Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:30 AM GMT

PDB ID	:	3ANZ
Title	:	Crystal Structure of alpha-hemolysin
Authors	:	Yamashita, K.; Kawauchi, H.; Tanaka, Y.; Yao, M.; Tanaka, I.
Deposited on	:	2010-09-16
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

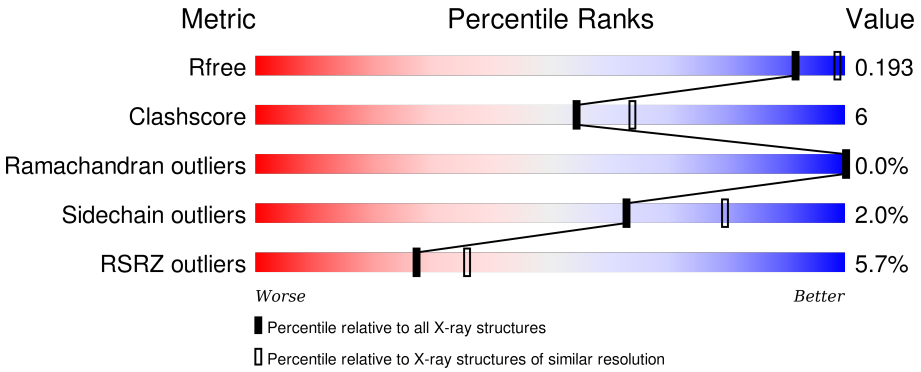
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	302	3% 84% 13%
1	B	302	5% 81% 16%
1	C	302	5% 81% 16%
1	D	302	5% 83% 13%
1	E	302	11% 82% 14%

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Mol	Chain	Length	Quality of chain
1	F	302	8% 83% 14%
1	G	302	6% 85% 12%
1	H	302	3% 85% 12%
1	I	302	4% 87% 10%
1	J	302	5% 85% 11%
1	K	302	4% 86% 11%
1	L	302	4% 85% 11%
1	M	302	9% 83% 14%
1	N	302	5% 84% 13%
1	O	302	7% 84% 13%
1	P	302	4% 85% 12%
1	Q	302	7% 82% 14%
1	R	302	5% 85% 12%
1	S	302	6% 85% 11%
1	T	302	5% 84% 13%
1	U	302	5% 82% 16%
1	V	302	5% 82% 15%
1	W	302	8% 80% 16%
1	X	302	6% 82% 15%
1	Y	302	7% 83% 14%
1	Z	302	5% 87% 10%
1	a	302	5% 95%
1	b	302	5% 95%

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	MPD	A	302	-	-	X	X
2	MPD	B	302	-	-	X	X
2	MPD	B	303	-	-	X	X
2	MPD	E	302	-	-	X	-
2	MPD	E	303	-	-	-	X
2	MPD	F	303	-	-	X	X
2	MPD	G	302	-	-	-	X
2	MPD	H	302	-	-	-	X
2	MPD	H	303	-	-	-	X
2	MPD	I	302	-	-	-	X
2	MPD	I	303	-	-	-	X
2	MPD	J	302	-	-	-	X
2	MPD	J	303	-	-	-	X
2	MPD	K	302	-	-	-	X
2	MPD	K	303	-	-	X	-
2	MPD	L	303	-	-	-	X
2	MPD	M	303	-	-	-	X
2	MPD	N	302	-	-	X	-
2	MPD	O	302	-	-	-	X
2	MPD	O	303	-	-	-	X
2	MPD	P	303	-	-	-	X
2	MPD	Q	302	-	-	X	X
2	MPD	Q	303	-	-	-	X
2	MPD	R	303	-	-	X	-
2	MPD	S	302	-	-	-	X
2	MPD	S	303	-	-	-	X
2	MPD	T	302	-	-	-	X
2	MPD	T	303	-	-	-	X
2	MPD	U	302	-	-	-	X
2	MPD	U	303	-	-	-	X
2	MPD	V	303	-	-	X	X
2	MPD	X	302	-	-	-	X
2	MPD	X	303	-	-	-	X
2	MPD	X	304	-	-	-	X
2	MPD	Y	302	-	-	-	X
2	MPD	Y	303	-	-	-	X
2	MPD	Z	302	-	-	-	X
2	MPD	a	302	-	-	-	X
2	MPD	a	303	-	-	-	X
2	MPD	b	302	-	-	-	X
2	MPD	b	303	-	-	-	X
3	ACY	A	305	-	-	-	X
3	ACY	D	304	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	E	304	-	-	-	X
3	ACY	H	305	-	-	-	X
3	ACY	J	304	-	-	-	X
3	ACY	K	304	-	-	-	X
3	ACY	L	304	-	-	-	X
3	ACY	M	304	-	-	-	X
3	ACY	O	304	-	-	-	X
3	ACY	O	305	-	-	-	X
3	ACY	Q	304	-	-	-	X
3	ACY	S	304	-	-	-	X
3	ACY	S	305	-	-	-	X
3	ACY	T	304	-	-	-	X
3	ACY	V	304	-	-	-	X
3	ACY	X	305	-	-	-	X
3	ACY	Y	304	-	-	-	X
3	ACY	Z	303	-	-	-	X
3	ACY	a	304	-	-	-	X
3	ACY	b	304	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 68607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	B	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	C	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	D	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	E	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	F	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	G	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	H	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	I	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	J	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	K	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	L	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	M	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	N	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	O	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	P	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	R	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	S	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	T	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	U	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	V	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	W	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	X	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	Y	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	Z	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	a	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	b	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q99UU6
A	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
A	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
A	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	0	MET	-	EXPRESSION TAG	UNP Q99UU6
B	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
B	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
B	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	298	HIS	-	EXPRESSION TAG	UNP Q99UU6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	0	MET	-	EXPRESSION TAG	UNP Q99UU6
C	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
C	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
C	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	0	MET	-	EXPRESSION TAG	UNP Q99UU6
D	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
D	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
D	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	0	MET	-	EXPRESSION TAG	UNP Q99UU6
E	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
E	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
E	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	0	MET	-	EXPRESSION TAG	UNP Q99UU6
F	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
F	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
F	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	0	MET	-	EXPRESSION TAG	UNP Q99UU6
G	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
G	295	GLU	-	EXPRESSION TAG	UNP Q99UU6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	0	MET	-	EXPRESSION TAG	UNP Q99UU6
H	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
H	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
H	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	0	MET	-	EXPRESSION TAG	UNP Q99UU6
I	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
I	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
I	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	0	MET	-	EXPRESSION TAG	UNP Q99UU6
J	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
J	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
J	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	0	MET	-	EXPRESSION TAG	UNP Q99UU6
K	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
K	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
K	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	301	HIS	-	EXPRESSION TAG	UNP Q99UU6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	EXPRESSION TAG	UNP Q99UU6
L	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
L	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
L	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	0	MET	-	EXPRESSION TAG	UNP Q99UU6
M	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
M	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
M	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	0	MET	-	EXPRESSION TAG	UNP Q99UU6
N	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
N	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
N	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	0	MET	-	EXPRESSION TAG	UNP Q99UU6
O	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
O	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
O	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	0	MET	-	EXPRESSION TAG	UNP Q99UU6
P	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
P	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
P	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	298	HIS	-	EXPRESSION TAG	UNP Q99UU6

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Chain	Residue	Modelled	Actual	Comment	Reference
P	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	0	MET	-	EXPRESSION TAG	UNP Q99UU6
Q	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
Q	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
Q	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	0	MET	-	EXPRESSION TAG	UNP Q99UU6
R	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
R	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
R	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	0	MET	-	EXPRESSION TAG	UNP Q99UU6
S	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
S	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
S	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	0	MET	-	EXPRESSION TAG	UNP Q99UU6
T	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
T	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
T	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	0	MET	-	EXPRESSION TAG	UNP Q99UU6
U	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
U	295	GLU	-	EXPRESSION TAG	UNP Q99UU6

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Chain	Residue	Modelled	Actual	Comment	Reference
U	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	0	MET	-	EXPRESSION TAG	UNP Q99UU6
V	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
V	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
V	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	0	MET	-	EXPRESSION TAG	UNP Q99UU6
W	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
W	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
W	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	0	MET	-	EXPRESSION TAG	UNP Q99UU6
X	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
X	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
X	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	0	MET	-	EXPRESSION TAG	UNP Q99UU6
Y	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
Y	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
Y	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	301	HIS	-	EXPRESSION TAG	UNP Q99UU6

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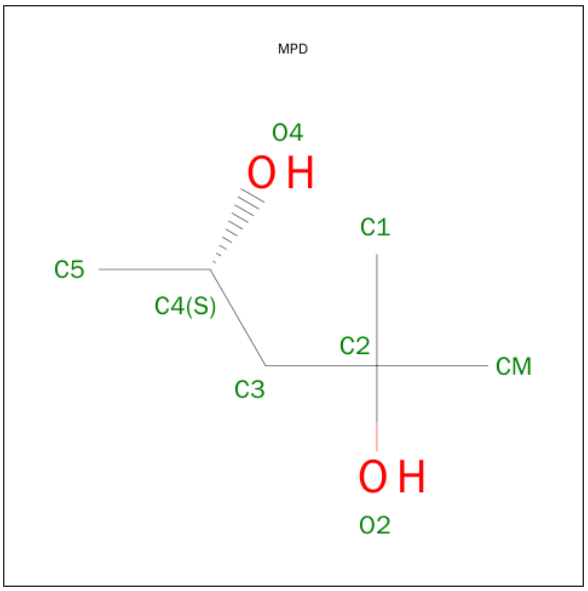
Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	MET	-	EXPRESSION TAG	UNP Q99UU6
Z	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
Z	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
Z	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	0	MET	-	EXPRESSION TAG	UNP Q99UU6
a	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
a	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
a	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	0	MET	-	EXPRESSION TAG	UNP Q99UU6
b	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
b	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
b	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	301	HIS	-	EXPRESSION TAG	UNP Q99UU6

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C O 8 6 2	0	0
2	H	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	J	1	Total C O 8 6 2	0	0
2	J	1	Total C O 8 6 2	0	0
2	K	1	Total C O 8 6 2	0	0
2	K	1	Total C O 8 6 2	0	0
2	L	1	Total C O 8 6 2	0	0
2	L	1	Total C O 8 6 2	0	0
2	M	1	Total C O 8 6 2	0	0
2	M	1	Total C O 8 6 2	0	0
2	N	1	Total C O 8 6 2	0	0
2	N	1	Total C O 8 6 2	0	0
2	O	1	Total C O 8 6 2	0	0
2	O	1	Total C O 8 6 2	0	0
2	P	1	Total C O 8 6 2	0	0
2	P	1	Total C O 8 6 2	0	0
2	Q	1	Total C O 8 6 2	0	0
2	Q	1	Total C O 8 6 2	0	0
2	R	1	Total C O 8 6 2	0	0

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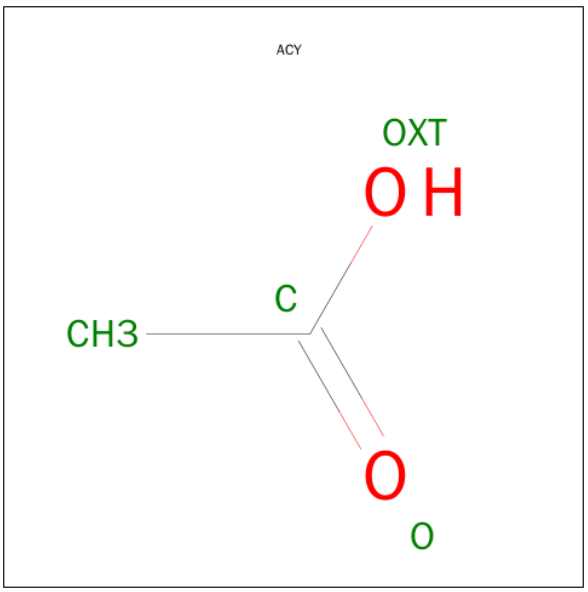
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	1	Total C O 8 6 2	0	0
2	S	1	Total C O 8 6 2	0	0
2	S	1	Total C O 8 6 2	0	0
2	T	1	Total C O 8 6 2	0	0
2	T	1	Total C O 8 6 2	0	0
2	U	1	Total C O 8 6 2	0	0
2	U	1	Total C O 8 6 2	0	0
2	V	1	Total C O 8 6 2	0	0
2	V	1	Total C O 8 6 2	0	0
2	W	1	Total C O 8 6 2	0	0
2	W	1	Total C O 8 6 2	0	0
2	X	1	Total C O 8 6 2	0	0
2	X	1	Total C O 8 6 2	0	0
2	X	1	Total C O 8 6 2	0	0
2	Y	1	Total C O 8 6 2	0	0
2	Y	1	Total C O 8 6 2	0	0
2	Z	1	Total C O 8 6 2	0	0
2	a	1	Total C O 8 6 2	0	0
2	a	1	Total C O 8 6 2	0	0
2	b	1	Total C O 8 6 2	0	0
2	b	1	Total C O 8 6 2	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	P	1	Total C O 4 2 2	0	0
3	Q	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0
3	V	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	X	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	Z	1	Total C O 4 2 2	0	0
3	a	1	Total C O 4 2 2	0	0
3	b	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	94	Total O 94 94	0	0
4	B	79	Total O 79 79	0	0
4	C	73	Total O 73 73	0	0
4	D	66	Total O 66 66	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	54	Total O 54 54	0	0
4	F	46	Total O 46 46	0	0
4	G	70	Total O 70 70	0	0
4	H	89	Total O 89 89	0	0
4	I	87	Total O 87 87	0	0
4	J	86	Total O 86 86	0	0
4	K	97	Total O 97 97	0	0
4	L	71	Total O 71 71	0	0
4	M	61	Total O 61 61	0	0
4	N	73	Total O 73 73	0	0
4	O	91	Total O 91 91	0	0
4	P	73	Total O 73 73	0	0
4	Q	61	Total O 61 61	0	0
4	R	73	Total O 73 73	0	0
4	S	69	Total O 69 69	0	0
4	T	82	Total O 82 82	0	0
4	U	85	Total O 85 85	0	0
4	V	82	Total O 82 82	0	0
4	W	50	Total O 50 50	0	0
4	X	46	Total O 46 46	0	0
4	Y	53	Total O 53 53	0	0

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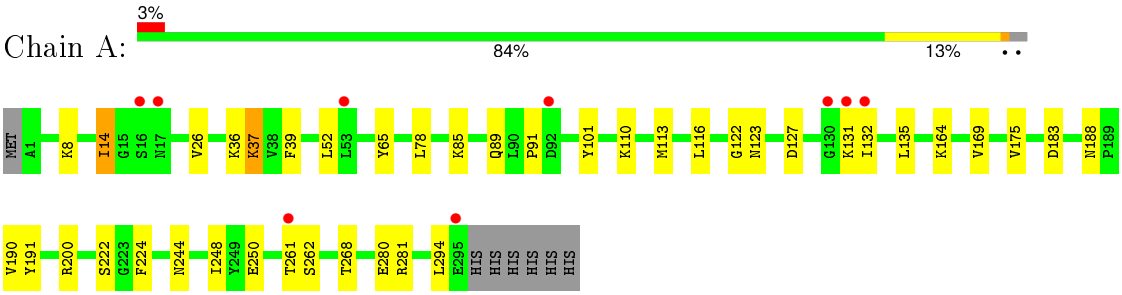
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Z	82	Total O 82 82	0	0
4	a	99	Total O 99 99	0	0
4	b	72	Total O 72 72	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

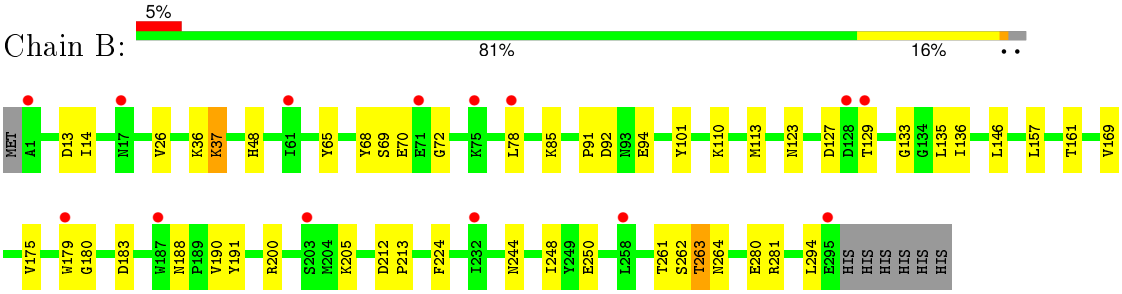
- Molecule 1: Alpha-hemolysin

Chain A:



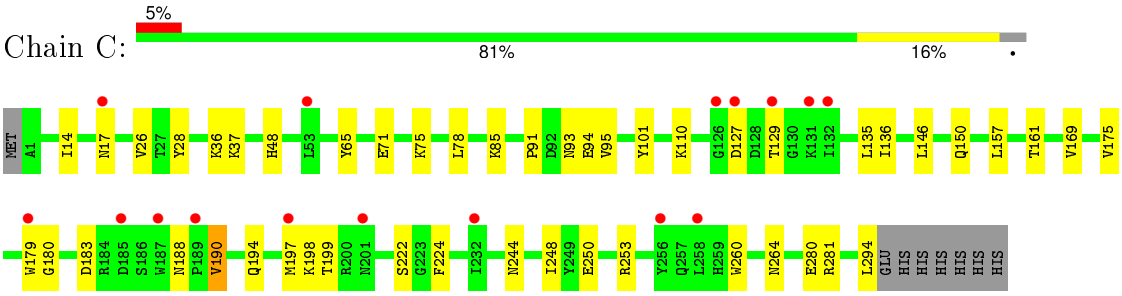
- Molecule 1: Alpha-hemolysin

Chain B:



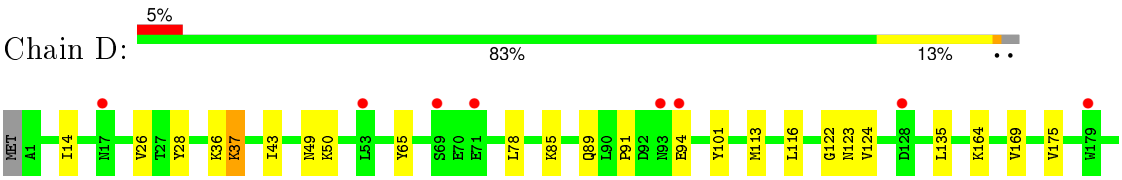
- Molecule 1: Alpha-hemolysin

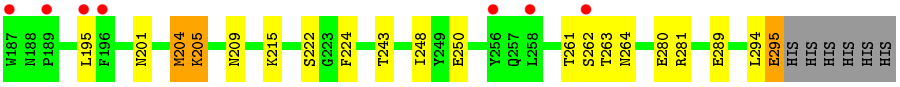
Chain C:



- Molecule 1: Alpha-hemolysin

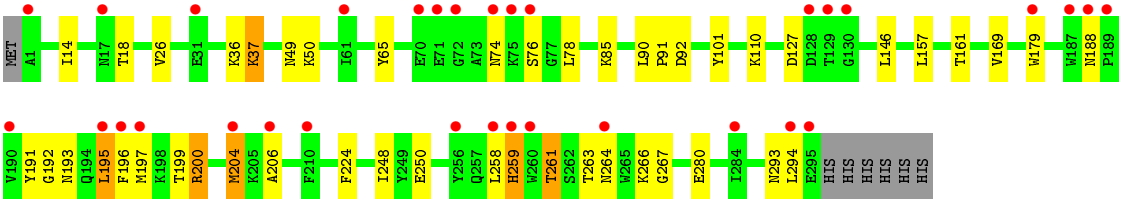
Chain D:





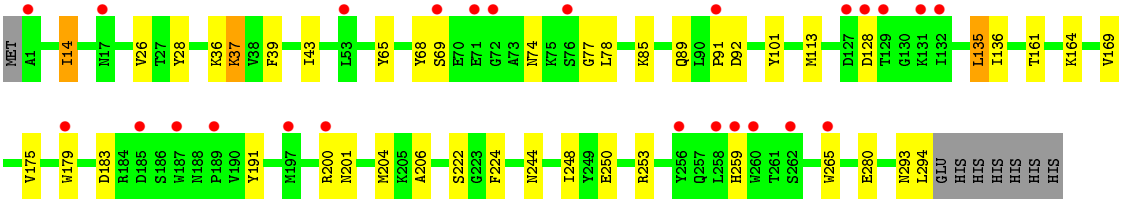
• Molecule 1: Alpha-hemolysin

Chain E:



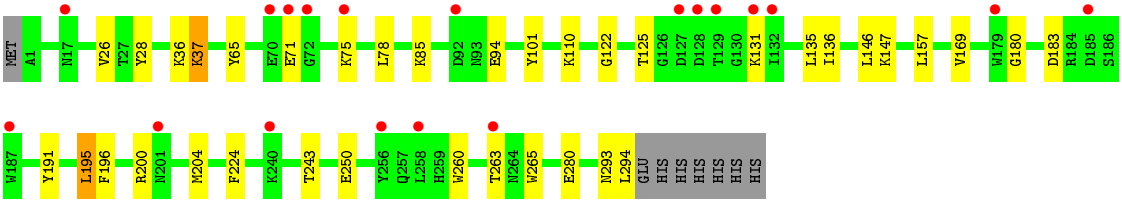
• Molecule 1: Alpha-hemolysin

Chain F:



