.40
1:B:237:LYS:HD3	1:B:299:VAL:CG1	2.51	0.40
1:E:146:HIS:ND1	1:E:260:ASP:OD2	2.50	0.40
1:E:254:LEU:HB3	1:E:315:LEU:HB3	2.03	0.40
1:B:282:VAL:HG12	1:B:283:LYS:HG3	2.04	0.40
1:E:226:TRP:O	1:E:313:SER:HA	2.20	0.40
1:F:71:PHE:O	1:F:71:PHE:CD1	2.74	0.40
1:H:259:VAL:O	1:H:285:HIS:NE2	2.53	0.40
1:A:264:TYR:CD2	1:A:273:LYS:HA	2.56	0.40
1:B:61:GLN:HB2	1:B:130:TYR:CE2	2.56	0.40
1:C:163:LEU:HD23	1:C:163:LEU:C	2.42	0.40
1:D:156:TYR:OH	1:D:184:GLU:OE1	2.29	0.40
1:D:321:LEU:O	1:D:322:VAL:C	2.59	0.40
1:F:163:LEU:C	1:F:163:LEU:HD13	2.42	0.40
1:H:114:ILE:HD13	1:H:158:LEU:HG	2.02	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	283/348 (81%)	278 (98%)	5 (2%)	0	100	100
1	B	284/348 (82%)	280 (99%)	4 (1%)	0	100	100
1	C	284/348 (82%)	278 (98%)	6 (2%)	0	100	100
1	D	284/348 (82%)	277 (98%)	7 (2%)	0	100	100
1	E	286/348 (82%)	278 (97%)	8 (3%)	0	100	100
1	F	284/348 (82%)	273 (96%)	11 (4%)	0	100	100
1	G	283/348 (81%)	278 (98%)	5 (2%)	0	100	100
1	H	281/348 (81%)	271 (96%)	10 (4%)	0	100	100
All	All	2269/2784 (82%)	2213 (98%)	56 (2%)	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/299 (83%)	247 (100%)	0	100	100
1	B	247/299 (83%)	247 (100%)	0	100	100
1	C	249/299 (83%)	249 (100%)	0	100	100
1	D	249/299 (83%)	249 (100%)	0	100	100
1	E	251/299 (84%)	251 (100%)	0	100	100
1	F	247/299 (83%)	247 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	248/299 (83%)	248 (100%)	0	100	100
1	H	248/299 (83%)	248 (100%)	0	100	100
All	All	1986/2392 (83%)	1986 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	218	ASN
1	G	148	ASN
1	H	295	GLN

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)

110 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	E	409	-	5,5,5	0.88	0	5,5,5	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	F	408	-	5,5,5	1.19	1 (20%)	5,5,5	1.42	1 (20%)
3	GOL	E	407	-	5,5,5	1.02	0	5,5,5	1.10	1 (20%)
3	GOL	D	414	-	5,5,5	0.90	0	5,5,5	1.00	0
3	GOL	B	414	-	5,5,5	0.87	0	5,5,5	1.28	1 (20%)
3	GOL	D	411	-	5,5,5	0.95	0	5,5,5	1.05	0
3	GOL	F	412	-	5,5,5	0.87	0	5,5,5	0.97	0
4	MES	E	411	-	12,12,12	2.21	1 (8%)	14,16,16	1.97	4 (28%)
3	GOL	G	412	-	5,5,5	1.05	0	5,5,5	1.07	0
3	GOL	A	413	-	5,5,5	0.87	0	5,5,5	1.05	0
3	GOL	B	415	-	5,5,5	1.02	0	5,5,5	1.14	1 (20%)
3	GOL	H	403	-	5,5,5	0.88	0	5,5,5	1.01	0
3	GOL	D	410	-	5,5,5	0.85	0	5,5,5	0.97	0
3	GOL	A	410	-	5,5,5	0.90	0	5,5,5	1.00	0
2	PO4	E	402	-	4,4,4	0.93	0	6,6,6	0.45	0
3	GOL	H	402	-	5,5,5	0.87	0	5,5,5	1.01	0
3	GOL	F	409	-	5,5,5	1.06	0	5,5,5	1.22	1 (20%)
3	GOL	G	408	-	5,5,5	1.10	1 (20%)	5,5,5	1.16	1 (20%)
2	PO4	A	401	-	4,4,4	0.92	0	6,6,6	0.42	0
3	GOL	B	419	-	5,5,5	0.93	0	5,5,5	1.09	1 (20%)
3	GOL	C	412	-	5,5,5	1.29	1 (20%)	5,5,5	1.48	1 (20%)
