Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2021 – 08:27 PM EST

PDB ID	:	3LTE
Title	:	CRYSTAL STRUCTURE OF RESPONSE REGULATOR (SIGNAL RECEIVER DOMAIN) FROM Bermanella marisrubri
Authors	:	Patskovsky, Y.; Toro, R.; Gilmore, M.; Miller, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-02-15
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

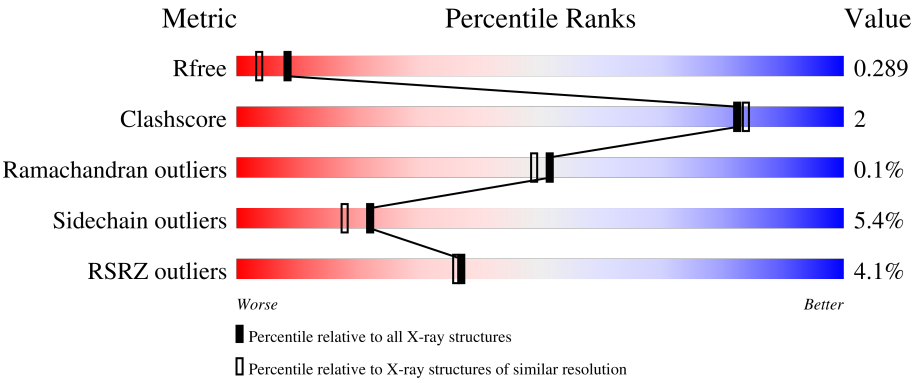
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	132	11% 73% 14% • 11%
1	B	132	2% 83% 8% • 9%
1	C	132	3% 86% • 10%
1	D	132	2% 86% 7% • 7%
1	E	132	4% 83% 8% • 7%

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Mol	Chain	Length	Quality of chain
1	F	132	2% 84% 8% 7%
1	G	132	4% 83% 8% 8%
1	H	132	% 80% 13% 7%
1	I	132	8% 77% 11% 10%
1	J	132	82% 9% 9%
1	K	132	5% 84% 7% 9%
1	L	132	2% 80% 9% 11%
1	M	132	4% 73% 15% 11%
1	N	132	% 84% 5% 10%
1	O	132	5% 81% 8% 11%
1	P	132	2% 85% 8% 7%
1	Q	132	12% 81% 6% 11%
1	R	132	81% 8% 11%
1	S	132	2% 84% 6% 9%
1	T	132	2% 80% 10% 10%
1	U	132	2% 77% 12% 10%
1	V	132	5% 86% 11%
1	W	132	4% 86% 9%
1	X	132	6% 76% 14% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23428 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 Response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			926	583	163	177	3			
1	B	120	Total	C	N	O	S	0	6	0
			980	618	175	184	3			
1	C	119	Total	C	N	O	S	0	1	0
			937	589	164	181	3			
1	D	123	Total	C	N	O	S	0	1	0
			967	608	170	186	3			
1	E	123	Total	C	N	O	S	0	4	0
			986	623	174	186	3			
1	F	123	Total	C	N	O	S	0	3	0
			984	621	175	185	3			
1	G	121	Total	C	N	O	S	0	1	0
			953	598	167	185	3			
1	H	123	Total	C	N	O	S	0	5	0
			986	623	171	189	3			
1	I	119	Total	C	N	O	S	0	0	0
			930	585	164	178	3			
1	J	120	Total	C	N	O	S	0	4	0
			963	605	172	183	3			
1	K	120	Total	C	N	O	S	0	2	0
			953	599	169	182	3			
1	L	118	Total	C	N	O	S	0	1	0
			927	584	162	178	3			
1	M	118	Total	C	N	O	S	0	1	0
			927	584	162	178	3			
1	N	119	Total	C	N	O	S	0	5	0
			957	603	168	183	3			
1	O	117	Total	C	N	O	S	0	1	0
			924	584	162	175	3			
1	P	123	Total	C	N	O	S	0	1	0
			967	608	170	186	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	117	Total	C	N	O	S	0	1	0
			923	581	162	177	3			
1	R	118	Total	C	N	O	S	0	3	0
			944	596	167	178	3			
1	S	120	Total	C	N	O	S	0	0	0
			941	591	166	181	3			
1	T	119	Total	C	N	O	S	0	0	0
			932	586	164	179	3			
1	U	119	Total	C	N	O	S	0	2	0
			942	593	164	182	3			
1	V	118	Total	C	N	O	S	0	1	0
			927	584	162	178	3			
1	W	120	Total	C	N	O	S	0	1	0
			944	593	166	182	3			
1	X	118	Total	C	N	O	S	0	1	0
			932	587	165	177	3			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	MET	-	expression tag	UNP Q1N036
A	63	SER	-	expression tag	UNP Q1N036
A	186	GLU	-	expression tag	UNP Q1N036
A	187	GLY	-	expression tag	UNP Q1N036
A	188	HIS	-	expression tag	UNP Q1N036
A	189	HIS	-	expression tag	UNP Q1N036
A	190	HIS	-	expression tag	UNP Q1N036
A	191	HIS	-	expression tag	UNP Q1N036
A	192	HIS	-	expression tag	UNP Q1N036
A	193	HIS	-	expression tag	UNP Q1N036
B	62	MET	-	expression tag	UNP Q1N036
B	63	SER	-	expression tag	UNP Q1N036
B	186	GLU	-	expression tag	UNP Q1N036
B	187	GLY	-	expression tag	UNP Q1N036
B	188	HIS	-	expression tag	UNP Q1N036
B	189	HIS	-	expression tag	UNP Q1N036
B	190	HIS	-	expression tag	UNP Q1N036
B	191	HIS	-	expression tag	UNP Q1N036
B	192	HIS	-	expression tag	UNP Q1N036
B	193	HIS	-	expression tag	UNP Q1N036
C	62	MET	-	expression tag	UNP Q1N036
C	63	SER	-	expression tag	UNP Q1N036
C	186	GLU	-	expression tag	UNP Q1N036

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Chain	Residue	Modelled	Actual	Comment	Reference
C	187	GLY	-	expression tag	UNP Q1N036
C	188	HIS	-	expression tag	UNP Q1N036
C	189	HIS	-	expression tag	UNP Q1N036
C	190	HIS	-	expression tag	UNP Q1N036
C	191	HIS	-	expression tag	UNP Q1N036
C	192	HIS	-	expression tag	UNP Q1N036
C	193	HIS	-	expression tag	UNP Q1N036
D	62	MET	-	expression tag	UNP Q1N036
D	63	SER	-	expression tag	UNP Q1N036
D	186	GLU	-	expression tag	UNP Q1N036
D	187	GLY	-	expression tag	UNP Q1N036
D	188	HIS	-	expression tag	UNP Q1N036
D	189	HIS	-	expression tag	UNP Q1N036
D	190	HIS	-	expression tag	UNP Q1N036
D	191	HIS	-	expression tag	UNP Q1N036
D	192	HIS	-	expression tag	UNP Q1N036
D	193	HIS	-	expression tag	UNP Q1N036
E	62	MET	-	expression tag	UNP Q1N036
E	63	SER	-	expression tag	UNP Q1N036
E	186	GLU	-	expression tag	UNP Q1N036
E	187	GLY	-	expression tag	UNP Q1N036
E	188	HIS	-	expression tag	UNP Q1N036
E	189	HIS	-	expression tag	UNP Q1N036
E	190	HIS	-	expression tag	UNP Q1N036
E	191	HIS	-	expression tag	UNP Q1N036
E	192	HIS	-	expression tag	UNP Q1N036
E	193	HIS	-	expression tag	UNP Q1N036
F	62	MET	-	expression tag	UNP Q1N036
F	63	SER	-	expression tag	UNP Q1N036
F	186	GLU	-	expression tag	UNP Q1N036
F	187	GLY	-	expression tag	UNP Q1N036
F	188	HIS	-	expression tag	UNP Q1N036
F	189	HIS	-	expression tag	UNP Q1N036
F	190	HIS	-	expression tag	UNP Q1N036
F	191	HIS	-	expression tag	UNP Q1N036
F	192	HIS	-	expression tag	UNP Q1N036
F	193	HIS	-	expression tag	UNP Q1N036
G	62	MET	-	expression tag	UNP Q1N036
G	63	SER	-	expression tag	UNP Q1N036
G	186	GLU	-	expression tag	UNP Q1N036
G	187	GLY	-	expression tag	UNP Q1N036
G	188	HIS	-	expression tag	UNP Q1N036