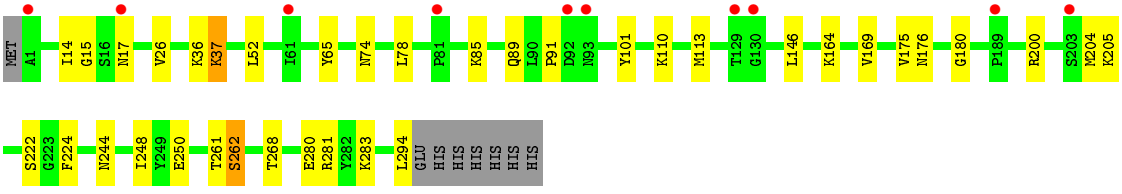
• Molecule 1: Alpha-hemolysin

Chain G:



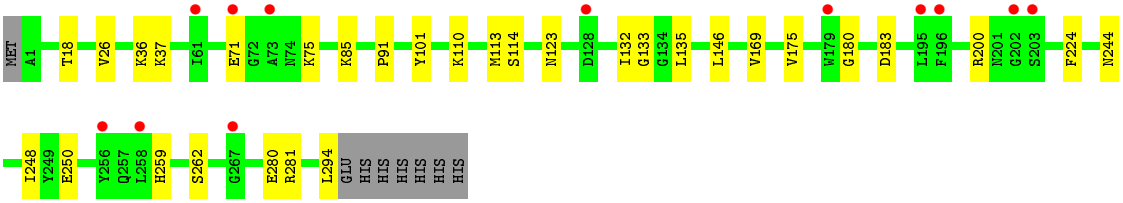
• Molecule 1: Alpha-hemolysin

Chain H:



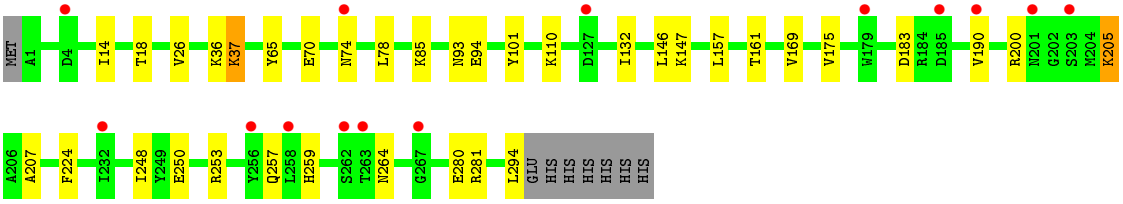
• Molecule 1: Alpha-hemolysin

Chain I:



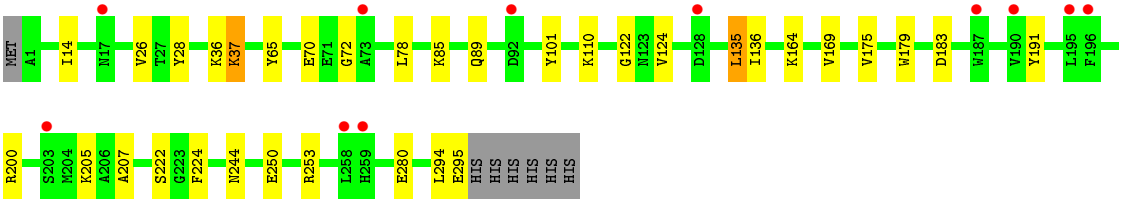
• Molecule 1: Alpha-hemolysin

Chain J:



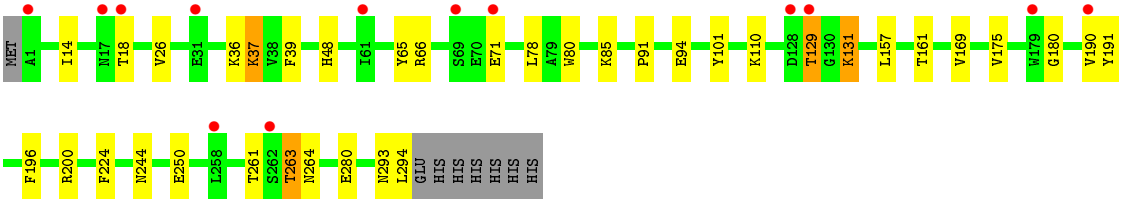
• Molecule 1: Alpha-hemolysin

Chain K:



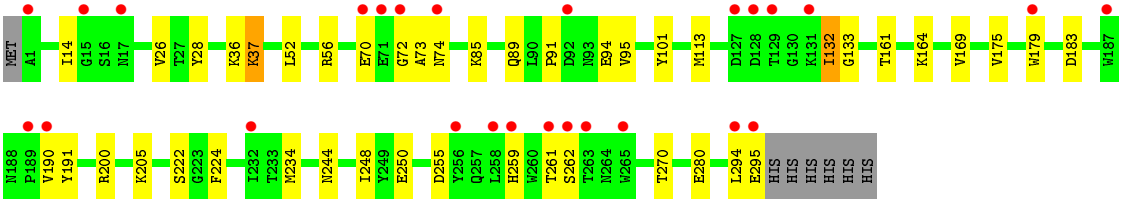
• Molecule 1: Alpha-hemolysin

Chain L:



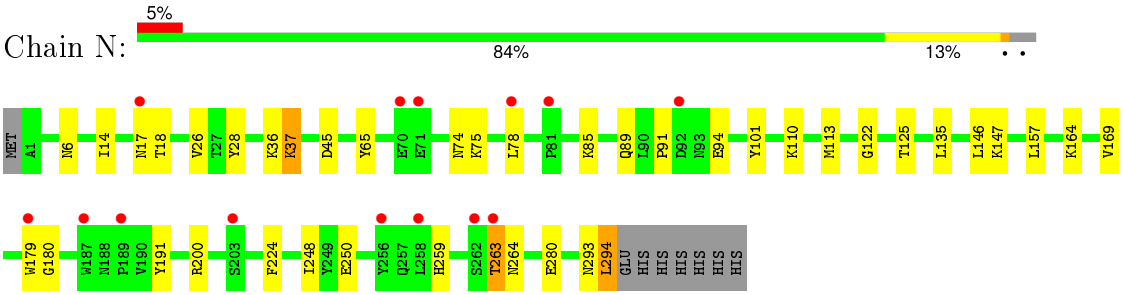
• Molecule 1: Alpha-hemolysin

Chain M:



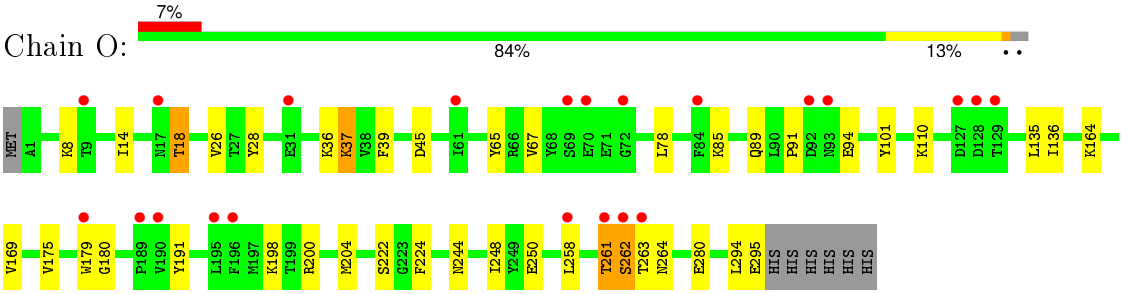
• Molecule 1: Alpha-hemolysin

Chain N:



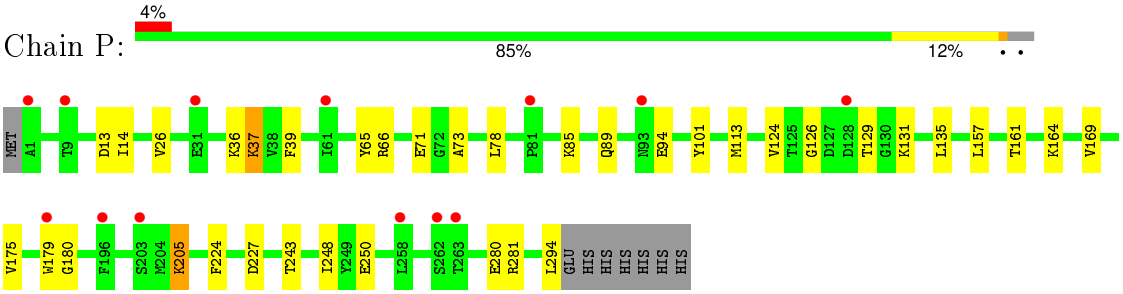
• Molecule 1: Alpha-hemolysin

Chain O:



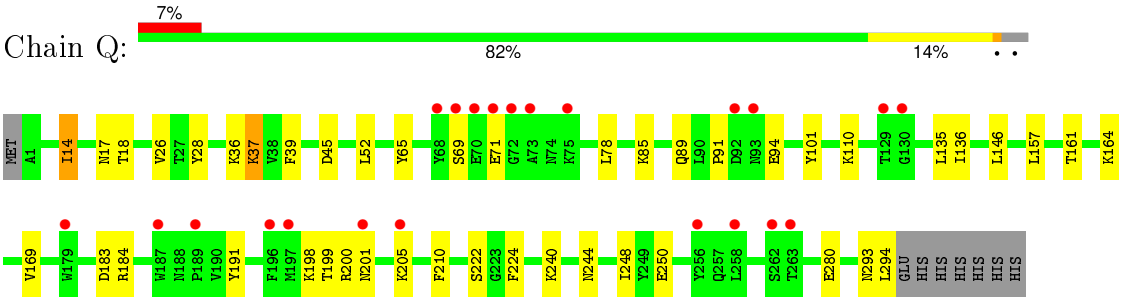
• Molecule 1: Alpha-hemolysin

Chain P:



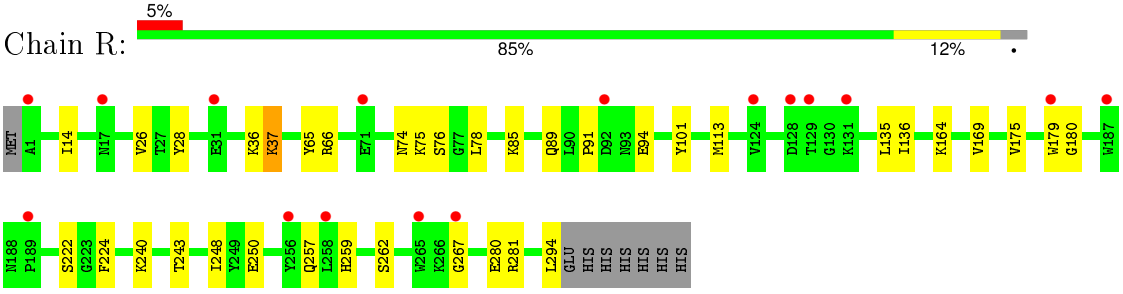
• Molecule 1: Alpha-hemolysin

Chain Q:



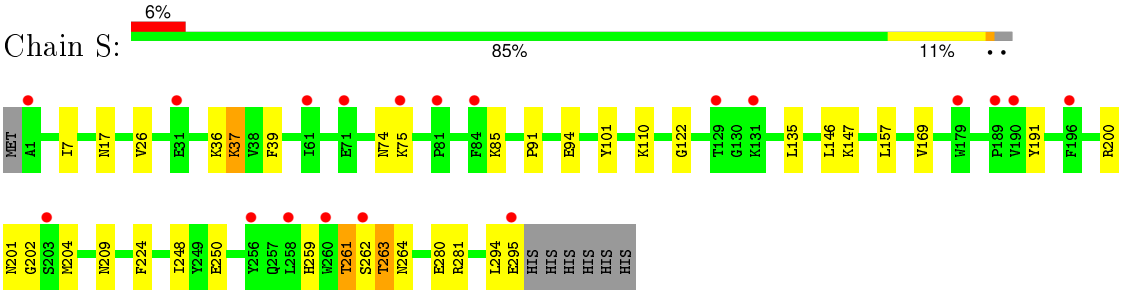
• Molecule 1: Alpha-hemolysin

Chain R:



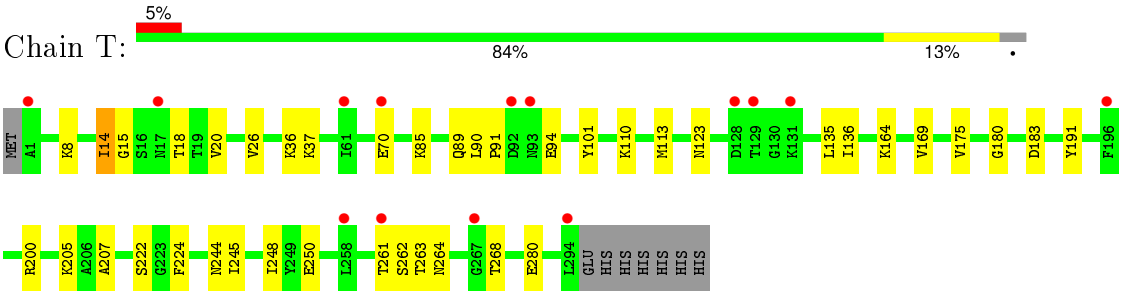
• Molecule 1: Alpha-hemolysin

Chain S:



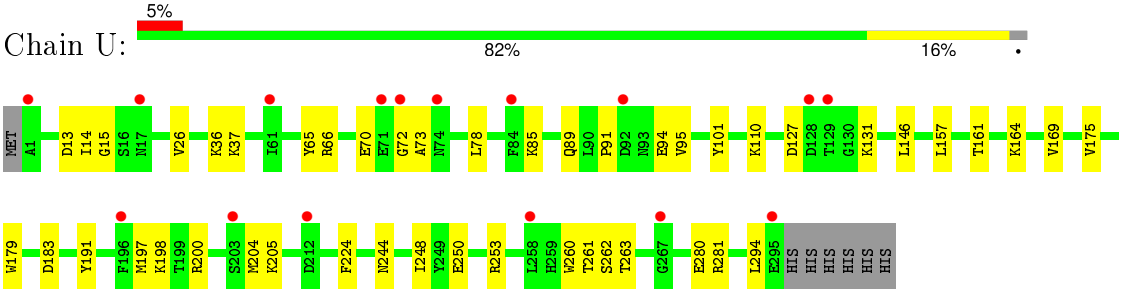
• Molecule 1: Alpha-hemolysin

Chain T:



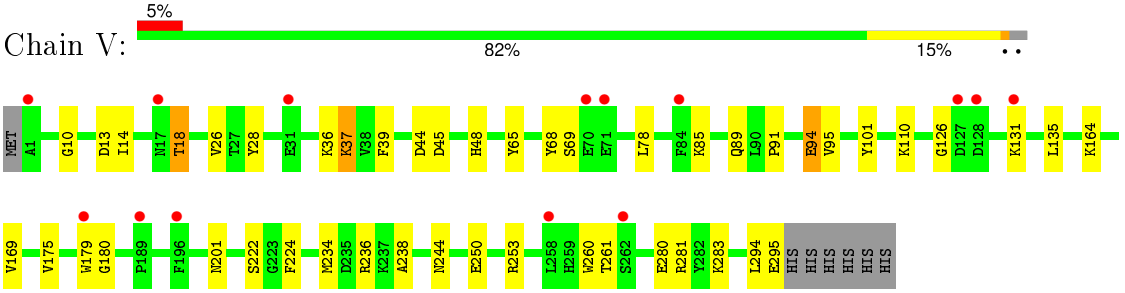
• Molecule 1: Alpha-hemolysin

Chain U:



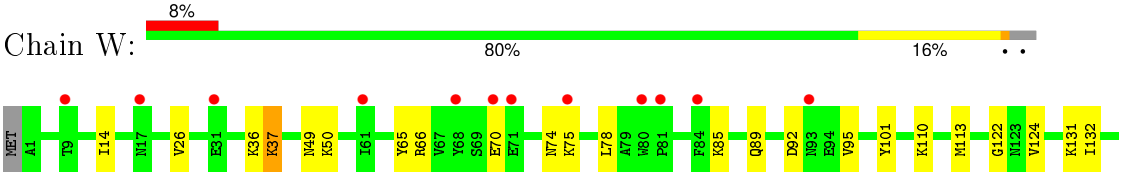
• Molecule 1: Alpha-hemolysin

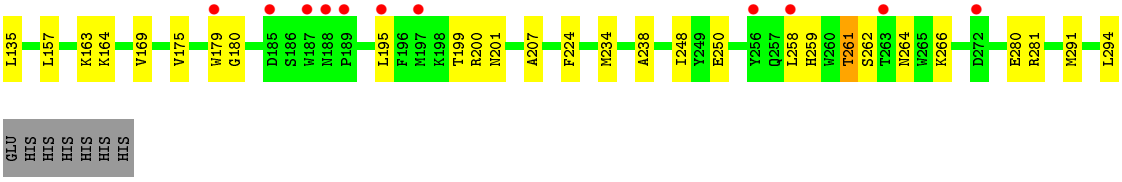
Chain V:



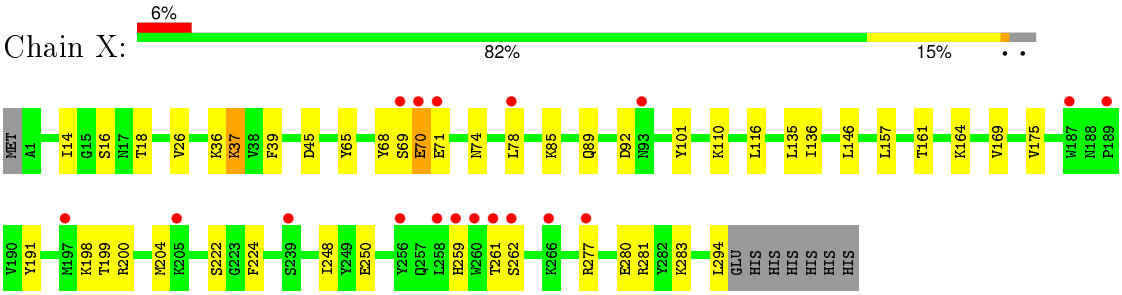
• Molecule 1: Alpha-hemolysin

Chain W:

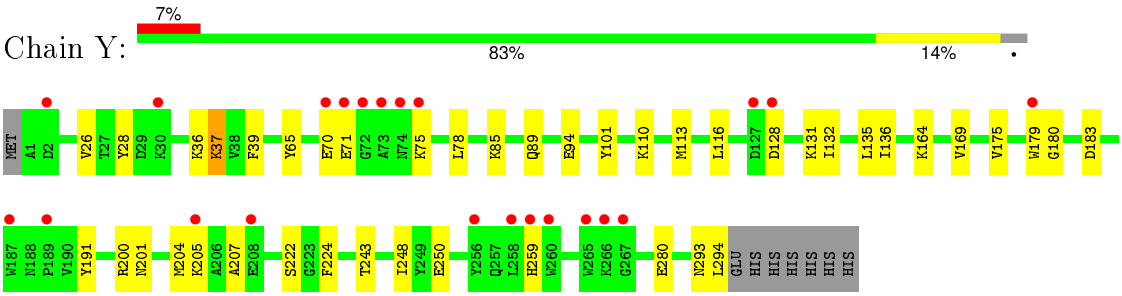




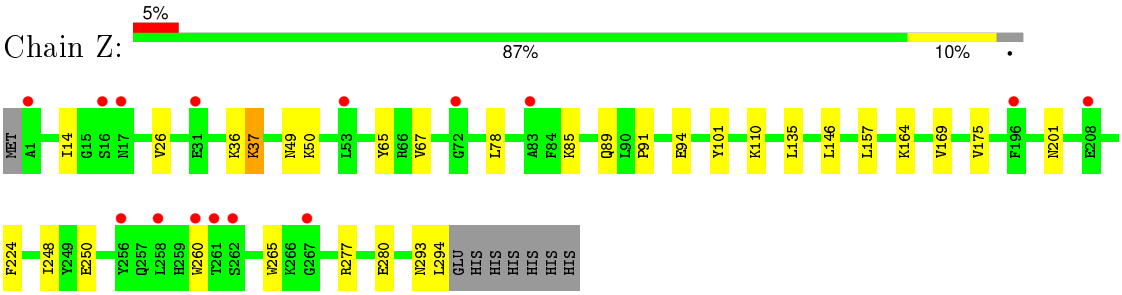
• Molecule 1: Alpha-hemolysin



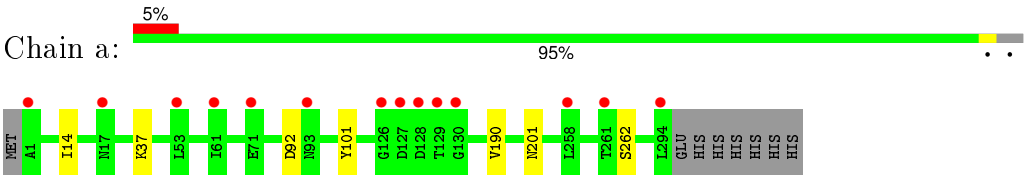
• Molecule 1: Alpha-hemolysin



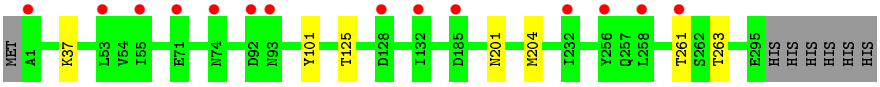
• Molecule 1: Alpha-hemolysin



• Molecule 1: Alpha-hemolysin



• Molecule 1: Alpha-hemolysin


MET
A1
K37
L53
V54
I55
E71
N74
D92
N93
Y101
T125
D128
I132
D185
N201
M204
I232
Y256
Q257
L258
T261
S262
T263
E295
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.82Å 293.88Å 170.54Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.98-2.30) 98.0 (19.98-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.77 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.193 , 0.226 0.192 , 0.193	Depositor DCC
R_{free} test set	31003 reflections (7.15%)	DCC
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.2	EDS
Estimated twinning fraction	0.010 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	2 of 434611 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	68607	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 61.01 % 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 1.3976e-05.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, 0.375 respectively for untwinned datasets, and 0.333, 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: ACY, MPD