3	GOL	A	417	-	5,5,5	0.93	0	5,5,5	1.08	0
3	GOL	C	413	-	5,5,5	0.85	0	5,5,5	1.00	0
2	PO4	B	402	-	4,4,4	0.82	0	6,6,6	0.46	0
3	GOL	B	405	-	5,5,5	0.88	0	5,5,5	1.01	0
2	PO4	F	401	-	4,4,4	0.93	0	6,6,6	0.43	0
3	GOL	F	406	-	5,5,5	0.87	0	5,5,5	1.03	0
3	GOL	D	402	-	5,5,5	0.90	0	5,5,5	0.99	0
3	GOL	B	410	-	5,5,5	0.88	0	5,5,5	1.01	0
3	GOL	D	407	-	5,5,5	0.94	0	5,5,5	0.98	0
2	PO4	H	401	-	4,4,4	0.93	0	6,6,6	0.45	0
3	GOL	D	404	-	5,5,5	0.89	0	5,5,5	0.98	0
3	GOL	A	415	-	5,5,5	0.90	0	5,5,5	1.08	0
3	GOL	F	404	-	5,5,5	0.94	0	5,5,5	0.99	0
3	GOL	A	409	-	5,5,5	0.95	0	5,5,5	0.96	0
3	GOL	F	403	-	5,5,5	0.93	0	5,5,5	0.98	0
3	GOL	A	411	-	5,5,5	0.93	0	5,5,5	0.98	0
3	GOL	C	410	-	5,5,5	0.98	0	5,5,5	1.08	0
3	GOL	A	420	-	5,5,5	1.00	0	5,5,5	1.16	1 (20%)
3	GOL	C	409	-	5,5,5	0.95	0	5,5,5	0.83	0
3	GOL	C	403	-	5,5,5	0.89	0	5,5,5	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	416	-	5,5,5	1.12	0	5,5,5	1.31	1 (20%)
3	GOL	F	411	-	5,5,5	1.05	0	5,5,5	1.15	1 (20%)
3	GOL	A	412	-	5,5,5	0.85	0	5,5,5	1.00	0
3	GOL	G	405	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	G	411	-	5,5,5	1.15	0	5,5,5	1.28	1 (20%)
3	GOL	G	404	-	5,5,5	0.91	0	5,5,5	0.99	0
4	MES	B	422	-	12,12,12	2.24	1 (8%)	14,16,16	1.76	5 (35%)
2	PO4	B	401	-	4,4,4	0.92	0	6,6,6	0.42	0
3	GOL	C	408	-	5,5,5	1.00	0	5,5,5	1.29	1 (20%)
3	GOL	D	413	-	5,5,5	0.91	0	5,5,5	0.97	0
3	GOL	D	405	-	5,5,5	0.95	0	5,5,5	0.96	0
3	GOL	B	420	-	5,5,5	0.96	0	5,5,5	0.98	0
3	GOL	A	405	-	5,5,5	0.87	0	5,5,5	1.00	0
3	GOL	E	403	-	5,5,5	1.00	0	5,5,5	0.96	0
3	GOL	F	402	-	5,5,5	0.91	0	5,5,5	0.99	0
2	PO4	B	403	-	4,4,4	0.94	0	6,6,6	0.43	0
3	GOL	B	408	-	5,5,5	0.89	0	5,5,5	1.03	0
2	PO4	D	401	-	4,4,4	0.94	0	6,6,6	0.44	0
3	GOL	B	409	-	5,5,5	0.88	0	5,5,5	1.00	0
3	GOL	B	411	-	5,5,5	0.92	0	5,5,5	1.01	0
2	PO4	A	403	-	4,4,4	0.93	0	6,6,6	0.43	0
3	GOL	A	416	-	5,5,5	0.94	0	5,5,5	1.18	1 (20%)
3	GOL	E	408	-	5,5,5	1.13	0	5,5,5	1.18	1 (20%)
3	GOL	E	406	-	5,5,5	0.94	0	5,5,5	1.15	1 (20%)
3	GOL	D	403	-	5,5,5	0.93	0	5,5,5	1.00	0
3	GOL	B	417	-	5,5,5	0.98	0	5,5,5	1.19	1 (20%)
3	GOL	G	406	-	5,5,5	0.91	0	5,5,5	0.98	0
4	MES	E	410	-	12,12,12	2.25	1 (8%)	14,16,16	1.81	4 (28%)
3	GOL	C	405	-	5,5,5	0.88	0	5,5,5	0.99	0
3	GOL	C	402	-	5,5,5	0.97	0	5,5,5	1.01	0
3	GOL	C	406	-	5,5,5	0.92	0	5,5,5	0.95	0
3	GOL	G	410	-	5,5,5	1.03	0	5,5,5	1.13	1 (20%)
3	GOL	G	409	-	5,5,5	0.99	0	5,5,5	1.13	1 (20%)
3	GOL	G	407	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	A	414	-	5,5,5	0.78	0	5,5,5	0.95	0
2	PO4	G	402	-	4,4,4	0.88	0	6,6,6	0.43	0
3	GOL	G	403	-	5,5,5	0.91	0	5,5,5	1.03	0
4	MES	G	414	-	12,12,12	2.22	1 (8%)	14,16,16	1.73	4 (28%)
2	PO4	C	401	-	4,4,4	0.93	0	6,6,6	0.42	0