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Chain	Residue	Modelled	Actual	Comment	Reference
G	189	HIS	-	expression tag	UNP Q1N036
G	190	HIS	-	expression tag	UNP Q1N036
G	191	HIS	-	expression tag	UNP Q1N036
G	192	HIS	-	expression tag	UNP Q1N036
G	193	HIS	-	expression tag	UNP Q1N036
H	62	MET	-	expression tag	UNP Q1N036
H	63	SER	-	expression tag	UNP Q1N036
H	186	GLU	-	expression tag	UNP Q1N036
H	187	GLY	-	expression tag	UNP Q1N036
H	188	HIS	-	expression tag	UNP Q1N036
H	189	HIS	-	expression tag	UNP Q1N036
H	190	HIS	-	expression tag	UNP Q1N036
H	191	HIS	-	expression tag	UNP Q1N036
H	192	HIS	-	expression tag	UNP Q1N036
H	193	HIS	-	expression tag	UNP Q1N036
I	62	MET	-	expression tag	UNP Q1N036
I	63	SER	-	expression tag	UNP Q1N036
I	186	GLU	-	expression tag	UNP Q1N036
I	187	GLY	-	expression tag	UNP Q1N036
I	188	HIS	-	expression tag	UNP Q1N036
I	189	HIS	-	expression tag	UNP Q1N036
I	190	HIS	-	expression tag	UNP Q1N036
I	191	HIS	-	expression tag	UNP Q1N036
I	192	HIS	-	expression tag	UNP Q1N036
I	193	HIS	-	expression tag	UNP Q1N036
J	62	MET	-	expression tag	UNP Q1N036
J	63	SER	-	expression tag	UNP Q1N036
J	186	GLU	-	expression tag	UNP Q1N036
J	187	GLY	-	expression tag	UNP Q1N036
J	188	HIS	-	expression tag	UNP Q1N036
J	189	HIS	-	expression tag	UNP Q1N036
J	190	HIS	-	expression tag	UNP Q1N036
J	191	HIS	-	expression tag	UNP Q1N036
J	192	HIS	-	expression tag	UNP Q1N036
J	193	HIS	-	expression tag	UNP Q1N036
K	62	MET	-	expression tag	UNP Q1N036
K	63	SER	-	expression tag	UNP Q1N036
K	186	GLU	-	expression tag	UNP Q1N036
K	187	GLY	-	expression tag	UNP Q1N036
K	188	HIS	-	expression tag	UNP Q1N036
K	189	HIS	-	expression tag	UNP Q1N036
K	190	HIS	-	expression tag	UNP Q1N036

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Chain	Residue	Modelled	Actual	Comment	Reference
K	191	HIS	-	expression tag	UNP Q1N036
K	192	HIS	-	expression tag	UNP Q1N036
K	193	HIS	-	expression tag	UNP Q1N036
L	62	MET	-	expression tag	UNP Q1N036
L	63	SER	-	expression tag	UNP Q1N036
L	186	GLU	-	expression tag	UNP Q1N036
L	187	GLY	-	expression tag	UNP Q1N036
L	188	HIS	-	expression tag	UNP Q1N036
L	189	HIS	-	expression tag	UNP Q1N036
L	190	HIS	-	expression tag	UNP Q1N036
L	191	HIS	-	expression tag	UNP Q1N036
L	192	HIS	-	expression tag	UNP Q1N036
L	193	HIS	-	expression tag	UNP Q1N036
M	62	MET	-	expression tag	UNP Q1N036
M	63	SER	-	expression tag	UNP Q1N036
M	186	GLU	-	expression tag	UNP Q1N036
M	187	GLY	-	expression tag	UNP Q1N036
M	188	HIS	-	expression tag	UNP Q1N036
M	189	HIS	-	expression tag	UNP Q1N036
M	190	HIS	-	expression tag	UNP Q1N036
M	191	HIS	-	expression tag	UNP Q1N036
M	192	HIS	-	expression tag	UNP Q1N036
M	193	HIS	-	expression tag	UNP Q1N036
N	62	MET	-	expression tag	UNP Q1N036
N	63	SER	-	expression tag	UNP Q1N036
N	186	GLU	-	expression tag	UNP Q1N036
N	187	GLY	-	expression tag	UNP Q1N036
N	188	HIS	-	expression tag	UNP Q1N036
N	189	HIS	-	expression tag	UNP Q1N036
N	190	HIS	-	expression tag	UNP Q1N036
N	191	HIS	-	expression tag	UNP Q1N036
N	192	HIS	-	expression tag	UNP Q1N036
N	193	HIS	-	expression tag	UNP Q1N036
O	62	MET	-	expression tag	UNP Q1N036
O	63	SER	-	expression tag	UNP Q1N036
O	186	GLU	-	expression tag	UNP Q1N036
O	187	GLY	-	expression tag	UNP Q1N036
O	188	HIS	-	expression tag	UNP Q1N036
O	189	HIS	-	expression tag	UNP Q1N036
O	190	HIS	-	expression tag	UNP Q1N036
O	191	HIS	-	expression tag	UNP Q1N036
O	192	HIS	-	expression tag	UNP Q1N036

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Chain	Residue	Modelled	Actual	Comment	Reference
O	193	HIS	-	expression tag	UNP Q1N036
P	62	MET	-	expression tag	UNP Q1N036
P	63	SER	-	expression tag	UNP Q1N036
P	186	GLU	-	expression tag	UNP Q1N036
P	187	GLY	-	expression tag	UNP Q1N036
P	188	HIS	-	expression tag	UNP Q1N036
P	189	HIS	-	expression tag	UNP Q1N036
P	190	HIS	-	expression tag	UNP Q1N036
P	191	HIS	-	expression tag	UNP Q1N036
P	192	HIS	-	expression tag	UNP Q1N036
P	193	HIS	-	expression tag	UNP Q1N036
Q	62	MET	-	expression tag	UNP Q1N036
Q	63	SER	-	expression tag	UNP Q1N036
Q	186	GLU	-	expression tag	UNP Q1N036
Q	187	GLY	-	expression tag	UNP Q1N036
Q	188	HIS	-	expression tag	UNP Q1N036
Q	189	HIS	-	expression tag	UNP Q1N036
Q	190	HIS	-	expression tag	UNP Q1N036
Q	191	HIS	-	expression tag	UNP Q1N036
Q	192	HIS	-	expression tag	UNP Q1N036
Q	193	HIS	-	expression tag	UNP Q1N036
R	62	MET	-	expression tag	UNP Q1N036
R	63	SER	-	expression tag	UNP Q1N036
R	186	GLU	-	expression tag	UNP Q1N036
R	187	GLY	-	expression tag	UNP Q1N036
R	188	HIS	-	expression tag	UNP Q1N036
R	189	HIS	-	expression tag	UNP Q1N036
R	190	HIS	-	expression tag	UNP Q1N036
R	191	HIS	-	expression tag	UNP Q1N036
R	192	HIS	-	expression tag	UNP Q1N036
R	193	HIS	-	expression tag	UNP Q1N036
S	62	MET	-	expression tag	UNP Q1N036
S	63	SER	-	expression tag	UNP Q1N036
S	186	GLU	-	expression tag	UNP Q1N036
S	187	GLY	-	expression tag	UNP Q1N036
S	188	HIS	-	expression tag	UNP Q1N036
S	189	HIS	-	expression tag	UNP Q1N036
S	190	HIS	-	expression tag	UNP Q1N036
S	191	HIS	-	expression tag	UNP Q1N036
S	192	HIS	-	expression tag	UNP Q1N036
S	193	HIS	-	expression tag	UNP Q1N036
T	62	MET	-	expression tag	UNP Q1N036