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	0.33	0/2414	0.50	1/3267 (0.0%)
1	B	0.32	0/2414	0.47	0/3267
1	C	0.32	0/2405	0.48	0/3255
1	D	0.32	0/2414	0.47	0/3267
1	E	0.32	0/2414	0.47	0/3267
1	F	0.31	0/2405	0.47	0/3255
1	G	0.32	0/2405	0.48	0/3255
1	H	0.33	0/2405	0.50	1/3255 (0.0%)
1	I	0.32	0/2405	0.48	0/3255
1	J	0.33	0/2405	0.47	0/3255
1	K	0.34	0/2414	0.48	0/3267
1	L	0.34	0/2405	0.48	0/3255
1	M	0.32	0/2414	0.47	0/3267
1	N	0.32	0/2405	0.47	0/3255
1	O	0.33	0/2414	0.47	0/3267
1	P	0.32	0/2405	0.48	0/3255
1	Q	0.32	0/2405	0.46	0/3255
1	R	0.33	0/2405	0.48	0/3255
1	S	0.32	0/2414	0.47	0/3267
1	T	0.33	0/2405	0.48	0/3255
1	U	0.32	0/2414	0.47	0/3267
1	V	0.32	0/2414	0.48	0/3267
1	W	0.32	0/2405	0.46	0/3255
1	X	0.31	0/2405	0.46	0/3255
1	Y	0.31	0/2405	0.47	0/3255
1	Z	0.32	0/2405	0.47	0/3255
1	a	0.33	0/2405	0.48	0/3255
1	b	0.33	0/2414	0.48	0/3267
All	All	0.32	0/67439	0.48	2/91272 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	261	THR	N-CA-C	-5.25	96.82	111.00
1	A	261	THR	N-CA-C	-5.19	96.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2362	0	2289	45	0
1	B	2362	0	2289	58	0
1	C	2353	0	2283	33	0
1	D	2362	0	2289	31	0
1	E	2362	0	2289	36	0
1	F	2353	0	2283	38	0
1	G	2353	0	2283	29	0
1	H	2353	0	2283	28	0
1	I	2353	0	2283	25	0
1	J	2353	0	2283	23	0
1	K	2362	0	2289	29	0
1	L	2353	0	2283	27	0
1	M	2362	0	2289	31	0
1	N	2353	0	2283	39	0
1	O	2362	0	2289	33	0
1	P	2353	0	2283	28	0
1	Q	2353	0	2283	35	0
1	R	2353	0	2283	29	0
1	S	2362	0	2289	28	0
1	T	2353	0	2283	35	0
1	U	2362	0	2289	36	0
1	V	2362	0	2289	40	0
1	W	2353	0	2283	40	0
1	X	2353	0	2283	39	0
1	Y	2353	0	2283	30	0
1	Z	2353	0	2283	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	2353	0	2283	0	0
1	b	2362	0	2289	0	0
2	A	16	0	28	12	0
2	B	16	0	28	14	0
2	C	16	0	28	6	0
2	D	16	0	28	2	0
2	E	16	0	28	8	0
2	F	16	0	28	10	0
2	G	16	0	28	7	0
2	H	16	0	28	5	0
2	I	16	0	28	7	0
2	J	16	0	28	5	0
2	K	16	0	28	11	0
2	L	16	0	28	5	0
2	M	16	0	28	4	0
2	N	16	0	28	11	0
2	O	16	0	28	10	0
2	P	16	0	28	4	0
2	Q	16	0	28	9	0
2	R	16	0	28	6	0
2	S	16	0	28	4	0
2	T	16	0	28	4	0
2	U	16	0	28	5	0
2	V	16	0	28	8	0
2	W	16	0	28	9	0
2	X	24	0	42	6	0
2	Y	16	0	28	6	0
2	Z	8	0	14	1	0
2	a	16	0	28	0	0
2	b	16	0	28	0	0
3	A	8	0	6	0	0
3	C	4	0	3	0	0
3	D	8	0	6	0	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
3	H	8	0	6	0	0
3	J	4	0	3	0	0
3	K	8	0	6	0	0
3	L	4	0	3	0	0
3	M	4	0	3	0	0
3	O	8	0	6	0	0
3	P	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	4	0	3	0	0
3	S	8	0	6	0	0
3	T	4	0	3	0	0
3	V	4	0	3	0	0
3	W	4	0	3	0	0
3	X	4	0	3	0	0
3	Y	4	0	3	0	0
3	Z	4	0	3	0	0
3	a	4	0	3	0	0
3	b	4	0	3	0	0
4	A	94	0	0	1	0
4	B	79	0	0	1	0
4	C	73	0	0	6	0
4	D	66	0	0	1	0
4	E	54	0	0	1	0
4	F	46	0	0	3	0
4	G	70	0	0	1	0
4	H	89	0	0	1	0
4	I	87	0	0	1	0
4	J	86	0	0	3	0
4	K	97	0	0	4	0
4	L	71	0	0	0	0
4	M	61	0	0	2	0
4	N	73	0	0	3	0
4	O	91	0	0	0	0
4	P	73	0	0	1	0
4	Q	61	0	0	2	0
4	R	73	0	0	0	0
4	S	69	0	0	0	0
4	T	82	0	0	3	0
4	U	85	0	0	3	0
4	V	82	0	0	7	0
4	W	50	0	0	1	0
4	X	46	0	0	1	0
4	Y	53	0	0	1	0
4	Z	82	0	0	2	0
4	a	99	0	0	0	0
4	b	72	0	0	0	0
All	All	68607	0	64858	839	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 6.

