wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 08:36 PM EDT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

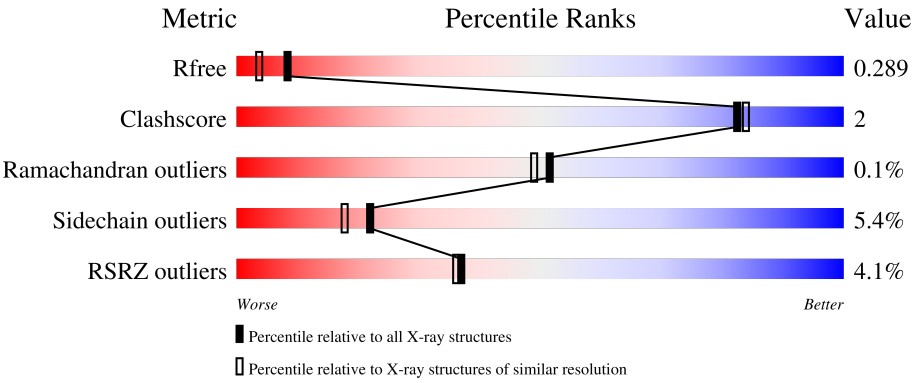
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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%

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Mol	Chain	Length	Quality of chain
1	E	132	4% 83% 8% • 7%
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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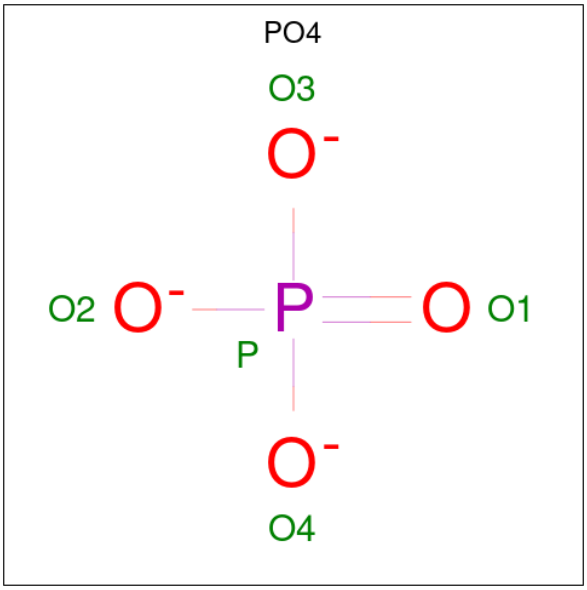
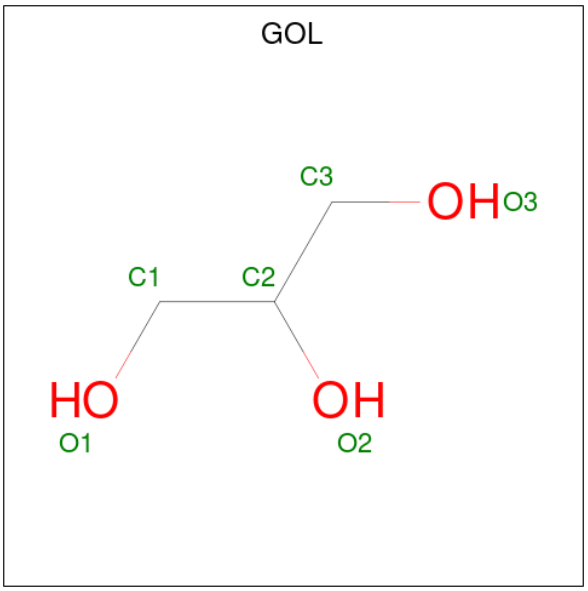
Chain	Residue	Modelled	Actual	Comment	Reference
X	187	GLY	-	expression tag	UNP Q1N036
X	188	HIS	-	expression tag	UNP Q1N036
X	189	HIS	-	expression tag	UNP Q1N036
X	190	HIS	-	expression tag	UNP Q1N036
X	191	HIS	-	expression tag	UNP Q1N036
X	192	HIS	-	expression tag	UNP Q1N036
X	193	HIS	-	expression tag	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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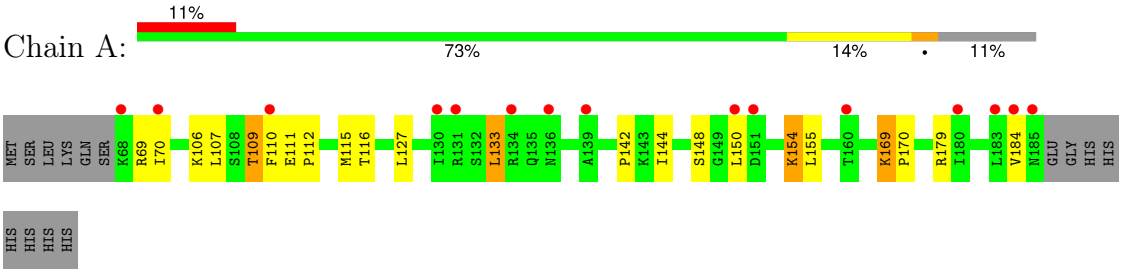
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	26	Total O 26 26	0	0
4	M	21	Total O 21 21	0	0
4	N	42	Total O 42 42	0	0
4	O	12	Total O 12 12	0	0
4	P	31	Total O 31 31	0	0
4	Q	12	Total O 12 12	0	0
4	R	38	Total O 38 38	0	0
4	S	45	Total O 45 45	0	0
4	T	16	Total O 16 16	0	0
4	U	18	Total O 18 18	0	0
4	V	16	Total 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 (i)