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Chain	Residue	Modelled	Actual	Comment	Reference
T	63	SER	-	expression tag	UNP Q1N036
T	186	GLU	-	expression tag	UNP Q1N036
T	187	GLY	-	expression tag	UNP Q1N036
T	188	HIS	-	expression tag	UNP Q1N036
T	189	HIS	-	expression tag	UNP Q1N036
T	190	HIS	-	expression tag	UNP Q1N036
T	191	HIS	-	expression tag	UNP Q1N036
T	192	HIS	-	expression tag	UNP Q1N036
T	193	HIS	-	expression tag	UNP Q1N036
U	62	MET	-	expression tag	UNP Q1N036
U	63	SER	-	expression tag	UNP Q1N036
U	186	GLU	-	expression tag	UNP Q1N036
U	187	GLY	-	expression tag	UNP Q1N036
U	188	HIS	-	expression tag	UNP Q1N036
U	189	HIS	-	expression tag	UNP Q1N036
U	190	HIS	-	expression tag	UNP Q1N036
U	191	HIS	-	expression tag	UNP Q1N036
U	192	HIS	-	expression tag	UNP Q1N036
U	193	HIS	-	expression tag	UNP Q1N036
V	62	MET	-	expression tag	UNP Q1N036
V	63	SER	-	expression tag	UNP Q1N036
V	186	GLU	-	expression tag	UNP Q1N036
V	187	GLY	-	expression tag	UNP Q1N036
V	188	HIS	-	expression tag	UNP Q1N036
V	189	HIS	-	expression tag	UNP Q1N036
V	190	HIS	-	expression tag	UNP Q1N036
V	191	HIS	-	expression tag	UNP Q1N036
V	192	HIS	-	expression tag	UNP Q1N036
V	193	HIS	-	expression tag	UNP Q1N036
W	62	MET	-	expression tag	UNP Q1N036
W	63	SER	-	expression tag	UNP Q1N036
W	186	GLU	-	expression tag	UNP Q1N036
W	187	GLY	-	expression tag	UNP Q1N036
W	188	HIS	-	expression tag	UNP Q1N036
W	189	HIS	-	expression tag	UNP Q1N036
W	190	HIS	-	expression tag	UNP Q1N036
W	191	HIS	-	expression tag	UNP Q1N036
W	192	HIS	-	expression tag	UNP Q1N036
W	193	HIS	-	expression tag	UNP Q1N036
X	62	MET	-	expression tag	UNP Q1N036
X	63	SER	-	expression tag	UNP Q1N036
X	186	GLU	-	expression tag	UNP Q1N036

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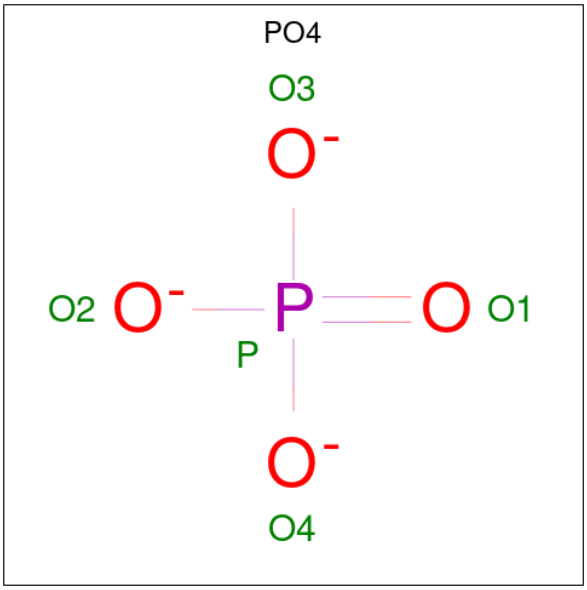
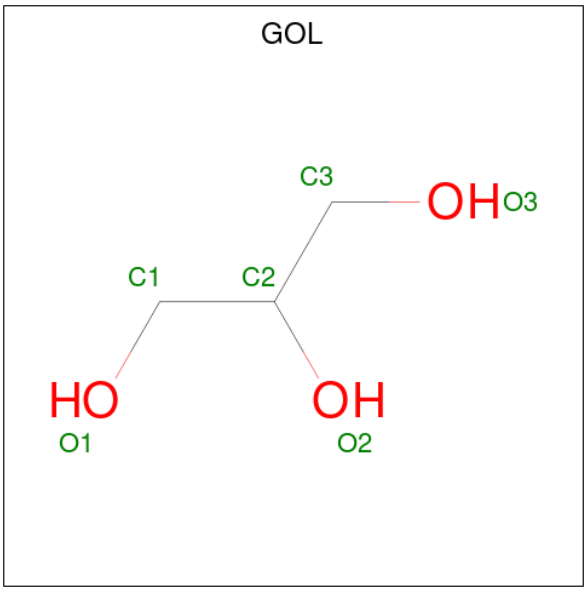
Chain	Residue	Modelled	Actual	Comment	Reference
X	187	GLY	-	expression tag	UNP Q1N036
X	188	HIS	-	expression tag	UNP Q1N036
X	189	HIS	-	expression tag	UNP Q1N036
X	190	HIS	-	expression tag	UNP Q1N036
X	191	HIS	-	expression tag	UNP Q1N036
X	192	HIS	-	expression tag	UNP Q1N036
X	193	HIS	-	expression tag	UNP Q1N036

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	20	Total O 20 20	0	0
4	B	43	Total O 43 43	0	0
4	C	19	Total O 19 19	0	0
4	D	31	Total O 31 31	0	0
4	E	28	Total O 28 28	0	0
4	F	36	Total O 36 36	0	0
4	G	19	Total O 19 19	0	0
4	H	31	Total O 31 31	0	0
4	I	20	Total O 20 20	0	0
4	J	56	Total O 56 56	0	0
4	K	40	Total O 40 40	0	0

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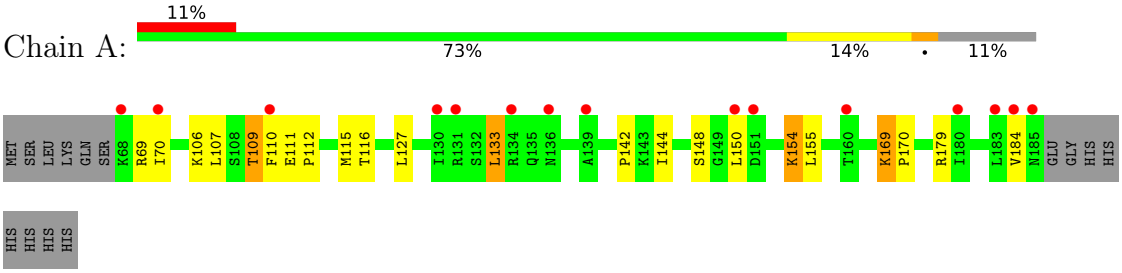
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	26	Total O 26 26	0	0
4	M	21	Total O 21 21	0	0
4	N	42	Total O 42 42	0	0
4	O	12	Total O 12 12	0	0
4	P	31	Total O 31 31	0	0
4	Q	12	Total O 12 12	0	0
4	R	38	Total O 38 38	0	0
4	S	45	Total O 45 45	0	0
4	T	16	Total O 16 16	0	0
4	U	18	Total O 18 18	0	0
4	V	16	Total O 16 16	0	0
4	W	24	Total O 24 24	0	0
4	X	16	Total O 16 16	0	0

3 Residue-property plots

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

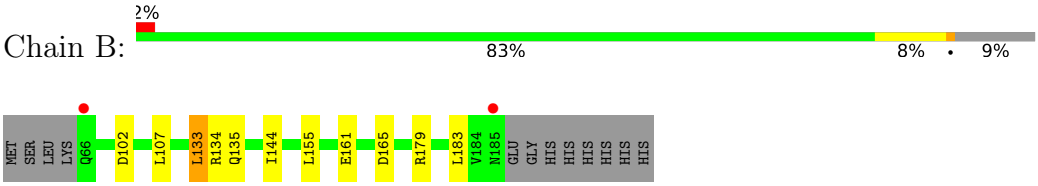
• Molecule 1: Response regulator

Chain A:



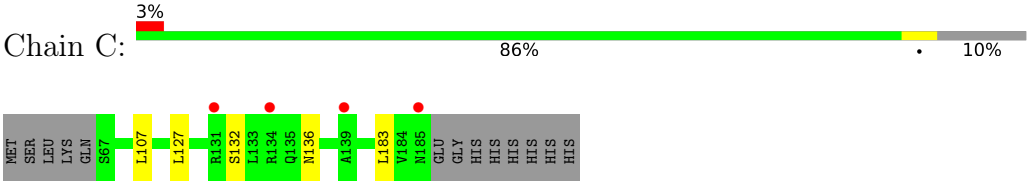
• Molecule 1: Response regulator

Chain B:



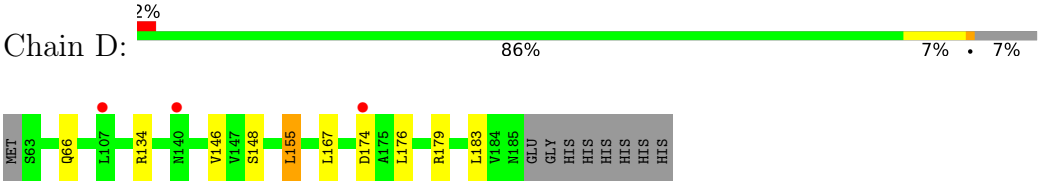
• Molecule 1: Response regulator

Chain C:



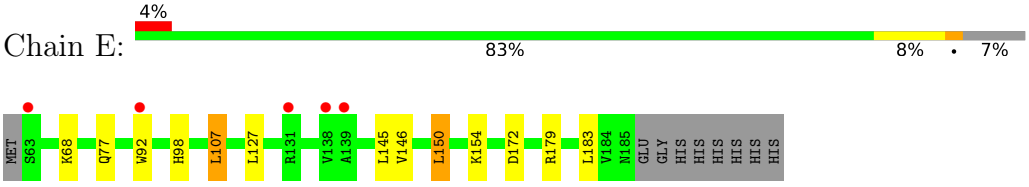
• Molecule 1: Response regulator

Chain D:



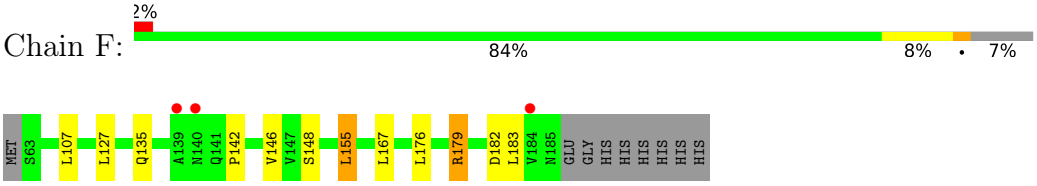
• Molecule 1: Response regulator

Chain E:



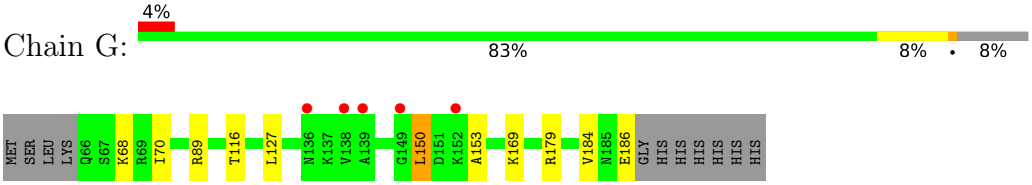
• Molecule 1: Response regulator

Chain F:



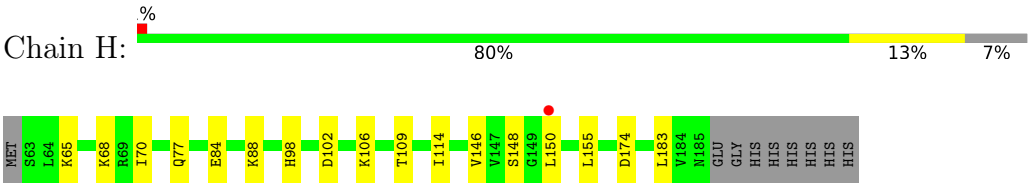
• Molecule 1: Response regulator

Chain G:



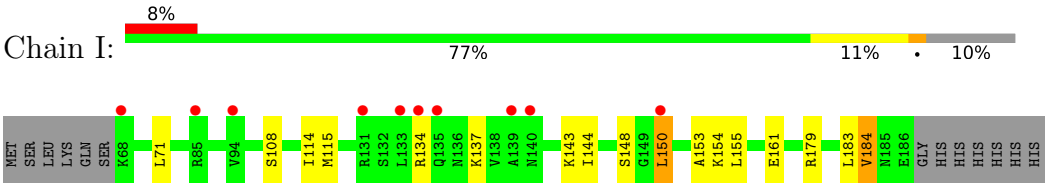
• Molecule 1: Response regulator

Chain H:



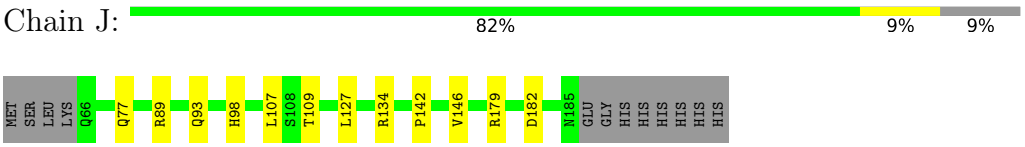
• Molecule 1: Response regulator

Chain I:



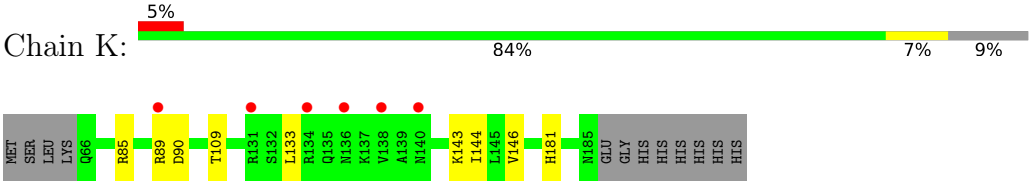
• Molecule 1: Response regulator

Chain J:



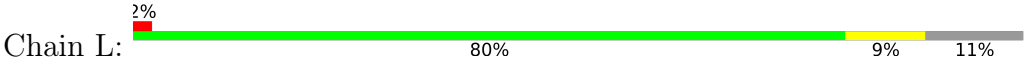
• Molecule 1: Response regulator

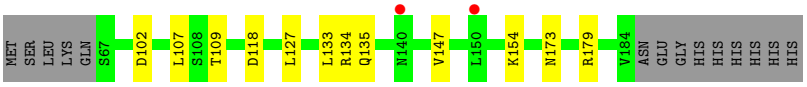
Chain K:



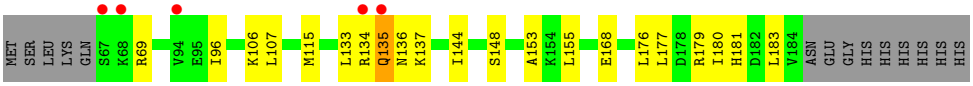
• Molecule 1: Response regulator

Chain L:

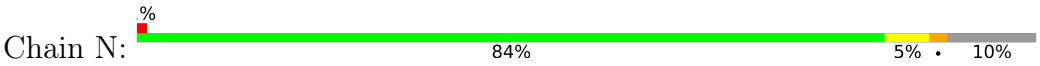


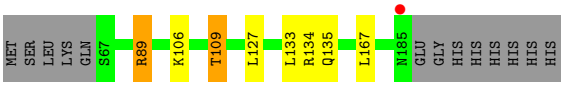


• Molecule 1: Response regulator

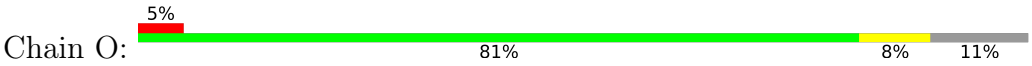


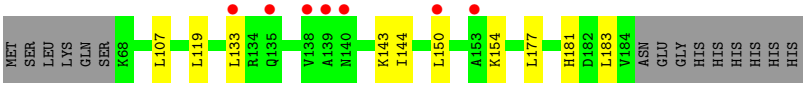
• Molecule 1: Response regulator



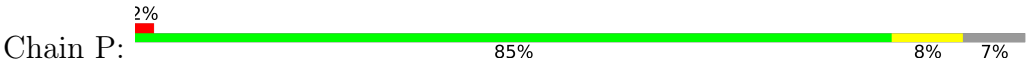


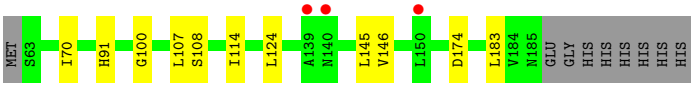
• Molecule 1: Response regulator



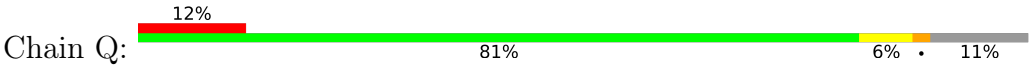


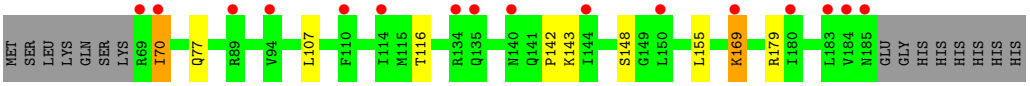
• Molecule 1: Response regulator



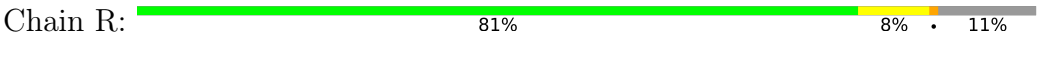


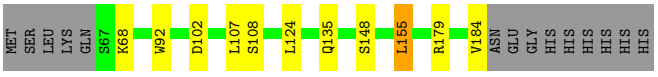
• Molecule 1: Response regulator





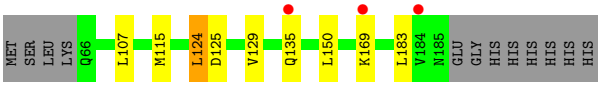
• Molecule 1: Response regulator





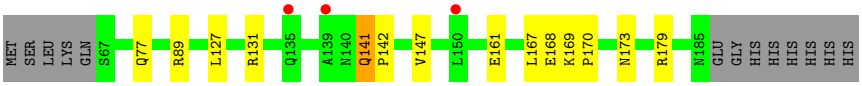
• Molecule 1: Response regulator

Chain S:



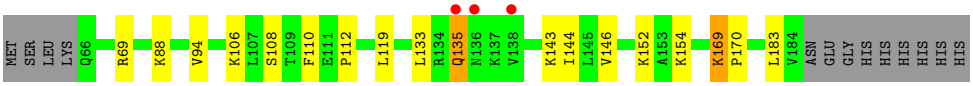
• Molecule 1: Response regulator

Chain T:



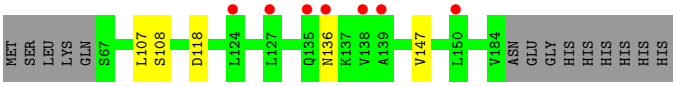
• Molecule 1: Response regulator

Chain U:



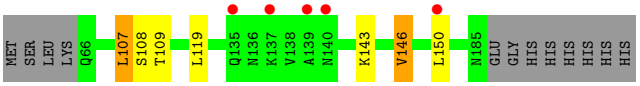
• Molecule 1: Response regulator

Chain V:



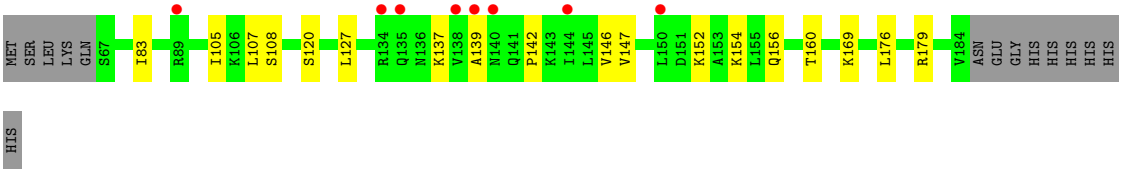
• Molecule 1: Response regulator

Chain W:



• Molecule 1: Response regulator

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.71Å 149.72Å 281.07Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 40.13 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-2.00) 87.8 (40.13-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.239 , 0.282 0.249 , 0.289	Depositor DCC
R_{free} test set	6835 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 19.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.087 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.086 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.059 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.065 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.070 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23428	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/938	0.59	0/1268
1	B	0.40	0/1010	0.59	0/1362
1	C	0.34	0/952	0.54	0/1287
1	D	0.39	0/982	0.61	0/1326
1	E	0.40	0/1010	0.62	1/1362 (0.1%)
1	F	0.41	0/1005	0.63	0/1354
1	G	0.40	0/968	0.58	0/1308
1	H	0.42	0/1013	0.63	0/1367
1	I	0.40	0/942	0.64	0/1273
1	J	0.41	0/987	0.61	0/1332
1	K	0.41	0/971	0.59	0/1312
1	L	0.37	0/942	0.59	0/1273
1	M	0.36	0/942	0.57	0/1273
1	N	0.43	0/984	0.61	0/1329
1	O	0.37	0/939	0.57	0/1268
1	P	0.41	0/982	0.63	0/1326
1	Q	0.37	0/938	0.58	0/1269
1	R	0.39	0/965	0.60	0/1303
1	S	0.41	0/953	0.62	0/1288
1	T	0.37	0/944	0.59	0/1276
1	U	0.44	0/960	0.64	0/1297
1	V	0.38	0/942	0.58	0/1273
1	W	0.40	0/959	0.57	0/1296
1	X	0.41	0/947	0.62	0/1279
All	All	0.40	0/23175	0.60	1/31301 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	172	ASP	N-CA-CB	-5.26	101.13	110.60