All (839) 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)
2:B:303:MPD:H53	2:B:303:MPD:H11	1.27	1.09
1:R:180:GLY:O	2:R:303:MPD:H11	1.52	1.06
1:E:199:THR:HA	2:E:302:MPD:H51	1.38	1.04
1:I:180:GLY:O	2:I:303:MPD:H12	1.60	1.01
2:S:303:MPD:H53	2:S:303:MPD:H12	1.44	0.98
2:Y:303:MPD:H12	2:Y:303:MPD:H53	1.49	0.93
2:H:303:MPD:H52	2:H:303:MPD:H13	1.51	0.91
2:A:302:MPD:HM3	2:A:302:MPD:H52	1.58	0.86
1:F:179:TRP:CE3	2:F:303:MPD:C5	2.61	0.83
1:P:180:GLY:O	2:P:303:MPD:H13	1.79	0.82
1:O:91:PRO:HG2	1:O:94:GLU:CG	2.08	0.82
1:F:179:TRP:HA	2:F:303:MPD:H53	1.61	0.81
1:U:91:PRO:HB2	1:U:94:GLU:HG2	1.61	0.81
1:M:179:TRP:CE3	2:M:303:MPD:H51	2.16	0.80
1:C:281:ARG:HG2	1:C:294:LEU:HD12	1.61	0.80
1:W:200:ARG:HG3	2:W:302:MPD:H52	1.62	0.80
1:D:91:PRO:HG2	1:D:94:GLU:HB2	1.63	0.79
2:A:303:MPD:H53	2:A:303:MPD:H12	1.65	0.79
2:G:303:MPD:H53	2:G:303:MPD:H12	1.63	0.79
1:B:127:ASP:HB2	1:V:131:LYS:HE2	160.90	0.76
1:F:179:TRP:CD2	2:F:303:MPD:C5	2.69	0.76
1:T:91:PRO:HB2	1:T:94:GLU:HG2	1.67	0.75
1:E:199:THR:CA	2:E:302:MPD:H51	2.14	0.75
1:O:91:PRO:HG2	1:O:94:GLU:HG2	1.68	0.75
1:G:180:GLY:O	2:G:303:MPD:H13	1.86	0.75
2:I:302:MPD:H11	2:I:302:MPD:O4	1.86	0.75
1:B:179:TRP:CE3	2:B:303:MPD:H51	2.23	0.74
2:A:302:MPD:CM	2:A:302:MPD:H52	2.17	0.74
1:F:179:TRP:CE3	2:F:303:MPD:H52	2.22	0.74
1:B:91:PRO:HB2	1:B:94:GLU:HG2	1.99	0.74
2:B:303:MPD:H12	2:B:303:MPD:H52	3.92	0.74
1:Q:199:THR:CA	2:Q:302:MPD:H51	2.18	0.74
1:Z:91:PRO:HG2	1:Z:94:GLU:CG	2.18	0.74
1:O:179:TRP:HA	2:O:303:MPD:H53	1.71	0.72
2:W:303:MPD:H53	2:W:303:MPD:H12	1.71	0.72
1:K:179:TRP:HA	2:K:303:MPD:H52	1.70	0.72
1:E:179:TRP:CG	2:E:302:MPD:HM3	2.24	0.72
1:F:179:TRP:CE3	2:F:303:MPD:H51	2.24	0.72
2:A:302:MPD:H11	2:A:302:MPD:O4	4.42	0.71
1:V:179:TRP:HA	2:V:303:MPD:H53	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:302:MPD:O4	2:G:302:MPD:H11	1.89	0.71
1:T:91:PRO:HG2	1:T:94:GLU:HG3	1.73	0.71
4:C:1969:HOH:O	1:D:215:LYS:HE2	1.89	0.71
2:L:303:MPD:H53	2:L:303:MPD:H12	1.73	0.70
1:O:91:PRO:HG2	1:O:94:GLU:HG3	1.73	0.70
1:U:91:PRO:HG2	1:U:94:GLU:HG3	1.74	0.70
1:A:268:THR:HG21	1:H:262:SER:HB2	91.95	0.69
1:F:179:TRP:CD2	2:F:303:MPD:H51	2.27	0.69
2:R:303:MPD:H12	2:R:303:MPD:H52	1.74	0.69
1:N:180:GLY:O	2:N:303:MPD:H13	1.92	0.69
1:K:200:ARG:CZ	2:K:302:MPD:C1	2.71	0.69
2:O:302:MPD:O4	2:O:302:MPD:H11	1.91	0.68
1:B:262:SER:HB3	1:K:124:VAL:HG11	60.27	0.68
2:K:303:MPD:H11	2:K:303:MPD:H52	1.75	0.68
2:B:303:MPD:C5	2:B:303:MPD:H11	2.13	0.68
2:N:303:MPD:H53	2:N:303:MPD:H12	1.76	0.68
1:C:179:TRP:CE3	2:C:303:MPD:H51	2.29	0.67
1:V:281:ARG:HG2	1:V:294:LEU:HD12	1.76	0.67
1:J:281:ARG:HG2	1:J:294:LEU:HD12	1.77	0.67
2:K:303:MPD:C5	2:K:303:MPD:H11	2.23	0.67
2:J:302:MPD:O4	2:J:302:MPD:HM1	1.95	0.67
2:M:303:MPD:H12	2:M:303:MPD:H53	1.76	0.67
1:S:91:PRO:HB2	1:S:94:GLU:HG2	1.77	0.66
1:X:116:LEU:HB2	2:X:304:MPD:HM1	1.76	0.66
1:B:200:ARG:HE	2:B:302:MPD:C1	2.55	0.66
2:B:302:MPD:O4	2:B:302:MPD:H11	1.95	0.66
1:J:200:ARG:HD2	2:J:302:MPD:H32	1.77	0.66
1:E:65:TYR:CE1	1:E:78:LEU:HD21	2.31	0.65
1:Y:180:GLY:O	2:Y:303:MPD:H13	1.97	0.65
1:W:179:TRP:CE3	2:W:303:MPD:H51	2.32	0.65
2:A:303:MPD:H11	1:Y:116:LEU:HB2	127.71	0.65
1:E:204:MET:N	4:E:1879:HOH:O	2.28	0.65
1:S:75:LYS:HE3	1:S:259:HIS:HB2	1.78	0.65
1:W:261:THR:HG22	1:W:264:ASN:O	1.96	0.64
1:B:91:PRO:HG2	1:B:94:GLU:HG3	1.78	0.64
1:S:281:ARG:HG2	1:S:294:LEU:HD12	1.80	0.64
1:S:191:TYR:CE1	1:S:200:ARG:HB3	2.32	0.64
1:B:281:ARG:HG2	1:B:294:LEU:HD12	1.79	0.64
1:Q:14:ILE:HD11	1:Q:52:LEU:HD22	1.78	0.64
1:B:261:THR:HG22	1:B:264:ASN:H	5.21	0.63
1:E:74:ASN:O	1:E:259:HIS:HA	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:180:GLY:O	2:T:303:MPD:H12	1.98	0.63
1:G:200:ARG:HE	2:G:302:MPD:C1	2.11	0.63
1:Z:91:PRO:HG2	1:Z:94:GLU:HG3	1.80	0.63
1:W:261:THR:HG23	1:W:262:SER:N	2.13	0.63
2:B:303:MPD:C1	2:B:303:MPD:H53	2.15	0.63
1:I:262:SER:HB3	1:W:124:VAL:HG11	1.79	0.63
1:B:180:GLY:O	2:B:303:MPD:H13	3.50	0.63
1:D:94:GLU:HG2	1:D:243:THR:HG23	1.80	0.63
1:O:179:TRP:CE3	2:O:303:MPD:H51	2.34	0.63
1:G:200:ARG:HE	2:G:302:MPD:H13	1.63	0.62
1:N:293:ASN:O	1:N:294:LEU:HB2	1.99	0.62
1:S:200:ARG:HE	2:S:302:MPD:H13	1.64	0.62
1:Q:14:ILE:CD1	1:Q:52:LEU:HD22	2.30	0.62
1:Z:94:GLU:HB2	4:Z:738:HOH:O	1.99	0.62
2:E:303:MPD:H12	2:E:303:MPD:H52	1.82	0.62
1:F:65:TYR:CE2	1:F:78:LEU:HD21	2.34	0.62
2:P:302:MPD:H13	2:P:302:MPD:O4	1.98	0.62
1:Q:199:THR:HA	2:Q:302:MPD:H51	1.82	0.62
1:Q:18:THR:HG21	1:Q:45:ASP:HA	1.82	0.62
2:V:302:MPD:HM3	2:V:302:MPD:O4	1.97	0.62
2:T:302:MPD:HM1	2:T:302:MPD:O4	1.99	0.62
1:D:261:THR:HG22	1:D:263:THR:H	1.65	0.61
2:Q:303:MPD:H52	2:Q:303:MPD:H12	1.82	0.61
1:J:183:ASP:HB2	4:J:309:HOH:O	2.01	0.61
1:A:268:THR:HG21	1:T:262:SER:HB2	1.83	0.61
1:C:150:GLN:HG2	4:C:508:HOH:O	1.99	0.61
1:K:200:ARG:NH2	2:K:302:MPD:H11	2.16	0.60
1:H:14:ILE:HG22	1:N:6:ASN:O	2.01	0.60
1:O:110:LYS:HD2	1:P:175:VAL:HG23	1.84	0.60
1:G:195:LEU:HD13	1:G:196:PHE:CE2	2.36	0.60
2:C:302:MPD:O4	2:C:302:MPD:H11	2.02	0.60
1:N:191:TYR:CZ	1:N:200:ARG:HD3	2.37	0.60
1:D:281:ARG:HG2	1:D:294:LEU:HD12	1.84	0.60
1:X:281:ARG:HG2	1:X:294:LEU:HD12	1.83	0.60
1:P:14:ILE:HD11	1:Q:39:PHE:HE1	1.66	0.60
1:Q:200:ARG:HE	2:Q:302:MPD:CM	2.14	0.59
1:A:262:SER:HB2	1:H:268:THR:HG21	105.86	0.59
2:O:302:MPD:O4	2:O:302:MPD:HM3	2.02	0.59
1:X:65:TYR:CE2	1:X:78:LEU:HD21	2.37	0.59
1:L:261:THR:HG22	1:L:264:ASN:O	2.02	0.59
2:K:303:MPD:HM2	2:K:303:MPD:H53	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:TRP:HA	2:C:303:MPD:H53	1.84	0.59
1:I:200:ARG:CZ	2:I:302:MPD:C1	2.81	0.59
1:T:205:LYS:HG2	4:T:1509:HOH:O	2.03	0.59
1:O:200:ARG:CZ	2:O:302:MPD:C1	2.81	0.58
1:L:261:THR:HG23	1:L:263:THR:H	1.67	0.58
1:V:85:LYS:HB2	1:V:250:GLU:HB3	1.85	0.58
1:N:18:THR:HG22	4:N:1336:HOH:O	2.03	0.58
1:A:14:ILE:CD1	1:A:52:LEU:HD22	2.32	0.58
1:B:85:LYS:HB2	1:B:250:GLU:HB3	1.85	0.58
1:M:85:LYS:HB2	1:M:250:GLU:HB3	1.86	0.58
1:E:192:GLY:N	1:E:266:LYS:HG3	2.17	0.58
1:S:91:PRO:HG2	1:S:94:GLU:HG3	1.85	0.58
1:W:281:ARG:HG2	1:W:294:LEU:HD12	1.84	0.58
1:F:293:ASN:O	1:F:294:LEU:HB2	2.02	0.58
1:F:200:ARG:HE	2:F:302:MPD:C1	2.15	0.58
1:J:205:LYS:HD2	1:J:205:LYS:N	2.17	0.58
1:D:65:TYR:CE1	1:D:78:LEU:HD21	2.39	0.58
1:Y:191:TYR:CE1	1:Y:200:ARG:HB3	2.38	0.58
1:G:71:GLU:HB2	1:G:75:LYS:HB2	1.86	0.58
1:O:200:ARG:CZ	2:O:302:MPD:H13	2.33	0.58
1:A:262:SER:HB2	1:T:268:THR:HG21	1.84	0.58
1:X:70:GLU:HG3	1:X:70:GLU:O	2.04	0.58
1:I:91:PRO:HD3	1:I:244:ASN:O	2.04	0.57
1:B:129:THR:HG23	1:V:131:LYS:HE3	163.94	0.57
1:Q:198:LYS:C	2:Q:302:MPD:H53	2.25	0.57
1:F:91:PRO:HD3	1:F:244:ASN:O	2.05	0.57
2:P:303:MPD:H52	2:P:303:MPD:O2	2.03	0.57
1:Q:200:ARG:HE	2:Q:302:MPD:HM1	1.68	0.57
1:Q:199:THR:C	2:Q:302:MPD:H51	2.24	0.57
1:L:65:TYR:CE2	1:L:78:LEU:HD21	2.40	0.57
1:I:183:ASP:HB2	4:I:1915:HOH:O	2.04	0.57
1:Y:94:GLU:OE1	1:Y:243:THR:HG23	2.04	0.57
2:C:303:MPD:H52	2:C:303:MPD:O2	2.05	0.57
1:T:180:GLY:O	2:T:303:MPD:C1	2.53	0.57
1:R:85:LYS:HB2	1:R:250:GLU:HB3	1.87	0.57
2:D:302:MPD:C5	2:D:302:MPD:HM1	2.35	0.57
1:W:258:LEU:HD12	1:W:258:LEU:O	2.05	0.57
1:T:183:ASP:HB2	4:T:1635:HOH:O	2.03	0.57
1:C:14:ILE:HD11	1:C:48:HIS:CE1	2.40	0.57
1:B:262:SER:HB3	1:P:124:VAL:HG11	1.85	0.57
1:N:91:PRO:HB2	1:N:94:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:91:PRO:HG2	1:R:94:GLU:HB2	1.87	0.57
1:B:261:THR:HG22	1:B:264:ASN:O	4.50	0.57
1:K:244:ASN:HB2	4:K:1399:HOH:O	2.05	0.57
1:B:91:PRO:CG	1:B:94:GLU:HG3	2.35	0.56
2:O:303:MPD:C5	2:O:303:MPD:H12	2.35	0.56
1:U:85:LYS:HB2	1:U:250:GLU:HB3	1.87	0.56
1:P:71:GLU:O	1:P:71:GLU:HG2	2.05	0.56
1:Y:85:LYS:HB2	1:Y:250:GLU:HB3	1.87	0.56
1:I:85:LYS:HB2	1:I:250:GLU:HB3	1.87	0.56
1:A:14:ILE:HD13	1:A:52:LEU:HD22	1.87	0.56
1:F:85:LYS:HB2	1:F:250:GLU:HB3	1.88	0.56
1:V:179:TRP:CE3	2:V:303:MPD:H51	2.41	0.56
1:G:191:TYR:CE2	1:G:200:ARG:HB3	2.41	0.56
1:B:65:TYR:CE2	1:B:78:LEU:HD21	3.70	0.56
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.41	0.56
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.43	0.56
1:O:169:VAL:HG21	1:O:224:PHE:CZ	2.41	0.56
1:V:169:VAL:HG21	1:V:224:PHE:CZ	2.41	0.56
1:U:65:TYR:CE1	1:U:78:LEU:HD21	2.41	0.56
1:Y:94:GLU:CD	1:Y:243:THR:HG23	2.25	0.56
1:L:85:LYS:HB2	1:L:250:GLU:HB3	1.88	0.56
1:F:169:VAL:HG21	1:F:224:PHE:CZ	2.41	0.56
1:X:85:LYS:HB2	1:X:250:GLU:HB3	1.88	0.56
1:G:85:LYS:HB2	1:G:250:GLU:HB3	1.88	0.56
1:X:14:ILE:HD11	1:Y:39:PHE:HE1	1.70	0.56
1:L:180:GLY:O	2:L:303:MPD:H12	2.06	0.56
1:Q:191:TYR:CZ	1:Q:200:ARG:HD2	2.40	0.55
1:H:85:LYS:HB2	1:H:250:GLU:HB3	1.87	0.55
1:N:169:VAL:HG21	1:N:224:PHE:CZ	2.41	0.55
1:E:200:ARG:CZ	2:E:302:MPD:C1	2.84	0.55
1:N:200:ARG:HG3	2:N:302:MPD:HM3	1.88	0.55
1:N:200:ARG:CG	2:N:302:MPD:HM3	2.37	0.55
1:F:74:ASN:O	1:F:259:HIS:HA	2.06	0.55
1:Q:85:LYS:HB2	1:Q:250:GLU:HB3	1.89	0.55
1:O:180:GLY:O	2:O:303:MPD:H13	2.07	0.55
1:D:294:LEU:O	1:D:295:GLU:HB2	2.07	0.55
1:A:294:LEU:C	1:A:294:LEU:HD12	5.14	0.55
2:Y:303:MPD:H12	2:Y:303:MPD:C5	2.28	0.55
1:R:14:ILE:HD11	1:S:39:PHE:HE1	1.71	0.55
1:N:85:LYS:HB2	1:N:250:GLU:HB3	1.88	0.55
1:I:281:ARG:HG2	1:I:294:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:TYR:CZ	1:F:200:ARG:HD3	2.41	0.55
1:H:169:VAL:HG21	1:H:224:PHE:CZ	2.42	0.55
1:N:91:PRO:HG2	1:N:94:GLU:HG3	1.89	0.55
1:G:260:TRP:HB2	1:G:265:TRP:CZ3	2.42	0.55
1:S:85:LYS:HB2	1:S:250:GLU:HB3	1.88	0.55
1:W:65:TYR:CE1	1:W:78:LEU:HD21	2.42	0.55
1:O:85:LYS:HB2	1:O:250:GLU:HB3	1.89	0.54
1:I:180:GLY:O	2:I:303:MPD:C1	2.45	0.54
1:N:179:TRP:CE3	2:N:303:MPD:H51	2.42	0.54
1:W:261:THR:HG22	1:W:264:ASN:H	1.72	0.54
1:W:14:ILE:HD11	1:X:39:PHE:HE1	1.72	0.54
1:M:183:ASP:HB2	4:M:869:HOH:O	2.07	0.54
1:I:169:VAL:HG21	1:I:224:PHE:CZ	2.41	0.54
1:P:85:LYS:HB2	1:P:250:GLU:HB3	1.90	0.54
1:Y:65:TYR:CE1	1:Y:78:LEU:HD21	2.42	0.54
1:B:200:ARG:HE	2:B:302:MPD:H13	1.73	0.54
1:T:85:LYS:HB2	1:T:250:GLU:HB3	1.89	0.54
1:A:175:VAL:HG23	1:Z:110:LYS:HD2	129.24	0.54
1:R:169:VAL:HG21	1:R:224:PHE:CZ	2.43	0.54
1:P:169:VAL:HG21	1:P:224:PHE:CZ	2.42	0.54
1:U:91:PRO:CG	1:U:94:GLU:HG3	2.36	0.54
1:A:85:LYS:HB2	1:A:250:GLU:HB3	1.92	0.54
1:U:253:ARG:NH2	4:U:702:HOH:O	2.34	0.54
1:W:85:LYS:HB2	1:W:250:GLU:HB3	1.90	0.54
1:Q:169:VAL:HG21	1:Q:224:PHE:CZ	2.43	0.54
1:A:169:VAL:HG21	1:A:224:PHE:CZ	2.43	0.54
1:C:180:GLY:O	2:C:303:MPD:H13	2.08	0.54
1:Y:169:VAL:HG21	1:Y:224:PHE:CZ	2.43	0.54
1:L:190:VAL:HG13	1:L:191:TYR:CD2	2.42	0.54
1:V:253:ARG:CZ	4:V:731:HOH:O	2.55	0.54
1:J:190:VAL:HG12	1:J:264:ASN:ND2	2.23	0.54
1:G:169:VAL:HG21	1:G:224:PHE:CZ	2.42	0.54
1:D:204:MET:HE3	1:D:209:ASN:HB2	1.89	0.54
1:E:261:THR:HG22	1:E:264:ASN:O	2.08	0.54
2:T:303:MPD:H52	2:T:303:MPD:O2	2.08	0.53
1:E:293:ASN:OD1	1:E:294:LEU:N	2.42	0.53
1:W:199:THR:HA	2:W:302:MPD:H53	1.90	0.53
1:F:200:ARG:HE	2:F:302:MPD:H13	1.72	0.53
1:E:85:LYS:HB2	1:E:250:GLU:HB3	1.91	0.53
1:M:74:ASN:O	1:M:259:HIS:HA	2.08	0.53
1:F:135:LEU:C	1:F:135:LEU:HD12	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:302:MPD:O4	2:U:302:MPD:HM3	2.08	0.53
1:A:268:THR:CG2	1:H:262:SER:HB2	92.83	0.53
2:Y:302:MPD:H11	2:Y:302:MPD:O4	2.08	0.53
1:X:169:VAL:HG21	1:X:224:PHE:CZ	2.44	0.53
1:Z:85:LYS:HB2	1:Z:250:GLU:HB3	1.90	0.53
2:Y:302:MPD:HM3	2:Y:302:MPD:O4	2.07	0.53
1:G:293:ASN:O	1:G:294:LEU:HB2	2.09	0.53
1:M:179:TRP:HA	2:M:303:MPD:H53	1.90	0.53
1:Z:169:VAL:HG21	1:Z:224:PHE:CZ	2.43	0.53
1:C:110:LYS:HD2	1:D:175:VAL:HG23	1.90	0.53
1:E:76:SER:HB2	1:E:206:ALA:HB3	1.90	0.53
1:K:169:VAL:HG21	1:K:224:PHE:CZ	2.44	0.53
2:U:303:MPD:H12	2:U:303:MPD:C5	2.39	0.53
2:N:303:MPD:O2	2:N:303:MPD:H52	2.09	0.53
1:P:94:GLU:OE1	1:P:243:THR:HG23	2.09	0.53
1:C:169:VAL:HG21	1:C:224:PHE:CZ	2.43	0.53
1:L:169:VAL:HG21	1:L:224:PHE:CZ	2.44	0.53
2:F:302:MPD:HM3	2:F:302:MPD:O4	2.09	0.53
1:I:75:LYS:HD3	1:I:259:HIS:HB3	1.91	0.53
1:M:91:PRO:HD3	1:M:244:ASN:O	2.09	0.53
1:M:169:VAL:HG21	1:M:224:PHE:CZ	2.45	0.53
1:B:91:PRO:HB2	1:B:94:GLU:CG	2.39	0.52
1:N:293:ASN:OD1	1:N:294:LEU:HD23	2.09	0.52
1:W:169:VAL:HG21	1:W:224:PHE:CZ	2.44	0.52
1:T:70:GLU:OE2	1:T:205:LYS:HE3	2.09	0.52
1:F:135:LEU:HD12	1:F:136:ILE:N	2.24	0.52
1:B:180:GLY:O	2:B:303:MPD:H12	2.10	0.52
1:S:200:ARG:NE	2:S:302:MPD:H13	2.24	0.52
1:C:85:LYS:HB2	1:C:250:GLU:HB3	1.90	0.52
1:J:85:LYS:HB2	1:J:250:GLU:HB3	1.91	0.52
1:L:129:THR:HG22	1:L:131:LYS:H	1.74	0.52
1:B:70:GLU:OE2	1:B:205:LYS:HE3	4.54	0.52
1:G:65:TYR:CE1	1:G:78:LEU:HD21	2.44	0.52
1:U:169:VAL:HG21	1:U:224:PHE:CZ	2.45	0.52
1:E:14:ILE:HD11	1:F:39:PHE:HE1	1.74	0.52
1:O:191:TYR:CZ	1:O:200:ARG:HD3	2.44	0.52
1:U:179:TRP:HA	2:U:303:MPD:H53	1.91	0.52
1:R:281:ARG:HG2	1:R:294:LEU:HD12	1.90	0.52
2:J:303:MPD:C1	2:J:303:MPD:H52	2.39	0.52
1:S:169:VAL:HG21	1:S:224:PHE:CZ	2.44	0.52
2:J:302:MPD:CM	2:J:302:MPD:O4	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:HD11	1:B:48:HIS:CE1	2.44	0.52
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.44	0.52
1:B:68:TYR:CE2	1:B:69:SER:HB2	2.44	0.52
1:A:200:ARG:NH2	2:A:302:MPD:H11	4.98	0.52
1:Q:293:ASN:O	1:Q:294:LEU:HB2	2.09	0.52
1:D:85:LYS:HB2	1:D:250:GLU:HB3	1.91	0.52
1:A:127:ASP:HA	1:B:133:GLY:HA2	1.92	0.52
1:X:198:LYS:HG2	1:X:199:THR:HG23	1.92	0.52
1:E:188:ASN:HB3	1:E:191:TYR:O	2.10	0.52
1:N:125:THR:HG23	4:N:1671:HOH:O	2.10	0.52
2:W:303:MPD:C5	2:W:303:MPD:H12	2.39	0.51
1:X:68:TYR:CG	1:X:69:SER:N	2.77	0.51
1:N:200:ARG:HE	2:N:302:MPD:CM	2.24	0.51
1:B:26:VAL:HG22	1:B:37:LYS:HG2	1.92	0.51
1:H:200:ARG:NH2	2:H:302:MPD:C1	2.73	0.51
1:U:91:PRO:HB2	1:U:94:GLU:CG	2.38	0.51
1:V:294:LEU:O	1:V:295:GLU:CB	2.59	0.51
1:A:91:PRO:HD3	1:A:244:ASN:O	2.09	0.51
1:O:198:LYS:O	2:O:302:MPD:H52	2.10	0.51
1:D:261:THR:HB	1:D:264:ASN:O	2.10	0.51
1:T:169:VAL:HG21	1:T:224:PHE:CZ	2.44	0.51
1:Z:91:PRO:CG	1:Z:94:GLU:HG3	2.41	0.51
1:T:135:LEU:HD23	1:T:136:ILE:N	2.26	0.51
1:D:135:LEU:C	1:D:135:LEU:HD23	2.31	0.51
1:P:179:TRP:CE3	2:P:303:MPD:H51	2.46	0.51
1:B:261:THR:HG23	1:B:263:THR:H	4.80	0.51
1:C:188:ASN:OD1	1:C:190:VAL:HG13	2.11	0.51
2:U:303:MPD:H12	2:U:303:MPD:H53	1.93	0.51
1:R:257:GLN:O	1:R:267:GLY:HA2	2.11	0.51
1:M:261:THR:HG22	1:M:262:SER:N	2.26	0.51
1:Q:91:PRO:HD3	1:Q:244:ASN:O	2.11	0.51
1:R:94:GLU:OE2	1:R:240:LYS:HE3	2.10	0.50
1:X:200:ARG:HG3	2:X:302:MPD:H13	1.92	0.50
1:A:116:LEU:HB3	2:V:303:MPD:HM1	132.86	0.50
1:V:180:GLY:O	2:V:303:MPD:H12	2.12	0.50
1:B:190:VAL:HG23	1:B:191:TYR:CD1	2.45	0.50
1:N:191:TYR:CE1	1:N:200:ARG:HB3	2.47	0.50
1:U:73:ALA:HB2	1:U:205:LYS:HE3	1.94	0.50
1:D:124:VAL:HG11	1:U:262:SER:HB3	1.93	0.50
1:K:135:LEU:HD13	1:K:136:ILE:N	2.26	0.50
2:L:302:MPD:H52	2:L:302:MPD:O2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:263:THR:HG23	1:S:264:ASN:OD1	2.12	0.50
1:V:94:GLU:HG3	4:V:1657:HOH:O	2.11	0.50
1:G:94:GLU:CD	1:G:243:THR:HG23	2.32	0.50
1:B:161:THR:HG22	1:V:28:TYR:CZ	146.91	0.50
1:Y:293:ASN:O	1:Y:294:LEU:HB2	2.12	0.50
1:F:113:MET:HA	1:G:146:LEU:O	2.12	0.50
1:Q:198:LYS:HE3	1:Q:210:PHE:O	2.12	0.50
1:W:95:VAL:HG11	1:W:238:ALA:HB1	1.94	0.50
1:V:44:ASP:HB3	4:V:2007:HOH:O	2.11	0.50
1:K:110:LYS:HD2	1:L:175:VAL:HG23	1.92	0.50
1:W:74:ASN:O	1:W:259:HIS:HA	2.12	0.50
1:U:281:ARG:HG2	1:U:294:LEU:HD12	1.92	0.50
1:Y:71:GLU:HB3	1:Y:75:LYS:HB2	1.94	0.50
1:S:26:VAL:HG22	1:S:37:LYS:HG2	1.93	0.50
1:R:113:MET:HA	1:S:146:LEU:O	2.12	0.50
1:V:253:ARG:HD3	4:V:731:HOH:O	2.11	0.49
1:B:135:LEU:HD23	1:B:136:ILE:N	2.48	0.49
1:P:73:ALA:HB1	1:P:205:LYS:HG3	1.94	0.49
1:G:36:LYS:NZ	1:G:280:GLU:HG2	2.27	0.49
1:J:253:ARG:NH2	4:J:1212:HOH:O	2.44	0.49
1:E:293:ASN:O	1:E:294:LEU:HB2	2.12	0.49
1:J:132:ILE:HG21	1:R:262:SER:HB3	1.94	0.49
1:B:157:LEU:O	1:V:222:SER:HB3	138.07	0.49
1:J:169:VAL:HG21	1:J:224:PHE:CZ	2.46	0.49
1:H:281:ARG:HG2	1:H:294:LEU:HD12	1.94	0.49
1:I:114:SER:CB	2:K:303:MPD:HM2	2.42	0.49
1:V:135:LEU:HD23	1:V:135:LEU:C	2.32	0.49
1:O:8:LYS:HD2	1:P:13:ASP:HB2	1.93	0.49
1:L:200:ARG:NH2	2:L:302:MPD:C3	2.75	0.49
1:A:135:LEU:HD13	1:A:135:LEU:C	2.32	0.49
1:F:68:TYR:CE2	1:F:69:SER:HB3	2.47	0.49
1:B:191:TYR:CZ	1:B:200:ARG:HD3	2.51	0.49
1:N:191:TYR:CE1	1:N:200:ARG:HD3	2.47	0.49
1:N:91:PRO:HG2	1:N:94:GLU:CG	2.42	0.49
1:K:85:LYS:HB2	1:K:250:GLU:HB3	1.94	0.49
1:I:114:SER:HB3	2:K:303:MPD:HM2	1.93	0.49
1:U:191:TYR:CZ	1:U:200:ARG:HD3	2.47	0.49
1:M:113:MET:HA	1:N:146:LEU:O	2.12	0.49
1:J:110:LYS:HD2	1:K:175:VAL:HG23	1.94	0.49
1:Q:110:LYS:HD2	1:R:175:VAL:HG23	1.94	0.49
1:E:26:VAL:HG22	1:E:37:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:65:TYR:CE2	1:P:78:LEU:HD21	2.47	0.49
1:A:8:LYS:HD2	1:B:13:ASP:HB2	2.08	0.49
1:T:36:LYS:NZ	1:T:280:GLU:HG2	2.28	0.49
1:I:36:LYS:NZ	1:I:280:GLU:HG2	2.28	0.49
1:A:268:THR:CG2	1:T:262:SER:HB2	2.43	0.49
1:B:191:TYR:CE2	1:B:200:ARG:HB3	2.92	0.49
1:N:125:THR:CG2	4:N:1671:HOH:O	2.60	0.49
1:X:68:TYR:CE1	1:X:69:SER:HB2	2.48	0.49
1:F:37:LYS:NZ	4:F:794:HOH:O	2.41	0.49
1:J:65:TYR:CE1	1:J:78:LEU:HD21	2.48	0.49
1:B:110:LYS:HD2	1:V:175:VAL:HG23	137.56	0.49
1:H:110:LYS:HD2	1:I:175:VAL:HG23	1.95	0.49
1:R:94:GLU:OE2	1:R:243:THR:HA	2.13	0.49
1:C:260:TRP:CZ3	1:C:264:ASN:HA	2.48	0.49
1:V:26:VAL:HG22	1:V:37:LYS:HG2	1.94	0.49
1:T:205:LYS:HE2	1:T:207:ALA:HB3	1.94	0.49
1:B:65:TYR:CE1	1:B:78:LEU:HD21	2.48	0.49
1:E:110:LYS:HD2	1:F:175:VAL:HG23	1.94	0.49
1:K:253:ARG:NH2	4:K:1974:HOH:O	2.45	0.49
1:R:135:LEU:HD23	1:R:136:ILE:N	2.28	0.49
1:N:135:LEU:C	1:N:135:LEU:HD23	2.33	0.49
1:L:261:THR:HG22	1:L:264:ASN:H	1.78	0.48
1:L:200:ARG:NH2	2:L:302:MPD:H32	2.28	0.48
1:C:71:GLU:OE1	1:C:75:LYS:HE3	2.13	0.48
1:X:110:LYS:HD2	1:Y:175:VAL:HG23	1.95	0.48
1:A:175:VAL:HG23	1:G:110:LYS:HD2	1.95	0.48
1:B:183:ASP:HB2	4:B:1231:HOH:O	2.13	0.48
1:O:26:VAL:HG22	1:O:37:LYS:HG2	1.94	0.48
1:L:91:PRO:HD3	1:L:244:ASN:O	2.13	0.48
1:P:135:LEU:C	1:P:135:LEU:HD23	2.34	0.48
1:V:110:LYS:HD2	1:W:175:VAL:HG23	1.95	0.48
1:E:188:ASN:O	1:E:191:TYR:O	2.31	0.48
1:A:222:SER:HB3	1:G:157:LEU:O	2.14	0.48
1:F:36:LYS:NZ	1:F:280:GLU:HG2	2.29	0.48
1:Q:69:SER:OG	1:Q:71:GLU:HG2	2.13	0.48
1:P:281:ARG:HG2	1:P:294:LEU:HD12	1.95	0.48
2:N:302:MPD:H13	2:N:302:MPD:H52	1.96	0.48
1:K:183:ASP:HB2	4:K:309:HOH:O	2.13	0.48
1:U:36:LYS:NZ	1:U:280:GLU:HG2	2.29	0.48
2:O:303:MPD:H53	2:O:303:MPD:H12	1.95	0.48
1:X:283:LYS:HB2	1:X:294:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:75:LYS:HE3	1:W:259:HIS:HB2	1.96	0.48
1:C:36:LYS:NZ	1:C:280:GLU:HG2	2.28	0.48
1:R:26:VAL:HG22	1:R:37:LYS:HG2	1.95	0.48
1:O:175:VAL:HG23	1:U:110:LYS:HD2	1.95	0.48
1:T:91:PRO:HB2	1:T:94:GLU:CG	2.41	0.48
1:Y:26:VAL:HG22	1:Y:37:LYS:HG2	1.94	0.48
1:L:110:LYS:HD2	1:M:175:VAL:HG23	1.94	0.48
1:T:26:VAL:HG22	1:T:37:LYS:HG2	1.94	0.48
1:C:194:GLN:HG2	1:C:197:MET:HE2	1.96	0.48
1:V:236:ARG:O	4:V:374:HOH:O	2.20	0.48
1:U:37:LYS:NZ	4:U:1357:HOH:O	2.45	0.48
2:A:303:MPD:H11	1:Y:116:LEU:CB	127.29	0.48
1:S:191:TYR:HE1	1:S:200:ARG:HB3	1.77	0.48
1:W:26:VAL:HG22	1:W:37:LYS:HG2	1.95	0.48
1:P:113:MET:HA	1:Q:146:LEU:O	2.13	0.48
1:A:113:MET:HA	1:B:146:LEU:O	2.21	0.48
1:C:183:ASP:HB2	4:C:1668:HOH:O	2.13	0.48
1:D:36:LYS:NZ	1:D:280:GLU:HG2	2.29	0.48
1:X:16:SER:O	1:X:18:THR:HG23	2.13	0.48
1:A:36:LYS:NZ	1:A:280:GLU:HG2	2.29	0.48
1:B:36:LYS:NZ	1:B:280:GLU:HG2	2.30	0.48
1:H:222:SER:HB3	1:N:157:LEU:O	2.14	0.48
1:A:262:SER:HB2	1:H:268:THR:CG2	105.13	0.48
1:W:36:LYS:NZ	1:W:280:GLU:HG2	2.29	0.48
1:B:262:SER:CB	1:K:124:VAL:HG11	60.65	0.47
1:V:68:TYR:O	1:V:69:SER:HB3	2.14	0.47
1:A:26:VAL:HG22	1:A:37:LYS:HG2	1.96	0.47
1:K:26:VAL:HG22	1:K:37:LYS:HG2	1.95	0.47
1:M:26:VAL:HG22	1:M:37:LYS:HG2	1.95	0.47
1:N:26:VAL:HG22	1:N:37:LYS:HG2	1.96	0.47
1:H:175:VAL:HG23	1:N:110:LYS:HD2	1.95	0.47
1:N:36:LYS:NZ	1:N:280:GLU:HG2	2.29	0.47
1:P:26:VAL:HG22	1:P:37:LYS:HG2	1.95	0.47
1:Z:91:PRO:CG	1:Z:94:GLU:CG	2.91	0.47
1:U:260:TRP:NE1	1:U:262:SER:HA	2.29	0.47
1:D:26:VAL:HG22	1:D:37:LYS:HG2	1.95	0.47
1:Q:36:LYS:NZ	1:Q:280:GLU:HG2	2.30	0.47
1:C:95:VAL:HG12	4:C:712:HOH:O	2.14	0.47
1:Z:260:TRP:HB2	1:Z:265:TRP:CZ3	2.50	0.47
1:J:93:ASN:OD1	1:J:94:GLU:HG3	2.14	0.47
1:O:294:LEU:O	1:O:295:GLU:CB	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:GLY:HA3	1:E:267:GLY:O	2.15	0.47
1:E:90:LEU:HB3	1:E:91:PRO:HD2	1.96	0.47
1:L:14:ILE:HD11	1:L:48:HIS:CE1	2.50	0.47
1:Z:26:VAL:HG22	1:Z:37:LYS:HG2	1.95	0.47
1:M:200:ARG:HE	2:M:302:MPD:HM2	1.79	0.47
1:O:65:TYR:CE2	1:O:78:LEU:HD21	2.49	0.47
1:B:91:PRO:HB2	1:B:94:GLU:HG3	1.97	0.47
1:E:261:THR:HG22	1:E:264:ASN:H	1.79	0.47
1:G:94:GLU:OE2	1:G:243:THR:HG23	2.14	0.47
1:F:26:VAL:HG22	1:F:37:LYS:HG2	1.96	0.47
1:G:26:VAL:HG22	1:G:37:LYS:HG2	1.96	0.47
1:Z:36:LYS:NZ	1:Z:280:GLU:HG2	2.30	0.47
1:M:56:ARG:NH2	4:M:315:HOH:O	2.47	0.47
1:W:113:MET:HA	1:X:146:LEU:O	2.15	0.47
1:A:200:ARG:CZ	2:A:302:MPD:C1	4.68	0.47
1:D:116:LEU:HB2	2:F:303:MPD:HM3	1.96	0.47
2:D:302:MPD:H53	2:D:302:MPD:HM1	1.96	0.47
1:W:14:ILE:HD11	1:X:39:PHE:CE1	2.50	0.47
1:V:18:THR:HG21	1:V:45:ASP:HA	1.96	0.47
1:L:26:VAL:HG22	1:L:37:LYS:HG2	1.97	0.47
1:H:17:ASN:N	4:H:1998:HOH:O	2.45	0.47
1:C:129:THR:O	1:C:129:THR:HG22	2.14	0.47
1:N:75:LYS:HD2	1:N:259:HIS:CB	2.45	0.47
1:O:39:PHE:HE1	1:U:14:ILE:HD11	1.80	0.47
1:T:90:LEU:HD12	1:T:245:ILE:HG13	1.95	0.47
1:Q:135:LEU:HD23	1:Q:136:ILE:N	2.30	0.47
1:S:110:LYS:HD2	1:T:175:VAL:HG23	1.97	0.47
1:X:161:THR:HG22	1:Y:28:TYR:CZ	2.50	0.47
1:X:191:TYR:CZ	1:X:200:ARG:HD3	2.50	0.47
1:X:36:LYS:NZ	1:X:280:GLU:HG2	2.30	0.47
1:I:132:ILE:HG22	1:I:133:GLY:N	2.30	0.47
1:R:36:LYS:NZ	1:R:280:GLU:HG2	2.29	0.47
1:E:197:MET:O	2:E:302:MPD:H52	2.15	0.47
1:A:116:LEU:CB	2:V:303:MPD:HM1	132.04	0.47
1:U:191:TYR:CE1	1:U:200:ARG:HD3	2.50	0.47
1:O:14:ILE:HD11	1:P:39:PHE:HE1	1.80	0.47
1:V:179:TRP:HA	2:V:303:MPD:C5	2.41	0.46
1:W:258:LEU:HA	1:W:266:LYS:O	2.15	0.46
1:E:36:LYS:NZ	1:E:280:GLU:HG2	2.30	0.46
1:P:227:ASP:OD1	4:P:2010:HOH:O	2.21	0.46
1:V:126:GLY:HA2	1:V:131:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASN:OD1	1:B:190:VAL:HG22	2.14	0.46
1:H:14:ILE:HG12	1:H:15:GLY:N	2.31	0.46
1:D:294:LEU:O	1:D:295:GLU:CB	2.63	0.46
1:X:200:ARG:CZ	2:X:302:MPD:H11	2.45	0.46
1:U:26:VAL:HG22	1:U:37:LYS:HG2	1.97	0.46
1:A:110:LYS:HD2	1:B:175:VAL:HG23	1.98	0.46
1:U:197:MET:HE1	1:U:200:ARG:HG2	1.96	0.46
1:C:26:VAL:HG22	1:C:37:LYS:HG2	1.95	0.46
1:M:72:GLY:C	1:M:205:LYS:HZ1	2.18	0.46
1:Q:183:ASP:HB2	4:Q:1535:HOH:O	2.13	0.46
1:N:263:THR:HG23	1:N:264:ASN:OD1	2.16	0.46
1:M:36:LYS:NZ	1:M:280:GLU:HG2	2.31	0.46
1:C:157:LEU:O	1:D:222:SER:HB3	2.15	0.46
1:P:36:LYS:NZ	1:P:280:GLU:HG2	2.31	0.46
1:I:26:VAL:HG22	1:I:37:LYS:HG2	1.97	0.46
1:Q:26:VAL:HG22	1:Q:37:LYS:HG2	1.96	0.46
1:J:36:LYS:HD2	4:J:527:HOH:O	2.16	0.46
1:B:14:ILE:HD11	1:V:39:PHE:HE1	178.46	0.46
1:L:36:LYS:NZ	1:L:280:GLU:HG2	2.31	0.46
2:R:303:MPD:C5	2:R:303:MPD:H12	2.41	0.46
1:R:179:TRP:CE3	2:R:303:MPD:H51	2.51	0.46
2:Q:302:MPD:H4	2:Q:302:MPD:HM1	1.69	0.46
1:E:192:GLY:H	1:E:266:LYS:HG3	1.80	0.46
1:V:253:ARG:NE	4:V:731:HOH:O	2.48	0.46
1:K:36:LYS:NZ	1:K:280:GLU:HG2	2.31	0.46
1:X:277:ARG:NE	4:X:728:HOH:O	2.45	0.46
1:A:183:ASP:HB2	4:A:313:HOH:O	2.15	0.46
1:A:188:ASN:OD1	1:A:190:VAL:HG13	5.21	0.46
1:H:36:LYS:NZ	1:H:280:GLU:HG2	2.30	0.46
2:A:302:MPD:C5	2:A:302:MPD:HM3	2.37	0.46
1:A:122:GLY:HA2	1:A:135:LEU:O	2.16	0.46
1:Q:161:THR:HG22	1:R:28:TYR:CZ	2.51	0.46
1:X:74:ASN:O	1:X:259:HIS:HA	2.15	0.46
1:H:14:ILE:HD13	1:H:52:LEU:HD22	1.97	0.46
1:V:253:ARG:CD	4:V:731:HOH:O	2.64	0.46
1:J:36:LYS:NZ	1:J:280:GLU:HG2	2.31	0.46
1:W:49:ASN:OD1	1:W:50:LYS:HG2	2.16	0.46
1:J:26:VAL:HG22	1:J:37:LYS:HG2	1.96	0.46
1:H:26:VAL:HG22	1:H:37:LYS:HG2	1.98	0.46
2:S:303:MPD:C5	2:S:303:MPD:H12	2.27	0.46
1:D:49:ASN:OD1	1:D:50:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:161:THR:HG22	1:Q:28:TYR:CZ	2.51	0.46
1:Z:65:TYR:CE2	1:Z:78:LEU:HD21	2.51	0.46
2:W:303:MPD:H52	2:W:303:MPD:O2	2.16	0.45
1:Q:157:LEU:O	1:R:222:SER:HB3	2.16	0.45
2:N:302:MPD:C1	2:N:302:MPD:H52	2.46	0.45
1:Y:179:TRP:CZ3	1:Y:200:ARG:NH1	2.84	0.45
1:W:122:GLY:HA2	1:W:135:LEU:O	2.15	0.45
1:H:65:TYR:CE1	1:H:78:LEU:HD21	2.52	0.45
2:A:302:MPD:HM3	2:A:302:MPD:O4	4.21	0.45
1:S:74:ASN:C	1:S:75:LYS:HD2	2.37	0.45
1:Y:36:LYS:NZ	1:Y:280:GLU:HG2	2.31	0.45
1:E:248:ILE:N	1:E:248:ILE:HD12	2.32	0.45
1:H:176:ASN:ND2	2:H:302:MPD:HM1	2.32	0.45
1:S:157:LEU:O	1:T:222:SER:HB3	2.16	0.45
1:C:65:TYR:CE1	1:C:78:LEU:HD21	2.51	0.45
1:B:113:MET:HA	1:C:146:LEU:O	2.16	0.45
1:P:157:LEU:O	1:Q:222:SER:HB3	2.16	0.45
1:V:10:GLY:HA2	1:V:13:ASP:OD2	2.16	0.45
1:D:113:MET:HA	1:E:146:LEU:O	2.16	0.45
1:B:91:PRO:HD3	1:B:244:ASN:O	2.20	0.45
1:N:200:ARG:HE	2:N:302:MPD:HM3	1.81	0.45
1:S:261:THR:O	1:S:262:SER:C	2.54	0.45
1:X:26:VAL:HG22	1:X:37:LYS:HG2	1.97	0.45
1:H:91:PRO:HD3	1:H:244:ASN:O	2.16	0.45
1:K:205:LYS:HG2	1:K:207:ALA:H	1.81	0.45
1:W:74:ASN:O	1:W:75:LYS:HD2	2.16	0.45
1:M:73:ALA:HA	1:M:205:LYS:CE	2.46	0.45
1:J:70:GLU:HG3	1:J:207:ALA:HB2	1.99	0.45
1:Y:110:LYS:HD2	1:Z:175:VAL:HG23	1.99	0.45
1:Z:67:VAL:HG23	1:Z:67:VAL:O	2.16	0.45
2:J:303:MPD:H52	2:J:303:MPD:H12	1.98	0.45
1:P:66:ARG:C	1:P:78:LEU:HD12	2.37	0.45
1:A:39:PHE:HE1	1:Z:14:ILE:HD11	155.90	0.45
1:A:65:TYR:CE2	1:A:78:LEU:HD21	2.52	0.45
2:Z:302:MPD:H52	2:Z:302:MPD:H13	1.99	0.45
1:S:7:ILE:HA	1:T:14:ILE:O	2.17	0.45
1:L:293:ASN:O	1:L:294:LEU:HB2	2.16	0.45
1:T:261:THR:HG22	1:T:263:THR:H	1.81	0.45
1:J:161:THR:HG22	1:K:28:TYR:CZ	2.51	0.45
1:V:283:LYS:HB2	1:V:294:LEU:HD21	1.99	0.45
1:N:18:THR:HG21	1:N:45:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:14:ILE:HD11	1:Y:39:PHE:CE1	2.49	0.45
1:O:294:LEU:O	1:O:295:GLU:HB2	2.17	0.45
1:M:70:GLU:OE2	1:M:205:LYS:HE2	2.17	0.45
1:D:14:ILE:CD1	1:D:43:ILE:HG21	2.47	0.45
1:V:36:LYS:NZ	1:V:280:GLU:HG2	2.32	0.45
1:K:200:ARG:NH2	2:K:302:MPD:C1	2.80	0.45
2:N:303:MPD:C5	2:N:303:MPD:H12	2.44	0.45
1:S:36:LYS:NZ	1:S:280:GLU:HG2	2.32	0.45
1:Y:113:MET:HA	1:Z:146:LEU:O	2.17	0.45
1:A:89:GLN:HG3	1:A:164:LYS:HG2	1.99	0.45
1:B:127:ASP:HB2	1:V:131:LYS:CE	160.58	0.44
1:I:36:LYS:HZ1	1:I:280:GLU:HG2	1.82	0.44
1:Z:277:ARG:NE	4:Z:1846:HOH:O	2.50	0.44
1:L:71:GLU:HG3	1:L:71:GLU:O	2.16	0.44
1:E:261:THR:HG23	1:E:263:THR:H	1.83	0.44
1:M:261:THR:HG22	1:M:262:SER:H	1.80	0.44
1:O:18:THR:HG21	1:O:45:ASP:HA	1.98	0.44
1:C:95:VAL:HG22	4:C:1924:HOH:O	2.17	0.44
1:X:261:THR:O	1:X:262:SER:C	2.55	0.44
1:K:294:LEU:O	1:K:295:GLU:CB	2.65	0.44
1:V:18:THR:HG21	1:V:44:ASP:O	2.18	0.44
1:R:135:LEU:C	1:R:135:LEU:HD23	2.38	0.44
1:O:28:TYR:CZ	1:U:161:THR:HG22	2.52	0.44
1:B:191:TYR:CE2	1:B:200:ARG:HD3	2.86	0.44
1:A:281:ARG:HG2	1:A:294:LEU:HD12	2.00	0.44
1:B:157:LEU:O	1:C:222:SER:HB3	2.18	0.44
1:W:89:GLN:HG3	1:W:164:LYS:HG2	1.99	0.44
2:G:302:MPD:O4	2:G:302:MPD:HM3	2.17	0.44
1:R:74:ASN:O	1:R:259:HIS:HA	2.17	0.44
1:T:191:TYR:CZ	1:T:200:ARG:HD3	2.52	0.44
1:Y:205:LYS:HG3	1:Y:207:ALA:H	1.83	0.44
1:Q:200:ARG:NE	2:Q:302:MPD:HM1	2.33	0.44
1:G:191:TYR:CZ	1:G:200:ARG:HD3	2.53	0.44
1:R:91:PRO:CG	1:R:94:GLU:HG3	2.48	0.44
1:U:261:THR:O	1:U:263:THR:N	2.51	0.44
1:F:293:ASN:O	1:F:294:LEU:CB	2.65	0.44
1:W:74:ASN:C	1:W:75:LYS:HD2	2.37	0.44
1:J:74:ASN:O	1:J:259:HIS:HA	2.17	0.44
1:S:261:THR:HG22	1:S:264:ASN:H	1.83	0.44
1:W:70:GLU:HB3	1:W:207:ALA:HB2	2.00	0.44
2:A:303:MPD:H13	2:A:303:MPD:H52	3.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:70:GLU:O	1:X:71:GLU:C	2.55	0.43
1:A:135:LEU:HD23	1:G:125:THR:CG2	2.47	0.43
1:N:65:TYR:CE1	1:N:78:LEU:HD21	2.53	0.43
1:O:222:SER:HB3	1:U:157:LEU:O	2.18	0.43
1:K:14:ILE:HD11	1:L:39:PHE:HE1	1.83	0.43
1:X:135:LEU:C	1:X:135:LEU:HD23	2.38	0.43
1:G:135:LEU:HD23	1:G:135:LEU:C	2.38	0.43
1:A:262:SER:HB2	1:T:268:THR:CG2	2.47	0.43
1:B:68:TYR:CD2	1:B:69:SER:HB2	2.53	0.43
1:V:37:LYS:HD2	1:V:37:LYS:C	2.38	0.43
1:X:18:THR:HG21	1:X:45:ASP:HA	2.00	0.43
1:C:93:ASN:ND2	1:C:94:GLU:HG3	2.33	0.43
1:R:75:LYS:HG2	1:R:76:SER:N	2.33	0.43
1:Y:200:ARG:HE	2:Y:302:MPD:H11	1.82	0.43
1:D:289:GLU:O	4:D:311:HOH:O	2.21	0.43
1:O:135:LEU:C	1:O:135:LEU:HD23	2.39	0.43
1:F:14:ILE:CD1	1:F:43:ILE:HG21	2.48	0.43
1:T:20:VAL:O	4:T:611:HOH:O	2.21	0.43
1:A:131:LYS:HE2	1:A:131:LYS:HB3	4.61	0.43
2:I:303:MPD:HM1	2:I:303:MPD:H4	1.90	0.43
1:K:191:TYR:CZ	1:K:200:ARG:HD3	2.53	0.43
2:V:303:MPD:O2	2:V:303:MPD:H52	2.19	0.43
1:R:91:PRO:HG2	1:R:94:GLU:HG3	2.00	0.43
1:F:253:ARG:NH2	4:F:741:HOH:O	2.44	0.43
1:C:135:LEU:HD23	1:C:136:ILE:N	2.33	0.43
1:V:95:VAL:HG11	1:V:238:ALA:HB1	2.00	0.43
1:Z:135:LEU:HD23	1:Z:135:LEU:C	2.38	0.43
1:N:248:ILE:HD12	1:N:248:ILE:N	2.33	0.43
1:X:116:LEU:HB2	2:X:304:MPD:CM	2.45	0.43
1:Y:89:GLN:HG3	1:Y:164:LYS:HG2	1.99	0.43
1:B:200:ARG:HE	2:B:302:MPD:H11	2.77	0.43
1:R:113:MET:SD	1:S:147:LYS:HE2	2.58	0.43
1:H:283:LYS:HB2	1:H:294:LEU:HD21	2.01	0.43
1:G:122:GLY:HA2	1:G:135:LEU:O	2.17	0.43
1:E:49:ASN:OD1	1:E:50:LYS:HG2	2.18	0.43
1:S:122:GLY:HA2	1:S:135:LEU:O	2.19	0.43
1:U:248:ILE:HD12	1:U:248:ILE:N	2.34	0.43
1:E:200:ARG:NH1	2:E:302:MPD:H12	2.34	0.43
1:T:261:THR:HB	1:T:264:ASN:O	2.18	0.43
1:D:261:THR:CG2	1:D:262:SER:N	2.82	0.43
1:U:197:MET:CE	1:U:200:ARG:HG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:75:LYS:HD2	1:N:259:HIS:HB3	2.00	0.43
1:Y:135:LEU:HD23	1:Y:136:ILE:N	2.33	0.43
1:Q:248:ILE:N	1:Q:248:ILE:HD12	2.34	0.43
1:R:180:GLY:O	2:R:303:MPD:C1	2.44	0.43
1:A:14:ILE:HD11	1:A:52:LEU:HD22	2.04	0.43
1:X:199:THR:HA	2:X:302:MPD:C4	2.48	0.43
1:B:36:LYS:HZ1	1:B:280:GLU:HG2	1.84	0.43
1:H:146:LEU:O	1:N:113:MET:HA	2.19	0.43
1:T:110:LYS:HD2	1:U:175:VAL:HG23	2.01	0.43
1:R:65:TYR:CE1	1:R:78:LEU:HD21	2.53	0.43
1:C:198:LYS:HG2	1:C:199:THR:HG23	2.01	0.43
1:W:131:LYS:O	1:W:132:ILE:HD12	2.19	0.43
1:E:161:THR:HG22	1:F:28:TYR:CZ	2.54	0.43
1:F:248:ILE:N	1:F:248:ILE:HD12	2.34	0.43
1:A:248:ILE:N	1:A:248:ILE:HD12	2.33	0.43
1:H:248:ILE:HD12	1:H:248:ILE:N	2.33	0.43
1:U:91:PRO:HD3	1:U:244:ASN:O	2.18	0.43
2:I:302:MPD:O4	2:I:302:MPD:HM3	2.19	0.43
1:W:180:GLY:O	2:W:303:MPD:H13	2.19	0.43
1:K:244:ASN:ND2	4:K:1399:HOH:O	2.51	0.43
1:K:70:GLU:HG2	1:K:72:GLY:O	2.19	0.43
1:C:253:ARG:NH2	4:C:1548:HOH:O	2.51	0.43
1:U:183:ASP:HB2	4:U:1063:HOH:O	2.18	0.43
1:U:89:GLN:HG3	1:U:164:LYS:HG2	2.01	0.42
1:W:110:LYS:HD2	1:X:175:VAL:HG23	2.01	0.42
1:D:89:GLN:HG3	1:D:164:LYS:HG2	2.01	0.42
1:P:37:LYS:C	1:P:37:LYS:HD2	2.40	0.42
1:U:14:ILE:HG22	1:U:15:GLY:N	2.34	0.42
1:B:212:ASP:OD1	1:B:213:PRO:HD2	2.20	0.42
1:G:183:ASP:HB2	4:G:1948:HOH:O	2.19	0.42
1:L:91:PRO:HB2	1:L:94:GLU:HG3	2.00	0.42
1:H:204:MET:HG2	1:H:205:LYS:O	2.19	0.42
1:Z:89:GLN:HG3	1:Z:164:LYS:HG2	2.02	0.42
1:E:179:TRP:CB	2:E:302:MPD:HM3	2.49	0.42
1:I:200:ARG:NH2	2:I:302:MPD:H11	2.33	0.42
1:K:179:TRP:CD1	2:K:302:MPD:HM3	2.54	0.42
1:M:255:ASP:HB3	1:M:270:THR:HB	2.00	0.42
1:K:89:GLN:HG3	1:K:164:LYS:HG2	2.02	0.42
1:M:14:ILE:HD12	1:M:52:LEU:HD22	2.01	0.42
1:R:248:ILE:N	1:R:248:ILE:HD12	2.35	0.42
1:W:200:ARG:NH2	2:W:302:MPD:C1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:91:PRO:HD3	1:T:244:ASN:O	2.20	0.42
2:B:302:MPD:O4	2:B:302:MPD:C1	2.62	0.42
1:W:95:VAL:HG13	1:W:234:MET:SD	2.59	0.42
1:Z:36:LYS:HZ1	1:Z:280:GLU:HG2	1.84	0.42
1:L:37:LYS:HD2	1:L:37:LYS:C	2.39	0.42
1:M:89:GLN:HG3	1:M:164:LYS:HG2	2.01	0.42
1:Z:293:ASN:O	1:Z:294:LEU:HB2	2.19	0.42
1:T:248:ILE:HD12	1:T:248:ILE:N	2.35	0.42
1:P:14:ILE:HD11	1:Q:39:PHE:CE1	2.50	0.42
1:D:122:GLY:HA2	1:D:135:LEU:O	2.20	0.42
1:F:113:MET:SD	1:G:147:LYS:HE2	2.60	0.42
1:O:135:LEU:HD23	1:O:136:ILE:N	2.35	0.42
1:Y:131:LYS:C	1:Y:132:ILE:HD12	2.40	0.42
1:C:161:THR:HG22	1:D:28:TYR:CZ	2.54	0.42
1:X:248:ILE:HD12	1:X:248:ILE:N	2.35	0.42
1:Y:248:ILE:N	1:Y:248:ILE:HD12	2.35	0.42
2:C:303:MPD:H12	2:C:303:MPD:H53	2.00	0.42
1:P:89:GLN:HG3	1:P:164:LYS:HG2	2.01	0.42
1:W:248:ILE:N	1:W:248:ILE:HD12	2.34	0.42
1:A:191:TYR:CZ	1:A:200:ARG:HD3	2.54	0.42
1:P:71:GLU:O	1:P:71:GLU:CG	2.67	0.42
2:H:302:MPD:O4	2:H:302:MPD:H13	2.19	0.42
1:B:161:THR:HG22	1:C:28:TYR:CZ	2.55	0.42
1:Y:75:LYS:HG2	1:Y:259:HIS:HB2	2.00	0.42
1:N:74:ASN:O	1:N:259:HIS:HA	2.19	0.42
1:Y:70:GLU:HG3	1:Y:70:GLU:O	2.19	0.42
1:M:95:VAL:HG23	1:M:234:MET:SD	2.60	0.42
1:B:70:GLU:HG2	1:B:72:GLY:O	4.47	0.42
1:W:37:LYS:HD2	1:W:37:LYS:C	2.40	0.42
1:X:157:LEU:O	1:Y:222:SER:HB3	2.20	0.42
1:W:157:LEU:O	1:X:222:SER:HB3	2.19	0.42
1:Z:248:ILE:N	1:Z:248:ILE:HD12	2.35	0.42
1:M:132:ILE:HD12	1:M:133:GLY:N	2.35	0.42
1:A:200:ARG:CZ	2:A:302:MPD:H11	5.07	0.42
1:H:14:ILE:CD1	1:H:52:LEU:HD22	2.49	0.42
1:D:37:LYS:C	1:D:37:LYS:HD2	2.40	0.42
1:W:291:MET:O	4:W:1028:HOH:O	2.21	0.42
1:B:37:LYS:HD2	1:B:37:LYS:C	2.41	0.41
1:P:126:GLY:HA2	1:P:131:LYS:O	2.20	0.41
1:O:36:LYS:NZ	1:O:280:GLU:HG2	2.35	0.41
1:B:248:ILE:N	1:B:248:ILE:HD12	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD23	1:G:125:THR:HG22	2.02	0.41
1:K:37:LYS:HD2	1:K:37:LYS:C	2.41	0.41
1:Q:205:LYS:HB2	1:Q:205:LYS:HE3	1.87	0.41
1:O:91:PRO:HD3	1:O:244:ASN:O	2.20	0.41
1:E:193:ASN:N	1:E:267:GLY:O	2.53	0.41
1:K:122:GLY:HA2	1:K:135:LEU:O	2.19	0.41
1:M:72:GLY:C	1:M:205:LYS:NZ	2.74	0.41
1:N:89:GLN:HG3	1:N:164:LYS:HG2	2.02	0.41
1:F:161:THR:HG22	1:G:28:TYR:CZ	2.56	0.41
1:Z:49:ASN:OD1	1:Z:50:LYS:HG2	2.21	0.41
1:V:260:TRP:CD1	1:V:261:THR:O	2.73	0.41
1:A:123:ASN:OD1	1:A:123:ASN:C	2.59	0.41
1:P:248:ILE:N	1:P:248:ILE:HD12	2.35	0.41
1:W:66:ARG:C	1:W:78:LEU:HD12	2.41	0.41
1:T:113:MET:HA	1:U:146:LEU:O	2.19	0.41
1:Q:65:TYR:CE2	1:Q:78:LEU:HD21	2.54	0.41
1:I:110:LYS:HD2	1:J:175:VAL:HG23	2.01	0.41
1:L:66:ARG:C	1:L:78:LEU:HD12	2.40	0.41
1:F:37:LYS:C	1:F:37:LYS:HD2	2.41	0.41
1:M:161:THR:HG22	1:N:28:TYR:CZ	2.56	0.41
1:Q:94:GLU:OE2	1:Q:240:LYS:HE3	2.21	0.41
1:D:205:LYS:H	1:D:205:LYS:HG3	1.64	0.41
1:L:261:THR:CG2	1:L:264:ASN:H	2.34	0.41
1:U:200:ARG:CZ	2:U:302:MPD:H13	2.51	0.41
1:Z:37:LYS:HD2	1:Z:37:LYS:C	2.41	0.41
1:M:248:ILE:N	1:M:248:ILE:HD12	2.36	0.41
1:I:248:ILE:HD12	1:I:248:ILE:N	2.34	0.41
1:C:248:ILE:HD12	1:C:248:ILE:N	2.35	0.41
1:H:180:GLY:O	2:H:303:MPD:O2	2.38	0.41
1:N:293:ASN:O	1:N:294:LEU:CB	2.68	0.41
1:O:39:PHE:CE1	1:U:14:ILE:HD11	2.55	0.41
1:Q:184:ARG:HG3	4:Q:1535:HOH:O	2.20	0.41
1:X:135:LEU:HD23	1:X:136:ILE:N	2.35	0.41
1:I:113:MET:HA	1:J:146:LEU:O	2.21	0.41
1:V:65:TYR:CE2	1:V:78:LEU:HD21	2.56	0.41
1:C:91:PRO:HD3	1:C:244:ASN:O	2.20	0.41
1:D:123:ASN:OD1	1:D:123:ASN:C	2.59	0.41
1:T:135:LEU:HD23	1:T:135:LEU:C	2.40	0.41
1:M:113:MET:SD	1:N:147:LYS:HE2	2.61	0.41
1:N:122:GLY:HA2	1:N:135:LEU:O	2.20	0.41
1:T:14:ILE:HA	1:T:15:GLY:HA2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:89:GLN:HG3	1:T:164:LYS:HG2	2.01	0.41
1:V:89:GLN:HG3	1:V:164:LYS:HG2	2.02	0.41
1:Q:89:GLN:HG3	1:Q:164:LYS:HG2	2.03	0.41
2:G:303:MPD:C5	2:G:303:MPD:H12	2.43	0.41
1:Z:91:PRO:HG2	1:Z:94:GLU:HG2	1.97	0.41
1:S:37:LYS:HD2	1:S:37:LYS:C	2.41	0.41
1:M:190:VAL:HG13	1:M:191:TYR:CD1	2.56	0.41
1:S:202:GLY:HA3	1:S:204:MET:HE2	2.03	0.41
1:J:248:ILE:N	1:J:248:ILE:HD12	2.36	0.41
1:D:248:ILE:HD12	1:D:248:ILE:N	2.34	0.41
1:H:113:MET:HA	1:I:146:LEU:O	2.21	0.41
1:V:14:ILE:HD11	1:V:48:HIS:CE1	2.54	0.41
1:F:206:ALA:HA	1:F:265:TRP:CH2	2.56	0.41
1:W:92:ASP:O	1:W:163:LYS:NZ	2.50	0.41
1:O:261:THR:HG22	1:O:263:THR:H	1.86	0.41
1:O:248:ILE:N	1:O:248:ILE:HD12	2.36	0.41
1:R:180:GLY:H	2:R:303:MPD:H53	1.86	0.41
1:S:191:TYR:CZ	1:S:200:ARG:HD3	2.56	0.41
1:X:199:THR:HA	2:X:302:MPD:H4	2.02	0.41
1:C:127:ASP:OD2	1:C:129:THR:HB	2.20	0.41
1:X:37:LYS:HD2	1:X:37:LYS:C	2.41	0.41
1:I:113:MET:SD	1:J:147:LYS:HE2	2.61	0.41
1:H:89:GLN:HG3	1:H:164:LYS:HG2	2.03	0.41
1:Y:183:ASP:HB2	4:Y:858:HOH:O	2.21	0.41
1:T:8:LYS:HD2	1:U:13:ASP:CB	2.51	0.41
1:X:89:GLN:HG3	1:X:164:LYS:HG2	2.03	0.41
1:F:89:GLN:HG3	1:F:164:LYS:HG2	2.03	0.41
1:L:157:LEU:O	1:M:222:SER:HB3	2.21	0.41
2:B:302:MPD:O4	2:B:302:MPD:HM3	2.20	0.40
1:E:204:MET:HE2	1:E:204:MET:H	1.86	0.40
1:F:68:TYR:CE1	1:F:77:GLY:HA3	2.56	0.40
1:B:110:LYS:HD2	1:C:175:VAL:HG23	2.02	0.40
1:E:195:LEU:HD13	1:E:196:PHE:CE1	2.56	0.40
1:O:89:GLN:HG3	1:O:164:LYS:HG2	2.02	0.40
1:F:183:ASP:HB2	4:F:625:HOH:O	2.22	0.40
1:E:157:LEU:O	1:F:222:SER:HB3	2.21	0.40
1:T:123:ASN:C	1:T:123:ASN:OD1	2.60	0.40
1:B:123:ASN:C	1:B:123:ASN:OD1	2.60	0.40
2:K:302:MPD:H4	2:K:302:MPD:H11	1.83	0.40
1:B:263:THR:HG23	1:B:264:ASN:OD1	2.70	0.40
1:A:135:LEU:HD23	1:A:135:LEU:C	4.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:SER:HB3	1:Z:157:LEU:O	137.60	0.40
1:V:95:VAL:HG13	1:V:234:MET:SD	2.61	0.40
1:K:65:TYR:CE1	1:K:78:LEU:HD21	2.57	0.40
1:S:248:ILE:N	1:S:248:ILE:HD12	2.36	0.40
1:I:123:ASN:C	1:I:123:ASN:OD1	2.60	0.40
1:I:135:LEU:HD23	1:I:135:LEU:C	2.42	0.40
1:G:294:LEU:HD23	1:G:294:LEU:HA	1.96	0.40
1:L:161:THR:HG22	1:M:28:TYR:CZ	2.56	0.40
1:M:294:LEU:O	1:M:295:GLU:HG2	2.21	0.40
1:L:80:TRP:CE2	1:L:196:PHE:HE2	2.40	0.40
1:R:89:GLN:HG3	1:R:164:LYS:HG2	2.02	0.40
1:W:200:ARG:H	2:W:302:MPD:H52	1.86	0.40
1:G:135:LEU:HD23	1:G:136:ILE:N	2.36	0.40
1:O:261:THR:O	1:O:262:SER:C	2.60	0.40
1:V:91:PRO:HD3	1:V:244:ASN:O	2.21	0.40
2:B:303:MPD:H12	2:B:303:MPD:C5	3.62	0.40
1:S:204:MET:HE1	1:S:209:ASN:OD1	2.22	0.40
1:U:70:GLU:HG2	1:U:72:GLY:O	2.22	0.40
1:J:157:LEU:O	1:K:222:SER:HB3	2.21	0.40
1:F:128:ASP:OD1	1:G:131:LYS:HA	2.21	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	293/302 (97%)	280 (96%)	13 (4%)	0	100	100
1	B	293/302 (97%)	278 (95%)	15 (5%)	0	100	100
1	C	292/302 (97%)	282 (97%)	10 (3%)	0	100	100
1	D	293/302 (97%)	282 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	293/302 (97%)	275 (94%)	18 (6%)	0	100	100
1	F	292/302 (97%)	280 (96%)	12 (4%)	0	100	100
1	G	292/302 (97%)	279 (96%)	13 (4%)	0	100	100
1	H	292/302 (97%)	278 (95%)	13 (4%)	1 (0%)	46	57
1	I	292/302 (97%)	280 (96%)	12 (4%)	0	100	100
1	J	292/302 (97%)	278 (95%)	14 (5%)	0	100	100
1	K	293/302 (97%)	284 (97%)	9 (3%)	0	100	100
1	L	292/302 (97%)	277 (95%)	15 (5%)	0	100	100
1	M	293/302 (97%)	282 (96%)	11 (4%)	0	100	100
1	N	292/302 (97%)	281 (96%)	11 (4%)	0	100	100
1	O	293/302 (97%)	278 (95%)	14 (5%)	1 (0%)	46	57
1	P	292/302 (97%)	281 (96%)	11 (4%)	0	100	100
1	Q	292/302 (97%)	282 (97%)	10 (3%)	0	100	100
1	R	292/302 (97%)	279 (96%)	13 (4%)	0	100	100
1	S	293/302 (97%)	280 (96%)	13 (4%)	0	100	100
1	T	292/302 (97%)	276 (94%)	16 (6%)	0	100	100
1	U	293/302 (97%)	283 (97%)	10 (3%)	0	100	100
1	V	293/302 (97%)	282 (96%)	11 (4%)	0	100	100
1	W	292/302 (97%)	279 (96%)	13 (4%)	0	100	100
1	X	292/302 (97%)	281 (96%)	11 (4%)	0	100	100
1	Y	292/302 (97%)	277 (95%)	15 (5%)	0	100	100
1	Z	292/302 (97%)	280 (96%)	12 (4%)	0	100	100
1	a	292/302 (97%)	279 (96%)	12 (4%)	1 (0%)	46	57
1	b	293/302 (97%)	282 (96%)	11 (4%)	0	100	100
All	All	8187/8456 (97%)	7835 (96%)	349 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	262	SER
1	a	262	SER
1	H	262	SER