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

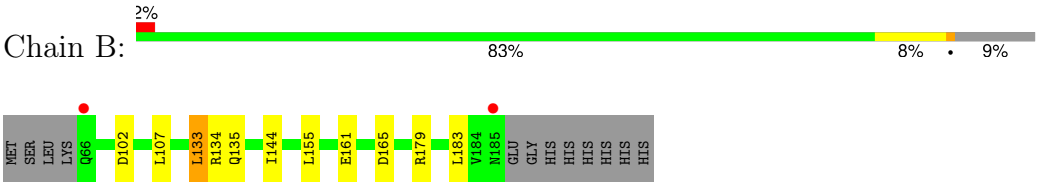
• Molecule 1: Response regulator

Chain A:



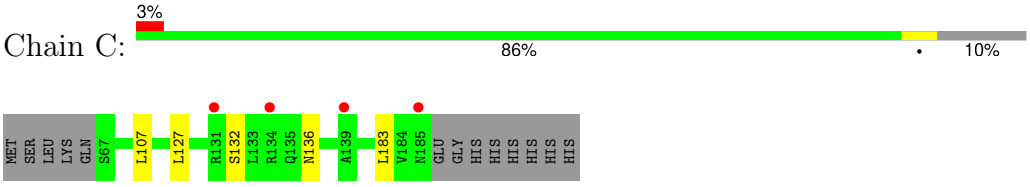
• Molecule 1: Response regulator

Chain B:



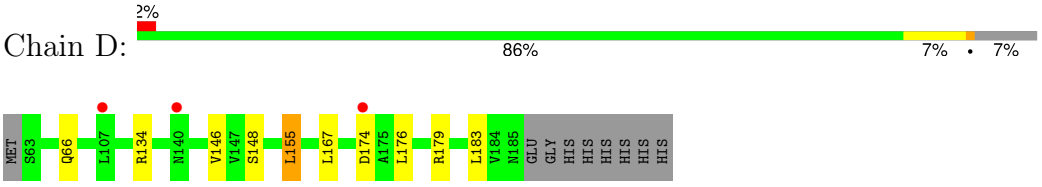
• Molecule 1: Response regulator

Chain C:



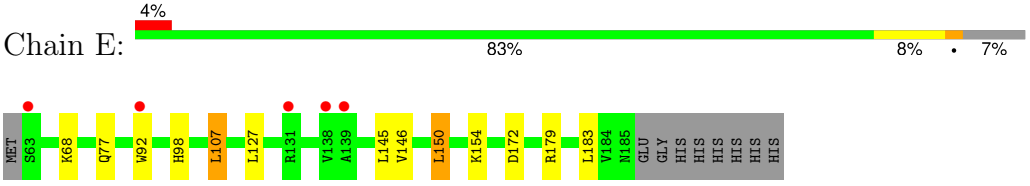
• Molecule 1: Response regulator

Chain D:



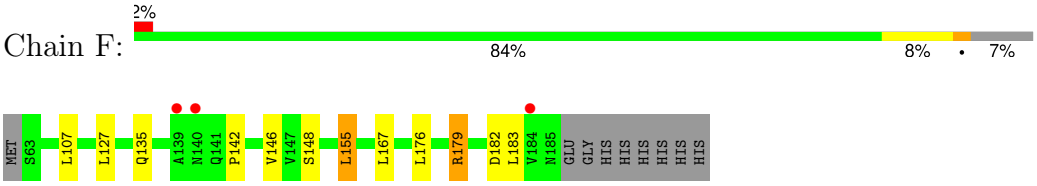
• Molecule 1: Response regulator

Chain E:



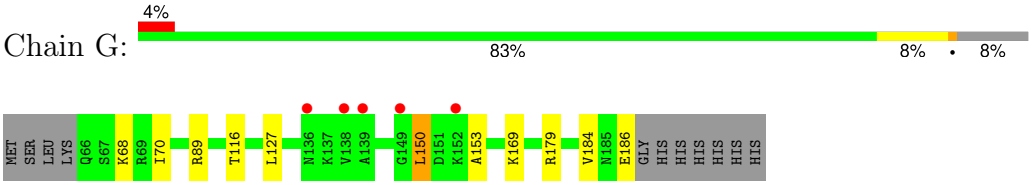
• Molecule 1: Response regulator

Chain F:



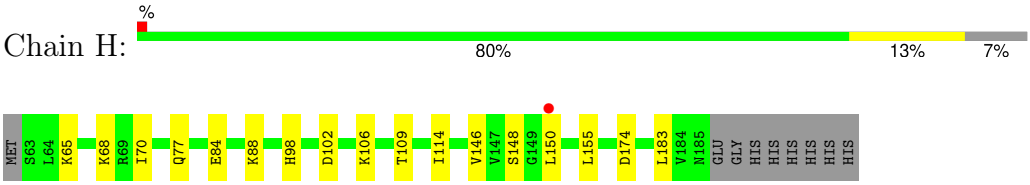
• Molecule 1: Response regulator

Chain G:



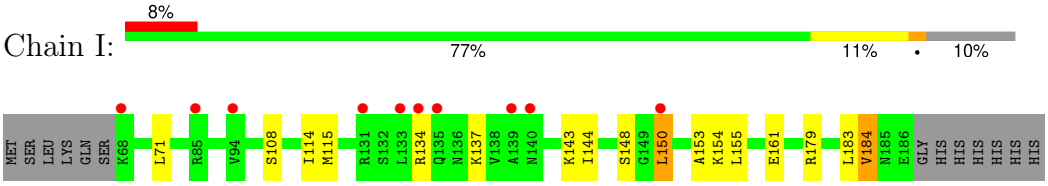
• Molecule 1: Response regulator

Chain H:



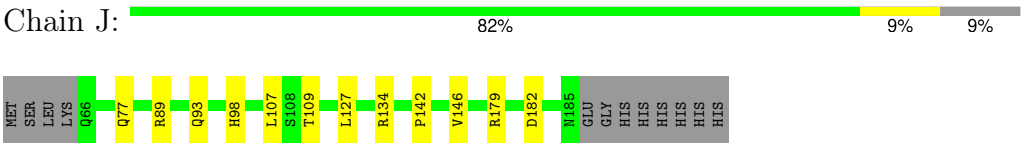
• Molecule 1: Response regulator

Chain I:



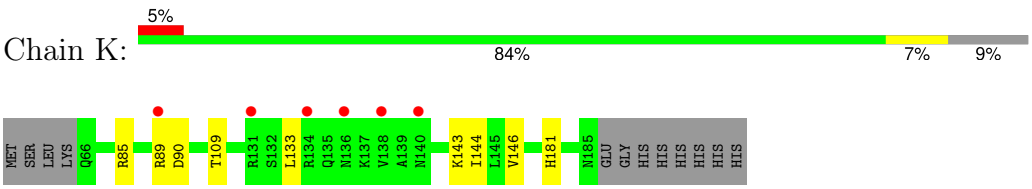
• Molecule 1: Response regulator

Chain J:



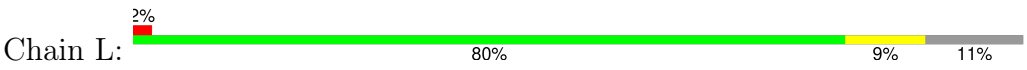
• Molecule 1: Response regulator

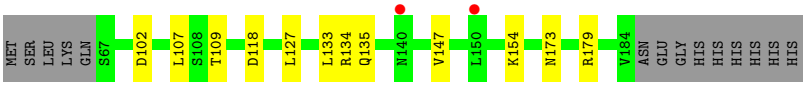
Chain K:



• Molecule 1: Response regulator

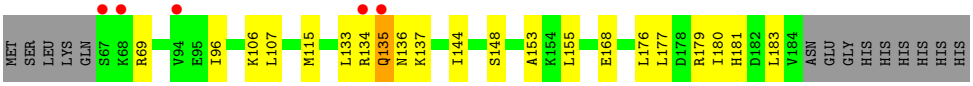
Chain L:





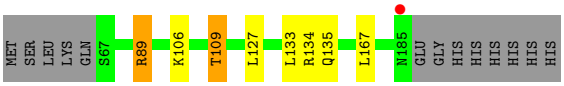
• Molecule 1: Response regulator

Chain M:



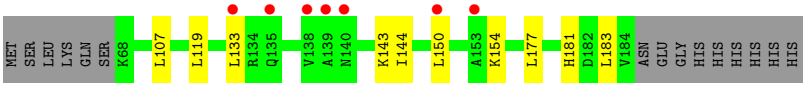
• Molecule 1: Response regulator

Chain N:



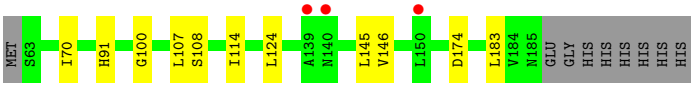
• Molecule 1: Response regulator

Chain O:



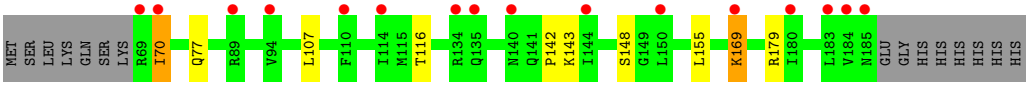
• Molecule 1: Response regulator

Chain P:



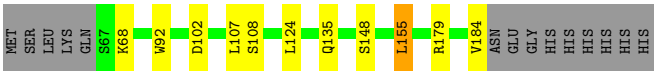
• Molecule 1: Response regulator

Chain Q:



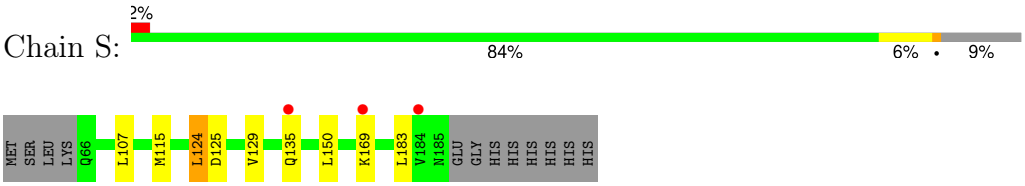
• Molecule 1: Response regulator

Chain R:



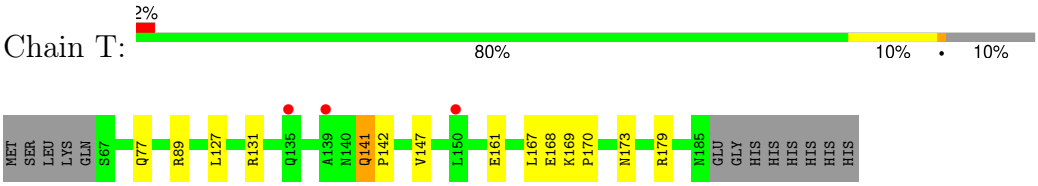
• Molecule 1: Response regulator

Chain S:



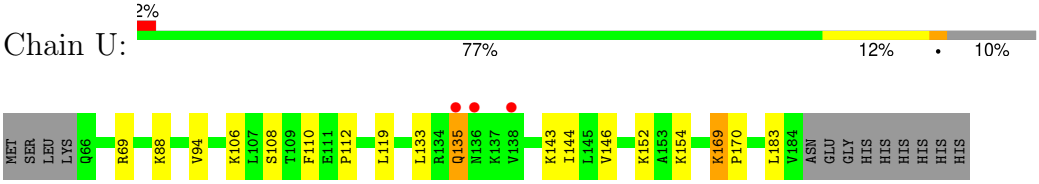
• Molecule 1: Response regulator

Chain T:



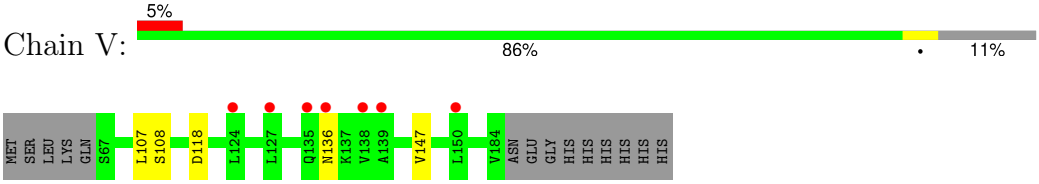
• Molecule 1: Response regulator

Chain U:



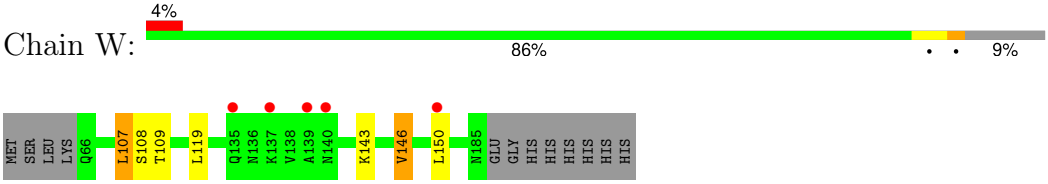
• Molecule 1: Response regulator

Chain V:



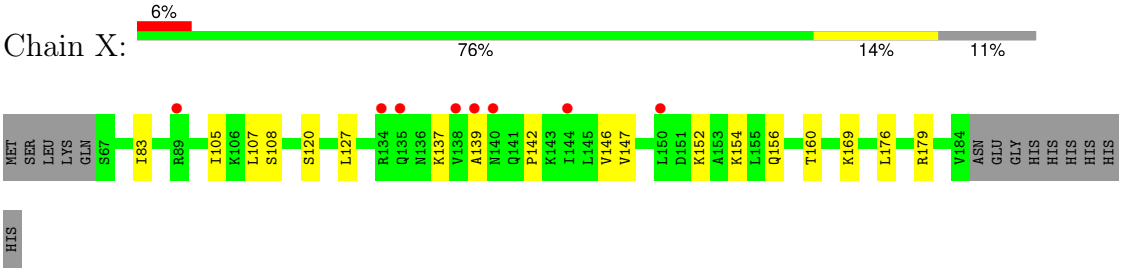
• Molecule 1: Response regulator

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 (i)

5.1 Standard geometry (i)

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.

The worst 5 of 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:HA	1:R:179[B]:ARG:HE	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:HA	1:R:179[B]:ARG:NE	1.95	0.77
1:N:106:LYS:HA	1:N:109:THR:HG22	1.69	0.75

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	161	GLU
1	U	135	GLN
1	W	146	VAL
1	H	102[B]	ASP
1	H	102[A]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	135	GLN
1	V	98	HIS
1	R	156	GLN
1	X	93	GLN
1	U	66	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	GOL	R	1	-	5,5,5	0.41	0	5,5,5	0.30	0
2	PO4	L	2	-	4,4,4	0.99	0	6,6,6	0.42	0
2	PO4	F	1	-	4,4,4	0.91	0	6,6,6	0.47	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 (i)

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%)	0.47	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

The worst 5 of 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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.