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	926	0	943	12	0
1	B	980	0	1020	3	0
1	C	937	0	952	1	0
1	D	967	0	990	3	0
1	E	986	0	1027	5	0
1	F	984	0	1024	4	0
1	G	953	0	967	5	0
1	H	986	0	1023	5	0
1	I	930	0	944	8	0
1	J	963	0	992	5	0
1	K	953	0	976	3	0
1	L	927	0	947	3	0
1	M	927	0	947	13	0
1	N	957	0	988	3	0
1	O	924	0	950	3	0
1	P	967	0	990	3	0
1	Q	923	0	938	5	0
1	R	944	0	976	6	0
1	S	941	0	956	7	0
1	T	932	0	948	5	0
1	U	942	0	961	9	0
1	V	927	0	947	3	0
1	W	944	0	961	2	0
1	X	932	0	955	6	0
2	F	5	0	0	0	0
2	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	6	0	8	0	0
4	A	20	0	0	0	0
4	B	43	0	0	0	0
4	C	19	0	0	0	0
4	D	31	0	0	0	0
4	E	28	0	0	0	0
4	F	36	0	0	0	0
4	G	19	0	0	0	0
4	H	31	0	0	0	0
4	I	20	0	0	0	0
4	J	56	0	0	0	0
4	K	40	0	0	0	0
4	L	26	0	0	0	0
4	M	21	0	0	1	0
4	N	42	0	0	0	0
4	O	12	0	0	0	0
4	P	31	0	0	0	0
4	Q	12	0	0	0	0
4	R	38	0	0	0	0
4	S	45	0	0	0	0
4	T	16	0	0	0	0
4	U	18	0	0	0	0
4	V	16	0	0	0	0
4	W	24	0	0	0	0
4	X	16	0	0	0	0
All	All	23428	0	23330	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:179[B]:ARG:HE	1:R:179[B]:ARG:HA	1.36	0.90
1:G:150:LEU:HB2	1:I:153:ALA:HB2	1.58	0.82
1:G:153:ALA:HB2	1:I:150:LEU:HB2	1.67	0.77
1:R:179[B]:ARG:NE	1:R:179[B]:ARG:HA	1.95	0.77
1:N:106:LYS:HA	1:N:109:THR:HG22	1.69	0.75
1:A:106:LYS:HA	1:A:109:THR:HG22	1.70	0.72
1:X:107:LEU:HD11	1:X:142:PRO:HG3	1.73	0.70
1:S:124:LEU:HD22	1:S:125:ASP:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:69:ARG:HB2	1:U:110:PHE:CZ	2.35	0.61
1:I:71:LEU:HD23	1:I:115:MET:HE2	1.83	0.61
1:S:124:LEU:HD21	1:S:129:VAL:CG2	2.30	0.60
1:M:135:GLN:C	1:M:137:LYS:H	2.06	0.59
1:S:124:LEU:C	1:S:124:LEU:HD22	2.24	0.58
1:E:150:LEU:HB2	1:M:153:ALA:HB2	1.86	0.58
1:K:90:ASP:OD2	1:K:181:HIS:HE1	1.87	0.57
1:M:107:LEU:HD13	1:M:115:MET:HE3	1.85	0.57
1:U:106:LYS:HE3	1:V:136:ASN:HD21	1.68	0.57
1:U:133:LEU:HD23	1:U:144:ILE:HD11	1.87	0.56
1:O:177:LEU:O	1:O:181:HIS:ND1	2.38	0.56
1:N:134:ARG:HD3	1:N:135:GLN:OE1	2.07	0.55
1:M:135:GLN:O	1:M:137:LYS:N	2.39	0.55
1:A:133:LEU:HD23	1:A:144:ILE:HD11	1.89	0.54
1:I:148:SER:HB2	1:I:155:LEU:HD13	1.89	0.54
1:R:179[B]:ARG:NE	1:R:179[B]:ARG:CA	2.71	0.53
1:T:89:ARG:HH22	1:T:173:ASN:HD22	1.56	0.53
1:A:107:LEU:HD11	1:A:142:PRO:HG3	1.91	0.53
1:M:148:SER:HB3	1:M:168:GLU:HA	1.91	0.53
1:U:69:ARG:HG3	1:U:112:PRO:HA	1.91	0.53
1:F:148:SER:HB2	1:F:155:LEU:HG	1.90	0.53
1:R:148:SER:HB2	1:R:155:LEU:HG	1.91	0.53
1:M:133:LEU:HD23	1:M:144:ILE:HD11	1.91	0.52
1:S:124:LEU:HD21	1:S:129:VAL:HG23	1.92	0.52
1:A:69:ARG:HG2	1:A:110:PHE:CZ	2.46	0.51
1:P:70:ILE:HG12	1:P:114:ILE:HB	1.93	0.51
1:A:148:SER:HB2	1:A:155:LEU:HD13	1.93	0.50
1:X:147:VAL:HG12	1:X:169:LYS:HE2	1.92	0.50
1:M:148:SER:HB2	1:M:155:LEU:HD13	1.93	0.50
1:X:156:GLN:NE2	1:X:160:THR:OG1	2.44	0.50
1:T:127:LEU:HB3	1:T:131:ARG:HH21	1.77	0.50
1:M:135:GLN:C	1:M:137:LYS:N	2.65	0.50
1:W:107:LEU:HD13	1:X:105:ILE:HD11	1.94	0.50
1:Q:107:LEU:HD11	1:Q:142:PRO:HG3	1.94	0.49
1:A:70:ILE:HD11	1:A:116:THR:HG23	1.94	0.49
1:I:134:ARG:HE	1:I:144:ILE:HD12	1.76	0.49
1:M:176:LEU:O	1:M:180:ILE:HG12	2.13	0.48
1:F:167:LEU:HG	1:F:179:ARG:HG2	1.95	0.48
1:Q:70:ILE:HD11	1:Q:116:THR:HG23	1.95	0.48
1:O:133:LEU:HD23	1:O:144:ILE:HD11	1.95	0.48
1:P:100:GLY:HA2	1:P:124:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:134[B]:ARG:HH11	1:K:85[B]:ARG:HE	1.60	0.48
1:I:114:ILE:HD11	1:I:184:VAL:HG13	1.96	0.47
1:F:167:LEU:HD11	1:F:176:LEU:HA	1.97	0.47
1:B:134[B]:ARG:HH22	1:B:161:GLU:HG2	1.80	0.47
1:A:107:LEU:HD13	1:A:115:MET:HE3	1.97	0.47
1:D:167:LEU:HG	1:D:179:ARG:HG3	1.96	0.46
1:U:119:LEU:HG	1:U:146:VAL:HG13	1.96	0.46
1:L:118:ASP:HA	1:L:147:VAL:HB	1.97	0.46
1:J:77:GLN:HG2	1:J:98:HIS:CE1	2.51	0.45
1:T:147:VAL:HG12	1:T:169:LYS:HE2	1.98	0.45
1:Q:169:LYS:HB3	1:Q:169:LYS:HE2	1.82	0.45
1:V:118:ASP:HA	1:V:147:VAL:HB	1.99	0.45
1:A:111:GLU:N	1:A:112:PRO:HD3	2.32	0.45
1:H:77:GLN:HG2	1:H:98:HIS:CE1	2.51	0.45
1:D:167:LEU:HD11	1:D:176:LEU:HA	1.99	0.45
1:M:96:ILE:O	1:M:106:LYS:NZ	2.47	0.45
1:O:119:LEU:HB3	1:O:154:LYS:HD3	1.98	0.45
1:R:124:LEU:HA	1:R:124:LEU:HD12	1.68	0.45
1:T:141:GLN:HA	1:T:142:PRO:HD2	1.88	0.45
1:G:70:ILE:HD11	1:G:116:THR:HG23	1.98	0.44
1:K:133:LEU:HD23	1:K:144:ILE:HD11	2.00	0.44
1:I:137:LYS:HB3	1:J:109:THR:HG21	1.99	0.44
1:Q:148:SER:HB2	1:Q:155:LEU:HD13	2.00	0.44
1:B:133:LEU:HD23	1:B:144:ILE:HD11	1.99	0.43
1:X:127:LEU:HD13	1:X:154:LYS:HE3	2.00	0.43
1:B:165:ASP:HB2	1:B:183:LEU:HD21	2.00	0.43
1:H:84:GLU:HG2	1:H:88[B]:LYS:HD2	1.99	0.43
1:J:107:LEU:HD11	1:J:142:PRO:HG3	2.00	0.43
1:M:179:ARG:NH1	4:M:815:HOH:O	2.51	0.43
1:S:124:LEU:C	1:S:124:LEU:CD2	2.87	0.43
1:W:119:LEU:HG	1:W:146:VAL:HG13	2.01	0.43
1:A:127:LEU:HD13	1:A:154:LYS:HD3	2.01	0.43
1:E:68:LYS:HB2	1:E:92:TRP:HZ3	1.83	0.43
1:S:107:LEU:HA	1:S:107:LEU:HD12	1.85	0.43
1:S:107:LEU:HD13	1:S:115:MET:HE3	2.00	0.43
1:N:89[A]:ARG:HA	1:N:89[A]:ARG:HD3	1.59	0.43
1:X:83:ILE:HG23	1:X:176:LEU:HD21	2.00	0.43
1:C:132:SER:O	1:C:136:ASN:HB2	2.18	0.42
1:A:169:LYS:HA	1:A:170:PRO:HA	1.90	0.42
1:F:107:LEU:HD11	1:F:142:PRO:HG3	2.00	0.42
1:U:88:LYS:HE2	1:U:94:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:NE	1:A:110:PHE:CE1	2.85	0.42
1:Q:179:ARG:HA	1:Q:179:ARG:HD3	1.83	0.42
1:M:177:LEU:O	1:M:181:HIS:ND1	2.53	0.42
1:R:92:TRP:HH2	1:R:184:VAL:HG21	1.85	0.42
1:G:68:LYS:HA	1:G:68:LYS:HD3	1.87	0.42
1:A:110:PHE:O	1:A:111:GLU:HB2	2.20	0.42
1:M:135:GLN:O	1:M:137:LYS:HG3	2.20	0.42
1:G:150:LEU:H	1:G:150:LEU:HG	1.65	0.41
1:U:135:GLN:HG3	1:U:135:GLN:H	1.66	0.41
1:H:106:LYS:HA	1:H:109:THR:HB	2.01	0.41
1:L:127:LEU:HG	1:L:154:LYS:HE3	2.01	0.41
1:L:173:ASN:HD21	1:T:170:PRO:HD2	1.85	0.41
1:E:77:GLN:HG2	1:E:98:HIS:CE1	2.56	0.41
1:H:70:ILE:HG12	1:H:114:ILE:HB	2.03	0.41
1:I:150:LEU:HG	1:I:150:LEU:H	1.54	0.41
1:U:169:LYS:HA	1:U:170:PRO:HA	1.92	0.41
1:D:148:SER:HB2	1:D:155:LEU:HG	2.03	0.41
1:E:68:LYS:HB2	1:E:92:TRP:CZ3	2.55	0.41
1:U:108[A]:SER:HB3	1:V:108[A]:SER:HG	1.85	0.41
1:E:107:LEU:HA	1:E:107:LEU:HD12	1.88	0.41
1:H:148:SER:HB2	1:H:155:LEU:HD13	2.03	0.40
1:J:107:LEU:HA	1:J:107:LEU:HD12	1.96	0.40
1:P:145:LEU:HB2	1:P:183:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	116/132 (88%)	112 (97%)	4 (3%)	0	100	100
1	B	124/132 (94%)	123 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	118/132 (89%)	113 (96%)	5 (4%)	0	100	100
1	D	122/132 (92%)	121 (99%)	1 (1%)	0	100	100
1	E	125/132 (95%)	122 (98%)	3 (2%)	0	100	100
1	F	124/132 (94%)	123 (99%)	1 (1%)	0	100	100
1	G	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
1	H	126/132 (96%)	125 (99%)	1 (1%)	0	100	100
1	I	117/132 (89%)	113 (97%)	4 (3%)	0	100	100
1	J	122/132 (92%)	122 (100%)	0	0	100	100
1	K	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
1	L	117/132 (89%)	113 (97%)	4 (3%)	0	100	100
1	M	117/132 (89%)	112 (96%)	4 (3%)	1 (1%)	17	11
1	N	122/132 (92%)	122 (100%)	0	0	100	100
1	O	116/132 (88%)	112 (97%)	4 (3%)	0	100	100
1	P	122/132 (92%)	122 (100%)	0	0	100	100
1	Q	116/132 (88%)	109 (94%)	7 (6%)	0	100	100
1	R	119/132 (90%)	118 (99%)	1 (1%)	0	100	100
1	S	118/132 (89%)	115 (98%)	3 (2%)	0	100	100
1	T	117/132 (89%)	112 (96%)	4 (3%)	1 (1%)	17	11
1	U	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
1	V	117/132 (89%)	114 (97%)	3 (3%)	0	100	100
1	W	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
1	X	117/132 (89%)	115 (98%)	1 (1%)	1 (1%)	17	11
All	All	2870/3168 (91%)	2800 (98%)	67 (2%)	3 (0%)	51	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	136	ASN
1	X	139	ALA
1	T	141	GLN