3	GOL	B	406	-	5,5,5	0.88	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	D	409	-	5,5,5	1.12	1 (20%)	5,5,5	1.22	1 (20%)
2	PO4	A	404	-	4,4,4	0.93	0	6,6,6	0.43	0
3	GOL	A	418	-	5,5,5	1.01	0	5,5,5	1.18	1 (20%)
3	GOL	G	413	-	5,5,5	0.90	0	5,5,5	0.99	0
3	GOL	D	412	-	5,5,5	0.89	0	5,5,5	1.04	0
3	GOL	C	404	-	5,5,5	0.88	0	5,5,5	0.99	0
3	GOL	E	405	-	5,5,5	0.86	0	5,5,5	0.98	0
3	GOL	A	419	-	5,5,5	1.02	0	5,5,5	1.06	0
3	GOL	A	407	-	5,5,5	0.87	0	5,5,5	1.05	0
2	PO4	A	402	-	4,4,4	0.93	0	6,6,6	0.42	0
2	PO4	G	401	-	4,4,4	0.93	0	6,6,6	0.44	0
3	GOL	C	411	-	5,5,5	0.90	0	5,5,5	0.96	0
2	PO4	B	404	-	4,4,4	0.95	0	6,6,6	0.43	0
3	GOL	B	418	-	5,5,5	0.97	0	5,5,5	1.15	1 (20%)
2	PO4	E	401	-	4,4,4	0.94	0	6,6,6	0.43	0
3	GOL	B	421	-	5,5,5	0.89	0	5,5,5	0.98	0
3	GOL	F	405	-	5,5,5	0.91	0	5,5,5	1.02	0
3	GOL	D	408	-	5,5,5	0.87	0	5,5,5	1.03	0
3	GOL	C	407	-	5,5,5	0.91	0	5,5,5	1.00	0
3	GOL	A	406	-	5,5,5	0.92	0	5,5,5	0.99	0
3	GOL	B	412	-	5,5,5	0.92	0	5,5,5	1.00	0
3	GOL	F	410	-	5,5,5	1.07	0	5,5,5	1.22	1 (20%)
3	GOL	B	407	-	5,5,5	0.91	0	5,5,5	1.01	0
3	GOL	E	404	-	5,5,5	0.91	0	5,5,5	0.99	0
3	GOL	A	408	-	5,5,5	0.99	0	5,5,5	0.94	0
4	MES	H	404	-	12,12,12	2.24	1 (8%)	14,16,16	1.56	4 (28%)
3	GOL	F	407	-	5,5,5	0.93	0	5,5,5	1.03	0
3	GOL	B	413	-	5,5,5	0.90	0	5,5,5	1.01	0
3	GOL	D	406	-	5,5,5	0.91	0	5,5,5	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	409	-	-	1/4/4/4	-
3	GOL	F	408	-	-	0/4/4/4	-
3	GOL	E	407	-	-	2/4/4/4	-
3	GOL	D	414	-	-	0/4/4/4	-
3	GOL	B	414	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	411	-	-	2/4/4/4	-
3	GOL	F	412	-	-	2/4/4/4	-
4	MES	E	411	-	-	4/6/14/14	0/1/1/1
3	GOL	G	412	-	-	1/4/4/4	-
3	GOL	A	413	-	-	0/4/4/4	-
3	GOL	B	415	-	-	0/4/4/4	-
3	GOL	H	403	-	-	0/4/4/4	-
3	GOL	D	410	-	-	0/4/4/4	-
3	GOL	A	410	-	-	0/4/4/4	-
3	GOL	H	402	-	-	0/4/4/4	-
3	GOL	F	409	-	-	1/4/4/4	-
3	GOL	G	408	-	-	0/4/4/4	-
3	GOL	B	419	-	-	2/4/4/4	-
3	GOL	C	412	-	-	0/4/4/4	-
3	GOL	A	417	-	-	1/4/4/4	-
3	GOL	C	413	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	F	406	-	-	0/4/4/4	-
3	GOL	D	402	-	-	2/4/4/4	-
3	GOL	B	410	-	-	0/4/4/4	-
3	GOL	D	407	-	-	0/4/4/4	-
3	GOL	D	404	-	-	0/4/4/4	-
3	GOL	A	415	-	-	1/4/4/4	-
3	GOL	F	404	-	-	0/4/4/4	-
3	GOL	A	409	-	-	1/4/4/4	-
3	GOL	F	403	-	-	0/4/4/4	-
3	GOL	A	411	-	-	0/4/4/4	-
3	GOL	C	410	-	-	2/4/4/4	-
3	GOL	A	420	-	-	0/4/4/4	-
3	GOL	C	409	-	-	0/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	B	416	-	-	0/4/4/4	-
3	GOL	F	411	-	-	0/4/4/4	-
3	GOL	A	412	-	-	2/4/4/4	-
3	GOL	G	405	-	-	0/4/4/4	-
3	GOL	G	411	-	-	1/4/4/4	-
3	GOL	G	404	-	-	0/4/4/4	-
4	MES	B	422	-	-	0/6/14/14	0/1/1/1
3	GOL	C	408	-	-	1/4/4/4	-
3	GOL	D	413	-	-	0/4/4/4	-
3	GOL	D	405	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	420	-	-	0/4/4/4	-