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	261/268 (97%)	257 (98%)	4 (2%)	72 85
1	B	261/268 (97%)	257 (98%)	4 (2%)	72 85
1	C	260/268 (97%)	257 (99%)	3 (1%)	78 89
1	D	261/268 (97%)	254 (97%)	7 (3%)	52 70
1	E	261/268 (97%)	250 (96%)	11 (4%)	36 49
1	F	260/268 (97%)	253 (97%)	7 (3%)	52 70
1	G	260/268 (97%)	255 (98%)	5 (2%)	65 81
1	H	260/268 (97%)	257 (99%)	3 (1%)	78 89
1	I	260/268 (97%)	257 (99%)	3 (1%)	78 89
1	J	260/268 (97%)	254 (98%)	6 (2%)	58 75
1	K	261/268 (97%)	258 (99%)	3 (1%)	80 90
1	L	260/268 (97%)	254 (98%)	6 (2%)	58 75
1	M	261/268 (97%)	257 (98%)	4 (2%)	72 85
1	N	260/268 (97%)	254 (98%)	6 (2%)	58 75
1	O	261/268 (97%)	253 (97%)	8 (3%)	47 64
1	P	260/268 (97%)	256 (98%)	4 (2%)	72 85
1	Q	260/268 (97%)	255 (98%)	5 (2%)	65 81
1	R	260/268 (97%)	257 (99%)	3 (1%)	78 89
1	S	261/268 (97%)	254 (97%)	7 (3%)	52 70
1	T	260/268 (97%)	257 (99%)	3 (1%)	78 89
1	U	261/268 (97%)	254 (97%)	7 (3%)	52 70
1	V	261/268 (97%)	256 (98%)	5 (2%)	65 81
1	W	260/268 (97%)	255 (98%)	5 (2%)	65 81
1	X	260/268 (97%)	255 (98%)	5 (2%)	65 81
1	Y	260/268 (97%)	255 (98%)	5 (2%)	65 81
1	Z	260/268 (97%)	257 (99%)	3 (1%)	78 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	260/268 (97%)	254 (98%)	6 (2%)	58 75
1	b	261/268 (97%)	254 (97%)	7 (3%)	52 70
All	All	7291/7504 (97%)	7146 (98%)	145 (2%)	63 79