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	101/114 (89%)	94 (93%)	7 (7%)	15	11
1	B	109/114 (96%)	103 (94%)	6 (6%)	21	17
1	C	103/114 (90%)	100 (97%)	3 (3%)	42	43
1	D	107/114 (94%)	101 (94%)	6 (6%)	21	17
1	E	110/114 (96%)	101 (92%)	9 (8%)	11	7
1	F	109/114 (96%)	102 (94%)	7 (6%)	17	13
1	G	105/114 (92%)	98 (93%)	7 (7%)	16	11
1	H	111/114 (97%)	103 (93%)	8 (7%)	14	9
1	I	101/114 (89%)	93 (92%)	8 (8%)	12	8
1	J	107/114 (94%)	101 (94%)	6 (6%)	21	17
1	K	105/114 (92%)	100 (95%)	5 (5%)	25	22
1	L	102/114 (90%)	95 (93%)	7 (7%)	15	11
1	M	102/114 (90%)	98 (96%)	4 (4%)	32	30
1	N	107/114 (94%)	101 (94%)	6 (6%)	21	17
1	O	101/114 (89%)	97 (96%)	4 (4%)	31	29
1	P	107/114 (94%)	102 (95%)	5 (5%)	26	22
1	Q	101/114 (89%)	96 (95%)	5 (5%)	24	20
1	R	104/114 (91%)	98 (94%)	6 (6%)	20	15
1	S	103/114 (90%)	98 (95%)	5 (5%)	25	21
1	T	102/114 (90%)	97 (95%)	5 (5%)	25	21
1	U	104/114 (91%)	98 (94%)	6 (6%)	20	15
1	V	102/114 (90%)	101 (99%)	1 (1%)	76	81
1	W	104/114 (91%)	98 (94%)	6 (6%)	20	15
1	X	102/114 (90%)	96 (94%)	6 (6%)	19	15
All	All	2509/2736 (92%)	2371 (94%)	138 (6%)	22	17

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	THR
1	A	133	LEU
1	A	150	LEU
1	A	154	LYS
1	A	169	LYS
1	A	179	ARG
1	A	184	VAL
1	B	102	ASP
1	B	107	LEU
1	B	133	LEU
1	B	135	GLN
1	B	155	LEU
1	B	179	ARG
1	C	107	LEU
1	C	127	LEU
1	C	183	LEU
1	D	66	GLN
1	D	134	ARG
1	D	146	VAL
1	D	155	LEU
1	D	174	ASP
1	D	183	LEU
1	E	107	LEU
1	E	127	LEU
1	E	145	LEU
1	E	146	VAL
1	E	150	LEU
1	E	154	LYS
1	E	179[A]	ARG
1	E	179[B]	ARG
1	E	183	LEU
1	F	127	LEU
1	F	135	GLN
1	F	146	VAL
1	F	155	LEU
1	F	179	ARG
1	F	182	ASP
1	F	183	LEU
1	G	89	ARG
1	G	127	LEU
1	G	150	LEU
1	G	169	LYS
1	G	179	ARG

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Mol	Chain	Res	Type
1	G	184	VAL
1	G	186	GLU
1	H	65	LYS
1	H	68	LYS
1	H	102[A]	ASP
1	H	102[B]	ASP
1	H	146	VAL
1	H	150	LEU
1	H	174	ASP
1	H	183	LEU
1	I	108	SER
1	I	143	LYS
1	I	150	LEU
1	I	154	LYS
1	I	161	GLU
1	I	179	ARG
1	I	183	LEU
1	I	184	VAL
1	J	89	ARG
1	J	93	GLN
1	J	127	LEU
1	J	146	VAL
1	J	179	ARG
1	J	182	ASP
1	K	89	ARG
1	K	109[A]	THR
1	K	109[B]	THR
1	K	143	LYS
1	K	146	VAL
1	L	102	ASP
1	L	107	LEU
1	L	109	THR
1	L	133	LEU
1	L	134	ARG
1	L	135	GLN
1	L	179	ARG
1	M	69	ARG
1	M	134	ARG
1	M	135	GLN
1	M	183	LEU
1	N	89[A]	ARG
1	N	89[B]	ARG

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Mol	Chain	Res	Type
1	N	109	THR
1	N	127	LEU
1	N	133	LEU
1	N	167	LEU
1	O	107	LEU
1	O	143	LYS
1	O	150	LEU
1	O	183	LEU
1	P	91	HIS
1	P	107	LEU
1	P	108	SER
1	P	146	VAL
1	P	174	ASP
1	Q	70	ILE
1	Q	77[A]	GLN
1	Q	77[B]	GLN
1	Q	143	LYS
1	Q	169	LYS
1	R	68	LYS
1	R	102	ASP
1	R	107	LEU
1	R	108	SER
1	R	135	GLN
1	R	155	LEU
1	S	124	LEU
1	S	135	GLN
1	S	150	LEU
1	S	169	LYS
1	S	183	LEU
1	T	77	GLN
1	T	161	GLU
1	T	167	LEU
1	T	168	GLU
1	T	179	ARG
1	U	135	GLN
1	U	143	LYS
1	U	152	LYS
1	U	154	LYS
1	U	169	LYS
1	U	183	LEU
1	V	107	LEU
1	W	107	LEU