3	GOL	A	405	-	-	0/4/4/4	-
3	GOL	E	403	-	-	0/4/4/4	-
3	GOL	F	402	-	-	0/4/4/4	-
3	GOL	B	408	-	-	0/4/4/4	-
3	GOL	B	409	-	-	0/4/4/4	-
3	GOL	B	411	-	-	0/4/4/4	-
3	GOL	A	416	-	-	0/4/4/4	-
3	GOL	E	408	-	-	4/4/4/4	-
3	GOL	E	406	-	-	0/4/4/4	-
3	GOL	D	403	-	-	0/4/4/4	-
3	GOL	B	417	-	-	0/4/4/4	-
3	GOL	G	406	-	-	0/4/4/4	-
4	MES	E	410	-	-	1/6/14/14	0/1/1/1
3	GOL	C	405	-	-	0/4/4/4	-
3	GOL	C	402	-	-	2/4/4/4	-
3	GOL	C	406	-	-	1/4/4/4	-
3	GOL	G	410	-	-	2/4/4/4	-
3	GOL	G	409	-	-	2/4/4/4	-
3	GOL	G	407	-	-	2/4/4/4	-
3	GOL	A	414	-	-	0/4/4/4	-
3	GOL	G	403	-	-	0/4/4/4	-
4	MES	G	414	-	-	3/6/14/14	0/1/1/1
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	D	409	-	-	3/4/4/4	-
3	GOL	A	418	-	-	0/4/4/4	-
3	GOL	G	413	-	-	0/4/4/4	-
3	GOL	D	412	-	-	2/4/4/4	-
3	GOL	C	404	-	-	1/4/4/4	-
3	GOL	E	405	-	-	2/4/4/4	-
3	GOL	A	419	-	-	2/4/4/4	-
3	GOL	A	407	-	-	0/4/4/4	-
3	GOL	C	411	-	-	2/4/4/4	-
3	GOL	B	418	-	-	0/4/4/4	-
3	GOL	B	421	-	-	0/4/4/4	-
3	GOL	F	405	-	-	0/4/4/4	-
3	GOL	D	408	-	-	0/4/4/4	-
3	GOL	C	407	-	-	4/4/4/4	-
3	GOL	A	406	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	412	-	-	0/4/4/4	-
3	GOL	F	410	-	-	2/4/4/4	-
3	GOL	B	407	-	-	0/4/4/4	-
3	GOL	E	404	-	-	0/4/4/4	-
3	GOL	A	408	-	-	0/4/4/4	-
4	MES	H	404	-	-	0/6/14/14	0/1/1/1
3	GOL	F	407	-	-	0/4/4/4	-
3	GOL	B	413	-	-	0/4/4/4	-
3	GOL	D	406	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	410	MES	C8-S	-7.50	1.66	1.77
4	B	422	MES	C8-S	-7.49	1.66	1.77
4	H	404	MES	C8-S	-7.47	1.66	1.77
4	G	414	MES	C8-S	-7.45	1.66	1.77
4	E	411	MES	C8-S	-7.40	1.67	1.77
3	C	412	GOL	O2-C2	-2.26	1.36	1.43
3	D	409	GOL	O2-C2	-2.03	1.37	1.43
3	F	408	GOL	O2-C2	-2.02	1.37	1.43
3	G	408	GOL	O2-C2	-2.00	1.37	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	411	MES	C2-C3-N4	-3.89	104.21	110.10
4	E	410	MES	O2S-S-C8	3.53	111.17	106.92
4	E	411	MES	C5-N4-C3	3.52	116.74	108.83
4	B	422	MES	C2-C3-N4	-3.40	104.95	110.10
4	G	414	MES	O3S-S-C8	3.31	111.12	105.77
4	E	410	MES	C2-C3-N4	-3.21	105.24	110.10
3	C	412	GOL	C3-C2-C1	-2.94	100.27	111.70
4	G	414	MES	C6-C5-N4	-2.90	105.71	110.10
4	E	411	MES	O3S-S-C8	2.89	110.44	105.77
4	B	422	MES	C5-N4-C3	2.85	115.23	108.83
4	H	404	MES	O2S-S-C8	2.84	110.34	106.92
3	F	408	GOL	C3-C2-C1	-2.76	100.96	111.70
4	G	414	MES	C5-N4-C3	2.75	115.02	108.83
4	B	422	MES	O3S-S-C8	2.49	109.79	105.77
3	G	411	GOL	C3-C2-C1	-2.45	102.19	111.70
3	B	416	GOL	C3-C2-C1	-2.43	102.27	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	408	GOL	C3-C2-C1	-2.38	102.43	111.70
3	D	409	GOL	C3-C2-C1	-2.32	102.69	111.70
4	E	410	MES	O3S-S-C8	2.32	109.51	105.77
4	G	414	MES	O2S-S-C8	2.30	109.68	106.92
4	H	404	MES	O1S-S-C8	2.28	109.67	106.92
3	B	414	GOL	C3-C2-C1	-2.28	102.85	111.70