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	37	LYS
1	A	101	TYR
1	A	132	ILE
1	B	37	LYS
1	B	92	ASP
1	B	101	TYR
1	B	263	THR
1	C	17	ASN
1	C	101	TYR
1	C	190	VAL
1	D	37	LYS
1	D	101	TYR
1	D	195	LEU
1	D	201	ASN
1	D	204	MET
1	D	205	LYS
1	D	295	GLU
1	E	18	THR
1	E	37	LYS
1	E	92	ASP
1	E	101	TYR
1	E	127	ASP
1	E	195	LEU
1	E	200	ARG
1	E	204	MET
1	E	258	LEU
1	E	259	HIS
1	E	261	THR
1	F	14	ILE
1	F	37	LYS
1	F	92	ASP
1	F	101	TYR
1	F	135	LEU

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Mol	Chain	Res	Type
1	F	201	ASN
1	F	204	MET
1	G	37	LYS
1	G	101	TYR
1	G	195	LEU
1	G	204	MET
1	G	263	THR
1	H	37	LYS
1	H	74	ASN
1	H	101	TYR
1	I	18	THR
1	I	71	GLU
1	I	101	TYR
1	J	14	ILE
1	J	18	THR
1	J	37	LYS
1	J	101	TYR
1	J	205	LYS
1	J	257	GLN
1	K	37	LYS
1	K	101	TYR
1	K	135	LEU
1	L	18	THR
1	L	37	LYS
1	L	101	TYR
1	L	129	THR
1	L	131	LYS
1	L	263	THR
1	M	37	LYS
1	M	94	GLU
1	M	101	TYR
1	M	132	ILE
1	N	14	ILE
1	N	17	ASN
1	N	37	LYS
1	N	101	TYR
1	N	263	THR
1	N	294	LEU
1	O	18	THR
1	O	37	LYS
1	O	67	VAL
1	O	101	TYR

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Mol	Chain	Res	Type
1	O	204	MET
1	O	258	LEU
1	O	261	THR
1	O	264	ASN
1	P	37	LYS
1	P	101	TYR
1	P	129	THR
1	P	205	LYS
1	Q	14	ILE
1	Q	17	ASN
1	Q	37	LYS
1	Q	101	TYR
1	Q	201	ASN
1	R	37	LYS
1	R	66	ARG
1	R	101	TYR
1	S	17	ASN
1	S	37	LYS
1	S	101	TYR
1	S	201	ASN
1	S	261	THR
1	S	263	THR
1	S	295	GLU
1	T	14	ILE
1	T	18	THR
1	T	101	TYR
1	U	66	ARG
1	U	95	VAL
1	U	101	TYR
1	U	127	ASP
1	U	131	LYS
1	U	198	LYS
1	U	204	MET
1	V	18	THR
1	V	37	LYS
1	V	94	GLU
1	V	101	TYR
1	V	201	ASN
1	W	37	LYS
1	W	101	TYR
1	W	195	LEU
1	W	201	ASN