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Mol	Chain	Res	Type
1	W	108	SER
1	W	109	THR
1	W	143	LYS
1	W	146	VAL
1	W	150	LEU
1	X	108	SER
1	X	120	SER
1	X	137	LYS
1	X	146	VAL
1	X	152	LYS
1	X	179	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	C	98	HIS
1	D	98	HIS
1	D	173	ASN
1	F	66	GLN
1	F	173	ASN
1	H	98	HIS
1	I	93	GLN
1	J	140	ASN
1	K	93	GLN
1	K	157	GLN
1	L	98	HIS
1	L	173	ASN
1	M	98	HIS
1	M	135	GLN
1	N	140	ASN
1	O	93	GLN
1	R	156	GLN
1	S	93	GLN
1	S	135	GLN
1	S	157	GLN
1	T	77	GLN
1	T	93	GLN
1	T	98	HIS
1	U	66	GLN
1	U	93	GLN
1	U	136	ASN

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Mol	Chain	Res	Type
1	V	98	HIS
1	V	136	ASN
1	X	93	GLN
1	X	173	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 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	PO4	L	2	-	4,4,4	0.95	0	6,6,6	0.39	0
3	GOL	R	1	-	5,5,5	0.40	0	5,5,5	0.26	0
2	PO4	F	1	-	4,4,4	0.87	0	6,6,6	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	R	1	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	1	GOL	O1-C1-C2-O2
3	R	1	GOL	O1-C1-C2-C3
3	R	1	GOL	C1-C2-C3-O3
3	R	1	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	118/132 (89%)	0.88	15 (12%) 3 3	12, 28, 45, 50	0
1	B	120/132 (90%)	0.24	2 (1%) 70 68	14, 21, 28, 42	0
1	C	119/132 (90%)	0.67	4 (3%) 45 44	12, 24, 44, 52	0
1	D	123/132 (93%)	0.44	3 (2%) 59 57	13, 21, 32, 43	0
1	E	123/132 (93%)	0.34	5 (4%) 37 36	12, 21, 38, 51	0
1	F	123/132 (93%)	0.29	3 (2%) 59 57	12, 21, 32, 44	0
1	G	121/132 (91%)	0.48	5 (4%) 37 36	10, 22, 44, 53	0
1	H	123/132 (93%)	0.25	1 (0%) 86 85	13, 19, 31, 43	0
1	I	119/132 (90%)	0.55	10 (8%) 11 10	9, 22, 44, 49	0
1	J	120/132 (90%)	0.15	0 100 100	12, 19, 28, 40	0
1	K	120/132 (90%)	0.32	6 (5%) 28 28	13, 21, 40, 46	0
1	L	118/132 (89%)	0.32	2 (1%) 70 68	11, 23, 32, 35	0
1	M	118/132 (89%)	0.57	5 (4%) 36 35	8, 25, 36, 41	0
1	N	119/132 (90%)	0.30	1 (0%) 86 85	10, 19, 28, 42	0
1	O	117/132 (88%)	0.66	7 (5%) 21 20	13, 24, 43, 57	0
1	P	123/132 (93%)	0.28	3 (2%) 59 57	12, 22, 33, 43	0
1	Q	117/132 (88%)	0.94	16 (13%) 3 2	10, 27, 44, 52	0
1	R	118/132 (89%)	0.23	0 100 100	13, 20, 29, 34	0
1	S	120/132 (90%)	0.40	3 (2%) 57 56	13, 21, 39, 47	0
1	T	119/132 (90%)	0.51	3 (2%) 57 56	12, 23, 38, 48	0
1	U	119/132 (90%)	0.36	3 (2%) 57 56	12, 22, 39, 45	0
1	V	118/132 (89%)	0.74	7 (5%) 22 21	13, 24, 38, 48	0
1	W	120/132 (90%)	0.45	5 (4%) 36 35	14, 22, 41, 53	0
1	X	118/132 (89%)	0.71	8 (6%) 17 16	10, 24, 47, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2873/3168 (90%)	0.46	117 (4%)	37	36	8, 22, 38, 57	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	139	ALA	7.7
1	X	139	ALA	6.8
1	Q	134	ARG	6.7
1	W	139	ALA	6.5
1	V	139	ALA	6.5
1	O	138	VAL	5.8
1	T	150	LEU	5.7
1	A	184	VAL	5.6
1	X	134	ARG	5.0
1	V	150	LEU	4.9
1	I	134	ARG	4.7
1	X	140	ASN	4.5
1	Q	135	GLN	4.4
1	E	139	ALA	4.4
1	C	185	ASN	4.1
1	I	85	ARG	3.9
1	A	150	LEU	3.9
1	F	139	ALA	3.9
1	X	138	VAL	3.8
1	X	135	GLN	3.8
1	A	185	ASN	3.7
1	D	140	ASN	3.7
1	Q	150	LEU	3.6
1	Q	185	ASN	3.6
1	F	140	ASN	3.6
1	X	150	LEU	3.6
1	G	149	GLY	3.6
1	G	138	VAL	3.6
1	P	150	LEU	3.5
1	M	67	SER	3.5
1	I	140	ASN	3.4
1	P	140	ASN	3.4
1	A	110	PHE	3.4
1	U	138	VAL	3.3
1	M	68	LYS	3.3
1	A	134	ARG	3.3
1	G	139	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	S	135	GLN	3.3
1	C	139	ALA	3.2
1	T	135	GLN	3.2
1	M	134	ARG	3.1
1	F	184	VAL	3.1
1	Q	94	VAL	3.1
1	O	140	ASN	3.1
1	W	137	LYS	3.1
1	Q	183	LEU	3.1
1	A	136	ASN	3.0
1	O	153	ALA	2.9
1	I	94	VAL	2.9
1	A	68	LYS	2.9
1	L	140	ASN	2.9
1	Q	70	ILE	2.8
1	G	136	ASN	2.8
1	P	139	ALA	2.8
1	U	135	GLN	2.8
1	I	131	ARG	2.8
1	I	135	GLN	2.8
1	B	185	ASN	2.8
1	K	134	ARG	2.7
1	V	127	LEU	2.7
1	Q	180	ILE	2.6
1	E	138	VAL	2.6
1	I	139	ALA	2.6
1	Q	110	PHE	2.6
1	Q	69	ARG	2.6
1	V	135	GLN	2.6
1	V	138	VAL	2.6
1	L	150	LEU	2.6
1	K	89	ARG	2.5
1	A	70	ILE	2.5
1	E	92	TRP	2.5
1	Q	144	ILE	2.5
1	A	130	ILE	2.4
1	V	136	ASN	2.4
1	A	183	LEU	2.4
1	I	68	LYS	2.4
1	N	185	ASN	2.4
1	T	139	ALA	2.4
1	Q	169	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	107	LEU	2.4
1	I	150	LEU	2.4
1	K	138	VAL	2.4
1	A	139	ALA	2.4
1	A	131	ARG	2.3
1	M	94	VAL	2.3
1	A	160	THR	2.3
1	W	140	ASN	2.3
1	C	134	ARG	2.3
1	E	63	SER	2.3
1	K	136	ASN	2.3
1	Q	140	ASN	2.3
1	Q	114	ILE	2.3
1	A	151	ASP	2.2
1	D	174	ASP	2.2
1	C	131	ARG	2.2
1	W	150	LEU	2.2
1	O	133	LEU	2.2
1	I	133	LEU	2.2
1	O	150	LEU	2.2
1	X	144	ILE	2.1
1	V	124	LEU	2.1
1	B	66	GLN	2.1
1	M	135	GLN	2.1
1	O	135	GLN	2.1
1	W	135	GLN	2.1
1	Q	184	VAL	2.1
1	S	169	LYS	2.1
1	U	136	ASN	2.1
1	G	152	LYS	2.1
1	E	131	ARG	2.1
1	A	180	ILE	2.0
1	K	131	ARG	2.0
1	X	89[A]	ARG	2.0
1	H	150	LEU	2.0
1	K	140	ASN	2.0
1	Q	89	ARG	2.0
1	S	184	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	R	1	6/6	0.88	0.11	61,63,63,65	0
2	PO4	L	2	5/5	0.90	0.17	51,51,51,52	5
2	PO4	F	1	5/5	0.94	0.11	64,64,65,67	0

6.5 Other polymers (i)

There are no such residues in this entry.