3	F	409	GOL	C3-C2-C1	-2.27	102.87	111.70
3	F	410	GOL	C3-C2-C1	-2.25	102.97	111.70
4	B	422	MES	O2S-S-C8	2.24	109.61	106.92
4	H	404	MES	C6-C5-N4	-2.24	106.71	110.10
3	B	417	GOL	C3-C2-C1	-2.23	103.04	111.70
3	A	420	GOL	C3-C2-C1	-2.19	103.19	111.70
3	B	418	GOL	C3-C2-C1	-2.18	103.24	111.70
3	E	408	GOL	C3-C2-C1	-2.18	103.24	111.70
3	A	418	GOL	C3-C2-C1	-2.18	103.24	111.70
4	E	411	MES	O2S-S-C8	2.16	109.52	106.92
3	A	416	GOL	C3-C2-C1	-2.15	103.35	111.70
3	E	407	GOL	C3-C2-C1	-2.12	103.48	111.70
4	H	404	MES	O3S-S-C8	2.12	109.19	105.77
4	E	410	MES	C7-N4-C3	2.11	116.63	111.23
3	G	408	GOL	C3-C2-C1	-2.09	103.57	111.70
3	B	419	GOL	C3-C2-C1	-2.09	103.58	111.70
3	G	410	GOL	C3-C2-C1	-2.08	103.63	111.70
3	G	409	GOL	C3-C2-C1	-2.07	103.64	111.70
4	B	422	MES	O1S-S-C8	2.07	109.41	106.92
3	B	415	GOL	C3-C2-C1	-2.07	103.67	111.70
3	F	411	GOL	C3-C2-C1	-2.06	103.69	111.70
3	E	406	GOL	C3-C2-C1	-2.05	103.73	111.70

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	419	GOL	C1-C2-C3-O3
3	C	410	GOL	C1-C2-C3-O3
3	C	411	GOL	C1-C2-C3-O3
3	F	410	GOL	C1-C2-C3-O3
3	G	407	GOL	C1-C2-C3-O3
3	G	410	GOL	C1-C2-C3-O3
4	E	411	MES	C7-C8-S-O2S
4	G	414	MES	C7-C8-S-O2S
4	E	411	MES	C7-C8-S-O3S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	414	MES	C7-C8-S-O3S
3	A	412	GOL	C1-C2-C3-O3
3	B	414	GOL	O1-C1-C2-C3
3	C	402	GOL	O1-C1-C2-C3
3	C	406	GOL	C1-C2-C3-O3
3	C	407	GOL	O1-C1-C2-C3
3	C	408	GOL	O1-C1-C2-C3
3	D	402	GOL	O1-C1-C2-C3
3	D	409	GOL	O1-C1-C2-C3
3	D	412	GOL	O1-C1-C2-C3
3	B	419	GOL	O2-C2-C3-O3
3	C	411	GOL	O2-C2-C3-O3
3	A	412	GOL	O2-C2-C3-O3
3	C	410	GOL	O2-C2-C3-O3
3	F	410	GOL	O2-C2-C3-O3
3	G	407	GOL	O2-C2-C3-O3
3	G	410	GOL	O2-C2-C3-O3
3	A	406	GOL	O1-C1-C2-C3
3	F	412	GOL	O1-C1-C2-C3
3	G	412	GOL	O1-C1-C2-C3
3	A	419	GOL	O2-C2-C3-O3
3	C	407	GOL	O2-C2-C3-O3
3	A	415	GOL	O2-C2-C3-O3
3	C	404	GOL	O2-C2-C3-O3
3	D	411	GOL	O2-C2-C3-O3
3	E	405	GOL	O2-C2-C3-O3
3	E	408	GOL	O1-C1-C2-O2
3	E	408	GOL	O2-C2-C3-O3
3	G	409	GOL	O2-C2-C3-O3
3	E	405	GOL	C1-C2-C3-O3
3	E	407	GOL	C1-C2-C3-O3
3	E	408	GOL	O1-C1-C2-C3
3	E	408	GOL	C1-C2-C3-O3
4	E	411	MES	C7-C8-S-O1S
4	G	414	MES	C7-C8-S-O1S
3	A	417	GOL	O1-C1-C2-C3
3	C	407	GOL	O1-C1-C2-O2
3	D	412	GOL	O1-C1-C2-O2
4	E	411	MES	C8-C7-N4-C5
3	G	411	GOL	O2-C2-C3-O3
3	D	411	GOL	C1-C2-C3-O3
3	E	409	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	409	GOL	C1-C2-C3-O3
3	D	402	GOL	O1-C1-C2-O2
3	D	409	GOL	O1-C1-C2-O2
3	E	407	GOL	O2-C2-C3-O3
3	A	409	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-O2
3	F	409	GOL	O2-C2-C3-O3
3	F	412	GOL	O1-C1-C2-O2
3	A	419	GOL	C1-C2-C3-O3
3	C	407	GOL	C1-C2-C3-O3
4	E	410	MES	C7-C8-S-O1S
3	D	409	GOL	O2-C2-C3-O3

There are no ring outliers.