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Mol	Chain	Res	Type
1	W	261	THR
1	X	37	LYS
1	X	70	GLU
1	X	92	ASP
1	X	101	TYR
1	X	204	MET
1	Y	37	LYS
1	Y	101	TYR
1	Y	128	ASP
1	Y	201	ASN
1	Y	204	MET
1	Z	37	LYS
1	Z	101	TYR
1	Z	201	ASN
1	a	14	ILE
1	a	37	LYS
1	a	92	ASP
1	a	101	TYR
1	a	190	VAL
1	a	201	ASN
1	b	37	LYS
1	b	101	TYR
1	b	125	THR
1	b	201	ASN
1	b	204	MET
1	b	261	THR
1	b	263	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	C	177	GLN
1	J	97	GLN
1	O	264	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

84 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MPD	A	302	-	6,7,7	0.28	0	7,10,10	0.66	0
2	MPD	A	303	-	6,7,7	0.35	0	7,10,10	0.37	0
3	ACY	A	304	-	1,3,3	1.48	0	0,3,3	0.00	-
3	ACY	A	305	-	1,3,3	1.46	0	0,3,3	0.00	-
2	MPD	B	302	-	6,7,7	0.28	0	7,10,10	0.44	0
2	MPD	B	303	-	6,7,7	0.33	0	7,10,10	0.42	0
2	MPD	C	302	-	6,7,7	0.28	0	7,10,10	0.38	0
2	MPD	C	303	-	6,7,7	0.33	0	7,10,10	0.22	0
3	ACY	C	304	-	1,3,3	1.36	0	0,3,3	0.00	-
2	MPD	D	302	-	6,7,7	0.35	0	7,10,10	0.54	0
2	MPD	D	303	-	6,7,7	0.30	0	7,10,10	0.35	0
3	ACY	D	304	-	1,3,3	1.31	0	0,3,3	0.00	-
3	ACY	D	305	-	1,3,3	1.37	0	0,3,3	0.00	-
2	MPD	E	302	-	6,7,7	0.24	0	7,10,10	0.56	0
2	MPD	E	303	-	6,7,7	0.35	0	7,10,10	0.39	0
3	ACY	E	304	-	1,3,3	1.28	0	0,3,3	0.00	-
2	MPD	F	302	-	6,7,7	0.31	0	7,10,10	0.41	0
2	MPD	F	303	-	6,7,7	0.19	0	7,10,10	0.42	0
3	ACY	F	304	-	1,3,3	1.40	0	0,3,3	0.00	-
2	MPD	G	302	-	6,7,7	0.29	0	7,10,10	0.40	0
2	MPD	G	303	-	6,7,7	0.36	0	7,10,10	0.29	0
2	MPD	H	302	-	6,7,7	0.27	0	7,10,10	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MPD	H	303	-	6,7,7	0.27	0	7,10,10	0.37	0
3	ACY	H	304	-	1,3,3	1.43	0	0,3,3	0.00	-
3	ACY	H	305	-	1,3,3	1.42	0	0,3,3	0.00	-
2	MPD	I	302	-	6,7,7	0.29	0	7,10,10	0.45	0
2	MPD	I	303	-	6,7,7	0.30	0	7,10,10	0.42	0
2	MPD	J	302	-	6,7,7	0.38	0	7,10,10	0.73	0
2	MPD	J	303	-	6,7,7	0.30	0	7,10,10	0.53	0
3	ACY	J	304	-	1,3,3	1.31	0	0,3,3	0.00	-
2	MPD	K	302	-	6,7,7	0.25	0	7,10,10	0.47	0
2	MPD	K	303	-	6,7,7	0.32	0	7,10,10	0.48	0
3	ACY	K	304	-	1,3,3	1.28	0	0,3,3	0.00	-
3	ACY	K	305	-	1,3,3	1.01	0	0,3,3	0.00	-
2	MPD	L	302	-	6,7,7	0.29	0	7,10,10	0.38	0
2	MPD	L	303	-	6,7,7	0.30	0	7,10,10	0.54	0
3	ACY	L	304	-	1,3,3	1.17	0	0,3,3	0.00	-
2	MPD	M	302	-	6,7,7	0.27	0	7,10,10	0.44	0
2	MPD	M	303	-	6,7,7	0.36	0	7,10,10	0.26	0
3	ACY	M	304	-	1,3,3	1.37	0	0,3,3	0.00	-
2	MPD	N	302	-	6,7,7	0.26	0	7,10,10	0.43	0
2	MPD	N	303	-	6,7,7	0.36	0	7,10,10	0.37	0
2	MPD	O	302	-	6,7,7	0.24	0	7,10,10	0.54	0
2	MPD	O	303	-	6,7,7	0.34	0	7,10,10	0.32	0
3	ACY	O	304	-	1,3,3	1.12	0	0,3,3	0.00	-
3	ACY	O	305	-	1,3,3	1.36	0	0,3,3	0.00	-
2	MPD	P	302	-	6,7,7	0.25	0	7,10,10	0.45	0
2	MPD	P	303	-	6,7,7	0.30	0	7,10,10	0.23	0
3	ACY	P	304	-	1,3,3	1.37	0	0,3,3	0.00	-
2	MPD	Q	302	-	6,7,7	0.19	0	7,10,10	0.67	0
2	MPD	Q	303	-	6,7,7	0.32	0	7,10,10	0.19	0
3	ACY	Q	304	-	1,3,3	1.14	0	0,3,3	0.00	-
2	MPD	R	302	-	6,7,7	0.30	0	7,10,10	0.52	0
2	MPD	R	303	-	6,7,7	0.30	0	7,10,10	0.34	0
2	MPD	S	302	-	6,7,7	0.33	0	7,10,10	0.46	0
2	MPD	S	303	-	6,7,7	0.35	0	7,10,10	0.31	0
3	ACY	S	304	-	1,3,3	1.16	0	0,3,3	0.00	-
3	ACY	S	305	-	1,3,3	1.30	0	0,3,3	0.00	-
2	MPD	T	302	-	6,7,7	0.32	0	7,10,10	0.35	0
2	MPD	T	303	-	6,7,7	0.29	0	7,10,10	0.55	0
3	ACY	T	304	-	1,3,3	1.42	0	0,3,3	0.00	-
2	MPD	U	302	-	6,7,7	0.32	0	7,10,10	0.44	0
2	MPD	U	303	-	6,7,7	0.37	0	7,10,10	0.34	0
2	MPD	V	302	-	6,7,7	0.28	0	7,10,10	0.43	0
2	MPD	V	303	-	6,7,7	0.29	0	7,10,10	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACY	V	304	-	1,3,3	1.41	0	0,3,3	0.00	-
2	MPD	W	302	-	6,7,7	0.30	0	7,10,10	0.33	0
2	MPD	W	303	-	6,7,7	0.33	0	7,10,10	0.28	0
3	ACY	W	304	-	1,3,3	1.51	0	0,3,3	0.00	-
2	MPD	X	302	-	6,7,7	0.29	0	7,10,10	0.28	0
2	MPD	X	303	-	6,7,7	0.30	0	7,10,10	0.35	0
2	MPD	X	304	-	6,7,7	0.32	0	7,10,10	0.49	0
3	ACY	X	305	-	1,3,3	1.28	0	0,3,3	0.00	-
2	MPD	Y	302	-	6,7,7	0.26	0	7,10,10	0.48	0
2	MPD	Y	303	-	6,7,7	0.36	0	7,10,10	0.41	0
3	ACY	Y	304	-	1,3,3	1.07	0	0,3,3	0.00	-
2	MPD	Z	302	-	6,7,7	0.30	0	7,10,10	0.38	0
3	ACY	Z	303	-	1,3,3	1.45	0	0,3,3	0.00	-
2	MPD	a	302	-	6,7,7	0.26	0	7,10,10	0.40	0
2	MPD	a	303	-	6,7,7	0.27	0	7,10,10	0.60	0
3	ACY	a	304	-	1,3,3	1.45	0	0,3,3	0.00	-
2	MPD	b	302	-	6,7,7	0.28	0	7,10,10	0.35	0
2	MPD	b	303	-	6,7,7	0.34	0	7,10,10	0.27	0
3	ACY	b	304	-	1,3,3	1.24	0	0,3,3	0.00	-

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
2	MPD	A	302	-	-	0/5/5/5	0/0/0/0
2	MPD	A	303	-	-	0/5/5/5	0/0/0/0
3	ACY	A	304	-	-	0/0/0/0	0/0/0/0
3	ACY	A	305	-	-	0/0/0/0	0/0/0/0
2	MPD	B	302	-	-	0/5/5/5	0/0/0/0
2	MPD	B	303	-	-	0/5/5/5	0/0/0/0
2	MPD	C	302	-	-	0/5/5/5	0/0/0/0
2	MPD	C	303	-	-	0/5/5/5	0/0/0/0
3	ACY	C	304	-	-	0/0/0/0	0/0/0/0
2	MPD	D	302	-	-	0/5/5/5	0/0/0/0
2	MPD	D	303	-	-	0/5/5/5	0/0/0/0
3	ACY	D	304	-	-	0/0/0/0	0/0/0/0
3	ACY	D	305	-	-	0/0/0/0	0/0/0/0
2	MPD	E	302	-	-	0/5/5/5	0/0/0/0
2	MPD	E	303	-	-	0/5/5/5	0/0/0/0
3	ACY	E	304	-	-	0/0/0/0	0/0/0/0
2	MPD	F	302	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	F	303	-	-	0/5/5/5	0/0/0/0
3	ACY	F	304	-	-	0/0/0/0	0/0/0/0
2	MPD	G	302	-	-	0/5/5/5	0/0/0/0
2	MPD	G	303	-	-	0/5/5/5	0/0/0/0
2	MPD	H	302	-	-	0/5/5/5	0/0/0/0
2	MPD	H	303	-	-	0/5/5/5	0/0/0/0
3	ACY	H	304	-	-	0/0/0/0	0/0/0/0
3	ACY	H	305	-	-	0/0/0/0	0/0/0/0
2	MPD	I	302	-	-	0/5/5/5	0/0/0/0
2	MPD	I	303	-	-	0/5/5/5	0/0/0/0
2	MPD	J	302	-	-	0/5/5/5	0/0/0/0
2	MPD	J	303	-	-	0/5/5/5	0/0/0/0
3	ACY	J	304	-	-	0/0/0/0	0/0/0/0
2	MPD	K	302	-	-	0/5/5/5	0/0/0/0
2	MPD	K	303	-	-	0/5/5/5	0/0/0/0
3	ACY	K	304	-	-	0/0/0/0	0/0/0/0
3	ACY	K	305	-	-	0/0/0/0	0/0/0/0
2	MPD	L	302	-	-	0/5/5/5	0/0/0/0
2	MPD	L	303	-	-	0/5/5/5	0/0/0/0
3	ACY	L	304	-	-	0/0/0/0	0/0/0/0
2	MPD	M	302	-	-	0/5/5/5	0/0/0/0
2	MPD	M	303	-	-	0/5/5/5	0/0/0/0
3	ACY	M	304	-	-	0/0/0/0	0/0/0/0
2	MPD	N	302	-	-	0/5/5/5	0/0/0/0
2	MPD	N	303	-	-	0/5/5/5	0/0/0/0
2	MPD	O	302	-	-	0/5/5/5	0/0/0/0
2	MPD	O	303	-	-	0/5/5/5	0/0/0/0
3	ACY	O	304	-	-	0/0/0/0	0/0/0/0
3	ACY	O	305	-	-	0/0/0/0	0/0/0/0
2	MPD	P	302	-	-	0/5/5/5	0/0/0/0
2	MPD	P	303	-	-	0/5/5/5	0/0/0/0
3	ACY	P	304	-	-	0/0/0/0	0/0/0/0
2	MPD	Q	302	-	-	0/5/5/5	0/0/0/0
2	MPD	Q	303	-	-	0/5/5/5	0/0/0/0
3	ACY	Q	304	-	-	0/0/0/0	0/0/0/0
2	MPD	R	302	-	-	0/5/5/5	0/0/0/0
2	MPD	R	303	-	-	0/5/5/5	0/0/0/0
2	MPD	S	302	-	-	0/5/5/5	0/0/0/0
2	MPD	S	303	-	-	0/5/5/5	0/0/0/0
3	ACY	S	304	-	-	0/0/0/0	0/0/0/0
3	ACY	S	305	-	-	0/0/0/0	0/0/0/0
2	MPD	T	302	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	T	303	-	-	0/5/5/5	0/0/0/0
3	ACY	T	304	-	-	0/0/0/0	0/0/0/0
2	MPD	U	302	-	-	0/5/5/5	0/0/0/0
2	MPD	U	303	-	-	0/5/5/5	0/0/0/0
2	MPD	V	302	-	-	0/5/5/5	0/0/0/0
2	MPD	V	303	-	-	0/5/5/5	0/0/0/0
3	ACY	V	304	-	-	0/0/0/0	0/0/0/0
2	MPD	W	302	-	-	0/5/5/5	0/0/0/0
2	MPD	W	303	-	-	0/5/5/5	0/0/0/0
3	ACY	W	304	-	-	0/0/0/0	0/0/0/0
2	MPD	X	302	-	-	0/5/5/5	0/0/0/0
2	MPD	X	303	-	-	0/5/5/5	0/0/0/0
2	MPD	X	304	-	-	0/5/5/5	0/0/0/0
3	ACY	X	305	-	-	0/0/0/0	0/0/0/0
2	MPD	Y	302	-	-	0/5/5/5	0/0/0/0
2	MPD	Y	303	-	-	0/5/5/5	0/0/0/0
3	ACY	Y	304	-	-	0/0/0/0	0/0/0/0
2	MPD	Z	302	-	-	0/5/5/5	0/0/0/0
3	ACY	Z	303	-	-	0/0/0/0	0/0/0/0
2	MPD	a	302	-	-	0/5/5/5	0/0/0/0
2	MPD	a	303	-	-	0/5/5/5	0/0/0/0
3	ACY	a	304	-	-	0/0/0/0	0/0/0/0
2	MPD	b	302	-	-	0/5/5/5	0/0/0/0
2	MPD	b	303	-	-	0/5/5/5	0/0/0/0
3	ACY	b	304	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

49 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	MPD	8	0
2	A	303	MPD	4	0
2	B	302	MPD	6	0
2	B	303	MPD	8	0
2	C	302	MPD	1	0
2	C	303	MPD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	MPD	2	0
2	E	302	MPD	7	0
2	E	303	MPD	1	0
2	F	302	MPD	3	0
2	F	303	MPD	7	0
2	G	302	MPD	4	0
2	G	303	MPD	3	0
2	H	302	MPD	3	0
2	H	303	MPD	2	0
2	I	302	MPD	4	0
2	I	303	MPD	3	0
2	J	302	MPD	3	0
2	J	303	MPD	2	0
2	K	302	MPD	5	0
2	K	303	MPD	6	0
2	L	302	MPD	3	0
2	L	303	MPD	2	0
2	M	302	MPD	1	0
2	M	303	MPD	3	0
2	N	302	MPD	6	0
2	N	303	MPD	5	0
2	O	302	MPD	5	0
2	O	303	MPD	5	0
2	P	302	MPD	1	0
2	P	303	MPD	3	0
2	Q	302	MPD	8	0
2	Q	303	MPD	1	0
2	R	303	MPD	6	0
2	S	302	MPD	2	0
2	S	303	MPD	2	0
2	T	302	MPD	1	0
2	T	303	MPD	3	0
2	U	302	MPD	2	0
2	U	303	MPD	3	0
2	V	302	MPD	1	0
2	V	303	MPD	7	0
2	W	302	MPD	4	0
2	W	303	MPD	5	0
2	X	302	MPD	4	0
2	X	304	MPD	2	0
2	Y	302	MPD	3	0
2	Y	303	MPD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	302	MPD	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	295/302 (97%)	0.04	9 (3%)	52	62	27, 45, 75, 108	0
1	B	295/302 (97%)	0.18	14 (4%)	35	44	27, 48, 82, 119	0
1	C	294/302 (97%)	0.22	16 (5%)	29	38	31, 50, 82, 108	0
1	D	295/302 (97%)	0.19	15 (5%)	32	41	33, 53, 83, 118	0
1	E	295/302 (97%)	0.44	32 (10%)	8	11	33, 54, 109, 151	0
1	F	294/302 (97%)	0.35	25 (8%)	13	19	30, 52, 95, 147	0
1	G	294/302 (97%)	0.12	19 (6%)	22	30	27, 50, 89, 127	0
1	H	294/302 (97%)	0.04	10 (3%)	49	58	29, 46, 71, 100	0
1	I	294/302 (97%)	0.17	12 (4%)	41	50	27, 47, 75, 106	0
1	J	294/302 (97%)	0.13	14 (4%)	34	43	24, 46, 80, 122	0
1	K	295/302 (97%)	0.09	11 (3%)	45	54	27, 45, 76, 111	0
1	L	294/302 (97%)	0.16	13 (4%)	38	47	30, 47, 75, 131	0
1	M	295/302 (97%)	0.34	26 (8%)	12	18	29, 52, 92, 149	0
1	N	294/302 (97%)	0.17	14 (4%)	34	43	28, 51, 87, 117	0
1	O	295/302 (97%)	0.15	22 (7%)	17	24	30, 48, 78, 117	0
1	P	294/302 (97%)	0.16	13 (4%)	38	47	29, 48, 75, 131	0
1	Q	294/302 (97%)	0.27	22 (7%)	17	24	30, 51, 95, 140	0
1	R	294/302 (97%)	0.23	16 (5%)	29	38	32, 49, 77, 99	0
1	S	295/302 (97%)	0.27	19 (6%)	23	31	30, 52, 92, 118	0
1	T	294/302 (97%)	0.12	14 (4%)	34	43	30, 47, 76, 106	0
1	U	295/302 (97%)	0.20	16 (5%)	29	38	28, 49, 85, 128	0
1	V	295/302 (97%)	0.11	14 (4%)	35	44	29, 50, 81, 123	0
1	W	294/302 (97%)	0.27	23 (7%)	16	22	33, 53, 94, 155	0
1	X	294/302 (97%)	0.24	18 (6%)	25	33	33, 53, 96, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	Y	294/302 (97%)	0.28	22 (7%)	17 24	29, 52, 102, 136	0
1	Z	294/302 (97%)	0.22	15 (5%)	32 41	28, 51, 87, 124	0
1	a	294/302 (97%)	0.07	14 (4%)	34 43	28, 45, 74, 123	0
1	b	295/302 (97%)	0.13	14 (4%)	35 44	28, 48, 84, 151	0
All	All	8243/8456 (97%)	0.19	472 (5%)	27 36	24, 49, 86, 155	0