52 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	409	GOL	1	0
3	F	408	GOL	1	0
3	E	407	GOL	1	0
3	D	414	GOL	2	0
3	D	411	GOL	3	0
4	E	411	MES	2	0
3	G	412	GOL	1	0
3	B	415	GOL	1	0
3	H	403	GOL	2	0
3	D	410	GOL	1	0
3	A	410	GOL	2	0
3	H	402	GOL	1	0
3	F	409	GOL	2	0
3	G	408	GOL	2	0
3	B	419	GOL	4	0
3	A	417	GOL	1	0
3	C	413	GOL	2	0
2	F	401	PO4	1	0
3	B	410	GOL	2	0
3	D	407	GOL	1	0
3	D	404	GOL	3	0
3	F	404	GOL	1	0
3	F	403	GOL	1	0
3	C	410	GOL	2	0
3	A	420	GOL	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	416	GOL	2	0
3	G	405	GOL	2	0
3	D	413	GOL	3	0
3	B	420	GOL	1	0
3	A	405	GOL	1	0
3	B	411	GOL	1	0
2	A	403	PO4	1	0
3	E	406	GOL	2	0
3	D	403	GOL	3	0
3	B	417	GOL	3	0
3	G	406	GOL	1	0
4	E	410	MES	1	0
3	C	402	GOL	1	0
3	G	410	GOL	1	0
3	G	407	GOL	2	0
3	A	414	GOL	2	0
3	G	403	GOL	2	0
4	G	414	MES	2	0
3	D	412	GOL	1	0
3	C	404	GOL	1	0
3	A	419	GOL	1	0
2	B	404	PO4	1	0
3	D	408	GOL	1	0
3	B	412	GOL	4	0
3	E	404	GOL	1	0
3	B	413	GOL	1	0
3	D	406	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	285/348 (81%)	0.41	8 (2%) 53 60	30, 66, 113, 125	0
1	B	286/348 (82%)	0.24	1 (0%) 94 96	46, 61, 87, 171	0
1	C	286/348 (82%)	0.43	10 (3%) 44 51	46, 63, 110, 138	0
1	D	286/348 (82%)	0.36	7 (2%) 59 66	45, 59, 104, 147	0
1	E	287/348 (82%)	0.43	17 (5%) 22 29	47, 68, 125, 159	0
1	F	286/348 (82%)	0.61	27 (9%) 8 11	55, 80, 138, 179	0
1	G	285/348 (81%)	0.21	2 (0%) 87 91	51, 68, 101, 138	0
1	H	285/348 (81%)	0.82	34 (11%) 4 6	62, 91, 131, 258	0
All	All	2286/2784 (82%)	0.44	106 (4%) 32 40	30, 69, 121, 258	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	118	VAL	4.9
1	E	127	TYR	4.9
1	H	322	VAL	4.7
1	F	125	ASN	4.6
1	H	190	VAL	4.5
1	E	174	ILE	4.4
1	F	123	GLY	4.1
1	C	125	ASN	4.0
1	E	322	VAL	4.0
1	H	310	TYR	3.9
1	F	66	ASN	3.9
1	F	121	THR	3.8
1	G	268	PHE	3.7
1	H	214	ALA	3.7
1	E	124	PRO	3.7
1	F	71	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	268	PHE	3.7
1	A	189	THR	3.5
1	F	124	PRO	3.5
1	D	321	LEU	3.4
1	F	171	LEU	3.4
1	C	75	LEU	3.4
1	H	71	PHE	3.3
1	F	126	GLU	3.3
1	A	321	LEU	3.3
1	H	215	LEU	3.3
1	H	319	PHE	3.3
1	C	190	VAL	3.3
1	E	323	PRO	3.3
1	C	127	TYR	3.2
1	F	130	TYR	3.2
1	F	174	ILE	3.2
1	C	62	ILE	3.1
1	F	122	ALA	3.1
1	D	171	LEU	3.1
1	H	44	ILE	3.0
1	A	188	LEU	2.9
1	H	243	THR	2.9
1	H	248	GLY	2.9
1	F	62	ILE	2.9
1	C	124	PRO	2.8
1	F	219	PRO	2.8
1	E	125	ASN	2.8
1	H	224	TYR	2.8
1	F	119	SER	2.7
1	H	166	THR	2.7
1	E	65	PRO	2.7
1	F	163	LEU	2.7
1	G	190	VAL	2.7
1	C	171	LEU	2.7
1	H	291	LEU	2.6
1	E	168	ALA	2.6
1	H	209	LEU	2.6
1	F	120	THR	2.6
1	H	320	GLY	2.6
1	H	289	ILE	2.6
1	H	178	SER	2.5
1	D	125	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	189	THR	2.5
1	F	68	THR	2.5
1	H	317	GLN	2.5
1	H	321	LEU	2.5
1	E	122	ALA	2.5
1	H	43	VAL	2.5
1	D	124	PRO	2.5
1	H	251	TYR	2.5
1	H	125	ASN	2.4
1	A	190	VAL	2.4
1	F	58	VAL	2.4
1	H	211	LEU	2.4
1	D	190	VAL	2.4
1	F	118	VAL	2.4
1	E	123	GLY	2.4
1	H	168	ALA	2.4
1	H	253	ILE	2.3
1	F	127	TYR	2.3
1	F	129	TYR	2.3
1	H	75	LEU	2.3
1	D	66	ASN	2.3
1	E	169	ASP	2.3
1	F	117	SER	2.3
1	A	132	VAL	2.2
1	E	121	THR	2.2
1	A	268	PHE	2.2
1	B	263	ILE	2.2
1	C	122	ALA	2.2
1	F	168	ALA	2.2
1	E	118	VAL	2.2
1	H	210	ASN	2.1
1	D	127	TYR	2.1
1	C	118	VAL	2.1
1	F	69	GLY	2.1
1	E	219	PRO	2.1
1	H	50	TRP	2.1
1	C	66	ASN	2.1
1	E	171	LEU	2.1
1	E	58	VAL	2.1
1	F	70	THR	2.1
1	E	129	TYR	2.1
1	H	102	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	129	TYR	2.1
1	A	163	LEU	2.0
1	F	75	LEU	2.0
1	F	263	ILE	2.0
1	H	208	ARG	2.0
1	A	114	ILE	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	B-factors(Å^2)	Q<0.9
3	GOL	D	407	6/6	0.38	0.27	90,103,108,110	0
3	GOL	F	403	6/6	0.38	0.29	100,123,126,127	0
3	GOL	B	420	6/6	0.41	0.38	101,117,131,141	0
3	GOL	C	402	6/6	0.53	0.29	79,84,103,109	0
3	GOL	B	419	6/6	0.54	0.40	102,125,155,155	0
4	MES	E	411	12/12	0.56	0.51	167,200,219,234	0
4	MES	E	410	12/12	0.59	0.45	165,204,223,245	0
4	MES	G	414	12/12	0.60	0.44	145,190,236,245	0
3	GOL	B	412	6/6	0.62	0.40	81,114,119,119	0
3	GOL	B	413	6/6	0.63	0.38	85,106,112,112	0
3	GOL	B	415	6/6	0.63	0.53	103,132,158,159	0
2	PO4	A	404	5/5	0.63	0.47	182,184,188,193	0
3	GOL	D	409	6/6	0.63	0.37	83,118,142,157	0
3	GOL	C	412	6/6	0.64	0.24	76,100,120,120	0
3	GOL	F	402	6/6	0.64	0.19	77,96,112,115	0
3	GOL	D	408	6/6	0.66	0.27	76,93,109,115	0
3	GOL	D	410	6/6	0.68	0.44	134,161,172,178	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	G	408	6/6	0.69	0.30	109,134,162,162	0
3	GOL	E	408	6/6	0.69	0.32	97,134,152,166	0
3	GOL	F	410	6/6	0.70	0.32	83,119,143,145	0
3	GOL	E	407	6/6	0.70	0.45	94,119,143,143	0
3	GOL	C	405	6/6	0.70	0.30	111,113,115,120	0
3	GOL	A	420	6/6	0.70	0.43	117,154,172,196	0
3	GOL	E	406	6/6	0.70	0.20	118,142,159,170	0
4	MES	H	404	12/12	0.70	0.39	141,192,218,232	0
3	GOL	F	405	6/6	0.71	0.29	90,107,109,113	0
3	GOL	F	408	6/6	0.71	0.29	119,142,167,171	0
2	PO4	B	403	5/5	0.71	0.44	154,157,170,176	0
3	GOL	C	406	6/6	0.71	0.20	116,121,122,126	0
3	GOL	C	407	6/6	0.72	0.31	91,104,108,112	0
3	GOL	B	408	6/6	0.73	0.19	93,108,116,116	0
3	GOL	D	413	6/6	0.73	0.20	78,115,138,138	0
2	PO4	C	401	5/5	0.73	0.25	156,165,168,171	0
3	GOL	B	411	6/6	0.74	0.27	88,98,103,106	0
2	PO4	F	401	5/5	0.75	0.34	157,161,162,165	0
4	MES	B	422	12/12	0.75	0.43	132,164,196,200	0
3	GOL	A	408	6/6	0.75	0.39	100,107,115,123	0
3	GOL	G	412	6/6	0.76	0.30	121,145,154,157	0
3	GOL	C	403	6/6	0.76	0.22	97,101,103,110	0
3	GOL	F	404	6/6	0.76	0.17	105,111,118,120	0
3	GOL	G	405	6/6	0.76	0.30	111,115,121,122	0
2	PO4	D	401	5/5	0.76	0.28	158,164,168,175	0
3	GOL	G	411	6/6	0.76	0.35	108,129,139,142	0
3	GOL	H	402	6/6	0.77	0.25	81,102,107,121	0
3	GOL	D	405	6/6	0.77	0.16	96,120,130,131	0
3	GOL	G	409	6/6	0.77	0.40	104,135,159,163	0
3	GOL	F	411	6/6	0.78	0.27	92,117,138,141	0
2	PO4	B	401	5/5	0.78	0.29	173,176,178,185	0