All (472) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	71	GLU	8.0
1	M	295	GLU	8.0
1	E	295	GLU	6.8
1	X	258	LEU	6.8
1	E	258	LEU	5.9
1	Q	262	SER	5.8
1	E	74	ASN	5.8
1	M	258	LEU	5.5
1	Y	258	LEU	5.5
1	A	132	ILE	5.4
1	Z	258	LEU	5.2
1	O	17	ASN	5.2
1	M	263	THR	5.1
1	F	17	ASN	5.1
1	V	17	ASN	5.0
1	F	71	GLU	4.9
1	M	179	TRP	4.7
1	A	295	GLU	4.7
1	R	92	ASP	4.7
1	Q	258	LEU	4.5
1	F	187	TRP	4.5
1	M	17	ASN	4.4
1	a	127	ASP	4.3
1	C	127	ASP	4.3
1	D	258	LEU	4.3
1	W	75	LYS	4.3
1	P	258	LEU	4.3
1	R	179	TRP	4.3
1	E	259	HIS	4.2
1	E	71	GLU	4.2
1	L	17	ASN	4.2
1	N	263	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	R	1	ALA	4.2
1	Z	262	SER	4.2
1	U	71	GLU	4.2
1	O	262	SER	4.1
1	R	189	PRO	4.1
1	F	76	SER	4.1
1	S	295	GLU	4.1
1	C	126	GLY	4.0
1	Y	189	PRO	4.0
1	N	258	LEU	4.0
1	Q	72	GLY	4.0
1	R	128	ASP	4.0
1	N	262	SER	3.9
1	W	263	THR	3.9
1	F	260	TRP	3.9
1	P	262	SER	3.9
1	X	256	TYR	3.8
1	T	258	LEU	3.7
1	K	73	ALA	3.7
1	P	128	ASP	3.7
1	O	258	LEU	3.7
1	M	92	ASP	3.6
1	M	262	SER	3.6
1	D	71	GLU	3.6
1	U	72	GLY	3.6
1	b	71	GLU	3.6
1	O	72	GLY	3.6
1	D	189	PRO	3.6
1	a	128	ASP	3.6
1	M	265	TRP	3.6
1	N	92	ASP	3.6
1	L	128	ASP	3.6
1	E	70	GLU	3.6
1	O	263	THR	3.5
1	P	1	ALA	3.5
1	C	131	LYS	3.5
1	F	258	LEU	3.5
1	K	203	SER	3.5
1	M	189	PRO	3.5
1	G	132	ILE	3.5
1	P	93	ASN	3.5
1	H	1	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	U	128	ASP	3.4
1	X	187	TRP	3.5
1	Y	187	TRP	3.5
1	Z	260	TRP	3.5
1	A	131	LYS	3.4
1	T	61	ILE	3.4
1	I	203	SER	3.4
1	S	196	PHE	3.4
1	Y	256	TYR	3.4
1	L	71	GLU	3.4
1	M	72	GLY	3.4
1	Z	256	TYR	3.4
1	B	295	GLU	3.4
1	W	31	GLU	3.4
1	S	258	LEU	3.4
1	D	93	ASN	3.4
1	K	258	LEU	3.3
1	J	262	SER	3.3
1	X	69	SER	3.3
1	S	31	GLU	3.3
1	a	129	THR	3.3
1	a	17	ASN	3.3
1	I	258	LEU	3.3
1	U	1	ALA	3.3
1	W	258	LEU	3.3
1	G	71	GLU	3.3
1	Q	256	TYR	3.3
1	a	258	LEU	3.3
1	U	196	PHE	3.3
1	Q	179	TRP	3.3
1	F	262	SER	3.3
1	W	70	GLU	3.2
1	E	179	TRP	3.2
1	N	179	TRP	3.2
1	G	17	ASN	3.2
1	T	128	ASP	3.2
1	M	187	TRP	3.2
1	b	128	ASP	3.2
1	S	203	SER	3.2
1	C	232	ILE	3.2
1	L	1	ALA	3.2
1	P	81	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	131	LYS	3.2
1	B	129	THR	3.2
1	B	258	LEU	3.1
1	X	71	GLU	3.1
1	E	17	ASN	3.1
1	M	129	THR	3.1
1	A	130	GLY	3.1
1	J	258	LEU	3.1
1	E	75	LYS	3.1
1	S	260	TRP	3.1
1	N	203	SER	3.1
1	P	203	SER	3.1
1	R	187	TRP	3.1
1	S	81	PRO	3.1
1	F	259	HIS	3.1
1	M	259	HIS	3.1
1	O	92	ASP	3.1
1	V	1	ALA	3.1
1	V	258	LEU	3.1
1	P	31	GLU	3.1
1	Y	267	GLY	3.1
1	H	92	ASP	3.1
1	S	1	ALA	3.0
1	E	204	MET	3.0
1	O	190	VAL	3.0
1	F	132	ILE	3.0
1	S	131	LYS	3.0
1	Y	260	TRP	3.0
1	L	69	SER	3.0
1	L	262	SER	3.0
1	V	196	PHE	3.0
1	G	258	LEU	3.0
1	Q	187	TRP	3.0
1	T	129	THR	3.0
1	S	256	TYR	3.0
1	W	179	TRP	3.0
1	A	17	ASN	3.0
1	U	74	ASN	3.0
1	G	256	TYR	3.0
1	L	258	LEU	3.0
1	U	258	LEU	3.0
1	F	128	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	T	1	ALA	3.0
1	W	68	TYR	3.0
1	B	71	GLU	3.0
1	W	61	ILE	2.9
1	E	195	LEU	2.9
1	W	81	PRO	2.9
1	Q	130	GLY	2.9
1	Y	179	TRP	2.9
1	J	74	ASN	2.9
1	N	189	PRO	2.9
1	O	128	ASP	2.9
1	T	17	ASN	2.9
1	Y	71	GLU	2.9
1	Z	208	GLU	2.9
1	C	187	TRP	2.9
1	O	196	PHE	2.9
1	J	201	ASN	2.9
1	Y	128	ASP	2.9
1	F	265	TRP	2.9
1	a	261	THR	2.9
1	C	256	TYR	2.9
1	H	130	GLY	2.8
1	S	189	PRO	2.8
1	S	190	VAL	2.8
1	I	61	ILE	2.8
1	U	92	ASP	2.8
1	J	263	THR	2.8
1	C	185	ASP	2.8
1	J	256	TYR	2.8
1	B	203	SER	2.8
1	a	126	GLY	2.8
1	E	256	TYR	2.8
1	Q	205	LYS	2.8
1	Q	75	LYS	2.8
1	E	61	ILE	2.8
1	b	258	LEU	2.8
1	F	72	GLY	2.8
1	L	179	TRP	2.8
1	Q	73	ALA	2.8
1	H	203	SER	2.8
1	Q	69	SER	2.8
1	C	258	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	260	TRP	2.8
1	R	129	THR	2.8
1	S	129	THR	2.8
1	a	71	GLU	2.8
1	N	17	ASN	2.7
1	Q	71	GLU	2.7
1	G	131	LYS	2.7
1	L	190	VAL	2.7
1	Q	196	PHE	2.7
1	M	131	LYS	2.7
1	G	127	ASP	2.7
1	C	17	ASN	2.7
1	F	127	ASP	2.7
1	Q	93	ASN	2.7
1	R	71	GLU	2.7
1	R	267	GLY	2.7
1	E	187	TRP	2.7
1	b	92	ASP	2.7
1	O	31	GLU	2.7
1	R	256	TYR	2.7
1	E	72	GLY	2.7
1	W	80	TRP	2.7
1	G	75	LYS	2.7
1	G	201	ASN	2.7
1	B	187	TRP	2.7
1	C	53	LEU	2.6
1	D	196	PHE	2.6
1	D	128	ASP	2.6
1	X	205	LYS	2.6
1	E	264	ASN	2.6
1	D	195	LEU	2.6
1	E	294	LEU	2.6
1	G	179	TRP	2.6
1	H	61	ILE	2.6
1	Y	73	ALA	2.6
1	V	131	LYS	2.6
1	W	256	TYR	2.6
1	K	195	LEU	2.6
1	R	31	GLU	2.6
1	V	71	GLU	2.6
1	X	266	LYS	2.6
1	H	129	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	187	TRP	2.6
1	I	179	TRP	2.6
1	O	189	PRO	2.6
1	W	197	MET	2.6
1	O	261	THR	2.6
1	P	9	THR	2.6
1	D	17	ASN	2.6
1	H	93	ASN	2.6
1	F	189	PRO	2.6
1	W	71	GLU	2.6
1	J	190	VAL	2.6
1	a	93	ASN	2.6
1	B	1	ALA	2.5
1	O	129	THR	2.5
1	M	232	ILE	2.5
1	B	179	TRP	2.5
1	F	179	TRP	2.5
1	V	179	TRP	2.5
1	X	260	TRP	2.5
1	T	93	ASN	2.5
1	X	93	ASN	2.5
1	M	1	ALA	2.5
1	M	127	ASP	2.5
1	O	127	ASP	2.5
1	T	261	THR	2.5
1	K	196	PHE	2.5
1	P	196	PHE	2.5
1	W	17	ASN	2.5
1	b	74	ASN	2.5
1	P	263	THR	2.5
1	U	129	THR	2.5
1	D	94	GLU	2.5
1	Q	189	PRO	2.5
1	Q	201	ASN	2.5
1	J	179	TRP	2.5
1	A	53	LEU	2.5
1	b	185	ASP	2.5
1	X	70	GLU	2.5
1	A	261	THR	2.5
1	C	129	THR	2.5
1	F	129	THR	2.5
1	J	203	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	Q	92	ASP	2.5
1	O	70	GLU	2.5
1	Z	72	GLY	2.4
1	Y	259	HIS	2.4
1	F	256	TYR	2.4
1	S	71	GLU	2.4
1	V	127	ASP	2.4
1	M	190	VAL	2.4
1	B	61	ILE	2.4
1	V	31	GLU	2.4
1	Y	74	ASN	2.4
1	Z	1	ALA	2.4
1	b	93	ASN	2.4
1	V	128	ASP	2.4
1	F	197	MET	2.4
1	O	195	LEU	2.4
1	Q	197	MET	2.4
1	E	284	ILE	2.4
1	G	72	GLY	2.4
1	Q	70	GLU	2.4
1	J	127	ASP	2.4
1	K	259	HIS	2.4
1	Y	2	ASP	2.4
1	M	256	TYR	2.4
1	I	71	GLU	2.4
1	N	71	GLU	2.4
1	F	69	SER	2.4
1	Z	16	SER	2.4
1	Y	30	LYS	2.4
1	C	189	PRO	2.4
1	V	189	PRO	2.4
1	X	78	LEU	2.4
1	G	128	ASP	2.4
1	M	74	ASN	2.4
1	T	131	LYS	2.4
1	K	187	TRP	2.4
1	P	179	TRP	2.4
1	E	31	GLU	2.4
1	Z	17	ASN	2.4
1	a	130	GLY	2.4
1	J	232	ILE	2.4
1	L	61	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	61	ILE	2.4
1	Y	208	GLU	2.4
1	K	128	ASP	2.3
1	S	75	LYS	2.3
1	X	189	PRO	2.3
1	b	1	ALA	2.3
1	B	128	ASP	2.3
1	M	128	ASP	2.3
1	K	17	ASN	2.3
1	C	132	ILE	2.3
1	E	128	ASP	2.3
1	F	91	PRO	2.3
1	Z	261	THR	2.3
1	I	196	PHE	2.3
1	X	197	MET	2.3
1	G	92	ASP	2.3
1	W	272	ASP	2.3
1	E	188	ASN	2.3
1	Y	75	LYS	2.3
1	Z	196	PHE	2.3
1	D	69	SER	2.3
1	D	262	SER	2.3
1	S	262	SER	2.3
1	X	262	SER	2.3
1	Y	70	GLU	2.3
1	M	294	LEU	2.3
1	R	17	ASN	2.3
1	E	189	PRO	2.3
1	Y	72	GLY	2.3
1	E	76	SER	2.3
1	G	187	TRP	2.3
1	Y	205	LYS	2.3
1	Q	263	THR	2.3
1	T	267	GLY	2.3
1	U	267	GLY	2.3
1	D	256	TYR	2.3
1	E	1	ALA	2.3
1	L	18	THR	2.3
1	b	256	TYR	2.3
1	Y	266	LYS	2.3
1	L	31	GLU	2.3
1	I	202	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	131	LYS	2.2
1	O	69	SER	2.2
1	N	78	LEU	2.2
1	Q	129	THR	2.2
1	I	128	ASP	2.2
1	O	61	ILE	2.2
1	b	132	ILE	2.2
1	X	259	HIS	2.2
1	F	53	LEU	2.2
1	H	81	PRO	2.2
1	V	70	GLU	2.2
1	b	261	THR	2.2
1	O	179	TRP	2.2
1	R	265	TRP	2.2
1	S	179	TRP	2.2
1	b	55	ILE	2.2
1	E	196	PHE	2.2
1	D	53	LEU	2.2
1	T	294	LEU	2.2
1	Y	127	ASP	2.2
1	E	129	THR	2.2
1	C	179	TRP	2.2
1	G	70	GLU	2.2
1	M	261	THR	2.2
1	a	61	ILE	2.2
1	N	187	TRP	2.2
1	A	92	ASP	2.2
1	E	130	GLY	2.2
1	U	212	ASP	2.2
1	B	75	LYS	2.2
1	L	129	THR	2.2
1	X	261	THR	2.2
1	X	277	ARG	2.1
1	b	232	ILE	2.1
1	M	15	GLY	2.1
1	W	187	TRP	2.1
1	H	189	PRO	2.1
1	N	81	PRO	2.1
1	B	17	ASN	2.1
1	W	84	PHE	2.1
1	W	93	ASN	2.1
1	G	185	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	61	ILE	2.1
1	C	201	ASN	2.1
1	W	188	ASN	2.1
1	B	78	LEU	2.1
1	C	197	MET	2.1
1	G	263	THR	2.1
1	J	185	ASP	2.1
1	U	17	ASN	2.1
1	R	124	VAL	2.1
1	Q	68	TYR	2.1
1	W	9	THR	2.1
1	a	53	LEU	2.1
1	F	1	ALA	2.1
1	W	185	ASP	2.1
1	T	196	PHE	2.1
1	G	129	THR	2.1
1	N	256	TYR	2.1
1	W	195	LEU	2.1
1	I	73	ALA	2.1
1	Z	83	ALA	2.1
1	Z	267	GLY	2.1
1	O	93	ASN	2.1
1	Z	31	GLU	2.1
1	F	185	ASP	2.1
1	K	92	ASP	2.1
1	U	203	SER	2.1
1	E	190	VAL	2.1
1	O	84	PHE	2.1
1	U	84	PHE	2.1
1	E	197	MET	2.1
1	I	267	GLY	2.1
1	I	256	TYR	2.1
1	N	70	GLU	2.1
1	b	53	LEU	2.1
1	D	179	TRP	2.1
1	Y	265	TRP	2.1
1	A	16	SER	2.1
1	B	232	ILE	2.1
1	T	70	GLU	2.0
1	U	295	GLU	2.0
1	O	9	THR	2.0
1	S	84	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	a	294	LEU	2.0
1	a	1	ALA	2.0
1	J	4	ASP	2.0
1	G	240	LYS	2.0
1	W	189	PRO	2.0
1	X	239	SER	2.0
1	U	61	ILE	2.0
1	H	17	ASN	2.0
1	E	210	PHE	2.0
1	E	206	ALA	2.0
1	R	258	LEU	2.0
1	V	84	PHE	2.0
1	M	70	GLU	2.0
1	V	262	SER	2.0
1	F	200	ARG	2.0
1	J	267	GLY	2.0
1	K	190	VAL	2.0
1	T	92	ASP	2.0
1	I	195	LEU	2.0
1	Z	53	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	ACY	X	305	4/4	0.89	0.41	15.26	58,74,85,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ACY	D	304	4/4	0.82	0.33	14.54	58,71,73,80	0
3	ACY	E	304	4/4	0.89	0.42	12.96	56,70,75,77	0
3	ACY	S	304	4/4	0.74	0.45	11.94	51,79,87,101	0
3	ACY	O	305	4/4	0.74	0.30	10.97	65,78,84,87	0
2	MPD	X	304	8/8	0.71	0.44	10.09	68,86,88,93	0
3	ACY	M	304	4/4	0.92	0.20	7.50	53,58,79,84	0
2	MPD	Z	302	8/8	0.62	0.40	7.49	56,82,97,102	0
3	ACY	V	304	4/4	0.75	0.33	7.43	60,72,75,91	0
3	ACY	Q	304	4/4	0.92	0.28	6.94	60,64,80,87	0
2	MPD	B	303	8/8	0.81	0.42	6.87	78,85,100,101	0
3	ACY	Y	304	4/4	0.96	0.30	6.71	64,75,79,82	0
2	MPD	X	303	8/8	0.80	0.29	6.39	60,74,85,90	0
3	ACY	L	304	4/4	0.87	0.27	6.36	62,70,82,90	0
3	ACY	S	305	4/4	0.83	0.24	6.26	70,73,79,80	0
2	MPD	U	303	8/8	0.77	0.29	5.57	52,76,87,93	0
3	ACY	A	305	4/4	0.68	0.34	5.48	52,72,90,99	0
3	ACY	O	304	4/4	0.87	0.24	5.42	59,68,77,86	0
3	ACY	K	304	4/4	0.94	0.21	5.35	52,67,72,73	0
2	MPD	Q	303	8/8	0.69	0.43	5.32	60,78,87,88	0
3	ACY	H	305	4/4	0.74	0.27	5.24	65,73,81,83	0
2	MPD	F	303	8/8	0.69	0.38	5.13	68,77,84,91	0
2	MPD	U	302	8/8	0.68	0.39	4.87	66,82,90,90	0
2	MPD	a	303	8/8	0.86	0.24	4.35	55,80,89,93	0
3	ACY	T	304	4/4	0.84	0.21	4.34	57,65,76,81	0
2	MPD	T	302	8/8	0.90	0.29	4.25	64,68,76,78	0
2	MPD	O	303	8/8	0.87	0.28	4.22	58,75,89,93	0
2	MPD	b	303	8/8	0.89	0.26	4.21	64,82,86,87	0
2	MPD	J	303	8/8	0.64	0.32	4.12	59,79,92,96	0
2	MPD	V	303	8/8	0.84	0.28	3.90	65,82,90,91	0
2	MPD	A	302	8/8	0.89	0.24	3.80	58,69,77,81	0
2	MPD	E	303	8/8	0.66	0.36	3.71	61,80,89,100	0
2	MPD	Y	303	8/8	0.83	0.31	3.57	64,82,87,93	0
2	MPD	H	302	8/8	0.92	0.24	3.50	58,64,75,78	0
2	MPD	I	302	8/8	0.88	0.30	3.41	64,68,73,82	0
2	MPD	G	302	8/8	0.85	0.32	3.32	66,72,80,81	0
2	MPD	Q	302	8/8	0.79	0.38	3.24	69,76,88,103	0
2	MPD	a	302	8/8	0.91	0.23	3.07	60,74,83,89	0
2	MPD	B	302	8/8	0.87	0.30	3.06	65,71,79,82	0
2	MPD	O	302	8/8	0.85	0.31	3.05	68,74,80,82	0
2	MPD	Y	302	8/8	0.89	0.29	2.88	58,76,88,90	0
2	MPD	L	303	8/8	0.81	0.27	2.86	67,72,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MPD	S	303	8/8	0.86	0.25	2.82	64,74,81,94	0
2	MPD	I	303	8/8	0.83	0.25	2.80	61,80,92,99	0
2	MPD	M	303	8/8	0.76	0.36	2.74	69,75,81,97	0
3	ACY	Z	303	4/4	0.87	0.18	2.73	56,71,71,75	0
3	ACY	a	304	4/4	0.78	0.26	2.71	67,68,82,87	0
2	MPD	b	302	8/8	0.91	0.26	2.64	71,74,83,88	0
2	MPD	J	302	8/8	0.77	0.27	2.62	63,72,87,93	0
2	MPD	S	302	8/8	0.86	0.34	2.62	68,80,81,85	0
2	MPD	K	302	8/8	0.87	0.25	2.61	66,73,83,90	0
2	MPD	X	302	8/8	0.80	0.28	2.40	70,85,88,89	0
2	MPD	H	303	8/8	0.82	0.20	2.39	62,70,86,88	0
3	ACY	J	304	4/4	0.79	0.18	2.27	61,65,78,90	0
2	MPD	T	303	8/8	0.91	0.22	2.26	56,72,85,89	0
2	MPD	P	303	8/8	0.77	0.21	2.16	59,79,86,88	0
3	ACY	b	304	4/4	0.91	0.17	2.02	66,69,91,92	0
2	MPD	N	302	8/8	0.89	0.28	1.97	64,77,82,92	0
3	ACY	C	304	4/4	0.90	0.19	1.92	63,66,74,78	0
2	MPD	F	302	8/8	0.88	0.31	1.90	71,79,91,103	0
2	MPD	R	302	8/8	0.77	0.28	1.87	60,73,83,86	0
3	ACY	F	304	4/4	0.94	0.17	1.77	69,76,84,85	0
2	MPD	A	303	8/8	0.88	0.18	1.71	59,72,85,90	0
2	MPD	C	302	8/8	0.92	0.24	1.69	67,73,79,82	0
2	MPD	R	303	8/8	0.85	0.25	1.58	64,77,82,87	0
2	MPD	D	303	8/8	0.85	0.19	1.48	51,71,79,80	0
2	MPD	G	303	8/8	0.84	0.20	1.37	59,75,86,97	0
2	MPD	K	303	8/8	0.87	0.18	1.14	63,78,80,88	0
2	MPD	M	302	8/8	0.89	0.27	1.14	64,73,79,82	0
2	MPD	W	303	8/8	0.86	0.18	1.10	60,80,89,91	0
2	MPD	C	303	8/8	0.83	0.18	1.08	65,76,87,88	0
2	MPD	P	302	8/8	0.90	0.20	1.08	54,76,79,80	0
2	MPD	N	303	8/8	0.86	0.18	0.98	66,79,90,95	0
3	ACY	K	305	4/4	0.94	0.12	0.98	45,68,72,82	0
3	ACY	D	305	4/4	0.93	0.12	0.79	70,71,78,78	0
2	MPD	V	302	8/8	0.93	0.20	0.77	49,61,75,80	0
3	ACY	P	304	4/4	0.93	0.16	0.60	63,63,82,97	0
2	MPD	D	302	8/8	0.90	0.18	0.59	65,73,83,85	0
2	MPD	W	302	8/8	0.79	0.22	0.58	68,75,83,84	0
2	MPD	L	302	8/8	0.90	0.17	0.55	59,65,80,89	0
2	MPD	E	302	8/8	0.86	0.16	-0.44	72,81,85,87	0
3	ACY	A	304	4/4	0.92	0.09	-0.70	54,61,73,74	0
3	ACY	H	304	4/4	0.95	0.08	-0.90	53,60,76,79	0
3	ACY	W	304	4/4	0.75	0.18	-	49,65,70,83	0

6.5 Other polymers (i)

There are no such residues in this entry.