3	GOL	C	409	6/6	0.78	0.28	79,123,141,157	0
3	GOL	A	413	6/6	0.79	0.27	94,101,105,107	0
3	GOL	A	417	6/6	0.79	0.20	100,129,154,156	0
2	PO4	B	404	5/5	0.79	0.41	158,161,163,174	0
2	PO4	E	402	5/5	0.79	0.45	162,167,170,189	0
3	GOL	B	418	6/6	0.80	0.37	123,148,163,163	0
3	GOL	G	407	6/6	0.80	0.14	125,150,163,170	0
3	GOL	C	404	6/6	0.80	0.27	88,92,99,115	0
3	GOL	B	421	6/6	0.80	0.29	99,111,117,125	0
3	GOL	A	409	6/6	0.80	0.20	80,87,91,102	0
3	GOL	D	406	6/6	0.80	0.18	94,107,110,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	419	6/6	0.81	0.45	88,118,142,162	0
2	PO4	A	402	5/5	0.81	0.38	138,144,161,169	0
3	GOL	G	404	6/6	0.82	0.28	85,100,103,106	0
3	GOL	D	404	6/6	0.82	0.37	101,105,112,112	0
3	GOL	B	414	6/6	0.82	0.41	85,118,142,156	0
3	GOL	G	413	6/6	0.82	0.20	94,103,107,109	0
2	PO4	H	401	5/5	0.82	0.49	171,176,181,193	0
3	GOL	A	415	6/6	0.83	0.25	84,108,130,141	0
2	PO4	G	401	5/5	0.83	0.24	138,139,142,146	0
3	GOL	C	408	6/6	0.85	0.29	94,117,143,152	0
3	GOL	D	412	6/6	0.86	0.27	85,109,144,144	0
3	GOL	A	416	6/6	0.86	0.24	87,108,136,141	0
3	GOL	G	406	6/6	0.86	0.23	92,97,105,120	0
3	GOL	B	410	6/6	0.86	0.19	82,90,101,112	0
3	GOL	A	410	6/6	0.86	0.30	93,102,108,112	0
2	PO4	E	401	5/5	0.87	0.16	162,162,165,179	0
3	GOL	F	406	6/6	0.87	0.19	100,102,105,105	0
3	GOL	B	409	6/6	0.87	0.21	75,83,86,89	0
3	GOL	A	418	6/6	0.87	0.19	107,129,138,139	0
3	GOL	F	412	6/6	0.88	0.12	70,76,91,96	0
3	GOL	D	411	6/6	0.88	0.39	86,126,151,179	0
3	GOL	G	410	6/6	0.88	0.44	115,139,150,155	0
3	GOL	D	402	6/6	0.88	0.15	78,86,91,108	0
3	GOL	B	417	6/6	0.88	0.25	103,131,164,164	0
3	GOL	E	409	6/6	0.88	0.21	83,87,104,105	0
3	GOL	A	411	6/6	0.89	0.28	77,104,105,108	0
3	GOL	A	406	6/6	0.89	0.22	69,75,99,108	0
3	GOL	E	403	6/6	0.89	0.25	76,90,109,120	0
3	GOL	C	410	6/6	0.89	0.46	84,117,147,147	0
3	GOL	B	405	6/6	0.89	0.22	91,99,106,113	0
3	GOL	B	416	6/6	0.89	0.37	100,120,135,142	0
3	GOL	D	403	6/6	0.89	0.24	73,91,102,108	0
3	GOL	A	405	6/6	0.89	0.18	82,90,91,96	0
3	GOL	F	407	6/6	0.90	0.19	98,118,135,136	0
2	PO4	A	403	5/5	0.90	0.40	125,135,143,146	0
3	GOL	A	407	6/6	0.90	0.21	71,87,92,94	0
3	GOL	E	404	6/6	0.90	0.24	93,103,104,106	0
3	GOL	B	407	6/6	0.90	0.24	121,123,127,129	0
3	GOL	C	413	6/6	0.90	0.17	71,79,91,109	0
2	PO4	B	402	5/5	0.90	0.16	85,90,98,110	0
3	GOL	F	409	6/6	0.91	0.23	104,125,142,150	0
3	GOL	D	414	6/6	0.91	0.16	71,78,89,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	H	403	6/6	0.92	0.22	84,93,104,110	0
3	GOL	B	406	6/6	0.92	0.28	79,90,92,99	0
2	PO4	G	402	5/5	0.94	0.20	85,86,98,109	0
3	GOL	E	405	6/6	0.94	0.13	79,104,111,124	0
3	GOL	G	403	6/6	0.94	0.23	101,104,105,107	0
3	GOL	A	414	6/6	0.94	0.31	97,117,132,140	0
2	PO4	A	401	5/5	0.95	0.20	121,127,132,136	0
3	GOL	A	412	6/6	0.95	0.22	72,86,92,98	0
3	GOL	C	411	6/6	0.95	0.25	84,101,116,135	0

6.5 Other polymers (i)

There are no such residues in this entry.